

# Rough Draft of Supplemental Material

Bradley Hintze

November 2014

## Contents

<b>1</b>	<b>Filtered Top8000 Residue Counts</b>	<b>2</b>
<b>2</b>	<b>Outlier counts: Top500 vs. Top8000</b>	<b>3</b>
<b>3</b>	<b><math>\chi</math> and Covalent Bond Angle Central Values</b>	<b>4</b>
3.1	SER . . . . .	4
3.2	THR . . . . .	5
3.3	VAL . . . . .	6
3.4	PRO . . . . .	7
3.5	CYS . . . . .	8
3.6	MET . . . . .	9
3.7	GLU . . . . .	13
3.8	GLN . . . . .	15
3.9	ASP . . . . .	18
3.10	ASN . . . . .	19
3.11	ILE . . . . .	20
3.12	LEU . . . . .	22
3.13	HIS . . . . .	24
3.14	TRP . . . . .	26
3.15	TYR . . . . .	29
3.16	PHE . . . . .	30
3.17	LYS . . . . .	31
3.18	ARG . . . . .	39
<b>4</b>	<b>Filtered Top8000 PDB Chains and Filtered Residue Counts</b>	<b>54</b>

# 1 Filtered Top8000 Residue Counts

Residue Type	No Filter	Filter	%Kept
LYS	69143	33746	48.81%
GLU	87622	55932	63.83%
ARG	63627	45310	71.21%
GLN	49542	36232	73.13%
ASP	87840	70701	80.49%
ASN	62843	52494	83.53%
MET	21458	18004	83.90%
HIS	33464	29179	87.20%
SER	83647	74623	89.21%
LEU	126255	112888	89.41%
PRO	64297	58207	90.53%
THR	81210	73532	90.55%
ILE	77630	70312	90.57%
TYR	51018	46264	90.68%
PHE	59573	55141	92.56%
VAL	102509	95222	92.89%
TRP	19744	18355	92.96%
CYS	17586	16387	93.18%
<b>Total</b>	<b>1159008</b>	<b>962529</b>	<b>83.05%</b>

**Table 1:** Residue counts with and without residue-level filters ordered by % kept after filtering. 'No Filter' means no RSCC, 2mF<sub>o</sub>-DF<sub>c</sub> sigma, and B filters but all other residue-level filters applied.

## 2 Outlier counts: Top500 vs. Top8000

Residue	n	Top500 $\leq 0.3\%$	Top8000 $\leq 1.0\%$	$\Delta$
ARG	193295	7631	6034	-1597
ASN	161814	2243	2122	-121
ASP	225302	3934	2998	-936
CYS	50824	630	537	-93
GLN	140651	2845	3034	189
GLU	255560	4991	6973	1982
HIS	91316	1347	878	-469
ILE	222518	1870	3511	1641
LEU	347449	8447	10311	1864
LYS	209811	6590	8232	1642
MET	69395	1901	1963	62
PHE	153564	1972	799	-1173
PRO	174910	948	898	-50
SER	236825	2730	2874	144
THR	214960	2305	3015	710
TRP	53869	750	301	-449
TYR	134580	1848	812	-1036
VAL	280539	1720	3576	1856

**Table 2:** Showing differences between outlier counts in the Top500-analyzed and Top8000-analyzed unfiltered dataset.

### 3 $\chi$ and Covalent Bond Angle Central Values

#### 3.1 SER

SER new.fd new.fd p n = 36176			SER m n = 21102		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	65.916	8.591	chi1	-63.982	7.656
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -OG	111.000	1.336	C $\alpha$ -C $\beta$ -OG	110.523	1.454
C $\alpha$ -C-O	120.456	0.915	C $\alpha$ -C-O	120.486	0.847
C $\beta$ -C $\alpha$ -C	109.926	1.388	C $\beta$ -C $\alpha$ -C	109.477	1.441
N-C $\alpha$ -C	111.619	2.525	N-C $\alpha$ -C	111.468	2.445
N-C $\alpha$ -C $\beta$	110.665	1.115	N-C $\alpha$ -C $\beta$	110.561	1.027

