

Rough Draft of Supplemental Material

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S1 Top500 vs. Top8000 Reference Contours

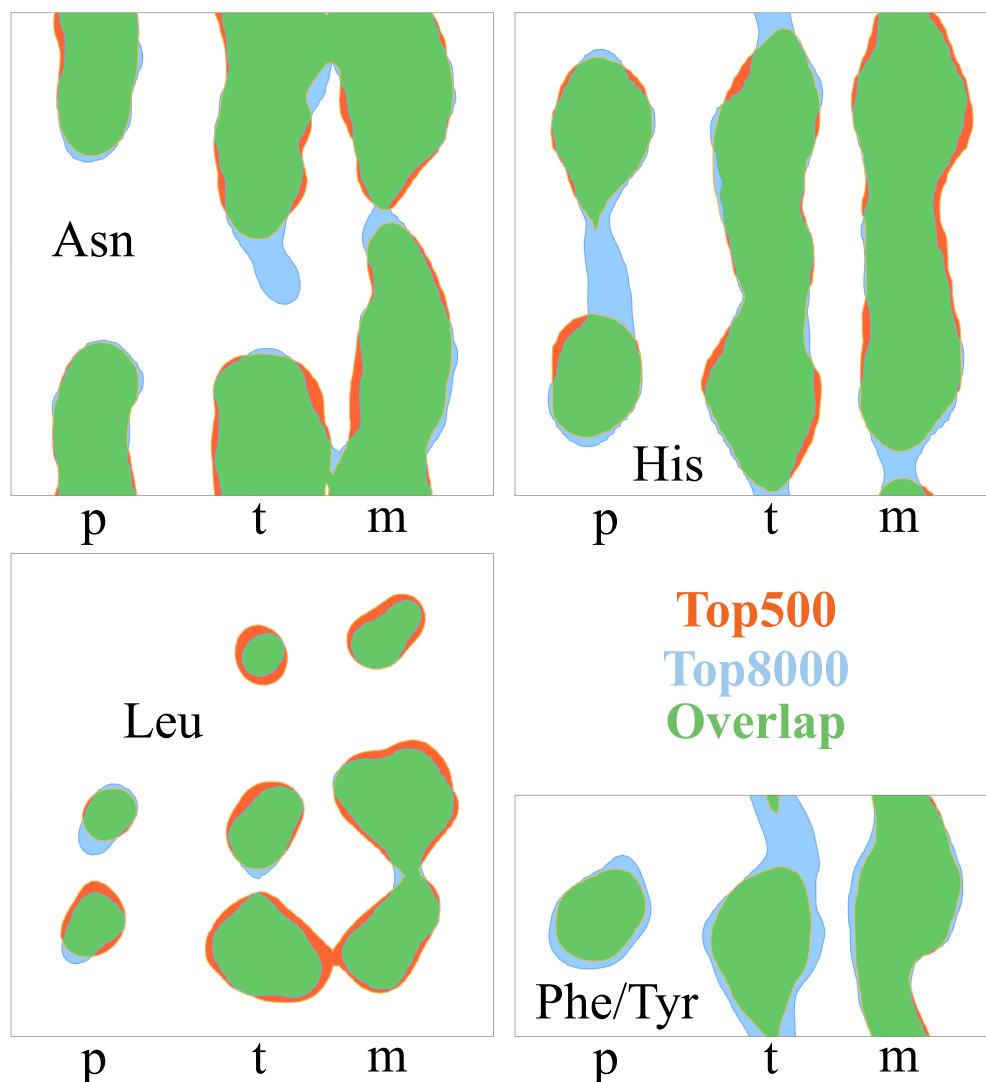


Figure S1: Areas in orange (from Top500 data) and in blue (from Top8000) fill the allowed regions for AsN, His, Leu, and Phe/Tyr. Phe and Tyr were done together as no significant difference was detected between their distributions. The extensive areas in green are where the two systems both declare allowed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

S2 Filtered Top8000 Residue Counts

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

Table S1: Residue counts with and without residue-level filters ordered by % kept after filtering. 'No Filter' means no RSCC, 2mF_o-DF_c sigma, and B filters but all other residue-level filters applied.

S3 Outlier Counts: Top500 vs. Top8000 Reference Contours

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

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

S4 Top8000 Filtered Dataset: Rotamer Frequency

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

residue	rotamer	n	%	rarity
SER : TOTAL N = 76186				
SER	p	36901	48.44	-
SER	t	17502	22.97	-
SER	m	21558	28.30	-
SER	OUTLIER	225	0.30	-
CYS : TOTAL N = 16708				
CYS	p	2962	17.73	-
CYS	t	4399	26.33	-
CYS	m	9301	55.67	-
CYS	OUTLIER	46	0.28	-
THR : TOTAL N = 75180				
THR	p	36195	48.14	-
THR	t	5197	6.91	-
THR	m	33559	44.64	-
THR	OUTLIER	229	0.30	-
VAL : TOTAL N = 97050				
VAL	p	6015	6.20	-
VAL	t	73329	75.56	-
VAL	m	17410	17.94	-
VAL	OUTLIER	296	0.30	-
PRO : TOTAL N = 59515				
PRO	Cg_exo	30128	50.62	-
PRO	Cg_endo	29192	49.05	-
PRO	OUTLIER	195	0.33	-
LEU : TOTAL N = 115053				
LEU	pp	521	0.45	✓
LEU	pt	378	0.33	✓
LEU	tp	34655	30.12	-
LEU	tt	1576	1.37	-
LEU	tm	143	0.12	✓✓
LEU	mp	2711	2.36	-
LEU	mt	74252	64.54	-
LEU	mm	484	0.42	✓
LEU	OUTLIER	333	0.29	-
ILE : TOTAL N = 71693				
ILE	pp	254	0.35	✓
ILE	pt	8837	12.33	-
ILE	tp	1869	2.61	-
ILE	tt	4163	5.81	-
ILE	mp	623	0.87	✓
ILE	mt	44470	62.03	-
ILE	mm	11258	15.70	-
ILE	OUTLIER	219	0.31	-
ASN : TOTAL N = 53650				
ASN	p0	7513	14.00	-

residue	rotamer	n	%	rarity
ASN	t0	15610	29.10	-
ASN	t160	61	0.11	✓✓
ASN	m110	4003	7.46	-
ASN	m-40	26292	49.01	-
ASN	OUTLIER	171	0.32	-
ASP : TOTAL N = 72336				
ASP	p0	11746	16.24	-
ASP	t0	17107	23.65	-
ASP	t70	6029	8.33	-
ASP	m-30	37239	51.48	-
ASP	OUTLIER	215	0.30	-
HIS : TOTAL N = 29791				
HIS	p90	1492	5.01	-
HIS	p-80	2203	7.39	-
HIS	t70	5068	17.01	-
HIS	t-170	1332	4.47	-
HIS	t-90	3553	11.93	-
HIS	m170	2695	9.05	-
HIS	m90	3914	13.14	-
HIS	m-70	9453	31.73	-
HIS	OUTLIER	81	0.27	-
PHE : TOTAL N = 56282				
PHE	p90	6289	11.17	-
PHE	t80	19289	34.27	-
PHE	m-10	3880	6.89	-
PHE	m-80	26665	47.38	-
PHE	OUTLIER	159	0.28	-
TYR : TOTAL N = 47243				
TYR	p90	5466	11.57	-
TYR	t80	16312	34.53	-
TYR	m-10	2623	5.55	-
TYR	m-80	22683	48.01	-
TYR	OUTLIER	159	0.34	-
TRP : TOTAL N = 18715				
TRP	p90	971	5.19	-
TRP	p-90	1937	10.35	-
TRP	t60	3385	18.09	-
TRP	t-100	2893	15.46	-
TRP	m100	6319	33.76	-
TRP	m-10	2196	11.73	-
TRP	m-90	961	5.13	-
TRP	OUTLIER	53	0.28	-
MET : TOTAL N = 16794				
MET	ppp	50	0.30	✓
MET	pp-130	27	0.16	✓

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

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

residue	rotamer	n	%	rarity
LYS	tppp	37	0.11	✓
LYS	tppt	272	0.78	-
LYS	tptp	409	1.17	-
LYS	tptt	1228	3.53	-
LYS	tptm	197	0.57	-
LYS	tttp	229	0.66	-
LYS	ttpt	883	2.54	-
LYS	ttpm	4	0.01	✓✓
LYS	tttp	1233	3.54	-
LYS	tttt	5043	14.48	-
LYS	tttm	1176	3.38	-
LYS	ttmp	9	0.03	✓
LYS	ttmt	674	1.94	-
LYS	ttmm	197	0.57	-
LYS	tmtp	11	0.03	✓
LYS	tmtt	82	0.24	-
LYS	tmtm	20	0.06	✓
LYS	tmmt	33	0.09	✓
LYS	tmmm	8	0.02	✓
LYS	mppt	31	0.09	✓
LYS	mptp	26	0.07	✓
LYS	mppt	124	0.36	-
LYS	mptm	11	0.03	✓
LYS	mtpm	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	mmtm	463	1.33	-
LYS	mmtt	3137	9.01	-
LYS	mmtm	727	2.09	-
LYS	mmmt	544	1.56	-
LYS	mmmm	90	0.26	-
LYS	OUTLIER	114	0.33	-

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

S5 χ and Covalent Bond Angle Central Values

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

S5.1 SER

SER p n = 36901			SER t n = 17502		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65.916	8.614	chi1	178.650	9.008
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -OG	111.001	1.348	C α -C β -OG	110.709	1.422
C α -C-O	120.458	0.922	C α -C-O	120.567	0.818
C β -C α -C	109.930	1.393	C β -C α -C	109.799	1.449
N-C α -C	111.621	2.519	N-C α -C	110.491	2.405
N-C α -C β	110.666	1.118	N-C α -C β	110.057	1.210

SER m n = 21558		
χ	Smooth COM	StdDev
chi1	-63.982	7.667
Bond Angle	Mean	StdDev
C α -C β -OG	110.527	1.459
C α -C-O	120.485	0.850
C β -C α -C	109.476	1.447
N-C α -C	111.471	2.440
N-C α -C β	110.563	1.028

S5.2 CYS

CYS p n = 2962		
χ	Smooth COM	StdDev
chi1	64.543	8.969
Bond Angle	Mean	StdDev
C α -C β -SG	114.646	1.684
C α -C-O	120.521	0.978
C β -C α -C	110.473	1.502
N-C α -C	111.297	2.778
N-C α -C β	110.904	1.232
CYS m n = 9301		
χ	Smooth COM	StdDev
chi1	-65.374	8.203
Bond Angle	Mean	StdDev
C α -C β -SG	113.554	1.864
C α -C-O	120.431	0.871
C β -C α -C	109.474	1.632
N-C α -C	111.518	2.424
N-C α -C β	110.613	1.065

CYS t n = 4399		
χ	Smooth COM	StdDev
chi1	-177.599	8.222
Bond Angle	Mean	StdDev
C α -C β -SG	113.679	1.938
C α -C-O	120.488	0.861
C β -C α -C	110.333	1.295
N-C α -C	109.702	2.435
N-C α -C β	110.020	1.370

S5.3 THR

THR p n = 36195			THR t n = 5197		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61.450	7.652	chi1	-172.707	7.389
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ 2	110.976	1.009	C α -C β -C γ 2	111.729	1.103
C α -C β -OG1	109.502	0.971	C α -C β -OG1	109.533	0.990
C α -C-O	120.473	0.956	C α -C-O	120.619	0.834
C β -C α -C	108.833	1.702	C β -C α -C	110.967	1.904
N-C α -C	111.374	2.770	N-C α -C	110.117	2.331
N-C α -C β	111.784	1.258	N-C α -C β	111.298	1.337
OG1-C β -C γ 2	109.207	1.712	OG1-C β -C γ 2	109.060	1.810

THR m n = 33559		
χ	Smooth COM	StdDev
chi1	-60.109	6.107
Bond Angle	Mean	StdDev
C α -C β -C γ 2	111.146	0.939
C α -C β -OG1	108.916	0.972
C α -C-O	120.533	0.810
C β -C α -C	110.050	1.532
N-C α -C	110.213	2.307
N-C α -C β	110.718	1.188
OG1-C β -C γ 2	108.767	1.669

S5.4 VAL

VAL p n = 6015			VAL t n = 73329		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64.912	7.166	chi1	175.704	6.352
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ 1	111.517	1.091	C α -C β -C γ 1	110.746	0.936
C α -C β -C γ 2	110.755	1.020	C α -C β -C γ 2	110.161	0.946
C α -C-O	120.598	0.828	C α -C-O	120.549	0.788
C β -C α -C	111.418	1.568	C β -C α -C	110.193	1.510
C γ 1-C β -C γ 2	111.030	1.204	C γ 1-C β -C γ 2	110.464	1.126
N-C α -C	110.312	2.482	N-C α -C	109.421	2.363
N-C α -C β	111.580	1.263	N-C α -C β	111.340	1.112

VAL m n = 17410		
χ	Smooth COM	StdDev
chi1	-61.900	5.694
Bond Angle	Mean	StdDev
C α -C β -C γ 1	110.354	0.917
C α -C β -C γ 2	111.323	1.023
C α -C-O	120.553	0.913
C β -C α -C	109.824	1.600
C γ 1-C β -C γ 2	110.892	1.165
N-C α -C	111.118	2.687
N-C α -C β	112.271	1.177

S5.5 PRO

PRO Cg _{exo} n = 30128			PRO Cg _{endo} n = 29192		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-24.512	7.169	chi1	26.645	7.653
chi2	35.520	7.825	chi2	-34.137	8.897
chi3	-31.747	7.122	chi3	27.789	9.234
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	104.229	1.397	C α -C β -C γ	104.233	1.468
C α -C-O	120.180	1.031	C α -C-O	120.227	1.070
C α -N-C δ	111.654	0.806	C α -N-C δ	111.798	0.843
C β -C α -C	110.809	1.300	C β -C α -C	110.911	1.411
C β -C γ -C δ	104.701	2.311	C β -C γ -C δ	105.301	2.361
N-C α -C	112.655	2.417	N-C α -C	112.933	2.596
N-C α -C β	103.312	0.589	N-C α -C β	103.192	0.719
N-C δ -C γ	102.715	0.876	N-C δ -C γ	103.063	0.876

S5.6 LEU

LEU pp n = 521			LEU pt n = 378		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61.357	8.227	chi1	72.738	8.508
chi2	83.113	9.465	chi2	164.797	10.798
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	119.083	2.531	C α -C β -C γ	118.709	2.155
C α -C-O	120.578	0.835	C α -C-O	120.802	0.831
C β -C α -C	111.537	1.381	C β -C α -C	110.423	1.451
C β -C γ -C δ 1	111.539	1.890	C β -C γ -C δ 1	109.794	1.542
C β -C γ -C δ 2	109.789	1.678	C β -C γ -C δ 2	111.556	1.845
C δ 1-C γ -C δ 2	109.695	1.226	C δ 1-C γ -C δ 2	110.437	1.240
N-C α -C	110.691	2.359	N-C α -C	110.447	2.450
N-C α -C β	111.107	1.151	N-C α -C β	111.556	1.184
LEU tp n = 34655			LEU tt n = 1576		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177.276	8.235	chi1	-172.476	8.492
chi2	62.594	6.963	chi2	153.401	10.535
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.491	2.056	C α -C β -C γ	117.300	2.706
C α -C-O	120.525	0.788	C α -C-O	120.592	0.860
C β -C α -C	110.192	1.205	C β -C α -C	111.070	1.256
C β -C γ -C δ 1	111.069	1.554	C β -C γ -C δ 1	110.121	1.530
C β -C γ -C δ 2	109.781	1.495	C β -C γ -C δ 2	111.610	1.837
C δ 1-C γ -C δ 2	110.707	1.134	C δ 1-C γ -C δ 2	110.437	1.320
N-C α -C	110.165	2.380	N-C α -C	109.108	2.499
N-C α -C β	110.303	1.147	N-C α -C β	110.213	1.253
LEU tm n = 143			LEU mp n = 2711		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-171.753	5.901	chi1	-77.359	12.530
chi2	-75.044	6.356	chi2	71.504	15.741
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	120.365	2.303	C α -C β -C γ	116.579	2.638
C α -C-O	120.583	0.802	C α -C-O	120.462	0.850
C β -C α -C	111.264	1.174	C β -C α -C	109.681	1.568
C β -C γ -C δ 1	112.297	1.918	C β -C γ -C δ 1	111.644	2.035
C β -C γ -C δ 2	111.622	1.690	C β -C γ -C δ 2	109.937	1.583
C δ 1-C γ -C δ 2	111.421	1.438	C δ 1-C γ -C δ 2	110.503	1.455
N-C α -C	108.547	2.317	N-C α -C	110.165	2.644
N-C α -C β	109.930	1.129	N-C α -C β	111.085	1.027

