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

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Top500 vs. Top8000 Reference Contours

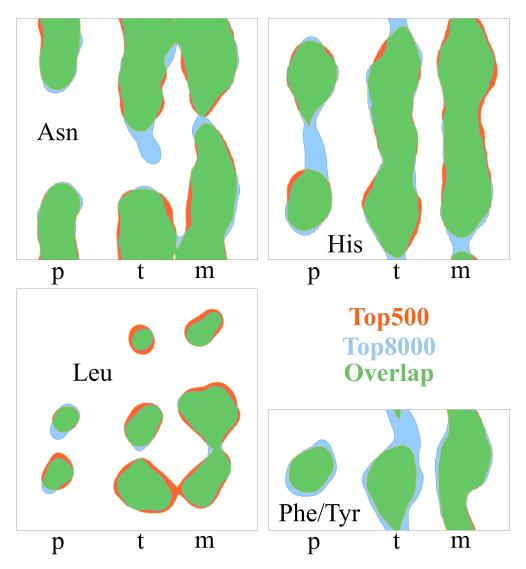


Figure S1: Areas in orange (from Top500 data) and in blue (from Top8000) fill the allowed regions for AsN, His, Leu, and Phe/Tyr. Phe and Tyr were done together as no significant difference was detected between their distributions. The extensive areas in green are where the two systems both declare allowed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

 $\textbf{Table S2:} \ \ \text{Showing differences between outlier counts in the unfiltered dataset using the Top 500 and Top 8000 reference contours.}$

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, marked with a 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% of the *expected rotamer count* then the rarity is marked with a checkmark.

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 checkmark.

These numbers, along with central angle values, are available in CSV format on GitHub under Top8000/Top8000_rotamer_central_values at http://github.com/rlabduke/reference_data.

residue	rotamer	n	%	rarity
	SER: TOT	AL N =	76186	
SER	p	36901	48.44	
SER	t	17502	22.97	
SER	m	21558	28.30	
SER	OUTLIER	225	0.30	
	CYS: TOT.	AL N =	16708	
CYS	p	2962	17.73	
CYS	t	4399	26.33	
CYS	m	9301	55.67	
CYS	OUTLIER	46	0.28	
	THR: TOT	AL N =	75180	
THR	р	36195	48.14	
THR	t	5197	6.91	
THR	m	33559	44.64	
THR	OUTLIER	229	0.30	
	VAL : TOT	ALN =	97050	
VAL	р	6015	6.20	
VAL	t	73329	75.56	
VAL	m	17410	17.94	
VAL	OUTLIER	296	0.30	
	PRO : TOT	AL N =	59515	
PRO	Cg_exo	30128	50.62	
PRO	Cg_endo	29192	49.05	
PRO	OUTLIER	195	0.33	
	LEU: TOTA	L 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 : TOTA	L 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			%	
residue	rotamer	n A.T. D.T.		rarity
A CINT	ASN: TOT			
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: TOTA		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: TOTA	AL 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: TOT	AL 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 : TOT	AL 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 : TOT	AL 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	
1101	111-00	501	0.10	

residue	rotamer	n	%	rarity
TRP	OUTLIER	53	0.28	
	MET: TOT	AL 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	\checkmark
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 : TOT	-	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 : TOT		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 : TOT		46380	
ARG	ppp80	10	0.02	√
ARG	ppp-140	4	0.02	√
ARG	ppt170	57	0.01	<u>√</u>
ARG	ppt170	19	0.12	<u>√</u>
ARG	ppt-90	15	0.04	√
ARG	ptp90	223	0.03	
ARG	ptp-110	77	0.48	
AIG	h-h-110	1.1	0.11	

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residue ARG	rotamer	388	% 0.84	rarity
ARG	ptp-170 ptt180	820	1.77	
ARG	ptt180	814	1.76	
ARG	ptt-90	726	1.57	
ARG	ptm160	502	1.08	
ARG	ptm-80	215	0.46	
ARG	pmt100	4	0.40	√
ARG	pmt170	39	0.01	√
ARG	pmt-80	27	0.06	√
ARG	pmm150	12	0.03	√
ARG	pmm-80	19	0.03	
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	0.73	
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	ttt180	1057	2.28	
ARG	ttt-90	1380	2.28	
ARG	ttm110	725	1.56	
ARG	ttm170	1317	2.84	
ARG	ttm-80	1504	3.24	
ARG	tmt170	104	0.22	
ARG	tmt90	23	0.22	√
ARG	tmt-80	62	0.03	· ·
ARG	tmm160	92	0.13	
ARG	tmm-80	71	0.20	
ARG	mpp80	54	0.13	
ARG	mpp-170	64	0.12	· ·
ARG	mpt180	245	0.14	
ARG	mpt100	46	0.10	√
ARG	mpt-90	85	0.10	· ·
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	0.14	
ARG	mmp-170	123	0.33	
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 : TOTA		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 ✓ LYS tppp 37 0.11 ✓ LYS tppt 272 0.78 LYS tptp 409 1.17 LYS tpt 1228 3.53 LYS tptm 197 0.57 LYS tptm 197 0.57 LYS ttp 229 0.66 LYS ttp 1233 3.54 LYS ttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmtm 197 0.57 LYS ttmtm 197 0.57 LYS tmtm 190 0.06	residue	rotamer	n	%	rarity
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 ttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmm 1170 0.57 LYS ttmm 197 0.57 LYS tmtm 199 0.06 ✓<	LYS	pttm	268	0.77	
LYS pmtt 10 0.03 ✓ LYS tppp 37 0.11 ✓ LYS tptpt 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 tttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmm 1176 3.38 LYS ttmm 197 0.57 LYS ttmm 197 0.57 LYS ttmtm 197 0.57 LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmtm 20 0.06 ✓ LYS mpt 31	LYS	ptmt	187	0.54	
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 tttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmm 9 0.03 ✓ LYS ttmm 197 0.57 LYS ttmm 197 0.57 LYS tmtm 197 0.57 LYS tmtt 82 0.24 LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS mpt 31 0.09 ✓ LYS mpt 31 <	LYS	ptmm	80	0.23	
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 tttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmm 674 1.94 LYS ttmm 197 0.57 LYS tmtm 197 0.57 LYS tmtm 197 0.57 LYS tmtm 197 0.57 LYS tmtm 190 0.06 ✓ LYS tmtm 20 0.06 ✓ LYS tmtm 20 0.06 ✓ LYS mpt 31		pmtt	10	0.03	√
LYS tptp 409 1.17 LYS tptt 1228 3.53 LYS tptm 197 0.57 LYS ttpp 229 0.66 LYS tttpt 883 2.54 LYS ttttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmm 197 0.57 LYS ttmtm 197 0.57 LYS tmttp 11 0.03 ✓ LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmm 33 0.09 ✓ LYS tmm 8 0.02 ✓ LYS mptp 26 0.07 ✓ LYS mptp 124 0.36 LYS <td< td=""><td>LYS</td><td>tppp</td><td>37</td><td>0.11</td><td>√</td></td<>	LYS	tppp	37	0.11	√
LYS tptt 1228 3.53 LYS tptm 197 0.57 LYS ttpp 229 0.66 LYS tttpt 883 2.54 LYS ttttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmt 674 1.94 LYS ttmt 197 0.57 LYS tmtp 11 0.03 ✓ LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmtm 33 0.09 ✓ LYS tmmm 8 0.02 ✓ LYS mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mtpp 392 1.13 LY	LYS	tppt	272	0.78	
LYS tptm 197 0.57 LYS ttpp 229 0.66 LYS ttpt 883 2.54 LYS ttttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmm 197 0.57 LYS tmtp 11 0.03 ✓ LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmtm 20 0.06 ✓ ✓ LYS tmtm 8 0.02 ✓ LYS tmtm 8 0.02 ✓ ✓ LYS mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptp 10.03 ✓ LYS mptp 392 1.13 LYS mtp 1357 3.90 <	LYS	tptp	409	1.17	
LYS ttpp 229 0.66 LYS ttpt 883 2.54 LYS tttp 1233 3.54 LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ 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 mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptm 11 0.03 ✓ LYS mtpp 392 1.13 LYS mtp 1357 3.90 LYS mtp 17 0.05 ✓	LYS	tptt	1228	3.53	
LYS ttpt 883 2.54 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 tmtm 20 0.06 ✓ LYS tmtm 8 0.02 ✓ LYS tmtm 8 0.02 ✓ LYS mpt 31 0.09 ✓ LYS mpt 26 0.07 ✓ LYS mpt 124 0.36 LYS mpt 124 0.36 LYS mpt 1357 3.90 LYS mtp 1357 3.90 LYS mtp 1414	LYS	tptm	197	0.57	
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 L LYS tmtm 20 0.06 ✓ LYS tmmt 33 0.09 ✓ LYS tmmm 8 0.02 ✓ LYS mpt 31 0.09 ✓ LYS mpt 26 0.07 ✓ LYS mpt 124 0.36 LYS mtp 392 1.13 LYS mtp 392 1.13 LYS mtp 17 0.05 ✓ LYS mtp 17 0.05	LYS	ttpp	229	0.66	
LYS tttt 5043 14.48 LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmt 674 1.94 LYS ttmt 197 0.57 LYS tmtp 11 0.03 ✓ LYS tmtt 82 0.24 L LYS tmtm 20 0.06 ✓ LYS tmmt 33 0.09 ✓ LYS tmmm 8 0.02 ✓ LYS mpt 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mpt 124 0.36 LYS mtpp 392 1.13 LYS mtp 392 1.13 LYS mtp 17 0.05 ✓ LYS mtp 17 0.05 ✓ LYS mtt 1829 <	LYS	ttpt	883	2.54	
LYS tttm 1176 3.38 LYS ttmp 9 0.03 ✓ LYS ttmt 674 1.94 LYS ttmt 197 0.57 LYS tmtp 11 0.03 ✓ LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmmt 33 0.09 ✓ LYS tmptm 8 0.02 ✓ LYS mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptp 124 0.36 LYS mtpp 392 1.13 LYS mtpp 392 1.13 LYS mtp 1357 3.90 LYS mtp 17 0.05 ✓ LYS mtt 1829 5.25 LYS mtt 1829 5.25	LYS	tttp	1233	3.54	
LYS ttmp 9 0.03 ✓ LYS ttmt 674 1.94 LYS ttmt 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 mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptp 26 0.07 ✓ LYS mptm 11 0.03 ✓ LYS mtpp 392 1.13 LYS mtpp 392 1.13 LYS mtpm 17 0.05 ✓ LYS mtpm 17 0.05 ✓ LYS mtt 1829 5.25 LYS mtmt <td< td=""><td>LYS</td><td>tttt</td><td>5043</td><td>14.48</td><td></td></td<>	LYS	tttt	5043	14.48	
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 mptp 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptm 11 0.03 ✓ LYS mptm 11 0.03 ✓ LYS mtpp 392 1.13 LYS mtpp 392 1.13 LYS mtpm 17 0.05 ✓ LYS mtpm 17 0.05 ✓ LYS mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtm 1314	LYS	tttm	1176	3.38	
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 tmptm 8 0.02 ✓ LYS mppt 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mpt 124 0.36 LYS mpt 11 0.03 ✓ LYS mtpp 392 1.13 LYS mtp 1357 3.90 LYS mtp 1414 4.06 LYS mtt 18597 24.68 LYS mtt 1829 5.25 LYS mtm 1829 5.25 LYS mtm 1314 3.77 LYS mtm 1314 3.77	LYS	ttmp	9	0.03	√
LYS tmtp 11 0.03 ✓ LYS tmtt 82 0.24 LYS tmtm 20 0.06 ✓ LYS tmmt 33 0.09 ✓ LYS mppt 31 0.09 ✓ LYS mptp 26 0.07 ✓ LYS mptp 26 0.07 ✓ LYS mptm 11 0.03 ✓ LYS mtpp 392 1.13 LYS mtpp 392 1.13 LYS mtpp 1357 3.90 LYS mtpm 17 0.05 ✓ LYS mttp 1414 4.06 LYS mtt 1829 5.25 LYS mtm 1829 5.25 LYS mtm 1314 3.77 LYS mtm 1314 3.77 LYS mtm 131 0.09 ✓	LYS	ttmt	674	1.94	
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 mtpp 1357 3.90 LYS mtpm 17 0.05 ✓ LYS mttp 1414 4.06 LYS mtt 1829 5.25 LYS mtm 1829 5.25 LYS mtm 1314 3.77 LYS mtm 1314 3.77 LYS mtm 131 0.09 ✓ LYS mmt <	LYS	ttmm	197	0.57	
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 Incompany LYS mptm 11 0.03 ✓ LYS mtpp 392 1.13 Incompany LYS mtp 1357 3.90 Incompany LYS mtp 17 0.05 ✓ LYS mttp 1414 4.06 Incompany Incom	LYS	tmtp	11	0.03	✓
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 mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtm 1314 3.77 LYS mtm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtp 463 1.33 LYS mmtm 727 2.09	LYS	tmtt	82	0.24	
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 mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 17 LYS mtmt 1314 3.77 17 LYS mmpt 31 0.09 ✓ LYS mmtt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 <td>LYS</td> <td>tmtm</td> <td>20</td> <td>0.06</td> <td>✓</td>	LYS	tmtm	20	0.06	✓
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 mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 LYS mtm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	tmmt	33	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 mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 LYS mtmm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	tmmm	8	0.02	√
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 mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 LYS mtmm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mppt	31	0.09	✓
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 mtt 8597 24.68 LYS mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 LYS mtmm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mptp	26	0.07	√
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 mtm 1829 5.25 LYS mtmp 9 0.03 ✓ LYS mtmt 1314 3.77 LYS mtmm 424 1.22 LYS mmpt 31 0.09 ✓ LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS		124	0.36	
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 mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mptm	11	0.03	✓
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	mtpp	392	1.13	
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	mtpt	1357	3.90	
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	mtpm	17	0.05	√
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	mttp	1414	4.06	
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	mttt	8597	24.68	
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	mttm	1829	5.25	
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	mtmp	9	0.03	✓
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		mtmt	1314	3.77	
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	mtmm	424	1.22	
LYS mmtt 3137 9.01 LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mmpt	31	0.09	✓
LYS mmtm 727 2.09 LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mmtp	463	1.33	
LYS mmmt 544 1.56 LYS mmmm 90 0.26	LYS	mmtt	3137	9.01	
LYS mmmm 90 0.26	LYS	mmtm	727	2.09	
	LYS	mmmt	544	1.56	
LYS OUTLIER 114 0.33	LYS	mmmm	90	0.26	
	LYS	OUTLIER	114	0.33	

 ${\bf Table~S3:}~{\bf Rotamer~names,~number~of~examples~in~the~filtered~data~set,~and~frequency~in~its~residue~type.$

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. These numbers, along with rotamer occurrence frequencies, are available in CSV format on GitHub under Top8000/Top8000_rotamer_central_values at http://github.com/rlabduke/reference_data.

Table S4: SER Central Values

StdDev 9.0 StdDev 1.42 0.82 1.45 2.40 1.21

$SER \mathbf{p} = 36901$			SE	$CR \mathbf{t} n = 17502$
χ	Smooth COM	StdDev	χ	Smooth COM
chi1	66	8.6	chi1	179
Bond Angle	Mean	StdDev	Bond Angle	Mean
$\begin{array}{c} C\alpha_{-}C\beta_{-}OG \\ C\alpha_{-}C_{-}O \\ C\beta_{-}C\alpha_{-}C \\ N_{-}C\alpha_{-}C \\ N_{-}C\alpha_{-}C\beta \end{array}$	111.0 120.5 109.9 111.6 110.7	1.35 0.92 1.39 2.52 1.12	$C\alphaC\betaOG$ $C\alphaCO$ $C\betaC\alphaC$ $NC\alphaC$ $NC\alphaC\beta$	110.7 120.6 109.8 110.5 110.1

$SER \mathbf{m} n = 21558$					
χ	Smooth COM	StdDev			
chi1	-64	7.7			
Bond Angle	Mean	StdDev			
$C\alphaC\betaOG$	110.5	1.46			
$C\alphaCO$	120.5	0.85			
$C\betaC\alphaC$	109.5	1.45			
$N_{-}C\alpha_{-}C$	111.5	2.44			
$N_C\alpha_C\beta$	110.6	1.03			

Table S5: CYS Central Values

$CYS \mathbf{p} = 2962$					
χ	Smooth COM	StdDev			
chi1	65	9.0			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}SG$	114.6	1.68			
$C\alphaCO$	120.5	0.98			
$C\beta C\alpha C$	110.5	1.50			
$N_{-}C\alpha_{-}C$	111.3	2.78			
$N_{-}C\alpha_{-}C\beta$	110.9	1.23			

C	$YS \mathbf{t} n = 4399$	
χ	Smooth COM	StdDev
chi1	-178	8.2
Bond Angle	Mean	StdDev
$C\alphaC\betaSG$	113.7	1.94
$C\alphaCO$	120.5	0.86
$C\betaC\alphaC$	110.3	1.30
$N_{-}C\alpha_{-}C$	109.7	2.44
$N_{-}C\alpha_{-}C\beta$	110.0	1.37

$CYS \mathbf{m} n = 9301$				
χ	Smooth COM	StdDev		
chi1	-65	8.2		
Bond Angle	Mean	StdDev		
$C\alphaC\betaSG$	113.6	1.86		
$C\alphaCO$	120.4	0.87		
$C\betaC\alphaC$	109.5	1.63		
$N_{-}C\alpha_{-}C$	111.5	2.42		
$N_{-}C\alpha_{-}C\beta$	110.6	1.07		

Table S6: THR Central Values

THR $p = 36195$				
χ	Smooth COM	StdDev		
chi1	61	7.7		
Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.0	1.01		
$C\alphaC\betaOG1$	109.5	0.97		
$C\alphaCO$	120.5	0.96		
$C\beta C\alpha C$	108.8	1.70		
$N_{-}C\alpha_{-}C$	111.4	2.77		
$N_C\alpha_C\beta$	111.8	1.26		
$OG1_C\beta_C\gamma2$	109.2	1.71		

TH	THR $t = 5197$				
χ	Smooth COM	StdDev			
chi1	-173	7.4			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.7	1.10			
$C\alphaC\betaOG1$	109.5	0.99			
$C\alphaCO$	120.6	0.83			
$C\beta C\alpha C$	111.0	1.90			
$N_{-}C\alpha_{-}C$	110.1	2.33			
$N_C\alpha_C\beta$	111.3	1.34			
${\rm OG1_C}\beta_{\rm C}\gamma2$	109.1	1.81			

THR $m = 33559$					
χ	Smooth COM	StdDev			
chi1	-60	6.1			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.1	0.94			
$C\alphaC\betaOG1$	108.9	0.97			
$C\alphaCO$	120.5	0.81			
$C\beta C\alpha C$	110.0	1.53			
$N_C\alpha_C$	110.2	2.31			
$N_C\alpha_C\beta$	110.7	1.19			
$OG1_C\beta_C\gamma2$	108.8	1.67			

Table S7: VAL Central Values

VAL p n = 6015			
VP	TL p II = 0010		
χ	Smooth COM	StdDev	
chi1	65	7.2	
Bond Angle	Mean	StdDev	
$C\alphaC\betaC\gamma 1$	111.5	1.09	
$C\alphaC\betaC\gamma_2$	110.8	1.02	
$C\alphaCO$	120.6	0.83	
$C\beta C\alpha C$	111.4	1.57	
$C\gamma 1C\betaC\gamma 2$	111.0	1.20	
$N_{-}C\alpha_{-}C$	110.3	2.48	
$N_{-}C\alpha_{-}C\beta$	111.6	1.26	

VA	$VAL \mathbf{t} n = 73329$				
χ	Smooth COM	StdDev			
chi1	176	6.4			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}C\gamma 1$	110.7	0.94			
$C\alphaC\betaC\gamma_2$	110.2	0.95			
$C\alphaCO$	120.5	0.79			
$C\beta C\alpha C$	110.2	1.51			
$C\gamma 1C\betaC\gamma 2$	110.5	1.13			
$N_{-}C\alpha_{-}C$	109.4	2.36			
$N_{-}C\alpha_{-}C\beta$	111.3	1.11			

$VAL \mathbf{m} n = 17410$				
χ	Smooth COM	StdDev		
chi1	-62	5.7		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma 1$	110.4	0.92		
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.3	1.02		
$C\alphaCO$	120.6	0.91		
$C\beta C\alpha C$	109.8	1.60		
$C\gamma 1_C\beta_C\gamma 2$	110.9	1.16		
$N_{-}C\alpha_{-}C$	111.1	2.69		
$N_{-}C\alpha_{-}C\beta$	112.3	1.18		

Table S8: PRO Central Values

PRO	PRO \mathbf{Cg} - $\mathbf{exo} \ n = 30128$			PRO Cg_endo $n = 29192$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	-25	7.2	chi1	27	7.7	
chi2	36	7.8	chi2	-34	8.9	
chi3	-32	7.1	chi3	28	9.2	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	104.2	1.40	$C\alphaC\betaC\gamma$	104.2	1.47	
$C\alphaCO$	120.2	1.03	$C\alphaCO$	120.2	1.07	
$C\alphaNC\delta$	111.7	0.81	$C\alpha_N_C\delta$	111.8	0.84	
$C\beta_{-}C\alpha_{-}C$	110.8	1.30	$C\betaC\alphaC$	110.9	1.41	
$C\betaC\gammaC\delta$	104.7	2.31	$C\betaC\gammaC\delta$	105.3	2.36	
$N_{-}C\alpha_{-}C$	112.7	2.42	$N_{-}C\alpha_{-}C$	112.9	2.60	
$N_C\alpha_C\beta$	103.3	0.59	$N_C\alpha_C\beta$	103.2	0.72	
$N_C\delta_C\gamma$	102.7	0.88	$N_C\delta_C\gamma$	103.1	0.88	

Table S9: LEU Central Values

LE	$U \mathbf{pp} n = 521$		LE	U pt n = 378	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	8.2	chi1	73	8.5
chi2	83	9.5	chi2	165	10.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	119.1	2.53	$C\alpha_{-}C\beta_{-}C\gamma$	118.7	2.16
$C\alphaCO$	120.6	0.83	$C\alphaCO$	120.8	0.83
$C\betaC\alphaC$	111.5	1.38	$C\betaC\alphaC$	110.4	1.45
$C\betaC\gammaC\delta 1$	111.5	1.89	$C\betaC\gammaC\delta 1$	109.8	1.54
$C\betaC\gammaC\delta_2$	109.8	1.68	$C\betaC\gammaC\delta 2$	111.6	1.84
$C\delta1_C\gamma_C\delta2$	109.7	1.23	$C\delta1_C\gamma_C\delta2$	110.4	1.24
$N_{-}C\alpha_{-}C$	110.7	2.36	$N_{-}C\alpha_{-}C$	110.4	2.45
$N_{-}C\alpha_{-}C\beta$	111.1	1.15	$N_{-}C\alpha_{-}C\beta$	111.6	1.18
LE	$U \ \mathbf{tp} \ n = 34655$		LE	$U \ tt \ n = 1576$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	8.2	chi1	-172	8.5
chi2	63	7.0	chi2	153	10.5
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	116.5	2.06	$C\alpha_{-}C\beta_{-}C\gamma$	117.3	2.71
$C\alphaCO$	120.5	0.79	$C\alphaCO$	120.6	0.86
$C\beta_{-}C\alpha_{-}C$	110.2	1.21	$C\beta_{-}C\alpha_{-}C$	111.1	1.26
$C\betaC\gammaC\delta 1$	111.1	1.55	$C\beta_{-}C\gamma_{-}C\delta 1$	110.1	1.53
$C\betaC\gammaC\delta_2$	109.8	1.50	$C\betaC\gammaC\delta_2$	111.6	1.84
$C\delta1_C\gamma_C\delta2$	110.7	1.13	$C\delta1_C\gamma_C\delta2$	110.4	1.32
$N_C\alpha_C$	110.2	2.38	$N_C\alpha_C$	109.1	2.50
$N_{-}C\alpha_{-}C\beta$	110.3	1.15	$N_{-}C\alpha_{-}C\beta$	110.2	1.25
LE	$U \mathbf{tm} n = 143$		LEU	$\mathbf{J} \mathbf{mp} \; \mathbf{n} = 2711$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-172	5.9	chi1	-77	12.5
chi2	-75	6.4	chi2	72	15.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	120.4	2.30	$C\alpha_{-}C\beta_{-}C\gamma$	116.6	2.64
$C\alpha_{-}C_{-}O$	120.6	0.80	$C\alphaCO$	120.5	0.85
$C\betaC\alphaC$	111.3	1.17	$C\betaC\alphaC$	109.7	1.57
$C\beta C\gamma C\delta 1$	112.3	1.92	$C\betaC\gammaC\delta 1$	111.6	2.04
$C\betaC\gammaC\delta_2$	111.6	1.69	$C\betaC\gammaC\delta 2$	109.9	1.58
$C\delta1_C\gamma_C\delta2$	111.4	1.44	$C\delta1C\gammaC\delta2$	110.5	1.45
$NC\alphaC$	108.5	2.32	$NC\alphaC$	110.2	2.64
$N_{-}C\alpha_{-}C\beta$	109.9	1.13	$NC\alphaC\beta$	111.1	1.03

LEU $\mathbf{mt} \ \mathbf{n} = 74252$			LEU \mathbf{mm} n = 484		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66	8.2	chi1	-83	10.2
chi2	174	8.1	chi2	-64	10.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	115.9	2.17	$C\alpha_{-}C\beta_{-}C\gamma$	117.8	2.63
$C\alphaCO$	120.4	0.82	$C\alphaCO$	120.3	0.89
$C\beta C\alpha C$	109.8	1.42	$C\beta C\alpha C$	110.1	1.58
$C\beta_{-}C\gamma_{-}C\delta 1$	109.9	1.47	$C\beta_{-}C\gamma_{-}C\delta 1$	110.9	1.60
$C\beta_C\gamma_C\delta_2$	111.0	1.55	$C\betaC\gammaC\delta_2$	111.9	1.72
$C\delta1_C\gamma_C\delta2$	110.8	1.11	$C\delta1_C\gamma_C\delta2$	110.7	1.40
$N_{-}C\alpha_{-}C$	111.4	2.34	$N_{-}C\alpha_{-}C$	111.1	2.61
$N_{-}C\alpha_{-}C\beta$	110.6	0.99	$N_C\alpha_C\beta$	111.0	0.98

Table S10: ILE Central Values

IL	$\mathbf{E} \mathbf{p} \mathbf{p} \ \mathbf{n} = 254$		ILI	$\mathbf{E} \mathbf{pt} \ \mathbf{n} = 8837$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	58	7.7	chi1	62	6.1
chi2	84	12.8	chi2	170	7.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma 1$	112.5	1.28	$C\alphaC\betaC\gamma 1$	111.3	1.08
$C\alphaC\betaC\gamma_2$	109.9	1.15	$C\alphaC\betaC\gamma_2$	110.2	0.94
$C\alphaCO$	120.5	0.87	$C\alphaCO$	120.5	0.94
$C\betaC\alphaC$	111.3	1.61	$C\betaC\alphaC$	110.1	1.67
$C\betaC\gamma_1C\delta_1$	115.1	1.80	$C\betaC\gamma_1C\delta_1$	113.6	1.25
$C\gamma 1_C\beta_C\gamma 2$	110.0	1.96	$C\gamma 1_C\beta_C\gamma 2$	111.4	1.53
$N_{-}C\alpha_{-}C$	112.0	2.51	$N_{-}C\alpha_{-}C$	111.4	2.74
$N_{-}C\alpha_{-}C\beta$	112.3	1.25	$N_{-}C\alpha_{-}C\beta$	112.3	1.20
IL	$\mathbf{E} \; \mathbf{tp} \; \mathbf{n} = 1869$		IL	E tt $n = 4163$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-167	7.8	chi1	-170	7.7
chi2	66	7.3	chi2	167	6.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma 1$	111.1	1.13	$C\alphaC\betaC\gamma 1$	110.7	1.07
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.4	1.03	$C\alphaC\betaC\gamma_2$	111.4	1.04
$C\alphaCO$	120.4	0.82	$C\alphaCO$	120.6	0.83
$C\betaC\alphaC$	111.5	1.46	$C\beta C\alpha C$	111.6	1.48
$C\beta_{-}C\gamma_{1}C\delta_{1}$	114.2	1.15	$C\beta C\gamma 1C\delta 1$	113.5	1.27
$C\gamma 1_C\beta_C\gamma 2$	110.8	1.70	$C\gamma 1_C\beta_C\gamma 2$	111.7	1.61
$N_C\alpha_C$	111.6	2.33	$N_{-}C\alpha_{-}C$	110.1	2.52
$N_{-}C\alpha_{-}C\beta$	111.5	1.27	$N_{-}C\alpha_{-}C\beta$	111.4	1.32
IL	$E \mathbf{mp} n = 623$		ILE	mt n = 44470	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-63	11.6	chi1	-63	6.4
chi2	89	16.6	chi2	169	7.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma 1$	111.2	1.11	$C\alpha_{-}C\beta_{-}C\gamma 1$	110.0	1.08
$C\alpha_{-}C\beta_{-}C\gamma_{2}$	110.5	1.09	$C\alphaC\betaC\gamma_2$	110.6	0.92
$C\alphaCO$	120.5	0.81	$C\alpha_{-}C_{-}O$	120.5	0.79
$C\betaC\alphaC$	110.1	1.63	$C\betaC\alphaC$	110.4	1.58
$C\betaC\gamma_1C\delta_1$	114.6	1.67	$C\betaC\gamma_1C\delta_1$	114.0	1.22
$C\gamma 1_C\beta_C\gamma 2$	109.3	1.87	$C\gamma 1_C\beta_C\gamma 2$	110.8	1.44
$N_{-}C\alpha_{-}C$	108.3	2.26	$N_{C}\alpha_{C}$	109.4	2.34
$N_{-}C\alpha_{-}C\beta$	111.9	1.29	$N_{-}C\alpha_{-}C\beta$	111.2	1.15
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ILE	ILE $mm n = 11258$				
χ	Smooth COM	StdDev			
chi1	-59	7.1			
chi2	-61	7.3			
Bond Angle	Mean	StdDev			
$C\alphaC\betaC\gamma 1$	110.9	1.12			
$C\alphaC\betaC\gamma_2$	110.8	0.97			
$C\alphaCO$	120.5	0.80			
$C\betaC\alphaC$	109.8	1.61			
$C\betaC\gamma_1C\delta_1$	114.8	1.21			
$C\gamma 1_C\beta_C\gamma 2$	111.3	1.47			
$N_{-}C\alpha_{-}C$	109.4	2.45			
$N_C\alpha_C\beta$	111.3	1.15			

