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

Bradley J. Hintze, Steven M. Lewis, Jane S. Richardson, and David C. Richardson Department of Biochemistry, Duke University

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Top500 vs. Top8000 Reference Contours

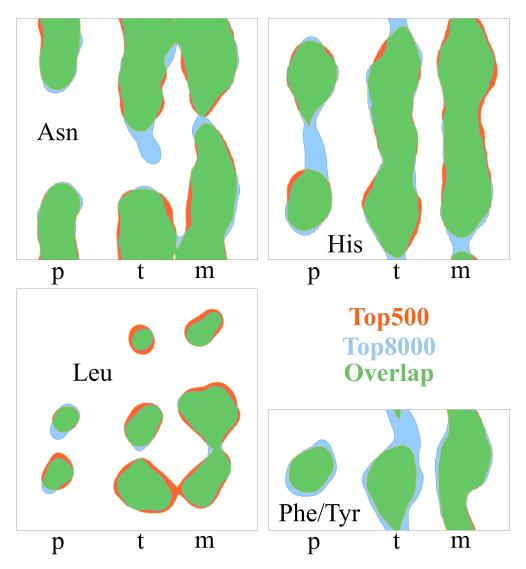


Figure S1: Areas in orange (from Top500 data) and in blue (from Top8000) fill the allowed regions for AsN, His, Leu, and Phe/Tyr. Phe and Tyr were done together as no significant difference was detected between their distributions. The extensive areas in green are where the two systems both declare allowed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

residue	rotamer	n	%	rarity
	SER: TOTA	AL N =	76186	
SER	p	36901	48.44	-
SER	t	17502	22.97	-
SER	m	21558	28.30	-
SER	OUTLIER	225	0.30	-
	CYS: TOTA	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	p	36195	48.14	-
THR	t	5197	6.91	-
THR	m	33559	44.64	-
THR	OUTLIER	229	0.30	-
	VAL: TOTA	AL N =	97050	
VAL	р	6015	6.20	_
VAL	t	73329	75.56	-
VAL	m	17410	17.94	-
VAL	OUTLIER	296	0.30	-
	PRO: TOTA	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	-
$\overline{\text{ASN}: \text{TOTAL N} = 53650}$				
ASN	p0	7513	14.00	-
	-			

residue	rotamer	n	%	rarity
ASN	t0	15610	29.10	-
ASN	t160	61	0.11	$\overline{\hspace{1cm}}$
ASN	m110	4003	7.46	-
ASN	m-40	26292	49.01	-
ASN	OUTLIER	171	0.32	-
	$\overline{\text{ASP}: \text{TOT}}$	AL N =	72336	
ASP	p0	11746	16.24	
ASP	t0	17107	23.65	-
ASP	t70	6029	8.33	-
ASP	m-30	37239	51.48	-
ASP	OUTLIER	215	0.30	-
	HIS: TOT.	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	
	$\overline{ ext{TYR}: ext{TOT}}$	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	_
	$\overline{\text{TRP}:\text{TOT}}$	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	_
TRP	OUTLIER	53	0.28	
		AL N =	16794	
MET	ppp	50	0.30	
MET	pp-130	27	0.16	
	rr			•

residue	rotamer	n	%	rarity
MET	ptp	404	2.41	-
MET	ptt	260	1.55	-
MET	ptm	375	2.23	-
MET	pmt	7	0.04	$\overline{}$
MET	pmm	42	0.25	$\overline{\hspace{1cm}}$
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	$\overline{}$
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	-
GLU	$\frac{\text{GLN:TOT.}}{\text{GLN:TOT.}}$		37119	
GLN	pp30	178	0.48	
GLN	pt0	1885	5.08	
GLN	pm20	487	1.31	
GLN	tp40	3618	9.75	-
GLN		534	1.44	
GLN	tp-100 tt0		18.69	
		6936		
GLN	tm130	55	0.15	
GLN	tm-30	547	1.47	-
GLN	mp10	1207	3.25	<u>-</u>
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	0.01	√
ARG	ppt170	57	0.12	<u>√</u>
ARG	ppt90	19	0.04	<u>√</u>
ARG	ppt-90	15	0.03	√
ARG	ptp90	223	0.48	
ARG	ptp-110	77	0.17	_
ARG	ptp-170	388	0.84	
ARG	ptt180	820	1.77	-
ARG	ptt90	814	1.76	-
ARG	ptt-90	726	1.57	-

residue	rotamer	n	%	rarity
ARG	ptm160	502	1.08	-
ARG	ptm-80	215	0.46	-
ARG	pmt100	4	0.01	✓
ARG	pmt170	39	0.08	√
ARG	pmt-80	27	0.06	√
ARG	pmm150	12	0.03	√
ARG	pmm-80	19	0.04	√
ARG	tpp80	363	0.78	-
ARG	tpp-160	496	1.07	-
ARG	tpt170	825	1.78	-
ARG	tpt90	652	1.41	-
ARG	tpt-90	365	0.79	-
ARG	tpm170	110	0.24	_
ARG	tpm-80	20	0.04	√
ARG	ttp80	1896	4.09	
ARG	ttp-110	623	1.34	
ARG	ttp-170	1533	3.31	_
ARG	ttt180	2339	5.04	
ARG	ttt90	$\frac{2339}{1057}$	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	0.05	√
ARG	tmt-80	62	0.13	-
ARG	tmm160	92	0.20	-
ARG	tmm-80	71	0.15	-
ARG	mpp80	54	0.12	✓
ARG	mpp-170	64	0.14	-
ARG	mpt180	245	0.53	-
ARG	mpt90	46	0.10	✓
ARG	mpt-90	85	0.18	-
ARG	mtp180	2504	5.40	-
ARG	mtp85	1857	4.00	-
ARG	mtp-110	470	1.01	-
ARG	mtt180	4592	9.90	-
ARG	mtt90	2460	5.30	-
ARG	mtt-85	2843	6.13	-
ARG	mtm110	781	1.68	-
ARG	mtm180	2407	5.19	-
ARG	mtm-85	2848	6.14	-
ARG	mmp80	164	0.35	-
ARG	mmp-170	123	0.27	-
ARG	mmt180	1203	2.59	-
ARG	mmt90	567	1.22	-
ARG	mmt-90	1428	3.08	-
ARG	mmm160	951	2.05	-
ARG	mmm-85	1022	2.20	-
ARG	OUTLIER	138	0.30	_
	YS : 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	0.34	-
LYS	pmtt	10	0.23	
шо	bine	10	0.05	٧

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

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

χ and Covalent Bond Angle Central Values

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

Table S4: SER Central Values

$SER \mathbf{p} = 36901$				
χ	Smooth COM	StdDev		
chi1	65	8.6		
Bond Angle	Mean	StdDev		
$C\alphaC\betaOG$	111.0	1.35		
$C\alphaCO$	120.5	0.92		
$C\beta C\alpha C$	109.9	1.39		
$N_C\alpha_C$	111.6	2.52		
$N_{-}C\alpha_{-}C\beta$	110.7	1.12		

SER \mathbf{t} n = 17502				
χ	Smooth COM	StdDev		
chi1	178	9.0		
Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}OG$	110.7	1.42		
$C\alphaCO$	120.6	0.82		
$C\betaC\alphaC$	109.8	1.45		
$N_{-}C\alpha_{-}C$	110.5	2.40		
$N_{-}C\alpha_{-}C\beta$	110.1	1.21		

SER \mathbf{m} n = 21558					
χ	Smooth COM	StdDev			
chi1	-63	7.7			
Bond Angle	Mean	StdDev			
$C\alphaC\betaOG$	110.5	1.46			
$C\alpha_{-}C_{-}O$	120.5	0.85			
$C\beta C\alpha C$	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	64	9.0			
Bond Angle	Mean	StdDev			
$C\alphaC\betaSG$	114.6	1.68			
$C\alphaCO$	120.5	0.98			
$C\betaC\alphaC$	110.5	1.50			
$N_{-}C\alpha_{-}C$	111.3	2.78			
$N_{-}C\alpha_{-}C\beta$	110.9	1.23			

C	CYS t n = 4399					
χ	Smooth COM	StdDev				
chi1	-177	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				
$NC\alphaC\beta$	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 \mathbf{p} n = 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			

THR $t = 5197$					
χ	Smooth COM	StdDev			
chi1	-172	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			
$OG1_C\beta_C\gamma2$	109.1	1.81			

THR m $n = 33559$						
χ	Smooth COM	StdDev				
chi1	-60	6.1				
Bond Angle	Mean	StdDev				
$C\alphaC\betaC\gamma_2$	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				
${\rm OG1_C}\beta_{\rm C}\gamma2$	108.8	1.67				

Table S7: VAL Central Values

VAL p n = 6015				
χ	Smooth COM	StdDev		
chi1	64	7.2		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma 1$	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		
$C\gamma 1_C\beta_C\gamma 2$	111.0	1.20		
$N_{-}C\alpha_{-}C$	110.3	2.48		
$N_C\alpha_C\beta$	111.6	1.26		

$VAL \mathbf{t} n = 73329$					
χ	Smooth COM	StdDev			
chi1	175	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	-61	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 Cg_exo n = 30128		28	PRO Cg_endo n = 29192		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-24	7.2	chi1	26	7.7
chi2	35	7.8	chi2	-34	8.9
chi3	-31	7.1	chi3	27	9.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	104.2	1.40	$C\alpha_{-}C\beta_{-}C\gamma$	104.2	1.47
$C\alphaCO$	120.2	1.03	$C\alphaCO$	120.2	1.07
$C\alpha_N_C\delta$	111.7	0.81	$C\alphaNC\delta$	111.8	0.84
$C\betaC\alphaC$	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	$U \mathbf{pp} n = 521$		L	EU pt n = 378	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	8.2	chi1	72	8.5
chi2	83	9.5	chi2	164	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	$C\beta C\alpha C$	110.4	1.45
$C\betaC\gammaC\delta 1$	111.5	1.89	$C\betaC\gammaC\delta 1$	109.8	1.54
$C\beta_{-}C\gamma_{-}C\delta_{2}$	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
LEV	$U \ \mathbf{tp} \ n = 34655$		LF	EU $\mathbf{tt} \; \mathbf{n} = 1576$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	8.2	chi1	-172	8.5
chi2	62	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
$C\alpha_{-}C_{-}O$	120.5	0.79	$C\alpha_{-}C_{-}O$	120.6	0.86
$C\betaC\alphaC$	110.2	1.21	$C\betaC\alphaC$	111.1	1.26
$C\betaC\gammaC\delta 1$	111.1	1.55	$C\betaC\gammaC\delta 1$	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	$C\delta 1_{-}C\gamma_{-}C\delta 2$	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	EU tm n = 143		LE	$U \mathbf{mp} \ n = 2711$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-171	5.9	chi1	-77	12.5
chi2	-75	6.4	chi2	71	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
$C\alphaCO$	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
$C\delta1C\gammaC\delta2$	111.4	1.44	$C\delta1_{-}C\gamma_{-}C\delta2$	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	$N_{-}C\alpha_{-}C\beta$	111.1	1.03

LEU $\mathbf{mt} \ \mathbf{n} = 74252$			LEU $\mathbf{mm} \ \mathbf{n} = 484$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-65	8.2	chi1	-82	10.2
chi2	174	8.1	chi2	-63	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
$C\betaC\alphaC$	109.8	1.42	$C\betaC\alphaC$	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	57	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
ILI	$\mathbf{E} \mathbf{tp} \mathbf{n} = 1869$		IL	E tt $n = 4163$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-167	7.8	chi1	-169	7.7
chi2	65	7.3	chi2	166	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	$C\alpha_{-}C\beta_{-}C\gamma_{2}$	111.4	1.04
$C\alphaCO$	120.4	0.82	$C\alphaCO$	120.6	0.83
$C\beta _C\alpha _C$	111.5	1.46	$C\beta _C\alpha _C$	111.6	1.48
$C\beta C\gamma 1C\delta 1$	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
ILI	$E \mathbf{mp} n = 623$		ILE	mt n = 44470	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-62	11.6	chi1	-62	6.4
chi2	88	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
$C\beta_{-}C\alpha_{-}C$	110.1	1.63	$C\betaC\alphaC$	110.4	1.58
$C\beta C\gamma 1C\delta 1$	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

ILE $\mathbf{mm} \ \mathbf{n} = 11258$				
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

ASN p0 n = 7513				
χ	Smooth COM	StdDev		
chi1	63	7.8		
chi2	6	43.3		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	113.1	0.88		
$C\alphaCO$	120.4	0.97		
$C\betaC\alphaC$	111.3	1.68		
$C\beta C\gamma N\delta 2$	116.3	0.91		
$C\betaC\gammaO\delta 1$	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		
AS	N t160 n = 61			