  

SER t n = 17121		
$\chi$	Smooth COM	StdDev
chi1	178.650	9.006
Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -OG	110.706	1.420
C $\alpha$ -C-O	120.567	0.814
C $\beta$ -C $\alpha$ -C	109.791	1.442
N-C $\alpha$ -C	110.492	2.404
N-C $\alpha$ -C $\beta$	110.059	1.206

### 3.2 THR

THR p n = 35387			THR m n = 32805		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	61.450	7.641	chi1	-60.109	6.112
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$ 2	110.969	1.002	C $\alpha$ _C $\beta$ _C $\gamma$ 2	111.143	0.934
C $\alpha$ _C $\beta$ _OG1	109.503	0.960	C $\alpha$ _C $\beta$ _OG1	108.916	0.967
C $\alpha$ _C_O	120.474	0.949	C $\alpha$ _C_O	120.534	0.805
C $\beta$ _C $\alpha$ _C	108.826	1.697	C $\beta$ _C $\alpha$ _C	110.047	1.529
N_C $\alpha$ _C	111.370	2.773	N_C $\alpha$ _C	110.211	2.312
N_C $\alpha$ _C $\beta$	111.785	1.255	N_C $\alpha$ _C $\beta$	110.720	1.184
OG1_C $\beta$ _C $\gamma$ 2	109.204	1.707	OG1_C $\beta$ _C $\gamma$ 2	108.771	1.662
THR t n = 5121					
$\chi$	Smooth COM	StdDev			
chi1	-172.707	7.394			
Bond Angle	Mean	StdDev			
C $\alpha$ _C $\beta$ _C $\gamma$ 2	111.717	1.088			
C $\alpha$ _C $\beta$ _OG1	109.534	0.984			
C $\alpha$ _C_O	120.615	0.828			
C $\beta$ _C $\alpha$ _C	110.961	1.905			
N_C $\alpha$ _C	110.122	2.334			
N_C $\alpha$ _C $\beta$	111.304	1.337			
OG1_C $\beta$ _C $\gamma$ 2	109.067	1.803			

### 3.3 VAL

VAL p n = 5892			VAL m n = 17054		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	64.912	7.171	chi1	-61.900	5.690
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$ 1	111.508	1.082	C $\alpha$ -C $\beta$ -C $\gamma$ 1	110.353	0.916
C $\alpha$ -C $\beta$ -C $\gamma$ 2	110.757	1.019	C $\alpha$ -C $\beta$ -C $\gamma$ 2	111.316	1.017
C $\alpha$ -C-O	120.600	0.821	C $\alpha$ -C-O	120.549	0.905
C $\beta$ -C $\alpha$ -C	111.407	1.565	C $\beta$ -C $\alpha$ -C	109.813	1.592
C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	111.028	1.203	C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	110.887	1.167
N-C $\alpha$ -C	110.309	2.481	N-C $\alpha$ -C	111.120	2.691
N-C $\alpha$ -C $\beta$	111.582	1.260	N-C $\alpha$ -C $\beta$	112.271	1.175

  

VAL t n = 71985		
$\chi$	Smooth COM	StdDev
chi1	175.704	6.347
Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$ 1	110.745	0.934
C $\alpha$ -C $\beta$ -C $\gamma$ 2	110.157	0.945
C $\alpha$ -C-O	120.547	0.786
C $\beta$ -C $\alpha$ -C	110.187	1.508
C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	110.461	1.126
N-C $\alpha$ -C	109.417	2.367
N-C $\alpha$ -C $\beta$	111.340	1.111