LEU mt n = 74252			LEU mm n = 484		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-65.787	8.164	chi1	-82.802	10.177
chi2	174.346	8.051	chi2	-63.907	9.998
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.859	2.169	C α -C β -C γ	117.810	2.626
C α -C-O	120.431	0.820	C α -C-O	120.323	0.893
C β -C α -C	109.811	1.421	C β -C α -C	110.092	1.579
C β -C γ -C δ 1	109.882	1.466	C β -C γ -C δ 1	110.866	1.604
C β -C γ -C δ 2	110.965	1.547	C β -C γ -C δ 2	111.876	1.719
C δ 1-C γ -C δ 2	110.777	1.107	C δ 1-C γ -C δ 2	110.701	1.403
N-C α -C	111.393	2.340	N-C α -C	111.081	2.614
N-C α -C β	110.599	0.985	N-C α -C β	111.033	0.983

S5.7 ILE

ILE pp n = 254			ILE pt n = 8837		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	57.851	7.686	chi1	62.073	6.094
chi2	84.312	12.800	chi2	170.331	7.581
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ 1	112.503	1.280	C α -C β -C γ 1	111.339	1.083
C α -C β -C γ 2	109.866	1.145	C α -C β -C γ 2	110.176	0.938
C α -C-O	120.547	0.873	C α -C-O	120.535	0.937
C β -C α -C	111.344	1.607	C β -C α -C	110.110	1.671
C β -C γ 1-C δ 1	115.059	1.803	C β -C γ 1-C δ 1	113.605	1.254
C γ 1-C β -C γ 2	110.044	1.960	C γ 1-C β -C γ 2	111.381	1.533
N-C α -C	112.012	2.513	N-C α -C	111.361	2.736
N-C α -C β	112.286	1.249	N-C α -C β	112.260	1.195
ILE tp n = 1869			ILE tt n = 4163		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-167.339	7.836	chi1	-169.614	7.748
chi2	65.770	7.313	chi2	166.622	6.871
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ 1	111.105	1.130	C α -C β -C γ 1	110.680	1.065
C α -C β -C γ 2	111.437	1.028	C α -C β -C γ 2	111.396	1.038
C α -C-O	120.365	0.819	C α -C-O	120.604	0.827
C β -C α -C	111.532	1.459	C β -C α -C	111.636	1.480
C β -C γ 1-C δ 1	114.167	1.154	C β -C γ 1-C δ 1	113.490	1.268
C γ 1-C β -C γ 2	110.819	1.695	C γ 1-C β -C γ 2	111.706	1.614
N-C α -C	111.577	2.333	N-C α -C	110.129	2.516
N-C α -C β	111.454	1.272	N-C α -C β	111.350	1.316
ILE mp n = 623			ILE mt n = 44470		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-62.667	11.611	chi1	-62.999	6.427
chi2	88.683	16.573	chi2	169.237	7.398
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ 1	111.150	1.110	C α -C β -C γ 1	109.984	1.081
C α -C β -C γ 2	110.473	1.090	C α -C β -C γ 2	110.617	0.918
C α -C-O	120.462	0.812	C α -C-O	120.542	0.790
C β -C α -C	110.134	1.635	C β -C α -C	110.366	1.581
C β -C γ 1-C δ 1	114.582	1.667	C β -C γ 1-C δ 1	113.966	1.223
C γ 1-C β -C γ 2	109.324	1.870	C γ 1-C β -C γ 2	110.762	1.437
N-C α -C	108.335	2.264	N-C α -C	109.405	2.337
N-C α -C β	111.949	1.287	N-C α -C β	111.245	1.145

ILE mm n = 11258		
χ	Smooth COM	StdDev
chi1	-59.020	7.075
chi2	-61.129	7.343
Bond Angle	Mean	StdDev
C α -C β -C γ 1	110.904	1.123
C α -C β -C γ 2	110.751	0.967
C α -C-O	120.513	0.804
C β -C α -C	109.837	1.605
C β -C γ 1-C δ 1	114.776	1.211
C γ 1-C β -C γ 2	111.277	1.468
N-C α -C	109.449	2.450
N-C α -C β	111.304	1.149

S5.8 ASN

ASN p0 n = 7513			ASN t0 n = 15610		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63.756	7.767	chi1	-171.473	10.505
chi2	6.662	43.284	chi2	-1.493	54.857
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.139	0.878	C α -C β -C γ	112.733	0.917
C α -C-O	120.389	0.966	C α -C-O	120.615	0.874
C β -C α -C	111.273	1.683	C β -C α -C	110.613	1.307
C β -C γ -N δ 2	116.347	0.911	C β -C γ -N δ 2	116.453	0.851
C β -C γ -O δ 1	121.130	0.982	C β -C γ -O δ 1	120.906	0.917
N-C α -C	111.973	2.774	N-C α -C	110.128	2.820
N-C α -C β	111.073	1.286	N-C α -C β	110.094	1.446
O δ 1-C γ -N δ 2	122.498	0.716	O δ 1-C γ -N δ 2	122.613	0.680
ASN t160 n = 61			ASN m110 n = 4003		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-161.337	7.377	chi1	-63.571	9.647
chi2	163.600	9.123	chi2	114.583	28.436
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.235	1.524	C α -C β -C γ	112.723	1.153
C α -C-O	120.433	0.848	C α -C-O	120.501	0.902
C β -C α -C	111.294	1.376	C β -C α -C	109.543	1.841
C β -C γ -N δ 2	117.029	2.099	C β -C γ -N δ 2	116.643	1.136
C β -C γ -O δ 1	120.496	2.021	C β -C γ -O δ 1	120.710	1.173
N-C α -C	110.034	1.950	N-C α -C	112.046	2.783
N-C α -C β	109.281	1.457	N-C α -C β	110.629	1.196
O δ 1-C γ -N δ 2	122.428	0.778	O δ 1-C γ -N δ 2	122.607	0.825
ASN m-40 n = 26292					
χ	Smooth COM	StdDev			
chi1	-69.790	9.121			
chi2	-41.669	26.314			
Bond Angle	Mean	StdDev			
C α -C β -C γ	112.457	0.918			
C α -C-O	120.432	0.869			
C β -C α -C	110.006	1.725			
C β -C γ -N δ 2	116.531	0.847			
C β -C γ -O δ 1	120.778	0.894			
N-C α -C	112.237	2.543			
N-C α -C β	110.546	1.096			
O δ 1-C γ -N δ 2	122.662	0.698			

S5.9 ASP

ASP p0 n = 11746			ASP t0 n = 17107		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62.914	7.504	chi1	-171.502	10.156
chi2	-2.097	31.033	chi2	-1.704	23.754
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.477	1.018	C α -C β -C γ	113.211	0.911
C α -C-O	120.397	0.909	C α -C-O	120.704	0.890
C β -C α -C	111.293	1.647	C β -C α -C	110.867	1.230
C β -C γ -O δ 1	119.658	1.560	C β -C γ -O δ 1	119.520	1.387
C β -C γ -O δ 2	118.192	1.768	C β -C γ -O δ 2	118.084	1.734
N-C α -C	112.193	2.551	N-C α -C	108.896	2.647
N-C α -C β	111.140	1.255	N-C α -C β	109.695	1.453
O δ 1-C γ -O δ 2	122.124	1.639	O δ 1-C γ -O δ 2	122.372	1.580
ASP t70 n = 6029			ASP m-30 n = 37239		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.210	9.206	chi1	-68.819	8.157
chi2	74.194	19.764	chi2	-29.214	22.379
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	112.428	0.833	C α -C β -C γ	112.905	0.946
C α -C-O	120.495	0.800	C α -C-O	120.451	0.856
C β -C α -C	110.144	1.274	C β -C α -C	109.353	1.669
C β -C γ -O δ 1	118.490	1.114	C β -C γ -O δ 1	119.179	1.363
C β -C γ -O δ 2	118.723	1.564	C β -C γ -O δ 2	118.242	1.703
N-C α -C	110.484	2.358	N-C α -C	111.690	2.296
N-C α -C β	110.212	1.370	N-C α -C β	110.769	1.055
O δ 1-C γ -O δ 2	122.747	1.537	O δ 1-C γ -O δ 2	122.553	1.556

S5.10 HIS

HIS p90 n = 1492			HIS p-80 n = 2203		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62.492	9.692	chi1	64.769	9.896
chi2	86.558	21.799	chi2	-80.838	16.239
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.189	1.053	C α -C β -C γ	114.073	1.065
C α -C-O	120.635	0.945	C α -C-O	120.392	0.980
C β -C α -C	110.826	1.567	C β -C α -C	110.369	1.531
C β -C γ -C δ 2	131.000	0.858	C β -C γ -C δ 2	131.015	0.802
C β -C γ -N δ 1	122.773	0.915	C β -C γ -N δ 1	122.746	0.806
C ϵ 1-N ϵ 2-C δ 2	108.808	0.592	C ϵ 1-N ϵ 2-C δ 2	108.828	0.584
C γ -C δ 2-N ϵ 2	107.271	0.501	C γ -C δ 2-N ϵ 2	107.240	0.521
C γ -N δ 1-C ϵ 1	109.201	0.717	C γ -N δ 1-C ϵ 1	109.201	0.610
N δ 1-C ϵ 1-N ϵ 2	108.528	0.659	N δ 1-C ϵ 1-N ϵ 2	108.521	0.605
N δ 1-C γ -C δ 2	106.170	0.534	N δ 1-C γ -C δ 2	106.187	0.514
N-C α -C	111.257	2.740	N-C α -C	112.010	2.426
N-C α -C β	110.998	1.361	N-C α -C β	111.016	1.324
HIS t70 n = 5068			HIS t-170 n = 1332		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.423	10.035	chi1	-173.314	9.701
chi2	73.865	17.323	chi2	-167.114	21.613
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.614	1.068	C α -C β -C γ	114.240	1.024
C α -C-O	120.573	0.830	C α -C-O	120.601	0.807
C β -C α -C	110.127	1.337	C β -C α -C	110.900	1.306
C β -C γ -C δ 2	131.028	0.815	C β -C γ -C δ 2	131.372	0.975
C β -C γ -N δ 1	122.666	0.792	C β -C γ -N δ 1	122.414	1.049
C ϵ 1-N ϵ 2-C δ 2	108.853	0.519	C ϵ 1-N ϵ 2-C δ 2	108.773	0.553
C γ -C δ 2-N ϵ 2	107.197	0.456	C γ -C δ 2-N ϵ 2	107.239	0.449
C γ -N δ 1-C ϵ 1	109.172	0.621	C γ -N δ 1-C ϵ 1	109.216	0.658
N δ 1-C ϵ 1-N ϵ 2	108.505	0.557	N δ 1-C ϵ 1-N ϵ 2	108.565	0.625
N δ 1-C γ -C δ 2	106.248	0.497	N δ 1-C γ -C δ 2	106.182	0.524
N-C α -C	110.682	2.354	N-C α -C	109.227	2.609
N-C α -C β	110.179	1.486	N-C α -C β	109.644	1.519

HIS t-90 n = 3553			HIS m170 n = 2695		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173.491	10.385	chi1	-67.985	8.200
chi2	-86.784	18.450	chi2	170.975	21.745
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.698	1.010	C α -C β -C γ	113.732	0.930
C α -C-O	120.474	0.846	C α -C-O	120.396	0.880
C β -C α -C	110.440	1.219	C β -C α -C	109.708	1.788
C β -C γ -C δ 2	130.907	0.830	C β -C γ -C δ 2	131.144	0.993
C β -C γ -N δ 1	122.790	0.749	C β -C γ -N δ 1	122.596	1.037
C ϵ 1-N ϵ 2-C δ 2	108.840	0.525	C ϵ 1-N ϵ 2-C δ 2	108.792	0.528
C γ -C δ 2-N ϵ 2	107.199	0.482	C γ -C δ 2-N ϵ 2	107.215	0.471
C γ -N δ 1-C ϵ 1	109.174	0.721	C γ -N δ 1-C ϵ 1	109.180	0.692
N δ 1-C ϵ 1-N ϵ 2	108.510	0.617	N δ 1-C ϵ 1-N ϵ 2	108.559	0.624
N δ 1-C γ -C δ 2	106.247	0.554	N δ 1-C γ -C δ 2	106.227	0.530
N-C α -C	109.908	2.468	N-C α -C	111.531	2.540
N-C α -C β	110.079	1.464	N-C α -C β	110.742	1.152
HIS m90 n = 3914			HIS m-70 n = 9453		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-65.658	9.782	chi1	-64.458	10.014
chi2	88.477	17.472	chi2	-75.228	19.348
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.467	1.110	C α -C β -C γ	113.370	1.064
C α -C-O	120.484	0.896	C α -C-O	120.407	0.875
C β -C α -C	109.759	1.956	C β -C α -C	109.866	1.886
C β -C γ -C δ 2	130.923	0.854	C β -C γ -C δ 2	131.054	0.818
C β -C γ -N δ 1	122.786	0.821	C β -C γ -N δ 1	122.620	0.801
C ϵ 1-N ϵ 2-C δ 2	108.852	0.557	C ϵ 1-N ϵ 2-C δ 2	108.856	0.517
C γ -C δ 2-N ϵ 2	107.207	0.499	C γ -C δ 2-N ϵ 2	107.184	0.469
C γ -N δ 1-C ϵ 1	109.189	0.640	C γ -N δ 1-C ϵ 1	109.178	0.630
N δ 1-C ϵ 1-N ϵ 2	108.501	0.615	N δ 1-C ϵ 1-N ϵ 2	108.498	0.562
N δ 1-C γ -C δ 2	106.226	0.511	N δ 1-C γ -C δ 2	106.259	0.532
N-C α -C	111.473	2.734	N-C α -C	111.715	2.840
N-C α -C β	110.637	1.176	N-C α -C β	110.397	1.175

S5.11 PHE

PHE p90 n = 6289			PHE t80 n = 19289		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63.561	9.566	chi1	-178.297	9.973
chi2	-89.699	9.411	chi2	75.767	17.432
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.408	0.965	C α -C β -C γ	113.786	1.072
C α -C-O	120.711	0.891	C α -C-O	120.598	0.802
C β -C α -C	110.881	1.459	C β -C α -C	110.336	1.300
C β -C γ -C δ 1	120.730	0.618	C β -C γ -C δ 1	120.648	0.723
C β -C γ -C δ 2	120.607	0.579	C β -C γ -C δ 2	120.537	0.684
C δ 1-C ϵ 1-C ζ	119.892	0.604	C δ 1-C ϵ 1-C ζ	119.859	0.588
C δ 1-C γ -C δ 2	118.617	0.534	C δ 1-C γ -C δ 2	118.764	0.551
C ϵ 1-C ζ -C ϵ 2	119.823	0.628	C ϵ 1-C ζ -C ϵ 2	119.922	0.630
C γ -C δ 1-C ϵ 1	120.858	0.589	C γ -C δ 1-C ϵ 1	120.767	0.581
C γ -C δ 2-C ϵ 2	120.855	0.575	C γ -C δ 2-C ϵ 2	120.790	0.589
C ζ -C ϵ 2-C δ 2	119.920	0.592	C ζ -C ϵ 2-C δ 2	119.864	0.587
N-C α -C	110.871	2.566	N-C α -C	110.337	2.307
N-C α -C β	111.393	1.319	N-C α -C β	110.203	1.503
PHE m-10 n = 3880			PHE m-80 n = 26665		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68.127	9.328	chi1	-66.760	10.140
chi2	-14.743	19.837	chi2	-80.589	16.828
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.792	0.955	C α -C β -C γ	113.517	1.023
C α -C-O	120.423	0.872	C α -C-O	120.453	0.861
C β -C α -C	108.945	1.776	C β -C α -C	109.811	1.992
C β -C γ -C δ 1	121.549	1.215	C β -C γ -C δ 1	120.579	0.602
C β -C γ -C δ 2	119.886	1.159	C β -C γ -C δ 2	120.569	0.590
C δ 1-C ϵ 1-C ζ	119.897	0.614	C δ 1-C ϵ 1-C ζ	119.862	0.580
C δ 1-C γ -C δ 2	118.521	0.565	C δ 1-C γ -C δ 2	118.798	0.527
C ϵ 1-C ζ -C ϵ 2	119.840	0.619	C ϵ 1-C ζ -C ϵ 2	119.894	0.607
C γ -C δ 1-C ϵ 1	120.784	0.600	C γ -C δ 1-C ϵ 1	120.768	0.562
C γ -C δ 2-C ϵ 2	120.989	0.612	C γ -C δ 2-C ϵ 2	120.766	0.570
C ζ -C ϵ 2-C δ 2	119.931	0.612	C ζ -C ϵ 2-C δ 2	119.878	0.579
N-C α -C	111.035	2.421	N-C α -C	111.240	2.815
N-C α -C β	111.200	1.109	N-C α -C β	110.549	1.107