ASN $t0 \text{ n} = 15610$				
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		
$C\beta C\alpha C$	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	ASN t160 n = 61				
χ	Smooth COM	StdDev			
chi1	-161	7.4			
chi2	163	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	-63	9.6		
chi2	114	28.4		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	112.7	1.15		
$C\alphaCO$	120.5	0.90		
$C\betaC\alphaC$	109.5	1.84		
$C\betaC\gammaN\delta 2$	116.6	1.14		
$C\betaC\gammaO\delta 1$	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 $m-40 \text{ n} = 26292$				
χ	Smooth COM	StdDev		
chi1	-69	9.1		
chi2	-41	26.3		
Bond Angle	Mean	StdDev		
$C\alpha_{-}C\beta_{-}C\gamma$	112.5	0.92		
$C\alphaCO$	120.4	0.87		
$C\betaC\alphaC$	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	62	7.5	chi1	-171	10.2
chi2	-2	31.0	chi2	-1	23.8
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	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
,			,		
ASI	P t70 n = 6029			m-30 n = 37239)
ASI χ	P t70 n = 6029 Smooth COM	StdDev		m-30 n = 37239 Smooth COM	StdDev
		StdDev 9.2	ASP		
χ	Smooth COM		ASP X	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -174	9.2	$\begin{array}{c} \text{ASP} \\ \chi \\ \text{chi1} \end{array}$	Smooth COM -68	StdDev 8.2
χ chi1 chi2	Smooth COM -174 74	9.2 19.8	$\begin{array}{c} \text{ASP} \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	Smooth COM -68 -29	8.2 22.4
χ chi1 chi2 Bond Angle	Smooth COM -174 74 Mean	9.2 19.8 StdDev	$\begin{array}{c} \text{ASP} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \end{array}$	Smooth COM -68 -29 Mean	StdDev 8.2 22.4 StdDev
χ chi1 chi2 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM -174 74 Mean 112.4	9.2 19.8 StdDev	$\begin{array}{c} \text{ASP} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{C}\alpha\text{-C}\beta\text{-C}\gamma \end{array}$	Smooth COM -68 -29 Mean 112.9	8.2 22.4 StdDev 0.95
χ chi1 chi2 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -174 74 Mean 112.4 120.5	9.2 19.8 StdDev 0.83 0.80	ASP $\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ \end{array}$	Smooth COM -68 -29 Mean 112.9 120.5	8.2 22.4 StdDev 0.95 0.86
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array}$	Smooth COM -174 74 Mean 112.4 120.5 110.1	9.2 19.8 StdDev 0.83 0.80 1.27	ASP $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi2}}$ Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}$	Smooth COM -68 -29 Mean 112.9 120.5 109.4	8.2 22.4 StdDev 0.95 0.86 1.67
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{C} \\ \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \\ \text{C}\beta_\text{C}\gamma_\text{O}\delta1 \\ \end{array}$	Smooth COM -174 74 Mean 112.4 120.5 110.1 118.5	9.2 19.8 StdDev 0.83 0.80 1.27 1.11	ASP $\frac{\chi}{\text{chi1}}$ $\frac{\text{chi2}}{\text{chi2}}$ Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{O}\delta 1}$	Smooth COM -68 -29 Mean 112.9 120.5 109.4 119.2	8.2 22.4 StdDev 0.95 0.86 1.67 1.36
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\alpha_\text{C} \end{array} $ $ \begin{array}{c} \text{C}\beta_\text{C}\gamma_\text{O}\delta 1 \\ \text{C}\beta_\text{C}\gamma_\text{O}\delta 2 \end{array} $	Smooth COM -68 -29 Mean 112.9 120.5 109.4 119.2 118.2	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	64	9.9
chi2	86	21.8	chi2	-80	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	$C\betaC\gammaN\delta 1$	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	$NC\alphaC\beta$	111.0	1.32
HIS	8 t70 n = 5068		HIS	t-170 n = 1332	
$\frac{\chi}{\chi}$	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 73	10.0 17.3	χ chi1 chi2	Smooth COM -173 -167	9.7 21.6
λ chi1 chi2 Bond Angle	Smooth COM -178 73 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \end{array}$	Smooth COM -178 73 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 73 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 73 Mean 113.6 120.6 110.1	10.0 17.3 StdDev 1.07 0.83 1.34	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha\text{_C}\beta\text{_C}\gamma \\ \\ \text{C}\alpha\text{_C_O} \\ \\ \text{C}\beta\text{_C}\alpha\text{_C} \\ \end{array}$	Smooth COM -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 73 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 \text{_$C} \gamma \\ \text{$C\alpha$_C_O} \\ \text{$C\beta$_C} \alpha \text{_$C} \\ \text{$C\beta$_$C$} \gamma \text{_$C$} \delta 2 \\ \text{$C\beta$_$C$} \gamma \text{_$N$} \delta 1 \\ \hline \end{array}$	Smooth COM -178 73 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$$\epsilon2$_$C}\delta2 \\ \text{$C\gamma$_$C}\delta2_\text{$N\epsilon2$} \\ \hline \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}-\text{$C} \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta 1 \\ \text{$C\epsilon 1.N}\epsilon 2.C}\delta 2 \\ \end{array}$	Smooth COM -178 73 Mean 113.6 120.6 110.1 131.0 122.7 108.9	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_\text{$C\gamma$} \\ \hline \\ \text{$C\alpha$_C_$O} \\ \hline \\ \text{$C\beta$_$Cα_$C} \\ \hline \\ \text{$C\beta$_$Cγ_C\delta2} \\ \hline \\ \text{$C\beta$_C\gamma$_$N$\delta1} \\ \hline \\ \text{$C\epsilon1$_N\epsilon2$_$C$\delta2} \\ \end{array}$	Smooth COM -173 -167 Mean 114.2 120.6 110.9 131.4 122.4 108.8	9.7 21.6 StdDev 1.02 0.81 1.31 0.98 1.05 0.55
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C}_0 \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta 1 \\ \text{$C\epsilon$1_N}\epsilon 2.C\delta 2 \\ \text{$C\gamma$_$C}\delta 2.N\epsilon 2 \\ \hline \end{array}$	Smooth COM -178 73 Mean 113.6 120.6 110.1 131.0 122.7 108.9 107.2	10.0 17.3 StdDev 1.07 0.83 1.34 0.82 0.79 0.52 0.46	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$O} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \text{$C\beta$_$C}\gamma_\text{$C\delta2$} \\ \text{$C\beta$_$C}\gamma_\text{$N\delta1$} \\ \text{$C\epsilon1$_$N$$\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\alpha_C$} \\ \hline \\ \text{$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 73 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 73 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{$C\alpha$_$C}-\text{CO} \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta2 \\ \text{$C\beta$_$C}\gamma$_$N}\delta1 \\ \text{$C\epsilon$1_$N}\epsilon2$_$C}\delta2 \\ \text{$C\gamma$_$C}\delta2 \\ \text{$N\delta$1_$C}\epsilon1 \\ \text{$N\delta$1_$C}\epsilon1 \\ \text{$N\delta$1_$C}\epsilon1 \\ \text{$N\delta$1_$C}\epsilon1 \\ \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		TITO	170 0001	
HIS	t-90 n = 3553		HIS	m170 n = 2695	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173	10.4	chi1	-67	8.2
chi2	-86	18.5	chi2	170	21.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.7	1.01	$C\alpha_{-}C\beta_{-}C\gamma$	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
			,		
HIS	m90 n = 3914		,	m-70 n = 9453	
ΗIS	m90 n = 3914 Smooth COM	StdDev	,		StdDev
		StdDev 9.8	HIS	m-70 n = 9453	StdDev 10.0
χ	Smooth COM		ΗIS	m-70 n = 9453 Smooth COM	
$\frac{\chi}{\text{chi1}}$	Smooth COM -65	9.8	$\frac{\chi}{\text{chi1}}$	m-70 n = 9453 Smooth COM -64	10.0
χ chi1 chi2	Smooth COM -65 88	9.8 17.5	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	m-70 n = 9453 Smooth COM -64 -75	10.0 19.3
χ chi1 chi2 Bond Angle	Smooth COM -65 88 Mean	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	10.0 19.3 StdDev
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{C}\alpha\text{-C}\beta\text{-C}\gamma \end{array}$	Smooth COM -65 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	10.0 19.3 StdDev 1.06
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$\text{$\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha$_$C-O} \end{array}$	Smooth COM -65 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	10.0 19.3 StdDev 1.06 0.87
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{Cα_C\beta$_$Cγ} \\ \hline \\ \text{Cα_C_$O} \\ \hline \\ \text{C$\beta$_$Cα_$C} \\ \end{array}$	Smooth COM -65 88 Mean 113.5 120.5 109.8	9.8 17.5 StdDev 1.11 0.90 1.96	HIS $ \frac{\chi}{\text{chi1}} $ chi2 $ \text{Bond Angle} $ $ \frac{C\alpha \text{-}C\beta \text{-}C\gamma}{C\alpha \text{-}C \text{-}O} $ $ \frac{C\beta \text{-}C\alpha \text{-}C}{C\beta \text{-}C\alpha \text{-}C} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9	10.0 19.3 StdDev 1.06 0.87 1.89
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -65 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	10.0 19.3 StdDev 1.06 0.87 1.89 0.82
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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 -65 88 Mean 113.5 120.5 109.8 130.9 122.8	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	10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \hline \\ \text{$C\alpha$_$C$_$O} \\ \hline \\ \text{$C\beta$_$C$$\alpha$_$C} \\ \hline \\ \text{$C\beta$_$C$$\gamma$_$C$$\delta2} \\ \hline \\ \text{$C\beta$_$C$$\gamma$_$N$$\delta1} \\ \hline \\ \text{$C\epsilon$1_$N$$\epsilon2$_$C$$\delta2} \\ \hline \end{array}$	Smooth COM -65 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9	9.8 17.5 StdDev 1.11 0.90 1.96 0.85 0.82 0.56	HIS $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \end{array} $ Bond Angle $ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta2 \\ \text{C}\beta_\text{C}\gamma_\text{N}\delta1 \\ \text{C}\epsilon1_\text{N}\epsilon2_\text{C}\delta2 \end{array} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9	10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \hline \\ \text{$C\alpha$_$C$_$C} \\ \text{$C\beta$_$C}\alpha_\text{$C$} \\ \hline \\ \text{$C\beta$_$C}\gamma_\text{$N\delta$1} \\ \hline \\ \text{$C\epsilon$1_$N$$\epsilon$2_$Cδ2} \\ \hline \\ \text{$C\gamma$_C\delta$2_$N$$\epsilon$2} \\ \hline \end{array}$	Smooth COM -65 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2	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}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{N}\delta 1 \\ \text{C}\epsilon 1_\text{N}\epsilon 2_\text{C}\delta 2 \\ \text{C}\gamma_\text{C}\delta 2_\text{N}\epsilon 2 \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	10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52 0.47
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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 \\ \text{$C\gamma$_$N}\delta 1.C\epsilon 1 \\ \hline \end{array}$	Smooth COM -65 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2 109.2	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	10.0 19.3 StdDev 1.06 0.87 1.89 0.82 0.80 0.52 0.47 0.63
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -65 88 Mean 113.5 120.5 109.8 130.9 122.8 108.9 107.2 109.2 108.5	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 _ C\beta _ C\gamma}{C\alpha _ C _ O} $ $ \frac{C\beta _ C\gamma _ C\delta 2}{C\beta _ C\gamma _ N\delta 1} $ $ \frac{C\epsilon 1_N\epsilon 2_C\delta 2}{C\gamma _ N\delta 1_C\epsilon 1} $ $ \frac{N\delta 1_C\epsilon 1_N\epsilon 2}{N\delta 1_C\epsilon 1} $	m-70 n = 9453 Smooth COM -64 -75 Mean 113.4 120.4 109.9 131.1 122.6 108.9 107.2 109.2 108.5	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	$\mathbf{E} \ \mathbf{p90} \ \mathbf{n} = 6289$		PHI	E t80 n = 19289	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63	9.6	chi1	-178	10.0
chi2	-89	9.4	chi2	75	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	$C\betaC\gammaC\delta 1$	120.6	0.72
$C\betaC\gammaC\delta 2$	120.6	0.58	$C\betaC\gammaC\delta 2$	120.5	0.68
$C\delta1_C\epsilon1_C\zeta$	119.9	0.60	$C\delta 1_C\epsilon 1_C\zeta$	119.9	0.59
$C\delta1_C\gamma_C\delta2$	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
$C\gamma C\delta 1C\epsilon 1$	120.9	0.59	$C\gamma_C\delta_1C\epsilon_1$	120.8	0.58
$C\gamma_C\delta_2C\epsilon_2$	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	m-10 n = 3880		PHE	m-80 n = 26665	5
<u>PHE</u> χ	m-10 n = 3880 Smooth COM	StdDev	PHE χ	m-80 n = 26665 Smooth COM	StdDev
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -68	StdDev 9.3	$\frac{\chi}{\text{chi1}}$	Smooth COM -66	StdDev 10.1
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha$-C\beta$-$C$\gamma} \end{array}$	Smooth COM -68 -14	9.3 19.8	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \end{array}$	Smooth COM -66 -80	StdDev 10.1 16.8
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -68 -14 Mean	9.3 19.8 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -66 -80 Mean	StdDev 10.1 16.8 StdDev
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha$-C\beta$-$C$\gamma} \end{array}$	Smooth COM -68 -14 Mean 114.8	9.3 19.8 StdDev 0.96	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5	StdDev 10.1 16.8 StdDev 1.02
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \hline \text{$\text{C}\alpha$_C_$O} \end{array}$	Smooth COM -68 -14 Mean 114.8 120.4	9.3 19.8 StdDev 0.96 0.87	χ chi1 chi2 Bond Angle $C\alphaC\betaC\gamma$ $C\alphaCO$	Smooth COM -66 -80 Mean 113.5 120.5	StdDev 10.1 16.8 StdDev 1.02 0.86
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -14 Mean 114.8 120.4 108.9	9.3 19.8 StdDev 0.96 0.87 1.78	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ \end{array}$	Smooth COM -68 -14 Mean 114.8 120.4 108.9 121.5	9.3 19.8 StdDev 0.96 0.87 1.78 1.22	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ C\beta_C\gamma_C\delta2 \\ \end{array}$	Smooth COM -68 -14 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \\ C\alpha_C\beta_C\gamma \\ \hline \\ C\alpha_C_O \\ \hline \\ C\beta_C\alpha_C \\ \hline \\ C\beta_C\gamma_C\delta1 \\ \hline \\ C\beta_C\gamma_C\delta2 \\ \hline \\ C\delta1_C\epsilon1_C\zeta \\ \end{array}$	Smooth COM -68 -14 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6 119.9	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_Cβ_Cγ} \\ \text{$C\alpha$_C$_O$} \\ \text{$C\beta$_Cα_C$} \\ \text{$C\beta$_C$\gamma$_C$\delta$1} \\ \text{$C\beta$_C$\gamma$_C$\delta$2} \\ \text{$C\delta1_Cς1$_C$\zeta$} \\ \text{$C\delta1_Cγ_Cδ2} \\ \hline \end{array}$	Smooth COM -68 -14 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\delta$1$_$C}\epsilon1$_$C}\zeta \\ \text{$C\delta$1$_$C}\gamma$_$C}\delta2 \\ \text{$C\epsilon$1$_$C}\zeta$_$C}\epsilon2 \\ \hline \end{array}$	Smooth COM -68 -14 Mean 114.8 120.4 108.9 121.5 119.9 118.5 119.8	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56 0.62	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53 0.61
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ C\beta_C\gamma_C\delta2 \\ C\delta1_C\epsilon1_C\zeta \\ C\delta1_C\gamma_C\delta2 \\ C\epsilon1_C\zeta_C\epsilon2 \\ C\gamma_C\delta1_C\epsilon1 \\ C\gamma_C\delta2_C\epsilon2 \\ C\gamma_C\delta1_C\epsilon2 \\ C\zeta_C\epsilon2_C\delta2 \\ C\zeta_C\epsilon2_C\delta2 \\ C\zeta_C\epsilon2_C\delta2 \\ \hline \end{array}$	Smooth COM -68 -14 Mean 114.8 120.4 108.9 121.5 119.9 118.5 119.8 120.8	9.3 19.8 StdDev 0.96 0.87 1.78 1.22 1.16 0.61 0.56 0.62 0.60	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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$} \\ \text{$C\gamma_C\delta1_C\epsilon1$} \\ \text{$C\gamma_C\delta2_C\epsilon2$} \\ \text{$C\gamma_C\delta2_C\epsilon2$} \\ \text{$C\zeta_C\epsilon2_C\delta2$} \\ \hline \end{array}$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9 120.8	StdDev 10.1 16.8 StdDev 1.02 0.86 1.99 0.60 0.59 0.58 0.53 0.61 0.56
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -14 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.5 120.5 109.8 120.6 120.6 119.9 118.8 119.9 120.8 120.8	StdDev 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

	R p90 n = 5466		TYI	R t80 n = 16312	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63	10.6	chi1	-178	10.5
chi2	-89	10.1	chi2	75	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
$C\betaC\alphaC$	110.6	1.41	$C\betaC\alphaC$	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	$C\delta 1_C\epsilon 1_C\zeta$	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
$C\epsilon 1_C\zeta_OH$	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	$C\gamma_{-}C\delta_{2}C\epsilon_{2}$	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	$\mathrm{OH}_{-}\mathrm{C}\zeta_{-}\mathrm{C}\epsilon 2$	119.7	1.28
TYR.	m-10 n = 2623		TVD	m-80 n = 22683)
			1110	m-80 ii = 22083)
χ	Smooth COM	StdDev	χ	Smooth COM	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 -66	StdDev 10.4
χ chi1 chi2 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -68 -14	9.9 20.2	χ chi1 chi2 Bond Angle $C\alphaC\betaC\gamma$	Smooth COM -66 -80	StdDev 10.4 16.8
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \end{array}$	Smooth COM -68 -14 Mean	StdDev 9.9 20.2 StdDev	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \hline \\ \hline \\ \text{C}\alpha_\text{C}_\text{O} \\ \end{array}$	Smooth COM -66 -80 Mean	StdDev 10.4 16.8 StdDev
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -14 Mean 115.8	9.9 20.2 StdDev 1.57	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 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 -14 Mean 115.8 120.4	9.9 20.2 StdDev 1.57 0.84	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \hline \\ \hline \\ \text{C}\alpha_\text{C}_\text{O} \\ \end{array}$	Smooth COM -66 -80 Mean 113.2 120.4	StdDev 10.4 16.8 StdDev 2.04 0.88
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{Cα_C\beta$_$Cγ} \\ \hline \\ \text{Cα_C_$O} \\ \hline \\ \text{C$\beta$_$Cα_$C} \\ \end{array}$	Smooth COM -68 -14 Mean 115.8 120.4 109.1	9.9 20.2 StdDev 1.57 0.84 1.75	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -66 -80 Mean 113.2 120.4 109.6	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -14 Mean 115.8 120.4 109.1 121.6	9.9 20.2 StdDev 1.57 0.84 1.75 1.01	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_O$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta1$} \\ \end{array}$	Smooth COM -66 -80 Mean 113.2 120.4 109.6 120.9	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -14 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 -66 -80 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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$} \\ \end{array}$	Smooth COM -68 -14 Mean 115.8 120.4 109.1 121.6 120.4 119.5	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} \\ \\ \hline \text{Bond Angle} \\ \hline \\ $	Smooth COM -66 -80 Mean 113.2 120.4 109.6 120.9 120.9 119.5	StdDev 10.4 16.8 StdDev 2.04 0.88 1.92 0.63 0.62 0.90
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{Cα_Cβ_Cγ} \\ \text{Cα_C$_O$} \\ \text{Cβ_Cα_C$} \\ \text{C$\beta$_C$\gamma$_C$\delta$1} \\ \text{C$\beta$_C$\gamma$_C$\delta$2} \\ \text{C$\delta1_Cϵ1$_C$\zeta$} \\ \text{C$\delta1_Cγ_Cδ2} \\ \hline \end{array}$	Smooth COM -68 -14 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 -66 -80 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$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\epsilon1_C\zeta$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\epsilon1_C\zeta_C\epsilon2$} \\ \hline \end{array}$	Smooth COM -68 -14 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} \\ \\ \hline \text{Bond Angle} \\ \hline \\ $	Smooth COM -66 -80 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\epsilon1_C\zeta$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\epsilon1_C\zeta_C\epsilon2$} \\ \hline \\ \text{$C\epsilon1_C\zeta_OH$} \\ \hline \end{array}$	Smooth COM -68 -14 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 -66 -80 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 -14 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 -66 -80 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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$} \\ \text{$C\epsilon1_C\zeta_OH$} \\ \text{$C\gamma_C\delta1_C\epsilon1$} \\ \text{$C\gamma_C\delta1_C\epsilon1$} \\ \text{$C\gamma_C\delta2_C\epsilon2$} \\ \hline \end{array}$	Smooth COM -68 -14 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 -66 -80 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} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	Smooth COM -68 -14 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 -66 -80 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