Table S11: ASN Central Values

AS	$N \ \mathbf{p0} \ n = 7513$	
χ	Smooth COM	StdDev
chi1	64	7.8
chi2	7	43.3
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	113.1	0.88
$C\alphaCO$	120.4	0.97
$C\beta C\alpha C$	111.3	1.68
$C\betaC\gammaN\delta 2$	116.3	0.91
$C\beta_C\gamma_O\delta 1$	121.1	0.98
$N_{-}C\alpha_{-}C$	112.0	2.77
$N_C\alpha_C\beta$	111.1	1.29
$O\delta1_C\gamma_N\delta2$	122.5	0.72
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ASI	N t0 n = 15610	
χ	Smooth COM	StdDev
chi1	-171	10.5
chi2	-1	54.9
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	112.7	0.92
$C\alphaCO$	120.6	0.87
$C\betaC\alphaC$	110.6	1.31
$C\betaC\gammaN\delta 2$	116.5	0.85
$C\betaC\gammaO\delta 1$	120.9	0.92
$N_{-}C\alpha_{-}C$	110.1	2.82
$N_C\alpha_C\beta$	110.1	1.45
$O\delta1_C\gamma_N\delta2$	122.6	0.68

AS	N t160 n = 61	
χ	Smooth COM	StdDev
chi1	-161	7.4
chi2	164	9.1
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.2	1.52
$C\alphaCO$	120.4	0.85
$C\beta C\alpha C$	111.3	1.38
$C\beta C\gamma N\delta 2$	117.0	2.10
$C\beta C\gamma O\delta 1$	120.5	2.02
$N_{-}C\alpha_{-}C$	110.0	1.95
$N_C\alpha_C\beta$	109.3	1.46
$O\delta1_C\gamma_N\delta2$	122.4	0.78

ASN	m110 n = 4003	
χ	Smooth COM	StdDev
chi1	-64	9.6
chi2	115	28.4
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	112.7	1.15
$C\alphaCO$	120.5	0.90
$C\beta C\alpha C$	109.5	1.84
$C\beta C\gamma N\delta 2$	116.6	1.14
$C\beta C\gamma O\delta 1$	120.7	1.17
$N_{-}C\alpha_{-}C$	112.0	2.78
$N_{-}C\alpha_{-}C\beta$	110.6	1.20
$O\delta1_C\gamma_N\delta2$	122.6	0.82

ASN	m-40 n = 26292),
χ	Smooth COM	StdDev
chi1	-70	9.1
chi2	-42	26.3
Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	112.5	0.92
$C\alphaCO$	120.4	0.87
$C\beta _C\alpha _C$	110.0	1.72
$C\beta C\gamma N\delta 2$	116.5	0.85
$C\beta C\gamma O\delta 1$	120.8	0.89
$N_{-}C\alpha_{-}C$	112.2	2.54
$N_{-}C\alpha_{-}C\beta$	110.5	1.10
$O\delta1_C\gamma_N\delta2$	122.7	0.70

Table S12: ASP Central Values

ASI	$\mathbf{p0} \ \mathbf{p0} \ \mathbf{n} = 11746$		AS	P t0 n = 17107	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63	7.5	chi1	-172	10.2
chi2	-2	31.0	chi2	-2	23.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.5	1.02	$C\alpha_{-}C\beta_{-}C\gamma$	113.2	0.91
$C\alphaCO$	120.4	0.91	$C\alphaCO$	120.7	0.89
$C\betaC\alphaC$	111.3	1.65	$C\betaC\alphaC$	110.9	1.23
$C\betaC\gammaO\delta 1$	119.7	1.56	$C\betaC\gammaO\delta 1$	119.5	1.39
$C\betaC\gammaO\delta 2$	118.2	1.77	$C\betaC\gammaO\delta 2$	118.1	1.73
$N_{-}C\alpha_{-}C$	112.2	2.55	$N_{-}C\alpha_{-}C$	108.9	2.65
$N_{-}C\alpha_{-}C\beta$	111.1	1.25	$N_{-}C\alpha_{-}C\beta$	109.7	1.45
$O\delta1_{-}C\gamma_{-}O\delta2$	122.1	1.64	$O\delta1_C\gamma_O\delta2$	122.4	1.58
			00000		
,	P t70 n = 6029			m-30 n = 37239	
,		StdDev			
ASI	P t70 n = 6029		ASP	m-30 n = 37239)
X ASI	P t70 n = 6029 Smooth COM	StdDev	ASP X	m-30 n = 37239 Smooth COM	StdDev
$\begin{array}{c} \text{ASI} \\ \chi \\ \text{chi1} \end{array}$	P t70 n = 6029 Smooth COM -174	StdDev 9.2	$\begin{array}{c} \text{ASP} \\ \hline \chi \\ \text{chi1} \end{array}$	m-30 n = 37239 Smooth COM -69	StdDev 8.2
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	P t70 n = 6029 Smooth COM -174 74	StdDev 9.2 19.8	ASP χ chi1 chi2	m-30 n = 37239 Smooth COM -69 -29	StdDev 8.2 22.4
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \end{array}$	P t70 n = 6029 Smooth COM -174 74 Mean	StdDev 9.2 19.8 StdDev	$\begin{array}{c} & \text{ASP} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \end{array}$	m-30 n = 37239 Smooth COM -69 -29 Mean	StdDev 8.2 22.4 StdDev
ASI $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{Bond Angle}}$ $\frac{\text{C}\alpha \cdot \text{C}\beta \cdot \text{C}\gamma}{\text{C}\gamma}$	P t70 n = 6029 Smooth COM -174 74 Mean 112.4	StdDev 9.2 19.8 StdDev 0.83	$\begin{array}{c} X \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \\ \end{array}$	m-30 n = 37239 Smooth COM -69 -29 Mean 112.9	StdDev 8.2 22.4 StdDev 0.95
ASI $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{Bond Angle}}$ $\frac{\text{C}\alpha \cdot \text{C}\beta \cdot \text{C}\gamma}{\text{C}\alpha \cdot \text{C} \cdot \text{O}}$	P t70 n = 6029 Smooth COM -174 74 Mean 112.4 120.5	StdDev 9.2 19.8 StdDev 0.83 0.80	ASP $\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ \end{array}$	m-30 n = 37239 Smooth COM -69 -29 Mean 112.9 120.5	StdDev 8.2 22.4 StdDev 0.95 0.86
ASI $\frac{\chi}{\text{chi1}}$ chi2 Bond Angle} $\frac{\text{C}\alpha \text{-}\text{C}\beta \text{-}\text{C}\gamma}{\text{C}\alpha \text{-}\text{C} \text{-}\text{O}}$ $\frac{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}$	P t70 n = 6029 Smooth COM -174 74 Mean 112.4 120.5 110.1	StdDev 9.2 19.8 StdDev 0.83 0.80 1.27	ASP $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{Bond Angle}}$ $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}$	m-30 n = 37239 Smooth COM -69 -29 Mean 112.9 120.5 109.4	StdDev 8.2 22.4 StdDev 0.95 0.86 1.67
ASI $\frac{\chi}{\text{chi1}}$ chi2 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{O}\delta 1}$	P t70 n = 6029 Smooth COM -174 74 Mean 112.4 120.5 110.1 118.5	StdDev 9.2 19.8 StdDev 0.83 0.80 1.27 1.11	ASP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{O}\delta1 \end{array} $	m-30 n = 37239 Smooth COM -69 -29 Mean 112.9 120.5 109.4 119.2	StdDev 8.2 22.4 StdDev 0.95 0.86 1.67 1.36
ASI $\frac{\chi}{\text{chi1}}$ chi2 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{C}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{O}\delta 1}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{O}\delta 2}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{O}\delta 2}$	P t70 n = 6029 Smooth COM -174 74 Mean 112.4 120.5 110.1 118.5 118.7	9.2 19.8 StdDev 0.83 0.80 1.27 1.11 1.56	ASP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{O}\delta1 \\ \text{C}\beta_\text{C}\gamma_\text{O}\delta2 \end{array} $	m-30 n = 37239 Smooth COM -69 -29 Mean 112.9 120.5 109.4 119.2 118.2	StdDev 8.2 22.4 StdDev 0.95 0.86 1.67 1.36 1.70

Table S13: HIS Central Values

HIS	$\mathbf{p90} \text{ n} = 1492$		HIS	p-80 n = 2203	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62	9.7	chi1	65	9.9
chi2	87	21.8	chi2	-81	16.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.2	1.05	$C\alphaC\betaC\gamma$	114.1	1.06
$C\alphaCO$	120.6	0.95	$C\alphaCO$	120.4	0.98
$C\beta C\alpha C$	110.8	1.57	$C\beta C\alpha C$	110.4	1.53
$C\betaC\gammaC\delta_2$	131.0	0.86	$C\betaC\gammaC\delta_2$	131.0	0.80
$C\betaC\gammaN\delta 1$	122.8	0.91	$C\beta_C\gamma_N\delta 1$	122.7	0.81
$C\epsilon 1_N\epsilon 2_C\delta 2$	108.8	0.59	$C\epsilon 1_N\epsilon 2_C\delta 2$	108.8	0.58
$C\gamma_C\delta_2N\epsilon_2$	107.3	0.50	$C\gamma_C\delta_2N\epsilon_2$	107.2	0.52
$C\gamma_N\delta_1C\epsilon_1$	109.2	0.72	$C\gamma_N\delta_1C\epsilon_1$	109.2	0.61
$N\delta 1_C\epsilon 1_N\epsilon 2$	108.5	0.66	$N\delta 1_C\epsilon 1_N\epsilon 2$	108.5	0.60
$N\delta1_{-}C\gamma_{-}C\delta2$	106.2	0.53	$N\delta1_{-}C\gamma_{-}C\delta2$	106.2	0.51
$N_{-}C\alpha_{-}C$	111.3	2.74	$N_{-}C\alpha_{-}C$	112.0	2.43
$N_{-}C\alpha_{-}C\beta$	111.0	1.36	$N_{-}C\alpha_{-}C\beta$	111.0	1.32
HIS	8 t70 n = 5068		HIS	t-170 n = 1332	
χ	S t70 n = 5068 Smooth COM	StdDev	χ	t-170 n = 1332 Smooth COM	StdDev
		StdDev 10.0			StdDev 9.7
χ	Smooth COM		χ	Smooth COM	
$\frac{\chi}{\text{chi1}}$	Smooth COM -178	10.0	$\frac{\chi}{\text{chi1}}$	Smooth COM -173	9.7
χ chi1 chi2	Smooth COM -178 74	10.0 17.3	χ chi1 chi2	Smooth COM -173 -167	9.7 21.6
λ chi1 chi2 Bond Angle	Smooth COM -178 74 Mean	10.0 17.3 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -173 -167 Mean	9.7 21.6 StdDev
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$-$\text{C}\beta$-$\text{C}\gamma$} \end{array}$	Smooth COM -178 74 Mean 113.6	10.0 17.3 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$-$\text{C}\beta$-$\text{C}\gamma$} \end{array}$	Smooth COM -173 -167 Mean 114.2	9.7 21.6 StdDev 1.02
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \end{array}$	Smooth COM -178 74 Mean 113.6 120.6	10.0 17.3 StdDev 1.07 0.83	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6	9.7 21.6 StdDev 1.02 0.81
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1	10.0 17.3 StdDev 1.07 0.83 1.34	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha\text{-}\text{C}\beta\text{-}\text{C}\gamma \\ \\ \text{C}\alpha\text{-}\text{C}\text{-}\text{O} \\ \\ \text{C}\beta\text{-}\text{C}\alpha\text{-}\text{C} \\ \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9	9.7 21.6 StdDev 1.02 0.81 1.31
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta2 \\ \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0	10.0 17.3 StdDev 1.07 0.83 1.34 0.82	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4	9.7 21.6 StdDev 1.02 0.81 1.31 0.98
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$-C\beta$-$Cγ} \\ \text{$C\alpha$-C-$O} \\ \text{$C\beta$-$Cα-C} \\ \text{$C\beta$-C\gamma$-$Cδ2} \\ \text{$C\beta$-C\gamma$-$Nδ1} \\ \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0 122.7	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$O} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta2$} \\ \text{$C\beta$_$C}\gamma_\text{$N\delta1$} \\ \text{$C\epsilon1$_$N$$\epsilon2$_$C}\delta2 \\ \text{$C\gamma$_$C}\delta2_\text{$N\epsilon2$} \\ \hline \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}-\text{$C} \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta 1 \\ \text{$C\epsilon 1.N}\epsilon 2.C}\delta 2 \\ \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0 122.7 108.9	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_\text{$C\gamma$} \\ \hline \\ \text{$C\alpha$_C_$O} \\ \hline \\ \text{$C\beta$_$Cα_$C} \\ \hline \\ \text{$C\beta$_$Cγ_C\delta2} \\ \hline \\ \text{$C\beta$_C\gamma$_$N$\delta1} \\ \hline \\ \text{$C\epsilon1$_N\epsilon2$_$C$\delta2} \\ \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4 108.8	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05 0.55
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}_0 \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta 1 \\ \text{$C\epsilon$1_N}\epsilon 2.C\delta 2 \\ \text{$C\gamma$_$C}\delta 2.N\epsilon 2 \\ \hline \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0 122.7 108.9 107.2	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52 0.46	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$O} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta2$} \\ \text{$C\beta$_$C}\gamma_\text{$N\delta1$} \\ \text{$C\epsilon1$_$N$$\epsilon2$_$C}\delta2 \\ \text{$C\gamma$_$C}\delta2_\text{$N\epsilon2$} \\ \hline \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4 108.8 107.2	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05 0.55 0.45
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\beta_C\gamma_N\delta1$} \\ \hline \\ \text{$C\epsilon1_N\epsilon2_C\delta2$} \\ \hline \\ \text{$C\gamma_C\delta2_N\epsilon2$} \\ \hline \\ \text{$C\gamma_N\delta1_C\epsilon1$} \\ \hline \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0 122.7 108.9 107.2 109.2	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52 0.46 0.62	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta2$} \\ \text{$C\beta_C\gamma_N\delta1$} \\ \text{$C\epsilon1_N\epsilon2_C\delta2$} \\ \text{$C\gamma_C\delta2_N\epsilon2$} \\ \text{$C\gamma_N\delta1_C\epsilon1$} \\ \hline \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4 108.8 107.2 109.2	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05 0.55 0.45 0.66
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta2$} \\ \text{$C\beta_C\gamma_N\delta1$} \\ \text{$C\epsilon1_N\epsilon2_C\delta2$} \\ \text{$C\gamma_C\delta2_N\epsilon2$} \\ \text{$C\gamma_N\delta1_C\epsilon1$} \\ \text{$N\delta1_C\epsilon1_N\epsilon2$} \\ \end{array}$	Smooth COM -178 74 Mean 113.6 120.6 110.1 131.0 122.7 108.9 107.2 109.2 108.5	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52 0.46 0.62 0.56	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}C \\ \text{$C\beta$_$C}\alpha$_$C \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta 1 \\ \text{$C\epsilon 1$_$N}\epsilon 2 _$C}\delta 2 \\ \text{$C\gamma$_$C}\delta 2 _$N}\epsilon 2 \\ \text{$C\gamma$_$N}\delta 1 _$C}\epsilon 1 \\ \text{$N\delta 1$_$C}\epsilon 1 _$N}\epsilon 2 \\ \hline \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4 108.8 107.2 109.2 108.6	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05 0.55 0.45 0.66 0.63

TITO	4.00 2552			150 0005	
HIS	t-90 n = 3553		HIS	m170 n = 2695	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173	10.4	chi1	-68	8.2
chi2	-87	18.5	chi2	171	21.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.7	1.01	$C\alphaC\betaC\gamma$	113.7	0.93
$C\alphaCO$	120.5	0.85	$C\alphaCO$	120.4	0.88
$C\beta C\alpha C$	110.4	1.22	$C\beta C\alpha C$	109.7	1.79
$C\betaC\gammaC\delta_2$	130.9	0.83	$C\betaC\gammaC\delta_2$	131.1	0.99
$C\beta C\gamma N\delta 1$	122.8	0.75	$C\betaC\gammaN\delta 1$	122.6	1.04
$C\epsilon 1_N\epsilon 2_C\delta 2$	108.8	0.52	$C\epsilon 1_N\epsilon 2_C\delta 2$	108.8	0.53
$C\gamma_C\delta_2N\epsilon_2$	107.2	0.48	$C\gamma_C\delta_2N\epsilon_2$	107.2	0.47
$C\gamma N\delta 1C\epsilon 1$	109.2	0.72	$C\gamma N\delta 1C\epsilon 1$	109.2	0.69
$N\delta1_{-}C\epsilon1_{-}N\epsilon2$	108.5	0.62	$N\delta1_C\epsilon1_N\epsilon2$	108.6	0.62
$N\delta1_{-}C\gamma_{-}C\delta2$	106.2	0.55	$N\delta1_{-}C\gamma_{-}C\delta2$	106.2	0.53
$N_{-}C\alpha_{-}C$	109.9	2.47	$N_{-}C\alpha_{-}C$	111.5	2.54
$N_{-}C\alpha_{-}C\beta$	110.1	1.46	$N_{-}C\alpha_{-}C\beta$	110.7	1.15
	m90 n = 3914			m-70 n = 9453	-
	m90 n = 3914 Smooth COM	StdDev			StdDev
HIS			HIS	m-70 n = 9453	
HIS χ	Smooth COM	StdDev	HIS χ	m-70 n = 9453 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -66	StdDev 9.8	HIS χ chi1	m-70 n = 9453 Smooth COM -64	StdDev 10.0
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM -66 88	StdDev 9.8 17.5	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	m-70 n = 9453 Smooth COM -64 -75	StdDev 10.0 19.3
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \end{array}$	Smooth COM -66 88 Mean	StdDev 9.8 17.5 StdDev	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{Bond Angle} \end{array}$	m-70 n = 9453 Smooth COM -64 -75 Mean	StdDev 10.0 19.3 StdDev
HIS $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{Bond Angle}}$ $\frac{\text{C}\alpha_{\text{-}}\text{C}\beta_{\text{-}}\text{C}\gamma}{\text{C}\gamma}$	Smooth COM -66 88 Mean 113.5	9.8 17.5 StdDev	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha\text{-}\text{C}\beta\text{-}\text{C}\gamma \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4	StdDev 10.0 19.3 StdDev 1.06
HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha\text{-C}\beta\text{-C}\gamma \\ \text{C}\alpha\text{-C-O} \end{array} $	Smooth COM -66 88 Mean 113.5 120.5	9.8 17.5 StdDev 1.11 0.90	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4	StdDev 10.0 19.3 StdDev 1.06 0.87
HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha\text{-C}\beta\text{-C}\gamma \\ \text{C}\alpha\text{-C}\text{-O} \\ \text{C}\beta\text{-C}\alpha\text{-C} \end{array} $	Smooth COM -66 88 Mean 113.5 120.5 109.8	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89
HIS $ \frac{\chi}{\text{chi1}} $ $ \frac{\text{chi2}}{\text{Bond Angle}} $ $ \frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}} $ $ \frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2}} $	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9	9.8 17.5 StdDev 1.11 0.90 1.96 0.85	HIS $ \frac{\chi}{\text{chi1}} $ chi2 $ \text{Bond Angle} $ $ \frac{C\alpha \text{-}C\beta \text{-}C\gamma}{C\alpha \text{-}C \text{-}C} $ $ \frac{C\beta \text{-}C\alpha \text{-}C}{C\beta \text{-}C\gamma \text{-}C\delta 2} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82
HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{N}\delta1 \end{array} $	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9 122.8	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta_{1} \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80
HIS $\frac{\chi}{\text{chi1}}$ chi2 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2}}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta_{1}}{\text{C}\epsilon_{1}.\text{N}\epsilon_{2}.\text{C}\delta_{2}}$	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82 0.56	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta2 \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta1 \\ \text{C}\epsilon1_{-}\text{N}\epsilon2_{-}\text{C}\delta2 \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52
HIS $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi2}}$ Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{C}}$ $\frac{\text{C}\alpha_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2}}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta_{1}}{\text{C}\epsilon_{1}\text{-N}\epsilon_{2}\text{-C}\delta_{2}}$ $\frac{\text{C}\gamma_{-}\text{C}\delta_{2}\text{-N}\epsilon_{2}}{\text{C}\gamma_{-}\text{C}\delta_{2}\text{-N}\epsilon_{2}}$	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82 0.56 0.50	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \\ \text{C}\beta_\text{C}\gamma_\text{N}\delta1 \\ \text{C}\epsilon1_\text{N}\epsilon2_\text{C}\delta2 \\ \text{C}\gamma_\text{C}\delta2_\text{N}\epsilon2 \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9 107.2	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52 0.47
HIS $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi2}}$ Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2}}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta_{1}}{\text{C}\epsilon_{1}.\text{N}\epsilon_{2}.\text{C}\delta_{2}.\text{N}\epsilon_{2}}$ $\frac{\text{C}\gamma_{-}\text{N}\delta_{1}.\text{C}\epsilon_{1}}{\text{C}\epsilon_{1}.\text{N}\epsilon_{1}.\text{C}\epsilon_{1}}$	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2 109.2	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82 0.56 0.50 0.64	HIS $ \frac{\chi}{\text{chi1}} $ chi2 $ \text{Bond Angle} $ $ \frac{C\alpha \text{_}C\beta \text{_}C\gamma}{C\alpha \text{_}C} $ $ \frac{C\alpha \text{_}C\beta \text{_}C\gamma \text{_}C\delta 2}{C\beta \text{_}C\gamma \text{_}C\delta 2} $ $ \frac{C\beta \text{_}C\gamma \text{_}C\delta 2}{C\gamma \text{_}C\delta 2} $ $ \frac{C\gamma \text{_}C\delta 2 \text{_}N\epsilon 2}{C\gamma \text{_}N\delta 1 \text{_}C\epsilon 1} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9 107.2 109.2	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52 0.47 0.63
HIS $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi2}}$ Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta_{2}}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{N}\delta_{1}}{\text{C}\epsilon_{1}\text{N}\epsilon_{2}\text{C}\delta_{2}}$ $\frac{\text{C}\gamma_{-}\text{C}\delta_{2}\text{N}\epsilon_{2}}{\text{C}\gamma_{-}\text{N}\delta_{1}\text{C}\epsilon_{1}}$ $\frac{\text{N}\delta_{1}\text{C}\epsilon_{1}\text{N}\epsilon_{2}}{\text{N}\epsilon_{2}\text{C}\epsilon_{1}\text{N}\epsilon_{2}}$	Smooth COM -66 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2 109.2 108.5	StdDev 9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82 0.56 0.50 0.64 0.61	HIS $ \frac{\chi}{\text{chi1}} $ chi2 $ \text{Bond Angle} $ $ \frac{C\alpha \text{_}C\beta \text{_}C\gamma}{C\alpha \text{_}C \text{_}C} $ $ \frac{C\beta \text{_}C\gamma \text{_}C\delta 2}{C\beta \text{_}C\gamma \text{_}N\delta 1} $ $ \frac{C\epsilon 1 \text{_}N\epsilon 2 \text{_}C\delta 2}{C\gamma \text{_}N\delta 1 \text{_}C\epsilon 1} $ $ \frac{N\delta 1 \text{_}C\epsilon 1 \text{_}N\epsilon 2}{N\delta 2} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9 107.2 109.2 108.5	StdDev 10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52 0.47 0.63 0.56

Table S14: PHE Central Values

PHI	E p90 n = 6289		PHI	E t80 n = 19289	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64	9.6	chi1	-178	10.0
chi2	-90	9.4	chi2	76	17.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.4	0.97	$C\alphaC\betaC\gamma$	113.8	1.07
$C\alphaCO$	120.7	0.89	$C\alphaCO$	120.6	0.80
$C\betaC\alphaC$	110.9	1.46	$C\betaC\alphaC$	110.3	1.30
$C\betaC\gammaC\delta 1$	120.7	0.62	$C\beta C\gamma C\delta 1$	120.6	0.72
$C\betaC\gammaC\delta_2$	120.6	0.58	$C\betaC\gammaC\delta_2$	120.5	0.68
$C\delta 1_C\epsilon 1_C\zeta$	119.9	0.60	$C\delta1_C\epsilon1_C\zeta$	119.9	0.59
$C\delta1C\gammaC\delta2$	118.6	0.53	$C\delta1C\gammaC\delta2$	118.8	0.55
$C\epsilon 1_C \zeta_C \epsilon 2$	119.8	0.63	$C\epsilon 1_C \zeta_C \epsilon 2$	119.9	0.63
$C\gamma C\delta 1 C\epsilon 1$	120.9	0.59	$C\gamma_C\delta_1C\epsilon_1$	120.8	0.58
$C\gammaC\delta_2C\epsilon_2$	120.9	0.58	$C\gammaC\delta_2C\epsilon_2$	120.8	0.59
$C\zetaC\epsilon_2C\delta_2$	119.9	0.59	$C\zetaC\epsilon_2C\delta_2$	119.9	0.59
$N_{-}C\alpha_{-}C$	110.9	2.57	$N_{-}C\alpha_{-}C$	110.3	2.31
$N_{-}C\alpha_{-}C\beta$	111.4	1.32	$N_C\alpha_C\beta$	110.2	1.50
PHE	2 m-10 n = 3880		PHE	m-80 n = 26665	ó
V	Smooth COM	~		0 1 0015	~
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	-68	StdDev 9.3	$\frac{\chi}{\text{chi1}}$	-67	StdDev 10.1
chi1	-68	9.3	chi1	-67	10.1
$\begin{array}{c} \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	-68 -15 Mean 114.8	9.3 19.8	chi1 chi2 Bond Angle $C\alpha$ - $C\beta$ - $C\gamma$	-67 -81 Mean 113.5	10.1 16.8
chi1 chi2 Bond Angle	-68 -15 Mean	9.3 19.8 StdDev	chi1 chi2 Bond Angle	-67 -81 Mean	10.1 16.8 StdDev
$\begin{array}{c} \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	-68 -15 Mean 114.8	9.3 19.8 StdDev	chi1 chi2 Bond Angle $C\alpha$ - $C\beta$ - $C\gamma$	-67 -81 Mean 113.5	10.1 16.8 StdDev 1.02
chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C O$	-68 -15 Mean 114.8 120.4	9.3 19.8 StdDev 0.96 0.87	chi1 chi2 Bond Angle $C\alpha \text{-}C\beta \text{-}C\gamma$ $C\alpha \text{-}C \text{-}O$	-67 -81 Mean 113.5 120.5	10.1 16.8 StdDev 1.02 0.86
chi1 chi2 Bond Angle $C\alpha \text{-}C\beta \text{-}C\gamma$ $C\alpha \text{-}C \text{-}O$ $C\beta \text{-}C\alpha \text{-}C$	-68 -15 Mean 114.8 120.4 108.9	9.3 19.8 StdDev 0.96 0.87 1.78	chi1 chi2 Bond Angle $C\alpha \cdot C\beta \cdot C\gamma$ $C\alpha \cdot C \cdot C$ $C\beta \cdot C\alpha \cdot C$	-67 -81 Mean 113.5 120.5 109.8	10.1 16.8 StdDev 1.02 0.86 1.99
chi1 chi2 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta 1$ $C\beta _C\gamma _C\delta 2$ $C\delta 1 _C\epsilon 1 _C\zeta$	-68 -15 Mean 114.8 120.4 108.9 121.5	9.3 19.8 StdDev 0.96 0.87 1.78 1.22	chi1 chi2 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta 1$ $C\beta _ C\gamma _ C\delta 2$ $C\delta 1_ C\epsilon 1_ C\zeta$	-67 -81 Mean 113.5 120.5 109.8 120.6	10.1 16.8 StdDev 1.02 0.86 1.99 0.60
chi1 chi2 Bond Angle $C\alpha \text{-}C\beta \text{-}C\gamma$ $C\alpha \text{-}C \text{-}O$ $C\beta \text{-}C\alpha \text{-}C$ $C\beta \text{-}C\gamma \text{-}C\delta 1$ $C\beta \text{-}C\gamma \text{-}C\delta 2$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16	chi1 chi2 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta 1$ $C\beta_{-}C\gamma_{-}C\delta 2$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59
chi1 chi2 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta 1$ $C\beta _C\gamma _C\delta 2$ $C\delta 1 _C\epsilon 1 _C\zeta$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9 119.9	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61	chi1 chi2 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta 1$ $C\beta _ C\gamma _ C\delta 2$ $C\delta 1_ C\epsilon 1_ C\zeta$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6 119.9	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58
chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\beta C\alpha C$ $C\beta C\gamma C\delta 1$ $C\beta C\gamma C\delta 2$ $C\delta 1 C\epsilon 1 C\zeta$ $C\delta 1 C\gamma C\delta 2$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9 119.9 118.5	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56	chi1 chi2 Bond Angle $C\alpha \text{-}C\beta \text{-}C\gamma$ $C\alpha \text{-}C\text{-}O$ $C\beta \text{-}C\alpha \text{-}C$ $C\beta \text{-}C\gamma \text{-}C\delta 1$ $C\beta \text{-}C\gamma \text{-}C\delta 2$ $C\delta 1 \text{-}C\epsilon 1 \text{-}C\zeta$ $C\delta 1 \text{-}C\gamma \text{-}C\delta 2$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53
chi1 chi2 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _C$ $C\beta _C\alpha _C$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta 1$ $C\beta _C\gamma _C\delta 2$ $C\delta 1 _C\epsilon 1 _C\epsilon$ $C\epsilon 1 _C\epsilon 2$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9 119.9 118.5 119.8	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56 0.62	chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\alpha C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta 1$ $C\beta C\gamma C\delta 2$ $C\delta 1.C\epsilon 1.C\zeta$ $C\delta 1.C\gamma C\delta 2$ $C\epsilon 1.C\zeta C\epsilon 2$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53 0.61
chi1 chi2 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta1$ $C\beta_C\gamma_C\delta2$ $C\delta1_C\epsilon1_C\zeta$ $C\delta1_C\gamma_C\delta2$ $C\epsilon1_C\zeta_C\epsilon2$ $C\gamma_C\delta1_C\epsilon1$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9 119.9 118.5 119.8 120.8	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56 0.62 0.60	chi1 chi2 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C\gamma$ $C\alpha_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta 1$ $C\beta_{-}C\gamma_{-}C\delta 2$ $C\delta 1_{-}C\delta 1_{-}C\zeta$ $C\delta 1_{-}C\gamma_{-}C\delta 2$ $C\epsilon 1_{-}C\zeta_{-}C\epsilon 2$ $C\gamma_{-}C\delta 1_{-}C\epsilon 1$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9 120.8	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53 0.61 0.56
chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C\gamma$ $C\alpha C C\gamma$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta 1$ $C\beta C\gamma C\delta 2$ $C\delta 1 C\gamma C\delta 2$	-68 -15 Mean 114.8 120.4 108.9 121.5 119.9 119.9 118.5 119.8 120.8 121.0	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56 0.62 0.60 0.61	chi1 chi2 Bond Angle $C\alpha = C\beta = C\gamma$ $C\alpha = CC$ $C\beta = C\alpha = C$ $C\beta = C\alpha = C$ $C\beta = C\alpha = C$ $C\beta = C\alpha = C\delta$ $C\delta$ $C\delta$ $C\delta$ $C\delta$ $C\delta$ $C\delta$ $C\delta$	-67 -81 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9 120.8 120.8	10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53 0.61 0.56 0.57