S5.12 TYR

TYR p90 n = 5466			TYR t80 n = 16312		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	63.561	10.553	chi1	-178.297	10.473
chi2	-89.699	10.123	chi2	75.767	16.674
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.846	1.875	C α -C β -C γ	113.708	2.135
C α -C-O	120.663	0.933	C α -C-O	120.621	0.799
C β -C α -C	110.645	1.410	C β -C α -C	110.305	1.253
C β -C γ -C δ 1	120.995	0.651	C β -C γ -C δ 1	120.905	0.663
C β -C γ -C δ 2	120.859	0.602	C β -C γ -C δ 2	120.836	0.646
C δ 1-C ϵ 1-C ζ	119.526	0.622	C δ 1-C ϵ 1-C ζ	119.513	0.600
C δ 1-C γ -C δ 2	118.104	0.554	C δ 1-C γ -C δ 2	118.209	0.523
C ϵ 1-C ζ -C ϵ 2	120.448	0.664	C ϵ 1-C ζ -C ϵ 2	120.505	0.653
C ϵ 1-C ζ -OH	119.792	1.246	C ϵ 1-C ζ -OH	119.748	1.279
C γ -C δ 1-C ϵ 1	121.166	0.582	C γ -C δ 1-C ϵ 1	121.095	0.555
C γ -C δ 2-C ϵ 2	121.163	0.550	C γ -C δ 2-C ϵ 2	121.137	0.560
C ζ -C ϵ 2-C δ 2	119.562	0.624	C ζ -C ϵ 2-C δ 2	119.508	0.628
N-C α -C	111.069	2.657	N-C α -C	110.391	2.248
N-C α -C β	111.212	1.224	N-C α -C β	110.211	1.442
OH-C ζ -C ϵ 2	119.743	1.241	OH-C ζ -C ϵ 2	119.729	1.278
TYR m-10 n = 2623			TYR m-80 n = 22683		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68.127	9.935	chi1	-66.760	10.437
chi2	-14.743	20.169	chi2	-80.589	16.848
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.769	1.568	C α -C β -C γ	113.205	2.043
C α -C-O	120.432	0.845	C α -C-O	120.442	0.877
C β -C α -C	109.056	1.746	C β -C α -C	109.633	1.925
C β -C γ -C δ 1	121.580	1.013	C β -C γ -C δ 1	120.859	0.627
C β -C γ -C δ 2	120.368	0.936	C β -C γ -C δ 2	120.851	0.617
C δ 1-C ϵ 1-C ζ	119.496	0.618	C δ 1-C ϵ 1-C ζ	119.505	0.900
C δ 1-C γ -C δ 2	118.010	0.570	C δ 1-C γ -C δ 2	118.240	0.580
C ϵ 1-C ζ -C ϵ 2	120.405	0.650	C ϵ 1-C ζ -C ϵ 2	120.500	0.733
C ϵ 1-C ζ -OH	120.080	1.320	C ϵ 1-C ζ -OH	119.719	1.238
C γ -C δ 1-C ϵ 1	121.075	0.598	C γ -C δ 1-C ϵ 1	121.099	0.856
C γ -C δ 2-C ϵ 2	121.325	0.575	C γ -C δ 2-C ϵ 2	121.096	0.860
C ζ -C ϵ 2-C δ 2	119.652	0.642	C ζ -C ϵ 2-C δ 2	119.515	0.903
N-C α -C	111.382	2.346	N-C α -C	111.429	2.763
N-C α -C β	111.006	1.145	N-C α -C β	110.557	1.100
OH-C ζ -C ϵ 2	119.496	1.345	OH-C ζ -C ϵ 2	119.764	1.250

S5.13 TRP

TRP p90 n = 971			TRP p-90 n = 1937		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	60.293	9.937	chi1	61.771	9.829
chi2	87.822	14.661	chi2	-89.374	12.891
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	115.031	2.042	C α _C β _C γ	115.039	1.903
C α _C_O	120.569	0.863	C α _C_O	120.457	0.933
C β _C α _C	110.664	1.413	C β _C α _C	110.457	1.434
C β _C γ _C δ 1	127.002	0.699	C β _C γ _C δ 1	126.859	0.673
C β _C γ _C δ 2	126.749	0.757	C β _C γ _C δ 2	126.898	0.711
C δ 1_C γ _C δ 2	106.201	0.376	C δ 1_C γ _C δ 2	106.193	0.435
C δ 1_N ϵ 1_C ϵ 2	108.926	0.597	C δ 1_N ϵ 1_C ϵ 2	108.956	0.459
C δ 2_C ϵ 2_C ζ 2	122.451	0.368	C δ 2_C ϵ 2_C ζ 2	122.437	0.342
C δ 2_C ϵ 3_C ζ 3	118.690	0.344	C δ 2_C ϵ 3_C ζ 3	118.715	0.472
C ϵ 2_C δ 2_C ϵ 3	118.827	0.360	C ϵ 2_C δ 2_C ϵ 3	118.806	0.387
C ϵ 2_C δ 2_C γ	107.259	0.313	C ϵ 2_C δ 2_C γ	107.248	0.330
C ϵ 3_C ζ 3_C η 2	121.028	0.417	C ϵ 3_C ζ 3_C η 2	121.029	0.457
C γ _C δ 1_N ϵ 1	110.152	0.498	C γ _C δ 1_N ϵ 1	110.152	0.461
C γ _C δ 2_C ϵ 3	133.896	0.337	C γ _C δ 2_C ϵ 3	133.932	0.413
C η 2_C ζ 2_C ϵ 2	117.467	0.446	C η 2_C ζ 2_C ϵ 2	117.524	0.444
C ζ 3_C η 2_C ζ 2	121.507	0.461	C ζ 3_C η 2_C ζ 2	121.463	0.462
N ϵ 1_C ϵ 2_C δ 2	107.442	0.366	N ϵ 1_C ϵ 2_C δ 2	107.431	0.341
N ϵ 1_C ϵ 2_C ζ 2	130.095	0.402	N ϵ 1_C ϵ 2_C ζ 2	130.118	0.406
N_C α _C	111.204	2.410	N_C α _C	112.137	2.597
N_C α _C β	111.115	1.260	N_C α _C β	111.096	1.241

TRP t60 n = 3385			TRP t-100 n = 2893		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.686	9.781	chi1	-177.069	11.596
chi2	64.773	32.759	chi2	-102.575	15.367
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.267	2.142	C α -C β -C γ	113.566	2.320
C α -C-O	120.658	0.805	C α -C-O	120.574	0.869
C β -C α -C	110.556	1.354	C β -C α -C	110.338	1.328
C β -C γ -C δ 1	127.131	0.791	C β -C γ -C δ 1	126.901	0.685
C β -C γ -C δ 2	126.521	0.816	C β -C γ -C δ 2	126.744	0.710
C δ 1-C γ -C δ 2	106.292	0.480	C δ 1-C γ -C δ 2	106.290	0.425
C δ 1-N ϵ 1-C ϵ 2	108.908	0.510	C δ 1-N ϵ 1-C ϵ 2	108.932	0.453
C δ 2-C ϵ 2-C ζ 2	122.396	0.397	C δ 2-C ϵ 2-C ζ 2	122.411	0.363
C δ 2-C ϵ 3-C ζ 3	118.696	0.418	C δ 2-C ϵ 3-C ζ 3	118.696	0.451
C ϵ 2-C δ 2-C ϵ 3	118.868	0.376	C ϵ 2-C δ 2-C ϵ 3	118.847	0.349
C ϵ 2-C δ 2-C γ	107.260	0.380	C ϵ 2-C δ 2-C γ	107.214	0.324
C ϵ 3-C ζ 3-C η 2	120.994	0.476	C ϵ 3-C ζ 3-C η 2	121.008	0.479
C γ -C δ 1-N ϵ 1	110.066	0.533	C γ -C δ 1-N ϵ 1	110.106	0.476
C γ -C δ 2-C ϵ 3	133.854	0.427	C γ -C δ 2-C ϵ 3	133.922	0.366
C η 2-C ζ 2-C ϵ 2	117.487	0.458	C η 2-C ζ 2-C ϵ 2	117.507	0.446
C ζ 3-C η 2-C ζ 2	121.531	0.477	C ζ 3-C η 2-C ζ 2	121.503	0.457
N ϵ 1-C ϵ 2-C δ 2	107.451	0.384	N ϵ 1-C ϵ 2-C δ 2	107.437	0.338
N ϵ 1-C ϵ 2-C ζ 2	130.137	0.461	N ϵ 1-C ϵ 2-C ζ 2	130.137	0.434
N-C α -C	110.136	2.153	N-C α -C	110.511	2.424
N-C α -C β	109.969	1.424	N-C α -C β	110.288	1.416

TRP m100 n = 6319			TRP m-10 n = 2196		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67.358	10.774	chi1	-68.163	8.989
chi2	97.262	16.989	chi2	-7.490	21.670
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.176	2.218	C α -C β -C γ	114.734	1.637
C α -C-O	120.433	0.860	C α -C-O	120.481	0.882
C β -C α -C	109.632	1.917	C β -C α -C	109.190	1.715
C β -C γ -C δ 1	127.022	0.664	C β -C γ -C δ 1	127.548	0.711
C β -C γ -C δ 2	126.590	0.685	C β -C γ -C δ 2	126.108	0.767
C δ 1-C γ -C δ 2	106.335	0.429	C δ 1-C γ -C δ 2	106.300	0.445
C δ 1-N ϵ 1-C ϵ 2	108.902	0.486	C δ 1-N ϵ 1-C ϵ 2	108.834	0.452
C δ 2-C ϵ 2-C ζ 2	122.401	0.364	C δ 2-C ϵ 2-C ζ 2	122.350	0.407
C δ 2-C ϵ 3-C ζ 3	118.699	0.455	C δ 2-C ϵ 3-C ζ 3	118.695	0.434
C ϵ 2-C δ 2-C ϵ 3	118.868	0.368	C ϵ 2-C δ 2-C ϵ 3	118.908	0.380
C ϵ 2-C δ 2-C γ	107.232	0.331	C ϵ 2-C δ 2-C γ	107.324	0.376
C ϵ 3-C ζ 3-C η 2	120.996	0.477	C ϵ 3-C ζ 3-C η 2	121.005	0.432
C γ -C δ 1-N ϵ 1	110.087	0.488	C γ -C δ 1-N ϵ 1	110.042	0.481
C γ -C δ 2-C ϵ 3	133.883	0.397	C γ -C δ 2-C ϵ 3	133.752	0.391
C η 2-C ζ 2-C ϵ 2	117.493	0.451	C η 2-C ζ 2-C ϵ 2	117.472	0.467
C ζ 3-C η 2-C ζ 2	121.514	0.456	C ζ 3-C η 2-C ζ 2	121.543	0.462
N ϵ 1-C ϵ 2-C δ 2	107.423	0.349	N ϵ 1-C ϵ 2-C δ 2	107.478	0.366
N ϵ 1-C ϵ 2-C ζ 2	130.160	0.431	N ϵ 1-C ϵ 2-C ζ 2	130.159	0.453
N-C α -C	111.436	2.636	N-C α -C	111.431	2.538
N-C α -C β	110.555	1.106	N-C α -C β	110.792	1.154

TRP m-90 n = 961		
χ	Smooth COM	StdDev
chi1	-67.780	12.415
chi2	-89.279	13.788
Bond Angle	Mean	StdDev
C α -C β -C γ	113.837	2.475
C α -C-O	120.475	0.855
C β -C α -C	109.396	2.035
C β -C γ -C δ 1	126.707	0.719
C β -C γ -C δ 2	126.952	0.778
C δ 1-C γ -C δ 2	106.279	0.441
C δ 1-N ϵ 1-C ϵ 2	108.930	0.474
C δ 2-C ϵ 2-C ζ 2	122.433	0.348
C δ 2-C ϵ 3-C ζ 3	118.702	0.453
C ϵ 2-C δ 2-C ϵ 3	118.842	0.382
C ϵ 2-C δ 2-C γ	107.196	0.323
C ϵ 3-C ζ 3-C η 2	121.019	0.460
C γ -C δ 1-N ϵ 1	110.124	0.496
C γ -C δ 2-C ϵ 3	133.947	0.378
C η 2-C ζ 2-C ϵ 2	117.505	0.430
C ζ 3-C η 2-C ζ 2	121.472	0.453
N ϵ 1-C ϵ 2-C δ 2	107.451	0.346
N ϵ 1-C ϵ 2-C ζ 2	130.101	0.430
N-C α -C	110.581	2.879
N-C α -C β	110.698	1.125

S5.14 MET

MET ppp n = 50			MET pp-130 n = 27		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61.248	9.313	chi1	64.331	7.151
chi2	78.960	10.968	chi2	82.303	4.909
chi3	70.700	9.878	chi3	-154.200	27.756
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.688	1.786	C α -C β -C γ	115.400	1.176
C α -C-O	120.690	0.904	C α -C-O	120.921	0.655
C β -C α -C	111.199	1.571	C β -C α -C	111.108	0.909
C β -C γ -SD	114.396	2.327	C β -C γ -SD	113.705	2.013
C γ -SD-C ϵ	100.530	4.023	C γ -SD-C ϵ	100.847	1.954
N-C α -C	111.830	2.718	N-C α -C	110.987	1.836
N-C α -C β	110.925	1.021	N-C α -C β	110.899	0.988
MET ptp n = 404			MET ptt n = 260		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64.508	8.469	chi1	65.361	8.250
chi2	-176.358	11.392	chi2	-178.195	9.143
chi3	73.220	11.597	chi3	179.354	15.601
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.589	1.803	C α -C β -C γ	114.719	1.689
C α -C-O	120.674	0.921	C α -C-O	120.592	0.945
C β -C α -C	110.290	1.464	C β -C α -C	110.343	1.486
C β -C γ -SD	112.889	2.185	C β -C γ -SD	111.033	2.395
C γ -SD-C ϵ	100.792	1.939	C γ -SD-C ϵ	99.817	2.318
N-C α -C	110.626	2.559	N-C α -C	111.139	2.697
N-C α -C β	111.047	1.233	N-C α -C β	111.125	1.299
MET ptm n = 375			MET pmt n = 7		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64.860	8.163	chi1	71.340	3.364
chi2	179.370	10.168	chi2	-74.720	3.186
chi3	-72.053	11.599	chi3	-162.328	4.884
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.625	1.646	C α -C β -C γ	114.786	0.770
C α -C-O	120.634	0.935	C α -C-O	120.997	0.636
C β -C α -C	110.349	1.438	C β -C α -C	111.122	1.130
C β -C γ -SD	112.773	2.109	C β -C γ -SD	111.744	2.285
C γ -SD-C ϵ	100.903	1.820	C γ -SD-C ϵ	100.246	1.914
N-C α -C	110.872	2.766	N-C α -C	109.009	1.550
N-C α -C β	111.166	1.207	N-C α -C β	111.648	1.281