TR	P p90 n = 971		TRP	p-90 n = 1937	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	60	9.9	chi1	61	9.8
chi2	87	14.7	chi2	-89	12.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.0	2.04	$C\alpha_{-}C\beta_{-}C\gamma$	115.0	1.90
$C\alphaCO$	120.6	0.86	$C\alphaCO$	120.5	0.93
$C\betaC\alphaC$	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
$C\delta1_N\epsilon_1_C\epsilon_2$	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
$C\delta2_C\epsilon3_C\zeta3$	118.7	0.34	$C\delta2_C\epsilon3_C\zeta3$	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	$C\zeta3_C\eta2_C\zeta2$	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
$N_{-}C\alpha_{-}C\beta$	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	-178	9.8	chi1	-177	11.6
chi2	64	32.8	chi2	-102	15.4
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	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	$C\beta_{-}C\gamma_{-}C\delta 1$	126.9	0.69
$C\betaC\gammaC\delta 2$	126.5	0.82	$C\betaC\gammaC\delta 2$	126.7	0.71
$C\delta1_C\gamma_C\delta2$	106.3	0.48	$C\delta1C\gammaC\delta2$	106.3	0.42
$C\delta1_N\epsilon1_C\epsilon2$	108.9	0.51	$C\delta1_N\epsilon1_C\epsilon2$	108.9	0.45
$C\delta2_C\epsilon2_C\zeta2$	122.4	0.40	$C\delta2_C\epsilon2_C\zeta2$	122.4	0.36
$C\delta 2_{-}C\epsilon 3_{-}C\zeta 3$	118.7	0.42	$C\delta 2_{-}C\epsilon 3_{-}C\zeta 3$	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	$C\epsilon 2C\delta 2C\gamma$	107.2	0.32
$C\epsilon 3 C\zeta 3C\eta 2$	121.0	0.48	$C\epsilon 3C\zeta 3C\eta 2$	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
$C\gammaC\delta_2C\epsilon_3$	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	$C\eta_2 C\zeta_2 C\epsilon_2$	117.5	0.45
$C\zeta3_C\eta2_C\zeta2$	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	$N_{-}C\alpha_{-}C$	110.5	2.42
$NC\alphaC\beta$	110.0	1.42	$NC\alphaC\beta$	110.3	1.42
	TRP $m100 \text{ n} = 6319$ TRP $m-10 \text{ s}$				
TRP	m100 n = 6319		TRP	m-10 n = 2196	
χ	m100 n = 6319 Smooth COM	StdDev	χ	m-10 n = 2196 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$		StdDev 10.8			StdDev 9.0
χ	Smooth COM		χ	Smooth COM	
$\frac{\chi}{\text{chi1}}$	Smooth COM -67	10.8	$\frac{\chi}{\text{chi1}}$	Smooth COM -68	9.0
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \text{Bond Angle} \\ \hline \text{C}\alpha\text{-}\text{C}\beta\text{-}\text{C}\gamma \end{array}$	Smooth COM -67 97	10.8 17.0	χ chi1 chi2 Bond Angle $C\alpha _ C\beta _ C\gamma$	Smooth COM -68 -7	9.0 21.7
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha\text{-}\text{C}\beta\text{-}\text{C}\gamma \\ \\ \text{C}\alpha\text{-}\text{C}\text{-}\text{O} \\ \end{array}$	Smooth COM -67 97 Mean 113.2 120.4	10.8 17.0 StdDev 2.22 0.86	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{C}\alpha\text{-C}\beta\text{-C}\gamma \\ \hline \\ \hline \\ \text{C}\alpha\text{-C-O} \\ \end{array}$	Smooth COM -68 -7 Mean 114.7 120.5	9.0 21.7 StdDev 1.64 0.88
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\alpha_C$} \\ \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6	10.8 17.0 StdDev 2.22 0.86 1.92	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -68 -7 Mean 114.7 120.5 109.2	9.0 21.7 StdDev 1.64 0.88 1.71
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0	10.8 17.0 StdDev 2.22 0.86 1.92 0.66	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ $	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5	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$_$C}\beta_\text{$C\gamma$} \\ \text{$C\alpha$_$C$_$O} \\ \text{$C\beta$_C\alpha$_$C} \\ \text{$C\beta$_C\gamma$_$C$\delta1} \\ \text{$C\beta$_$Cγ_C\delta2} \\ \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6	10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\delta$1} \\ \text{$C\beta$_$C$}\gamma_\text{$C\delta$2} \\ \end{array}$	Smooth COM -68 -7 Mean 114.7 120.5 109.2	9.0 21.7 StdDev 1.64 0.88 1.71
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C}\beta$_$C}\gamma \\ \text{$C\alpha$_$C$_$O} \\ \text{$C\beta$_$C}\alpha$_$C} \\ \text{$C\beta$_$C}\gamma$_$C}\delta 1 \\ \text{$C\beta$_$C}\gamma$_$C}\delta 2 \\ \text{$C\delta 1$_$C}\gamma$_$C}\delta 2 \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3	10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\gamma_C\delta2$} \\ \hline \end{array}$	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3	9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \text{$C\alpha_C_O$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_N\epsilon1_C\epsilon2$} \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9	10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ $	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8	9.0 21.7 StdDev 1.64 0.88 1.71 0.71 0.77 0.45 0.45
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_N\epsilon1_C\epsilon2$} \\ \hline \\ \text{$C\delta2_C\epsilon2_C\zeta2$} \\ \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4	10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C$$\beta$_$C$$\gamma$} \\ \hline \\ \text{$C\alpha$_$C$$-$C$$} \\ \text{$C\alpha$_$C$$-$C$$} \\ \text{$C\beta$_$C$$\alpha$_$C$} \\ \text{$C\beta$_$C$$\gamma$_$C$$\delta$1} \\ \hline \\ \text{$C\beta$_$C$$\gamma$_$C$$\delta$2} \\ \hline \\ \text{$C\delta1_$N$$\epsilon1_$C$$\epsilon$2} \\ \hline \\ \text{$C\delta2_$C$$\epsilon2_$C$$\zeta$2} \\ \hline \end{array}$	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3	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} \\ \\ \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\delta1$} \\ \hline \\ \text{$C\beta_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_C\gamma_C\delta2$} \\ \hline \\ \text{$C\delta1_N\epsilon1_C\epsilon2$} \\ \hline \\ \text{$C\delta2_C\epsilon2_C\zeta2$} \\ \hline \\ \text{$C\delta2_C\epsilon3_C\zeta3$} \\ \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	10.8 17.0 StdDev 2.22 0.86 1.92 0.66 0.69 0.43 0.49 0.36 0.46	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \hline \text{Bond Angle} \\ \hline \\ $	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7	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} \\ \\ \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\delta1 \\ \hline \\ C\beta_C\gamma_C\delta2 \\ \hline \\ C\delta1_C\gamma_C\delta2 \\ \hline \\ C\delta1_N\epsilon1_C\epsilon2 \\ \hline \\ C\delta2_C\epsilon2_C\zeta2 \\ \hline \\ C\delta2_C\epsilon3_C\zeta3 \\ \hline \\ C\epsilon2_C\delta2_C\epsilon3 \\ \hline \\ \hline \\ C\epsilon2_C\delta3_C\epsilon3 \\ \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	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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 \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ C\beta_C\gamma_C\delta2 \\ C\delta1_C\gamma_C\delta2 \\ C\delta1_N\epsilon1_C\epsilon2 \\ C\delta2_C\epsilon2_C\zeta2 \\ C\delta2_C\epsilon3_C\zeta3 \\ C\epsilon2_C\delta2_C\epsilon3 \\ C\epsilon2_C\delta2_C\epsilon3 \\ C\epsilon2_C\delta2_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	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	$\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\gamma_C\delta2$} \\ \text{$C\delta1_N\epsilon1_C\epsilon2$} \\ \text{$C\delta2_C\epsilon2_C\zeta2$} \\ \text{$C\delta2_C\epsilon3_C\zeta3$} \\ \text{$C\epsilon2_C\delta2_C\epsilon3$} \\ \text{$C\epsilon2_C\delta2_C\gamma$} \\ \hline \end{array}$	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	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} \\ \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\delta1 \\ C\beta_C\gamma_C\delta2 \\ C\delta1_C\gamma_C\delta2 \\ C\delta1_N\epsilon1_C\epsilon2 \\ C\delta2_C\epsilon2_C\epsilon2 \\ C\epsilon2_C\epsilon3_C\epsilon3 \\ C\epsilon2_C\epsilon3_C\epsilon3 \\ C\epsilon2_C\epsilon3_C\epsilon3 \\ C\epsilon2_C\epsilon3_C\epsilon3 \\ C\epsilon3_C\epsilon3_C\epsilon3 \\ C\epsilon3_C\epsilon3_C\epsilon3 \\ C\epsilon3_C\epsilon3_C\epsilon3 \\ C\epsilon3_C\epsilon3_C\epsilon3 \\ C\epsilon3_C\epsilon3_C\epsilon3 \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_C\beta$_$Cγ} \\ \text{$C\alpha$_C-C} \\ \text{$C\beta$_C\alpha$_$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$2.$Cϵ2.C\epsilon$2} \\ \text{$C\delta$2.$Cϵ3.C\epsilon$3} \\ \text{$C\epsilon$2.$Cδ2.C\epsilon$3} \\ \text{$C\epsilon$2.$Cδ2.C\gamma$} \\ \text{$C\epsilon$3.$Cζ3.C\eta$2} \\ \hline \end{array}$	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	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} \\ \\ \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\delta1 \\ \hline \\ C\beta_C\gamma_C\delta2 \\ \hline \\ C\delta1_C\gamma_C\delta2 \\ \hline \\ C\delta1_N\epsilon1_C\epsilon2 \\ \hline \\ C\delta2_C\epsilon2_C\zeta2 \\ \hline \\ C\delta2_C\epsilon3_C\zeta3 \\ \hline \\ C\epsilon2_C\delta2_C\gamma \\ \hline \\ C\epsilon3_C\zeta3_C\gamma \\ \hline \\ C\epsilon3_C\zeta3_C\gamma \\ \hline \\ C\epsilon3_C\zeta3_C\gamma \\ \hline \\ C\gamma_C\delta1_N\epsilon1 \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ $	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	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_$C$$\beta$_$C$$\gamma$} \\ \hline \\ \text{$C\alpha$_$C$$-$C$$O$} \\ \hline \\ \text{$C\beta$_$C$$\alpha$_$C} \\ \hline \\ \text{$C\beta$_$C$$\gamma$_$C$$\delta$1} \\ \hline \\ \text{$C\beta$_$C$$\gamma$_$C$$\delta$2} \\ \hline \\ \text{$C\delta$1}$_C\gamma$_$C$$\delta$2} \\ \hline \\ \text{$C\delta$1}$_C\gamma$_$C$$\delta$2} \\ \hline \\ \text{$C\delta2_$C$$\epsilon2_$C$$\zeta2} \\ \hline \\ \text{$C\delta$2$_$C$$\epsilon2_C\zeta3} \\ \hline \\ \text{$C\epsilon$2$_$C$$\delta2_C\zeta3} \\ \hline \\ \text{$C\epsilon$2$_$C$$\delta2_C\chi3} \\ \hline \\ \text{$C\gamma$_$C$$\delta1_$N$$\epsilon$1} \\ \hline \\ \text{$C\gamma$_$C$$\delta2_C\epsilon$3} \\ \hline \end{array}$	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	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 0.43 0.48
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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
$\begin{array}{ c c c }\hline \chi\\ \hline \text{chi1}\\ \hline \text{chi2}\\ \hline \\\hline $	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	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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 0.43 0.49 0.49
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5 121.5 107.4	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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 0.43 0.49 0.47 0.46 0.37
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta1 \\ C\beta_C\gamma_C\delta2 \\ C\delta1_C\gamma_C\delta2 \\ C\delta1_N\epsilon1_C\epsilon2 \\ C\delta2_C\epsilon2_C\zeta2 \\ C\delta2_C\epsilon3_C\zeta3 \\ C\epsilon2_C\delta2_C\epsilon3 \\ C\epsilon2_C\delta2_C\epsilon3 \\ C\epsilon2_C\delta2_C\gamma \\ C\epsilon3_C\zeta3_C\eta2 \\ C\gamma_C\delta1_N\epsilon1 \\ C\gamma_C\delta2_C\epsilon2 \\ C\gamma_C\delta1_N\epsilon1 \\ C\gamma_C\delta2_C\epsilon2 \\ C\gamma_C\delta1_C\epsilon2 \\ C\gamma_C\delta2_C\epsilon2 \\ C\gamma_C\delta2_C\epsilon2 \\ C\gamma_C\zeta2_C\epsilon2 \\ C\zeta3_C\eta2_C\zeta2 \\ N\epsilon1_C\epsilon2_C\zeta2 \\ N\epsilon1_C\epsilon2_C\zeta2 \\ \hline \\ N\epsilon1_C\epsilon2_C\zeta2 \\ \hline \\ \\ \hline \end{array}$	Smooth COM -67 97 Mean 113.2 120.4 109.6 127.0 126.6 106.3 108.9 122.4 118.7 118.9 107.2 121.0 110.1 133.9 117.5 121.5 107.4 130.2	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 0.43	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	Smooth COM -68 -7 Mean 114.7 120.5 109.2 127.5 126.1 106.3 108.8 122.3 118.7 118.9 107.3 121.0 110.0 133.8 117.5 121.5 107.5 130.2	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 0.45
$\begin{array}{ c c c }\hline \chi\\ \hline \text{chi1}\\ \hline \text{chi2}\\ \hline \\\hline $	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	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	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	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 0.43 0.49 0.47 0.46 0.37

TRP m-90 n = 961				
χ	Smooth COM	StdDev		
chi1	-67	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
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	9.3	chi1	64	7.2
chi2	78	11.0	chi2	82	4.9
chi3	70	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
$C\beta C\alpha C$	111.2	1.57	$C\beta C\alpha C$	111.1	0.91
$C\beta_C\gamma_SD$	114.4	2.33	$C\beta C\gamma SD$	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	$ET \mathbf{ptp} \ n = 404$		ME	ET ptt $n = 260$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64	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
$C\beta C\alpha C$	110.3	1.46	$C\beta _C\alpha _C$	110.3	1.49
$C\beta C\gamma SD$	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	64	8.2	chi1	71	3.4
chi2	179	10.2	chi2	-74	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	$C\alpha_{-}C\beta_{-}C\gamma$	114.8	0.77
$C\alphaCO$	120.6	0.93	$C\alphaCO$	121.0	0.64
$C\betaC\alphaC$	110.3	1.44	$C\beta C\alpha C$	111.1	1.13
$C\beta C\gamma SD$	112.8	2.11	$C\beta C\gamma SD$	111.7	2.28
$C\gammaSDC\epsilon$	100.9	1.82	$C\gammaSDC\epsilon$	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
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ME	$T \mathbf{pmm} \ n = 42$		•	ME	$T \mathbf{tpp} \ n = 1138$	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	72	7.8		chi1	-174	9.4
chi2	-68	6.7		chi2	63	8.0
chi3	-68	8.1		chi3	72	12.0
Bond Angle	Mean	StdDev	•	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	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
$C\beta C\gamma SD$	115.2	2.54		$C\beta C\gamma SD$	113.7	2.02
$C\gamma_SD_C\epsilon$	101.1	1.58		$C\gamma_SD_C\epsilon$	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
MH	ET $\mathbf{tpt} \ n = 388$			ME	$T \mathbf{ttp} \ n = 1246$	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-173	8.7		chi1	-177	8.6
chi2	65	7.8		chi2	179	11.4
chi3	-156	31.2		chi3	71	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		$C\betaC\alphaC$	110.0	1.17
$C\betaC\gammaSD$	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	-176	8.8		chi1	-175	9.3
chi2	176	9.5		chi2	179	8.2
chi3	176	15.5		chi3	-71	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
$C\beta _C\alpha _C$	110.1	1.31		$C\beta C\alpha C$	110.0	1.17
$C\beta C\gamma SD$	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		$N_{-}C\alpha_{-}C$	110.1	2.40
$N_{-}C\alpha_{-}C\beta$	110.1	1.39		$N_{-}C\alpha_{-}C\beta$	110.4	1.33

$MET \mathbf{tmt} \ n = 34$		•	$\frac{}{\text{MET tmm n}} = 276$			
$\overline{\chi}$	Smooth COM	StdDev	•	χ	Smooth COM	StdDev
chi1	-179	6.7		chi1	-177	7.3
chi2	-85	7.6		chi2	-81	6.8
chi3	173	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
$C\beta C\gamma SD$	112.8	1.77		$C\beta_C\gamma_SD$	114.0	2.12
$C\gamma_SD_C\epsilon$	100.3	1.37		$C\gammaSDC\epsilon$	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	ET mpp $n = 74$			ME	ET mpt $n = 34$	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-76	13.7		chi1	-69	11.7
chi2	73	12.3		chi2	74	11.0
chi3	73	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
$C\beta C\alpha C$	109.9	1.63		$C\beta C\alpha C$	109.3	1.40
$C\beta C\gamma SD$	114.3	2.25		$C\betaC\gammaSD$	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	Γ mtp n = 2815	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-77	5.1		chi1	-66	7.1
chi2	63	5.5		chi2	177	9.3
chi3	-101	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		$C\beta_{-}C\alpha_{-}C$	110.0	1.59
$C\betaC\gammaSD$	115.9	2.31		$C\betaC\gammaSD$	112.8	2.08
$C\gammaSDC\epsilon$	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

$MET \mathbf{mtt} \ n = 1542$				
χ	Smooth COM	StdDev		
chi1	-67	7.7		
chi2	179	8.7		
chi3	-176	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		
$C\beta C\gamma SD$	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_Cα_Cβ	110.7	1.00		
MET mmp $n = 520$				
χ	Smooth COM	StdDev		
chi1	-65	5.3		
chi2	-61	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		
$C\beta C\gamma SD$	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 mmm $n = 3354$				
χ	Smooth COM	StdDev		
chi1	-65	8.9		
chi2	-60	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		
$C\gammaSDC\epsilon$	100.9	1.74		
$N_{-}C\alpha_{-}C$	111.6	2.38		
$N_{-}C\alpha_{-}C\beta$	110.7	1.02		

$MET \mathbf{mtm} \ n = 1851$				
χ	Smooth COM	StdDev		
chi1	-66	7.9		
chi2	-177	10.7		
chi3	-73	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 $\mathbf{mmt} \ \mathbf{n} = 597$				
χ	Smooth COM	StdDev		
chi1	-64	8.7		
chi2	-63	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		
$C\betaC\gammaSD$	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	U pp20 n = 159		GLU	U pt0 n = 2800	
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	8.1	chi1	65	8.4
chi2	85	8.0	chi2	-177	10.1
chi3	19	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
$C\alphaCO$	120.4	0.85	$C\alphaCO$	120.5	0.93
$C\betaC\alphaC$	111.6	1.84	$C\betaC\alphaC$	110.5	1.50
$C\betaC\gammaC\delta$	114.1	1.30	$C\betaC\gammaC\delta$	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
GLU	pm20 n = 1485		GLI	5 tp30 n = 4616	
$\frac{\alpha}{\chi}$	Smooth COM	StdDev	$\frac{\partial \mathcal{L}}{\chi}$	Smooth COM	StdDev
chi1	69	8.8	chi1	-178	9.8
chi2	-84	8.6	chi2	64	9.2
chi3	15	21.7	chi3	25	26.1
Bond Angle	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
$C\alphaCO$	120.2	0.83	$C\alphaCO$	120.5	0.80
$C\betaC\alphaC$	110.5	1.25	$C\betaC\alphaC$	110.6	1.21
$C\betaC\gammaC\delta$	114.5	1.45	$C\betaC\gammaC\delta$	113.8	1.35
$C\gammaC\deltaO\epsilon 1$	119.8	1.71	$C\gammaC\deltaO\epsilon 1$	119.3	1.46
$C\gamma C\delta O\epsilon 2$	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
GLU	U tt0 n = 13610		GLU	tm-30 n = 862	
$\frac{1}{\chi}$	Smooth COM	StdDev	$\frac{1}{\chi}$	Smooth COM	StdDev
chi1	-176	8.6	chi1	-170	8.6
chi2	177	10.3	chi2	-83	9.2
chi3	1	41.4	chi3	-28	17.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.5	1.74	$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.35
$C\alpha_{-}C_{-}O$	120.6	0.77	$C\alpha_{-}C_{-}O$	120.5	0.84
$C\betaC\alphaC$	110.1	1.17	$C\betaC\alphaC$	111.0	1.33
$C\beta$ _ $C\gamma$ _ $C\delta$	113.1	1.50	$C\beta$ _ $C\gamma$ _ $C\delta$	113.8	1.47
$C\gamma_{-}C\delta_{-}O\epsilon 1$	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
$O\epsilon 1 C\delta O\epsilon 2$	123.1	1.07	$O\epsilon 1 C\delta O\epsilon 2$	122.8	1.17

$GLU \ mp0 \ n = 3671$				
χ	Smooth COM	StdDev		
chi1	-66	7.3		
chi2	82	9.4		
chi3	3	27.5		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	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		
$C\gammaC\deltaO\epsilon 2$	117.8	1.47		
$N_{-}C\alpha_{-}C$	112.0	2.00		
$N_{-}C\alpha_{-}C\beta$	110.6	1.06		
$O\epsilon 1_C\delta_O\epsilon 2$	122.4	1.18		

GLU mt-10 $n = 21021$				
χ	Smooth COM	StdDev		
chi1	-66	7.7		
chi2	179	11.4		
chi3	-6	37.3		
Bond Angle	Mean	StdDev		
$C\alphaC\betaC\gamma$	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		
$C\gammaC\deltaO\epsilon 2$	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	GLU mm-30 $n = 9080$				
χ	Smooth COM	StdDev			
chi1	-66	8.7			
chi2	-66	10.6			
chi3	-31	26.9			
Bond Angle	Mean	StdDev			
$C\alpha_{-}C\beta_{-}C\gamma$	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

GLN pp30 n = 178		•	GLN pt0 $n = 1885$			
χ	Smooth COM	StdDev	•	χ	Smooth COM	StdDev
chi1	62	7.8		chi1	64	8.1
chi2	83	8.5		chi2	-177	11.3
chi3	29	20.9		chi3	-2	75.2
Bond Angle	Mean	StdDev	-	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.9	1.28	-	$C\alphaC\betaC\gamma$	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
$C\betaC\gammaC\delta$	113.6	1.40		$C\betaC\gammaC\delta$	112.5	1.47
$C\gamma_C\delta_N\epsilon_2$	116.4	0.89		$C\gamma_C\delta_N\epsilon_2$	116.5	0.95
$C\gammaC\deltaO\epsilon 1$	120.9	0.95		$C\gamma_{-}C\delta_{-}O\epsilon 1$	120.8	0.97
$N_{-}C\alpha_{-}C$	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
GLN	$N \ pm20 \ n = 487$			GLN	V tp40 n = 3618	
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	69	9.9		chi1	-176	8.7
chi2	-84	9.3		chi2	66	8.2
chi3	16	32.3		chi3	41	24.2
Bond Angle	Mean	StdDev	_	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	115.7	1.41		$C\alphaC\betaC\gamma$	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		$C\betaC\gammaC\delta$	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			GLN $\mathbf{tt0}$ n = 6936		
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev
chi1	-176	8.7		chi1	-176	8.5
chi2	62	8.8		chi2	177	10.8
chi3	-104	27.5	_	chi3	2	60.9
Bond Angle	Mean	StdDev	_	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.4	1.57		$C\alphaC\betaC\gamma$	113.6	1.80
$C\alphaCO$	120.6	0.83		$C\alphaCO$	120.6	0.76
$C\betaC\alphaC$	110.5	1.24		$C\betaC\alphaC$	110.1	1.18
$C\betaC\gammaC\delta$	113.0	1.31		$C\betaC\gammaC\delta$	112.6	1.50
$C\gamma_C\delta_N\epsilon_2$	116.6	0.95		$C\gamma_C\delta_N\epsilon_2$	116.5	0.84
$C\gammaC\deltaO\epsilon 1$	120.9	0.85		$C\gammaC\deltaO\epsilon 1$	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

GLN	V tm 130 n = 55		GLN	$\sqrt{\text{tm-30 n}} = 547$,
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-171	9.7		-171	10.1
chi2	-75	10.4	chi2	-85	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
$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	117.1	1.28	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.5	0.71
$C\gammaC\deltaO\epsilon 1$	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			mp-120 n = 87	
$\frac{\alpha}{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66	9.0	chi1	-72	10.0
chi2	81	11.4	chi2	69	10.0 11.4
chi3	17	37.5	chi3	-119	13.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.2	1.36	$C\alpha_{-}C\beta_{-}C\gamma$	114.4	1.55
$C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	120.4	0.84	$C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	120.5	0.88
$C\betaC\alphaC$	109.8	1.52	$C\beta_{-}C\alpha_{-}C$	109.7	1.79
$C\beta$ _ $C\alpha$ _ $C\delta$	113.4	1.32 1.29	$C\beta C\alpha C$ $C\beta C\gamma C\delta$	113.6	1.79 1.57
$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.3	0.82	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$	116.6	0.65
$C\gamma_{-}C\delta_{-}N\epsilon_{2}$ $C\gamma_{-}C\delta_{-}O\epsilon_{1}$	121.1	0.82 0.95	$C\gamma_{-}C\delta_{-}N\epsilon_{2}$ $C\gamma_{-}C\delta_{-}O\epsilon_{1}$	120.6	1.09
$N_{-}C\alpha_{-}C$	111.6	2.35	N_Cα_C	111.6	2.76
$N_{-}C\alpha_{-}C\beta$	111.0	2.33 1.10	$N_{C}\alpha_{C}$	111.0	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
OET_CO_INEZ	122.0	0.00			
GLN	mt0 n = 14370		GLN mm110 n = 1147		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66	7.5	chi1	-65	8.6
chi2	179	11.2	chi2	-62	10.9
chi3	-3	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	GLN mm-40 $n = 5959$					
χ	Smooth COM	StdDev				
chi1	-63	8.6				
chi2	-66	10.4				
chi3	-38	24.7				
Bond Angle	Mean	StdDev				
$C\alpha_{-}C\beta_{-}C\gamma$	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				
$C\gammaC\deltaN\epsilon_2$	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				
$O\epsilon 1C\deltaN\epsilon 2$	122.6	0.78				