### 3.4 PRO

PRO Cg_exo n = 29437			PRO Cg_endo n = 28580		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-24.564	7.168	chi1	26.880	7.644
chi2	35.608	7.827	chi2	-34.515	8.879
chi3	-31.827	7.125	chi3	28.146	9.221
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	104.221	1.395	C $\alpha$ -C $\beta$ -C $\gamma$	104.230	1.466
C $\alpha$ -C-O	120.177	1.025	C $\alpha$ -C-O	120.221	1.058
C $\alpha$ -N-C $\delta$	111.653	0.807	C $\alpha$ -N-C $\delta$	111.798	0.844
C $\beta$ -C $\alpha$ -C	110.805	1.304	C $\beta$ -C $\alpha$ -C	110.911	1.412
C $\beta$ -C $\gamma$ -C $\delta$	104.694	2.311	C $\beta$ -C $\gamma$ -C $\delta$	105.294	2.360
N-C $\alpha$ -C	112.651	2.419	N-C $\alpha$ -C	112.935	2.599
N-C $\alpha$ -C $\beta$	103.313	0.588	N-C $\alpha$ -C $\beta$	103.192	0.716
N-C $\delta$ -C $\gamma$	102.712	0.872	N-C $\delta$ -C $\gamma$	103.060	0.874

### 3.5 CYS

CYS p n = 2895			CYS m n = 9132		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	64.543	8.968	chi1	-65.374	8.192
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -SG	114.644	1.686	C $\alpha$ -C $\beta$ -SG	113.550	1.865
C $\alpha$ -C-O	120.523	0.976	C $\alpha$ -C-O	120.433	0.868
C $\beta$ -C $\alpha$ -C	110.467	1.507	C $\beta$ -C $\alpha$ -C	109.469	1.635
N-C $\alpha$ -C	111.265	2.785	N-C $\alpha$ -C	111.517	2.435
N-C $\alpha$ -C $\beta$	110.915	1.235	N-C $\alpha$ -C $\beta$	110.612	1.065
CYS t n = 4315					
$\chi$	Smooth COM	StdDev			
chi1	-177.599	8.230			
Bond Angle	Mean	StdDev			
C $\alpha$ -C $\beta$ -SG	113.682	1.935			
C $\alpha$ -C-O	120.482	0.858			
C $\beta$ -C $\alpha$ -C	110.328	1.288			
N-C $\alpha$ -C	109.690	2.446			
N-C $\alpha$ -C $\beta$	110.020	1.366			



### 3.6 MET

MET pmt n = 7			MET ptm n = 373		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	71.340	3.364	chi1	64.860	8.164
chi2	-74.720	3.186	chi2	179.370	10.213
chi3	-162.328	4.884	chi3	-72.053	11.283
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.786	0.770	C $\alpha$ -C $\beta$ -C $\gamma$	114.669	1.690
C $\alpha$ -C-O	120.997	0.636	C $\alpha$ -C-O	120.624	0.934
C $\beta$ -C $\alpha$ -C	111.122	1.130	C $\beta$ -C $\alpha$ -C	110.368	1.454
C $\beta$ -C $\gamma$ -SD	111.744	2.285	C $\beta$ -C $\gamma$ -SD	112.721	2.135
C $\gamma$ -SD-C $\epsilon$	100.246	1.914	C $\gamma$ -SD-C $\epsilon$	100.857	1.773
N-C $\alpha$ -C	109.009	1.550	N-C $\alpha$ -C	110.855	2.783
N-C $\alpha$ -C $\beta$	111.648	1.281	N-C $\alpha$ -C $\beta$	111.162	1.208
MET ttp n = 1225			MET ttt n = 560		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.766	8.548	chi1	-176.725	8.829
chi2	179.141	11.453	chi2	176.823	9.573
chi3	71.790	10.513	chi3	176.456	15.731
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.541	1.658	C $\alpha$ -C $\beta$ -C $\gamma$	113.714	1.721
C $\alpha$ -C-O	120.615	0.850	C $\alpha$ -C-O	120.589	0.934
C $\beta$ -C $\alpha$ -C	110.040	1.160	C $\beta$ -C $\alpha$ -C	110.145	1.310
C $\beta$ -C $\gamma$ -SD	112.814	2.099	C $\beta$ -C $\gamma$ -SD	110.585	2.192
C $\gamma$ -SD-C $\epsilon$	100.721	2.113	C $\gamma$ -SD-C $\epsilon$	100.100	1.669
N-C $\alpha$ -C	110.277	2.151	N-C $\alpha$ -C	110.195	2.426
N-C $\alpha$ -C $\beta$	110.374	1.307	N-C $\alpha$ -C $\beta$	110.070	1.382
MET ppp n = 48			MET ttm n = 1075		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	61.248	9.401	chi1	-175.045	9.403
chi2	78.960	11.124	chi2	179.637	8.195
chi3	70.700	9.854	chi3	-71.855	12.995
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.591	1.641	C $\alpha$ -C $\beta$ -C $\gamma$	113.528	1.721
C $\alpha$ -C-O	120.670	0.854	C $\alpha$ -C-O	120.509	0.788
C $\beta$ -C $\alpha$ -C	111.148	1.562	C $\beta$ -C $\alpha$ -C	109.946	1.162
C $\beta$ -C $\gamma$ -SD	114.342	2.359	C $\beta$ -C $\gamma$ -SD	112.755	2.173
C $\gamma$ -SD-C $\epsilon$	100.371	4.017	C $\gamma$ -SD-C $\epsilon$	100.802	1.740
N-C $\alpha$ -C	111.809	2.731	N-C $\alpha$ -C	110.143	2.369
N-C $\alpha$ -C $\beta$	110.937	1.040	N-C $\alpha$ -C $\beta$	110.404	1.330