MET pmm n = 42			MET tpp n = 1138		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	72.629	7.847	chi1	-174.981	9.366
chi2	-68.668	6.731	chi2	63.633	7.983
chi3	-68.863	8.148	chi3	72.405	12.028
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.484	0.858	C α -C β -C γ	114.191	1.355
C α -C-O	120.618	0.788	C α -C-O	120.501	0.842
C β -C α -C	110.176	1.220	C β -C α -C	110.324	1.130
C β -C γ -SD	115.246	2.537	C β -C γ -SD	113.667	2.023
C γ -SD-C ϵ	101.108	1.585	C γ -SD-C ϵ	100.683	1.769
N-C α -C	112.287	2.688	N-C α -C	110.665	2.235
N-C α -C β	110.768	1.207	N-C α -C β	110.488	1.169
MET tpt n = 388			MET ttp n = 1246		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173.452	8.736	chi1	-177.766	8.645
chi2	65.814	7.811	chi2	179.141	11.418
chi3	-156.289	31.222	chi3	71.790	10.585
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.077	1.391	C α -C β -C γ	113.559	1.653
C α -C-O	120.521	0.742	C α -C-O	120.611	0.853
C β -C α -C	110.486	1.134	C β -C α -C	110.039	1.168
C β -C γ -SD	112.447	1.994	C β -C γ -SD	112.805	2.114
C γ -SD-C ϵ	100.425	2.088	C γ -SD-C ϵ	100.741	2.073
N-C α -C	110.446	2.248	N-C α -C	110.270	2.150
N-C α -C β	110.324	1.364	N-C α -C β	110.378	1.313
MET ttt n = 569			MET ttm n = 1124		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.725	8.762	chi1	-175.045	9.346
chi2	176.823	9.513	chi2	179.637	8.225
chi3	176.456	15.483	chi3	-71.855	13.081
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.692	1.716	C α -C β -C γ	113.533	1.706
C α -C-O	120.590	0.958	C α -C-O	120.521	0.803
C β -C α -C	110.139	1.307	C β -C α -C	109.956	1.173
C β -C γ -SD	110.615	2.198	C β -C γ -SD	112.759	2.157
C γ -SD-C ϵ	100.115	1.656	C γ -SD-C ϵ	100.808	1.735
N-C α -C	110.201	2.431	N-C α -C	110.136	2.395
N-C α -C β	110.091	1.385	N-C α -C β	110.414	1.331

MET tmt n = 34			MET tmm n = 276		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-179.131	6.701	chi1	-177.257	7.306
chi2	-85.941	7.575	chi2	-81.707	6.798
chi3	173.719	24.401	chi3	-72.167	10.514
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.856	1.126	C α -C β -C γ	114.995	1.371
C α -C-O	120.669	0.563	C α -C-O	120.520	0.782
C β -C α -C	110.695	1.236	C β -C α -C	111.023	1.239
C β -C γ -SD	112.753	1.775	C β -C γ -SD	114.026	2.121
C γ -SD-C ϵ	100.340	1.369	C γ -SD-C ϵ	100.840	1.640
N-C α -C	110.002	2.892	N-C α -C	109.902	2.105
N-C α -C β	110.086	1.223	N-C α -C β	110.096	1.162
MET mpp n = 74			MET mpt n = 34		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-76.610	13.735	chi1	-69.557	11.736
chi2	73.172	12.266	chi2	74.032	10.961
chi3	73.993	11.907	chi3	167.387	18.642
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.617	1.359	C α -C β -C γ	114.581	0.956
C α -C-O	120.531	0.886	C α -C-O	120.388	0.881
C β -C α -C	109.865	1.627	C β -C α -C	109.316	1.399
C β -C γ -SD	114.327	2.245	C β -C γ -SD	113.183	2.024
C γ -SD-C ϵ	101.176	2.262	C γ -SD-C ϵ	100.105	2.397
N-C α -C	110.743	2.686	N-C α -C	110.123	2.780
N-C α -C β	110.760	1.199	N-C α -C β	110.956	1.118
MET mpm n = 13			MET mtp n = 2815		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-77.183	5.132	chi1	-66.650	7.058
chi2	63.994	5.469	chi2	177.074	9.262
chi3	-101.774	5.027	chi3	70.464	10.090
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.136	1.018	C α -C β -C γ	113.148	1.645
C α -C-O	120.662	0.735	C α -C-O	120.492	0.844
C β -C α -C	109.135	1.274	C β -C α -C	109.955	1.587
C β -C γ -SD	115.853	2.314	C β -C γ -SD	112.850	2.081
C γ -SD-C ϵ	100.367	1.563	C γ -SD-C ϵ	100.766	1.731
N-C α -C	110.742	1.813	N-C α -C	111.257	2.348
N-C α -C β	111.036	1.046	N-C α -C β	110.469	1.007

MET mtt n = 1542		
χ	Smooth COM	StdDev
chi1	-67.154	7.717
chi2	179.723	8.705
chi3	-176.816	16.539
Bond Angle	Mean	StdDev
C α -C β -C γ	113.586	1.708
C α -C-O	120.527	0.825
C β -C α -C	109.380	1.673
C β -C γ -SD	110.388	2.192
C γ -SD-C ϵ	100.144	1.974
N-C α -C	111.150	2.271
N-C α -C β	110.658	0.996

MET mmp n = 520		
χ	Smooth COM	StdDev
chi1	-65.195	5.298
chi2	-61.634	6.333
chi3	102.180	9.255
Bond Angle	Mean	StdDev
C α -C β -C γ	114.212	1.410
C α -C-O	120.324	0.802
C β -C α -C	110.229	1.552
C β -C γ -SD	113.849	2.144
C γ -SD-C ϵ	101.224	2.184
N-C α -C	111.490	2.153
N-C α -C β	110.838	1.099

MET mmm n = 3354		
χ	Smooth COM	StdDev
chi1	-65.551	8.867
chi2	-60.977	8.775
chi3	-69.165	10.156
Bond Angle	Mean	StdDev
C α -C β -C γ	114.003	1.286
C α -C-O	120.359	0.857
C β -C α -C	110.042	1.527
C β -C γ -SD	113.654	1.948
C γ -SD-C ϵ	100.895	1.737
N-C α -C	111.629	2.379
N-C α -C β	110.711	1.020

MET mtm n = 1851		
χ	Smooth COM	StdDev
chi1	-66.363	7.865
chi2	-177.825	10.672
chi3	-73.985	10.774
Bond Angle	Mean	StdDev
C α -C β -C γ	113.170	1.716
C α -C-O	120.494	0.902
C β -C α -C	109.943	1.631
C β -C γ -SD	112.920	2.146
C γ -SD-C ϵ	100.758	1.779
N-C α -C	111.074	2.323
N-C α -C β	110.665	1.072

MET mmt n = 597		
χ	Smooth COM	StdDev
chi1	-64.971	8.734
chi2	-63.753	9.443
chi3	172.207	18.496
Bond Angle	Mean	StdDev
C α -C β -C γ	113.918	1.444
C α -C-O	120.423	0.802
C β -C α -C	109.926	1.551
C β -C γ -SD	112.060	2.042
C γ -SD-C ϵ	100.263	1.993
N-C α -C	111.450	2.253
N-C α -C β	110.610	0.944

S5.15 GLU

GLU pp20 n = 159			GLU pt0 n = 2800		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61.255	8.074	chi1	65.363	8.357
chi2	85.644	7.983	chi2	-177.309	10.089
chi3	19.654	17.191	chi3	1.201	51.015
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.555	1.282	C α -C β -C γ	114.597	1.602
C α -C-O	120.440	0.848	C α -C-O	120.524	0.927
C β -C α -C	111.591	1.836	C β -C α -C	110.513	1.498
C β -C γ -C δ	114.078	1.297	C β -C γ -C δ	112.902	1.527
C γ -C δ -O ϵ 1	119.034	1.429	C γ -C δ -O ϵ 1	118.928	1.384
C γ -C δ -O ϵ 2	118.356	1.340	C γ -C δ -O ϵ 2	118.169	1.352
N-C α -C	110.829	2.541	N-C α -C	111.272	2.667
N-C α -C β	111.446	1.254	N-C α -C β	111.061	1.180
O ϵ 1-C δ -O ϵ 2	122.590	1.020	O ϵ 1-C δ -O ϵ 2	122.878	1.149
GLU pm20 n = 1485			GLU tp30 n = 4616		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	69.039	8.839	chi1	-178.170	9.848
chi2	-84.712	8.551	chi2	64.992	9.169
chi3	15.811	21.665	chi3	25.784	26.065
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.558	1.350	C α -C β -C γ	114.624	1.386
C α -C-O	120.191	0.834	C α -C-O	120.486	0.798
C β -C α -C	110.506	1.246	C β -C α -C	110.645	1.209
C β -C γ -C δ	114.466	1.447	C β -C γ -C δ	113.769	1.354
C γ -C δ -O ϵ 1	119.771	1.714	C γ -C δ -O ϵ 1	119.284	1.459
C γ -C δ -O ϵ 2	117.692	1.688	C γ -C δ -O ϵ 2	118.037	1.380
N-C α -C	112.900	1.826	N-C α -C	110.857	2.089
N-C α -C β	110.887	1.055	N-C α -C β	110.284	1.123
O ϵ 1-C δ -O ϵ 2	122.520	1.102	O ϵ 1-C δ -O ϵ 2	122.658	1.073
GLU tt0 n = 13610			GLU tm-30 n = 862		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.677	8.634	chi1	-170.330	8.580
chi2	177.900	10.314	chi2	-83.400	9.158
chi3	1.122	41.445	chi3	-28.718	17.284
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.479	1.738	C α -C β -C γ	114.520	1.347
C α -C-O	120.579	0.766	C α -C-O	120.511	0.838
C β -C α -C	110.135	1.168	C β -C α -C	110.969	1.333
C β -C γ -C δ	113.090	1.500	C β -C γ -C δ	113.819	1.465
C γ -C δ -O ϵ 1	118.950	1.273	C γ -C δ -O ϵ 1	119.014	1.362
C γ -C δ -O ϵ 2	117.962	1.269	C γ -C δ -O ϵ 2	118.207	1.249
N-C α -C	110.583	2.260	N-C α -C	110.226	2.465
N-C α -C β	110.351	1.366	N-C α -C β	110.236	1.156
O ϵ 1-C δ -O ϵ 2	123.063	1.067	O ϵ 1-C δ -O ϵ 2	122.755	1.171

GLU mp0 n = 3671			GLU mt-10 n = 21021		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66.877	7.274	chi1	-66.989	7.750
chi2	82.550	9.362	chi2	179.213	11.417
chi3	3.347	27.520	chi3	-6.596	37.250
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.352	1.344	C α _C β _C γ	113.038	1.846
C α _C_O	120.431	0.818	C α _C_O	120.491	0.823
C β _C α _C	109.695	1.424	C β _C α _C	110.020	1.731
C β _C γ _C δ	114.166	1.404	C β _C γ _C δ	113.253	1.500
C γ _C δ _O ϵ 1	119.771	1.659	C γ _C δ _O ϵ 1	119.081	1.288
C γ _C δ _O ϵ 2	117.760	1.471	C γ _C δ _O ϵ 2	117.940	1.286
N_C α _C	112.041	1.999	N_C α _C	111.364	2.321
N_C α _C β	110.602	1.057	N_C α _C β	110.595	1.004
O ϵ 1_C δ _O ϵ 2	122.450	1.179	O ϵ 1_C δ _O ϵ 2	122.955	1.064

GLU mm-30 n = 9080		
χ	Smooth COM	StdDev
chi1	-66.002	8.689
chi2	-66.544	10.569
chi3	-31.662	26.859
Bond Angle	Mean	StdDev
C α _C β _C γ	114.037	1.414
C α _C_O	120.415	0.828
C β _C α _C	109.927	1.502
C β _C γ _C δ	113.361	1.338
C γ _C δ _O ϵ 1	119.153	1.345
C γ _C δ _O ϵ 2	118.206	1.265
N_C α _C	111.483	2.356
N_C α _C β	110.748	1.014
O ϵ 1_C δ _O ϵ 2	122.622	1.092

S5.16 GLN

GLN pp30 n = 178			GLN pt0 n = 1885		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62.991	7.802	chi1	64.891	8.125
chi2	83.801	8.473	chi2	-177.468	11.284
chi3	29.841	20.903	chi3	-2.755	75.227
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.880	1.278	C α -C β -C γ	114.518	1.528
C α -C-O	120.321	0.946	C α -C-O	120.546	0.962
C β -C α -C	111.398	1.618	C β -C α -C	110.361	1.519
C β -C γ -C δ	113.604	1.401	C β -C γ -C δ	112.497	1.466
C γ -C δ -N ϵ 2	116.446	0.892	C γ -C δ -N ϵ 2	116.505	0.954
C γ -C δ -O ϵ 1	120.885	0.949	C γ -C δ -O ϵ 1	120.841	0.973
N-C α -C	111.003	2.550	N-C α -C	111.263	2.631
N-C α -C β	111.519	1.154	N-C α -C β	110.949	1.178
O ϵ 1-C δ -N ϵ 2	122.630	0.669	O ϵ 1-C δ -N ϵ 2	122.629	0.748
GLN pm20 n = 487			GLN tp40 n = 3618		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	69.577	9.904	chi1	-176.823	8.734
chi2	-84.394	9.313	chi2	66.430	8.230
chi3	16.576	32.336	chi3	41.056	24.195
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.686	1.408	C α -C β -C γ	113.949	1.419
C α -C-O	120.304	0.925	C α -C-O	120.428	0.793
C β -C α -C	110.423	1.352	C β -C α -C	110.237	1.153
C β -C γ -C δ	113.925	1.430	C β -C γ -C δ	112.883	1.238
C γ -C δ -N ϵ 2	116.256	0.863	C γ -C δ -N ϵ 2	116.593	0.838
C γ -C δ -O ϵ 1	121.254	0.986	C γ -C δ -O ϵ 1	120.792	0.874
N-C α -C	112.420	2.222	N-C α -C	111.017	2.005
N-C α -C β	111.150	1.131	N-C α -C β	110.571	1.130
O ϵ 1-C δ -N ϵ 2	122.470	0.718	O ϵ 1-C δ -N ϵ 2	122.594	0.646
GLN tp-100 n = 534			GLN tt0 n = 6936		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.963	8.680	chi1	-176.317	8.500
chi2	62.135	8.823	chi2	177.556	10.804
chi3	-104.704	27.530	chi3	2.032	60.871
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.443	1.567	C α -C β -C γ	113.566	1.797
C α -C-O	120.563	0.834	C α -C-O	120.576	0.762
C β -C α -C	110.517	1.240	C β -C α -C	110.144	1.180
C β -C γ -C δ	113.047	1.311	C β -C γ -C δ	112.612	1.504
C γ -C δ -N ϵ 2	116.553	0.949	C γ -C δ -N ϵ 2	116.455	0.840
C γ -C δ -O ϵ 1	120.860	0.852	C γ -C δ -O ϵ 1	120.819	0.883
N-C α -C	110.364	2.260	N-C α -C	110.448	2.271
N-C α -C β	110.382	1.236	N-C α -C β	110.304	1.362
O ϵ 1-C δ -N ϵ 2	122.560	0.637	O ϵ 1-C δ -N ϵ 2	122.701	0.714

GLN tm130 n = 55			GLN tm-30 n = 547		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-171.730	9.735	chi1	-171.950	10.144
chi2	-75.893	10.370	chi2	-85.646	10.982
chi3	127.247	16.058	chi3	-29.401	20.284
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.897	1.440	C α -C β -C γ	114.618	1.348
C α -C-O	120.546	0.938	C α -C-O	120.534	0.826
C β -C α -C	111.262	1.629	C β -C α -C	110.944	1.310
C β -C γ -C δ	114.423	2.701	C β -C γ -C δ	113.510	1.404
C γ -C δ -N ϵ 2	117.082	1.285	C γ -C δ -N ϵ 2	116.459	0.713
C γ -C δ -O ϵ 1	120.469	1.172	C γ -C δ -O ϵ 1	120.874	0.812
N-C α -C	108.797	3.399	N-C α -C	110.153	2.506
N-C α -C β	110.136	1.370	N-C α -C β	110.287	1.242
O ϵ 1-C δ -N ϵ 2	122.423	0.743	O ϵ 1-C δ -N ϵ 2	122.641	0.676
GLN mp10 n = 1207			GLN mp-120 n = 87		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66.517	8.985	chi1	-72.531	9.965
chi2	81.837	11.441	chi2	69.333	11.372
chi3	17.344	37.547	chi3	-119.632	13.002
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.240	1.363	C α -C β -C γ	114.359	1.549
C α -C-O	120.433	0.836	C α -C-O	120.487	0.882
C β -C α -C	109.775	1.525	C β -C α -C	109.672	1.790
C β -C γ -C δ	113.448	1.294	C β -C γ -C δ	113.610	1.567
C γ -C δ -N ϵ 2	116.318	0.819	C γ -C δ -N ϵ 2	116.625	0.650
C γ -C δ -O ϵ 1	121.139	0.951	C γ -C δ -O ϵ 1	120.632	1.086
N-C α -C	111.608	2.346	N-C α -C	111.577	2.757
N-C α -C β	110.830	1.095	N-C α -C β	110.738	1.006
O ϵ 1-C δ -N ϵ 2	122.522	0.603	O ϵ 1-C δ -N ϵ 2	122.722	0.842
GLN mt0 n = 14370			GLN mm110 n = 1147		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66.588	7.494	chi1	-65.092	8.598
chi2	179.220	11.203	chi2	-62.550	10.868
chi3	-3.560	62.564	chi3	109.265	24.134
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.241	1.815	C α -C β -C γ	113.964	1.562
C α -C-O	120.494	0.850	C α -C-O	120.379	0.849
C β -C α -C	109.919	1.708	C β -C α -C	109.984	1.528
C β -C γ -C δ	112.644	1.530	C β -C γ -C δ	112.879	1.429
C γ -C δ -N ϵ 2	116.444	0.847	C γ -C δ -N ϵ 2	116.587	0.920
C γ -C δ -O ϵ 1	120.849	0.897	C γ -C δ -O ϵ 1	120.788	0.941
N-C α -C	111.415	2.256	N-C α -C	111.589	2.280
N-C α -C β	110.567	1.042	N-C α -C β	110.721	1.066
O ϵ 1-C δ -N ϵ 2	122.680	0.696	O ϵ 1-C δ -N ϵ 2	122.597	0.683