Table S20: ARG Central Values

ARC	$\frac{1}{2}$ 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	86	7.0	chi2	91	4.6
chi3	57	3.8	chi3	62	10.6
chi4	79	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
$C\gamma_C\delta_N\epsilon$	112.5	1.08	$C\gammaC\deltaN\epsilon$	113.8	2.26
$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.6	0.68	$N\epsilon C\zeta \eta 1$	121.0	1.24
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.8	0.63	$N\epsilon C\zeta \eta 2$	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	$N_{-}C\alpha_{-}C$	113.6	2.34
$N_{-}C\alpha_{-}C\beta$	111.9	1.19	$N_{-}C\alpha_{-}C\beta$	111.2	1.26
ARG	5 ppt170 n = 57		ARC	G ppt90 n = 19	
$\frac{\Lambda RG}{\chi}$	$\frac{\text{S ppt170 n} = 57}{\text{Smooth COM}}$	StdDev	ARC	G ppt90 n = 19 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM 59	StdDev 9.9	χ chi1	Smooth COM	5.9
χ chi1 chi2	Smooth COM 59 87	9.9 12.3	χ chi1 chi2	Smooth COM 63 99	5.9 8.0
χ chi1 chi2 chi3	Smooth COM 59 87 173	9.9 12.3 12.3	χ chi1 chi2 chi3	Smooth COM	5.9
χ chi1 chi2	Smooth COM 59 87	9.9 12.3	χ chi1 chi2	Smooth COM 63 99	5.9 8.0
χ chi1 chi2 chi3	Smooth COM 59 87 173	9.9 12.3 12.3	χ chi1 chi2 chi3	Smooth COM 63 99 -179	5.9 8.0 9.8
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 59 87 173 173 Mean 116.2	9.9 12.3 12.3 17.3 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM 63 99 -179 87 Mean 115.4	5.9 8.0 9.8 13.0 StdDev 1.89
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \end{array}$	Smooth COM 59 87 173 173 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 $C\alpha C\beta C\gamma$ $C\alpha CO$	Smooth COM 63 99 -179 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$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \hline \end{array}$	Smooth COM 59 87 173 173 Mean 116.2 120.4 111.9	9.9 12.3 12.3 17.3 StdDev 1.39 1.04 1.37	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array}$	Smooth COM 63 99 -179 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 87 173 173 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 63 99 -179 87 Mean 115.4 120.8	5.9 8.0 9.8 13.0 StdDev 1.89 0.83
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline \text{$\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$} \\ \end{array}$	Smooth COM 59 87 173 173 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 63 99 -179 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$-C\beta$-$Cγ} \\ \text{$C\alpha$-C-C0} \\ \text{$C\beta$-C\alpha$-$C$} \\ \text{$C\beta$-$Cγ-C\delta$} \\ \text{$C\delta$-$Nϵ-C\zeta$} \\ \text{$C\gamma$-$Cδ-N\epsilon$} \\ \end{array}$	Smooth COM 59 87 173 173 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \hline \end{array}$	Smooth COM 63 99 -179 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline \text{$\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$} \\ \end{array}$	Smooth COM 59 87 173 173 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM 63 99 -179 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$-C\beta$-$Cγ} \\ \text{$C\alpha$-C-C0} \\ \text{$C\beta$-C\alpha$-$C$} \\ \text{$C\beta$-$Cγ-C\delta$} \\ \text{$C\delta$-$Nϵ-C\zeta$} \\ \text{$C\gamma$-$Cδ-N\epsilon$} \\ \end{array}$	Smooth COM 59 87 173 173 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \hline \end{array}$	Smooth COM 63 99 -179 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$} \\ \hline \\ \text{$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$} \\ \hline \\ \text{$N\epsilon_C\zeta$} \\ \hline \\ \text{$N\eta1$} \\ \hline \end{array}$	Smooth COM 59 87 173 173 Mean 116.2 120.4 111.9 112.4 124.2 111.4 120.5 119.8 119.7	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 0.70	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta 1 \\ \\ \end{array}$	Smooth COM 63 99 -179 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_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$} \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM 59 87 173 173 Mean 116.2 120.4 111.9 112.4 124.2 111.4 120.5 119.8	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM 63 99 -179 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

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ARC	ARG ppt-90 $n = 15$		$ARG \mathbf{ptp90} \text{ n} = 223$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61	9.1	chi1	65	9.4
chi2	90	11.1	chi2	178	11.3
chi3	177	5.5	chi3	64	8.6
chi4	-92	14.4	chi4	87	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
$C\betaC\gammaC\delta$	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	$N\epsilon C\zeta \eta 1$	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	ptp-110 n = 77	7	ARG ptp-170 n = 388		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	67	8.2	chi1	67	7.7
chi2					
CHIZ	-179	11.9	chi2	-175	12.2
chi3	-179 64	11.9 10.0		-175 68	
			chi2		12.2
chi3	64	10.0	chi2 chi3	68	$12.2 \\ 9.7$
chi3 chi4	64 -108	10.0 9.9	chi2 chi3 chi4	68 -172	12.2 9.7 16.0
chi3 chi4 Bond Angle	64 -108 Mean	10.0 9.9 StdDev	chi2 chi3 chi4 Bond Angle	68 -172 Mean	12.2 9.7 16.0 StdDev
chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	64 -108 Mean 114.8	10.0 9.9 StdDev 1.93	chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	68 -172 Mean 114.5	12.2 9.7 16.0 StdDev 1.46
chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$ $C\alphaCO$	64 -108 Mean 114.8 120.7	10.0 9.9 StdDev 1.93 1.22	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 -172 Mean 114.5 120.6	12.2 9.7 16.0 StdDev 1.46 0.96
chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C CO$ $C\beta C\alpha C$	64 -108 Mean 114.8 120.7 110.4	10.0 9.9 StdDev 1.93 1.22 1.42	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$	68 -172 Mean 114.5 120.6 110.4	12.2 9.7 16.0 StdDev 1.46 0.96 1.57
chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$	64 -108 Mean 114.8 120.7 110.4 111.9	10.0 9.9 StdDev 1.93 1.22 1.42 1.47	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 -172 Mean 114.5 120.6 110.4 111.3	12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74
chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\beta _N\epsilon _C\zeta$	64 -108 Mean 114.8 120.7 110.4 111.9 125.6	10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44	chi2 chi3 chi4 Bond Angle $C\alpha . C\beta . C\gamma$ $C\alpha . C . O$ $C\beta . C\alpha . C$ $C\beta . C\gamma . C\delta$ $C\delta . N\epsilon . C\zeta$	68 -172 Mean 114.5 120.6 110.4 111.3 124.6	12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14
chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$	64 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7	10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29	chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$	68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4	12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63
chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$	64 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7 121.0	10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29 1.42	chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$	68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4 120.5	12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63 0.94
chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	64 -108 Mean 114.8 120.7 110.4 111.9 125.6 111.7 121.0 119.6	10.0 9.9 StdDev 1.93 1.22 1.42 1.47 1.44 2.29 1.42 1.57	chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	68 -172 Mean 114.5 120.6 110.4 111.3 124.6 111.4 120.5 119.8	12.2 9.7 16.0 StdDev 1.46 0.96 1.57 1.74 1.14 1.63 0.94 0.93