Table S15: TYR Central Values

TYI	R p90 n = 5466		TYI	R t80 n = 16312	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64	10.6	chi1	-178	10.5
chi2	-90	10.1	chi2	76	16.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.8	1.88	$C\alphaC\betaC\gamma$	113.7	2.14
$C\alphaCO$	120.7	0.93	$C\alphaCO$	120.6	0.80
$C\beta C\alpha C$	110.6	1.41	$C\beta C\alpha C$	110.3	1.25
$C\betaC\gammaC\delta 1$	121.0	0.65	$C\betaC\gammaC\delta 1$	120.9	0.66
$C\betaC\gammaC\delta_2$	120.9	0.60	$C\betaC\gammaC\delta 2$	120.8	0.65
$C\delta1_C\epsilon1_C\zeta$	119.5	0.62	$C\delta1_C\epsilon1_C\zeta$	119.5	0.60
$C\delta1_C\gamma_C\delta2$	118.1	0.55	$C\delta1C\gammaC\delta2$	118.2	0.52
$C\epsilon 1 C\zeta C\epsilon 2$	120.4	0.66	$C\epsilon 1_C \zeta_C \epsilon 2$	120.5	0.65
$C\epsilon 1_C \zeta_O H$	119.8	1.25	$C\epsilon 1_C\zeta_OH$	119.7	1.28
$C\gamma C\delta 1C\epsilon 1$	121.2	0.58	$C\gamma C\delta 1C\epsilon 1$	121.1	0.55
$C\gamma C\delta 2C\epsilon 2$	121.2	0.55	$C\gamma_C\delta_2C\epsilon_2$	121.1	0.56
$C\zetaC\epsilon_2C\delta_2$	119.6	0.62	$C\zetaC\epsilon_2C\delta_2$	119.5	0.63
$N_{-}C\alpha_{-}C$	111.1	2.66	$N_{-}C\alpha_{-}C$	110.4	2.25
$N_C\alpha_C\beta$	111.2	1.22	$N_{-}C\alpha_{-}C\beta$	110.2	1.44
$OH_C\zeta_C\epsilon 2$	119.7	1.24	$OH_C\zeta_C\epsilon 2$	119.7	1.28
TYR	m-10 n = 2623		TYR	m-80 n = 22683	3
χ	m-10 n = 2623 Smooth COM	StdDev	ΥΥR	m-80 n = 22683 Smooth COM	3 StdDev
			•		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -68	StdDev 9.9	$\frac{\chi}{\text{chi1}}$	Smooth COM -67	StdDev 10.4
χ chi1 chi2	Smooth COM -68 -15	StdDev 9.9 20.2	χ chi1 chi2	Smooth COM -67 -81	StdDev 10.4 16.8
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -68 -15 Mean	StdDev 9.9 20.2 StdDev	χ chi1 chi2 Bond Angle	Smooth COM -67 -81 Mean	StdDev 10.4 16.8 StdDev
χ chi1 chi2 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -68 -15 Mean 115.8	9.9 20.2 StdDev 1.57	χ chi1 chi2 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM -67 -81 Mean 113.2	StdDev 10.4 16.8 StdDev 2.04
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4	9.9 20.2 StdDev 1.57 0.84	χ chi1 chi2 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -67 -81 Mean 113.2 120.4	StdDev 10.4 16.8 StdDev 2.04 0.88
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha\text{_C}\beta\text{_C}\gamma \\ \\ \text{C}\alpha\text{_C_O} \\ \\ \text{C}\beta\text{_C}\alpha\text{_C} \\ \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4 109.1	9.9 20.2 StdDev 1.57 0.84 1.75	χ chi1 chi2 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$	Smooth COM -67 -81 Mean 113.2 120.4 109.6	10.4 16.8 StdDev 2.04 0.88 1.92
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha$_C\beta$_$Cγ} \\ \text{$C\alpha$_C_$C} \\ \text{$C\beta$_$Cα_C} \\ \text{$C\beta$_C\alpha$_$C$} \\ \text{$C\beta$_$Cγ_C\delta$1} \\ \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6	9.9 20.2 StdDev 1.57 0.84 1.75 1.01	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_C\beta$_$Cγ} \\ \text{$C\alpha$_C-C0} \\ \text{$C\beta$_C\alpha$_$C$} \\ \text{$C\beta$_$Cγ_C\delta$1} \\ \text{$C\beta$_$Cγ_C\delta$2} \\ \text{$C\delta1_C\varsigma1_C\zeta$} \\ \text{$C\delta1_C\gamma$_$Cδ2} \\ \hline \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2 120.5	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C_$O} \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta1 \\ \text{$C\beta$_$C}\gamma$_$C}\delta2 \\ \text{$C\delta1$_$C}\epsilon1.C\zeta \\ \text{$C\delta1$_$C}\gamma$_$C}\delta2 \\ \hline \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta1$} \\ \text{$C\beta_C\gamma_C\delta2$} \\ \text{$C\delta1_C\epsilon1_C\zeta$} \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \text{$C\epsilon1_C\zeta_C\epsilon2$} \\ \hline \end{array}$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57 0.65	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2 120.5	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58 0.73
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4 120.1	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57 0.65 1.32	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2 120.5 119.7	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58 0.73 1.24
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4 120.1 121.1	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57 0.65 1.32 0.60	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2 120.5 119.7 121.1	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58 0.73 1.24 0.86
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4 120.1 121.1 121.3	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57 0.65 1.32 0.60 0.57	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 120.9 119.5 118.2 120.5 119.7 121.1 121.1	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58 0.73 1.24 0.86 0.86
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -15 Mean 115.8 120.4 109.1 121.6 120.4 119.5 118.0 120.4 120.1 121.1 121.3 119.7	9.9 20.2 StdDev 1.57 0.84 1.75 1.01 0.94 0.62 0.57 0.65 1.32 0.60 0.57 0.64	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 -81 Mean 113.2 120.4 109.6 120.9 119.5 118.2 120.5 119.7 121.1 121.1 119.5	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90 0.58 0.73 1.24 0.86 0.86 0.90

Table S16: TRP Central Values

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TR	P p90 n = 971		TRP	\mathbf{p} -90 n = 1937	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	60	9.9	chi1	62	9.8
chi2	88	14.7	chi2	-89	12.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	115.0	2.04	$C\alphaC\betaC\gamma$	115.0	1.90
$C\alphaCO$	120.6	0.86	$C\alphaCO$	120.5	0.93
$C\beta C\alpha C$	110.7	1.41	$C\beta C\alpha C$	110.5	1.43
$C\betaC\gammaC\delta 1$	127.0	0.70	$C\beta C\gamma C\delta 1$	126.9	0.67
$C\betaC\gammaC\delta 2$	126.7	0.76	$C\betaC\gammaC\delta_2$	126.9	0.71
$C\delta1_C\gamma_C\delta2$	106.2	0.38	$C\delta1_C\gamma_C\delta2$	106.2	0.44
$C\delta1_N\epsilon1_C\epsilon2$	108.9	0.60	$C\delta1_N\epsilon1_C\epsilon2$	109.0	0.46
$C\delta2_C\epsilon2_C\zeta2$	122.5	0.37	$C\delta2_C\epsilon2_C\zeta2$	122.4	0.34
$C\delta 2_{-}C\epsilon 3_{-}C\zeta 3$	118.7	0.34	$C\delta 2_C\epsilon 3_C\zeta 3$	118.7	0.47
$C\epsilon 2_C\delta 2_C\epsilon 3$	118.8	0.36	$C\epsilon 2_C\delta 2_C\epsilon 3$	118.8	0.39
$C\epsilon 2_C\delta 2_C\gamma$	107.3	0.31	$C\epsilon 2_C\delta 2_C\gamma$	107.2	0.33
$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.42	$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.46
$C\gamma_C\delta_1N\epsilon_1$	110.2	0.50	$C\gamma_C\delta_1N\epsilon_1$	110.2	0.46
$C\gamma_C\delta_2C\epsilon_3$	133.9	0.34	$C\gamma_C\delta_2C\epsilon_3$	133.9	0.41
$C\eta 2_C\zeta 2_C\epsilon 2$	117.5	0.45	$C\eta_2C\zeta_2C\epsilon_2$	117.5	0.44
$C\zeta_3 C\eta_2 C\zeta_2$	121.5	0.46	$C\zeta_3C\eta_2C\zeta_2$	121.5	0.46
$N\epsilon 1_C\epsilon 2_C\delta 2$	107.4	0.37	$N\epsilon 1_C\epsilon 2_C\delta 2$	107.4	0.34
$N\epsilon 1_C\epsilon 2_C\zeta 2$	130.1	0.40	$N\epsilon 1_C\epsilon 2_C\zeta 2$	130.1	0.41
$N_{-}C\alpha_{-}C$	111.2	2.41	$N_{-}C\alpha_{-}C$	112.1	2.60
$NC\alphaC\beta$	111.1	1.26	$N_{-}C\alpha_{-}C\beta$	111.1	1.24

TRI	P t60 n = 3385		TRP	t-100 n = 2893	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-179	9.8	chi1	-177	11.6
chi2	65	32.8	chi2	-103	15.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.3	2.14	$C\alphaC\betaC\gamma$	113.6	2.32
$C\alphaCO$	120.7	0.81	$C\alphaCO$	120.6	0.87
$C\betaC\alphaC$	110.6	1.35	$C\betaC\alphaC$	110.3	1.33
$C\betaC\gammaC\delta 1$	127.1	0.79	$C\betaC\gammaC\delta 1$	126.9	0.69
$C\betaC\gammaC\delta_2$	126.5	0.82	$C\betaC\gammaC\delta_2$	126.7	0.71
$C\delta1C\gammaC\delta2$	106.3	0.48	$C\delta1C\gammaC\delta2$	106.3	0.42
$C\delta 1_N\epsilon 1_C\epsilon 2$	108.9	0.51	$C\delta1_N\epsilon1_C\epsilon2$	108.9	0.45
$C\delta 2_{-}C\epsilon 2_{-}C\zeta 2$	122.4	0.40	$C\delta2_C\epsilon2_C\zeta2$	122.4	0.36
$C\delta2_C\epsilon3_C\zeta3$	118.7	0.42	$C\delta2_C\epsilon3_C\zeta3$	118.7	0.45
$C\epsilon 2_C\delta 2_C\epsilon 3$	118.9	0.38	$C\epsilon 2_C\delta 2_C\epsilon 3$	118.8	0.35
$C\epsilon 2_C\delta 2_C\gamma$	107.3	0.38	$C\epsilon 2_C\delta 2_C\gamma$	107.2	0.32
$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.48	$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.48
$C\gamma_C\delta_1N\epsilon_1$	110.1	0.53	$C\gamma_C\delta_1N\epsilon_1$	110.1	0.48
$C\gamma_C\delta_2C\epsilon_3$	133.9	0.43	$C\gamma_C\delta_2C\epsilon_3$	133.9	0.37
$C\eta_2C\zeta_2C\epsilon_2$	117.5	0.46	$C\eta_2C\zeta_2C\epsilon_2$	117.5	0.45
$C\zeta_3 C\eta_2 C\zeta_2$	121.5	0.48	$C\zeta_3 C\eta_2 C\zeta_2$	121.5	0.46
$N\epsilon 1_C\epsilon 2_C\delta 2$	107.5	0.38	$N\epsilon 1_C\epsilon 2_C\delta 2$	107.4	0.34
$N\epsilon 1_C\epsilon 2_C\zeta 2$	130.1	0.46	$N\epsilon 1_C\epsilon 2_C\zeta 2$	130.1	0.43
$N_{-}C\alpha_{-}C$	110.1	2.15	$NC\alphaC$	110.5	2.42
$N_{-}C\alpha_{-}C\beta$	110.0	1.42	$N_{-}C\alpha_{-}C\beta$	110.3	1.42
			,		
TRP	m100 n = 6319			m-10 n = 2196	
χ	m100 n = 6319 Smooth COM	StdDev			StdDev
			TRP	m-10 n = 2196	
χ	Smooth COM	StdDev	χ	m-10 n = 2196 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -67	StdDev 10.8	χ chi1	m-10 n = 2196 Smooth COM -68	StdDev 9.0
χ chi1 chi2	Smooth COM -67 97	StdDev 10.8 17.0	$\begin{array}{c} \text{TRP} \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	m-10 n = 2196 Smooth COM -68 -7	StdDev 9.0 21.7
χ chi1 chi2 Bond Angle	Smooth COM -67 97 Mean	StdDev 10.8 17.0 StdDev	$\begin{array}{c} \text{TRP} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \end{array}$	m-10 n = 2196 Smooth COM -68 -7 Mean	StdDev 9.0 21.7 StdDev 1.64
χ chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM -67 97 Mean 113.2	StdDev 10.8 17.0 StdDev 2.22	$\begin{array}{c} \text{TRP} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \end{array}$	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7	StdDev 9.0 21.7 StdDev
χ chi1 chi2 Bond Angle $C\alpha \text{-}C\beta \text{-}C\gamma$ $C\alpha \text{-}C\text{-}O$ $C\beta \text{-}C\alpha \text{-}C$	Smooth COM -67 97 Mean 113.2 120.4	StdDev 10.8 17.0 StdDev 2.22 0.86	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5	StdDev 9.0 21.7 StdDev 1.64 0.88
χ chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C-O$	Smooth COM -67 97 Mean 113.2 120.4 109.6	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92	$\begin{array}{c} \text{TRP} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ \end{array}$	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{C}\delta1 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{C}\delta1 \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1	9.0 21.7 StdDev 1.64 0.88 1.71 0.71
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta1 \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \\ \text{C}\delta1_\text{C}\gamma_\text{C}\delta2 \\ \hline \\ \text{C}\delta1_\text{C}\gamma_\text{C}\delta2 \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C_ O \\ C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 1 \\ C\beta _ C\gamma _ C\delta 2 \end{array} $ $ \begin{array}{c} C\delta _ C\gamma _ C\delta 2 \\ C\delta _ C\gamma _ C\delta 2 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha \text{_}C\beta \text{_}C\gamma \\ C\alpha \text{_}C\text{_}O \\ C\beta \text{_}C\alpha \text{_}C \end{array} $ $ \begin{array}{c} C\beta \text{_}C\gamma \text{_}C\delta 1 \\ C\beta \text{_}C\gamma \text{_}C\delta 2 \\ C\delta 1 \text{_}C\gamma \text{_}C\delta 2 \end{array} $ $ \begin{array}{c} C\delta 1 \text{_}C\gamma \text{_}C\delta 2 \\ C\delta 1 \text{_}N\epsilon 1 \text{_}C\epsilon 2 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha \text{_}C\beta \text{_}C\gamma \\ C\alpha \text{_}C \text{_}C\gamma \\ C\beta \text{_}C\alpha \text{_}C \end{array} $ $ \begin{array}{c} C\beta \text{_}C\gamma \text{_}C\delta 1 \\ C\beta \text{_}C\gamma \text{_}C\delta 2 \\ C\delta 1 \text{_}N\epsilon 1 \text{_}C\epsilon 2 \\ C\delta 2 \text{_}C\epsilon 2 \text{_}C\zeta 2 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta1 \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \end{array} $ $ \begin{array}{c} \text{C}\delta1_\text{C}\gamma_\text{C}\delta2 \end{array} $ $ \begin{array}{c} \text{C}\delta1_\text{N}\epsilon1_\text{C}\epsilon2 \end{array} $ $ \begin{array}{c} \text{C}\delta2_\text{C}\epsilon2_\text{C}\zeta2 \end{array} $ $ \begin{array}{c} \text{C}\delta2_\text{C}\epsilon3_\text{C}\zeta3 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.41 0.43
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C _ O \\ C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 1 \\ C\beta _ C\gamma _ C\delta 2 \\ C\delta 1 _ N\epsilon 1 _ C\epsilon 2 \\ C\delta 2 _ C\epsilon 2 _ C\zeta 2 \\ C\delta 2 _ C\epsilon 3 _ C\zeta 3 \\ C\epsilon 2 _ C\delta 2 _ C\epsilon 3 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_C\beta$_$Cγ} \\ \text{$C\alpha$_C-$O} \\ \text{$C\beta$_$Cα_$C} \\ \text{$C\beta$_$Cγ_C\delta$1} \\ \text{$C\beta$_$Cγ_C\delta$2} \\ \text{$C\delta$1.$Nϵ1.C\epsilon$2} \\ \text{$C\delta$1.$Nϵ1.C\epsilon$2} \\ \text{$C\delta$2.$Cϵ2.C\zeta$2} \\ \text{$C\delta$2.$Cϵ2.C\zeta$2} \\ \text{$C\epsilon$2.$Cδ2.C\epsilon$3} \\ \text{$C\epsilon$2.$Cδ2.C\epsilon$3} \\ \text{$C\epsilon$2.$Cδ2.C\epsilon$3} \\ \hline \\ \text{$C\epsilon$2.$Cδ2.C\gamma$} \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C _ O \\ C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 1 \\ C\beta _ C\gamma _ C\delta 2 \\ C\delta 1 _ C\gamma _ C\delta 2 \\ C\delta 1 _ N\epsilon 1 _ C\epsilon 2 \\ C\delta 2 _ C\epsilon 2 _ C\zeta 2 \\ C\delta 2 _ C\epsilon 3 _ C\zeta 3 \\ C\epsilon 2 _ C\delta 2 _ C\epsilon 3 \\ C\epsilon 2 _ C\delta 2 _ C\epsilon 3 \\ C\epsilon 2 _ C\delta 2 _ C\gamma \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48	TRP $ \frac{\chi}{\text{chi1}} $ chi2 Bond Angle $ \frac{C\alpha . C\beta . C\gamma}{C\alpha . C} $ $ \frac{C\alpha . C}{C\beta . C\gamma} $ $ \frac{C\beta . C\gamma . C\delta 1}{C\beta . C\gamma . C\delta 2} $ $ \frac{C\delta 1 . N\epsilon 1 . C\epsilon 2}{C\delta 2 . C\epsilon 2 . C\epsilon 2} $ $ \frac{C\delta 2 . C\epsilon 3 . C\epsilon 3}{C\epsilon 2 . C\epsilon 3} $ $ \frac{C\epsilon 2 . C\delta 2 . C\epsilon 3}{C\epsilon 3 . C\epsilon 3} $ $ \frac{C\epsilon 3 . C\epsilon 3 . C\epsilon 3}{C\epsilon 3} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38 0.43
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48 0.49	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C _ O \end{array} $ $ \begin{array}{c} C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 1 \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 2 \end{array} $ $ \begin{array}{c} C\delta 1 _ N\epsilon 1 _ C\epsilon 2 \end{array} $ $ \begin{array}{c} C\delta 2 _ C\epsilon 2 _ C\epsilon 2 \end{array} $ $ \begin{array}{c} C\delta 2 _ C\epsilon 3 _ C\epsilon 3 \end{array} $ $ \begin{array}{c} C\epsilon 2 _ C\delta 2 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\epsilon 3 _ C\gamma \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38 0.43 0.48
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48 0.49 0.40	TRP $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C _ O \end{array} $ $ \begin{array}{c} C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta 1 \end{array} $ $ \begin{array}{c} C\delta 1 _ C\gamma _ C\delta 2 \end{array} $ $ \begin{array}{c} C\delta 1 _ N\epsilon 1 _ C\epsilon 2 \end{array} $ $ \begin{array}{c} C\delta 2 _ C\epsilon 2 _ C\zeta 2 \end{array} $ $ \begin{array}{c} C\delta 2 _ C\epsilon 3 _ C\zeta 3 \end{array} $ $ \begin{array}{c} C\epsilon 2 _ C\delta 2 _ C\epsilon 3 \end{array} $ $ \begin{array}{c} C\epsilon 2 _ C\delta 2 _ C\gamma \end{array} $ $ \begin{array}{c} C\epsilon 3 _ C\zeta 3 _ C\eta 2 \end{array} $ $ \begin{array}{c} C\gamma _ C\delta 1 _ N\epsilon 1 \end{array} $ $ \begin{array}{c} C\gamma _ C\delta 1 _ N\epsilon 1 \end{array} $ $ \begin{array}{c} C\gamma _ C\delta 2 _ C\epsilon 3 \end{array} $	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0 133.8	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38 0.48 0.39
$\frac{\chi}{\text{chi1}}$ $\frac{\chi}{\text{chi2}}$ Bond Angle $\frac{\chi}{\chi}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48 0.49 0.40 0.45	TRP	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0 133.8 117.5	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.41 0.43 0.38 0.38 0.48 0.39 0.47
$\frac{\chi}{\text{chi1}}$ $\frac{\chi}{\text{chi2}}$ Bond Angle $\frac{\chi}{\chi}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5 121.5	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48 0.49 0.40 0.45 0.46	TRP	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0 133.8 117.5 121.5	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38 0.48 0.39 0.47 0.46
$\frac{\chi}{\text{chi1}}$ $\frac{\chi}{\text{chi2}}$ Bond Angle $\frac{\chi}{\chi}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5 121.5 107.4	StdDev 10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46 0.37 0.33 0.48 0.49 0.40 0.45 0.46 0.35	TRP	m-10 n = 2196 Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0 133.8 117.5 121.5 107.5	StdDev 9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45 0.41 0.43 0.38 0.38 0.43 0.48 0.39 0.47 0.46 0.37

TRP m-90 n = 961					
χ	Smooth COM	StdDev			
chi1	-68	12.4			
chi2	-89	13.8			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}C\gamma$	113.8	2.48			
$C\alphaCO$	120.5	0.86			
$C\betaC\alphaC$	109.4	2.04			
$C\betaC\gammaC\delta 1$	126.7	0.72			
$C\betaC\gammaC\delta 2$	127.0	0.78			
$C\delta1_C\gamma_C\delta2$	106.3	0.44			
$C\delta1_N\epsilon1_C\epsilon2$	108.9	0.47			
$C\delta 2_C\epsilon 2_C\zeta 2$	122.4	0.35			
$C\delta 2_C\epsilon 3_C\zeta 3$	118.7	0.45			
$C\epsilon 2_C\delta 2_C\epsilon 3$	118.8	0.38			
$C\epsilon 2_C\delta 2_C\gamma$	107.2	0.32			
$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.46			
$C\gamma_{-}C\delta_{1}N\epsilon_{1}$	110.1	0.50			
$C\gamma_{-}C\delta_{-}C\epsilon_{3}$	133.9	0.38			
$C\eta_2$ _ $C\zeta_2$ _ $C\epsilon_2$	117.5	0.43			
$C\zeta_3 C\eta_2 C\zeta_2$	121.5	0.45			
$N\epsilon 1_C\epsilon 2_C\delta 2$	107.5	0.35			
$N\epsilon 1_C\epsilon 2_C\zeta 2$	130.1	0.43			
$N_{-}C\alpha_{-}C$	110.6	2.88			
$N_{-}C\alpha_{-}C\beta$	110.7	1.12			

Table S17: MET Central Values

MI	ET ppp n = 50		MET	Γ pp-130 n = 27	7
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	9.3	chi1	64	7.2
chi2	79	11.0	chi2	82	4.9
chi3	71	9.9	chi3	-154	27.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.7	1.79	$C\alpha_{-}C\beta_{-}C\gamma$	115.4	1.18
$C\alphaCO$	120.7	0.90	$C\alphaCO$	120.9	0.65
$C\betaC\alphaC$	111.2	1.57	$C\beta C\alpha C$	111.1	0.91
$C\beta_C\gamma_SD$	114.4	2.33	$C\betaC\gammaSD$	113.7	2.01
$C\gamma_SD_C\epsilon$	100.5	4.02	$C\gamma_SD_C\epsilon$	100.8	1.95
$N_{-}C\alpha_{-}C$	111.8	2.72	$N_{-}C\alpha_{-}C$	111.0	1.84
$N_{-}C\alpha_{-}C\beta$	110.9	1.02	$N_C\alpha_C\beta$	110.9	0.99
ME	$T \mathbf{ptp} \ n = 404$		MH	ET ptt $n = 260$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	8.5	chi1	65	8.2
chi2	-176	11.4	chi2	-178	9.1
chi3	73	11.6	chi3	179	15.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.6	1.80	$C\alphaC\betaC\gamma$	114.7	1.69
$C\alphaCO$	120.7	0.92	$C\alphaCO$	120.6	0.94
$C\betaC\alphaC$	110.3	1.46	$C\betaC\alphaC$	110.3	1.49
$C\betaC\gammaSD$	112.9	2.19	$C\beta C\gamma SD$	111.0	2.39
$C\gammaSDC\epsilon$	100.8	1.94	$C\gammaSDC\epsilon$	99.8	2.32
$N_{-}C\alpha_{-}C$	110.6	2.56	$N_{-}C\alpha_{-}C$	111.1	2.70
$N_{-}C\alpha_{-}C\beta$	111.0	1.23	$N_{-}C\alpha_{-}C\beta$	111.1	1.30
ME	T ptm $n = 375$		M	ET pmt $n = 7$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	8.2	chi1	71	3.4
chi2	179	10.2	chi2	-75	3.2
chi3	-72	11.6	chi3	-162	4.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.65	$C\alphaC\betaC\gamma$	114.8	0.77
$C\alphaCO$	120.6	0.93	$C\alphaCO$	121.0	0.64
$C\betaC\alphaC$	110.3	1.44	$C\betaC\alphaC$	111.1	1.13
$C\beta C\gamma SD$	112.8	2.11	$C\beta C\gamma SD$	111.7	2.28
$C\gamma_SD_C\epsilon$	100.9	1.82	$C\gamma_SD_C\epsilon$	100.2	1.91
$N_{-}C\alpha_{-}C$	110.9	2.77	$N_{-}C\alpha_{-}C$	109.0	1.55
$N_{-}C\alpha_{-}C\beta$	111.2	1.21	$N_{-}C\alpha_{-}C\beta$	111.6	1.28