GLN mm-40 n = 5959		
χ	Smooth COM	StdDev
chi1	-63.698	8.629
chi2	-66.032	10.427
chi3	-38.665	24.730
Bond Angle	Mean	StdDev
C α _C β _C γ	113.884	1.423
C α _C_O	120.457	0.869
C β _C α _C	109.908	1.491
C β _C γ _C δ	112.838	1.280
C γ _C δ _N ϵ 2	116.518	0.909
C γ _C δ _O ϵ 1	120.856	0.911
N_C α _C	111.383	2.451
N_C α _C β	110.631	1.036
O ϵ 1_C δ _N ϵ 2	122.604	0.776

S5.17 ARG

ARG ppp80 n = 10			ARG ppp-140 n = 4		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	62.201	5.082	chi1	58.431	3.025
chi2	86.595	6.961	chi2	91.756	4.604
chi3	57.216	3.753	chi3	62.263	10.579
chi4	79.687	8.472	chi4	-143.455	12.578
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.109	0.884	C α -C β -C γ	115.223	0.896
C α -C-O	120.837	0.551	C α -C-O	120.687	0.538
C β -C α -C	111.013	1.509	C β -C α -C	111.973	1.456
C β -C γ -C δ	113.944	0.819	C β -C γ -C δ	112.231	1.497
C δ -N ϵ -C ζ	125.029	0.341	C δ -N ϵ -C ζ	125.872	1.184
C γ -C δ -N ϵ	112.507	1.082	C γ -C δ -N ϵ	113.783	2.259
N ϵ -C ζ -N η 1	120.628	0.683	N ϵ -C ζ -N η 1	120.992	1.242
N ϵ -C ζ -N η 2	119.754	0.628	N ϵ -C ζ -N η 2	120.128	1.383
N η 1-C ζ -N η 2	119.607	0.318	N η 1-C ζ -N η 2	118.855	0.611
N-C α -C	111.134	2.176	N-C α -C	113.626	2.343
N-C α -C β	111.870	1.188	N-C α -C β	111.211	1.258
ARG ppt170 n = 57			ARG ppt90 n = 19		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	59.128	9.858	chi1	63.537	5.887
chi2	87.628	12.300	chi2	99.251	7.971
chi3	173.545	12.300	chi3	-179.890	9.835
chi4	173.353	17.309	chi4	87.261	12.995
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.237	1.393	C α -C β -C γ	115.366	1.885
C α -C-O	120.372	1.040	C α -C-O	120.762	0.834
C β -C α -C	111.948	1.371	C β -C α -C	110.804	1.700
C β -C γ -C δ	112.408	1.628	C β -C γ -C δ	111.852	2.407
C δ -N ϵ -C ζ	124.240	1.282	C δ -N ϵ -C ζ	125.397	1.126
C γ -C δ -N ϵ	111.386	1.601	C γ -C δ -N ϵ	113.143	2.891
N ϵ -C ζ -N η 1	120.500	1.081	N ϵ -C ζ -N η 1	120.860	1.089
N ϵ -C ζ -N η 2	119.821	0.871	N ϵ -C ζ -N η 2	119.873	1.094
N η 1-C ζ -N η 2	119.657	0.701	N η 1-C ζ -N η 2	119.235	0.792
N-C α -C	110.844	2.504	N-C α -C	111.026	2.141
N-C α -C β	111.575	1.315	N-C α -C β	110.842	1.298

ARG ppt-90 n = 15			ARG ptp90 n = 223		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	61.770	9.125	chi1	65.165	9.396
chi2	90.213	11.134	chi2	178.845	11.322
chi3	177.663	5.499	chi3	64.039	8.635
chi4	-92.246	14.372	chi4	87.873	11.117
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	115.763	1.382	C α _C β _C γ	114.956	1.706
C α _C_O	120.637	0.931	C α _C_O	120.464	0.957
C β _C α _C	111.235	1.747	C β _C α _C	110.461	1.385
C β _C γ _C δ	113.040	1.278	C β _C γ _C δ	111.807	1.560
C δ _N ϵ _C ζ	124.988	0.738	C δ _N ϵ _C ζ	124.916	1.152
C γ _C δ _N ϵ	111.689	1.956	C γ _C δ _N ϵ	112.153	2.179
N ϵ _C ζ _N η 1	120.569	1.315	N ϵ _C ζ _N η 1	120.771	1.065
N ϵ _C ζ _N η 2	119.890	1.166	N ϵ _C ζ _N η 2	119.714	0.970
N η 1_C ζ _N η 2	119.520	0.600	N η 1_C ζ _N η 2	119.498	0.797
N_C α _C	111.578	3.116	N_C α _C	110.918	2.815
N_C α _C β	111.579	1.236	N_C α _C β	111.106	1.187
ARG ptp-110 n = 77			ARG ptp-170 n = 388		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	67.597	8.250	chi1	67.375	7.654
chi2	-179.670	11.900	chi2	-175.630	12.219
chi3	64.784	10.049	chi3	68.232	9.651
chi4	-108.305	9.865	chi4	-172.286	15.957
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.792	1.933	C α _C β _C γ	114.528	1.455
C α _C_O	120.741	1.224	C α _C_O	120.563	0.963
C β _C α _C	110.403	1.416	C β _C α _C	110.408	1.567
C β _C γ _C δ	111.895	1.473	C β _C γ _C δ	111.291	1.743
C δ _N ϵ _C ζ	125.606	1.443	C δ _N ϵ _C ζ	124.582	1.140
C γ _C δ _N ϵ	111.728	2.285	C γ _C δ _N ϵ	111.416	1.628
N ϵ _C ζ _N η 1	120.996	1.421	N ϵ _C ζ _N η 1	120.454	0.937
N ϵ _C ζ _N η 2	119.559	1.566	N ϵ _C ζ _N η 2	119.760	0.930
N η 1_C ζ _N η 2	119.421	1.129	N η 1_C ζ _N η 2	119.756	0.920
N_C α _C	111.045	2.373	N_C α _C	111.331	2.560
N_C α _C β	110.983	1.300	N_C α _C β	110.785	1.148

ARG ptt180 n = 820			ARG ptt90 n = 814		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65.305	8.301	chi1	64.935	7.600
chi2	-177.454	10.432	chi2	178.802	12.292
chi3	-179.814	10.417	chi3	176.614	8.719
chi4	179.152	17.466	chi4	87.625	9.814
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.577	1.525	C α _C β _C γ	114.818	1.433
C α _C_O	120.578	1.008	C α _C_O	120.575	0.864
C β _C α _C	110.520	1.503	C β _C α _C	110.208	1.412
C β _C γ _C δ	111.129	2.013	C β _C γ _C δ	110.988	1.946
C δ _N ϵ _C ζ	124.433	1.099	C δ _N ϵ _C ζ	124.876	0.920
C γ _C δ _N ϵ	110.745	1.990	C γ _C δ _N ϵ	111.873	2.472
N ϵ _C ζ _N η 1	120.477	0.941	N ϵ _C ζ _N η 1	120.762	0.988
N ϵ _C ζ _N η 2	119.617	0.893	N ϵ _C ζ _N η 2	119.679	0.912
N η 1_C ζ _N η 2	119.887	0.877	N η 1_C ζ _N η 2	119.540	0.696
N_C α _C	111.325	2.492	N_C α _C	110.780	2.513
N_C α _C β	111.010	1.124	N_C α _C β	111.050	1.153
ARG ptt-90 n = 726			ARG ptm160 n = 502		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	66.303	7.908	chi1	63.484	8.731
chi2	-175.118	12.037	chi2	-179.108	14.966
chi3	-176.524	8.892	chi3	-67.148	9.716
chi4	-87.098	11.825	chi4	165.337	25.706
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.840	1.508	C α _C β _C γ	114.588	1.635
C α _C_O	120.486	0.935	C α _C_O	120.504	0.978
C β _C α _C	110.455	1.554	C β _C α _C	110.438	1.556
C β _C γ _C δ	110.983	2.037	C β _C γ _C δ	111.713	1.805
C δ _N ϵ _C ζ	124.865	1.144	C δ _N ϵ _C ζ	124.678	1.394
C γ _C δ _N ϵ	111.656	2.664	C γ _C δ _N ϵ	111.548	2.110
N ϵ _C ζ _N η 1	120.763	1.014	N ϵ _C ζ _N η 1	120.580	1.282
N ϵ _C ζ _N η 2	119.688	1.138	N ϵ _C ζ _N η 2	119.717	1.123
N η 1_C ζ _N η 2	119.527	1.027	N η 1_C ζ _N η 2	119.683	1.001
N_C α _C	111.666	2.550	N_C α _C	110.949	2.570
N_C α _C β	110.954	1.159	N_C α _C β	111.004	1.273

ARG ptm-80 n = 215			ARG pmt100 n = 4		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65.373	8.260	chi1	70.210	7.245
chi2	-178.472	14.370	chi2	-90.541	9.055
chi3	-66.034	10.269	chi3	-174.190	5.432
chi4	-84.515	10.828	chi4	97.849	2.006
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.564	1.281	C α _C β _C γ	115.830	0.421
C α _C_O	120.421	0.844	C α _C_O	120.581	0.283
C β _C α _C	110.304	1.382	C β _C α _C	110.812	0.494
C β _C γ _C δ	111.894	1.743	C β _C γ _C δ	112.728	0.575
C δ _N ϵ _C ζ	124.963	1.432	C δ _N ϵ _C ζ	125.083	0.125
C γ _C δ _N ϵ	112.362	2.279	C γ _C δ _N ϵ	111.181	0.920
N ϵ _C ζ _N η 1	120.717	1.214	N ϵ _C ζ _N η 1	120.967	0.288
N ϵ _C ζ _N η 2	119.898	1.456	N ϵ _C ζ _N η 2	119.634	0.266
N η 1_C ζ _N η 2	119.365	0.871	N η 1_C ζ _N η 2	119.397	0.052
N_C α _C	111.616	2.543	N_C α _C	110.231	1.442
N_C α _C β	110.971	1.307	N_C α _C β	111.390	0.423
ARG pmt170 n = 39			ARG pmt-80 n = 27		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	73.963	11.193	chi1	81.229	9.292
chi2	-78.972	15.367	chi2	-68.144	7.568
chi3	-169.420	10.139	chi3	-176.905	10.963
chi4	-169.441	15.119	chi4	-84.063	8.317
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	116.291	1.188	C α _C β _C γ	115.767	1.164
C α _C_O	120.751	0.702	C α _C_O	120.964	0.647
C β _C α _C	110.782	1.123	C β _C α _C	110.281	1.017
C β _C γ _C δ	112.734	1.257	C β _C γ _C δ	113.254	1.792
C δ _N ϵ _C ζ	124.390	1.048	C δ _N ϵ _C ζ	124.929	0.992
C γ _C δ _N ϵ	111.561	1.865	C γ _C δ _N ϵ	112.132	1.754
N ϵ _C ζ _N η 1	120.368	0.782	N ϵ _C ζ _N η 1	120.989	0.889
N ϵ _C ζ _N η 2	119.973	0.643	N ϵ _C ζ _N η 2	119.623	0.599
N η 1_C ζ _N η 2	119.646	0.558	N η 1_C ζ _N η 2	119.368	0.601
N_C α _C	110.725	2.400	N_C α _C	110.720	2.032
N_C α _C β	111.788	1.071	N_C α _C β	111.393	1.156

ARG pmm150 n = 12			ARG pmm-80 n = 19		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	75.579	3.166	chi1	73.642	12.608
chi2	-75.440	5.561	chi2	-75.958	11.183
chi3	-64.975	6.260	chi3	-56.789	8.115
chi4	151.999	15.442	chi4	-81.265	7.401
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	116.190	1.499	C α _C β _C γ	115.931	1.019
C α _C_O	120.267	0.926	C α _C_O	120.769	0.553
C β _C α _C	110.409	1.045	C β _C α _C	110.942	1.227
C β _C γ _C δ	112.425	1.153	C β _C γ _C δ	113.505	1.558
C δ _N ϵ _C ζ	125.348	2.473	C δ _N ϵ _C ζ	125.145	1.080
C γ _C δ _N ϵ	111.569	2.064	C γ _C δ _N ϵ	112.540	1.304
N ϵ _C ζ _N η 1	121.076	1.741	N ϵ _C ζ _N η 1	120.428	0.947
N ϵ _C ζ _N η 2	119.660	1.033	N ϵ _C ζ _N η 2	120.291	0.953
N η 1_C ζ _N η 2	119.218	1.385	N η 1_C ζ _N η 2	119.271	0.671
N_C α _C	109.038	0.995	N_C α _C	109.672	2.434
N_C α _C β	112.126	0.964	N_C α _C β	111.608	1.001
ARG tpp80 n = 363			ARG tpp-160 n = 496		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177.765	10.251	chi1	178.900	9.622
chi2	65.211	10.679	chi2	65.564	10.745
chi3	59.806	9.544	chi3	65.339	9.826
chi4	84.211	9.112	chi4	-167.680	19.748
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.925	1.369	C α _C β _C γ	114.753	1.301
C α _C_O	120.516	0.750	C α _C_O	120.521	0.835
C β _C α _C	110.476	1.234	C β _C α _C	110.424	1.291
C β _C γ _C δ	112.970	1.585	C β _C γ _C δ	112.686	1.753
C δ _N ϵ _C ζ	124.999	1.053	C δ _N ϵ _C ζ	124.533	1.383
C γ _C δ _N ϵ	112.587	2.062	C γ _C δ _N ϵ	111.868	1.817
N ϵ _C ζ _N η 1	120.720	0.868	N ϵ _C ζ _N η 1	120.495	1.034
N ϵ _C ζ _N η 2	119.749	0.827	N ϵ _C ζ _N η 2	119.796	1.090
N η 1_C ζ _N η 2	119.512	0.717	N η 1_C ζ _N η 2	119.690	0.837
N_C α _C	110.795	2.025	N_C α _C	110.619	2.297
N_C α _C β	110.349	1.121	N_C α _C β	110.242	1.093