chi1 65 8.3 chi1 64 7.6 chi2 -177 10.4 chi2 178 12.3 chi3 -179 10.4 chi3 176 8.7 chi4 179 17.5 chi4 87 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 114.6 1.53 $C\alpha_{-}C\beta_{-}C\gamma_{-}$ 114.6 1.53 $C\alpha_{-}C\beta_{-}C\gamma_{-}$ 114.8 1.43 $C\beta_{-}C\gamma_{-}C\delta_{-}$ 110.5 1.50 $C\beta_{-}C\alpha_{-}C$ 110.2 1.41 $C\beta_{-}C\gamma_{-}C\delta_{-}$ 111.1 2.01 $C\beta_{-}C\gamma_{-}C\delta_{-}$ 111.0 1.95 $C\delta_{-}N\epsilon_{-}C\zeta_{-}$ 124.4 1.10 $C\delta_{-}N\epsilon_{-}C\zeta_{-}$ 124.9 0.92 $C\gamma_{-}C\delta_{-}N\eta_{1}$ 120.5 0.94 $N\epsilon_{-}C\zeta_{-}N\eta_{2}$ 119.6 0.89 $N\epsilon_{-}C\zeta_{-}N\eta_{2}$ 119.9 0.88 $N\eta_{1}.C\zeta_{-}N\eta_{2}$ 119.9 0.88 $N\eta_{1}.C\zeta_{-}N\eta_{2}$ 119.9 0.88 $N\eta_{1}.C\zeta_{-}N\eta_{2}$ 119.9 0.88 $N\eta_{1}.C\zeta_{-}N\eta_{2}$ 119.5 0.70 $N.C\alpha_{-}C$ 111.0 1.12 $N.C\alpha_{-}C\beta_{-}$ 111.0 1.15 $N.C\alpha_{-}C\beta_{-}$ 111.0 1.15 $N.C\alpha_{-}C\beta_{-}$ 111.0 1.15 $N.C\alpha_{-}C\beta_{-}$ 111.0 1.15 $N.C\alpha_{-}C\beta_{-}$ 111.0 1.16 $S\delta_{-}S\delta_{$	ARG	ptt180 n = 820)	ARC	$\frac{1}{2}$ ptt90 n = 814	
chi2 -177 10.4 chi2 178 12.3 chi3 -179 10.4 chi3 176 8.7 chi4 179 17.5 chi4 87 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDe Cα_Cβ_Cγ_Cγ 114.6 1.53 Cα_Cβ_Cγ_C0 120.6 0.86 Cβ_Cγ_Cδ 110.5 1.50 Cβ_Cα_C 110.2 1.41 Cβ_Cγ_Cδ 111.1 2.01 Cβ_Cα_C 110.2 1.41 Nε_Cζ_Nη2 119.6 0.89 Nε_Cζ_Nη1 120.8 0.99 Nε_Cζ_Nη2 119.9 0.88 Nη1_Cζ_Nη2 119.7	χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi3 -179 10.4 chi3 176 8.7 chi4 179 17.5 chi4 87 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDe Cα_Cβ_Cγ 114.6 1.53 Cα_Cβ_Cγ 114.8 1.43 Cα_C C_O 120.6 1.01 Cα_C C_O 120.6 0.86 Cβ_Cα_C 110.5 1.50 Cβ_Cα_C 110.2 1.41 Cβ_Cγ_Cδ 111.1 2.01 Cβ_Cγ_Cδ 111.0 1.95 Cδ_Nε_Cζ 124.4 1.10 Cδ_Nε_Cζ 124.9 0.92 Cγ_Cδ_Nε 110.7 1.99 Cγ_Cδ_Nε 111.9 2.47 Nε_Cζ_Nη1 120.5 0.94 Nε_Cζ_Nη2 119.7 0.91 Nη1_Cζ_Nη2 119.6 0.89 Nε_Cζ_Nη2 119.7 0.91 Nη1_Cζ_Nη2 119.9 0.88 Nη1_Cζ_Nη2 119.5 0.70 N_Cα_C 111.0 1.12 N.Cα_C 110.8	chi1	65	8.3	chi1	64	7.6
chi4 179 17.5 chi4 87 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDe Cα_Cβ_Cγ 114.6 1.53 $Cα_Cβ_C^2$ 114.8 1.43 Cα_C, O 120.6 1.01 $Cα_C C_O$ 120.6 0.86 Cβ_Cα_C 110.5 1.50 $Cβ_Cα_C$ 110.2 1.41 Cβ_Cγ_Cδ 111.1 2.01 $Cβ_Cγ_Cδ$ 111.0 1.95 Cδ_Nε_Cζ 124.4 1.10 $Cδ_Nε_Cζ$ 124.9 0.92 $Cγ_Cδ_Nε$ 110.7 1.99 $Cγ_Cδ_Nε$ 111.9 2.47 Nε_Cζ_Nη1 120.5 0.94 Nε_Cζ_Nη2 119.7 0.91 Nβ_Cζ_Nη2 119.6 0.89 Nε_Cζ_Nη2 119.7 0.91 Nη1.Cζ_Nη2 119.9 0.88 Nη1.Cζ_Nη2 119.5 0.70 N.Cα_C 111.3 2.49 N.Cα_C 110.8 2.51 N.Cα_Cβ 111.0 1.12 N.Cα_C	chi2	-177	10.4	chi2	178	12.3
Bond Angle Mean StdDev Bond Angle Mean StdDe $C\alpha_{-}C\beta_{-}C\gamma$ 114.6 1.53 $C\alpha_{-}C\beta_{-}C\gamma$ 114.8 1.43 $C\alpha_{-}C_{-}C$ 120.6 1.01 $C\alpha_{-}C_{-}O$ 120.6 0.86 $C\beta_{-}C\alpha_{-}C$ 110.5 1.50 $C\beta_{-}C\alpha_{-}C$ 110.2 1.41 $C\beta_{-}C\gamma_{-}C\delta$ 111.1 2.01 $C\beta_{-}C\gamma_{-}C\delta$ 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 $N\epsilon_{-}C\zeta_{-}N\eta$ 1 120.5 0.94 $N\epsilon_{-}C\zeta_{-}N\eta$ 2 119.7 0.91 $N_{-}C\zeta_{-}N\eta$ 2 119.9 0.88 $N\eta_{-}C\zeta_{-}N\eta$ 2 119.7 0.91 $N_{-}C_{-}C\beta_{-}N\eta$ 2 119.9 0.88 $N\eta_{-}C\zeta_{-}N\eta$ 2 119.7 0.70 $N_{-}C\alpha_{-}C\beta$ 111.0 1.12 N	chi3	-179	10.4	chi3	176	8.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	chi4	179	17.5	chi4	87	9.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\alphaC\betaC\gamma$	114.6	1.53	$C\alpha_{-}C\beta_{-}C\gamma$	114.8	1.43
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\alphaCO$	120.6	1.01	$C\alphaCO$	120.6	0.86
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\betaC\alphaC$	110.5	1.50	$C\beta_{-}C\alpha_{-}C$	110.2	1.41
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C\beta C\gamma C\delta$	111.1	2.01	$C\betaC\gammaC\delta$	111.0	1.95
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\delta_N\epsilon_C\zeta$	124.4	1.10	$C\delta_N\epsilon_C\zeta$	124.9	0.92
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\gamma_C\delta_N\epsilon$	110.7	1.99	$C\gamma_C\delta_N\epsilon$	111.9	2.47
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.5	0.94	$N\epsilon_{-}C\zeta_{-}N\eta 1$	120.8	0.99
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	0.89	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.7	0.91
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		119.9	0.88		119.5	0.70
N_Cα_Cβ 111.0 1.12 N_Cα_Cβ 111.0 1.15 ARG ptt-90 n = 726 ARG ptm160 n = 502 ARG ptm160 n = 502 χ Smooth COM StdDev χ Smooth COM StdDe chi1 66 7.9 chi1 63 8.7 chi2 -175 12.0 chi2 -179 15.0 chi3 -176 8.9 chi3 -67 9.7 chi4 -87 11.8 chi4 165 25.7 Bond Angle Mean StdDev Bond Angle Mean StdDe $CαCβCγ$ 114.8 1.51 $CαCβCγ$ 114.6 1.63 $CαCβCγ$ 114.8 1.51 $CαCβCγ$ 114.6 1.63 $CαCβCγ$ 114.8 1.51 $CαCβCγ$ 114.6 1.63 $CαCβCγ$ 114.8 1.55 $CβCβCγ$ 110.4 1.56 $CβCβCγ$ 110.5 1.55 $CβCβCβ$ 111.7 1.80						2.51
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$N_{-}C\alpha_{-}C\beta$	111.0	1.12	$N_{-}C\alpha_{-}C\beta$	111.0	1.15
chi1 66 7.9 chi1 63 8.7 chi2 -175 12.0 chi2 -179 15.0 chi3 -176 8.9 chi3 -67 9.7 chi4 -87 11.8 chi4 165 25.7 Bond Angle Mean StdDev Bond Angle Mean StdDev $C\alpha_C\beta_C\gamma$ 114.8 1.51 $C\alpha_C\beta_C\gamma$ 114.6 1.63 $C\alpha_C_C$ 110.5 0.94 $C\alpha_C_C$ 110.5 1.55 $C\beta_C\alpha_C$ 110.4 1.56 $C\beta_C\gamma_C\delta$ 111.0 2.04 $C\beta_C\gamma_C\delta$ 111.7 1.80 $C\delta_N\epsilon_C\zeta$ 124.9 1.14 $C\delta_N\epsilon_C\zeta$ 124.7 1.39 $C\gamma_C\delta_N\epsilon$ 111.7 2.66 $C\gamma_C\delta_N\epsilon$ 111.5 2.11 $N\epsilon_C\zeta_N\eta$ 1 120.8 1.01 $N\epsilon_C\zeta_N\eta$ 1 120.6 1.28 $N\epsilon_C\zeta_N\eta$ 2 119.7 1.14 $N\epsilon_C\zeta_N\eta$ 2 119.7 1.12 $N\eta$ 1. $C\zeta_N\eta$ 2 119.5 1.03 $N\eta$ 1. $C\zeta_N\eta$ 2 119.7 1.00 $N_C\alpha_C$ 111.7 2.55 $N_C\alpha_C$ 110.9 2.57	A D.C					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ang	ptt-90 n = 726	<u> </u>	ARG	ptm160 n = 503	2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		-	_			$\frac{2}{\text{StdDev}}$
chi4 -87 11.8 chi4 165 25.7 Bond Angle Mean StdDev Bond Angle Mean StdDe $C\alpha_C\beta_C\gamma$ 114.8 1.51 $C\alpha_C\beta_C\gamma$ 114.6 1.63 $C\alpha_C \supseteq O$ 120.5 0.94 $C\alpha_C \supseteq O$ 120.5 0.98 $C\beta_C\alpha_C$ 110.5 1.55 $C\beta_C\alpha_C$ 110.4 1.56 $C\beta_C\gamma_C\delta$ 111.0 2.04 $C\beta_C\gamma_C\delta$ 111.7 1.80 $C\delta_N\epsilon_C\zeta$ 124.9 1.14 $C\delta_N\epsilon_C\zeta$ 124.7 1.39 $C\gamma_C\delta_N\epsilon$ 111.7 2.66 $C\gamma_C\delta_N\epsilon$ 111.5 2.11 $N\epsilon_C\zeta_N\eta1$ 120.8 1.01 $N\epsilon_C\zeta_N\eta1$ 120.6 1.28 $N\epsilon_C\zeta_N\eta2$ 119.7 1.14 $N\epsilon_C\zeta_N\eta2$ 119.7 1.12 $N\eta1_C\zeta_N\eta2$ 119.5 1.03 $N\eta1_C\zeta_N\eta2$ 119.7 1.00 $N_C\alpha_C$ 111.7 2.55 $N_C\alpha_C$ 110.9 2.57		Smooth COM	StdDev	χ	Smooth COM	StdDev
Bond Angle Mean StdDev Bond Angle Mean StdDe $C\alpha_C\beta_C\gamma$ 114.8 1.51 $C\alpha_C\beta_C\gamma$ 114.6 1.63 $C\alpha_C_O$ 120.5 0.94 $C\alpha_C_O$ 120.5 0.98 $C\beta_C\alpha_C$ 110.5 1.55 $C\beta_C\alpha_C$ 110.4 1.56 $C\beta_C\gamma_C\delta$ 111.0 2.04 $C\beta_C\gamma_C\delta$ 111.7 1.80 $C\delta_N\epsilon_C\zeta$ 124.9 1.14 $C\delta_N\epsilon_C\zeta$ 124.7 1.39 $C\gamma_C\delta_N\epsilon$ 111.7 2.66 $C\gamma_C\delta_N\epsilon$ 111.5 2.11 $N\epsilon_C\zeta_N\eta$ 120.8 1.01 $N\epsilon_C\zeta_N\eta$ 120.6 1.28 $N\epsilon_C\zeta_N\eta$ 119.7 1.14 $N\epsilon_C\zeta_N\eta$ 119.7 1.12 $N\eta$ $C\zeta_N\eta$ 119.7 1.00 N_1 $C\zeta_N\eta$ 119.7 1.00 N_2 111.7 2.55 N_2 110.9 2.57	χ	Smooth COM 66	StdDev 7.9	$\frac{\chi}{\text{chi1}}$	Smooth COM 63	StdDev 8.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	χ chi1	Smooth COM 66 -175	7.9 12.0	χ chi1 chi2	Smooth COM 63 -179	StdDev 8.7 15.0
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3	Smooth COM 66 -175 -176	7.9 12.0 8.9	χ chi1 chi2 chi3	Smooth COM 63 -179 -67	8.7 15.0 9.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3	Smooth COM 66 -175 -176 -87	7.9 12.0 8.9 11.8	chi1 chi2 chi3 chi4	Smooth COM 63 -179 -67 165	8.7 15.0 9.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 66 -175 -176 -87 Mean	7.9 12.0 8.9 11.8 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 63 -179 -67 165 Mean	8.7 15.0 9.7 25.7 StdDev
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 66 -175 -176 -87 Mean 114.8	7.9 12.0 8.9 11.8 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$	Smooth COM 63 -179 -67 165 Mean 114.6	8.7 15.0 9.7 25.7 StdDev 1.63
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5	7.9 12.0 8.9 11.8 StdDev 1.51 0.94	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	Smooth COM 63 -179 -67 165 Mean 114.6 120.5	8.7 15.0 9.7 25.7 StdDev 1.63 0.98
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \text{$\text{C}\beta_\text{C}\alpha_\text{C}$} \\ \end{array}$	Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4	8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\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 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7	8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0 124.9	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7	8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39
$Nη1_Cζ_Nη2$ 119.5 1.03 $Nη1_Cζ_Nη2$ 119.7 1.00 $N_Cα_C$ 111.7 2.55 $N_Cα_C$ 110.9 2.57	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14 2.66	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \hline \text{$C\alpha_C_\beta_C\gamma$} \\ \hline \\ \hline \text{$C\beta_C\alpha_C$} \\ \hline \\ \hline \\ \hline \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \hline \\ \hline \\ \hline \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ $	Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5	8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39 2.11
$N_{-}C\alpha_{-}C$ 111.7 2.55 $N_{-}C\alpha_{-}C$ 110.9 2.57	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _C$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7 120.8	7.9 12.0 8.9 11.8 StdDev 1.51 0.94 1.55 2.04 1.14 2.66 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$} \\ \hline \end{array}$	Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5 120.6	8.7 15.0 9.7 25.7 StdDev 1.63 0.98 1.56 1.80 1.39 2.11 1.28
	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$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 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7 120.8 119.7	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5 120.6 119.7	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
	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \text{N}\eta1_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM 66 -175 -176 -87 Mean 114.8 120.5 110.5 111.0 124.9 111.7 120.8 119.7 119.5	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 1.03	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_Cβ_C\gamma$} \\ \text{$C\alpha$_C$_O$} \\ \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$\delta_Nϵ} \\ \text{$N\epsilon$_Cζ_Nη1} \\ \text{$N\epsilon$_Cζ_Nη2} \\ \text{$N\eta$1_Cζ_Nη2} \\ \end{array}$	Smooth COM 63 -179 -67 165 Mean 114.6 120.5 110.4 111.7 124.7 111.5 120.6 119.7 119.7	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	ptm-80 n = 215	5	ARC	$\frac{1}{2}$ pmt100 n = 4	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	8.3	chi1	70	7.2
chi2	-178	14.4	chi2	-90	9.1
chi3	-66	10.3	chi3	-174	5.4
chi4	-84	10.8	chi4	97	2.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	1.28	$C\alphaC\betaC\gamma$	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
$C\betaC\gammaC\delta$	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
$N\epsilon C\zeta \eta 1$	120.7	1.21	$N\epsilon C\zeta N\eta 1$	121.0	0.29
$N\epsilon C\zeta \eta 2$	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	$N_{-}C\alpha_{-}C$	110.2	1.44
$N_{-}C\alpha_{-}C\beta$	111.0	1.31	$N_{-}C\alpha_{-}C\beta$	111.4	0.42
ADO					
AKG	pmt170 n = 39)	ARG	3 pmt-80 n = 27	•
$\frac{\lambda}{\chi}$	$\frac{\text{pmt170 n} = 39}{\text{Smooth COM}}$	StdDev	$\frac{\text{ARG}}{\chi}$	$\frac{\text{F pmt-80 n} = 27}{\text{Smooth COM}}$	StdDev
	-	_	-	-	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
χ chi1	Smooth COM 73	StdDev 11.2	χ chi1	Smooth COM 81	StdDev 9.3
χ chi1 chi2	Smooth COM 73 -78	StdDev 11.2 15.4	χ chi1 chi2	Smooth COM 81 -68	StdDev 9.3 7.6
χ chi1 chi2 chi3	Smooth COM 73 -78 -169	StdDev 11.2 15.4 10.1	χ chi1 chi2 chi3	Smooth COM 81 -68 -176	9.3 7.6 11.0
chi1 chi2 chi3 chi4	Smooth COM 73 -78 -169 -169	StdDev 11.2 15.4 10.1 15.1	chi1 chi2 chi3 chi4	Smooth COM 81 -68 -176 -84	9.3 7.6 11.0 8.3
chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 73 -78 -169 -169 Mean	StdDev 11.2 15.4 10.1 15.1 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 81 -68 -176 -84 Mean	9.3 7.6 11.0 8.3 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 73 -78 -169 -169 Mean 116.3	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 81 -68 -176 -84 Mean 115.8	9.3 7.6 11.0 8.3 StdDev 1.16
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM 73 -78 -169 -169 Mean 116.3 120.8	StdDev 11.2 15.4 10.1 15.1 StdDev 1.19 0.70	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 81 -68 -176 -84 Mean 115.8 121.0	9.3 7.6 11.0 8.3 StdDev 1.16 0.65
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$	Smooth COM 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\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 81 -68 -176 -84 Mean 115.8 121.0 110.3	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \text{$\text{C}\alpha$_$C$_$C} \\ \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \text{$\text{C}\beta$_$C}\gamma$_$C}\delta \end{array}$	Smooth COM 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 81 -68 -176 -84 Mean 115.8 121.0 110.3 113.3	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \hline \text{$C\alpha_C_O$} \\ \hline \\ \hline \text{$C\beta_C\alpha_C$} \\ \hline \\ \hline \\ \hline \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \hline \\ \hline \\ \hline \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \end{array}$	Smooth COM 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$C\alpha_C\beta_C\gamma$} \\ \text{$C\alpha_C_C$} \\ \text{$C\beta_C\alpha_C$} \\ \text{$C\beta_C\gamma_C\delta$} \\ \text{$C\beta_N\epsilon_C\zeta$} \\ \end{array}$	Smooth COM 81 -68 -176 -84 Mean 115.8 121.0 110.3 113.3 124.9	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\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$} \\ \hline \end{array}$	Smooth COM 81 -68 -176 -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
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 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\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 81 -68 -176 -84 Mean 115.8 121.0 110.3 113.3 124.9 112.1 121.0	9.3 7.6 11.0 8.3 StdDev 1.16 0.65 1.02 1.79 0.99 1.75 0.89
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$ $N\epsilon _C\zeta _N\eta 2$	Smooth COM 73 -78 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\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$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta2$} \\ \end{array}$	Smooth COM 81 -68 -176 -84 Mean 115.8 121.0 110.3 113.3 124.9 112.1 121.0 119.6	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 = 15	2	ARG	pmm-80 n = 19	 9
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	75	3.2	chi1	73	12.6
chi2	-75	5.6	chi2	-75	11.2
chi3	-64	6.3	chi3	-56	8.1
chi4	151	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
$C\beta_{-}C\alpha_{-}C$	110.4	1.04	$C\beta_{-}C\alpha_{-}C$	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	$C\gamma_C\delta_N\epsilon$	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	$N\epsilon C\zeta N\eta 2$	120.3	0.95
$N\eta 1_C C\zeta_N \eta 2$	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	tpp80 n = 363		ARG	tpp-160 n = 49	6
X ARG	Smooth COM	StdDev	$\frac{\lambda}{\chi}$	tpp-160 n = 49 Smooth COM	6 StdDev
		StdDev 10.3			
χ	Smooth COM		χ	Smooth COM 178 65	StdDev
$\frac{\chi}{\text{chi1}}$	Smooth COM -177	10.3	χ chi1	Smooth COM 178	StdDev 9.6
χ chi1 chi2	Smooth COM -177 65	10.3 10.7	χ chi1 chi2	Smooth COM 178 65	9.6 10.7
χ chi1 chi2 chi3	Smooth COM -177 65 59	10.3 10.7 9.5	χ chi1 chi2 chi3	Smooth COM 178 65 65	9.6 10.7 9.8
χ chi1 chi2 chi3 chi4	Smooth COM -177 65 59 84	10.3 10.7 9.5 9.1	chi1 chi2 chi3 chi4	Smooth COM 178 65 65 -167	9.6 10.7 9.8 19.7
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -177 65 59 84 Mean	10.3 10.7 9.5 9.1 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 178 65 65 -167 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 -177 65 59 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 178 65 65 -167 Mean 114.8	9.6 10.7 9.8 19.7 StdDev 1.30
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ \end{array}$	Smooth COM -177 65 59 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 178 65 65 -167 Mean 114.8 120.5 110.4 112.7	9.6 10.7 9.8 19.7 StdDev 1.30 0.84
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$C\alpha$_$C}\beta_\text{$C\gamma$} \\ \hline \\ \hline \text{$C\alpha$_$C}_2\text{$C\gamma$} \\ \hline \\ \hline \text{$C\beta$_$C}\alpha_\text{$C$} \\ \hline \\ \hline \\ \hline \text{$C\beta$_$C}\gamma_\text{$C\delta$} \\ \hline \\ \hline \\ \hline \text{$C\delta$_$N}\epsilon_\text{$C\zeta$} \\ \hline \end{array}$	Smooth COM -177 65 59 84 Mean 114.9 120.5 110.5	10.3 10.7 9.5 9.1 StdDev 1.37 0.75 1.23	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{Cα_C\beta$_$Cγ} \\ \text{Cα_C_CO} \\ \text{Cβ_C\alpha$_$C$} \\ \text{C$\beta$_$Cα_C\delta$} \\ \text{C$\delta$_$Nϵ_C\zeta$} \end{array}$	Smooth COM 178 65 65 -167 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 -177 65 59 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 178 65 65 -167 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$} \end{array}$	Smooth COM -177 65 59 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 178 65 65 -167 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} \\ \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 -177 65 59 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 178 65 65 -167 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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\beta_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$} \\ \hline \\ \text{$N\eta1_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM -177 65 59 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 178 65 65 -167 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_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_N\eta1$} \\ \text{$N\epsilon_C\zeta_N\eta2$} \\ \hline \end{array}$	Smooth COM -177 65 59 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 178 65 65 -167 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		ARC	6 tpt90 n = 652	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178	9.0	chi1	178	8.4
chi2	66	10.4	chi2	65	7.7
chi3	177	11.7	chi3	178	9.9
chi4	171	19.3	chi4	86	10.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	114.5	1.23	$C\alphaC\betaC\gamma$	114.7	1.27
$C\alphaCO$	120.5	0.74	$C\alphaCO$	120.5	0.80
$C\betaC\alphaC$	110.6	1.15	$C\beta_{-}C\alpha_{-}C$	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
$C\gamma_C\delta_N\epsilon$	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
$N\eta 1 C\zeta N\eta 2$	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
$N_{-}C\alpha_{-}C\beta$	110.2	1.19	$N_{-}C\alpha_{-}C\beta$	110.2	1.09
A D.C					
AKG	t tpt-90 n = 365		ARG	tpm170 n = 110	0
χ	$\frac{\text{tpt-90 n} = 365}{\text{Smooth COM}}$	StdDev	$\frac{\text{ARG}}{\chi}$	$\frac{\mathbf{tpm170} \text{ n} = 110}{\text{Smooth COM}}$	$\frac{0}{\text{StdDev}}$
	_	_		-	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
χ chi1	Smooth COM 179	StdDev 8.4	$\frac{\chi}{\text{chi1}}$	Smooth COM 178	StdDev
χ chi1 chi2	Smooth COM 179 67	StdDev 8.4 10.8	χ chi1 chi2	Smooth COM 178 70	StdDev 8.1 10.9
χ chi1 chi2 chi3	Smooth COM 179 67 -179	8.4 10.8 8.8	χ chi1 chi2 chi3	Smooth COM 178 70 -85	8.1 10.9 12.8
χ chi1 chi2 chi3 chi4	Smooth COM 179 67 -179 -89	8.4 10.8 8.8 12.2	χ chi1 chi2 chi3 chi4	Smooth COM 178 70 -85 171	8.1 10.9 12.8 18.6
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 179 67 -179 -89 Mean	8.4 10.8 8.8 12.2 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM 178 70 -85 171 Mean	8.1 10.9 12.8 18.6 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 179 67 -179 -89 Mean 114.7	8.4 10.8 8.8 12.2 StdDev 1.25	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM 178 70 -85 171 Mean 115.6	8.1 10.9 12.8 18.6 StdDev
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5	8.4 10.8 8.8 12.2 StdDev 1.25 0.72	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha$_$C}\beta$_$C}\gamma \\ \hline \text{$\text{C}\alpha$_$C}_2\text{CO} \end{array}$	Smooth COM 178 70 -85 171 Mean 115.6 120.6	8.1 10.9 12.8 18.6 StdDev 1.26 0.80
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5 110.6	8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \hline \end{array}$	Smooth COM 178 70 -85 171 Mean 115.6 120.6 110.6	8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5 110.6 112.4	8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\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 178 70 -85 171 Mean 115.6 120.6 110.6 112.8	8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5 110.6 112.4 124.9	8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM 178 70 -85 171 Mean 115.6 120.6 110.6 112.8 124.7	8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \end{array}$	Smooth COM 179 67 -179 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$C\alpha_C\beta_C\gamma$} \\ \hline \\ \hline \text{$C\alpha_C_C$} \\ \hline \\ \hline \text{$C\beta_C\alpha_C$} \\ \hline \\ \hline \\ \hline \text{$C\beta_C\gamma_C\delta$} \\ \hline \\ \hline \\ \hline \\ \hline \text{$C\delta_N\epsilon_C\zeta$} \\ \hline \\ $	Smooth COM 178 70 -85 171 Mean 115.6 120.6 110.6 112.8 124.7 112.0	8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25 2.15
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _C$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1 120.7	8.4 10.8 8.8 12.2 StdDev 1.25 0.72 1.20 1.62 1.15 2.52 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$} \\ \hline \\ \text{$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 178 70 -85 171 Mean 115.6 120.6 110.6 112.8 124.7 112.0 120.5	8.1 10.9 12.8 18.6 StdDev 1.26 0.80 1.33 2.17 2.25 2.15 1.05
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$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 179 67 -179 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1 120.7 119.7	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$C\alpha$_Cβ_C\gamma$} \\ \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$\delta_Nϵ} \\ \text{$N\epsilon$_Cζ_Nη1} \\ \text{$N\epsilon$_Cζ_Nη2} \\ \end{array}$	Smooth COM 178 70 -85 171 Mean 115.6 120.6 110.6 112.8 124.7 112.0 120.5 119.8	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
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta 1$ $N\epsilon_{-}C\zeta_{-}N\eta 2$ $N\eta 1_{-}C\zeta_{-}N\eta 2$	Smooth COM 179 67 -179 -89 Mean 114.7 120.5 110.6 112.4 124.9 111.1 120.7 119.7 119.6	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 0.73	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM 178 70 -85 171 Mean 115.6 120.6 110.6 112.8 124.7 112.0 120.5 119.8 119.7	8.1 10.9 12.8 18.6 StdDe 1.26 0.80 1.33 2.17 2.25 2.15 1.05 0.90 0.74