ME	$T \mathbf{pmm} \ n = 42$		ME	$T \mathbf{tpp} \ n = 1138$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	73	7.8	chi1	-175	9.4
chi2	-69	6.7	chi2	64	8.0
chi3	-69	8.1	chi3	72	12.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	115.5	0.86	$C\alphaC\betaC\gamma$	114.2	1.35
$C\alphaCO$	120.6	0.79	$C\alphaCO$	120.5	0.84
$C\betaC\alphaC$	110.2	1.22	$C\betaC\alphaC$	110.3	1.13
$C\betaC\gammaSD$	115.2	2.54	$C\betaC\gammaSD$	113.7	2.02
$C\gamma_SD_C\epsilon$	101.1	1.58	$C\gammaSDC\epsilon$	100.7	1.77
$N_{-}C\alpha_{-}C$	112.3	2.69	$N_{-}C\alpha_{-}C$	110.7	2.23
$N_C\alpha_C\beta$	110.8	1.21	$N_{-}C\alpha_{-}C\beta$	110.5	1.17
MI	ET $\mathbf{tpt} \ n = 388$		ME	$T \mathbf{ttp} \ n = 1246$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173	8.7	chi1	-178	8.6
chi2	66	7.8	chi2	179	11.4
chi3	-156	31.2	chi3	72	10.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.1	1.39	$C\alphaC\betaC\gamma$	113.6	1.65
$C\alphaCO$	120.5	0.74	$C\alphaCO$	120.6	0.85
$C\betaC\alphaC$	110.5	1.13	$C\beta _C\alpha _C$	110.0	1.17
$C\beta C\gamma SD$	112.4	1.99	$C\beta C\gamma SD$	112.8	2.11
$C\gammaSDC\epsilon$	100.4	2.09	$C\gammaSDC\epsilon$	100.7	2.07
$N_{-}C\alpha_{-}C$	110.4	2.25	$N_{-}C\alpha_{-}C$	110.3	2.15
$N_{-}C\alpha_{-}C\beta$	110.3	1.36	$N_{-}C\alpha_{-}C\beta$	110.4	1.31
MI	ET $\mathbf{ttt} \ \mathbf{n} = 569$		ME	$T \mathbf{ttm} \ n = 1124$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	8.8	chi1	-175	9.3
chi2	177	9.5	chi2	180	8.2
chi3	176	15.5	chi3	-72	13.1
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	113.7	1.72	$C\alphaC\betaC\gamma$	113.5	1.71
$C\alphaCO$	120.6	0.96	$C\alphaCO$	120.5	0.80
$C\betaC\alphaC$	110.1	1.31	$C\betaC\alphaC$	110.0	1.17
$C\betaC\gammaSD$	110.6	2.20	$C\beta _C\gamma _SD$	112.8	2.16
$C\gammaSDC\epsilon$	100.1	1.66	$C\gammaSDC\epsilon$	100.8	1.74
$N_{-}C\alpha_{-}C$	110.2	2.43	$NC\alphaC$	110.1	2.40
$N_{-}C\alpha_{-}C\beta$	110.1	1.39	$N_{-}C\alpha_{-}C\beta$	110.4	1.33

MI	$MET \mathbf{tmt} n = 34$			$\frac{}{\text{MET tmm n}} = 276$		
χ	Smooth COM	StdDev	•	χ	Smooth COM	StdDev
chi1	-179	6.7		chi1	-177	7.3
chi2	-86	7.6		chi2	-82	6.8
chi3	174	24.4		chi3	-72	10.5
Bond Angle	Mean	StdDev	•	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.9	1.13		$C\alphaC\betaC\gamma$	115.0	1.37
$C\alphaCO$	120.7	0.56		$C\alphaCO$	120.5	0.78
$C\betaC\alphaC$	110.7	1.24		$C\betaC\alphaC$	111.0	1.24
$C\betaC\gammaSD$	112.8	1.77		$C\betaC\gammaSD$	114.0	2.12
$C\gamma_SD_C\epsilon$	100.3	1.37		$C\gamma_SD_C\epsilon$	100.8	1.64
$N_C\alpha_C$	110.0	2.89		$N_{-}C\alpha_{-}C$	109.9	2.10
$N_{-}C\alpha_{-}C\beta$	110.1	1.22		$N_{-}C\alpha_{-}C\beta$	110.1	1.16
ME	$\text{TT} \mathbf{mpp} \ \text{n} = 74$		Ċ	MF	ET mpt $n = 34$	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-77	13.7		chi1	-70	11.7
chi2	73	12.3		chi2	74	11.0
chi3	74	11.9		chi3	167	18.6
Bond Angle	Mean	StdDev		Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.36		$C\alphaC\betaC\gamma$	114.6	0.96
$C\alphaCO$	120.5	0.89		$C\alphaCO$	120.4	0.88
$C\betaC\alphaC$	109.9	1.63		$C\beta C\alpha C$	109.3	1.40
$C\betaC\gammaSD$	114.3	2.25		$C\beta C\gamma SD$	113.2	2.02
$C\gammaSDC\epsilon$	101.2	2.26		$C\gammaSDC\epsilon$	100.1	2.40
$N_{-}C\alpha_{-}C$	110.7	2.69		$N_C\alpha_C$	110.1	2.78
$N_{-}C\alpha_{-}C\beta$	110.8	1.20		$N_{-}C\alpha_{-}C\beta$	111.0	1.12
ME	T mpm $n = 13$			ME	$\Gamma \mathbf{mtp} \ \mathrm{n} = 2815$	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-77	5.1		chi1	-67	7.1
chi2	64	5.5		chi2	177	9.3
chi3	-102	5.0		chi3	70	10.1
Bond Angle	Mean	StdDev		Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	116.1	1.02		$C\alphaC\betaC\gamma$	113.1	1.64
$C\alphaCO$	120.7	0.73		$C\alphaCO$	120.5	0.84
$C\betaC\alphaC$	109.1	1.27		$C\betaC\alphaC$	110.0	1.59
$C\beta C\gamma SD$	115.9	2.31		$C\betaC\gammaSD$	112.8	2.08
$C\gamma_SD_C\epsilon$	100.4	1.56		$C\gammaSDC\epsilon$	100.8	1.73
$N_{-}C\alpha_{-}C$	110.7	1.81		$N_{-}C\alpha_{-}C$	111.3	2.35
$NC\alphaC\beta$	111.0	1.05		$NC\alphaC\beta$	110.5	1.01

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MET $\mathbf{mtt} \ \mathbf{n} = 1542$				
χ	Smooth COM	StdDev		
chi1	-67	7.7		
chi2	180	8.7		
chi3	-177	16.5		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.6	1.71		
$C\alphaCO$	120.5	0.82		
$C\betaC\alphaC$	109.4	1.67		
$C\betaC\gammaSD$	110.4	2.19		
$C\gamma_SD_C\epsilon$	100.1	1.97		
$N_{-}C\alpha_{-}C$	111.1	2.27		
$N_{-}C\alpha_{-}C\beta$	110.7	1.00		

$N_{-}C\alpha_{-}C\beta$	110.7	1.00
ME'	Γ mmp $n = 520$	
χ	Smooth COM	StdDev
chi1	-65	5.3
chi2	-62	6.3
chi3	102	9.3
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.2	1.41
$C\alphaCO$	120.3	0.80
$C\beta C\alpha C$	110.2	1.55
$C\betaC\gammaSD$	113.8	2.14
$C\gammaSDC\epsilon$	101.2	2.18
$N_{-}C\alpha_{-}C$	111.5	2.15
$N_C\alpha_C\beta$	110.8	1.10

$MET \mathbf{mmm} \ n = 3354$				
χ	Smooth COM	StdDev		
chi1	-66	8.9		
chi2	-61	8.8		
chi3	-69	10.2		
Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	114.0	1.29		
$C\alphaCO$	120.4	0.86		
$C\beta C\alpha C$	110.0	1.53		
$C\beta C\gamma SD$	113.7	1.95		
$C\gamma_SD_C\epsilon$	100.9	1.74		
$N_{-}C\alpha_{-}C$	111.6	2.38		
$N_{-}C\alpha_{-}C\beta$	110.7	1.02		

MET	$MET \mathbf{mtm} \ n = 1851$				
χ	Smooth COM	StdDev			
chi1	-66	7.9			
chi2	-178	10.7			
chi3	-74	10.8			
Bond Angle	Mean	StdDev			
$C\alphaC\betaC\gamma$	113.2	1.72			
$C\alphaCO$	120.5	0.90			
$C\betaC\alphaC$	109.9	1.63			
$C\betaC\gammaSD$	112.9	2.15			
$C\gamma_SD_C\epsilon$	100.8	1.78			
$N_{-}C\alpha_{-}C$	111.1	2.32			
$N_{-}C\alpha_{-}C\beta$	110.7	1.07			

MET mmt $n = 597$					
χ	Smooth COM	StdDev			
chi1	-65	8.7			
chi2	-64	9.4			
chi3	172	18.5			
Bond Angle	Mean	StdDev			
$C\alphaC\betaC\gamma$	113.9	1.44			
$C\alphaCO$	120.4	0.80			
$C\beta C\alpha C$	109.9	1.55			
$C\beta C\gamma SD$	112.1	2.04			
$C\gammaSDC\epsilon$	100.3	1.99			
$N_{-}C\alpha_{-}C$	111.5	2.25			
$N_{-}C\alpha_{-}C\beta$	110.6	0.94			

Table S18: GLU Central Values

GLU	pp20 n = 159		GL	$U \mathbf{pt0} n = 2800$	
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	8.1	chi1	65	8.4
chi2	86	8.0	chi2	-177	10.1
chi3	20	17.2	chi3	1	51.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.6	1.28	$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.60
$C\alpha_{-}C_{-}O$	120.4	0.85	$C\alpha_{-}C_{-}O$	120.5	0.93
$C\beta C\alpha C$	111.6	1.84	$C\beta C\alpha C$	110.5	1.50
$C\beta C\gamma C\delta$	114.1	1.30	$C\beta C\gamma C\delta$	112.9	1.53
$C\gammaC\deltaO\epsilon 1$	119.0	1.43	$C\gammaC\deltaO\epsilon 1$	118.9	1.38
$C\gammaC\deltaO\epsilon_2$	118.4	1.34	$C\gammaC\deltaO\epsilon_2$	118.2	1.35
$N_{-}C\alpha_{-}C$	110.8	2.54	$N_{-}C\alpha_{-}C$	111.3	2.67
$N_{-}C\alpha_{-}C\beta$	111.4	1.25	$N_{-}C\alpha_{-}C\beta$	111.1	1.18
$O\epsilon 1 C\delta O\epsilon 2$	122.6	1.02	$O\epsilon 1 C\delta O\epsilon 2$	122.9	1.15
CIII	pm20 n = 1485	,	CII	U tp30 n = 4616	
$\frac{\alpha}{\chi}$	Smooth COM	StdDev	${\chi}$	$\frac{\text{Smooth COM}}{\text{Smooth COM}}$	StdDev
chi1	69	8.8	chi1	-178	9.8
chi2	-85	8.6	chi2	65	9.2
chi3	16	21.7	chi3	26	26.1
	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.6	1.35	$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.39
$C\alpha_{-}C_{-}O$	120.2	0.83	$C\alpha_{-}C\beta_{-}C\gamma$	120.5	0.80
$C\betaC\alphaC$	110.5	1.25	$C\beta_{-}C\alpha_{-}C$	110.6	1.21
$C\beta$ _ $C\gamma$ _ $C\delta$	114.5	1.45	$C\beta$ _ $C\alpha$ _ $C\delta$	113.8	1.35
$C\gammaC\deltaO\epsilon 1$	119.8	1.71	$C\gamma_{-}C\delta_{-}O\epsilon 1$	119.3	1.46
$C\gammaC\deltaO\epsilon_2$	117.7	1.69	$C\gamma_{-}C\delta_{-}O\epsilon_{2}$	118.0	1.38
$N_{-}C\alpha_{-}C$	112.9	1.83	$N_{-}C\alpha_{-}C$	110.9	2.09
$N_{-}C\alpha_{-}C\beta$	110.9	1.05	$N_{-}C\alpha_{-}C\beta$	110.3	1.12
$O\epsilon 1 C\delta O\epsilon 2$	122.5	1.10	$O\epsilon 1 C\delta O\epsilon 2$	122.7	1.07
	tt0 n = 13610			J tm-30 n = 862	
	$\frac{\text{Cto II} = 13010}{\text{Smooth COM}}$	StdDev		$\frac{\text{Smooth COM}}{\text{Smooth COM}}$	StdDev
χ			χ		
chi1	-177	8.6	chi1	-170	8.6
chi2	178	10.3	chi2	-83	9.2
chi3	1	41.4	chi3	-29	17.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	113.5	1.74	$C\alphaC\betaC\gamma$	114.5	1.35
$C\alphaCO$	120.6	0.77	$C\alphaCO$	120.5	0.84
$C\betaC\alphaC$	110.1	1.17	$C\beta C\alpha C$	111.0	1.33
$C\betaC\gammaC\delta$	113.1	1.50	$C\betaC\gammaC\delta$	113.8	1.47
$C\gammaC\deltaO\epsilon 1$	119.0	1.27	$C\gammaC\deltaO\epsilon 1$	119.0	1.36
$C\gammaC\deltaO\epsilon 2$	118.0	1.27	$C\gammaC\deltaO\epsilon 2$	118.2	1.25
$N_{-}C\alpha_{-}C$	110.6	2.26	$N_{-}C\alpha_{-}C$	110.2	2.46
$N_{-}C\alpha_{-}C\beta$	110.4	1.37	$N_{-}C\alpha_{-}C\beta$	110.2	1.16
$O\epsilon1_C\delta_O\epsilon2$	123.1	1.07	$O\epsilon 1 C\delta O\epsilon 2$	122.8	1.17

GLU	$J \ \mathbf{mp0} \ n = 3671$	
χ	Smooth COM	StdDev
chi1	-67	7.3
chi2	83	9.4
chi3	3	27.5
Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.4	1.34
$C\alphaCO$	120.4	0.82
$C\betaC\alphaC$	109.7	1.42
$C\betaC\gammaC\delta$	114.2	1.40
$C\gammaC\deltaO\epsilon 1$	119.8	1.66
$C\gamma_C\delta_O\epsilon_2$	117.8	1.47
$N_C\alpha_C$	112.0	2.00
$N_C\alpha_C\beta$	110.6	1.06
$O\epsilon 1C\deltaO\epsilon 2$	122.4	1.18

GLU mt-10 $n = 21021$				
χ	Smooth COM	StdDev		
chi1	-67	7.7		
chi2	179	11.4		
chi3	-7	37.3		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.0	1.85		
$C\alphaCO$	120.5	0.82		
$C\betaC\alphaC$	110.0	1.73		
$C\betaC\gammaC\delta$	113.3	1.50		
$C\gammaC\deltaO\epsilon 1$	119.1	1.29		
$C\gamma C\delta O\epsilon 2$	117.9	1.29		
$N_{-}C\alpha_{-}C$	111.4	2.32		
$N_{-}C\alpha_{-}C\beta$	110.6	1.00		
$O\epsilon 1_C\delta_O\epsilon 2$	123.0	1.06		

GLU mm-30 $n = 9080$				
χ	Smooth COM	StdDev		
chi1	-66	8.7		
chi2	-67	10.6		
chi3	-32	26.9		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	114.0	1.41		
$C\alphaCO$	120.4	0.83		
$C\beta C\alpha C$	109.9	1.50		
$C\betaC\gammaC\delta$	113.4	1.34		
$C\gammaC\deltaO\epsilon 1$	119.2	1.35		
$C\gammaC\deltaO\epsilon 2$	118.2	1.26		
$N_{-}C\alpha_{-}C$	111.5	2.36		
$N_C\alpha_C\beta$	110.7	1.01		
$O\epsilon 1_C\delta_O\epsilon 2$	122.6	1.09		

Table S19: GLN Central Values

GLI	$\sqrt{pp30} n = 178$		GL	N pt0 n = 1885	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63	7.8	chi1	65	8.1
chi2	84	8.5	chi2	-177	11.3
chi3	30	20.9	chi3	-3	75.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.9	1.28	$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.53
$C\alphaCO$	120.3	0.95	$C\alphaCO$	120.5	0.96
$C\betaC\alphaC$	111.4	1.62	$C\betaC\alphaC$	110.4	1.52
$C\beta$ _ $C\gamma$ _ $C\delta$	113.6	1.40	$C\beta C\gamma C\delta$	112.5	1.47
$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.4	0.89	$C\gammaC\deltaN\epsilon_2$	116.5	0.95
$C\gammaC\deltaO\epsilon 1$	120.9	0.95	$C\gammaC\deltaO\epsilon 1$	120.8	0.97
N_Cα_C	111.0	2.55	$N_{-}C\alpha_{-}C$	111.3	2.63
$N_{-}C\alpha_{-}C\beta$	111.5	1.15	$N_{-}C\alpha_{-}C\beta$	110.9	1.18
$O\epsilon 1 C\delta N\epsilon 2$	122.6	0.67	$O\epsilon 1 C\delta N\epsilon 2$	122.6	0.75
	V pm20 n = 487			N tp40 n = 3618	
$\frac{\alpha}{\chi}$	Smooth COM	StdDev	$\frac{\alpha}{\chi}$	Smooth COM	StdDev
chi1	70	9.9	chi1	-177	8.7
chi2	-84	9.3	chi2	66	8.2
chi3	17	32.3	chi3	41	24.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.7	1.41	$C\alpha_{-}C\beta_{-}C\gamma$	113.9	1.42
$C\alphaCO$	120.3	0.93	$C\alphaCO$	120.4	0.79
$C\betaC\alphaC$	110.4	1.35	$C\betaC\alphaC$	110.2	1.15
$C\betaC\gammaC\delta$	113.9	1.43	$\overset{'}{\mathrm{C}eta}_{-}\mathrm{C}\gamma_{-}\mathrm{C}\delta$	112.9	1.24
$C\gamma_C\delta_N\epsilon_2$	116.3	0.86	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.6	0.84
$C\gammaC\deltaO\epsilon 1$	121.3	0.99	$C\gammaC\deltaO\epsilon 1$	120.8	0.87
$N_{-}C\alpha_{-}C$	112.4	2.22	$N_{-}C\alpha_{-}C$	111.0	2.01
$N_C\alpha_C\beta$	111.2	1.13	$N_C\alpha_C\beta$	110.6	1.13
$O\epsilon 1_C\delta_N\epsilon 2$	122.5	0.72	$O\epsilon 1 C\delta N\epsilon 2$	122.6	0.65
GLN	tp-100 n = 534		GL	N tt0 n = 6936	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	8.7	chi1	-176	8.5
chi2	62	8.8	chi2	178	10.8
chi3	-105	27.5	chi3	2	60.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.4	1.57	$C\alpha_{-}C\beta_{-}C\gamma$	113.6	1.80
$C\alphaCO$	120.6	0.83	$C\alphaCO$	120.6	0.76
$C\beta C\alpha C$	110.5	1.24	$C\betaC\alphaC$	110.1	1.18
$C\beta C\gamma C\delta$,		1.50
$C\gammaC\deltaN\epsilon_2$	116.6	0.95	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.5	0.84
$C\gamma C\delta O\epsilon 1$	120.9	0.85	$C\gamma_{-}C\delta_{-}O\epsilon 1$	120.8	0.88
$N_{-}C\alpha_{-}C$	110.4	2.26	$N_{-}C\alpha_{-}C$	110.4	2.27
$N_C\alpha_C\beta$	110.4	1.24	$N_C\alpha_C\beta$	110.3	1.36
$O\epsilon 1 C\delta N\epsilon 2$	122.6	0.64	$O\epsilon 1_C\delta_N\epsilon 2$	122.7	0.71
chi3 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\alpha C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\gamma C\delta N\epsilon 2$ $C\gamma C\delta C\epsilon N$ $C\alpha C$ $C\alpha C\beta C\alpha C$	-105 Mean 114.4 120.6 110.5 113.0 116.6 120.9 110.4 110.4	27.5 StdDev 1.57 0.83 1.24 1.31 0.95 0.85 2.26 1.24	chi3 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C\beta_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C\delta$ $C\gamma_{-}C\delta_{-}N\epsilon_{2}$ $C\gamma_{-}C\delta_{-}O\epsilon_{1}$ $N_{-}C\alpha_{-}C$ $N_{-}C\alpha_{-}C\beta$	Mean 113.6 120.6 110.1 112.6 116.5 120.8 110.4 110.3	5tdDev 1.80 0.76 1.18 1.50 0.84 0.88 2.27 1.36

GLN	V tm130 n = 55		GLN	1 tm-30 n = 547	
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-172	9.7	chi1	-172	10.1
chi2	-76	10.4	chi2	-86	11.0
chi3	127	16.1	chi3	-29	20.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.9	1.44	$C\alphaC\betaC\gamma$	114.6	1.35
$C\alphaCO$	120.5	0.94	$C\alphaCO$	120.5	0.83
$C\betaC\alphaC$	111.3	1.63	$C\betaC\alphaC$	110.9	1.31
$C\betaC\gammaC\delta$	114.4	2.70	$C\betaC\gammaC\delta$	113.5	1.40
$C\gammaC\deltaN\epsilon_2$	117.1	1.28	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.5	0.71
$C\gamma_{-}C\delta_{-}O\epsilon 1$	120.5	1.17	$C\gammaC\deltaO\epsilon 1$	120.9	0.81
$N_{-}C\alpha_{-}C$	108.8	3.40	$N_{-}C\alpha_{-}C$	110.2	2.51
$N_{-}C\alpha_{-}C\beta$	110.1	1.37	$N_C\alpha_C\beta$	110.3	1.24
$O\epsilon 1 C\delta N\epsilon 2$	122.4	0.74	$O\epsilon 1 C\delta N\epsilon 2$	122.6	0.68
GLN	mp10 n = 1207	7	GLN	mp-120 n = 87	7
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67	9.0	chi1	-73	10.0
chi2	82	11.4	chi2	69	11.4
chi3	17	37.5	chi3	-120	13.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.2	1.36	$C\alphaC\betaC\gamma$	114.4	1.55
$C\alphaCO$	120.4	0.84	$C\alphaCO$	120.5	0.88
$C\betaC\alphaC$	109.8	1.52	$C\betaC\alphaC$	109.7	1.79
$C\betaC\gammaC\delta$	113.4	1.29	$C\betaC\gammaC\delta$	113.6	1.57
$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.3	0.82	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.6	0.65
$C\gammaC\deltaO\epsilon 1$	121.1	0.95	$C\gammaC\deltaO\epsilon 1$	120.6	1.09
$N_{-}C\alpha_{-}C$	111.6	2.35	$N_{-}C\alpha_{-}C$	111.6	2.76
$N_{-}C\alpha_{-}C\beta$	110.8	1.10	$N_{-}C\alpha_{-}C\beta$	110.7	1.01
$O\epsilon 1 C\delta N\epsilon 2$	122.5	0.60	$O_{\epsilon}1_{-}C\delta_{-}N_{\epsilon}2$	122.7	0.84
	$\sqrt{\mathbf{mt0}} \; \mathbf{n} = 14370$			mm110 n = 114	17
	$\frac{\text{Into } n = 14570}{\text{Smooth COM}}$	StdDev		$\frac{\text{Minition} = 114}{\text{Smooth COM}}$	StdDev
χ			χ		
chi1	-67	7.5	chi1	-65	8.6
chi2	179	11.2	chi2	-63	10.9
chi3	-4	62.6	chi3	109	24.1
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	113.2	1.82	$C\alphaC\betaC\gamma$	114.0	1.56
$C\alphaCO$	120.5	0.85	$C\alphaCO$	120.4	0.85
$C\betaC\alphaC$	109.9	1.71	$C\betaC\alphaC$	110.0	1.53
$C\betaC\gammaC\delta$	112.6	1.53	$C\betaC\gammaC\delta$	112.9	1.43
$C\gammaC\deltaN\epsilon_2$	116.4	0.85	$C\gammaC\deltaN\epsilon_2$	116.6	0.92
$C\gammaC\deltaO\epsilon 1$	120.8	0.90	$C\gammaC\deltaO\epsilon 1$	120.8	0.94
$N_{-}C\alpha_{-}C$	111.4	2.26	$N_{-}C\alpha_{-}C$	111.6	2.28
$N_{-}C\alpha_{-}C\beta$	110.6	1.04	$N_{-}C\alpha_{-}C\beta$	110.7	1.07
$O\epsilon 1_C\delta_N\epsilon 2$	122.7	0.70	$O\epsilon 1_C\delta_N\epsilon 2$	122.6	0.68

GLN mm-40 $n = 5959$					
χ	Smooth COM	StdDev			
chi1	-64	8.6			
chi2	-66	10.4			
chi3	-39	24.7			
Bond Angle	Mean	StdDev			
$C\alphaC\betaC\gamma$	113.9	1.42			
$C\alphaCO$	120.5	0.87			
$C\betaC\alphaC$	109.9	1.49			
$C\betaC\gammaC\delta$	112.8	1.28			
$C\gamma_C\delta_N\epsilon_2$	116.5	0.91			
$C\gammaC\deltaO\epsilon 1$	120.9	0.91			
$N_{-}C\alpha_{-}C$	111.4	2.45			
$N_C\alpha_C\beta$	110.6	1.04			
$O\epsilon 1_C\delta_N\epsilon 2$	122.6	0.78			

Table S20: ARG Central Values

ARC	$\frac{G}{r}$ ppp80 n = 10		ARG	ppp-140 n = 4	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62	5.1	chi1	58	3.0
chi2	87	7.0	chi2	92	4.6
chi3	57	3.8	chi3	62	10.6
chi4	80	8.5	chi4	-143	12.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	116.1	0.88	$C\alphaC\betaC\gamma$	115.2	0.90
$C\alphaCO$	120.8	0.55	$C\alphaCO$	120.7	0.54
$C\betaC\alphaC$	111.0	1.51	$C\betaC\alphaC$	112.0	1.46
$C\betaC\gammaC\delta$	113.9	0.82	$C\betaC\gammaC\delta$	112.2	1.50
$C\delta_N\epsilon_C\zeta$	125.0	0.34	$C\delta_N\epsilon_C\zeta$	125.9	1.18
$C\gammaC\deltaN\epsilon$	112.5	1.08	$C\gammaC\deltaN\epsilon$	113.8	2.26
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.6	0.68	$N\epsilon_{-}C\zeta_{-}N\eta 1$	121.0	1.24
$N\epsilon_{-}C\zeta_{-}N\eta 2$	119.8	0.63	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	120.1	1.38
$N\eta_1 C\zeta N\eta_2$	119.6	0.32	$N\eta 1_C\zeta N\eta 2$	118.9	0.61
$N_{-}C\alpha_{-}C$	111.1	2.18	$NC\alphaC$	113.6	2.34
$N_{-}C\alpha_{-}C\beta$	111.9	1.19	$N_{-}C\alpha_{-}C\beta$	111.2	1.26
ARG	ppt170 n = 57		ARC	G ppt90 n = 19	
χ	$\frac{1}{2} \frac{\mathbf{ppt170} \ \mathbf{n} = 57}{\mathbf{Smooth COM}}$	StdDev	ARC	G ppt90 n = 19 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM 59	StdDev 9.9	$\frac{\chi}{\text{chi1}}$	Smooth COM 64	5.9
χ chi1 chi2	Smooth COM	9.9 12.3	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM	
χ chi1 chi2 chi3	Smooth COM 59 88 174	9.9 12.3 12.3	χ chi1 chi2 chi3	Smooth COM 64 99 -180	5.9 8.0 9.8
χ chi1 chi2	Smooth COM 59 88	9.9 12.3	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM 64 99	5.9 8.0
χ chi1 chi2 chi3	Smooth COM 59 88 174	9.9 12.3 12.3	χ chi1 chi2 chi3	Smooth COM 64 99 -180	5.9 8.0 9.8
chi1 chi2 chi3 chi4	59 88 174 173	9.9 12.3 12.3 17.3	chi1 chi2 chi3 chi4	Smooth COM 64 99 -180 87	5.9 8.0 9.8 13.0
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM 59 88 174 173 Mean	9.9 12.3 12.3 17.3 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM 64 99 -180 87 Mean	5.9 8.0 9.8 13.0 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM 59 88 174 173 Mean 116.2	9.9 12.3 12.3 17.3 StdDev 1.39	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 64 99 -180 87 Mean 115.4	5.9 8.0 9.8 13.0 StdDev 1.89
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	59 88 174 173 Mean 116.2 120.4	9.9 12.3 12.3 17.3 StdDev 1.39 1.04	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$	Smooth COM 64 99 -180 87 Mean 115.4 120.8	5.9 8.0 9.8 13.0 StdDev 1.89 0.83
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9	9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9 112.4	9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37 1.63	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8 111.9	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70 2.41
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9 112.4 124.2	9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37 1.63 1.28	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \text{$\text{C}\alpha_\text{C}_{-}\text{C}$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \end{array}$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8 111.9 125.4	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70 2.41 1.13
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9 112.4 124.2 111.4	9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37 1.63 1.28 1.60	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \hline \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \hline \end{array}$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8 111.9 125.4 113.1	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70 2.41 1.13 2.89
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta-N\eta1$} \\ \hline \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9 112.4 124.2 111.4 120.5	StdDev 9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37 1.63 1.28 1.60 1.08	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \text{$\text{C}\alpha_\text{C}_{-}\text{C}$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \end{array}$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8 111.9 125.4 113.1 120.9	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70 2.41 1.13 2.89 1.09
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM 59 88 174 173 Mean 116.2 120.4 111.9 112.4 124.2 111.4 120.5 119.8	StdDev 9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37 1.63 1.28 1.60 1.08 0.87	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \text{$\text{C}\alpha$_$C$_$C} \\ \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \text{$\text{C}\beta$_$C}\gamma$_$C} \\ \text{$\text{N}\epsilon$_$C}\zeta$_$N}\epsilon$_$N}\epsilon$_$C}\zeta$	Smooth COM 64 99 -180 87 Mean 115.4 120.8 110.8 111.9 125.4 113.1 120.9 119.9	5.9 8.0 9.8 13.0 StdDev 1.89 0.83 1.70 2.41 1.13 2.89 1.09