MET tpp n = 1101			MET pmm n = 40		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.981	9.422	chi1	72.629	7.836
chi2	63.633	7.967	chi2	-68.668	6.494
chi3	72.405	12.004	chi3	-68.863	8.290
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.203	1.349	C $\alpha$ -C $\beta$ -C $\gamma$	115.519	0.864
C $\alpha$ -C-O	120.501	0.844	C $\alpha$ -C-O	120.611	0.806
C $\beta$ -C $\alpha$ -C	110.321	1.131	C $\beta$ -C $\alpha$ -C	110.189	1.248
C $\beta$ -C $\gamma$ -SD	113.644	2.028	C $\beta$ -C $\gamma$ -SD	115.342	2.562
C $\gamma$ -SD-C $\epsilon$	100.676	1.734	C $\gamma$ -SD-C $\epsilon$	101.094	1.623
N-C $\alpha$ -C	110.663	2.226	N-C $\alpha$ -C	112.130	2.289
N-C $\alpha$ -C $\beta$	110.492	1.157	N-C $\alpha$ -C $\beta$	110.813	1.156
MET ptt n = 255			MET ptp n = 404		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	65.361	8.183	chi1	64.508	8.538
chi2	-178.195	9.115	chi2	-176.358	11.433
chi3	179.354	15.498	chi3	73.220	11.523
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.739	1.694	C $\alpha$ -C $\beta$ -C $\gamma$	114.610	1.803
C $\alpha$ -C-O	120.597	0.953	C $\alpha$ -C-O	120.653	0.918
C $\beta$ -C $\alpha$ -C	110.343	1.471	C $\beta$ -C $\alpha$ -C	110.327	1.470
C $\beta$ -C $\gamma$ -SD	111.018	2.372	C $\beta$ -C $\gamma$ -SD	112.878	2.187
C $\gamma$ -SD-C $\epsilon$	99.772	2.342	C $\gamma$ -SD-C $\epsilon$	100.802	1.967
N-C $\alpha$ -C	111.182	2.724	N-C $\alpha$ -C	110.657	2.574
N-C $\alpha$ -C $\beta$	111.147	1.301	N-C $\alpha$ -C $\beta$	111.057	1.243
MET tmt n = 33			MET pp-130 n = 25		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-179.131	6.802	chi1	64.331	7.216
chi2	-85.941	7.670	chi2	82.303	4.913
chi3	173.719	24.069	chi3	-154.200	27.945
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.931	1.056	C $\alpha$ -C $\beta$ -C $\gamma$	115.459	1.202
C $\alpha$ -C-O	120.666	0.571	C $\alpha$ -C-O	120.981	0.586
C $\beta$ -C $\alpha$ -C	110.722	1.244	C $\beta$ -C $\alpha$ -C	111.112	0.943
C $\beta$ -C $\gamma$ -SD	112.722	1.792	C $\beta$ -C $\gamma$ -SD	113.811	2.038
C $\gamma$ -SD-C $\epsilon$	100.439	1.266	C $\gamma$ -SD-C $\epsilon$	100.809	2.026
N-C $\alpha$ -C	110.032	2.930	N-C $\alpha$ -C	110.846	1.804
N-C $\alpha$ -C $\beta$	110.055	1.229	N-C $\alpha$ -C $\beta$	110.961	0.993