ARG	t tpm-80 n = 20	1	ARG	ttp80 n = 1896	;
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	5.2	chi1	-177	8.2
chi2	78	8.2	chi2	179	13.4
chi3	-80	10.4	chi3	62	9.9
chi4	-79	9.1	chi4	82	9.6
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.2	1.38	$C\alphaC\betaC\gamma$	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	$N\epsilon C\zeta N\eta 1$	120.7	0.95
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	120.1	0.92	$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	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
,		1110	11_0α_0ρ	110.1	
,	ttp-110 n = 625		,	ttp-170 n = 153	
,			,		
ARG	ttp-110 n = 623	3	ARG	ttp-170 n = 153	3
ARG	ttp-110 n = 623 Smooth COM	3 StdDev	$\frac{\lambda}{\chi}$	ttp-170 n = 153 Smooth COM	StdDev
$\frac{\chi}{\text{chi1}}$	ttp-110 n = 623 Smooth COM -174	3 StdDev 8.5	$\frac{\chi}{\text{chi1}}$	ttp-170 n = 153 Smooth COM -175	StdDev 9.3
ARG χ chi1 chi2	ttp-110 n = 623 Smooth COM -174 177	StdDev 8.5 13.0	ARG χ chi1 chi2	ttp-170 n = 153 Smooth COM -175 179	9.3 13.2
ARG $\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	ttp-110 n = 623 Smooth COM -174 177 64	StdDev 8.5 13.0 10.7	ARG	Smooth COM -175 179 66	9.3 13.2 9.0
ARG $\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array}$	ttp-110 n = 623 Smooth COM -174 177 64 -113	StdDev 8.5 13.0 10.7 9.9	ARG	Smooth COM -175 179 66 -171	StdDev 9.3 13.2 9.0 17.3
$\begin{array}{c} \text{ARG} \\ \hline \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \end{array}$	ttp-110 n = 623 Smooth COM -174 177 64 -113 Mean	StdDev 8.5 13.0 10.7 9.9 StdDev	ARG χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -175 179 66 -171 Mean	StdDev 9.3 13.2 9.0 17.3 StdDev
ARG $ \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} $	ttp-110 n = 623 Smooth COM -174 177 64 -113 Mean 113.8	StdDev 8.5 13.0 10.7 9.9 StdDev 1.63	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma$	Smooth COM -175 179 66 -171 Mean 113.7	StdDev 9.3 13.2 9.0 17.3 StdDev 1.65
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} $	ttp-110 n = 623 Smooth COM -174 177 64 -113 Mean 113.8 120.6	8.5 13.0 10.7 9.9 StdDev 1.63 0.80	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}-\text{O}}$	Smooth COM -175 179 66 -171 Mean 113.7 120.6	9.3 13.2 9.0 17.3 StdDev 1.65 0.76
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$	ttp-110 n = 623 Smooth COM -174 177 64 -113 Mean 113.8 120.6 110.2	8.5 13.0 10.7 9.9 StdDev 1.63 0.80 1.23	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}O}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\alpha_{-}C}$	Smooth COM -175 179 66 -171 Mean 113.7 120.6 110.0	9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_C$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$	ttp-110 n = 623 Smooth COM -174 177 64 -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	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 \end{array} $	Smooth COM -175 179 66 -171 Mean 113.7 120.6 110.0 111.6	StdDev 9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68
ARG χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha . C\beta . C\gamma$ $C\beta . C\alpha . C$ $C\beta . C\alpha . C$ $C\beta . C\gamma . C\delta$ $C\delta . N\epsilon . C\zeta$	ttp-110 n = 623 Smooth COM -174 177 64 -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	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} $	Smooth COM -175 179 66 -171 Mean 113.7 120.6 110.0 111.6 124.5	StdDev 9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17
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} $	ttp-110 n = 623 Smooth COM -174 177 64 -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	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 -175 179 66 -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
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} $	ttp-110 n = 623 Smooth COM -174 177 64 -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	ARG $\frac{\chi}{\chi}$ chi1 chi2 chi3 chi4 Bond Angle $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\gamma_{-}C\delta}{C\delta_{-}N\epsilon_{-}C\zeta}$ $\frac{C\gamma_{-}C\delta_{-}N\epsilon}{N\epsilon_{-}C\zeta_{-}N\eta_{1}}$	Smooth COM -175 179 66 -171 Mean 113.7 120.6 110.0 111.6 124.5 111.5 120.5	StdDev 9.3 13.2 9.0 17.3 StdDev 1.65 0.76 1.24 1.68 1.17 1.58 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{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} $	ttp-110 n = 623 Smooth COM -174 177 64 -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	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}\beta_{\text{-}}\text{C}\gamma \\ \text{C}\alpha_{\text{-}}\text{C}\beta_{\text{-}}\text{C}\zeta \\ \text{C}\beta_{\text{-}}\text{C}\alpha_{\text{-}}\text{C}\zeta \\ \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} $	ttp-170 n = 153 Smooth COM -175 179 66 -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 178 11.5 chi3 176 9.6 chi4 179 18.7 chi4 86 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ_Cγ 113.5 1.78 Cα_Cβ_Cγ_Cγ 113.9 1.70 Cα_Cβ_Cα_C 120.6 0.81 Cα_Cβ_Cα_C 120.6 0.79 Cβ_Cα_Cβ_Cγ_Cδ 110.2 1.17 Cβ_Cα_Cβ_Cγ_Cδ 110.2 1.25 Cβ_Cγ_Cβ_Cβ_Cβ 111.4 2.19 Cβ_Cβ_Cγ_Cδ 111.3 2.08 Cδ_Nε_Cζ 124.3 1.19 Cδ_Nε_Cζ 124.8 1.01 Cγ_Cδ_Nε 110.7 1.92 Cγ_Cδ_Nε_Cβ 111.6 2.62 Nε_Cζ_Nη1 120.4 0.90 Nε_Cζ_Nη1 120.7 1.02 Nε_Cζ_Nη2 119.6 0.92 Nε_Cζ_Nη2 <t< th=""><th>ARG</th><th>ttt180 n = 2339</th><th>9</th><th>ARG</th><th>ttt90 n = 1057</th><th></th></t<>	ARG	ttt180 n = 2339	9	ARG	ttt90 n = 1057	
chi2 176 11.2 chi2 176 10.8 chi3 178 11.5 chi3 176 9.6 chi4 179 18.7 chi3 176 9.6 chi4 179 18.7 chi3 176 9.6 chi4 179 18.7 chi3 176 9.6 chi4 186 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Co.CA.CD 110.6 0.81 Ca.CG.CD 110.6 0.79 Cβ.CA.CD 120.6 0.81 Ca.CA.CD 120.6 0.79 Cβ.CA.CD 110.2 1.17 Cβ.CA.CD 110.2 1.25 Cβ.Ne.CZ 124.3 1.19 Cβ.CA.CD 111.3 2.08 Ne.CZ <nη1< th=""> 120.4 0.90 Ne.CZ.Nη1 120.7 1.02 Ne.CC,Nη2 119.6 0.92 Ne.CA.Nη2 119.6 1.00 Nη1.CZ.Nη2 120.0</nη1<>	χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	chi1	-176	9.1	chi1	-176	9.3
chi4 179 18.7 chi4 86 10.8 Bond Angle Mean StdDev Bond Angle Mean StdDev Cα_Cβ_Cγ 113.5 1.78 $Cα_Cβ_C$ Cγ 113.9 1.70 Cα_C,C 120.6 0.81 $Cα_C$ CO 120.6 0.79 Cβ_Cα_C 110.2 1.17 $Cβ_Cα_C$ C 110.2 1.25 Cβ_Cγ_Cδ 111.4 2.19 $Cβ_Cα_C$ C 110.2 1.25 Cβ_Nε_Cζ 124.3 1.19 $Cβ_Cα_C$ C 111.3 2.08 Cδ_Nε_Cζ 124.8 1.01 1.02 1.25 1.02 1.25 Nε_Cζ_Nη1 120.4 0.90 Nε_Cζ_Nη1 120.7 1.02 1	chi2	176	11.2	chi2	176	10.8
Bond Angle Mean StdDev Bond Angle Mean StdDev $C\alpha_{-}C\beta_{-}C\gamma$ 113.5 1.78 $C\alpha_{-}C\beta_{-}C\gamma$ 113.9 1.70 $C\alpha_{-}C_{-}C$ 120.6 0.81 $C\alpha_{-}C_{-}O$ 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 $C\gamma_{-}C\delta_{-}N\epsilon_{-}C\zeta$ 124.3 1.19 $C\delta_{-}N\epsilon_{-}C\zeta$ 124.8 1.01 $N_{-}C\zeta_{-}N\eta^{2}$ 119.6 0.90 $N\epsilon_{-}C\zeta_{-}N\eta^{2}$ 119.6 1.00 $N_{-}C\zeta_{-}N\eta^{2}$ 119.6 <td< td=""><td>chi3</td><td>178</td><td>11.5</td><td>chi3</td><td>176</td><td>9.6</td></td<>	chi3	178	11.5	chi3	176	9.6
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	chi4	179	18.7	chi4	86	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
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\alphaCO$	120.6	0.81	$C\alphaCO$	120.6	0.79
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\betaC\alphaC$	110.2	1.17	$C\betaC\alphaC$	110.2	1.25
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C\beta C\gamma C\delta$	111.4	2.19	$C\betaC\gammaC\delta$	111.3	2.08
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C\delta_N\epsilon_C\zeta$	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	$C\gamma_C\delta_N\epsilon$	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 StdDev chi1 -176 9.4 chi1 -175 9.0 chi2 177 11.5 chi2 178 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -89 12.5 chi4 112 9.8 Bond Angle Mean StdDev Bond Angle Mean StdDe $Cα.Cβ.Cγ$ 114.0 1.62 $Cα.Cβ.Cγ$ 113.9 1.64 $Cα.Cβ.Cγ$ 110.3 1.26 $Cβ.Cβ.Cγ$ 110.3 1.23 $Cβ.Cα.C$ 110.3 1.26 $Cβ.Cα.C$ 110.3 1.23 $Cβ.Cγ.Cδ$ 110.9 2.08 $Cβ.Cα.C$ 112.2 1.69 $Cδ.Nε.Cζ$ 124.8 </td <td></td> <td>120.0</td> <td>0.81</td> <td></td> <td>119.6</td> <td>0.74</td>		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 StdDev chi1 -176 9.4 chi1 -175 9.0 chi2 177 11.5 chi2 178 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -89 12.5 chi4 112 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_C 110.3 1.23 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 <						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 -176 9.4 chi1 -175 9.0 chi2 177 11.5 chi2 178 9.5 chi3 -178 9.9 chi3 -64 10.7 chi4 -89 12.5 chi4 112 9.8 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 $C\alpha_{-}C\beta_{-}C\gamma$ 114.0 1.62 $C\alpha_{-}C\beta_{-}C\gamma$ 113.9 1.64 $C\alpha_{-}C\beta_{-}C\gamma$ 114.0 1.62 $C\alpha_{-}C\beta_{-}C\gamma$ 113.9 1.64 $C\alpha_{-}C\beta_{-}C\gamma$ 110.3 1.26 $C\beta_{-}C\alpha_{-}C$ 110.3 1.23 $C\beta_{-}C\alpha_{-}C$ 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 $C\gamma_{-}C\delta_{-}N\epsilon_{-}C$ <td>ADC</td> <td>111 00 1990</td> <td></td> <td></td> <td></td> <td></td>	ADC	111 00 1990				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ANG	ttt-90 n = 1380)	ARG	ttm110 n = 725	Ď
$\begin{array}{cccccccccccccccccccccccccccccccccccc$						StdDev
chi4 -89 12.5 chi4 112 9.8 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 $C\gamma_C\delta_N\epsilon$ 111.8 2.58 $C\gamma_C\delta_N\epsilon$ 111.6 1.93 $N\epsilon_C\zeta_N\eta1$ 120.8 1.08 $N\epsilon_C\zeta_N\eta1$ 121.0 1.24 $N\epsilon_C\zeta_N\eta2$ 119.6 1.01 $N\epsilon_C\zeta_N\eta2$ 119.5 1.12 $N\eta1_C\zeta_N\eta2$ 119.6 0.87 $N\eta1_C\zeta_N\eta2$ 119.4 0.82 $N_C\alpha_C$ 110.4 2.30 $N_C\alpha_C$ 110.5 2.14	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 $C\gamma_C\delta_N\epsilon$ 111.8 2.58 $C\gamma_C\delta_N\epsilon$ 111.6 1.93 $N\epsilon_C\zeta_N\eta$ 120.8 1.08 $N\epsilon_C\zeta_N\eta$ 111.6 1.93 $N\epsilon_C\zeta_N\eta$ 120.8 1.01 $N\epsilon_C\zeta_N\eta$ 119.5 1.12 $N\eta$ N_0	χ chi1	Smooth COM -176	StdDev 9.4	χ chi1	Smooth COM -175	StdDev 9.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	χ chi1 chi2	Smooth COM -176 177	9.4 11.5	χ chi1 chi2	Smooth COM -175 178	9.0 9.5
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3	Smooth COM -176 177 -178	9.4 11.5 9.9	χ chi1 chi2 chi3	Smooth COM -175 178 -64	9.0 9.5 10.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4	Smooth COM -176 177 -178 -89	9.4 11.5 9.9 12.5	chi1 chi2 chi3 chi4	Smooth COM -175 178 -64 112	9.0 9.5 10.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -176 177 -178 -89 Mean	9.4 11.5 9.9 12.5 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -175 178 -64 112 Mean	9.0 9.5 10.7 9.8 StdDev
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -176 177 -178 -89 Mean 114.0	9.4 11.5 9.9 12.5 StdDev 1.62	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -175 178 -64 112 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 -176 177 -178 -89 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 $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$	Smooth COM -175 178 -64 112 Mean 113.9 120.6	9.0 9.5 10.7 9.8 StdDev 1.64 0.78
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$	Smooth COM -176 177 -178 -89 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 -175 178 -64 112 Mean 113.9 120.6 110.3	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \begin{array}{c} \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -176 177 -178 -89 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -175 178 -64 112 Mean 113.9 120.6 110.3 112.2	9.0 9.5 10.7 9.8 StdDev 1.64 0.78 1.23 1.69
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C_O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$	Smooth COM -176 177 -178 -89 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$\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$} \\ \end{array}$	Smooth COM -175 178 -64 112 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 1.23
$Nη1_Cζ_Nη2$ 119.6 0.87 $Nη1_Cζ_Nη2$ 119.4 0.82 $N_Cα_C$ 110.4 2.30 $N_Cα_C$ 110.5 2.14	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \end{array}$	Smooth COM -176 177 -178 -89 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\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$} \\ \end{array}$	Smooth COM -175 178 -64 112 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 1.93
$N_{-}C\alpha_{-}C$ 110.4 2.30 $N_{-}C\alpha_{-}C$ 110.5 2.14	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$ $C\gamma_C\delta_N\epsilon$ $N\epsilon_C\zeta_N\eta1$	Smooth COM -176 177 -178 -89 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\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 -175 178 -64 112 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 1.24
	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -176 177 -178 -89 Mean 114.0 120.5 110.3 110.9 124.8 111.8 120.8 119.6	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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\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$} \\ \text{$\text{N}\epsilon_\text{C}\zeta_\text{N}\eta2$} \\ \end{array}$	Smooth COM -175 178 -64 112 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 1.12
	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline \\ C\alpha_C\beta_C\gamma \\ \\ C\alpha_C_O \\ \hline \\ C\beta_C\alpha_C \\ \\ C\beta_C\gamma_C\delta \\ \\ \hline \\ C\delta_N\epsilon_C\zeta \\ \\ \hline \\ C\gamma_C\delta_N\epsilon \\ \\ N\epsilon_C\zeta_N\eta1 \\ \\ N\epsilon_C\zeta_N\eta2 \\ \\ \hline \\ N\eta1_C\zeta_N\eta2 \\ \\ \end{array}$	Smooth COM -176 177 -178 -89 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \text{N}\eta1_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -175 178 -64 112 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 0.82

ARG	ttm170 n = 131	7	ARG	ttm-80 n = 150	4
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	9.9	chi1	-174	9.4
chi2	176	12.4	chi2	179	9.9
chi3	-67	9.9	chi3	-64	10.6
chi4	171	17.6	chi4	-84	9.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.8	1.74	$C\alphaC\betaC\gamma$	113.7	1.66
$C\alphaCO$	120.6	0.81	$C\alphaCO$	120.5	0.79
$C\beta_{-}C\alpha_{-}C$	110.1	1.16	$C\betaC\alphaC$	110.2	1.24
$C\betaC\gammaC\delta$	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
$N\epsilon_{-}C\zeta_{-}N\eta 1$	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	$N\epsilon C\zeta \eta 2$	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	$N_{-}C\alpha_{-}C$	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	tmt170 n = 104 Smooth COM	4 StdDev	ARC	G tmt90 n = 23 Smooth COM	StdDev
			-		StdDev 9.2
χ	Smooth COM	StdDev	χ	Smooth COM	
$\frac{\chi}{\text{chi1}}$	Smooth COM -173	StdDev 12.3	$\frac{\chi}{\text{chi1}}$	Smooth COM -178	9.2
χ chi1 chi2	Smooth COM -173 -91	StdDev 12.3 12.7	χ chi1 chi2	Smooth COM -178 -93	9.2 9.1
χ chi1 chi2 chi3	Smooth COM -173 -91 -173	StdDev 12.3 12.7 9.4	χ chi1 chi2 chi3	Smooth COM -178 -93 -177	9.2 9.1 11.2
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \text{Bond Angle} \\ \hline C\alpha_C\beta_C\gamma \end{array}$	Smooth COM -173 -91 -173 -170	StdDev 12.3 12.7 9.4 17.5	chi1 chi2 chi3 chi4	Smooth COM -178 -93 -177 87	9.2 9.1 11.2 12.0
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -173 -91 -173 -170 Mean	StdDev 12.3 12.7 9.4 17.5 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -178 -93 -177 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 -173 -91 -173 -170 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 -93 -177 87 Mean 115.2	9.2 9.1 11.2 12.0 StdDev 1.49
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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 -173 -91 -173 -170 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -178 -93 -177 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\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 -173 -91 -173 -170 Mean 115.0 120.6 110.9	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -178 -93 -177 87 Mean 115.2 120.6 110.5	9.2 9.1 11.2 12.0 StdDev 1.49 0.98 1.33
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline C\alpha_C\beta_C\gamma \\ \hline C\alpha_C_O \\ \hline C\beta_C\alpha_C \\ \hline C\beta_C\gamma_C\delta \\ \hline C\beta_C\gamma_C\delta \\ \hline C\delta_N\epsilon_C\zeta \\ \hline C\gamma_C\delta_N\epsilon \\ \hline \end{array}$	Smooth COM -173 -91 -173 -170 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \text{$\text{C}\alpha_\text{C}_\text{C}$} \\ \hline \text{$\text{C}\alpha_\text{C}_{-}\text{C}$} \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \text{$\text{C}\beta_\text{N}\epsilon_\text{C}\zeta$} \\ \hline \text{$\text{C}\gamma_\text{C}\delta_\text{N}\epsilon$} \\ \hline \end{array}$	Smooth COM -178 -93 -177 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$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 -173 -91 -173 -170 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \hline \end{array}$	Smooth COM -178 -93 -177 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 -173 -91 -173 -170 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\text{C}0$} \\ \hline \\ \hline \text{$\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 -178 -93 -177 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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ N\eta1_C\zeta_N\eta2 \\ \hline \end{array}$	Smooth COM -173 -91 -173 -170 Mean 115.0 120.6 110.9 112.7 124.5 110.7 120.7 119.6 119.7	StdDev 12.3 12.7 9.4 17.5 StdDev 1.33 0.74 1.07 1.72 0.90 1.62 1.03 0.80 0.72	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -178 -93 -177 87 Mean 115.2 120.6 110.5 112.9 125.1 111.4 120.9 119.6 119.4	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 0.74
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta \\ C\gamma_C\delta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -173 -91 -173 -170 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}\text{C}0$} \\ \hline \\ \hline \text{$\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 -178 -93 -177 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	-92	11.4	chi2	-90	11.1
chi3	-177	10.0	chi3	-61	11.3
chi4	-84	11.5	chi4	163	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
,		1.00	11200208	11011	1.10
	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 -76 81	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 -76 81 57	StdDev 11.8 12.0 7.4
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \end{array}$	tmm-80 n = 71 Smooth COM -174 -86 -56 -82	StdDev 9.2 8.8 10.7 8.5	ARC χ chi1 chi2 chi3 chi4	Smooth COM -76 81 57 84	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 -76 81 57 84 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	ARC χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	Smooth COM -76 81 57 84 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	StdDev 9.2 8.8 10.7 8.5 StdDev 1.32 0.78	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 -76 81 57 84 Mean 115.5 120.4	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 -76 81 57 84 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 -76 81 57 84 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 -76 81 57 84 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 $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle $\frac{C\alpha - C\beta - C\gamma}{C\alpha - C - C}$ $\frac{C\beta - C\alpha - C}{C\beta - C\gamma - C\delta}$ $\frac{C\beta - C\gamma - C\delta}{C\delta - N\epsilon - C\zeta}$ $\frac{C\gamma - C\delta - N\epsilon}{C\gamma - C\delta - N\epsilon}$	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 -76 81 57 84 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 -76 81 57 84 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 $ \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{N}\epsilon_{-}\text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta 1 \\ \text{N}\epsilon_{-}\text{C}\zeta_{-}\text{N}\eta 2 \end{array} $	tmm-80 n = 71 Smooth COM -174 -86 -56 -82 Mean 115.3 120.6 111.1 113.7 124.9 112.6 120.9 119.7	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 $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C\gamma$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	Smooth COM -76 81 57 84 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