ARG tpt170 n = 825			ARG tpt90 n = 652		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.826	8.985	chi1	178.926	8.381
chi2	66.313	10.376	chi2	65.741	7.685
chi3	177.963	11.716	chi3	178.589	9.896
chi4	171.354	19.311	chi4	86.350	10.296
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.515	1.233	C α _C β _C γ	114.718	1.274
C α _C_O	120.510	0.735	C α _C_O	120.469	0.802
C β _C α _C	110.571	1.154	C β _C α _C	110.288	1.182
C β _C γ _C δ	112.241	1.705	C β _C γ _C δ	112.118	1.671
C δ _N ϵ _C ζ	124.487	1.136	C δ _N ϵ _C ζ	124.798	0.923
C γ _C δ _N ϵ	110.851	1.868	C γ _C δ _N ϵ	111.919	2.267
N ϵ _C ζ _N η 1	120.532	0.938	N ϵ _C ζ _N η 1	120.812	0.967
N ϵ _C ζ _N η 2	119.674	0.880	N ϵ _C ζ _N η 2	119.714	0.888
N η 1_C ζ _N η 2	119.775	0.857	N η 1_C ζ _N η 2	119.453	0.822
N_C α _C	110.743	1.989	N_C α _C	111.449	2.056
N_C α _C β	110.225	1.192	N_C α _C β	110.205	1.088
ARG tpt-90 n = 365			ARG tpm170 n = 110		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	179.343	8.403	chi1	178.317	8.113
chi2	67.144	10.829	chi2	70.416	10.901
chi3	-179.669	8.849	chi3	-85.345	12.809
chi4	-89.385	12.210	chi4	171.668	18.570
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.741	1.251	C α _C β _C γ	115.637	1.263
C α _C_O	120.494	0.717	C α _C_O	120.626	0.802
C β _C α _C	110.562	1.204	C β _C α _C	110.602	1.333
C β _C γ _C δ	112.371	1.618	C β _C γ _C δ	112.785	2.167
C δ _N ϵ _C ζ	124.855	1.145	C δ _N ϵ _C ζ	124.702	2.252
C γ _C δ _N ϵ	111.131	2.518	C γ _C δ _N ϵ	111.970	2.147
N ϵ _C ζ _N η 1	120.736	1.033	N ϵ _C ζ _N η 1	120.476	1.046
N ϵ _C ζ _N η 2	119.671	1.050	N ϵ _C ζ _N η 2	119.776	0.905
N η 1_C ζ _N η 2	119.568	0.730	N η 1_C ζ _N η 2	119.734	0.745
N_C α _C	110.867	2.153	N_C α _C	111.099	1.434
N_C α _C β	110.203	1.187	N_C α _C β	109.942	1.120

ARG tpm-80 n = 20			ARG ttp80 n = 1896		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177.264	5.162	chi1	-177.383	8.162
chi2	78.524	8.234	chi2	179.646	13.425
chi3	-80.359	10.382	chi3	62.978	9.944
chi4	-79.824	9.071	chi4	82.895	9.577
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	115.170	1.379	C α _C β _C γ	113.686	1.495
C α _C_O	120.653	1.054	C α _C_O	120.681	0.798
C β _C α _C	110.318	1.131	C β _C α _C	110.045	1.208
C β _C γ _C δ	113.047	1.221	C β _C γ _C δ	112.080	1.526
C δ _N ϵ _C ζ	125.229	1.191	C δ _N ϵ _C ζ	124.882	1.039
C γ _C δ _N ϵ	113.709	2.206	C γ _C δ _N ϵ	112.575	1.938
N ϵ _C ζ _N η 1	120.646	0.958	N ϵ _C ζ _N η 1	120.750	0.949
N ϵ _C ζ _N η 2	120.052	0.924	N ϵ _C ζ _N η 2	119.766	0.857
N η 1_C ζ _N η 2	119.284	0.631	N η 1_C ζ _N η 2	119.465	0.753
N_C α _C	110.800	1.483	N_C α _C	110.748	2.056
N_C α _C β	109.849	1.128	N_C α _C β	110.433	1.201
ARG ttp-110 n = 623			ARG ttp-170 n = 1533		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.744	8.457	chi1	-175.447	9.345
chi2	177.160	12.953	chi2	179.359	13.232
chi3	64.599	10.746	chi3	66.850	8.993
chi4	-113.458	9.867	chi4	-171.036	17.274
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.826	1.633	C α _C β _C γ	113.660	1.651
C α _C_O	120.605	0.798	C α _C_O	120.595	0.757
C β _C α _C	110.158	1.233	C β _C α _C	110.009	1.236
C β _C γ _C δ	112.012	1.748	C β _C γ _C δ	111.642	1.683
C δ _N ϵ _C ζ	125.367	1.360	C δ _N ϵ _C ζ	124.480	1.169
C γ _C δ _N ϵ	111.876	2.159	C γ _C δ _N ϵ	111.497	1.581
N ϵ _C ζ _N η 1	121.079	1.283	N ϵ _C ζ _N η 1	120.455	0.896
N ϵ _C ζ _N η 2	119.474	1.161	N ϵ _C ζ _N η 2	119.763	0.881
N η 1_C ζ _N η 2	119.427	0.887	N η 1_C ζ _N η 2	119.764	0.703
N_C α _C	110.684	2.176	N_C α _C	110.456	2.209
N_C α _C β	110.314	1.287	N_C α _C β	110.433	1.313

ARG ttt180 n = 2339			ARG ttt90 n = 1057		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.225	9.097	chi1	-176.157	9.260
chi2	176.468	11.186	chi2	176.118	10.807
chi3	178.543	11.535	chi3	176.454	9.628
chi4	179.245	18.746	chi4	86.745	10.847
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.475	1.785	C α _C β _C γ	113.859	1.696
C α _C_O	120.570	0.812	C α _C_O	120.572	0.794
C β _C α _C	110.176	1.171	C β _C α _C	110.230	1.247
C β _C γ _C δ	111.351	2.189	C β _C γ _C δ	111.326	2.078
C δ _N ϵ _C ζ	124.329	1.194	C δ _N ϵ _C ζ	124.757	1.007
C γ _C δ _N ϵ	110.653	1.920	C γ _C δ _N ϵ	111.615	2.616
N ϵ _C ζ _N η 1	120.399	0.902	N ϵ _C ζ _N η 1	120.741	1.016
N ϵ _C ζ _N η 2	119.608	0.915	N ϵ _C ζ _N η 2	119.607	0.998
N η 1_C ζ _N η 2	119.974	0.814	N η 1_C ζ _N η 2	119.628	0.738
N_C α _C	110.517	2.410	N_C α _C	110.528	2.396
N_C α _C β	110.183	1.389	N_C α _C β	110.355	1.373
ARG ttt-90 n = 1380			ARG ttm110 n = 725		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.754	9.438	chi1	-175.260	8.991
chi2	177.849	11.450	chi2	178.639	9.463
chi3	-178.261	9.915	chi3	-64.314	10.708
chi4	-89.587	12.519	chi4	112.805	9.769
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.964	1.616	C α _C β _C γ	113.881	1.635
C α _C_O	120.540	0.793	C α _C_O	120.589	0.780
C β _C α _C	110.272	1.256	C β _C α _C	110.255	1.228
C β _C γ _C δ	110.941	2.077	C β _C γ _C δ	112.165	1.691
C δ _N ϵ _C ζ	124.821	1.167	C δ _N ϵ _C ζ	125.322	1.226
C γ _C δ _N ϵ	111.802	2.580	C γ _C δ _N ϵ	111.648	1.927
N ϵ _C ζ _N η 1	120.801	1.078	N ϵ _C ζ _N η 1	121.010	1.241
N ϵ _C ζ _N η 2	119.565	1.015	N ϵ _C ζ _N η 2	119.531	1.123
N η 1_C ζ _N η 2	119.613	0.869	N η 1_C ζ _N η 2	119.435	0.817
N_C α _C	110.382	2.296	N_C α _C	110.499	2.138
N_C α _C β	110.230	1.313	N_C α _C β	110.380	1.239

ARG t_{tm}170 n = 1317			ARG t_{tm}-80 n = 1504		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-177.285	9.924	chi1	-174.135	9.435
chi2	176.943	12.449	chi2	179.281	9.905
chi3	-67.797	9.912	chi3	-64.732	10.575
chi4	171.206	17.554	chi4	-84.522	9.745
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.752	1.740	C α -C β -C γ	113.668	1.664
C α -C-O	120.583	0.815	C α -C-O	120.532	0.789
C β -C α -C	110.105	1.164	C β -C α -C	110.241	1.238
C β -C γ -C δ	111.482	1.826	C β -C γ -C δ	111.990	1.645
C δ -N ϵ -C ζ	124.437	1.166	C δ -N ϵ -C ζ	124.859	1.304
C γ -C δ -N ϵ	111.263	1.652	C γ -C δ -N ϵ	112.437	2.033
N ϵ -C ζ -N η 1	120.519	0.959	N ϵ -C ζ -N η 1	120.726	1.016
N ϵ -C ζ -N η 2	119.735	0.929	N ϵ -C ζ -N η 2	119.733	1.037
N η 1-C ζ -N η 2	119.728	0.835	N η 1-C ζ -N η 2	119.521	0.763
N-C α -C	110.279	2.382	N-C α -C	110.578	2.257
N-C α -C β	110.267	1.337	N-C α -C β	110.372	1.356
ARG t_{mt}170 n = 104			ARG t_{mt}90 n = 23		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-173.869	12.307	chi1	-178.402	9.228
chi2	-91.306	12.725	chi2	-93.565	9.120
chi3	-173.542	9.380	chi3	-177.879	11.168
chi4	-170.971	17.524	chi4	87.027	11.977
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.031	1.334	C α -C β -C γ	115.152	1.485
C α -C-O	120.633	0.742	C α -C-O	120.604	0.982
C β -C α -C	110.891	1.069	C β -C α -C	110.471	1.327
C β -C γ -C δ	112.702	1.716	C β -C γ -C δ	112.863	2.341
C δ -N ϵ -C ζ	124.499	0.904	C δ -N ϵ -C ζ	125.096	1.261
C γ -C δ -N ϵ	110.712	1.619	C γ -C δ -N ϵ	111.403	2.847
N ϵ -C ζ -N η 1	120.677	1.032	N ϵ -C ζ -N η 1	120.873	1.858
N ϵ -C ζ -N η 2	119.571	0.805	N ϵ -C ζ -N η 2	119.647	1.458
N η 1-C ζ -N η 2	119.736	0.716	N η 1-C ζ -N η 2	119.441	0.740
N-C α -C	108.533	3.170	N-C α -C	110.308	1.542
N-C α -C β	109.989	1.249	N-C α -C β	109.926	1.134

ARG tmt-80 n = 62			ARG tmm160 n = 92		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.441	10.751	chi1	-172.150	10.890
chi2	-92.932	11.363	chi2	-90.073	11.146
chi3	-177.757	10.023	chi3	-61.282	11.279
chi4	-84.998	11.504	chi4	163.764	18.601
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.665	1.340	C α _C β _C γ	114.825	1.323
C α _C_O	120.545	0.772	C α _C_O	120.627	0.803
C β _C α _C	111.341	1.330	C β _C α _C	111.278	1.113
C β _C γ _C δ	112.460	1.924	C β _C γ _C δ	112.552	1.822
C δ _N ϵ _C ζ	124.688	1.117	C δ _N ϵ _C ζ	124.630	1.190
C γ _C δ _N ϵ	111.211	2.142	C γ _C δ _N ϵ	111.887	1.925
N ϵ _C ζ _N η 1	120.610	0.908	N ϵ _C ζ _N η 1	120.655	1.000
N ϵ _C ζ _N η 2	119.729	0.896	N ϵ _C ζ _N η 2	119.705	0.893
N η 1_C ζ _N η 2	119.637	0.627	N η 1_C ζ _N η 2	119.616	0.813
N_C α _C	110.062	2.449	N_C α _C	109.950	2.048
N_C α _C β	110.064	1.027	N_C α _C β	110.061	1.132
ARG tmm-80 n = 71			ARG mpp80 n = 54		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.294	9.153	chi1	-76.744	11.753
chi2	-86.372	8.784	chi2	81.853	11.964
chi3	-56.434	10.717	chi3	57.995	7.391
chi4	-82.108	8.527	chi4	84.630	10.143
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	115.257	1.317	C α _C β _C γ	115.469	1.724
C α _C_O	120.621	0.778	C α _C_O	120.418	1.087
C β _C α _C	111.061	1.008	C β _C α _C	109.200	1.982
C β _C γ _C δ	113.720	2.294	C β _C γ _C δ	113.558	1.616
C δ _N ϵ _C ζ	124.893	1.247	C δ _N ϵ _C ζ	124.998	1.163
C γ _C δ _N ϵ	112.553	1.891	C γ _C δ _N ϵ	113.125	2.284
N ϵ _C ζ _N η 1	120.861	1.095	N ϵ _C ζ _N η 1	120.782	1.174
N ϵ _C ζ _N η 2	119.709	0.923	N ϵ _C ζ _N η 2	119.773	1.129
N η 1_C ζ _N η 2	119.397	0.720	N η 1_C ζ _N η 2	119.423	0.733
N_C α _C	109.672	1.698	N_C α _C	109.653	2.541
N_C α _C β	110.067	1.009	N_C α _C β	111.451	1.261

ARG mpp-170 n = 64			ARG mpt180 n = 245		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-78.876	12.884	chi1	-84.592	7.996
chi2	81.734	17.402	chi2	69.331	13.073
chi3	65.059	7.427	chi3	173.629	9.351
chi4	-166.895	16.426	chi4	174.437	16.771
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.639	1.431	C α _C β _C γ	114.779	1.423
C α _C_O	120.527	0.677	C α _C_O	120.561	0.858
C β _C α _C	109.707	1.574	C β _C α _C	109.479	1.658
C β _C γ _C δ	112.675	1.744	C β _C γ _C δ	113.013	1.809
C δ _N ϵ _C ζ	124.456	1.194	C δ _N ϵ _C ζ	124.423	1.453
C γ _C δ _N ϵ	111.467	1.342	C γ _C δ _N ϵ	110.690	1.999
N ϵ _C ζ _N η 1	120.599	1.057	N ϵ _C ζ _N η 1	120.410	1.021
N ϵ _C ζ _N η 2	119.723	0.761	N ϵ _C ζ _N η 2	119.733	0.916
N η 1_C ζ _N η 2	119.659	0.703	N η 1_C ζ _N η 2	119.829	0.881
N_C α _C	109.974	3.124	N_C α _C	109.972	2.748
N_C α _C β	111.366	1.108	N_C α _C β	111.150	1.151
ARG mpt90 n = 46			ARG mpt-90 n = 85		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-76.133	12.907	chi1	-78.778	13.914
chi2	84.673	13.588	chi2	74.660	16.331
chi3	170.244	9.730	chi3	177.663	9.619
chi4	93.427	11.198	chi4	-87.847	13.667
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.631	1.635	C α _C β _C γ	114.921	1.261
C α _C_O	120.402	0.642	C α _C_O	120.436	0.752
C β _C α _C	109.251	1.434	C β _C α _C	109.954	1.553
C β _C γ _C δ	112.529	1.552	C β _C γ _C δ	112.861	2.301
C δ _N ϵ _C ζ	125.102	0.846	C δ _N ϵ _C ζ	124.891	0.998
C γ _C δ _N ϵ	111.041	2.030	C γ _C δ _N ϵ	111.632	2.525
N ϵ _C ζ _N η 1	121.088	0.907	N ϵ _C ζ _N η 1	120.590	1.067
N ϵ _C ζ _N η 2	119.381	0.679	N ϵ _C ζ _N η 2	119.828	0.834
N η 1_C ζ _N η 2	119.512	0.586	N η 1_C ζ _N η 2	119.561	0.667
N_C α _C	109.965	2.682	N_C α _C	110.431	2.708
N_C α _C β	111.296	1.245	N_C α _C β	110.866	1.019

ARG mtp180 n = 2504			ARG mtp85 n = 1857		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-66.448	8.145	chi1	-66.328	8.550
chi2	178.975	13.041	chi2	177.775	11.188
chi3	66.423	9.133	chi3	64.643	9.713
chi4	-171.573	16.500	chi4	87.715	10.960
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.196	1.788	C α _C β _C γ	113.275	1.819
C α _C_O	120.474	0.834	C α _C_O	120.493	0.910
C β _C α _C	110.040	1.648	C β _C α _C	110.136	1.676
C β _C γ _C δ	111.714	1.807	C β _C γ _C δ	112.055	1.715
C δ _N ϵ _C ζ	124.376	1.212	C δ _N ϵ _C ζ	124.893	1.199
C γ _C δ _N ϵ	111.554	1.558	C γ _C δ _N ϵ	112.285	1.990
N ϵ _C ζ _N η 1	120.437	0.999	N ϵ _C ζ _N η 1	120.785	1.055
N ϵ _C ζ _N η 2	119.768	0.969	N ϵ _C ζ _N η 2	119.683	1.040
N η 1_C ζ _N η 2	119.779	0.774	N η 1_C ζ _N η 2	119.513	0.811
N_C α _C	111.426	2.415	N_C α _C	111.102	2.410
N_C α _C β	110.537	1.046	N_C α _C β	110.598	1.049
ARG mtp-110 n = 470			ARG mtt180 n = 4592		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-65.062	8.129	chi1	-67.383	7.802
chi2	179.092	10.812	chi2	179.853	11.020
chi3	66.411	11.580	chi3	-179.128	10.659
chi4	-109.636	9.635	chi4	177.093	17.916
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.354	1.662	C α _C β _C γ	112.906	1.753
C α _C_O	120.369	0.947	C α _C_O	120.449	0.847
C β _C α _C	110.075	1.684	C β _C α _C	109.969	1.657
C β _C γ _C δ	112.354	1.634	C β _C γ _C δ	111.523	2.022
C δ _N ϵ _C ζ	125.306	2.055	C δ _N ϵ _C ζ	124.359	1.101
C γ _C δ _N ϵ	111.671	1.878	C γ _C δ _N ϵ	110.625	1.820
N ϵ _C ζ _N η 1	121.057	1.200	N ϵ _C ζ _N η 1	120.426	0.894
N ϵ _C ζ _N η 2	119.441	1.295	N ϵ _C ζ _N η 2	119.625	0.896
N η 1_C ζ _N η 2	119.478	0.895	N η 1_C ζ _N η 2	119.931	0.794
N_C α _C	111.125	2.585	N_C α _C	111.576	2.328
N_C α _C β	110.743	1.052	N_C α _C β	110.570	1.047