	1 4 00 17		150	1 4 00 000		
ARC	$\frac{1}{2} \text{ ppt-90 } \text{n} = 15$		ARG ptp90 n = 223			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	62	9.1	chi1	65	9.4	
chi2	90	11.1	chi2	179	11.3	
chi3	178	5.5	chi3	64	8.6	
chi4	-92	14.4	chi4	88	11.1	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	115.8	1.38	$C\alphaC\betaC\gamma$	115.0	1.71	
$C\alphaCO$	120.6	0.93	$C\alphaCO$	120.5	0.96	
$C\betaC\alphaC$	111.2	1.75	$C\betaC\alphaC$	110.5	1.39	
$C\beta C\gamma C\delta$	113.0	1.28	$C\betaC\gammaC\delta$	111.8	1.56	
$C\delta_N\epsilon_C\zeta$	125.0	0.74	$C\delta_N\epsilon_C\zeta$	124.9	1.15	
$C\gamma_C\delta_N\epsilon$	111.7	1.96	$C\gamma_C\delta_N\epsilon$	112.2	2.18	
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.6	1.31	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.8	1.06	
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.9	1.17	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.97	
$N\eta 1_{-}C\zeta_{-}N\eta 2$	119.5	0.60	$N\eta 1_C \zeta_N \eta 2$	119.5	0.80	
$N_{-}C\alpha_{-}C$	111.6	3.12	$N_{-}C\alpha_{-}C$	110.9	2.82	
$N_C\alpha_C\beta$	111.6	1.24	$N_C\alpha_C\beta$	111.1	1.19	
$ARG \mathbf{ptp-110} \ n = 77$			•			
ARG	ptp-110 n = 77	7	ARG	ptp-170 n = 38	8	
χ	ptp-110 n = 77 Smooth COM	StdDev	χ	ptp-170 n = 38 Smooth COM	8 StdDev	
•			•			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
$\frac{\chi}{\text{chi1}}$	Smooth COM 68	StdDev 8.2	$\frac{\chi}{\text{chi1}}$	Smooth COM 67	StdDev 7.7	
χ chi1 chi2	Smooth COM 68 -180	StdDev 8.2 11.9	χ chi1 chi2	Smooth COM 67 -176	StdDev 7.7 12.2	
chi1 chi2 chi3	Smooth COM 68 -180 65	8.2 11.9 10.0	χ chi1 chi2 chi3	Smooth COM 67 -176 68	7.7 12.2 9.7	
chi1 chi2 chi3 chi4	Smooth COM 68 -180 65 -108	8.2 11.9 10.0 9.9	chi1 chi2 chi3 chi4	Smooth COM 67 -176 68 -172	7.7 12.2 9.7 16.0	
chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 68 -180 65 -108 Mean	8.2 11.9 10.0 9.9 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM 67 -176 68 -172 Mean	7.7 12.2 9.7 16.0 StdDev	
χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM 68 -180 65 -108 Mean 114.8	8.2 11.9 10.0 9.9 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$	Smooth COM 67 -176 68 -172 Mean 114.5	7.7 12.2 9.7 16.0 StdDev 1.46	
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7	8.2 11.9 10.0 9.9 StdDev 1.93 1.22	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6	7.7 12.2 9.7 16.0 StdDev 1.46 0.96	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4	8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array}$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4	7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4 111.9	StdDev 8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42 1.47	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \end{array}$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4 111.3	StdDev 7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline C\alpha_C\beta_C\gamma \\ \hline C\alpha_C_O \\ \hline C\beta_C\alpha_C \\ \hline C\beta_C\gamma_C\delta \\ \hline C\beta_C\gamma_C\delta \\ \hline C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4 111.9 125.6	8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42 1.47	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \hline \text{$C\alpha_C,C\rangle$} \\ \hline \\ \hline \\ \hline \text{$C\beta_C\alpha_C$} \\ \hline \\ $	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4 111.3 124.6	7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7	8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4	7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta-N\eta1$} \\ \hline \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7 121.0	8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29 1.42	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\alpha_C$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \hline \end{array}$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4 120.5	7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63 0.94	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM 68 -180 65 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7 121.0 119.6	8.2 11.9 10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29 1.42 1.57	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$C} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta$} \\ \text{$C\delta$_$N$$\epsilon$_$C}\zeta \\ \text{$C\gamma$_C\delta$_$N$$\epsilon$_$C}\zeta \\ \text{$C\gamma$_C\delta$_$N$$\epsilon$} \\ \text{$N\epsilon$_$Cζ_$N$$\eta$1} \\ \text{$N\epsilon$_$Cζ_$N$$\eta$2} \\ \end{array}$	Smooth COM 67 -176 68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4 120.5 119.8	7.7 12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63 0.94 0.93	

				N00 01.1	
ARG	ptt180 n = 820		ARC	$\frac{1}{2}$ ptt90 n = 814	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	8.3	chi1	65	7.6
chi2	-177	10.4	chi2	179	12.3
chi3	-180	10.4	chi3	177	8.7
chi4	179	17.5	chi4	88	9.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.53	$C\alpha C\beta C\gamma$	114.8	1.43
$C\alphaCO$	120.6	1.01	$C\alphaCO$	120.6	0.86
$C\betaC\alphaC$	110.5	1.50	$C\beta_{-}C\alpha_{-}C$	110.2	1.41
$C\beta C\gamma C\delta$	111.1	2.01	$C\betaC\gammaC\delta$	111.0	1.95
$C\delta_N\epsilon_C\zeta$	124.4	1.10	$C\delta_N\epsilon_C\zeta$	124.9	0.92
$C\gamma_C\delta_N\epsilon$	110.7	1.99	$C\gamma_C\delta_N\epsilon$	111.9	2.47
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.5	0.94	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.8	0.99
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	0.89	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.91
$N\eta 1_{-}C\zeta_{-}N\eta 2$	119.9	0.88	$N\eta 1_C \zeta_N \eta 2$	119.5	0.70
$N_{-}C\alpha_{-}C$	111.3	2.49	$N_{-}C\alpha_{-}C$	110.8	2.51
$N_C\alpha_C\beta$	111.0	1.12	$N_{-}C\alpha_{-}C\beta$	111.0	1.15
			11204208	111.0	1110
	ptt-90 n = 726		,	ptm160 n = 50	
			,		
ARG	ptt-90 n = 726		ARG	ptm160 n = 50	2
ARG X	ptt-90 n = 726 Smooth COM	StdDev	$\frac{\lambda}{\chi}$	$\frac{\mathbf{ptm160} \text{ n} = 509}{\text{Smooth COM}}$	2 StdDev
χ chi1	ptt-90 n = 726 Smooth COM	StdDev 7.9	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \end{array}$	ptm160 n = 500 Smooth COM	2 StdDev 8.7
ARG χ chi1 chi2	F ptt-90 n = 726 Smooth COM 66 -175	StdDev 7.9 12.0	ARG χ chi1 chi2	ptm160 n = 500 Smooth COM 63 -179	2 StdDev 8.7 15.0
ARG χ chi1 chi2 chi3	Smooth COM 66 -175 -177	StdDev 7.9 12.0 8.9	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3	ptm160 n = 509 Smooth COM 63 -179 -67	2 StdDev 8.7 15.0 9.7
ARG x chi1 chi2 chi3 chi4	Smooth COM 66 -175 -177 -87	StdDev 7.9 12.0 8.9 11.8	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4	ptm160 n = 502 Smooth COM 63 -179 -67 165	2 StdDev 8.7 15.0 9.7 25.7
$\begin{array}{c} \text{ARG} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM 66 -175 -177 -87 Mean	7.9 12.0 8.9 11.8 StdDev	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \end{array}$	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean	StdDev 8.7 15.0 9.7 25.7 StdDev
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM 66 -175 -177 -87 Mean 114.8	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha\text{-C}\beta\text{-C}\gamma \end{array} $	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \end{array} $	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 110.5	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha \text{-}\text{C}\beta \text{-}\text{C}\gamma}{\text{C}\alpha \text{-}\text{C}\text{-}\text{C}}$ $\frac{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}$	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 110.5 111.0	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	ptm160 n = 500 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \end{array} $	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 110.5 111.0 124.9	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C _ C$ $C\beta _ C\alpha _ C$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$ $C\delta _ N\epsilon _ C\zeta$	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \end{array} $	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14 2.66	ARG $\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39 2.11
ARG $ \chi $ chi1 chi2 chi3 chi4 Bond Angle $ C\alpha_{-}C\beta_{-}C\gamma $ $ C\alpha_{-}C_{-}CO $ $ C\beta_{-}C\alpha_{-}C $ $ C\beta_{-}C\gamma_{-}C\delta $ $ C\delta_{-}N\epsilon_{-}C\zeta $ $ C\gamma_{-}C\delta_{-}N\epsilon $ $ N\epsilon_{-}C\zeta_{-}N\eta_{1}$	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 111.0 124.9 111.7 120.8	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14 2.66 1.01	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \end{array} $ $ \begin{array}{c} \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \end{array} $	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5 120.6	2 StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39 2.11 1.28
ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	Smooth COM 66 -175 -177 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7 120.8 119.7	StdDev 7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14 2.66 1.01 1.14	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1} \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{2} \end{array} $	ptm160 n = 502 Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5 120.6 119.7	StdDev 8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39 2.11 1.28 1.12

ARG	ARG ptm-80 n = 215		ARC	$\frac{1}{5}$ pmt100 n = 4	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	8.3	chi1	70	7.2
chi2	-178	14.4	chi2	-91	9.1
chi3	-66	10.3	chi3	-174	5.4
chi4	-85	10.8	chi4	98	2.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.28	$C\alpha_{-}C\beta_{-}C\gamma$	115.8	0.42
$C\alphaCO$	120.4	0.84	$C\alphaCO$	120.6	0.28
$C\betaC\alphaC$	110.3	1.38	$C\betaC\alphaC$	110.8	0.49
$C\beta C\gamma C\delta$	111.9	1.74	$C\betaC\gammaC\delta$	112.7	0.57
$C\delta_N\epsilon_C\zeta$	125.0	1.43	$C\delta_N\epsilon_C\zeta$	125.1	0.12
$C\gamma_C\delta_N\epsilon$	112.4	2.28	$C\gamma_C\delta_N\epsilon$	111.2	0.92
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.7	1.21	$N\epsilon C\zeta N\eta 1$	121.0	0.29
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.9	1.46	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	0.27
$N\eta_1 C\zeta N\eta_2$	119.4	0.87	$N\eta 1_C\zeta N\eta 2$	119.4	0.05
$N_{-}C\alpha_{-}C$	111.6	2.54	$NC\alphaC$	110.2	1.44
$N_C\alpha_C\beta$	111.0	1.31	$N_{-}C\alpha_{-}C\beta$	111.4	0.42
<u> </u>			/-		
	pmt170 n = 39		,	pmt-80 n = 27	
	pmt170 n = 39 Smooth COM		,		
ARG)	ARG	pmt-80 n = 27	
$\frac{\lambda}{\chi}$	Smooth COM	StdDev	$\frac{\lambda}{\chi}$	pmt-80 n = 27 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM 74	StdDev 11.2	$\frac{\chi}{\text{chi1}}$	pmt-80 n = 27 Smooth COM 81	StdDev 9.3
$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM 74 -79	StdDev 11.2 15.4	$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	pmt-80 n = 27 Smooth COM 81 -68	StdDev 9.3 7.6
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	Smooth COM 74 -79 -169	StdDev 11.2 15.4 10.1	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \end{array}$	9 pmt-80 n = 27 Smooth COM 81 -68 -177	StdDev 9.3 7.6 11.0
ARG $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi3}}$ $\frac{\text{chi4}}{\text{chi4}}$	Smooth COM 74 -79 -169 -169	StdDev 11.2 15.4 10.1 15.1	$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array}$	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84	StdDev 9.3 7.6 11.0 8.3
$\begin{array}{c} X \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM 74 -79 -169 -169 Mean	StdDev 11.2 15.4 10.1 15.1 StdDev	$\begin{array}{c} \text{ARG} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean	StdDev 9.3 7.6 11.0 8.3 StdDev
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\text{C}\alpha\text{-C}\beta\text{-C}\gamma$	Smooth COM 74 -79 -169 -169 Mean 116.3	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \end{array} $	9mt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8	9.3 7.6 11.0 8.3 StdDev 1.16
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70	ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0	9.3 7.6 11.0 8.3 StdDev 1.16 0.65
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha \text{-}\text{C}\beta \text{-}\text{C}\gamma}{\text{C}\alpha \text{-}\text{C}\text{-}\text{C}}$ $\frac{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}{\text{C}\beta \text{-}\text{C}\alpha \text{-}\text{C}}$	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8 112.7	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12 1.26	ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\gamma_{-}C\delta}$	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3 113.3	StdDev 9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\alpha C$ $C\beta C\alpha C$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8 112.7 124.4	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12 1.26 1.05	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \end{array} $	9 pmt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3 113.3 124.9	StdDev 9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99
ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8 112.7 124.4 111.6	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12 1.26 1.05 1.87	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}_{\alpha} \text{-C}_{\beta} \text{-C}_{\gamma} \\ \text{C}_{\alpha} \text{-C}_{-0} \\ \text{C}_{\beta} \text{-C}_{\alpha} \text{-C} \\ \text{C}_{\beta} \text{-C}_{\gamma} \text{-C}_{\delta} \\ \text{C}_{\delta} \text{-N}_{\epsilon} \text{-C}_{\zeta} \\ \text{C}_{\gamma} \text{-C}_{\delta} \text{-N}_{\epsilon} \end{array} $	mt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3 113.3 124.9 112.1	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99 1.75
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1} \end{array} $	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8 112.7 124.4 111.6 120.4	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12 1.26 1.05 1.87 0.78	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha \text{C}\beta \text{C}\gamma \\ \text{C}\alpha \text{C} \text{C}\zeta \\ \text{C}\beta \text{C}\alpha \text{C}\zeta \\ \text{C}\gamma \text{C}\delta \text{N}\epsilon \\ \text{N}\epsilon \text{C}\zeta \text{N}\eta \text{1} \end{array} $	mt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3 113.3 124.9 112.1 121.0	StdDev 9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99 1.75 0.89
ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	Smooth COM 74 -79 -169 -169 Mean 116.3 120.8 110.8 112.7 124.4 111.6 120.4 120.0	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70 1.12 1.26 1.05 1.87 0.78 0.64	ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha C\beta C\gamma}{C\alpha C C}$ $\frac{C\beta C\alpha C}{C\beta C\alpha C}$ $\frac{C\beta C\alpha C}{C\beta N\epsilon C}$ $\frac{C\delta N\epsilon C\zeta}{C\gamma C\delta N\epsilon}$ $\frac{N\epsilon C\zeta N\eta 1}{N\epsilon C\zeta N\eta 2}$	mt-80 n = 27 Smooth COM 81 -68 -177 -84 Mean 115.8 121.0 110.3 113.3 124.9 112.1 121.0 119.6	StdDev 9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99 1.75 0.89 0.60

ARG pmm150 n = 12		ARG	pmm-80 n = 19	9	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	76	3.2	chi1	74	12.6
chi2	-75	5.6	chi2	-76	11.2
chi3	-65	6.3	chi3	-57	8.1
chi4	152	15.4	chi4	-81	7.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	116.2	1.50	$C\alphaC\betaC\gamma$	115.9	1.02
$C\alphaCO$	120.3	0.93	$C\alphaCO$	120.8	0.55
$C\betaC\alphaC$	110.4	1.04	$C\betaC\alphaC$	110.9	1.23
$C\betaC\gammaC\delta$	112.4	1.15	$C\betaC\gammaC\delta$	113.5	1.56
$C\delta_N\epsilon_C\zeta$	125.3	2.47	$C\delta_N\epsilon_C\zeta$	125.1	1.08
$C\gamma_C\delta_N\epsilon$	111.6	2.06	$C\gammaC\deltaN\epsilon$	112.5	1.30
$N\epsilon_{-}C\zeta_{-}N\eta 1$	121.1	1.74	$N\epsilon C\zeta \eta 1$	120.4	0.95
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	1.03	$N\epsilon C\zeta \eta 2$	120.3	0.95
$N\eta_1 C\zeta N\eta_2$	119.2	1.39	$N\eta 1_C\zeta_N\eta 2$	119.3	0.67
$N_{-}C\alpha_{-}C$	109.0	1.00	$NC\alphaC$	109.7	2.43
$N_C\alpha_C\beta$	112.1	0.96	$N_C\alpha_C\beta$	111.6	1.00
·			,		
ARG	t tpp80 n = 363		ARG	tpp-160 n = 49	6
ARC X	Smooth COM	StdDev	χ	tpp-160 n = 49 Smooth COM	6 StdDev
		StdDev 10.3			
χ	Smooth COM		χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -178	10.3	χ chi1	Smooth COM 179	StdDev 9.6
χ chi1 chi2	Smooth COM -178 65	10.3 10.7	χ chi1 chi2	Smooth COM 179 66	9.6 10.7
χ chi1 chi2 chi3	Smooth COM -178 65 60	10.3 10.7 9.5	χ chi1 chi2 chi3	Smooth COM 179 66 65	9.6 10.7 9.8
χ chi1 chi2 chi3 chi4	Smooth COM -178 65 60 84	10.3 10.7 9.5 9.1	chi1 chi2 chi3 chi4	Smooth COM 179 66 65 -168	9.6 10.7 9.8 19.7
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -178 65 60 84 Mean	10.3 10.7 9.5 9.1 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 179 66 65 -168 Mean	9.6 10.7 9.8 19.7 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -178 65 60 84 Mean 114.9	10.3 10.7 9.5 9.1 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM 179 66 65 -168 Mean 114.8	9.6 10.7 9.8 19.7 StdDev 1.30
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7	9.6 10.7 9.8 19.7 StdDev 1.30 0.84
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\beta_N\epsilon_C\zeta$} \\ \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\beta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0 125.0 112.6	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59 1.05 2.06	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \hline \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7 124.5 111.9	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29 1.75
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta-N\eta1$} \\ \hline \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0 125.0 112.6 120.7	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59 1.05 2.06 0.87	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7 124.5 111.9 120.5	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29 1.75 1.38 1.82 1.03
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}_2\text{$C\gamma$_$C} \\ \text{$C\beta$_$C}\gamma$_$C} \\ \text{$C\beta$_$C}\gamma$_$C} \\ \text{$C\beta$_$C}\gamma$_$C} \\ \text{$C\delta$_$N}\epsilon$_$C} \\ \text{$C\delta$_$N}\epsilon$_$C} \\ \text{$C\gamma$_$C}\delta$_$N}\epsilon \\ \text{$N\epsilon$_$C}\zeta$_$N}\eta 1 \\ \text{$N\epsilon$_$C}\zeta$_$N}\eta 2 \\ \hline \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0 125.0 112.6 120.7 119.7	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59 1.05 2.06 0.87 0.83	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7 124.5 111.9 120.5 119.8	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29 1.75 1.38 1.82 1.03 1.09
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ N\eta1_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0 125.0 112.6 120.7 119.7 119.5	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59 1.05 2.06 0.87 0.83 0.72	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \hline \\ \text{C}\alpha_\text{C}_\text{C} \\ \hline \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \hline \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \hline \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \hline \\ \hline \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \hline \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \hline \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \hline \\ \text{N}\eta1_\text{C}\zeta_\text{N}\eta2 \\ \hline \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7 124.5 111.9 120.5 119.8 119.7	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29 1.75 1.38 1.82 1.03 1.09 0.84
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}_2\text{$C} \\ \text{$C\alpha$_$C}_2\text{$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta \\ \text{$C\delta$_$N}\epsilon$_$C}\zeta \\ \text{$C\delta$_$N}\epsilon$_$C}\zeta \\ \text{$C\gamma$_$C}\delta$_$N}\epsilon \\ \text{$N\epsilon$_$C}\zeta \\ \text{$N\eta1} \\ \text{$N\epsilon$_$C}\zeta \\ \text{$N\eta2} \\ \hline \end{array}$	Smooth COM -178 65 60 84 Mean 114.9 120.5 110.5 113.0 125.0 112.6 120.7 119.7	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23 1.59 1.05 2.06 0.87 0.83	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM 179 66 65 -168 Mean 114.8 120.5 110.4 112.7 124.5 111.9 120.5 119.8	9.6 10.7 9.8 19.7 StdDev 1.30 0.84 1.29 1.75 1.38 1.82 1.03 1.09

ARG	tpt170 n = 825	<u> </u>	ARC	3 tpt90 n = 652	
$\frac{\gamma}{\chi}$	Smooth COM	StdDev	$\frac{11100}{\chi}$	Smooth COM	StdDev
chi1	-179	9.0	chi1	179	8.4
chi2	66	10.4	chi2	66	7.7
chi3	178	11.7	chi3	179	9.9
chi4	171	19.3	chi4	86	10.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.23	$C\alphaC\betaC\gamma$	114.7	1.27
$C\alphaCO$	120.5	0.74	$C\alpha_{-}C_{-}O$	120.5	0.80
$C\betaC\alphaC$	110.6	1.15	$C\betaC\alphaC$	110.3	1.18
$C\beta_{-}C\gamma_{-}C\delta$	112.2	1.71	$C\betaC\gammaC\delta$	112.1	1.67
$C\delta_N\epsilon_C\zeta$	124.5	1.14	$C\delta_N\epsilon_C\zeta$	124.8	0.92
$C\gammaC\deltaN\epsilon$	110.9	1.87	$C\gamma_C\delta_N\epsilon$	111.9	2.27
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.5	0.94	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.8	0.97
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.88	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.89
$N\eta 1 \vec{C} \zeta \vec{N} \eta 2$	119.8	0.86	$N\eta 1 C\zeta N\eta 2$	119.5	0.82
$N_{-}C\alpha_{-}C$	110.7	1.99	$N_{-}C\alpha_{-}C$	111.4	2.06
$N C \alpha C \beta$		1.19	$N_C\alpha_C\beta$	110.2	1.09
$N_{-}C\alpha_{-}C\beta$ 110.2		1110	11_0α_0ρ	110. -	1.00
	tpt-90 n = 365		,	tpm170 n = 110	
			,		
ARG	tpt-90 n = 365		ARG	tpm170 n = 110	0
ARG	tpt-90 n = 365 Smooth COM	StdDev	$\frac{\lambda}{\chi}$	tpm170 n = 110 Smooth COM	0 StdDev
$\frac{\chi}{\text{chi1}}$	tpt-90 n = 365 Smooth COM	StdDev 8.4 10.8	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \end{array}$	tpm170 n = 110 Smooth COM	O StdDev 8.1
$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM 179 67	StdDev 8.4	$\begin{array}{c} \text{ARG} \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	tpm170 n = 110 Smooth COM 178 70	StdDev 8.1 10.9
ARG x chi1 chi2 chi3	Smooth COM 179 67 -180	StdDev 8.4 10.8 8.8	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3	tpm170 n = 110 Smooth COM 178 70 -85	StdDev 8.1 10.9 12.8
ARG x chi1 chi2 chi3 chi4	Smooth COM 179 67 -180 -89	StdDev 8.4 10.8 8.8 12.2	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \end{array}$	tpm170 n = 110 Smooth COM 178 70 -85 172	StdDev 8.1 10.9 12.8 18.6
$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	F tpt-90 n = 365 Smooth COM 179 67 -180 -89 Mean	StdDev 8.4 10.8 8.8 12.2 StdDev	$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \end{array}$	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean	StdDev 8.1 10.9 12.8 18.6 StdDev
ARG $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi3}}$ $\frac{\text{chi4}}{\text{Bond Angle}}$ $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\gamma}$	Smooth COM 179 67 -180 -89 Mean 114.7	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$	Smooth COM 179 67 -180 -89 Mean 114.7 120.5	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}$	Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$	F tpt-90 n = 365 Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6 112.4	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6 112.8	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}{\text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta}$ $\frac{\text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon}{\text{C}\delta_{-}\text{N}\epsilon}$	Francisco (12.4) Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6 112.4 124.9	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6 112.8 124.7	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{C}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}{\text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta}$	# tpt-90 n = 365 Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15 2.52	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6 112.8 124.7 112.0	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25 2.15
ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	# tpt-90 n = 365 Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1 120.7	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15 2.52 1.03	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1} \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{2} \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6 112.8 124.7 112.0 120.5	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25 2.15 1.05
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$ $\frac{\text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta}{\text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon}$ $\frac{\text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1}}{\text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1}}$	# tpt-90 n = 365 Smooth COM 179 67 -180 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1 120.7 119.7	StdDev 8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15 2.52 1.03 1.05	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \end{array} $	tpm170 n = 110 Smooth COM 178 70 -85 172 Mean 115.6 120.6 110.6 112.8 124.7 112.0 120.5 119.8	StdDev 8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25 2.15 1.05 0.90

A D C	tpm-80 n = 20		A D.C	ttp80 n = 1896	<u> </u>
ANG	_		ANG		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	5.2	chi1	-177	8.2
chi2	79	8.2	chi2	180	13.4
chi3	-80	10.4	chi3	63	9.9
chi4	-80	9.1	chi4	83	9.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.2	1.38	$C\alpha_{-}C\beta_{-}C\gamma$	113.7	1.50
$C\alphaCO$	120.7	1.05	$C\alphaCO$	120.7	0.80
$C\betaC\alphaC$	110.3	1.13	$C\betaC\alphaC$	110.0	1.21
$C\betaC\gammaC\delta$	113.0	1.22	$C\betaC\gammaC\delta$	112.1	1.53
$C\delta_N\epsilon_C\zeta$	125.2	1.19	$C\delta_N\epsilon_C\zeta$	124.9	1.04
$C\gamma_C\delta_N\epsilon$	113.7	2.21	$C\gamma_C\delta_N\epsilon$	112.6	1.94
$N\epsilon C\zeta N\eta 1$	120.6	0.96	$N\epsilon C\zeta \eta 1$	120.7	0.95
$N\epsilon C\zeta N\eta 2$	120.1	0.92	$N\epsilon C\zeta \eta 2$	119.8	0.86
$N\eta 1_C\zeta N\eta 2$	119.3	0.63	$N\eta 1_C\zeta_N\eta 2$	119.5	0.75
$N_{-}C\alpha_{-}C$	110.8	1.48	$NC\alphaC$	110.7	2.06
$N_{-}C\alpha_{-}C\beta$	109.8	1.13	$N_{-}C\alpha_{-}C\beta$	110.4	1.20
ARG	ttp-110 n = 625	3	ARG	ttp-170 n = 153	3
χ	ttp-110 n = 623 Smooth COM	3 StdDev	ARG χ	ttp-170 n = 153 Smooth COM	StdDev
			-	_	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -175	StdDev 8.5	χ chi1	Smooth COM -175	StdDev 9.3
χ chi1 chi2	Smooth COM -175 177	8.5 13.0	χ chi1 chi2	Smooth COM -175 179	StdDev 9.3 13.2
χ chi1 chi2 chi3	Smooth COM -175 177 65	8.5 13.0 10.7	χ chi1 chi2 chi3	Smooth COM -175 179 67	9.3 13.2 9.0
χ chi1 chi2 chi3 chi4	Smooth COM -175 177 65 -113	8.5 13.0 10.7 9.9	chi1 chi2 chi3 chi4	Smooth COM -175 179 67 -171	9.3 13.2 9.0 17.3
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -175 177 65 -113 Mean	8.5 13.0 10.7 9.9 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -175 179 67 -171 Mean	9.3 13.2 9.0 17.3 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -175 177 65 -113 Mean 113.8	8.5 13.0 10.7 9.9 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM -175 179 67 -171 Mean 113.7	9.3 13.2 9.0 17.3 StdDev 1.65
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -175 177 65 -113 Mean 113.8 120.6	8.5 13.0 10.7 9.9 StdDev 1.63 0.80	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C CO$	Smooth COM -175 179 67 -171 Mean 113.7 120.6	9.3 13.2 9.0 17.3 StdDev 1.65 0.76
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2	8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2 112.0	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23 1.75	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0 111.6	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{Ca_C}\beta\text{C}\gamma$} \\ \text{$\text{Ca_C}\triangle\text{O}$} \\ \text{$\text{C}\beta\text{C}\gamma\text{C}\delta$} \\ \text{$\text{C}\beta\text{C}\gamma\text{C}\delta$} \\ \text{$\text{C}\delta\text{N}\epsilon\text{C}\zeta$} \\ \text{$\text{C}\gamma\text{C}\delta\text{N}\epsilon$} \\ \text{$\text{N}\epsilon\text{C}\zeta\text{N}\eta 1$} \\ \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2 112.0 125.4	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23 1.75 1.36	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0 111.6 124.5	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2 112.0 125.4 111.9	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23 1.75 1.36 2.16	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{O} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0 111.6 124.5 111.5	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17 1.58
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{Ca_C}\beta\text{C}\gamma$} \\ \text{$\text{Ca_C}\triangle\text{O}$} \\ \text{$\text{C}\beta\text{C}\gamma\text{C}\delta$} \\ \text{$\text{C}\beta\text{C}\gamma\text{C}\delta$} \\ \text{$\text{C}\delta\text{N}\epsilon\text{C}\zeta$} \\ \text{$\text{C}\gamma\text{C}\delta\text{N}\epsilon$} \\ \text{$\text{N}\epsilon\text{C}\zeta\text{N}\eta 1$} \\ \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2 112.0 125.4 111.9 121.1	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23 1.75 1.36 2.16 1.28	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0 111.6 124.5 111.5 120.5	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17 1.58 0.90
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -175 177 65 -113 Mean 113.8 120.6 110.2 112.0 125.4 111.9 121.1 119.5	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23 1.75 1.36 2.16 1.28 1.16	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{O} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -175 179 67 -171 Mean 113.7 120.6 110.0 111.6 124.5 111.5 120.5 119.8	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17 1.58 0.90 0.88