	4 5 0 0		15.0	1400 **	
ARG	mpp-170 $n = 6$		ARG	mpt180 n = 24	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-78	12.9	chi1	-84	8.0
chi2	81	17.4	chi2	69	13.1
chi3	65	7.4	chi3	173	9.4
chi4	-166	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
$C\betaC\gammaC\delta$	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
$N\epsilon C\zeta \eta 1$	120.6	1.06	$N\epsilon C\zeta \eta 1$	120.4	1.02
$N\epsilon C\zeta N\eta 2$	119.7	0.76	$N\epsilonC\zetaN\eta_2$	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_0α_0ρ	111.1	1.10
	$G \mathbf{mpt90} \ \mathrm{n} = 46$			$\frac{111.1}{\text{mpt-90 n} = 85}$	
		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	$\begin{array}{c} ARG \\ \chi \\ chi1 \end{array}$	mpt-90 n = 85 Smooth COM -78	StdDev 13.9
$\begin{array}{c} \lambda \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	G mpt90 n = 46 Smooth COM -76 84	StdDev 12.9 13.6	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \end{array}$	mpt-90 n = 85 Smooth COM -78 74	StdDev 13.9 16.3
X chi1 chi2 chi3	Smooth COM -76 84 170	StdDev 12.9 13.6 9.7	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \end{array}$	Smooth COM -78 74 177	StdDev 13.9 16.3 9.6
ARC x chi1 chi2 chi3 chi4	F mpt90 n = 46 Smooth COM -76 84 170 93	StdDev 12.9 13.6 9.7 11.2	$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \end{array}$	mpt-90 n = 85 Smooth COM -78 74 177 -87	StdDev 13.9 16.3 9.6 13.7
$\begin{array}{c} \chi \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	Smooth COM -76 84 170 93 Mean	StdDev 12.9 13.6 9.7 11.2 StdDev	$\begin{array}{c} X \\ \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \end{array}$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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 84 170 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 -78 74 177 -87 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 84 170 93 Mean 114.6 120.4	StdDev 12.9 13.6 9.7 11.2 StdDev 1.63 0.64	ARG $\frac{\chi}{\text{chi1}}$ chi2 chi3 chi4 Bond Angle} $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{O}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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 $C\alphaC\betaC\gamma$ $C\alphaCO$ $C\betaC\alphaC$	F mpt90 n = 46 Smooth COM -76 84 170 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 -78 74 177 -87 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 $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$	Smooth COM -76 84 170 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 $\frac{\chi}{\text{chi1}}$ 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 mpt-90 n = 85 Smooth COM -78 74 177 -87 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 84 170 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} $\frac{C\alpha \cdot C\beta \cdot C\gamma}{C\alpha \cdot C \cdot C}$ $\frac{C\beta \cdot C\alpha \cdot C}{C\beta \cdot C\gamma \cdot C\delta}$ $\frac{C\beta \cdot N\epsilon \cdot C\zeta}{C\delta \cdot N\epsilon \cdot C\zeta}$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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 $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$ $C\delta _ N\epsilon _ C\zeta$ $C\gamma _ C\delta _ N\epsilon$	F mpt90 n = 46 Smooth COM -76 84 170 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 $\frac{\text{C}\alpha_{-}\text{C}\beta_{-}\text{C}\gamma}{\text{C}\alpha_{-}\text{C}_{-}\text{C}}$ $\frac{\text{C}\beta_{-}\text{C}\alpha_{-}\text{C}}{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}$ $\frac{\text{C}\beta_{-}\text{C}\gamma_{-}\text{C}\delta}{\text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta}$ $\frac{\text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon_{-}\text{C}\zeta}{\text{C}\gamma_{-}\text{C}\delta_{-}\text{N}\epsilon}$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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 84 170 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 $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C\alpha_{-}C}$ $\frac{C\beta_{-}C\alpha_{-}C}{C\beta_{-}C\gamma_{-}C\delta}$ $\frac{C\delta_{-}N\epsilon_{-}C\zeta}{C\gamma_{-}C\delta_{-}N\epsilon}$ $\frac{N\epsilon_{-}C\zeta_{-}N\eta_{1}}{N\epsilon_{-}C\zeta_{-}N\eta_{1}}$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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 $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\gamma_{-}C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon_{-}N\epsilon_{-}C\zeta$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	F mpt90 n = 46 Smooth COM -76 84 170 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 $\frac{C\alpha_{-}C\beta_{-}C\gamma}{C\alpha_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C_{-}C$	mpt-90 n = 85 Smooth COM -78 74 177 -87 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	mtp180 n = 250)4	ARG	mtp85 n = 185	7
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66	8.1	chi1	-66	8.6
chi2	178	13.0	chi2	177	11.2
chi3	66	9.1	chi3	64	9.7
chi4	-171	16.5	chi4	87	11.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	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
$C\betaC\gammaC\delta$	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	$N\epsilon_{-}C\zeta_{-}N\eta 1$	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
ARC	mater 110 m 47	·0	ABG	11100 150	0
1110	mtp-110 n = 47	0	ARG	mtt180 n = 459	2
χ	Smooth COM	StdDev	$\frac{\text{ARG}}{\chi}$	$\frac{\text{mtt180 n} = 459}{\text{Smooth COM}}$	2 StdDev
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
χ chi1	Smooth COM -65	StdDev 8.1	$\frac{\chi}{\text{chi1}}$	Smooth COM -67	StdDev 7.8
χ chi1 chi2	Smooth COM -65 179	StdDev 8.1 10.8	χ chi1 chi2	Smooth COM -67 179	StdDev 7.8 11.0
χ chi1 chi2 chi3	Smooth COM -65 179 66	StdDev 8.1 10.8 11.6	χ chi1 chi2 chi3	Smooth COM -67 179 -179	7.8 11.0 10.7
χ chi1 chi2 chi3 chi4	Smooth COM -65 179 66 -109	8.1 10.8 11.6 9.6	chi1 chi2 chi3 chi4	Smooth COM -67 179 -179 177	7.8 11.0 10.7 17.9
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -65 179 66 -109 Mean	8.1 10.8 11.6 9.6 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -67 179 -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 -109 Mean 113.4	8.1 10.8 11.6 9.6 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$	Smooth COM -67 179 -179 177 Mean 112.9	7.8 11.0 10.7 17.9 StdDev 1.75
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 -65 179 66 -109 Mean 113.4 120.4	8.1 10.8 11.6 9.6 StdDev 1.66 0.95	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -67 179 -179 177 Mean 112.9 120.4	7.8 11.0 10.7 17.9 StdDev 1.75 0.85
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C\alpha C$ $C\beta C\alpha C$	Smooth COM -65 179 66 -109 Mean 113.4 120.4 110.1	8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68	χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$	Smooth COM -67 179 -179 177 Mean 112.9 120.4 110.0	7.8 11.0 10.7 17.9 StdDev 1.75 0.85 1.66
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 -65 179 66 -109 Mean 113.4 120.4 110.1 112.4	8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}_\text{O} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \end{array}$	Smooth COM -67 179 -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
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C_O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$	Smooth COM -65 179 66 -109 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{C} \\ \text{C}\beta_\text{C}\alpha_\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \end{array}$	Smooth COM -67 179 -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
χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C_O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$	Smooth COM -65 179 66 -109 Mean 113.4 120.4 110.1 112.4 125.3 111.7	8.1 10.8 11.6 9.6 StdDev 1.66 0.95 1.68 1.63 2.05 1.88	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \text{$\text{Ca_C}\beta\text{C}\gamma$} \\ \text{$\text{Ca_C}-\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$} \\ \end{array}$	Smooth COM -67 179 -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
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 -65 179 66 -109 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{$\text{C}\alpha_\text{C}\beta_\text{C}\gamma$} \\ \text{$\text{C}\alpha_\text{C}_\text{O}$} \\ \text{$\text{C}\beta_\text{C}\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 -67 179 -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
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \text{Bond Angle} \\ \\ \text{$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 -65 179 66 -109 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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 179 -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
$χ$ chi1 chi2 chi3 chi4 Bond Angle $Cα_{-}Cβ_{-}Cγ$ $Cα_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cβ_{-}Cα_{-}C$ $Cγ_{-}Cδ_{-}Nε_{-}Cζ$ $Cγ_{-}Cδ_{-}Nε_{-}Cζ$ $Nε_{-}Cζ_{-}Nη1$ $Nε_{-}Cζ_{-}Nη2$ $Nη1_{-}Cζ_{-}Nη2$	Smooth COM -65 179 66 -109 Mean 113.4 120.4 110.1 112.4 125.3 111.7 121.1 119.4 119.5	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 0.90	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Smooth COM -67 179 -179 177 Mean 112.9 120.4 110.0 111.5 124.4 110.6 120.4 119.6 119.9	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 0.79

1.5-~	1100 2:2		4.D.~	05	0
ARG	mtt90 n = 2460		ARG	mtt-85 n = 284	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67	7.5	chi1	-67	7.8
chi2	179	13.5	chi2	-178	10.6
chi3	178	10.6	chi3	-176	9.2
chi4	90	15.1	chi4	-88	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	$N\epsilon C\zeta N\eta 1$	120.8	1.02
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	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	$NC\alphaC$	111.4	2.30
$N_{-}C\alpha_{-}C\beta$	110.6	1.12	$N_{-}C\alpha_{-}C\beta$	110.6	1.04
ARG	mtm110 n = 78	1	ARG 1	mtm180 n = 240)7
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68	8.2	chi1	-66	8.1
chi2					
	-177	9.7	chi2	179	12.7
chi3	-177 -68	$9.7 \\ 10.2$	chi2 chi3	179 -67	
chi3 chi4					12.7
	-68	10.2	chi3	-67	12.7 8.8
chi4	-68 112	10.2 10.6	chi3 chi4	-67 172	12.7 8.8 15.2
chi4 Bond Angle	-68 112 Mean	10.2 10.6 StdDev	chi3 chi4 Bond Angle	-67 172 Mean	12.7 8.8 15.2 StdDev
$\begin{array}{c} \text{chi4} \\ \hline \text{Bond Angle} \\ \hline \hline \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \end{array}$	-68 112 Mean 113.1	10.2 10.6 StdDev	$\begin{array}{c} \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \end{array}$	-67 172 Mean 113.3	12.7 8.8 15.2 StdDev 1.63
chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$	-68 112 Mean 113.1 120.4	10.2 10.6 StdDev 1.81 0.90	chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$	-67 172 Mean 113.3 120.5	12.7 8.8 15.2 StdDev 1.63 0.89
chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$	-68 112 Mean 113.1 120.4 110.1	10.2 10.6 StdDev 1.81 0.90 1.76	$\begin{array}{c} \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \\ \text{C}\alpha_\text{C}_\text{O} \\ \\ \text{C}\beta_\text{C}\alpha_\text{C} \end{array}$	-67 172 Mean 113.3 120.5 109.9	12.7 8.8 15.2 StdDev 1.63 0.89 1.62
chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$	-68 112 Mean 113.1 120.4 110.1 112.4	10.2 10.6 StdDev 1.81 0.90 1.76 1.72	chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$	-67 172 Mean 113.3 120.5 109.9 111.6	12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68
chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\alpha C$ $C\beta C\alpha C$	-68 112 Mean 113.1 120.4 110.1 112.4 125.3	10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52	chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	-67 172 Mean 113.3 120.5 109.9 111.6 124.4	12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08
chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C\gamma$ $C\alpha C\gamma$ $C\beta C\alpha C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$	-68 112 Mean 113.1 120.4 110.1 112.4 125.3 112.1	10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88	chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$ $C\gamma_C\delta_N\epsilon$	-67 172 Mean 113.3 120.5 109.9 111.6 124.4 111.4	12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08 1.69
chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$	-68 112 Mean 113.1 120.4 110.1 112.4 125.3 112.1 121.1	10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88 1.28	chi3 chi4 Bond Angle $C\alpha _C\beta _C\gamma$ $C\alpha _C _O$ $C\beta _C\alpha _C$ $C\beta _C\gamma _C\delta$ $C\delta _N\epsilon _C\zeta$ $C\gamma _C\delta _N\epsilon$ $N\epsilon _C\zeta _N\eta 1$	-67 172 Mean 113.3 120.5 109.9 111.6 124.4 111.4 120.4	12.7 8.8 15.2 StdDev 1.63 0.89 1.62 1.68 1.08 1.69 0.90
chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\alpha C$ $C\gamma C\delta C\alpha C$ $C\gamma C\delta C\alpha C$ $C\gamma C\delta C\alpha C$ $C\gamma C\delta C\alpha C$	-68 112 Mean 113.1 120.4 110.1 112.4 125.3 112.1 121.1 119.4	10.2 10.6 StdDev 1.81 0.90 1.76 1.72 1.52 1.88 1.28 1.12	chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}O$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$ $C\gamma_{-}C\delta_{-}N\epsilon$ $N\epsilon_{-}C\zeta_{-}N\eta_{1}$ $N\epsilon_{-}C\zeta_{-}N\eta_{2}$	-67 172 Mean 113.3 120.5 109.9 111.6 124.4 111.4 120.4 119.8	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	mtm-85 n = 284	18	ARG	mmp80 n = 164	4
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68	8.1	chi1	-62	6.7
chi2	-171	9.3	chi2	-75	12.7
chi3	-63	9.5	chi3	74	11.7
chi4	-88	8.9	chi4	77	6.9
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.5	1.56	$C\alphaC\betaC\gamma$	114.8	1.39
$C\alphaCO$	120.5	0.81	$C\alphaCO$	120.4	0.95
$C\betaC\alphaC$	110.0	1.49	$C\betaC\alphaC$	109.8	1.49
$C\betaC\gammaC\delta$	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
$N\epsilon C\zeta \eta 1$	120.8	1.03	$N\epsilon C\zeta \eta 1$	120.6	0.99
$N\epsilon C\zeta \eta 2$	119.7	1.00	$N\epsilon C\zeta \eta 2$	120.0	0.86
$N\eta_1 C\zeta N\eta_2$	119.5	0.78	$N\eta 1_C\zeta_N\eta 2$	119.5	0.64
$N_{-}C\alpha_{-}C$	111.3	1.97	$NC\alphaC$	111.4	1.82
$N_C\alpha_C\beta$	111.1	1.03	$N_C\alpha_C\beta$	110.9	0.93
			11200209	110.0	
	nmp-170 n = 12			mmt180 n = 120	
ARG r	nmp-170 n = 12	23	ARG 1	mmt180 n = 120)3
ARG r	mmp-170 n = 12 Smooth COM	23 StdDev	ARG 1	mmt180 n = 120 Smooth COM	O3 StdDev
ARG r χ chi1	mmp-170 n = 12 Smooth COM -64	23 StdDev 7.2	χ chi1	mmt180 n = 120 Smooth COM -61	StdDev 9.1
ARG r χ chi1 chi2	mmp-170 n = 12 Smooth COM -64 -65	23 StdDev 7.2 14.3	ARG 1 χ chi1 chi2	mmt180 n = 120 Smooth COM -61 -68	9.1 12.9
ARG r chi1 chi2 chi3	mmp-170 n = 12 Smooth COM -64 -65 85	23 StdDev 7.2 14.3 9.7	ARG 1 χ chi1 chi2 chi3	mmt180 n = 120 Smooth COM -61 -68 -176	9.1 12.9 11.3
ARG r x chi1 chi2 chi3 chi4	mmp-170 n = 19 Smooth COM -64 -65 85 -167	23 StdDev 7.2 14.3 9.7 19.8	ARG 1 χ chi1 chi2 chi3 chi4	mmt180 n = 120 Smooth COM -61 -68 -176 -176	9.1 12.9 11.3 17.4
ARG r $ \begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \end{array} $ Bond Angle	mmp-170 n = 12 Smooth COM -64 -65 85 -167 Mean	23 StdDev 7.2 14.3 9.7 19.8 StdDev	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean	StdDev 9.1 12.9 11.3 17.4 StdDev
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5	9.1 12.9 11.3 17.4 StdDev 1.38
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alphaC\betaC\gamma$ $C\alphaCO$	mmp-170 n = 19 Smooth COM -64 -65 85 -167 Mean 115.5 120.4	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4	9.1 12.9 11.3 17.4 StdDev 1.38 0.87
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\alpha_C$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5 112.8	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C_ O$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4 112.0	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_C\beta_C\gamma$ $C\alpha_C_O$ $C\beta_C\alpha_C$ $C\beta_C\gamma_C\delta$ $C\beta_C\gamma_C\delta$ $C\delta_N\epsilon_C\zeta$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5 112.8 124.8	StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha_{-}C\beta_{-}C\gamma$ $C\alpha_{-}C_{-}C$ $C\beta_{-}C\alpha_{-}C$ $C\beta_{-}C\gamma_{-}C\delta$ $C\delta_{-}N\epsilon_{-}C\zeta$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4 112.0 124.4	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha _ C\beta _ C\gamma$ $C\alpha _ C _ C$ $C\beta _ C\alpha _ C$ $C\beta _ C\gamma _ C\delta$ $C\delta _ N\epsilon _ C\zeta$ $C\gamma _ C\delta _ N\epsilon$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$ $C\beta C\alpha C$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83
ARG r 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 $	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5 120.5	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61 1.21	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha . C\beta . C\gamma$ $C\alpha . C . C$ $C\beta . C\alpha . C$ $C\beta . C\alpha . C$ $C\beta . N\epsilon . C\zeta$ $C\gamma . C\delta . N\epsilon$ $N\epsilon . C\zeta . N\eta 1$	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0 120.5	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83 0.87
ARG r χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\gamma$ $C\alpha C C$ $C\beta C\gamma C\delta$ $C\delta N\epsilon C\zeta$ $C\gamma C\delta N\epsilon$ $N\epsilon C\zeta N\eta 1$ $N\epsilon C\zeta N\eta 2$	mmp-170 n = 19 Smooth COM -64 -65 -85 -167 Mean 115.5 120.4 109.5 112.8 124.8 111.5 120.5 119.8	23 StdDev 7.2 14.3 9.7 19.8 StdDev 1.27 0.99 1.52 1.74 1.32 1.61 1.21 1.10	ARG 1 χ chi1 chi2 chi3 chi4 Bond Angle $C\alpha C\beta C\gamma$ $C\alpha C C$ $C\beta C\gamma C\delta C$ $C\beta C\gamma C\delta $	mmt180 n = 120 Smooth COM -61 -68 -176 -176 Mean 114.5 120.4 109.4 112.0 124.4 111.0 120.5 119.7	9.1 12.9 11.3 17.4 StdDev 1.38 0.87 1.62 1.71 1.19 1.83 0.87 0.87

ARG mmt90 n = 567			ARG mmt-90 n = 1428			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	-60	8.8	chi1	-63	6.6	
chi2	-68	12.5	chi2	-68	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	
$C\alpha_{-}C\beta_{-}C\gamma$	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	$N\epsilonC\zetaN\eta 1$	120.9	1.00	
$N\epsilon_{-}C\zeta_{-}N\eta_{2}$	119.6	1.09	$N\epsilonC\zetaN\eta 2$	119.6	0.88	
$N\eta 1_C\zeta_N\eta 2$	119.6	0.72	$N\eta 1C\zetaN\eta 2$	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 -61	StdDev 9.2	χ chi1	Smooth COM -63	StdDev 9.2	
χ chi1 chi2	Smooth COM -61 -66	9.2 13.7	χ chi1 chi2	Smooth COM -63 -67	StdDev 9.2 10.9	
χ chi1 chi2 chi3	Smooth COM -61 -66 -64	9.2 13.7 9.9	χ chi1 chi2 chi3	Smooth COM -63 -67 -60	9.2 10.9 9.2	
χ chi1 chi2 chi3 chi4	-61 -66 -64 163	9.2 13.7 9.9 24.2	χ chi1 chi2 chi3 chi4	-63 -67 -60 -86	9.2 10.9 9.2 10.1	
χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -61 -66 -64 163 Mean	9.2 13.7 9.9 24.2 StdDev	χ chi1 chi2 chi3 chi4 Bond Angle	Smooth COM -63 -67 -60 -86 Mean	9.2 10.9 9.2 10.1 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 -61 -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 -67 -60 -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 \\ \hline \text{$\text{C}\alpha$_$C}.\text{CO} \end{array}$	Smooth COM -61 -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 -67 -60 -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$_$C}\beta$_$C}\gamma \\ \hline \\ \text{$\text{C}\alpha$_C_$C} \\ \hline \\ \text{$\text{C}\alpha$_$C$_$C} \\ \hline \\ \text{$\text{C}\beta$_$C}\alpha$_$C} \\ \end{array}$	Smooth COM -61 -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 -67 -60 -86 Mean 114.6 120.5 109.7	9.2 10.9 9.2 10.1 StdDev 1.52 0.88 1.54	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \\ \hline C\alpha_C\beta_C\gamma \\ \hline C\alpha_C_O \\ \hline C\beta_C\alpha_C \\ \hline C\beta_C\gamma_C\delta \\ \hline C\beta_C\gamma_C\delta \\ \hline C\delta_N\epsilon_C\zeta \\ \hline C\gamma_C\delta_N\epsilon \\ \hline \end{array}$	Smooth COM -61 -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 -67 -60 -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	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \text{Bond Angle} \\ \hline \hline C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ \end{array}$	Smooth COM -61 -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 -67 -60 -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	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta \\ C\gamma_C\delta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -61 -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}_{\beta}$-$\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}_{\beta}$-$\text{C}\gamma$-$\text{C}\delta$} \\ \hline \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \\ \hline \\ \hline \text{$\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 -67 -60 -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	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ N\eta1_C\zeta_N\eta2 \\ \hline \end{array}$	Smooth COM -61 -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	$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \\ \hline \\ \text{Bond Angle} \\ \hline \\ \text{C}\alpha_\text{C}\beta_\text{C}\gamma \\ \text{C}\alpha_\text{C}\text{C} \\ \text{C}\beta_\text{C}\gamma_\text{C}\delta \\ \text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon_\text{C}\zeta \\ \text{C}\gamma_\text{C}\delta_\text{N}\epsilon \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta1 \\ \text{N}\epsilon_\text{C}\zeta_\text{N}\eta2 \\ \text{N}\eta1_\text{C}\zeta_\text{N}\eta2 \\ \end{array}$	Smooth COM -63 -67 -60 -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	
$\begin{array}{c} \chi \\ \text{chi1} \\ \text{chi2} \\ \text{chi3} \\ \text{chi4} \\ \hline \\ \text{Bond Angle} \\ \hline \\ C\alpha_C\beta_C\gamma \\ C\alpha_C_O \\ C\beta_C\alpha_C \\ C\beta_C\gamma_C\delta \\ C\delta_N\epsilon_C\zeta \\ C\gamma_C\delta_N\epsilon \\ N\epsilon_C\zeta \\ C\gamma_C\delta_N\eta1 \\ N\epsilon_C\zeta_N\eta2 \\ \end{array}$	Smooth COM -61 -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}_{\beta}$-$\text{C}\gamma$} \\ \hline \\ \hline \text{$\text{C}\alpha_\text{C}_{\beta}$-$\text{C}\gamma$-$\text{C}\delta$} \\ \hline \\ \hline \text{$\text{C}\beta_\text{C}\gamma_\text{C}\delta$} \\ \hline \\ \hline \\ \hline \text{$\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 -67 -60 -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