ARG mtt90 n = 2460			ARG mtt-85 n = 2843		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67.677	7.504	chi1	-67.013	7.843
chi2	179.859	13.535	chi2	-178.550	10.650
chi3	178.901	10.625	chi3	-176.240	9.240
chi4	90.605	15.148	chi4	-88.795	11.677
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.347	1.719	C α _C β _C γ	113.460	1.703
C α _C_O	120.443	0.802	C α _C_O	120.445	0.822
C β _C α _C	109.894	1.726	C β _C α _C	109.838	1.651
C β _C γ _C δ	111.540	2.042	C β _C γ _C δ	111.361	1.969
C δ _N ϵ _C ζ	124.859	1.138	C δ _N ϵ _C ζ	124.795	1.053
C γ _C δ _N ϵ	111.010	2.492	C γ _C δ _N ϵ	111.412	2.434
N ϵ _C ζ _N η 1	120.854	1.069	N ϵ _C ζ _N η 1	120.794	1.020
N ϵ _C ζ _N η 2	119.529	1.057	N ϵ _C ζ _N η 2	119.578	0.926
N η 1_C ζ _N η 2	119.591	0.803	N η 1_C ζ _N η 2	119.609	0.768
N_C α _C	111.444	2.403	N_C α _C	111.436	2.299
N_C α _C β	110.565	1.121	N_C α _C β	110.636	1.045
ARG mtm110 n = 781			ARG mtm180 n = 2407		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68.128	8.152	chi1	-66.409	8.111
chi2	-177.015	9.719	chi2	179.025	12.715
chi3	-68.916	10.245	chi3	-67.433	8.823
chi4	112.867	10.583	chi4	172.922	15.154
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.128	1.811	C α _C β _C γ	113.294	1.630
C α _C_O	120.427	0.902	C α _C_O	120.456	0.891
C β _C α _C	110.057	1.759	C β _C α _C	109.865	1.623
C β _C γ _C δ	112.410	1.719	C β _C γ _C δ	111.632	1.675
C δ _N ϵ _C ζ	125.312	1.518	C δ _N ϵ _C ζ	124.437	1.082
C γ _C δ _N ϵ	112.087	1.885	C γ _C δ _N ϵ	111.358	1.691
N ϵ _C ζ _N η 1	121.057	1.278	N ϵ _C ζ _N η 1	120.426	0.896
N ϵ _C ζ _N η 2	119.445	1.122	N ϵ _C ζ _N η 2	119.771	0.882
N η 1_C ζ _N η 2	119.479	0.917	N η 1_C ζ _N η 2	119.785	0.768
N_C α _C	111.659	2.436	N_C α _C	111.291	2.634
N_C α _C β	110.673	1.037	N_C α _C β	110.532	1.054

ARG mtm-85 n = 2848			ARG mmp80 n = 164		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68.282	8.114	chi1	-62.526	6.654
chi2	-171.664	9.296	chi2	-75.134	12.697
chi3	-63.903	9.515	chi3	74.408	11.683
chi4	-88.066	8.888	chi4	77.834	6.858
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	113.529	1.560	C α _C β _C γ	114.756	1.393
C α _C_O	120.475	0.810	C α _C_O	120.405	0.951
C β _C α _C	110.037	1.494	C β _C α _C	109.795	1.486
C β _C γ _C δ	111.973	1.573	C β _C γ _C δ	113.417	1.619
C δ _N ϵ _C ζ	124.892	1.167	C δ _N ϵ _C ζ	125.034	1.158
C γ _C δ _N ϵ	112.687	1.963	C γ _C δ _N ϵ	113.473	2.231
N ϵ _C ζ _N η 1	120.777	1.028	N ϵ _C ζ _N η 1	120.554	0.995
N ϵ _C ζ _N η 2	119.743	1.003	N ϵ _C ζ _N η 2	119.976	0.857
N η 1_C ζ _N η 2	119.464	0.785	N η 1_C ζ _N η 2	119.450	0.642
N_C α _C	111.343	1.972	N_C α _C	111.399	1.818
N_C α _C β	111.054	1.026	N_C α _C β	110.883	0.931
ARG mmp-170 n = 123			ARG mmt180 n = 1203		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-64.124	7.185	chi1	-61.912	9.054
chi2	-65.485	14.262	chi2	-68.373	12.909
chi3	85.873	9.711	chi3	-176.971	11.256
chi4	-167.047	19.760	chi4	-176.339	17.437
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	115.470	1.274	C α _C β _C γ	114.493	1.380
C α _C_O	120.374	0.989	C α _C_O	120.394	0.872
C β _C α _C	109.451	1.525	C β _C α _C	109.365	1.625
C β _C γ _C δ	112.812	1.743	C β _C γ _C δ	112.048	1.715
C δ _N ϵ _C ζ	124.848	1.315	C δ _N ϵ _C ζ	124.422	1.187
C γ _C δ _N ϵ	111.535	1.611	C γ _C δ _N ϵ	110.995	1.829
N ϵ _C ζ _N η 1	120.505	1.207	N ϵ _C ζ _N η 1	120.487	0.873
N ϵ _C ζ _N η 2	119.752	1.096	N ϵ _C ζ _N η 2	119.663	0.872
N η 1_C ζ _N η 2	119.724	1.141	N η 1_C ζ _N η 2	119.830	0.740
N_C α _C	111.010	2.146	N_C α _C	111.227	2.571
N_C α _C β	111.080	1.123	N_C α _C β	110.702	1.071

ARG mmt90 n = 567			ARG mmt-90 n = 1428		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-60.697	8.808	chi1	-63.806	6.649
chi2	-68.408	12.498	chi2	-68.992	8.052
chi3	179.437	10.449	chi3	-175.179	7.656
chi4	90.018	12.895	chi4	-91.022	11.109
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.636	1.391	C α _C β _C γ	114.535	1.429
C α _C_O	120.470	0.870	C α _C_O	120.522	0.849
C β _C α _C	109.542	1.648	C β _C α _C	109.577	1.636
C β _C γ _C δ	112.219	1.613	C β _C γ _C δ	112.031	1.668
C δ _N ϵ _C ζ	124.948	1.236	C δ _N ϵ _C ζ	124.921	0.997
C γ _C δ _N ϵ	111.566	2.487	C γ _C δ _N ϵ	111.800	2.277
N ϵ _C ζ _N η 1	120.843	1.216	N ϵ _C ζ _N η 1	120.940	0.997
N ϵ _C ζ _N η 2	119.554	1.095	N ϵ _C ζ _N η 2	119.615	0.880
N η 1_C ζ _N η 2	119.578	0.717	N η 1_C ζ _N η 2	119.419	0.824
N_C α _C	111.367	2.715	N_C α _C	110.068	2.671
N_C α _C β	110.685	1.076	N_C α _C β	110.879	1.109
ARG mmm160 n = 951			ARG mmm-85 n = 1022		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-61.827	9.224	chi1	-63.497	9.155
chi2	-66.167	13.742	chi2	-67.585	10.864
chi3	-64.223	9.924	chi3	-60.741	9.180
chi4	163.153	24.183	chi4	-86.156	10.081
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α _C β _C γ	114.464	1.598	C α _C β _C γ	114.631	1.520
C α _C_O	120.403	0.880	C α _C_O	120.548	0.882
C β _C α _C	109.780	1.544	C β _C α _C	109.688	1.537
C β _C γ _C δ	112.547	1.734	C β _C γ _C δ	112.840	1.621
C δ _N ϵ _C ζ	124.581	1.313	C δ _N ϵ _C ζ	124.979	1.088
C γ _C δ _N ϵ	111.850	1.891	C γ _C δ _N ϵ	112.452	2.260
N ϵ _C ζ _N η 1	120.567	1.167	N ϵ _C ζ _N η 1	120.857	1.007
N ϵ _C ζ _N η 2	119.783	1.115	N ϵ _C ζ _N η 2	119.638	0.965
N η 1_C ζ _N η 2	119.627	0.771	N η 1_C ζ _N η 2	119.485	0.827
N_C α _C	111.421	2.426	N_C α _C	111.267	2.645
N_C α _C β	110.746	1.182	N_C α _C β	110.750	1.121

S5.18 LYS

LYS pttt n = 25			LYS ptpp n = 89		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64.183	7.527	chi1	65.327	6.803
chi2	89.871	8.334	chi2	178.405	8.068
chi3	175.578	11.861	chi3	72.033	9.721
chi4	179.092	7.380	chi4	66.034	8.135
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.057	1.244	C α -C β -C γ	114.569	1.201
C α -C-O	120.408	0.698	C α -C-O	120.169	0.968
C β -C α -C	111.303	1.430	C β -C α -C	110.070	1.280
C β -C γ -C δ	112.212	1.704	C β -C γ -C δ	112.209	1.294
C δ -C ϵ -N ζ	111.319	1.822	C δ -C ϵ -N ζ	112.484	1.716
C γ -C δ -C ϵ	110.556	1.940	C γ -C δ -C ϵ	112.719	1.335
N-C α -C	111.714	2.089	N-C α -C	111.895	2.034
N-C α -C β	111.577	1.190	N-C α -C β	110.924	1.307
LYS ptpt n = 148			LYS pttp n = 240		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	64.802	8.153	chi1	67.562	8.269
chi2	179.088	11.802	chi2	-179.054	10.390
chi3	72.966	10.396	chi3	178.259	11.216
chi4	174.545	11.210	chi4	66.699	12.279
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.721	1.636	C α -C β -C γ	114.794	1.433
C α -C-O	120.525	0.854	C α -C-O	120.380	0.901
C β -C α -C	110.518	1.433	C β -C α -C	110.362	1.449
C β -C γ -C δ	112.144	1.650	C β -C γ -C δ	110.892	1.675
C δ -C ϵ -N ζ	111.436	2.103	C δ -C ϵ -N ζ	112.359	2.336
C γ -C δ -C ϵ	112.378	1.854	C γ -C δ -C ϵ	111.720	1.424
N-C α -C	111.237	2.936	N-C α -C	111.801	2.552
N-C α -C β	111.124	1.321	N-C α -C β	110.983	1.091
LYS pttt n = 1385			LYS pttm n = 268		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	65.436	7.578	chi1	64.251	6.915
chi2	-178.083	8.650	chi2	-177.627	9.133
chi3	-179.332	9.673	chi3	-178.897	9.970
chi4	-179.680	9.634	chi4	-67.053	11.673
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.839	1.455	C α -C β -C γ	114.862	1.467
C α -C-O	120.431	0.948	C α -C-O	120.393	0.977
C β -C α -C	110.437	1.381	C β -C α -C	110.414	1.447
C β -C γ -C δ	110.833	1.793	C β -C γ -C δ	110.696	2.050
C δ -C ϵ -N ζ	111.334	2.005	C δ -C ϵ -N ζ	112.324	2.369
C γ -C δ -C ϵ	111.005	1.621	C γ -C δ -C ϵ	111.942	1.508
N-C α -C	111.317	2.768	N-C α -C	111.970	2.550
N-C α -C β	111.134	1.099	N-C α -C β	110.983	1.162

LYS ptmt n = 187			LYS ptmm n = 80		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	66.652	8.246	chi1	66.614	8.388
chi2	-175.856	12.044	chi2	-177.929	9.983
chi3	-71.430	11.735	chi3	-69.614	9.844
chi4	-175.836	10.337	chi4	-66.129	7.000
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.548	1.572	C α -C β -C γ	114.458	1.301
C α -C-O	120.513	0.972	C α -C-O	120.630	1.032
C β -C α -C	110.429	1.608	C β -C α -C	109.915	1.495
C β -C γ -C δ	112.146	1.576	C β -C γ -C δ	112.342	1.435
C δ -C ϵ -N ζ	111.541	2.110	C δ -C ϵ -N ζ	112.989	1.776
C γ -C δ -C ϵ	112.363	1.870	C γ -C δ -C ϵ	112.999	1.154
N-C α -C	111.050	2.718	N-C α -C	110.495	2.702
N-C α -C β	111.011	1.103	N-C α -C β	110.827	1.205
LYS pmmt n = 10			LYS tppp n = 37		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	73.156	8.365	chi1	-177.926	11.531
chi2	-74.065	10.515	chi2	62.258	10.078
chi3	-168.029	10.580	chi3	65.517	7.785
chi4	-174.606	10.738	chi4	67.940	11.330
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	116.445	1.641	C α -C β -C γ	115.134	1.503
C α -C-O	120.801	0.552	C α -C-O	120.707	0.872
C β -C α -C	110.351	1.279	C β -C α -C	110.330	0.746
C β -C γ -C δ	112.587	2.234	C β -C γ -C δ	113.479	1.870
C δ -C ϵ -N ζ	111.694	2.248	C δ -C ϵ -N ζ	112.983	1.698
C γ -C δ -C ϵ	111.327	1.312	C γ -C δ -C ϵ	113.390	1.737
N-C α -C	109.953	2.378	N-C α -C	110.891	1.930
N-C α -C β	112.145	2.128	N-C α -C β	110.228	1.115
LYS tppt n = 272			LYS tppt n = 409		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.194	7.887	chi1	-179.932	7.986
chi2	63.490	8.924	chi2	67.443	10.399
chi3	69.535	9.197	chi3	173.601	13.550
chi4	177.447	9.361	chi4	66.191	12.980
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.823	1.234	C α -C β -C γ	114.807	1.338
C α -C-O	120.535	0.743	C α -C-O	120.530	0.826
C β -C α -C	110.620	1.101	C β -C α -C	110.226	1.227
C β -C γ -C δ	113.177	1.543	C β -C γ -C δ	112.085	1.487
C δ -C ϵ -N ζ	111.201	1.842	C δ -C ϵ -N ζ	112.676	1.952
C γ -C δ -C ϵ	112.378	1.445	C γ -C δ -C ϵ	112.158	1.313
N-C α -C	110.638	2.080	N-C α -C	110.254	2.081
N-C α -C β	110.328	1.075	N-C α -C β	110.339	1.125