chi1 -176 9.1 chi1 -176 9.3 chi2 176 11.2 chi2 176 10.8 chi3 179 11.5 chi3 176 9.6 chi4 179 18.7 chi4 87 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev Cα.Cβ.Cγ 113.5 1.78 Cα.Cβ.Cγ 113.9 1.70 Cα.C.O 120.6 0.81 Cα.Cβ.Cγ 113.9 1.70 Cβ.Cα.C 110.2 1.17 Cβ.Cα.C 110.2 1.25 Cβ.Cα.C 111.4 2.19 Cβ.Cα.C 111.3 2.08 Cβ.Ελ.ε.Cζ 124.3 1.19 Cβ.Cα.C 124.8 1.01 Cγ.Cδ.Nε 110.7 1.92 Cγ.Cδ.Nε 111.6 2.62 Nε.Cζ.Nη2 119.6 0.92 Nε.Cζ.Nη2 119.6 1.00	ARG $ttt180 \text{ n} = 2339$			ARG ttt90 n = 1057		
chi2 176 11.2 chi2 176 10.8 chi3 179 11.5 chi3 176 9.6 chi4 179 18.7 chi4 87 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα.Cβ.Cγ 113.5 1.78 Cα.Cβ.Cγ 113.9 1.70 Cα.Cθ. 120.6 0.81 Cα.Cθ.O 120.6 0.79 Cβ.Cα.C 110.2 1.17 Cβ.Cα.C 110.2 1.20 Cβ.Cγ.Cδ 111.4 2.19 Cβ.Cα.C 110.2 1.20 Cβ.Cγ.Cδ 111.4 2.19 Cβ.Cα.C 110.2 1.20 Cβ.Λγ.Cδ 110.7 1.92 Cβ.Cγ.Cδ 111.6 2.62 Nε.Cζ.Nη1 120.4 0.90 Nε.Cζ.Nη1 120.7 1.02 Nε.Cγ.Πγ2 119.6 0.92 Nε.Cα.C 119.6 0.74 N.LCα.Cβ 110.2 1.39 N.Cα.Cβ 110.4 1.37 <th>χ</th> <th>Smooth COM</th> <th>StdDev</th> <th>χ</th> <th>Smooth COM</th> <th>StdDev</th>	χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi3 179 11.5 chi3 176 9.6 chi4 179 18.7 chi4 87 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev CαCβCγ 113.5 1.78 CαCβCγ 113.9 1.70 CβCα 120.6 0.81 CαCβCγ 112.6 0.79 CβCγ 110.2 1.17 CβCαC 110.2 1.25 CβCγCγ 111.4 2.19 CβCγCδ 111.3 2.08 CδNεCζ 124.3 1.19 CβCγCβ 111.6 2.06 NεCγΠη1 120.4 0.90 NεCγΝη1 120.7 1.02 NεCγΠη2 119.6 0.92 NεCγΝη2 119.6 0.74 NCαC 110.5 2.41 NCαC 110.5 2.40 NCαCβ 110.2	chi1	-176	9.1	chi1	-176	9.3
chi4 179 18.7 chi4 87 10.8 Bond Angle Mean StdDev Bond Angle Mean StdD $C\alpha . C\beta . C\gamma$ 113.5 1.78 $C\alpha . C\beta . C\gamma$ 113.9 1.70 $C\alpha . C$.0 120.6 0.81 $C\alpha . C$.0 120.6 0.79 $C\beta . C\alpha . C$ 110.2 1.17 $C\beta . C\alpha . C$ 110.2 1.25 $C\beta . C\gamma . C\delta$ 111.4 2.19 $C\beta . C\gamma . C\delta$ 111.3 2.08 $C\delta . N\epsilon . C\zeta$ 124.3 1.19 $C\delta . N\epsilon . C\zeta$ 124.8 1.01 $C\gamma . C\delta . N\epsilon$ 110.7 1.92 $C\gamma . C\delta . N\epsilon$ 111.6 2.62 $N\epsilon . C\zeta . N\eta$ 1 120.4 0.90 $N\epsilon . C\zeta . N\eta$ 1 120.7 1.02 $N\epsilon . C\zeta . N\eta$ 2 119.6 0.92 $N\epsilon . C\zeta . N\eta$ 2 119.6 0.74 $N.C\alpha . C$ 110.5 2.41 $N.C\alpha . C$ 110.5 2.40 $N.C\alpha . C\beta$ 110.2 1.39 $N.C\alpha . C\beta$ 110.4 1.37 <t< td=""><td>chi2</td><td>176</td><td>11.2</td><td>chi2</td><td>176</td><td>10.8</td></t<>	chi2	176	11.2	chi2	176	10.8
Bond Angle Mean StdDev Bond Angle Mean StdDev $C\alpha \bot C\beta \bot C\gamma$ 113.5 1.78 $C\alpha \bot C\beta \bot C\gamma$ 113.9 1.70 $C\alpha \bot C_0$ 120.6 0.81 $C\alpha \bot C_0$ 120.6 0.79 $C\beta \bot C\alpha \bot C$ 110.2 1.17 $C\beta \bot C\alpha \bot C$ 110.2 1.25 $C\beta \bot C\alpha \bot C$ 110.2 1.17 $C\beta \bot C\alpha \bot C$ 110.3 2.08 $C\delta \bot C\gamma \bot C\delta$ 111.4 2.19 $C\beta \bot C\gamma \bot C\delta$ 111.3 2.08 $C\delta \bot C\gamma \bot C\delta$ 111.4 2.19 $C\beta \bot C\gamma \bot C\delta$ 111.3 2.08 $C\delta \bot C\gamma \bot C\delta$ 110.1 1.92 $C\gamma \bot C\delta \bot C\gamma$ 111.6 2.62 $N \in \Box C\zeta \bot N\eta$ 110.7 1.92 $C\gamma \bot C\delta \bot C\gamma$ 111.6 2.62 $N \in \Box C\zeta \bot N\eta$ 120.4 0.90 $N \in \Box C\zeta \bot N\eta$ 120.7 1.02 $N \in \Box C\zeta \bot N\eta$ 120.0 0.81 $N\eta \bot \Box C\zeta \bot N\eta$ 19.6 0.70 $N \cup C\alpha \bot C$ 110.5 2.41 $N \bot \Box C\zeta \bot N\eta$ 119.6	chi3	179	11.5	chi3	176	9.6
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	chi4	179	18.7	chi4	87	10.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\alphaC\betaC\gamma$	113.5	1.78	$C\alphaC\betaC\gamma$	113.9	1.70
CβCγCδ 111.4 2.19 $CβCγCδ$ 111.3 2.08 $CδNεCζ$ 124.3 1.19 $CδNεCζ$ 124.8 1.01 $CγCδNε$ 110.7 1.92 $CγCδNε$ 111.6 2.62 $NεCζNη1$ 120.4 0.90 $NεCζNη1$ 120.7 1.02 $NεCζNη2$ 119.6 0.92 $NεCζNη2$ 119.6 1.00 $Nη1CζNη2$ 120.0 0.81 $Nη1CζNη2$ 119.6 0.74 $NCαC$ 110.5 2.41 $NCαC$ 110.5 2.40 $NCαCβ$ 110.2 1.39 $NCαCβ$ 110.4 1.37 ARG ttt-90 n = 1380	$C\alphaCO$	120.6	0.81	$C\alphaCO$	120.6	0.79
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\betaC\alphaC$	110.2	1.17	$C\beta_{-}C\alpha_{-}C$	110.2	1.25
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\betaC\gammaC\delta$	111.4	2.19	$C\betaC\gammaC\delta$	111.3	2.08
Nε_Cζ_Nη1 120.4 0.90 Nε_Cζ_Nη1 120.7 1.02 Nε_Cζ_Nη2 119.6 0.92 Nε_Cζ_Nη2 119.6 1.00 Nη1_Cζ_Nη2 120.0 0.81 Nη1_Cζ_Nη2 119.6 0.74 N_Cα_C 110.5 2.41 N_Cα_C 110.5 2.40 N_Cα_Cβ 110.2 1.39 N_Cα_Cβ 110.4 1.37 ARG ttt-90 n = 1380 ARG ttm110 n = 725 χ Smooth COM StdDev X Smooth COM StdDev chi1 -177 9.4 chi1 -175 9.0 chi2 178 11.5 chi2 179 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdD Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ_Cγ 113.9 1.64 Cα_Cβ_Cγ_Cγ <td>$C\delta_N\epsilon_C\zeta$</td> <td>124.3</td> <td>1.19</td> <td>$C\delta_N\epsilon_C\zeta$</td> <td>124.8</td> <td>1.01</td>	$C\delta_N\epsilon_C\zeta$	124.3	1.19	$C\delta_N\epsilon_C\zeta$	124.8	1.01
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\gamma_C\delta_N\epsilon$	110.7	1.92	$C\gammaC\deltaN\epsilon$	111.6	2.62
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.4	0.90	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.7	1.02
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	0.92	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	1.00
N.Cα.C 110.5 2.41 N.Cα.C 110.5 2.40 N.Cα.Cβ 110.2 1.39 N.Cα.Cβ 110.4 1.37 ARG ttt-90 n = 1380 ARG ttm110 n = 725 χ Smooth COM StdDev χ Smooth COM StdD chi1 -177 9.4 chi1 -175 9.0 chi2 178 11.5 chi2 179 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdD Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 110.3 1.26 Cβ_Cα_Cβ 110.3 1.23 Cβ_Cα_Cβ 110.3 1.26 Cβ_Cα_Cβ 112.2 1.69 Cβ_Cβ_Cγ 110.3 1.		120.0	0.81		119.6	0.74
N_Cα_Cβ 110.2 1.39 N_Cα_Cβ 110.4 1.37 ARG ttt-90 n = 1380 ARG ttm110 n = 725 χ Smooth COM StdDev χ Smooth COM StdDer chi1 -177 9.4 chi1 -175 9.0 chi2 178 11.5 chi2 179 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 110.3 1.26 Cβ_Cα_Cθ 110.3 1.23 Cβ_Cα_Cβ 110.3 1.26 Cβ_Cα_Cθ 110.3 1.23 Cβ_Cγ_Cδ 110.9 2.08 Cβ_Cγ_Cδ 112.2 1.69 Cβ_Nε_Cζ 124.8						2.40
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N_C\alpha_C\beta$	110.2	1.39	$N_{-}C\alpha_{-}C\beta$	110.4	1.37
chi1 -177 9.4 chi1 -175 9.0 chi2 178 11.5 chi2 179 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev C α _C β _C γ 114.0 1.62 α _C β _C γ 113.9 1.64 C α _C β _C γ 114.0 1.62 α _C β _C γ 113.9 1.64 C α _C β _C γ 114.0 1.62 α _C β _C γ 113.9 1.64 C α _C β _C γ 114.0 1.62 α _C β _C γ 113.9 1.64 C α _C β _C γ 113.9 1.64 α _C β _C γ 113.9 1.64 C α _C β _C γ 110.3 1.23 α _C β _C γ 110.3 1.23 C β _C α _C γ 110.3 1.26 α _C β _C γ _C δ 112.2 1.69 C β _C γ _C δ 110.9 <	ARG	$t+t_{-}00 n = 1380$		ADC	44110 701	-
chi2 178 11.5 chi2 179 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 114.0 1.62 Cα_Cβ_Cγ 113.9 1.64 Cα_Cβ_Cγ 113.9 1.64 0.78 0.78 0.72 0.72 0.78 Cβ_Cα_C 110.3 1.26 Cβ_Cα_C 110.3 1.23 1.23 Cβ_Cα_Cβ_Cα_C 110.3 1.26 Cβ_Cα_Cβ_Cα_C 110.3 1.23 Cβ_Cα_Cβ_Cα_C 110.9 2.08 Cβ_Cα_Cβ_Cα_C 112.2 1.69 Cδ_Nε_Cζ 124.8 1.17 Cδ_Nε_Cζ 125.3 1.23 Cγ_Cδ_Nε_C 111.6 <td></td> <td>ttt-90 II — 1360</td> <td>)</td> <td>ARG</td> <td>ttm110 n = 728</td> <td>)</td>		ttt-90 II — 1360)	ARG	ttm110 n = 728)
chi3 -178 9.9 chi3 -64 10.7 chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 114.0 1.62 $Cα_Cβ_Cγ$ 113.9 1.64 Cα_Cβ_Cγ 120.5 0.79 $Cα_C C_O$ 120.6 0.78 Cβ_Cα_C 110.3 1.26 $Cβ_Cα_C$ 110.3 1.23 Cβ_Cγ_Cδ 110.9 2.08 $Cβ_Cγ_Cδ$ 112.2 1.69 Cδ_Nϵ_Cζ 124.8 1.17 $Cδ_Nϵ_Cζ$ 125.3 1.23 Cγ_Cδ_Nϵ 111.8 2.58 $Cγ_Cδ_Nϵ$ 111.6 1.93 Nϵ_Cζ_Nη1 120.8 1.08 Nϵ_Cζ_Nη2 119.5 1.12 Nη1_Cζ_Nη2 119.6 1.01 Nϵ_Cζ_Nη2 119.5 1.12 Nη1_Cζ_Nη2 119.6 0.87 Nη1_Cζ_Nη2 119.4 0.82 N_Cα_C 110.4 2.30 N_Cα_C			-			StdDev
chi4 -90 12.5 chi4 113 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 114.0 1.62 $CαCβCγ$ 113.9 1.64 Cα_C_O 120.5 0.79 $CαCC$ 120.6 0.78 Cβ_Cα_C 110.3 1.26 $CβCαC$ 110.3 1.23 CβCγ_Cδ 110.9 2.08 $CβCγCδ$ 112.2 1.69 Cδ_Nϵ_Cζ 124.8 1.17 $Cδ_NϵCζ$ 125.3 1.23 Cγ_Cδ_Nϵ_C 124.8 1.17 $Cδ_NϵCζ$ 125.3 1.23 Cγ_Cδ_Nϵ_Nϵ 111.8 2.58 $CγCδ_NϵCζ$ 125.3 1.23 NϵCζ_Nη1 120.8 1.08 NϵCζ_Nη1 121.0 1.24 NϵCζ_Nη2 119.6 1.01 NϵCζ_Nη2 119.5 1.12 Nη1Cζ_Nη2 119.6 0.87 Nη1Cζ_Nη2 119.4 0.82 NCα_C 110.4 2.30<	χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
Bond Angle Mean StdDev Bond Angle Mean StdDev $C\alpha_C\beta_C\gamma$ 114.0 1.62 $C\alpha_C\beta_C\gamma$ 113.9 1.64 $C\alpha_C_O$ 120.5 0.79 $C\alpha_C_O$ 120.6 0.78 $C\beta_C\alpha_C$ 110.3 1.26 $C\beta_C\alpha_C$ 110.3 1.23 $C\beta_C\gamma_C\delta$ 110.9 2.08 $C\beta_C\gamma_C\delta$ 112.2 1.69 $C\delta_N\epsilon_C\zeta$ 124.8 1.17 $C\delta_N\epsilon_C\zeta$ 125.3 1.23 $C\gamma_C\delta_N\epsilon_C\zeta$ 124.8 1.17 $C\delta_N\epsilon_C\zeta$ 125.3 1.23 $C\gamma_C\delta_N\epsilon$ 111.8 2.58 $C\gamma_C\delta_N\epsilon$ 111.6 1.93 $N\epsilon_C\zeta_N\eta$ 120.8 1.08 $N\epsilon_C\zeta_N\eta$ 121.0 1.24 $N\epsilon_C\zeta_N\eta$ 119.6 1.01 $N\epsilon_C\zeta_N\eta$ 119.5 1.12 $N\eta$ $C\zeta_N\eta$ 119.4 0.82 $N_C\alpha_C$ 110.4 2.30 $N_C\alpha_C$ 110.5 2.14	χ chi1	Smooth COM -177	StdDev 9.4	$\frac{\chi}{\text{chi1}}$	Smooth COM -175	StdDev 9.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	χ chi1 chi2	Smooth COM -177 178	StdDev 9.4 11.5	χ chi1 chi2	Smooth COM -175 179	StdDev
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3	Smooth COM -177 178 -178	9.4 11.5 9.9	χ chi1 chi2 chi3	Smooth COM -175 179 -64	9.0 9.5 10.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4	Smooth COM -177 178 -178 -90	9.4 11.5 9.9 12.5	χ chi1 chi2 chi3 chi4	Smooth COM -175 179 -64 113	9.0 9.5 10.7 9.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -177 178 -178 -90 Mean	9.4 11.5 9.9 12.5 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -175 179 -64 113 Mean	9.0 9.5 10.7 9.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -177 178 -178 -90 Mean 114.0	9.4 11.5 9.9 12.5 StdDev 1.62	χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM -175 179 -64 113 Mean 113.9	9.0 9.5 10.7 9.8 StdDev
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5	9.4 11.5 9.9 12.5 StdDev 1.62 0.79	χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$ $C\alphaC$ -O	Smooth COM -175 179 -64 113 Mean 113.9 120.6	9.0 9.5 10.7 9.8 StdDev
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3	9.0 9.5 10.7 9.8 StdDev 1.64 0.78
N_{ϵ} _C ζ _N η 2 119.6 1.01 N_{ϵ} _C ζ _N η 2 119.5 1.12 N_{η} 1_C ζ _N η 2 119.6 0.87 N_{η} 1_C ζ _N η 2 119.4 0.82 N _C α _C 110.4 2.30 N _C α _C 110.5 2.14	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23
$N\epsilon_{-}C\zeta_{-}N\eta^{2}$ 119.6 1.01 $N\epsilon_{-}C\zeta_{-}N\eta^{2}$ 119.5 1.12 $N\eta_{1-}C\zeta_{-}N\eta^{2}$ 119.6 0.87 $N\eta_{1-}C\zeta_{-}N\eta^{2}$ 119.4 0.82 $N_{-}C\alpha_{-}C$ 110.4 2.30 $N_{-}C\alpha_{-}C$ 110.5 2.14	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9 124.8	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08 1.17	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline \text{$C\alpha_C\beta_C\gamma$} \\ \hline \text{$C\alpha_C_O$} \\ \hline \text{$C\beta_C\alpha_C$} \\ \hline \text{$C\beta_C\gamma_C\delta$} \\ \hline \text{$C\beta_N\epsilon_C\zeta$} \\ \hline \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2 125.3	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69
$N_{-}C\alpha_{-}C$ 110.4 2.30 $N_{-}C\alpha_{-}C$ 110.5 2.14	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9 124.8 111.8	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08 1.17 2.58	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$-C\beta$-$Cγ} \\ \text{$C\alpha$-C_{-}Cγ} \\ \text{$C\alpha$-C_{-}Cδ} \\ \text{$C\beta$-C\gamma$-$Cδ} \\ \text{$C\delta$-N\epsilon$-$Cζ} \\ \text{$C\gamma$-C\delta$-$Nϵ} \\ \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2 125.3 111.6	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69 1.23
$N_{-}C\alpha_{-}C$ 110.4 2.30 $N_{-}C\alpha_{-}C$ 110.5 2.14	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9 124.8 111.8 120.8	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08 1.17 2.58 1.08	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2 125.3 111.6 121.0	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69 1.23 1.93
$N_{-}C\alpha_{-}C\beta$ 110.2 1.31 $N_{-}C\alpha_{-}C\beta$ 110.4 1.24	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \end{array}$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9 124.8 111.8 120.8 119.6	StdDev 9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08 1.17 2.58 1.08 1.01	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_C\beta$_$Cγ} \\ \text{$C\alpha$_CC$O} \\ \text{$C\beta$_$Cα_C} \\ \text{$C\beta$_C\gamma$_$Cδ} \\ \text{$C\delta$_N\epsilon$_$Cζ} \\ \text{$C\gamma$_C\delta$_$Nϵ} \\ \text{$N\epsilon$_C\zeta$_$Nη1} \\ \text{$N\epsilon$_C\zeta$_$Nη2} \\ \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2 125.3 111.6 121.0 119.5	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69 1.23 1.93 1.24
	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline \\ C\alpha_C\beta_C\gamma \\ \\ C\alpha_C_O \\ \\ C\beta_C\alpha_C \\ \\ C\beta_C\gamma_C\delta \\ \\ C\delta_N\epsilon_C\zeta \\ \\ C\delta_N\epsilon_C\zeta \\ \\ C\gamma_C\delta_N\epsilon \\ \\ N\epsilon_C\zeta_N\eta1 \\ \\ N\epsilon_C\zeta_N\eta2 \\ \\ N\eta1_C\zeta_N\eta2 \\ \\ \end{array}$	Smooth COM -177 178 -178 -90 Mean 114.0 120.5 110.3 110.9 124.8 111.8 120.8 119.6 119.6	9.4 11.5 9.9 12.5 StdDev 1.62 0.79 1.26 2.08 1.17 2.58 1.08 1.01 0.87	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_C$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \text{$N\eta1_C\zeta_N\eta2$} \\ \end{array}$	Smooth COM -175 179 -64 113 Mean 113.9 120.6 110.3 112.2 125.3 111.6 121.0 119.5 119.4	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69 1.23 1.93 1.24 1.12

ARG ttm170 n = 1317		ARG	ARG ttm-80 n = 1504		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	9.9	chi1	-174	9.4
chi2	177	12.4	chi2	179	9.9
chi3	-68	9.9	chi3	-65	10.6
chi4	171	17.6	chi4	-85	9.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.8	1.74	$C\alpha_{-}C\beta_{-}C\gamma$	113.7	1.66
$C\alphaCO$	120.6	0.81	$C\alphaCO$	120.5	0.79
$C\betaC\alphaC$	110.1	1.16	$C\betaC\alphaC$	110.2	1.24
$C\beta C\gamma C\delta$	111.5	1.83	$C\betaC\gammaC\delta$	112.0	1.64
$C\delta_N\epsilon_C\zeta$	124.4	1.17	$C\delta_N\epsilon_C\zeta$	124.9	1.30
$C\gamma_C\delta_N\epsilon$	111.3	1.65	$C\gamma_C\delta_N\epsilon$	112.4	2.03
$N\epsilonC\zetaN\eta 1$	120.5	0.96	$N\epsilon C\zeta \eta 1$	120.7	1.02
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.93	$N\epsilon C\zeta N\eta 2$	119.7	1.04
$N\eta_1 C\zeta N\eta_2$	119.7	0.83	$N\eta 1_C\zeta N\eta 2$	119.5	0.76
$N_{-}C\alpha_{-}C$	110.3	2.38	$NC\alphaC$	110.6	2.26
$N_{-}C\alpha_{-}C\beta$	110.3	1.34	$N_{-}C\alpha_{-}C\beta$	110.4	1.36
,					
ARG	tmt170 n = 104	1	ARC	G tmt90 n = 23	
χ ARG	tmt170 n = 104 Smooth COM	StdDev	ARC	$\frac{G \text{ tmt90 n} = 23}{\text{Smooth COM}}$	StdDev
		_			StdDev 9.2
χ	Smooth COM	StdDev	χ	Smooth COM	
$\frac{\chi}{\text{chi1}}$	Smooth COM -174	StdDev 12.3	$\frac{\chi}{\text{chi1}}$	Smooth COM -178	9.2
χ chi1 chi2	Smooth COM -174 -91	StdDev 12.3 12.7	χ chi1 chi2	Smooth COM -178 -94	9.2 9.1
χ chi1 chi2 chi3	Smooth COM -174 -91 -174	StdDev 12.3 12.7 9.4	χ chi1 chi2 chi3	Smooth COM -178 -94 -178	9.2 9.1 11.2
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$	Smooth COM -174 -91 -174 -171	StdDev 12.3 12.7 9.4 17.5	chi1 chi2 chi3 chi4	Smooth COM -178 -94 -178 87	9.2 9.1 11.2 12.0
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -174 -91 -174 -171 Mean	StdDev 12.3 12.7 9.4 17.5 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -178 -94 -178 87 Mean	9.2 9.1 11.2 12.0 StdDev
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM -178 -94 -178 87 Mean 115.2	9.2 9.1 11.2 12.0 StdDev 1.49
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \hline \text{$\text{C}\alpha$_$C}_2\text{C}O \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha CO$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6	9.2 9.1 11.2 12.0 StdDev 1.49 0.98
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9 112.7	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5 112.9	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33 2.34
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9 112.7 124.5	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72 0.90	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5 112.9 125.1	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33 2.34 1.26
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta \\ C\gamma_C\delta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9 112.7 124.5 110.7	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72 0.90 1.62	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \hline \end{array}$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5 112.9 125.1 111.4	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33 2.34 1.26 2.85
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta-N\eta1$} \\ \hline \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9 112.7 124.5 110.7 120.7	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72 0.90 1.62 1.03	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \end{array}$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5 112.9 125.1 111.4 120.9	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33 2.34 1.26 2.85 1.86
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta \\ C\gamma_C\delta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -174 -91 -174 -171 Mean 115.0 120.6 110.9 112.7 124.5 110.7 120.7 119.6	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72 0.90 1.62 1.03 0.80	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -178 -94 -178 87 Mean 115.2 120.6 110.5 112.9 125.1 111.4 120.9 119.6	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33 2.34 1.26 2.85 1.86 1.46

ARC	f tmt-80 n = 62		ARG	tmm160 n = 92	2
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174	10.8	chi1	-172	10.9
chi2	-93	11.4	chi2	-90	11.1
chi3	-178	10.0	chi3	-61	11.3
chi4	-85	11.5	chi4	164	18.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha C\beta C\gamma$	114.7	1.34	$C\alpha C\beta C\gamma$	114.8	1.32
$C\alphaCO$	120.5	0.77	$C\alphaCO$	120.6	0.80
$C\betaC\alphaC$	111.3	1.33	$C\beta_{-}C\alpha_{-}C$	111.3	1.11
$C\betaC\gammaC\delta$	112.5	1.92	$C\betaC\gammaC\delta$	112.6	1.82
$C\delta_N\epsilon_C\zeta$	124.7	1.12	$C\delta_N\epsilon_C\zeta$	124.6	1.19
$C\gamma_C\delta_N\epsilon$	111.2	2.14	$C\gamma_C\delta_N\epsilon$	111.9	1.92
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.6	0.91	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.7	1.00
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.90	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.89
$N\eta 1 C\zeta N\eta 2$	119.6	0.63	$N\eta 1_{-}C\zeta_{-}N\eta 2$	119.6	0.81
$N_{-}C\alpha_{-}C$	110.1	2.45	$N_{-}C\alpha_{-}C$	110.0	2.05
$N_C\alpha_C\beta$	110.1	1.03	$N_C\alpha_C\beta$	110.1	1.13
$N_{-}C\alpha_{-}C\beta$ 110.1		1.00	1.200207	11011	
	tmm-80 n = 71			6 mpp80 n = 54	
ARG	tmm-80 n = 71		ARC	$\frac{1}{5}$ mpp80 n = 54	
χ	tmm-80 n = 71 Smooth COM	StdDev	ARC	Smooth COM	StdDev
$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \end{array}$	tmm-80 n = 71 Smooth COM -174	StdDev 9.2	$\begin{array}{c} \text{ARO} \\ \chi \\ \text{chi1} \end{array}$	S mpp80 n = 54 Smooth COM	StdDev 11.8
$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	tmm-80 n = 71 Smooth COM -174 -86	StdDev 9.2 8.8	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM -77 82	StdDev 11.8 12.0
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	tmm-80 n = 71 Smooth COM -174 -86 -56	StdDev 9.2 8.8 10.7	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	Smooth COM -77 82 58	StdDev 11.8 12.0 7.4
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4	tmm-80 n = 71 Smooth COM -174 -86 -56 -82	StdDev 9.2 8.8 10.7 8.5	ARO $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha \text{-}C\beta \text{-}C\gamma \end{array} $	Smooth COM -77 82 58 85	StdDev 11.8 12.0 7.4 10.1
$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \end{array}$	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean	StdDev 9.2 8.8 10.7 8.5 StdDev	$\begin{array}{c} \text{ARO} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -77 82 58 85 Mean	StdDev 11.8 12.0 7.4 10.1 StdDev
ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\text{C}\alpha\text{-C}\beta\text{-C}\gamma$	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32	ARO $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha \text{-}C\beta \text{-}C\gamma \end{array} $	Smooth COM -77 82 58 85 Mean 115.5	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha_{-}C\beta_{-}C\gamma \\ C\alpha_{-}C_{-}C \end{array} $ $ \begin{array}{c} C\beta_{-}C\alpha_{-}C \\ C\beta_{-}C\gamma_{-}C\delta \\ C\delta_{-}N\epsilon_{-}C\zeta \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_C$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98 1.62
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha_{-}C\beta_{-}C\gamma \\ C\alpha_{-}C_{-}C \end{array} $ $ \begin{array}{c} C\beta_{-}C\alpha_{-}C \\ C\beta_{-}C\gamma_{-}C\delta \\ C\delta_{-}N\epsilon_{-}C\zeta \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7 124.9	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29 1.25	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_C$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6 125.0	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98 1.62 1.16
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} C\alpha _ C\beta _ C\gamma \\ C\alpha _ C_ O \\ C\beta _ C\alpha _ C \end{array} $ $ \begin{array}{c} C\beta _ C\gamma _ C\delta \\ C\delta _ N\epsilon _ C\zeta \\ C\gamma _ C\delta _ N\epsilon $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7 124.9 112.6	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29 1.25 1.89	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C _ C$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$ $C\delta _ N\epsilon _ C\zeta$ $C\gamma _ C\delta _ N\epsilon$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6 125.0 113.1	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98 1.62 1.16 2.28
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta_{1} \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7 124.9 112.6 120.9	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29 1.25 1.89 1.10	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\gamma_{-}C\delta$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$	Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6 125.0 113.1 120.8	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98 1.62 1.16 2.28 1.17
ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\gamma_{-}C\delta}{C\delta_{-}N\epsilon_{-}C\zeta}$ $\frac{C\gamma_{-}C\delta_{-}N\epsilon_{-}C\zeta}{C\gamma_{-}C\delta_{-}N\eta_{1}}$ $\frac{N\epsilon_{-}C\zeta_{-}N\eta_{2}}{N\epsilon_{-}C\zeta_{-}N\eta_{2}}$	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7 124.9 112.6 120.9 119.7	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78 1.01 2.29 1.25 1.89 1.10 0.92	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	F mpp80 n = 54 Smooth COM -77 82 58 85 Mean 115.5 120.4 109.2 113.6 125.0 113.1 120.8 119.8	StdDev 11.8 12.0 7.4 10.1 StdDev 1.72 1.09 1.98 1.62 1.16 2.28 1.17 1.13