LY	$\overline{\text{S pptt n}} = 25$		LY	$\sqrt{S ptpp} n = 89$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64	7.5	chi1	65	6.8
chi2	89	8.3	chi2	178	8.1
chi3	175	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
$C\gammaC\deltaC\epsilon$	110.6	1.94	$C\gammaC\deltaC\epsilon$	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	$S \mathbf{pttp} n = 240$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64	8.2	chi1	67	8.3
chi2	179	11.8	chi2	-179	10.4
chi3	72	10.4	chi3	178	11.2
chi4	174	11.2	chi4	66	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	$8 \mathbf{pttt} \mathbf{n} = 1385$		LYS		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65	7.6	chi1	64	6.9
chi2	-178	8.7	chi2	-177	9.1
chi3	-179	9.7	chi3	-178	10.0
chi4	-179	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
$C\delta_{-}C\epsilon_{-}N\zeta$	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	$S \mathbf{ptmt} \ n = 187$		LYS	$8 \mathbf{ptmm} \ n = 80$	
$\overline{\chi}$	Smooth COM	StdDev	$\overline{\chi}$	Smooth COM	StdDev
chi1	66	8.2	chi1	66	8.4
chi2	-175	12.0	chi2	-177	10.0
chi3	-71	11.7	chi3	-69	9.8
chi4	-175	10.3	chi4	-66	7.0
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	114.5	1.57	$C\alphaC\betaC\gamma$	114.5	1.30
$C\alphaCO$	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 β _ $^{'}$ C γ _ $^{'}$ C δ	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
$C\gammaC\deltaC\overset{_{}_\circ}{\epsilon}$	112.4	1.87	$\text{C}\gamma_{-}\text{C}\delta_{-}\text{C}\overset{ ext{ iny }}{\epsilon}$	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	$\overline{\text{S pmtt n}} = 10$		LY	S tppp n = 37	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	73	8.4	chi1	-177	11.5
chi2	-74	10.5	chi2	62	10.1
chi3	-168	10.6	chi3	65	7.8
chi4	-174	10.7	chi4	67	11.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	116.4	1.64	$C\alpha_{-}C\beta_{-}C\gamma$	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
$C\deltaC\epsilonN\zeta$	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
$N_{-}C\alpha_{-}C\beta$	112.1	2.13	$N_{-}C\alpha_{-}C\beta$	110.2	1.12
LY	S tppt $n = 272$		LY	$\mathbf{tptp} \; n = 409$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178	7.9	chi1	-179	8.0
chi2	63	8.9	chi2	67	10.4
chi3	69	9.2	chi3	173	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 tptt $n = 1228$		LYS tptm $n = 197$			
$\overline{\chi}$	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178	9.1	chi1	-177	7.6
chi2	69	9.0	chi2	67	9.7
chi3	175	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
$C\deltaC\epsilonN\zeta$	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
$N_{-}C\alpha_{-}C\beta$	110.2	1.11	$N_{-}C\alpha_{-}C\beta$	110.3	1.14
LY	LYS ttpp $n = 229$		LY	S ttpt n = 883	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178	8.6	chi1	-178	8.1
chi2	174	14.5	chi2	174	12.1
chi3	71	11.2	chi3	73	11.9
chi4	68	10.5	chi4	175	11.3
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	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	S $\mathbf{tttp} \ \mathbf{n} = 1233$		LYS $tttt n = 5043$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177	8.1	chi1	-175	8.2
chi2	175	9.9	chi2	176	8.7
chi3	173	10.8	chi3	179	9.2
chi4	65	12.8	chi4	-179	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 tttm $n = 1176$		LYS ttmp n = 9			
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176	8.1	chi1	-174	4.2
chi2	177	9.7	chi2	-179	8.5
chi3	-176	10.5	chi3	-95	18.6
chi4	-67	12.1	chi4	76	25.2
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	113.9	1.60	$C\alphaC\betaC\gamma$	113.2	1.24
$C\alphaCO$	120.6	0.82	$C\alphaCO$	120.6	0.50
$C\beta_{-}C\alpha_{-}C$	110.3	1.14	$C\beta _C\alpha _C$	110.3	1.62
$C\betaC\gammaC\delta$	111.0	1.70	$C\betaC\gammaC\delta$	112.6	1.74
$C\delta_C\epsilon_N\zeta$	112.3	1.97	$C\deltaC\epsilonN\zeta$	114.0	1.36
$C\gammaC\deltaC\epsilon$	111.8	1.47	$C\gammaC\deltaC\epsilon$	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	LYS $ttmt n = 674$		LYS	$5 \mathbf{ttmm} \ \mathbf{n} = 197$	
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174	9.4	chi1	-174	8.5
chi2	-177	10.8	chi2	179	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
$C\alphaC\betaC\gamma$	113.7	1.55	$C\alphaC\betaC\gamma$	113.6	1.46
$C\alphaCO$	120.6	0.86	$C\alphaCO$	120.6	0.82
$C\betaC\alphaC$	110.2	1.18	$C\beta_{-}C\alpha_{-}C$	110.2	1.29
$C\betaC\gammaC\delta$	112.2	1.52	$C\betaC\gammaC\delta$	112.1	1.57
$C\delta_{-}C\epsilon_{-}N\zeta$	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 $\mathbf{tmtp} \ n = 11$		LY		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176	7.5	chi1	-172	8.5
chi2	-97	8.3	chi2	-91	9.6
chi3	-178	12.4	chi3	-176	11.7
chi4	65	7.8	chi4	-178	10.7
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
$C\alphaC\betaC\gamma$	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	$C\beta_{-}C\alpha_{-}C$	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	$C\gammaC\deltaC\epsilon$	111.0	1.37
$N_{-}C\alpha_{-}C$	110.1	3.05	$N_{-}C\alpha_{-}C$	110.2	1.89
$N_{-}C\alpha_{-}C\beta$	110.4	0.87	$N_{-}C\alpha_{-}C\beta$	110.1	0.81

LY	$8 \mathbf{tmtm} \ n = 20$			$LYS \mathbf{tmmt} n = 3$	 33
χ	Smooth COM	StdDev	χ	Smooth CON	M StdDev
chi1	-172	10.4	chi1	-179	10.0
chi2	-90	5.6	chi2	-93	12.1
chi3	-172	15.1	chi3	-70	8.9
chi4	-64	7.7	chi4	-179	10.2
Bond Angle	Mean	StdDev	Bond A	Angle Mean	StdDev
$C\alpha_{-}C\beta_{-}C\gamma$	115.5	1.62	$C\alpha_{-}C\beta$	_Cγ 115.0	1.85
$C\alphaCO$	120.6	0.65	$C\alphaC$	120.5	0.88
$C\betaC\alphaC$	111.0	0.85	$C\betaC\alpha$	_C 110.7	1.12
$C\betaC\gammaC\delta$	112.2	1.23	$C\betaC\gamma$	$C\delta$ 113.5	1.73
$C\delta_{-}C\epsilon_{-}N\zeta$	112.7	1.69	$C\deltaC\epsilon$	$N\zeta$ 110.8	2.86
$C\gammaC\deltaC\epsilon$	112.0	1.55	$C\gamma_{-}C\delta$	$C\epsilon$ 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	S tmmm $n = 8$			LYS mppt $n = 3$	31
χ	Smooth COM	StdDev	χ	Smooth CON	M StdDev
chi1	-177	11.9	chi1	-82	8.9
chi2	-81	7.5	chi2	73	14.9
chi3	-63	8.0	chi3	69	8.0
chi4	-64	4.9	chi4	177	5.4
Bond Angle	Mean	StdDev	Bond A	Angle Mean	StdDev
$C\alphaC\betaC\gamma$	116.2	2.69	$C\alpha C\beta$		1.99
$C\alphaCO$	120.3	0.85	$C\alphaCC$		0.89
$C\betaC\alphaC$	111.2	1.13	$C\beta_{-}C\alpha$		1.23
$C\betaC\gammaC\delta$	114.9	1.37	$C\betaC\gamma$		1.56
$C\deltaC\epsilonN\zeta$	113.1	1.48	$C\deltaC\epsilon$		1.92
$C\gammaC\deltaC\epsilon$	115.0	1.62	$C\gamma_{-}C\delta$		1.37
$N_{-}C\alpha_{-}C$	109.0	2.01	$N_{-}C\alpha_{-}$		1.97
$N_{-}C\alpha_{-}C\beta$	109.5	1.26	$N_{-}C\alpha_{-}$	$C\beta$ 110.9	0.92
LY	$S \mathbf{mptp} \ n = 26$			LYS $mptt n = 12$	
χ	Smooth COM	StdDev	χ	Smooth CON	M StdDev
chi1	-74	18.5	chi1	-79	13.3
chi2	86	18.2	chi2	72	17.3
chi3	171	9.0	chi3	176	12.4
chi4	65	12.1	chi4	175	11.9
Bond Angle	Mean	StdDev	Bond A	Angle Mean	StdDev
$C\alphaC\betaC\gamma$	114.7	1.56	$C\alpha C\beta$,	1.39
$C\alphaCO$	120.5	1.13	$C\alphaCC$		0.78
$C\betaC\alphaC$	110.1	1.43	$C\beta C\alpha$		1.53
$C\betaC\gammaC\delta$	113.2	2.50	$C\betaC\gamma$		2.03
$C\delta_{-}C\epsilon_{-}N\zeta$	113.4	2.26	$C\deltaC\epsilon$	~	2.27
$C\gammaC\deltaC\epsilon$	112.5	2.72	$C\gamma_{-}C\delta$		1.60
$N_{-}C\alpha_{-}C$	110.6	2.77	$N_{-}C\alpha_{-}$		2.59
$N_{-}C\alpha_{-}C\beta$	110.9	1.04	$N_{-}C\alpha_{-}$	$C\beta$ 110.8	1.10

LYS	S mptm n = 11			LYS $\mathbf{mtpp} \ n = 392$		
$\overline{\chi}$	Smooth COM	StdDev	$\overline{\chi}$	Smooth COM	StdDev	
chi1	-91	6.7	chi1	-68	7.5	
chi2	61	11.1	chi2	176	10.9	
chi3	-173	5.4	chi3	70	10.8	
chi4	-60	13.5	chi4	67	10.9	
Bond Angle	Mean	StdDev	Bond A	angle Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	114.6	0.81	$C\alpha C\beta$	_Cγ 113.2	1.66	
$C\alphaCO$	120.7	0.57	$C\alpha_{-}C_{-}C$	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	$C\beta_{-}C\gamma_{-}$	$C\delta$ 112.4	1.45	
$C\delta_C\epsilon_N\zeta$	113.4	1.68	$C\deltaC\epsilon$	$N\zeta$ 112.8	2.11	
$C\gammaC\deltaC\epsilon$	111.8	0.50	$C\gamma_{-}C\delta_{-}$	$C\epsilon$ 112.7	1.41	
$N_C\alpha_C$	110.8	2.19	$N_{C}\alpha_{C}$	C 111.4	2.53	
$NC\alphaC\beta$	110.6	0.91	$N_{-}C\alpha_{-}C$	$C\beta$ 110.5	1.01	
LYS	LYS mtpt $n = 1357$			LYS $mtpm n = 17$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	-69	8.1	chi1	-70	6.1	
chi2	174	11.3	chi2	174	15.5	
chi3	70	11.8	chi3	90	14.7	
chi4	175	10.4	chi4	-70	12.1	
Bond Angle	Mean	StdDev	Bond A	angle Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	113.3	1.54	$C\alpha C\beta$	_Cγ 113.5	2.14	
$C\alphaCO$	120.5	0.84	$C\alphaCC$		0.77	
$C\betaC\alphaC$	110.0	1.65	$C\beta C\alpha$	_C 109.8	2.27	
$C\betaC\gammaC\delta$	112.3	1.55	$C\beta_{-}C\gamma_{-}$	$C\delta$ 112.3	1.70	
$C\delta_{-}C\epsilon_{-}N\zeta$	110.8	2.15	$C\delta_{-}C\epsilon_{-}$		1.87	
$C\gammaC\deltaC\epsilon$	112.3	1.49	$C\gammaC\delta$	$C\epsilon$ 113.2	1.59	
$N_C\alpha_C$	111.4	2.21	$N_{C}\alpha_{C}$	C = 110.9	2.12	
$N_{C}\alpha_{C}\beta$	110.7	1.03	N_Cα_0	$C\beta$ 110.5	1.03	
LYS	$\mathbf{mttp} \ n = 1414$			LYS mttt $n = 8597$		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev	
chi1	-65	8.3	chi1	-67	7.1	
chi2	-179	10.7	chi2	-178	9.1	
chi3	176	11.2	chi3	-179	9.8	
chi4	66	13.6	chi4	179	10.3	
Bond Angle	Mean	StdDev	Bond A	angle Mean	StdDev	
$C\alphaC\betaC\gamma$	113.4	1.73	$C\alpha C\beta$	'	1.62	
$C\alphaCO$	120.5	0.84	$C\alphaCC$		0.83	
$C\betaC\alphaC$	110.1	1.63	$C\beta C\alpha$		1.56	
$C\betaC\gammaC\delta$	111.3	1.75	$C\beta_{-}C\gamma_{-}$		1.85	
$C\deltaC\epsilonN\zeta$	112.2	1.98	$C\delta_{-}C\epsilon_{-}$	•	2.10	
$C\gammaC\deltaC\epsilon$	111.8	1.47	$C\gammaC\delta$		1.60	
$N_{-}C\alpha_{-}C$	111.3	2.49	$N_{-}C\alpha_{-}C$		2.24	
$N_{-}C\alpha_{-}C\beta$	110.6	1.02	$N_{C}\alpha_{C}$	$C\beta$ 110.7	0.99	

LYS	LYS $\mathbf{mttm} \ \mathbf{n} = 1829$			$\frac{\text{LYS } \mathbf{mtmp} \ n = 9}{}$			
χ	Smooth COM	StdDev	•	χ	Smooth COM	StdDev	
chi1	-66	7.3		chi1	-67	5.8	
chi2	-177	10.0		chi2	-175	8.3	
chi3	-176	10.8		chi3	-95	7.4	
chi4	-67	12.8		chi4	73	12.3	
Bond Angle	Mean	StdDev		Bond Angle	Mean	StdDev	
$C\alpha_{-}C\beta_{-}C\gamma$	113.4	1.74		$C\alphaC\betaC\gamma$	113.8	1.23	
$C\alphaCO$	120.5	0.85		$C\alpha_{-}C_{-}O$	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		$C\beta C\gamma C\delta$	111.7	1.98	
$C\deltaC\epsilonN\zeta$	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	
$N_{-}C\alpha_{-}C\beta$	110.6	1.00		$N_{-}C\alpha_{-}C\beta$	110.8	0.91	
LYS mtmt $n = 1314$:		LYS	$\mathbf{mtmm} \ \mathbf{n} = 424$		
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev	
chi1	-66	6.9		chi1	-63	6.9	
chi2	-173	9.8		chi2	-177	10.1	
chi3	-73	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	
$C\alpha_{-}C_{-}O$	120.4	0.86		$C\alpha_{-}C_{-}O$	120.5	0.84	
$C\beta_{-}C\alpha_{-}C$	110.1	1.56		$C\beta_{-}C\alpha_{-}C$	109.8	1.56	
$C\beta C\gamma C\delta$	112.3	1.50 1.52		$C\beta C\gamma C\delta$	112.3	1.37	
$C\delta_{-}C\epsilon_{-}N\zeta$	111.0	$\frac{1.32}{2.18}$		$C\deltaC\epsilonN\zeta$	112.8	2.10	
C_{γ} _ C_{δ} _ C_{ϵ}	112.1	1.45		$C_{\gamma}C_{\delta}C_{\epsilon}$	112.9		
$N_{-}C\alpha_{-}C$	111.3	2.14		$N_{-}C\alpha_{-}C$	111.5	$1.50 \\ 2.39$	
	111.5						
N_Cα_Cβ	110.7	0.96		$N_{-}C\alpha_{-}C\beta$	110.6	1.03	
LYS	8 mmpt n = 31			LYS			
χ	Smooth COM	StdDev		χ	Smooth COM	StdDev	
chi1	-60	7.0		chi1	-61	8.2	
chi2	-70	19.5		chi2	-68	12.0	
chi3	93	14.5		chi3	179	11.9	
chi4	175	10.7		chi4	67	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		$C\beta_{-}C\alpha_{-}C$	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	
$NC\alphaC\beta$	111.2	1.39		$N_{-}C\alpha_{-}C\beta$	110.7	1.04	

LYS	LYS mmtt $n = 3137$			$LYS \mathbf{mmtm} \ n = 727$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdD		
chi1	-61	8.3	chi1	-60	8.2		
chi2	-67	9.8	chi2	-65	10.8		
chi3	-176	10.1	chi3	-173	11.2		
chi4	-178	11.0	chi4	-68	13.4		
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdD		
$C\alphaC\betaC\gamma$	114.5	1.32	$C\alpha_{-}C\beta_{-}C\gamma$	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	$C\gammaC\deltaC\epsilon$	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 $\mathbf{mmmm} \ n = 90$			
χ	Smooth COM	StdDev	χ	Smooth COM	StdD		
chi1	-62	7.7	chi1	-61	8.3		
chi2	-64	10.7	chi2	-61	10.4		
chi3	-70	9.7	chi3	-66	10.8		
chi4	-176	9.8	chi4	-64	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	$\mathrm{C}\delta_{-}\mathrm{C}\epsilon_{-}\mathrm{N}\zeta$	112.6	2.73		
$C\gammaC\deltaC\epsilon$	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	$^{'}$ C $lpha$ _C	111.7	2.47		
$N_{-}C\alpha_{-}C\beta$	110.7	1.05	$N_{-}C\alpha_{-}C\beta$	110.5	1.11		