LYS tppt n = 1228			LYS tpm n = 197		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.908	9.092	chi1	-177.928	7.615
chi2	69.056	9.015	chi2	67.158	9.702
chi3	175.565	10.063	chi3	-179.368	11.396
chi4	177.246	12.306	chi4	-66.243	13.423
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.773	1.314	C α -C β -C γ	114.983	1.451
C α -C-O	120.549	0.775	C α -C-O	120.391	0.767
C β -C α -C	110.423	1.219	C β -C α -C	110.392	1.099
C β -C γ -C δ	112.033	1.596	C β -C γ -C δ	111.930	1.409
C δ -C ϵ -N ζ	111.116	2.237	C δ -C ϵ -N ζ	112.550	2.065
C γ -C δ -C ϵ	111.028	1.474	C γ -C δ -C ϵ	111.891	1.350
N-C α -C	110.655	2.152	N-C α -C	110.288	2.061
N-C α -C β	110.224	1.113	N-C α -C β	110.274	1.138
LYS ttpp n = 229			LYS ttpt n = 883		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-178.427	8.557	chi1	-178.343	8.129
chi2	174.058	14.474	chi2	174.555	12.116
chi3	71.618	11.151	chi3	73.017	11.886
chi4	68.201	10.487	chi4	175.105	11.316
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.658	1.575	C α -C β -C γ	113.777	1.645
C α -C-O	120.629	0.777	C α -C-O	120.604	0.755
C β -C α -C	110.131	1.263	C β -C α -C	110.066	1.179
C β -C γ -C δ	112.134	1.677	C β -C γ -C δ	112.121	1.474
C δ -C ϵ -N ζ	112.810	2.349	C δ -C ϵ -N ζ	111.088	2.074
C γ -C δ -C ϵ	112.800	1.569	C γ -C δ -C ϵ	112.173	1.575
N-C α -C	110.229	2.480	N-C α -C	110.329	2.318
N-C α -C β	110.369	1.468	N-C α -C β	110.243	1.317
LYS ttpm n = 4			LYS tttp n = 1233		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-176.905	10.026	chi1	-177.650	8.068
chi2	175.311	6.851	chi2	175.444	9.877
chi3	87.099	18.038	chi3	173.929	10.830
chi4	-84.400	4.171	chi4	65.901	12.780
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.353	1.109	C α -C β -C γ	113.932	1.516
C α -C-O	120.752	0.322	C α -C-O	120.582	0.750
C β -C α -C	110.281	0.444	C β -C α -C	110.189	1.092
C β -C γ -C δ	111.616	0.992	C β -C γ -C δ	111.148	1.611
C δ -C ϵ -N ζ	113.892	1.178	C δ -C ϵ -N ζ	112.268	1.984
C γ -C δ -C ϵ	113.140	0.242	C γ -C δ -C ϵ	111.826	1.347
N-C α -C	110.149	1.306	N-C α -C	110.703	2.222
N-C α -C β	110.149	0.835	N-C α -C β	110.410	1.138

LYS tttt n = 5043			LYS tttm n = 1176		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-175.451	8.188	chi1	-176.393	8.096
chi2	176.592	8.732	chi2	177.818	9.663
chi3	179.677	9.233	chi3	-176.243	10.489
chi4	-179.889	10.261	chi4	-67.353	12.094
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.874	1.525	C α -C β -C γ	113.887	1.596
C α -C-O	120.583	0.778	C α -C-O	120.552	0.824
C β -C α -C	110.243	1.137	C β -C α -C	110.254	1.139
C β -C γ -C δ	111.148	1.744	C β -C γ -C δ	111.029	1.702
C δ -C ϵ -N ζ	111.156	1.986	C δ -C ϵ -N ζ	112.329	1.971
C γ -C δ -C ϵ	111.042	1.543	C γ -C δ -C ϵ	111.847	1.465
N-C α -C	110.545	2.283	N-C α -C	110.514	2.115
N-C α -C β	110.335	1.206	N-C α -C β	110.424	1.165
LYS ttmp n = 9			LYS ttmt n = 674		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.170	4.238	chi1	-174.573	9.441
chi2	-179.415	8.457	chi2	-177.288	10.835
chi3	-95.701	18.562	chi3	-73.479	11.719
chi4	76.743	25.218	chi4	-175.112	11.548
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.206	1.243	C α -C β -C γ	113.686	1.546
C α -C-O	120.593	0.500	C α -C-O	120.604	0.865
C β -C α -C	110.316	1.623	C β -C α -C	110.214	1.180
C β -C γ -C δ	112.630	1.745	C β -C γ -C δ	112.161	1.524
C δ -C ϵ -N ζ	114.038	1.362	C δ -C ϵ -N ζ	110.881	2.322
C γ -C δ -C ϵ	112.905	0.737	C γ -C δ -C ϵ	112.229	1.651
N-C α -C	110.754	1.510	N-C α -C	110.307	2.331
N-C α -C β	111.426	1.042	N-C α -C β	110.339	1.250
LYS ttmm n = 197			LYS tmtp n = 11		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-174.055	8.490	chi1	-176.649	7.525
chi2	179.742	9.943	chi2	-97.994	8.314
chi3	-71.028	11.891	chi3	-178.365	12.353
chi4	-67.045	11.420	chi4	65.083	7.821
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.643	1.459	C α -C β -C γ	114.616	1.223
C α -C-O	120.558	0.817	C α -C-O	120.800	0.413
C β -C α -C	110.229	1.285	C β -C α -C	110.486	0.704
C β -C γ -C δ	112.136	1.574	C β -C γ -C δ	112.010	1.506
C δ -C ϵ -N ζ	112.648	2.300	C δ -C ϵ -N ζ	113.099	3.033
C γ -C δ -C ϵ	112.487	1.564	C γ -C δ -C ϵ	111.842	1.204
N-C α -C	110.191	2.445	N-C α -C	110.140	3.054
N-C α -C β	110.327	1.394	N-C α -C β	110.368	0.871

LYS tmtt n = 82			LYS tmtm n = 20		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-172.661	8.464	chi1	-172.233	10.447
chi2	-91.117	9.621	chi2	-90.510	5.572
chi3	-176.853	11.750	chi3	-172.543	15.072
chi4	-178.511	10.695	chi4	-64.869	7.732
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.500	1.145	C α -C β -C γ	115.452	1.619
C α -C-O	120.778	0.610	C α -C-O	120.586	0.646
C β -C α -C	110.869	1.093	C β -C α -C	110.984	0.853
C β -C γ -C δ	111.882	1.443	C β -C γ -C δ	112.208	1.226
C δ -C ϵ -N ζ	110.842	2.070	C δ -C ϵ -N ζ	112.679	1.691
C γ -C δ -C ϵ	111.015	1.375	C γ -C δ -C ϵ	111.998	1.546
N-C α -C	110.180	1.891	N-C α -C	110.089	1.720
N-C α -C β	110.078	0.810	N-C α -C β	109.782	0.789
LYS tmmt n = 33			LYS tmmm n = 8		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-179.225	9.981	chi1	-177.527	11.864
chi2	-93.418	12.058	chi2	-81.761	7.499
chi3	-70.433	8.917	chi3	-63.102	8.026
chi4	-179.549	10.245	chi4	-64.475	4.939
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.020	1.846	C α -C β -C γ	116.243	2.695
C α -C-O	120.544	0.877	C α -C-O	120.272	0.848
C β -C α -C	110.741	1.116	C β -C α -C	111.246	1.126
C β -C γ -C δ	113.459	1.734	C β -C γ -C δ	114.871	1.367
C δ -C ϵ -N ζ	110.756	2.859	C δ -C ϵ -N ζ	113.141	1.476
C γ -C δ -C ϵ	112.411	2.864	C γ -C δ -C ϵ	114.998	1.617
N-C α -C	109.953	2.155	N-C α -C	108.983	2.013
N-C α -C β	109.895	1.083	N-C α -C β	109.523	1.258
LYS mppt n = 31			LYS mppt n = 26		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-82.599	8.918	chi1	-74.901	18.526
chi2	73.518	14.873	chi2	86.563	18.186
chi3	69.157	8.044	chi3	171.631	8.992
chi4	177.385	5.414	chi4	65.232	12.143
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	115.111	1.987	C α -C β -C γ	114.682	1.564
C α -C-O	120.424	0.890	C α -C-O	120.477	1.133
C β -C α -C	109.879	1.228	C β -C α -C	110.099	1.428
C β -C γ -C δ	113.688	1.564	C β -C γ -C δ	113.211	2.501
C δ -C ϵ -N ζ	111.358	1.922	C δ -C ϵ -N ζ	113.419	2.262
C γ -C δ -C ϵ	112.185	1.373	C γ -C δ -C ϵ	112.501	2.718
N-C α -C	108.768	1.973	N-C α -C	110.602	2.774
N-C α -C β	110.907	0.923	N-C α -C β	110.868	1.039

LYS mptt n = 124			LYS mptm n = 11		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-79.911	13.282	chi1	-91.748	6.662
chi2	72.964	17.284	chi2	61.180	11.061
chi3	176.124	12.429	chi3	-173.655	5.358
chi4	175.095	11.920	chi4	-60.981	13.466
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	114.896	1.389	C α -C β -C γ	114.614	0.809
C α -C-O	120.553	0.785	C α -C-O	120.670	0.565
C β -C α -C	109.748	1.534	C β -C α -C	110.693	0.842
C β -C γ -C δ	112.619	2.029	C β -C γ -C δ	112.838	0.654
C δ -C ϵ -N ζ	110.877	2.274	C δ -C ϵ -N ζ	113.434	1.681
C γ -C δ -C ϵ	111.162	1.603	C γ -C δ -C ϵ	111.830	0.502
N-C α -C	110.579	2.594	N-C α -C	110.770	2.188
N-C α -C β	110.815	1.103	N-C α -C β	110.642	0.906
LYS mtpp n = 392			LYS mtpt n = 1357		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-68.535	7.507	chi1	-69.197	8.061
chi2	176.954	10.868	chi2	174.242	11.340
chi3	70.471	10.847	chi3	70.524	11.811
chi4	67.722	10.865	chi4	175.197	10.445
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.235	1.656	C α -C β -C γ	113.256	1.539
C α -C-O	120.433	0.824	C α -C-O	120.481	0.839
C β -C α -C	110.157	1.514	C β -C α -C	109.985	1.646
C β -C γ -C δ	112.402	1.454	C β -C γ -C δ	112.293	1.551
C δ -C ϵ -N ζ	112.819	2.106	C δ -C ϵ -N ζ	110.841	2.155
C γ -C δ -C ϵ	112.704	1.415	C γ -C δ -C ϵ	112.343	1.491
N-C α -C	111.365	2.533	N-C α -C	111.357	2.211
N-C α -C β	110.495	1.009	N-C α -C β	110.670	1.031
LYS mtpm n = 17			LYS mttp n = 1414		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-70.323	6.135	chi1	-65.910	8.334
chi2	174.831	15.490	chi2	-179.442	10.679
chi3	90.638	14.675	chi3	176.319	11.179
chi4	-70.024	12.061	chi4	66.691	13.607
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.509	2.138	C α -C β -C γ	113.442	1.732
C α -C-O	120.306	0.769	C α -C-O	120.510	0.841
C β -C α -C	109.783	2.273	C β -C α -C	110.097	1.628
C β -C γ -C δ	112.290	1.700	C β -C γ -C δ	111.258	1.746
C δ -C ϵ -N ζ	113.385	1.869	C δ -C ϵ -N ζ	112.223	1.982
C γ -C δ -C ϵ	113.180	1.587	C γ -C δ -C ϵ	111.751	1.466
N-C α -C	110.870	2.120	N-C α -C	111.268	2.491
N-C α -C β	110.511	1.029	N-C α -C β	110.594	1.017

LYS mttt n = 8597			LYS mttm n = 1829		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67.654	7.111	chi1	-66.855	7.320
chi2	-178.811	9.067	chi2	-177.777	10.020
chi3	-179.106	9.781	chi3	-176.656	10.842
chi4	179.484	10.347	chi4	-67.384	12.838
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.453	1.623	C α -C β -C γ	113.406	1.737
C α -C-O	120.467	0.827	C α -C-O	120.484	0.849
C β -C α -C	109.998	1.557	C β -C α -C	110.086	1.544
C β -C γ -C δ	111.143	1.850	C β -C γ -C δ	111.204	1.726
C δ -C ϵ -N ζ	111.119	2.099	C δ -C ϵ -N ζ	112.211	2.034
C γ -C δ -C ϵ	111.049	1.601	C γ -C δ -C ϵ	111.752	1.469
N-C α -C	111.334	2.236	N-C α -C	111.378	2.375
N-C α -C β	110.665	0.988	N-C α -C β	110.611	1.003
LYS mtmp n = 9			LYS mtmt n = 1314		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-67.465	5.792	chi1	-66.838	6.886
chi2	-175.781	8.346	chi2	-173.335	9.847
chi3	-95.844	7.431	chi3	-73.733	11.654
chi4	73.531	12.322	chi4	-175.371	10.598
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.802	1.228	C α -C β -C γ	113.209	1.595
C α -C-O	120.633	0.607	C α -C-O	120.408	0.857
C β -C α -C	109.891	1.198	C β -C α -C	110.085	1.557
C β -C γ -C δ	111.699	1.976	C β -C γ -C δ	112.313	1.519
C δ -C ϵ -N ζ	113.681	2.374	C δ -C ϵ -N ζ	111.041	2.184
C γ -C δ -C ϵ	112.703	0.792	C γ -C δ -C ϵ	112.107	1.451
N-C α -C	110.375	2.291	N-C α -C	111.319	2.137
N-C α -C β	110.828	0.914	N-C α -C β	110.673	0.960
LYS mtmm n = 424			LYS mmpt n = 31		
χ	Smooth COM	StdDev	χ	Smooth COM	StdDev
chi1	-63.898	6.909	chi1	-60.371	7.013
chi2	-177.154	10.058	chi2	-70.556	19.521
chi3	-70.378	10.902	chi3	93.615	14.476
chi4	-66.004	9.830	chi4	175.537	10.679
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C α -C β -C γ	113.456	1.534	C α -C β -C γ	115.281	1.118
C α -C-O	120.488	0.838	C α -C-O	120.359	0.888
C β -C α -C	109.818	1.557	C β -C α -C	109.807	1.683
C β -C γ -C δ	112.288	1.374	C β -C γ -C δ	113.354	1.803
C δ -C ϵ -N ζ	112.759	2.097	C δ -C ϵ -N ζ	111.539	1.766
C γ -C δ -C ϵ	112.869	1.500	C γ -C δ -C ϵ	112.040	1.404
N-C α -C	111.524	2.392	N-C α -C	111.535	2.365
N-C α -C β	110.573	1.029	N-C α -C β	111.168	1.386

LYS mmtp n = 463		
χ	Smooth COM	StdDev
chi1	-61.499	8.157
chi2	-68.646	12.048
chi3	179.724	11.913
chi4	67.912	13.158
Bond Angle	Mean	StdDev
C α -C β -C γ	114.716	1.514
C α -C-O	120.405	0.904
C β -C α -C	109.563	1.559
C β -C γ -C δ	112.024	1.545
C δ -C ϵ -N ζ	112.649	2.339
C γ -C δ -C ϵ	111.879	1.343
N-C α -C	111.141	2.596
N-C α -C β	110.702	1.044

LYS mmtm n = 727		
χ	Smooth COM	StdDev
chi1	-60.188	8.246
chi2	-65.555	10.785
chi3	-173.090	11.157
chi4	-68.899	13.356
Bond Angle	Mean	StdDev
C α -C β -C γ	114.540	1.397
C α -C-O	120.538	0.866
C β -C α -C	109.750	1.568
C β -C γ -C δ	111.934	1.429
C δ -C ϵ -N ζ	112.437	1.969
C γ -C δ -C ϵ	111.964	1.439
N-C α -C	111.442	2.525
N-C α -C β	110.623	1.025

LYS mmmm n = 90		
χ	Smooth COM	StdDev
chi1	-61.396	8.320
chi2	-61.832	10.421
chi3	-66.893	10.843
chi4	-64.659	10.880
Bond Angle	Mean	StdDev
C α -C β -C γ	114.738	1.388
C α -C-O	120.417	1.064
C β -C α -C	109.517	1.525
C β -C γ -C δ	113.153	1.432
C δ -C ϵ -N ζ	112.644	2.734
C γ -C δ -C ϵ	113.176	1.865
N-C α -C	111.658	2.469
N-C α -C β	110.501	1.112

LYS mmtt n = 3137		
χ	Smooth COM	StdDev
chi1	-61.713	8.298
chi2	-67.230	9.794
chi3	-176.776	10.146
chi4	-178.237	10.966
Bond Angle	Mean	StdDev
C α -C β -C γ	114.531	1.322
C α -C-O	120.435	0.906
C β -C α -C	109.619	1.555
C β -C γ -C δ	111.910	1.487
C δ -C ϵ -N ζ	111.069	2.082
C γ -C δ -C ϵ	111.132	1.533
N-C α -C	111.465	2.473
N-C α -C β	110.691	1.009

LYS mmmt n = 544		
χ	Smooth COM	StdDev
chi1	-62.678	7.662
chi2	-64.116	10.733
chi3	-70.703	9.725
chi4	-176.812	9.766
Bond Angle	Mean	StdDev
C α -C β -C γ	114.613	1.313
C α -C-O	120.383	0.968
C β -C α -C	109.622	1.455
C β -C γ -C δ	113.105	1.508
C δ -C ϵ -N ζ	111.154	2.215
C γ -C δ -C ϵ	112.301	1.533
N-C α -C	111.767	2.314
N-C α -C β	110.671	1.052