MET tmm n = 272			MET mmt n = 595		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.257	7.464	chi1	-64.971	8.702
chi2	-81.707	6.828	chi2	-63.753	9.416
chi3	-72.167	10.584	chi3	172.207	18.621
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.016	1.345	C $\alpha$ -C $\beta$ -C $\gamma$	113.935	1.442
C $\alpha$ -C-O	120.520	0.784	C $\alpha$ -C-O	120.423	0.805
C $\beta$ -C $\alpha$ -C	111.006	1.229	C $\beta$ -C $\alpha$ -C	109.934	1.562
C $\beta$ -C $\gamma$ -SD	114.013	2.127	C $\beta$ -C $\gamma$ -SD	112.054	2.038
C $\gamma$ -SD-C $\epsilon$	100.852	1.655	C $\gamma$ -SD-C $\epsilon$	100.286	2.007
N-C $\alpha$ -C	109.933	2.108	N-C $\alpha$ -C	111.418	2.244
N-C $\alpha$ -C $\beta$	110.096	1.166	N-C $\alpha$ -C $\beta$	110.617	0.955
MET mpm n = 13			MET mmp n = 504		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-77.183	5.132	chi1	-65.195	5.225
chi2	63.994	5.469	chi2	-61.634	6.375
chi3	-101.774	5.027	chi3	102.180	9.173
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	116.136	1.018	C $\alpha$ -C $\beta$ -C $\gamma$	114.222	1.394
C $\alpha$ -C-O	120.662	0.735	C $\alpha$ -C-O	120.336	0.802
C $\beta$ -C $\alpha$ -C	109.135	1.274	C $\beta$ -C $\alpha$ -C	110.240	1.537
C $\beta$ -C $\gamma$ -SD	115.853	2.314	C $\beta$ -C $\gamma$ -SD	113.838	2.127
C $\gamma$ -SD-C $\epsilon$	100.367	1.563	C $\gamma$ -SD-C $\epsilon$	101.229	2.164
N-C $\alpha$ -C	110.742	1.813	N-C $\alpha$ -C	111.460	2.154
N-C $\alpha$ -C $\beta$	111.036	1.046	N-C $\alpha$ -C $\beta$	110.829	1.096
MET mmm n = 3277			MET mpt n = 33		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-65.551	8.899	chi1	-69.557	11.833
chi2	-60.977	8.698	chi2	74.032	11.118
chi3	-69.165	10.164	chi3	167.387	18.897
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.004	1.295	C $\alpha$ -C $\beta$ -C $\gamma$	114.616	0.948
C $\alpha$ -C-O	120.361	0.849	C $\alpha$ -C-O	120.404	0.889
C $\beta$ -C $\alpha$ -C	110.035	1.526	C $\beta$ -C $\alpha$ -C	109.302	1.417
C $\beta$ -C $\gamma$ -SD	113.636	1.954	C $\beta$ -C $\gamma$ -SD	113.338	1.846
C $\gamma$ -SD-C $\epsilon$	100.890	1.779	C $\gamma$ -SD-C $\epsilon$	100.190	2.382
N-C $\alpha$ -C	111.616	2.388	N-C $\alpha$ -C	110.160	2.814
N-C $\alpha$ -C $\beta$	110.713	1.014	N-C $\alpha$ -C $\beta$	110.955	1.135