450	150 0		150	1100 01	
ARG	mpp-170 $n = 64$		ARG	mpt180 n = 24	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-79	12.9	chi1	-85	8.0
chi2	82	17.4	chi2	69	13.1
chi3	65	7.4	chi3	174	9.4
chi4	-167	16.4	chi4	174	16.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.43	$C\alphaC\betaC\gamma$	114.8	1.42
$C\alphaCO$	120.5	0.68	$C\alphaCO$	120.6	0.86
$C\betaC\alphaC$	109.7	1.57	$C\betaC\alphaC$	109.5	1.66
$C\beta C\gamma C\delta$	112.7	1.74	$C\betaC\gammaC\delta$	113.0	1.81
$C\delta_N\epsilon_C\zeta$	124.5	1.19	$C\delta_N\epsilon_C\zeta$	124.4	1.45
$C\gamma_C\delta_N\epsilon$	111.5	1.34	$C\gamma_C\delta_N\epsilon$	110.7	2.00
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.6	1.06	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.4	1.02
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.76	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.92
$N\eta 1_{-}C\zeta_{-}N\eta 2$	119.7	0.70	$N\eta 1_C \zeta_N \eta 2$	119.8	0.88
$N_{-}C\alpha_{-}C$	110.0	3.12	$N_{-}C\alpha_{-}C$	110.0	2.75
$N_C\alpha_C\beta$	111.4	1.11	$N_C\alpha_C\beta$	111.1	1.15
·		1.11	11_{-} C α_{-} C β	111.1	1.10
	$\frac{1}{6}$ mpt90 n = 46	1.11		$\frac{111.1}{\text{mpt-90 n} = 85}$	
		StdDev			
ARC	$G \mathbf{mpt90} \ \mathrm{n} = 46$		ARG	mpt-90 n = 85	ı
ARC	G mpt90 n = 46 Smooth COM	StdDev	ARG	mpt-90 n = 85 Smooth COM	StdDev
χ chi1	G mpt90 n = 46 Smooth COM -76	StdDev 12.9	$\begin{array}{c} \text{ARG} \\ \chi \\ \text{chi1} \end{array}$	mpt-90 n = 85 Smooth COM	StdDev 13.9
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	G mpt90 n = 46 Smooth COM -76 85	StdDev 12.9 13.6	$\begin{array}{c} X \\ \text{chi1} \\ \text{chi2} \end{array}$	mpt-90 n = 85 Smooth COM -79 75	StdDev 13.9 16.3
ARC χ chi1 chi2 chi3	G mpt90 n = 46 Smooth COM -76 85 170	StdDev 12.9 13.6 9.7	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	Smooth COM -79 75 178	StdDev 13.9 16.3 9.6
ARC x chi1 chi2 chi3 chi4	F mpt90 n = 46 Smooth COM -76 85 170 93	StdDev 12.9 13.6 9.7 11.2	ARG x chi1 chi2 chi3 chi4	mpt-90 n = 85 Smooth COM -79 75 178 -88	StdDev 13.9 16.3 9.6 13.7
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	G mpt90 n = 46 Smooth COM -76 85 170 93 Mean	StdDev 12.9 13.6 9.7 11.2 StdDev	$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean	StdDev 13.9 16.3 9.6 13.7 StdDev
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\text{C}\alpha\text{-C}\beta\text{-C}\gamma$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C O$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\alpha C$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3 112.5	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43 1.55	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\alpha C$	F mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0 112.9	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55 2.30
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3 112.5 125.1	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43 1.55 0.85	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}O}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\gamma_{-}C\delta}$ $\frac{C\beta_{-}C\gamma_{-}C\delta}{C\delta_{-}N\epsilon_{-}C\zeta}$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0 112.9 124.9	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55 2.30 1.00
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C _ C$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$ $C\delta _ N\epsilon _ C\zeta$ $C\gamma _ C\delta _ N\epsilon$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3 112.5 125.1 111.0	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43 1.55 0.85 2.03	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0 112.9 124.9 111.6	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55 2.30 1.00 2.53
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\gamma C C$ $C\beta C\gamma C\delta C$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$ $N\epsilon C\zeta N\eta 1$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3 112.5 125.1 111.0 121.1	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43 1.55 0.85 2.03 0.91	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\gamma_{-}C\delta}$ $\frac{C\delta_{-}N\epsilon_{-}C\zeta}{C\gamma_{-}C\delta_{-}N\epsilon}$ $\frac{N\epsilon_{-}C\zeta}{N\epsilon_{-}C\zeta_{-}N\eta_{1}}$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0 112.9 124.9 111.6 120.6	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55 2.30 1.00 2.53 1.07
ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\gamma$ $C\alpha C C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$ $N\epsilon C\zeta N\eta 1$ $N\epsilon C\zeta N\eta 2$	F mpt90 n = 46 Smooth COM -76 85 170 93 Mean 114.6 120.4 109.3 112.5 125.1 111.0 121.1 119.4	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64 1.43 1.55 0.85 2.03 0.91 0.68	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\beta_{-}C\gamma}$ $\frac{C\alpha_{-}C\beta_{-}C\gamma_{-}C\delta}{C\beta_{-}C\gamma_{-}C\delta}$ $\frac{C\beta_{-}C\gamma_{-}C\delta_{-}C\delta_{-}N\epsilon_{-}C\zeta}{C\gamma_{-}C\delta_{-}N\epsilon_{-}C\zeta}$ $\frac{N\epsilon_{-}C\zeta_{-}N\eta_{1}}{N\epsilon_{-}C\zeta_{-}N\eta_{2}}$	mpt-90 n = 85 Smooth COM -79 75 178 -88 Mean 114.9 120.4 110.0 112.9 124.9 111.6 120.6 119.8	StdDev 13.9 16.3 9.6 13.7 StdDev 1.26 0.75 1.55 2.30 1.00 2.53 1.07 0.83

ARG	ARG mtp180 n = 2504		ARG	mtp85 n = 185'	7
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66	8.1	chi1	-66	8.6
chi2	179	13.0	chi2	178	11.2
chi3	66	9.1	chi3	65	9.7
chi4	-172	16.5	chi4	88	11.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.2	1.79	$C\alphaC\betaC\gamma$	113.3	1.82
$C\alphaCO$	120.5	0.83	$C\alphaCO$	120.5	0.91
$C\betaC\alphaC$	110.0	1.65	$C\betaC\alphaC$	110.1	1.68
$C\beta C\gamma C\delta$	111.7	1.81	$C\betaC\gammaC\delta$	112.1	1.71
$C\delta_N\epsilon_C\zeta$	124.4	1.21	$C\delta_N\epsilon_C\zeta$	124.9	1.20
$C\gamma_C\delta_N\epsilon$	111.6	1.56	$C\gamma_C\delta_N\epsilon$	112.3	1.99
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.4	1.00	$N\epsilon C\zeta \eta 1$	120.8	1.05
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.8	0.97	$N\epsilon C\zeta N\eta 2$	119.7	1.04
$N\eta_1 C\zeta N\eta_2$	119.8	0.77	$N\eta 1_C\zeta_N\eta 2$	119.5	0.81
$N_{-}C\alpha_{-}C$	111.4	2.42	$NC\alphaC$	111.1	2.41
$N_C\alpha_C\beta$	110.5	1.05	$N_C\alpha_C\beta$	110.6	1.05
,			/-		
ARG	mtp-110 $n = 47$,	mtt180 n = 459	2
ARG :			,		2 StdDev
		0	ARG	mtt180 n = 459	
χ	Smooth COM	StdDev	ARG	mtt180 n = 459 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -65	5tdDev 8.1	$\frac{\lambda}{\chi}$	mtt180 n = 459 Smooth COM -67	StdDev 7.8
χ chi1 chi2	Smooth COM -65 179	StdDev 8.1 10.8	ARG χ chi1 chi2	mtt180 n = 459 Smooth COM -67 180	7.8 11.0
χ chi1 chi2 chi3	Smooth COM -65 179 66	StdDev 8.1 10.8 11.6	ARG χ chi1 chi2 chi3	mtt180 n = 459 Smooth COM -67 180 -179	7.8 11.0 10.7
χ chi1 chi2 chi3 chi4	Smooth COM -65 179 66 -110	StdDev 8.1 10.8 11.6 9.6	ARG χ chi1 chi2 chi3 chi4	mtt180 n = 459 Smooth COM -67 180 -179 177	7.8 11.0 10.7 17.9
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -65 179 66 -110 Mean	StdDev 8.1 10.8 11.6 9.6 StdDev	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean	7.8 11.0 10.7 17.9 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$	Smooth COM -65 179 66 -110 Mean 113.4	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\text{C}\alpha\text{-C}\beta\text{-C}\gamma$	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9	7.8 11.0 10.7 17.9 StdDev 1.75
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \hline \text{$\text{C}\alpha$_$C}_2\text{CO} \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha \cdot \text{C}\beta \cdot \text{C}\gamma}{\text{C}\alpha \cdot \text{C} \cdot \text{O}}$	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4	7.8 11.0 10.7 17.9 StdDev 1.75 0.85
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \text{$\text{C}\alpha$_$C$_$O} \\ \text{$\text{C}\beta$_$C}\alpha_{\text{C}} \\ \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha \text{_C}\beta \text{_C}\gamma \\ \text{C}\alpha \text{_C}\text{_O} \\ \text{C}\beta \text{_C}\alpha \text{_C} \end{array} $	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$-C\beta$-$Cγ} \\ \text{$C\alpha$-C-$O} \\ \text{$C\beta$-$Cα-$C} \\ \text{$C\beta$-$Cγ-C\delta$} \\ \text{$C\delta$-$Nϵ-C\zeta$} \\ \text{$C\delta$-$Nϵ-C\zeta$} \\ \text{$C\gamma$-$Cδ-N\epsilon$} \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1 112.4	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63	ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0 111.5	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66 2.02
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1 112.4 125.3	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63 2.05	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \end{array} $	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0 111.5 124.4	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66 2.02 1.10
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$C} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta$} \\ \text{$C\delta$_N\epsilon$_$C$\zeta} \\ \text{$C\gamma$_$Cδ_N\epsilon$} \\ \text{$C\gamma$_$Cδ_N\epsilon$} \\ \text{$N\epsilon$_$Cζ_N\eta$1} \\ \text{$N\epsilon$_$Cζ_N\eta$2} \\ \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1 112.4 125.3 111.7	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63 2.05 1.88	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma \\ \text{C}\alpha_{-}\text{C}_{-}\text{O} \\ \text{C}\beta_{-}\text{C}\alpha_{-}\text{C} \\ \text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta \\ \text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta \\ \text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon \end{array} $	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0 111.5 124.4 110.6	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66 2.02 1.10 1.82
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1 112.4 125.3 111.7 121.1	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63 2.05 1.88 1.20	ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha \text{C}\beta \text{C}\gamma \\ \text{C}\alpha \text{C} \text{C}\zeta \\ \text{C}\beta \text{C}\alpha \text{C}\zeta \\ \text{C}\gamma \text{C}\delta \text{N}\epsilon \text{C}\zeta \\ \text{C}\gamma \text{C}\delta \text{N}\epsilon \text{N}\zeta \\ \text{N}\epsilon \text{C}\zeta \text{N}\eta 1 \end{array} $	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0 111.5 124.4 110.6 120.4	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66 2.02 1.10 1.82 0.89
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C_$C} \\ \text{$C\beta$_$C}\alpha_\text{C} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta$} \\ \text{$C\delta$_$N$$\epsilon$_$C$\zeta} \\ \text{$C\gamma$_$Cδ_N\epsilon$_$C$\zeta} \\ \text{$C\gamma$_$Cδ_N\epsilon$} \\ \text{$N\epsilon$_$Cζ_N\eta$1} \\ \text{$N\epsilon$_$Cζ_N\eta$2} \\ \end{array}$	Smooth COM -65 179 66 -110 Mean 113.4 120.4 110.1 112.4 125.3 111.7 121.1 119.4	StdDev 8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63 2.05 1.88 1.20 1.29	ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\gamma_{-}C\delta}{C\delta_{-}N\epsilon_{-}C\zeta}$ $\frac{C\gamma_{-}C\delta_{-}N\epsilon_{-}C\zeta}{C\gamma_{-}C\delta_{-}N\epsilon_{-}N\epsilon_{-}C\zeta_{-}N\eta_{1}}$ $\frac{N\epsilon_{-}C\zeta_{-}N\eta_{2}}{N\epsilon_{-}C\zeta_{-}N\eta_{2}}$	mtt180 n = 459 Smooth COM -67 180 -179 177 Mean 112.9 120.4 110.0 111.5 124.4 110.6 120.4 119.6	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66 2.02 1.10 1.82 0.89 0.90

	1100 0100		4.D.C	11.05 001	0
ARG	mtt90 n = 2460		ARG	mtt-85 n = 284	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68	7.5	chi1	-67	7.8
chi2	180	13.5	chi2	-179	10.6
chi3	179	10.6	chi3	-176	9.2
chi4	91	15.1	chi4	-89	11.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.3	1.72	$C\alphaC\betaC\gamma$	113.5	1.70
$C\alphaCO$	120.4	0.80	$C\alphaCO$	120.4	0.82
$C\betaC\alphaC$	109.9	1.73	$C\betaC\alphaC$	109.8	1.65
$C\betaC\gammaC\delta$	111.5	2.04	$C\betaC\gammaC\delta$	111.4	1.97
$C\delta_N\epsilon_C\zeta$	124.9	1.14	$C\delta_N\epsilon_C\zeta$	124.8	1.05
$C\gamma_C\delta_N\epsilon$	111.0	2.49	$C\gamma_C\delta_N\epsilon$	111.4	2.43
$N\epsilon C\zeta \eta 1$	120.9	1.07	$N\epsilon C\zeta \eta 1$	120.8	1.02
$N\epsilon C\zeta \eta 2$	119.5	1.06	$N\epsilon C\zeta N\eta 2$	119.6	0.93
$N\eta_1 C\zeta N\eta_2$	119.6	0.80	$N\eta_1 C\zeta N\eta_2$	119.6	0.77
$N_{-}C\alpha_{-}C$	111.4	2.40	$N_{-}C\alpha_{-}C$	111.4	2.30
$N_C\alpha_C\beta$	110.6	1.12	$N_C\alpha_C\beta$	110.6	1.04
·		1.12	Ν_Οα_Ορ	110.0	1.04
	$\mathbf{mtm110} \ \mathbf{n} = 78$			$\frac{110.0}{\text{mtm}180 \text{ n} = 240}$	
ARG	mtm110 n = 78	1	ARG 1	ntm180 n = 240)7
ARG X	mtm110 n = 78 Smooth COM	1 StdDev	ARG 1	mtm180 n = 240 Smooth COM	O7 StdDev
χ chi1	mtm110 n = 78 Smooth COM -68	StdDev 8.2	ARG 1 χ chi1	mtm180 n = 240 Smooth COM -66	07 StdDev 8.1
ARG χ chi1 chi2	mtm110 n = 78 Smooth COM -68 -177	1 StdDev 8.2 9.7	$\begin{array}{c} \text{ARG 1} \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	mtm180 n = 240 Smooth COM -66 179	07 StdDev 8.1 12.7
ARG	mtm110 n = 78 Smooth COM -68 -177 -69	1 StdDev 8.2 9.7 10.2	$\begin{array}{c} \text{ARG 1} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	mtm180 n = 240 Smooth COM -66 179 -67	StdDev 8.1 12.7 8.8
ARG	mtm110 n = 78 Smooth COM -68 -177 -69 113	1 StdDev 8.2 9.7 10.2 10.6	ARG 1 χ chi1 chi2 chi3 chi4	mtm180 n = 240 Smooth COM -66 179 -67 173	StdDev 8.1 12.7 8.8 15.2
$\begin{array}{c} \text{ARG} \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean	1 StdDev 8.2 9.7 10.2 10.6 StdDev	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean	StdDev 8.1 12.7 8.8 15.2 StdDev
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C-C$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C C\alpha C$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C\alpha C$ $C\beta C\alpha C$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1 112.4	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76 1.72	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9 111.6	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_C$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1 112.4 125.3	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9 111.6 124.4	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1 112.4 125.3 112.1	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9 111.6 124.4 111.4	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08 1.69
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\gamma C\delta C$ $C\beta C\gamma C\delta $	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1 112.4 125.3 112.1 121.1	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88 1.28	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\gamma_{-}C\delta$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9 111.6 124.4 111.4 120.4	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08 1.69 0.90
ARG $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_{\text{-}}\text{C}\beta_{\text{-}}\text{C}\gamma \\ \text{C}\alpha_{\text{-}}\text{C}_{\text{-}}\text{C} \\ \text{C}\beta_{\text{-}}\text{C}\alpha_{\text{-}}\text{C} \\ \text{C}\beta_{\text{-}}\text{C}\gamma_{\text{-}}\text{C}\delta \\ \text{C}\delta_{\text{-}}\text{N}\epsilon_{\text{-}}\text{C}\zeta \\ \text{C}\gamma_{\text{-}}\text{C}\delta_{\text{-}}\text{N}\epsilon \\ \text{N}\epsilon_{\text{-}}\text{C}\zeta_{\text{-}}\text{N}\eta_{\text{1}} \\ \text{N}\epsilon_{\text{-}}\text{C}\zeta_{\text{-}}\text{N}\eta_{\text{2}} \end{array} $	mtm110 n = 78 Smooth COM -68 -177 -69 113 Mean 113.1 120.4 110.1 112.4 125.3 112.1 121.1 119.4	1 StdDev 8.2 9.7 10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88 1.28 1.12	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	mtm180 n = 240 Smooth COM -66 179 -67 173 Mean 113.3 120.5 109.9 111.6 124.4 111.4 120.4 119.8	StdDev 8.1 12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08 1.69 0.90 0.88

ARG 1	ARG mtm-85 n = 2848			mmp80 n = 164	ARG mmp80 n = 164			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev			
chi1	-68	8.1	chi1	-63	6.7			
chi2	-172	9.3	chi2	-75	12.7			
chi3	-64	9.5	chi3	74	11.7			
chi4	-88	8.9	chi4	78	6.9			
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev			
$C\alphaC\betaC\gamma$	113.5	1.56	$C\alpha_{-}C\beta_{-}C\gamma$	114.8	1.39			
$C\alphaCO$	120.5	0.81	$C\alphaCO$	120.4	0.95			
$C\betaC\alphaC$	110.0	1.49	$C\beta_{-}C\alpha_{-}C$	109.8	1.49			
$C\beta C\gamma C\delta$	112.0	1.57	$C\betaC\gammaC\delta$	113.4	1.62			
$C\delta_N\epsilon_C\zeta$	124.9	1.17	$C\delta_N\epsilon_C\zeta$	125.0	1.16			
$C\gamma_C\delta_N\epsilon$	112.7	1.96	$C\gamma_C\delta_N\epsilon$	113.5	2.23			
$N\epsilon C\zeta N\eta 1$	120.8	1.03	$N\epsilon C\zeta N\eta 1$	120.6	0.99			
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	1.00	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	120.0	0.86			
$N\eta 1 C\zeta N\eta 2$	119.5	0.78	$N\eta 1 \underline{C}\zeta \underline{N}\eta 2$	119.5	0.64			
$N_{-}C\alpha_{-}C$	111.3	1.97	$N_{-}C\alpha_{-}C$	111.4	1.82			
$N_{-}C\alpha_{-}C\beta$	111.1	1.03	$N_{-}C\alpha_{-}C\beta$	110.9	0.93			
ARG r	mmp-170 n = 12	23	ARG 1	mmt180 n = 120)3			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev			
1 *4								
chi1	-64	7.2	chi1	-62	9.1			
chil chi2	-64 -65	7.2 14.3	chi1 chi2	-62 -68	9.1 12.9			
chi2	-65	14.3	chi2	-68	12.9			
chi2 chi3	-65 86	$14.3 \\ 9.7$	chi2 chi3	-68 -177	12.9 11.3			
chi2 chi3 chi4	-65 86 -167	14.3 9.7 19.8	chi2 chi3 chi4	-68 -177 -176	12.9 11.3 17.4			
chi2 chi3 chi4 Bond Angle	-65 86 -167 Mean	14.3 9.7 19.8 StdDev	chi2 chi3 chi4 Bond Angle	-68 -177 -176 Mean	12.9 11.3 17.4 StdDev			
chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	-65 86 -167 Mean 115.5	14.3 9.7 19.8 StdDev	chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	-68 -177 -176 Mean 114.5	12.9 11.3 17.4 StdDev			
chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C-O$	-65 86 -167 Mean 115.5 120.4	14.3 9.7 19.8 StdDev 1.27 0.99	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	-68 -177 -176 Mean 114.5 120.4	12.9 11.3 17.4 StdDev 1.38 0.87			
chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C CO$ $C\beta C\alpha C$	-65 86 -167 Mean 115.5 120.4 109.5	14.3 9.7 19.8 StdDev 1.27 0.99 1.52	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$	-68 -177 -176 Mean 114.5 120.4 109.4	12.9 11.3 17.4 StdDev 1.38 0.87 1.62			
chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$	-65 86 -167 Mean 115.5 120.4 109.5 112.8	14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$	-68 -177 -176 Mean 114.5 120.4 109.4 112.0	12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71			
chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$	-65 86 -167 Mean 115.5 120.4 109.5 112.8 124.8	14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32	chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\alpha C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$	-68 -177 -176 Mean 114.5 120.4 109.4 112.0 124.4	12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19			
chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$	-65 86 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5	14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$	-68 -177 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0	12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83			
chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$ $C\alphaCO$ $C\betaC\alphaC$ $C\betaC\gammaC\delta$ $C\deltaN\epsilonC\zeta$ $C\gammaC\deltaN\epsilon$ $N\epsilonC\zetaN\eta_1$ $N\epsilonC\zetaN\eta_2$	-65 86 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5 120.5	14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61 1.21	chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\alpha C\beta C\gamma$ $C\beta C\gamma C\delta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon N\epsilon C\zeta$ $C\gamma C\delta N\epsilon C\zeta N\eta 1$ $N\epsilon C\zeta N\eta 2$	-68 -177 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0 120.5	12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83 0.87			
chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\alpha C$ $C\beta C\alpha C$	-65 86 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5 120.5 119.8	14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61 1.21 1.10	chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\alpha C$ $C\beta C\alpha C$ $C\alpha C\alpha$	-68 -177 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0 120.5 119.7	12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83 0.87 0.87			

ARG	$\mathbf{mmt90} \ \mathbf{n} = 567$	7	ARG	mmt-90 n = 142	28
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-61	8.8	chi1	-64	6.6
chi2	-68	12.5	chi2	-69	8.1
chi3	179	10.4	chi3	-175	7.7
chi4	90	12.9	chi4	-91	11.1
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.6	1.39	$C\alphaC\betaC\gamma$	114.5	1.43
$C\alphaCO$	120.5	0.87	$C\alphaCO$	120.5	0.85
$C\betaC\alphaC$	109.5	1.65	$C\betaC\alphaC$	109.6	1.64
$C\betaC\gammaC\delta$	112.2	1.61	$C\betaC\gammaC\delta$	112.0	1.67
$C\delta_N\epsilon_C\zeta$	124.9	1.24	$C\delta_N\epsilon_C\zeta$	124.9	1.00
$C\gamma_C\delta_N\epsilon$	111.6	2.49	$C\gamma_C\delta_N\epsilon$	111.8	2.28
$N\epsilon C\zeta N\eta 1$	120.8	1.22	$N\epsilon C\zeta \eta 1$	120.9	1.00
$N\epsilon C\zeta N\eta 2$	119.6	1.09	$N\epsilon C\zeta \eta 2$	119.6	0.88
$N\eta 1_C\zeta_N\eta 2$	119.6	0.72	$N\eta 1_C\zeta_N\eta 2$	119.4	0.82
$N_{-}C\alpha_{-}C$	111.4	2.72	$N_{-}C\alpha_{-}C$	110.1	2.67
$N_{-}C\alpha_{-}C\beta$	110.7	1.08	$N_{-}C\alpha_{-}C\beta$	110.9	1.11
ARG 1	nmm160 n = 95	51	ARG n	nmm-85 n = 10	22
ARG 1	mmm160 n = 95 Smooth COM	51 StdDev	ARG n	nmm-85 n = 10 Smooth COM	22 StdDev
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -62	StdDev 9.2	χ chi1 chi2 chi3	Smooth COM -63	StdDev 9.2
χ chi1 chi2	Smooth COM -62 -66	9.2 13.7	χ chi1 chi2	Smooth COM -63 -68	StdDev 9.2 10.9
χ chi1 chi2 chi3	Smooth COM -62 -66 -64	9.2 13.7 9.9	χ chi1 chi2 chi3	Smooth COM -63 -68 -61	9.2 10.9 9.2
χ chi1 chi2 chi3 chi4	-62 -66 -64 163	9.2 13.7 9.9 24.2	χ chi1 chi2 chi3 chi4	-63 -68 -61 -86	9.2 10.9 9.2 10.1
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -62 -66 -64 163 Mean	9.2 13.7 9.9 24.2 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -63 -68 -61 -86 Mean	9.2 10.9 9.2 10.1 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$	Smooth COM -62 -66 -64 163 Mean 114.5	9.2 13.7 9.9 24.2 StdDev 1.60	χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM -63 -68 -61 -86 Mean 114.6	9.2 10.9 9.2 10.1 StdDev 1.52
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \text{$\text{C}\alpha$_$C$_$O} \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4	9.2 13.7 9.9 24.2 StdDev 1.60 0.88	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5	9.2 10.9 9.2 10.1 StdDev 1.52 0.88
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \hline \\ \hline \text{$\text{C}\alpha$_C_$C} \\ \hline \\ \hline \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \hline \\ \hline \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \hline \\ \hline \\ \hline \text{$\text{C}\beta$_$C}\gamma$_$C}\delta \\ \hline \\ \hline \\ \hline \text{$\text{C}\beta$_$C}\gamma$_$C}\delta \\ \hline \\ \hline \\ \hline \text{$\text{C}\beta$_$C}\gamma$_$C}\delta \\ \hline \\ \hline \\ \hline \\ \hline \text{$\text{C}\gamma$_$C}\delta$_$N}\epsilon \\ \hline \\ $	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8 112.5	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54 1.73	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \hline \\ \text{C}\alpha_\text{C}_\text{O} \\ \hline \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \hline \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7 112.8	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54 1.62
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{C} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8 112.5 124.6	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54 1.73 1.31	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7 112.8 125.0	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54 1.62 1.09
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\alpha_C$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8 112.5 124.6 111.9	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54 1.73 1.31 1.89	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}_{-}\text{C} \\ \text{$\text{C}\alpha_\text{C}_{-}\text{C}$} \\ \hline \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \\ \hline \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \hline \\ \hline \\ \hline \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \hline \\ \hline \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \\ \hline \\ \hline \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta2$} \\ \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7 112.8 125.0 112.5	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54 1.62 1.09 2.26
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8 112.5 124.6 111.9 120.6	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54 1.73 1.31 1.89 1.17	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7 112.8 125.0 112.5 120.9	StdDev 9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54 1.62 1.09 2.26 1.01
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\alpha_C$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ \text{$C\gamma_C\delta_N\epsilon$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta1$} \\ \hline \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM -62 -66 -64 163 Mean 114.5 120.4 109.8 112.5 124.6 111.9 120.6 119.8	9.2 13.7 9.9 24.2 StdDev 1.60 0.88 1.54 1.73 1.31 1.89 1.17 1.11	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}_{-}\text{C} \\ \text{$\text{C}\alpha_\text{C}_{-}\text{C}$} \\ \hline \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \\ \hline \text{$\text{C}\delta_\text{N}\epsilon_\text{C}\zeta$} \\ \hline \\ \hline \\ \hline \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \hline \\ \hline \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta1$} \\ \hline \\ \hline \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta2$} \\ \end{array}$	Smooth COM -63 -68 -61 -86 Mean 114.6 120.5 109.7 112.8 125.0 112.5 120.9 119.6	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54 1.62 1.09 2.26 1.01 0.96