MET mpp n = 73			MET mtp n = 2786		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-76.610	14.305	chi1	-66.650	7.093
chi2	73.172	12.244	chi2	177.074	9.224
chi3	73.993	11.779	chi3	70.464	10.141
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.613	1.338	C $\alpha$ -C $\beta$ -C $\gamma$	113.153	1.638
C $\alpha$ -C-O	120.560	0.909	C $\alpha$ -C-O	120.497	0.835
C $\beta$ -C $\alpha$ -C	109.864	1.628	C $\beta$ -C $\alpha$ -C	109.960	1.578
C $\beta$ -C $\gamma$ -SD	114.196	2.171	C $\beta$ -C $\gamma$ -SD	112.868	2.067
C $\gamma$ -SD-C $\epsilon$	101.069	2.291	C $\gamma$ -SD-C $\epsilon$	100.770	1.677
N-C $\alpha$ -C	110.683	2.689	N-C $\alpha$ -C	111.249	2.347
N-C $\alpha$ -C $\beta$	110.800	1.230	N-C $\alpha$ -C $\beta$	110.473	1.005
MET mtt n = 1506			MET tpt n = 390		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-67.154	7.781	chi1	-173.452	9.177
chi2	179.723	8.664	chi2	65.814	7.765
chi3	-176.816	16.565	chi3	-156.289	31.207
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.590	1.725	C $\alpha$ -C $\beta$ -C $\gamma$	114.091	1.456
C $\alpha$ -C-O	120.534	0.822	C $\alpha$ -C-O	120.527	0.740
C $\beta$ -C $\alpha$ -C	109.370	1.665	C $\beta$ -C $\alpha$ -C	110.472	1.138
C $\beta$ -C $\gamma$ -SD	110.372	2.190	C $\beta$ -C $\gamma$ -SD	112.463	2.079
C $\gamma$ -SD-C $\epsilon$	100.129	1.988	C $\gamma$ -SD-C $\epsilon$	100.438	2.106
N-C $\alpha$ -C	111.160	2.251	N-C $\alpha$ -C	110.444	2.253
N-C $\alpha$ -C $\beta$	110.661	0.990	N-C $\alpha$ -C $\beta$	110.318	1.375
MET mtm n = 1805					
$\chi$	Smooth COM	StdDev			
chi1	-66.363	7.887			
chi2	-177.825	10.720			
chi3	-73.985	10.892			
Bond Angle	Mean	StdDev			
C $\alpha$ -C $\beta$ -C $\gamma$	113.186	1.706			
C $\alpha$ -C-O	120.486	0.897			
C $\beta$ -C $\alpha$ -C	109.934	1.643			
C $\beta$ -C $\gamma$ -SD	112.910	2.147			
C $\gamma$ -SD-C $\epsilon$	100.768	1.772			
N-C $\alpha$ -C	111.046	2.320			
N-C $\alpha$ -C $\beta$	110.674	1.065			