Table S21: LYS Central Values

LYS pptt $n = 25$		LYS $\mathbf{ptpp} \ n = 89$					
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	64	7.5	chi1	65	6.8		
chi2	90	8.3	chi2	178	8.1		
chi3	176	11.9	chi3	72	9.7		
chi4	179	7.4	chi4	66	8.1		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	116.1	1.24	$C\alphaC\betaC\gamma$	114.6	1.20		
$C\alphaCO$	120.4	0.70	$C\alphaCO$	120.2	0.97		
$C\betaC\alphaC$	111.3	1.43	$C\betaC\alphaC$	110.1	1.28		
$C\betaC\gammaC\delta$	112.2	1.70	$C\betaC\gammaC\delta$	112.2	1.29		
$C\deltaC\epsilonN\zeta$	111.3	1.82	$C\deltaC\epsilonN\zeta$	112.5	1.72		
$C\gamma_{-}C\delta_{-}C\epsilon$	110.6	1.94	$C\gamma_{-}C\delta_{-}C\epsilon$	112.7	1.34		
$N_{-}C\alpha_{-}C$	111.7	2.09	$N_{-}C\alpha_{-}C$	111.9	2.03		
$N_{-}C\alpha_{-}C\beta$	111.6	1.19	$N_{-}C\alpha_{-}C\beta$	110.9	1.31		
LY	LYS $\mathbf{ptpt} \ n = 148$		LY	S pttp n = 240			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	65	8.2	chi1	68	8.3		
chi2	179	11.8	chi2	-179	10.4		
chi3	73	10.4	chi3	178	11.2		
chi4	175	11.2	chi4	67	12.3		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	114.7	1.64	$C\alphaC\betaC\gamma$	114.8	1.43		
$C\alphaCO$	120.5	0.85	$C\alphaCO$	120.4	0.90		
$C\betaC\alphaC$	110.5	1.43	$C\betaC\alphaC$	110.4	1.45		
$C\betaC\gammaC\delta$	112.1	1.65	$C\betaC\gammaC\delta$	110.9	1.68		
$C\deltaC\epsilonN\zeta$	111.4	2.10	$C\deltaC\epsilonN\zeta$	112.4	2.34		
$C\gammaC\deltaC\epsilon$	112.4	1.85	$C\gammaC\deltaC\epsilon$	111.7	1.42		
$N_C\alpha_C$	111.2	2.94	$N_{-}C\alpha_{-}C$	111.8	2.55		
$N_{-}C\alpha_{-}C\beta$	111.1	1.32	$N_{-}C\alpha_{-}C\beta$	111.0	1.09		
LYS	8 pttt n = 1385		LYS	LYS pttm $n = 268$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	65	7.6	chi1	64	6.9		
chi2	-178	8.7	chi2	-178	9.1		
chi3	-179	9.7	chi3	-179	10.0		
chi4	-180	9.6	chi4	-67	11.7		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	114.8	1.46	$C\alphaC\betaC\gamma$	114.9	1.47		
$C\alphaCO$	120.4	0.95	$C\alphaCO$	120.4	0.98		
$C\betaC\alphaC$	110.4	1.38	$C\betaC\alphaC$	110.4	1.45		
$C\betaC\gammaC\delta$	110.8	1.79	$C\betaC\gammaC\delta$	110.7	2.05		
$C\deltaC\epsilonN\zeta$	111.3	2.00	$C\deltaC\epsilonN\zeta$	112.3	2.37		
$C\gammaC\deltaC\epsilon$	111.0	1.62	$C\gammaC\deltaC\epsilon$	111.9	1.51		
$N_{-}C\alpha_{-}C$	111.3	2.77	$N_{-}C\alpha_{-}C$	112.0	2.55		
$N_{-}C\alpha_{-}C\beta$	111.1	1.10	$N_{-}C\alpha_{-}C\beta$	111.0	1.16		

LYS	$8 \mathbf{ptmt} \ n = 187$		LYS	$8 \mathbf{ptmm} \ n = 80$			
$\overline{\chi}$	Smooth COM	StdDev	$\overline{\chi}$	Smooth COM	StdDev		
chi1	67	8.2	chi1	67	8.4		
chi2	-176	12.0	chi2	-178	10.0		
chi3	-71	11.7	chi3	-70	9.8		
chi4	-176	10.3	chi4	-66	7.0		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.57	$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.30		
$C\alpha_{-}C_{-}O$	120.5	0.97	$C\alphaCO$	120.6	1.03		
$C\betaC\alphaC$	110.4	1.61	$C\betaC\alphaC$	109.9	1.49		
$C\betaC\gammaC\delta$	112.1	1.58	$C\betaC\gammaC\delta$	112.3	1.44		
$C\deltaC\epsilonN\zeta$	111.5	2.11	$C\deltaC\epsilonN\zeta$	113.0	1.78		
$\mathrm{C}\gamma\mathrm{C}\delta\mathrm{C}\dot{\epsilon}$	112.4	1.87	$C\gammaC\deltaC\epsilon$	113.0	1.15		
$N_{-}C\alpha_{-}C$	111.0	2.72	$N_{-}C\alpha_{-}C$	110.5	2.70		
$N_{-}C\alpha_{-}C\beta$	111.0	1.10	$N_{-}C\alpha_{-}C\beta$	110.8	1.21		
LY	S pmtt $n = 10$		LY	S tppp n = 37			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	73	8.4	chi1	-178	11.5		
chi2	-74	10.5	chi2	62	10.1		
chi3	-168	10.6	chi3	66	7.8		
chi4	-175	10.7	chi4	68	11.3		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	116.4	1.64	$C\alphaC\betaC\gamma$	115.1	1.50		
$C\alphaCO$	120.8	0.55	$C\alphaCO$	120.7	0.87		
$C\betaC\alphaC$	110.4	1.28	$C\betaC\alphaC$	110.3	0.75		
$C\betaC\gammaC\delta$	112.6	2.23	$C\betaC\gammaC\delta$	113.5	1.87		
$C\delta_{-}C\epsilon_{-}N\zeta$	111.7	2.25	$C\deltaC\epsilonN\zeta$	113.0	1.70		
$C\gammaC\deltaC\epsilon$	111.3	1.31	$C\gammaC\deltaC\epsilon$	113.4	1.74		
$N_{-}C\alpha_{-}C$	110.0	2.38	$N_{-}C\alpha_{-}C$	110.9	1.93		
$NC\alphaC\beta$	112.1	2.13	$N_{-}C\alpha_{-}C\beta$	110.2	1.12		
LY	S tppt $n = 272$		LY	LYS $\mathbf{tptp} \ n = 409$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	-178	7.9	chi1	-180	8.0		
chi2	63	8.9	chi2	67	10.4		
chi3	70	9.2	chi3	174	13.6		
chi4	177	9.4	chi4	66	13.0		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	114.8	1.23	$C\alphaC\betaC\gamma$	114.8	1.34		
$C\alphaCO$	120.5	0.74	$C\alphaCO$	120.5	0.83		
$C\betaC\alphaC$	110.6	1.10	$C\betaC\alphaC$	110.2	1.23		
$C\betaC\gammaC\delta$	113.2	1.54	$C\betaC\gammaC\delta$	112.1	1.49		
$C\deltaC\epsilonN\zeta$	111.2	1.84	$C\deltaC\epsilonN\zeta$	112.7	1.95		
$C\gammaC\deltaC\epsilon$	112.4	1.45	$C\gammaC\deltaC\epsilon$	112.2	1.31		
$N_{-}C\alpha_{-}C$	110.6	2.08	$N_{-}C\alpha_{-}C$	110.3	2.08		
$N_{-}C\alpha_{-}C\beta$	110.3	1.07	$N_{-}C\alpha_{-}C\beta$	110.3	1.12		

LYS	$8 \mathbf{tptt} \ n = 1228$		LYS	8 tptm n = 197			
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	-179	9.1	chi1	-178	7.6		
chi2	69	9.0	chi2	67	9.7		
chi3	176	10.1	chi3	-179	11.4		
chi4	177	12.3	chi4	-66	13.4		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	114.8	1.31	$C\alpha_{-}C\beta_{-}C\gamma$	115.0	1.45		
$C\alphaCO$	120.5	0.78	$C\alphaCO$	120.4	0.77		
$C\betaC\alphaC$	110.4	1.22	$C\betaC\alphaC$	110.4	1.10		
$C\betaC\gammaC\delta$	112.0	1.60	$C\betaC\gammaC\delta$	111.9	1.41		
$C\delta_C\epsilon_N\zeta$	111.1	2.24	$C\deltaC\epsilonN\zeta$	112.5	2.06		
$C\gammaC\deltaC\epsilon$	111.0	1.47	$C\gammaC\deltaC\epsilon$	111.9	1.35		
$N_C\alpha_C$	110.7	2.15	$N_{-}C\alpha_{-}C$	110.3	2.06		
$NC\alphaC\beta$	110.2	1.11	$N_{-}C\alpha_{-}C\beta$	110.3	1.14		
LY	LYS $\mathbf{ttpp} \ n = 229$		LY	S $\mathbf{ttpt} \ n = 883$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	-178	8.6	chi1	-178	8.1		
chi2	174	14.5	chi2	175	12.1		
chi3	72	11.2	chi3	73	11.9		
chi4	68	10.5	chi4	175	11.3		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.7	1.58	$C\alphaC\betaC\gamma$	113.8	1.64		
$C\alphaCO$	120.6	0.78	$C\alphaCO$	120.6	0.75		
$C\betaC\alphaC$	110.1	1.26	$C\betaC\alphaC$	110.1	1.18		
$C\betaC\gammaC\delta$	112.1	1.68	$C\betaC\gammaC\delta$	112.1	1.47		
$C\deltaC\epsilonN\zeta$	112.8	2.35	$C\deltaC\epsilonN\zeta$	111.1	2.07		
$C\gammaC\deltaC\epsilon$	112.8	1.57	$C\gammaC\deltaC\epsilon$	112.2	1.58		
$N_{-}C\alpha_{-}C$	110.2	2.48	$N_{-}C\alpha_{-}C$	110.3	2.32		
$N_{-}C\alpha_{-}C\beta$	110.4	1.47	$N_{-}C\alpha_{-}C\beta$	110.2	1.32		
LYS	8 tttp n = 1233		LYS	LYS tttt $n = 5043$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev		
chi1	-178	8.1	chi1	-175	8.2		
chi2	175	9.9	chi2	177	8.7		
chi3	174	10.8	chi3	180	9.2		
chi4	66	12.8	chi4	-180	10.3		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.9	1.52	$C\alphaC\betaC\gamma$	113.9	1.52		
$C\alphaCO$	120.6	0.75	$C\alphaCO$	120.6	0.78		
$C\betaC\alphaC$	110.2	1.09	$C\betaC\alphaC$	110.2	1.14		
$C\betaC\gammaC\delta$	111.1	1.61	$C\betaC\gammaC\delta$	111.1	1.74		
$C\deltaC\epsilonN\zeta$	112.3	1.98	$C\deltaC\epsilonN\zeta$	111.2	1.99		
$C\gammaC\deltaC\epsilon$	111.8	1.35	$C\gammaC\deltaC\epsilon$	111.0	1.54		
$N_{-}C\alpha_{-}C$	110.7	2.22	$N_{-}C\alpha_{-}C$	110.5	2.28		
$N_{-}C\alpha_{-}C\beta$	110.4	1.14	$N_{-}C\alpha_{-}C\beta$	110.3	1.21		

LYS	5 tttm n = 1176			7S ttmp n = 9	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176	8.1	chi1	-174	4.2
chi2	178	9.7	chi2	-179	8.5
chi3	-176	10.5	chi3	-96	18.6
chi4	-67	12.1	chi4	77	25.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.9	1.60	$C\alpha_{-}C\beta_{-}C\gamma$	113.2	1.24
$C\alphaCO$	120.6	0.82	$C\alphaCO$	120.6	0.50
$C\betaC\alphaC$	110.3	1.14	$C\betaC\alphaC$	110.3	1.62
$C\betaC\gammaC\delta$	111.0	1.70	$C\betaC\gammaC\delta$	112.6	1.74
$C\deltaC\epsilonN\zeta$	112.3	1.97	$C\deltaC\epsilonN\zeta$	114.0	1.36
$C\gammaC\deltaC\epsilon$	111.8	1.47	$\mathrm{C}\gamma\mathrm{C}\delta\mathrm{C}\epsilon$	112.9	0.74
$N_{-}C\alpha_{-}C$	110.5	2.11	$N_{-}C\alpha_{-}C$	110.8	1.51
$N_{-}C\alpha_{-}C\beta$	110.4	1.16	$N_{-}C\alpha_{-}C\beta$	111.4	1.04
LY	S $\mathbf{ttmt} \ \mathbf{n} = 674$		LYS ttmm $n = 197$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-175	9.4	chi1	-174	8.5
chi2	-177	10.8	chi2	180	9.9
chi3	-73	11.7	chi3	-71	11.9
chi4	-175	11.5	chi4	-67	11.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.7	1.55	$C\alpha_{-}C\beta_{-}C\gamma$	113.6	1.46
$C\alphaCO$	120.6	0.86	$C\alphaCO$	120.6	0.82
$C\betaC\alphaC$	110.2	1.18	$C\betaC\alphaC$	110.2	1.29
$^{'}_{\mathrm{C}\beta}_{\mathrm{-}\mathrm{C}\gamma_{\mathrm{-}}\mathrm{C}\delta}$	112.2	1.52	$^{'}\!$	112.1	1.57
$C\deltaC\epsilonN\zeta$	110.9	2.32	$C\deltaC\epsilonN\zeta$	112.6	2.30
$C\gammaC\deltaC\epsilon$	112.2	1.65	$C\gammaC\deltaC\epsilon$	112.5	1.56
$N_{-}C\alpha_{-}C$	110.3	2.33	$N_{-}C\alpha_{-}C$	110.2	2.45
$N_{-}C\alpha_{-}C\beta$	110.3	1.25	$N_{-}C\alpha_{-}C\beta$	110.3	1.39
LY	S tmtp n = 11		LY	TS tmtt $n = 82$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	7.5	chi1	-173	8.5
chi2	-98	8.3	chi2	-91	9.6
chi3	-178	12.4	chi3	-177	11.7
chi4	65	7.8	chi4	-179	10.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.22	$C\alphaC\betaC\gamma$	114.5	1.14
$C\alphaCO$	120.8	0.41	$C\alphaCO$	120.8	0.61
$C\betaC\alphaC$	110.5	0.70	$C\betaC\alphaC$	110.9	1.09
$C\betaC\gammaC\delta$	112.0	1.51	$C\betaC\gammaC\delta$	111.9	1.44
$C\deltaC\epsilonN\zeta$	113.1	3.03	$C\deltaC\epsilonN\zeta$	110.8	2.07
$C\gammaC\deltaC\epsilon$	111.8	1.20	$\mathrm{C}\gamma\mathrm{C}\delta\mathrm{C}\epsilon$	111.0	1.37
$N_{-}C\alpha_{-}C$	110.1	3.05	$N_{-}C\alpha_{-}C$	110.2	1.89
$NC\alphaC\beta$	110.4	0.87	$N_{-}C\alpha_{-}C\beta$	110.1	0.81

LY	$S \mathbf{tmtm} \ n = 20$		LY	S tmmt n = 33		
χ	Smooth COM	StdDev	$\overline{\chi}$	Smooth COM	StdDev	
chi1	-172	10.4	chi1	-179	10.0	
chi2	-91	5.6	chi2	-93	12.1	
chi3	-173	15.1	chi3	-70	8.9	
chi4	-65	7.7	chi4	-180	10.2	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	115.5	1.62	$C\alpha_{-}C\beta_{-}C\gamma$	115.0	1.85	
$C\alphaCO$	120.6	0.65	$C\alphaCO$	120.5	0.88	
$C\betaC\alphaC$	111.0	0.85	$C\betaC\alphaC$	110.7	1.12	
$^{'}\!\!eta_{-}\!$	112.2	1.23	$C\betaC\gammaC\delta$	113.5	1.73	
$C\deltaC\epsilonN\zeta$	112.7	1.69	$C\deltaC\epsilonN\zeta$	110.8	2.86	
$C\gammaC\deltaC\epsilon$	112.0	1.55	$\mathrm{C}\gamma\mathrm{C}\delta\mathrm{C}\epsilon$	112.4	2.86	
$N_{-}C\alpha_{-}C$	110.1	1.72	$N_{-}C\alpha_{-}C$	110.0	2.15	
$N_{-}C\alpha_{-}C\beta$	109.8	0.79	$N_{-}C\alpha_{-}C\beta$	109.9	1.08	
LYS tmmm $n = 8$ LYS mp		S mppt $n = 31$				
$\frac{1}{\chi}$	Smooth COM	StdDev	$\frac{1}{\chi}$	Smooth COM	StdDev	
chi1	-178	11.9	chi1	-83	8.9	
chi2	-82	7.5	chi2	74	14.9	
chi3	-63	8.0	chi3	69	8.0	
chi4	-64	4.9	chi4	177	5.4	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	116.2	2.69	$C\alpha_{-}C\beta_{-}C\gamma$	115.1	1.99	
$C\alpha_{-}C_{-}O$	120.3	0.85	$C\alpha_{-}C_{-}O$	120.4	0.89	
$C\beta_{-}C\alpha_{-}C$	111.2	1.13	$C\beta_{-}C\alpha_{-}C$	109.9	1.23	
$C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$	114.9	1.13 1.37	$C\beta C\alpha C\delta$	113.7	1.56	
$C\delta_{-}C\epsilon_{-}N\zeta$	113.1	1.48	$C\deltaC\epsilonN\zeta$	111.4	1.92	
$C\gammaC\deltaC\epsilon$	115.0	1.62	$C\gammaC\deltaC\epsilon$	112.2	1.32 1.37	
N_Cα_C	109.0	2.01	N_Cα_C	108.8	1.97	
$N_{-}C\alpha_{-}C\beta$	109.5	1.26	$N_{-}C\alpha_{-}C\beta$	110.9	0.92	
		1.20			0.32	
	$\frac{\text{S mptp n} = 26}{\text{Constant}}$	G. ID		LYS mptt n = 124 Smooth COM StdD		
<u>X</u>	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	-75	18.5	chi1	-80	13.3	
chi2	87	18.2	chi2	73	17.3	
chi3	172	9.0	chi3	176	12.4	
chi4	65	12.1	chi4	175	11.9	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev	
$C\alphaC\betaC\gamma$	114.7	1.56	$C\alphaC\betaC\gamma$	114.9	1.39	
$C\alphaCO$	120.5	1.13	$C\alphaCO$	120.6	0.78	
$C\betaC\alphaC$	110.1	1.43	$C\betaC\alphaC$	109.7	1.53	
$C\betaC\gammaC\delta$	113.2	2.50	$C\betaC\gammaC\delta$	112.6	2.03	
$C\deltaC\epsilonN\zeta$	113.4	2.26	$C\deltaC\epsilonN\zeta$	110.9	2.27	
$C\gammaC\deltaC\epsilon$	112.5	2.72	$C\gammaC\deltaC\epsilon$	111.2	1.60	
$N_{-}C\alpha_{-}C$	110.6	2.77	$N_{-}C\alpha_{-}C$	110.6	2.59	
$NC\alphaC\beta$	110.9	1.04	$NC\alphaC\beta$	110.8	1.10	

LYS	S mptm n = 11			LYS	6 mtpp n = 392			
χ	Smooth COM	StdDev	•	χ	Smooth COM	StdDev		
chi1	-92	6.7		chi1	-69	7.5		
chi2	61	11.1		chi2	177	10.9		
chi3	-174	5.4		chi3	70	10.8		
chi4	-61	13.5		chi4	68	10.9		
Bond Angle	Mean	StdDev		Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	0.81		$C\alphaC\betaC\gamma$	113.2	1.66		
$C\alpha_{-}C_{-}O$	120.7	0.57		$C\alpha_{-}C_{-}O$	120.4	0.82		
$C\beta_{-}C\alpha_{-}C$	110.7	0.84		$C\beta_{-}C\alpha_{-}C$	110.2	1.51		
$C\betaC\gammaC\delta$	112.8	0.65		$C\betaC\gammaC\delta$	112.4	1.45		
$C\delta_{-}C\epsilon_{-}N\zeta$	113.4	1.68		$C\deltaC\epsilonN\zeta$	112.8	2.11		
$C\gammaC\deltaC\epsilon$	111.8	0.50		$C\gammaC\deltaC\epsilon$	112.7	1.41		
$N_{-}C\alpha_{-}C$	110.8	2.19		$N_{-}C\alpha_{-}C$	111.4	2.53		
$N_{-}C\alpha_{-}C\beta$	110.6	0.91		$N_{-}C\alpha_{-}C\beta$	110.5	1.01		
LYS	LYS mtpt $n = 1357$			LYS	6 mtpm n = 17			
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev		
chi1	-69	8.1		chi1	-70	6.1		
chi2	174	11.3		chi2	175	15.5		
chi3	71	11.8		chi3	91	14.7		
chi4	175	10.4		chi4	-70	12.1		
Bond Angle	Mean	StdDev	•	Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	113.3	1.54		$C\alphaC\betaC\gamma$	113.5	2.14		
$C\alphaCO$	120.5	0.84		$C\alphaCO$	120.3	0.77		
$C\betaC\alphaC$	110.0	1.65		$C\betaC\alphaC$	109.8	2.27		
$C\betaC\gammaC\delta$	112.3	1.55		$C\betaC\gammaC\delta$	112.3	1.70		
$C\deltaC\epsilonN\zeta$	110.8	2.15		$C\delta_{-}C\epsilon_{-}N\zeta$	113.4	1.87		
$C\gammaC\deltaC\epsilon$	112.3	1.49		$C\gammaC\deltaC\epsilon$	113.2	1.59		
$N_C\alpha_C$	111.4	2.21		$N_{-}C\alpha_{-}C$	110.9	2.12		
$NC\alphaC\beta$	110.7	1.03		$N_{-}C\alpha_{-}C\beta$	110.5	1.03		
LYS	$\mathbf{mttp} \ \mathrm{n} = 1414$			LYS mttt $n = 8597$				
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev		
chi1	-66	8.3		chi1	-68	7.1		
chi2	-179	10.7		chi2	-179	9.1		
chi3	176	11.2		chi3	-179	9.8		
chi4	67	13.6		chi4	179	10.3		
Bond Angle	Mean	StdDev		Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.4	1.73		$C\alphaC\betaC\gamma$	113.5	1.62		
$C\alphaCO$	120.5	0.84		$C\alphaCO$	120.5	0.83		
$C\betaC\alphaC$	110.1	1.63		$C\beta_{-}C\alpha_{-}C$	110.0	1.56		
$C\betaC\gammaC\delta$	111.3	1.75		$C\betaC\gammaC\delta$	111.1	1.85		
$C\deltaC\epsilonN\zeta$	112.2	1.98		$C\deltaC\epsilonN\zeta$	111.1	2.10		
$C\gammaC\deltaC\epsilon$	111.8	1.47		$C\gammaC\deltaC\epsilon$	111.0	1.60		
$N_{-}C\alpha_{-}C$	111.3	2.49		$N_{-}C\alpha_{-}C$	111.3	2.24		
$N_{-}C\alpha_{-}C\beta$	110.6	1.02		$N_{-}C\alpha_{-}C\beta$	110.7	0.99		

LYS	$\mathbf{mttm} \ \mathbf{n} = 1829$	<u> </u>		$VS \mathbf{mtmp} \ n = 9$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67	7.3	chi1	-67	5.8
chi2	-178	10.0	chi2	-176	8.3
chi3	-177	10.8	chi3	-96	7.4
chi4	-67	12.8	chi4	74	12.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.4	1.74	$C\alpha_{-}C\beta_{-}C\gamma$	113.8	1.23
$C\alphaCO$	120.5	0.85	$C\alphaCO$	120.6	0.61
$C\betaC\alphaC$	110.1	1.54	$C\betaC\alphaC$	109.9	1.20
$C\betaC\gammaC\delta$	111.2	1.73	$C\betaC\gammaC\delta$	111.7	1.98
$C\delta_C\epsilon_N\zeta$	112.2	2.03	$C\deltaC\epsilonN\zeta$	113.7	2.37
$C\gammaC\deltaC\epsilon$	111.8	1.47	$C\gammaC\deltaC\epsilon$	112.7	0.79
$N_{-}C\alpha_{-}C$	111.4	2.37	$N_{-}C\alpha_{-}C$	110.4	2.29
$NC\alphaC\beta$	110.6	1.00	$NC\alphaC\beta$	110.8	0.91
LYS mtmt $n = 1314$		LYS	6 mtmm n = 424		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67	6.9	chi1	-64	6.9
chi2	-173	9.8	chi2	-177	10.1
chi3	-74	11.7	chi3	-70	10.9
chi4	-175	10.6	chi4	-66	9.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.2	1.59	$C\alpha_{-}C\beta_{-}C\gamma$	113.5	1.53
$C\alphaCO$	120.4	0.86	$C\alphaCO$	120.5	0.84
$C\betaC\alphaC$	110.1	1.56	$C\beta C\alpha C$	109.8	1.56
$C\betaC\gammaC\delta$	112.3	1.52	$C\betaC\gammaC\delta$	112.3	1.37
$C\delta_{-}C\epsilon_{-}N\zeta$	111.0	2.18	$C\deltaC\epsilonN\zeta$	112.8	2.10
$C\gamma_C\delta_C\epsilon$	112.1	1.45	$C\gammaC\deltaC\epsilon$	112.9	1.50
$N_{-}C\alpha_{-}C$	111.3	2.14	$N_{-}C\alpha_{-}C$	111.5	2.39
$N_{-}C\alpha_{-}C\beta$	110.7	0.96	$N_{-}C\alpha_{-}C\beta$	110.6	1.03
LYS	8 mmpt n = 31		LY	S mmtp $n = 463$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-60	7.0	chi1	-61	8.2
chi2	-71	19.5	chi2	-69	12.0
chi3	94	14.5	chi3	180	11.9
chi4	176	10.7	chi4	68	13.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	115.3	1.12	$C\alphaC\betaC\gamma$	114.7	1.51
$C\alphaCO$	120.4	0.89	$C\alphaCO$	120.4	0.90
$C\betaC\alphaC$	109.8	1.68	$C\betaC\alphaC$	109.6	1.56
$C\betaC\gammaC\delta$	113.4	1.80	$C\betaC\gammaC\delta$	112.0	1.55
$C\deltaC\epsilonN\zeta$	111.5	1.77	$C\deltaC\epsilonN\zeta$	112.6	2.34
$C\gammaC\deltaC\epsilon$	112.0	1.40	$C\gammaC\deltaC\epsilon$	111.9	1.34
$N_{-}C\alpha_{-}C$	111.5	2.37	$N_{-}C\alpha_{-}C$	111.1	2.60
$N_{-}C\alpha_{-}C\beta$	111.2	1.39	$NC\alphaC\beta$	110.7	1.04

LYS	mmtt n = 3137	, 	LYS	mmtm n = 727	,	
χ	Smooth COM	StdDev	χ	Smooth COM	StdD	
chi1	-62	8.3	chi1	-60	8.2	
chi2	-67	9.8	chi2	-66	10.8	
chi3	-177	10.1	chi3	-173	11.2	
chi4	-178	11.0	chi4	-69	13.4	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdD	
$C\alphaC\betaC\gamma$	114.5	1.32	$C\alphaC\betaC\gamma$	114.5	1.40	
$C\alphaCO$	120.4	0.91	$C\alphaCO$	120.5	0.87	
$C\betaC\alphaC$	109.6	1.56	$C\betaC\alphaC$	109.7	1.57	
$C\betaC\gammaC\delta$	111.9	1.49	$C\betaC\gammaC\delta$	111.9	1.43	
$C\delta_C\epsilon_N\zeta$	111.1	2.08	$C\deltaC\epsilonN\zeta$	112.4	1.97	
$C\gamma_C\delta_C\epsilon$	111.1	1.53	$C\gamma_{-}C\delta_{-}C\epsilon$	112.0	1.44	
$N_C\alpha_C$	111.5	2.47	$N_{-}C\alpha_{-}C$	111.4	2.53	
$N_{-}C\alpha_{-}C\beta$	110.7	1.01	$N_{-}C\alpha_{-}C\beta$	110.6	1.02	
LYS	mmmt n = 544		LYS	LYS mmmm $n = 90$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdD	
chi1	-63	7.7	chi1	-61	8.3	
chi2	-64	10.7	chi2	-62	10.4	
chi3	-71	9.7	chi3	-67	10.8	
chi4	-177	9.8	chi4	-65	10.9	
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdD	
$C\alphaC\betaC\gamma$	114.6	1.31	$C\alphaC\betaC\gamma$	114.7	1.39	
$C\alphaCO$	120.4	0.97	$C\alphaCO$	120.4	1.06	
$C\betaC\alphaC$	109.6	1.46	$C\betaC\alphaC$	109.5	1.53	
$C\betaC\gammaC\delta$	113.1	1.51	$C\betaC\gammaC\delta$	113.2	1.43	
$C\delta_{-}C\epsilon_{-}N\zeta$	111.2	2.21	$C\deltaC\epsilonN\zeta$	112.6	2.73	
$C\gamma_C\delta_C\epsilon$	112.3	1.53	$\mathrm{C}\gamma\mathrm{C}\delta\mathrm{C}\epsilon$	113.2	1.87	
$N_{-}C\alpha_{-}C$	111.8	2.31	$N_{-}C\alpha_{-}C$	111.7	2.47	
$N_C\alpha_C\beta$	110.7	1.05	$N_{-}C\alpha_{-}C\beta$	110.5	1.11	