### 3.7 GLU

GLU pp20 n = 154			GLU tt0 n = 13252		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	61.255	7.965	chi1	-176.677	8.640
chi2	85.644	8.039	chi2	177.900	10.316
chi3	19.654	17.432	chi3	1.122	41.331
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.526	1.295	C $\alpha$ -C $\beta$ -C $\gamma$	113.479	1.738
C $\alpha$ -C-O	120.432	0.854	C $\alpha$ -C-O	120.578	0.764
C $\beta$ -C $\alpha$ -C	111.610	1.873	C $\beta$ -C $\alpha$ -C	110.134	1.167
C $\beta$ -C $\gamma$ -C $\delta$	114.078	1.327	C $\beta$ -C $\gamma$ -C $\delta$	113.089	1.497
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	119.009	1.429	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	118.950	1.272
C $\gamma$ -C $\delta$ -O $\epsilon$ 2	118.383	1.360	C $\gamma$ -C $\delta$ -O $\epsilon$ 2	117.959	1.267
N-C $\alpha$ -C	110.806	2.534	N-C $\alpha$ -C	110.581	2.266
N-C $\alpha$ -C $\beta$	111.442	1.256	N-C $\alpha$ -C $\beta$	110.349	1.370
O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	122.588	1.027	O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	123.066	1.062
GLU mm-30 n = 8827			GLU tm-30 n = 834		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.002	8.684	chi1	-170.330	8.522
chi2	-66.544	10.539	chi2	-83.400	9.292
chi3	-31.662	26.892	chi3	-28.718	17.355
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.040	1.409	C $\alpha$ -C $\beta$ -C $\gamma$	114.512	1.350
C $\alpha$ -C-O	120.414	0.822	C $\alpha$ -C-O	120.511	0.830
C $\beta$ -C $\alpha$ -C	109.927	1.495	C $\beta$ -C $\alpha$ -C	110.950	1.298
C $\beta$ -C $\gamma$ -C $\delta$	113.359	1.332	C $\beta$ -C $\gamma$ -C $\delta$	113.802	1.459
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	119.157	1.337	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	119.005	1.342
C $\gamma$ -C $\delta$ -O $\epsilon$ 2	118.207	1.255	C $\gamma$ -C $\delta$ -O $\epsilon$ 2	118.200	1.230
N-C $\alpha$ -C	111.482	2.363	N-C $\alpha$ -C	110.251	2.444
N-C $\alpha$ -C $\beta$	110.749	1.014	N-C $\alpha$ -C $\beta$	110.249	1.161
O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	122.618	1.085	O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	122.771	1.168
GLU tp30 n = 4517			GLU mt-10 n = 20435		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-178.170	9.868	chi1	-66.989	7.734
chi2	64.992	9.194	chi2	179.213	11.391
chi3	25.784	26.056	chi3	-6.596	37.288
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.624	1.390	C $\alpha$ -C $\beta$ -C $\gamma$	113.034	1.847
C $\alpha$ -C-O	120.487	0.801	C $\alpha$ -C-O	120.491	0.820
C $\beta$ -C $\alpha$ -C	110.638	1.211	C $\beta$ -C $\alpha$ -C	110.013	1.730
C $\beta$ -C $\gamma$ -C $\delta$	113.765	1.352	C $\beta$ -C $\gamma$ -C $\delta$	113.251	1.498
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	119.283	1.461	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	119.080	1.288
C $\gamma$ -C $\delta$ -O $\epsilon$ 2	118.040	1.377	C $\gamma$ -C $\delta$ -O $\epsilon$ 2	117.941	1.283
N-C $\alpha$ -C	110.864	2.098	N-C $\alpha$ -C	111.369	2.319
N-C $\alpha$ -C $\beta$	110.284	1.125	N-C $\alpha$ -C $\beta$	110.592	1.005
O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	122.657	1.067	O $\epsilon$ 1-C $\delta$ -O $\epsilon$ 2	122.956	1.064

GLU mp0 n = 3570			GLU pm20 n = 1442		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.877	7.314	chi1	69.039	8.862
chi2	82.550	9.370	chi2	-84.712	8.530
chi3	3.347	27.571	chi3	15.811	21.596
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.363	1.328	C $\alpha$ _C $\beta$ _C $\gamma$	115.546	1.342
C $\alpha$ _C_O	120.434	0.809	C $\alpha$ _C_O	120.198	0.828
C $\beta$ _C $\alpha$ _C	109.686	1.410	C $\beta$ _C $\alpha$ _C	110.500	1.241
C $\beta$ _C $\gamma$ _C $\delta$	114.151	1.383	C $\beta$ _C $\gamma$ _C $\delta$	114.428	1.424
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	119.757	1.672	C $\gamma$ _C $\delta$ _O $\epsilon$ 1	119.754	1.696
C $\gamma$ _C $\delta$ _O $\epsilon$ 2	117.768	1.507	C $\gamma$ _C $\delta$ _O $\epsilon$ 2	117.707	1.688
N_C $\alpha$ _C	112.038	2.010	N_C $\alpha$ _C	112.894	1.830
N_C $\alpha$ _C $\beta$	110.605	1.052	N_C $\alpha$ _C $\beta$	110.902	1.048
O $\epsilon$ 1_C $\delta$ _O $\epsilon$ 2	122.455	1.156	O $\epsilon$ 1_C $\delta$ _O $\epsilon$ 2	122.522	1.102

  

GLU pt0 n = 2737		
$\chi$	Smooth COM	StdDev
chi1	65.363	8.368
chi2	-177.309	10.096
chi3	1.201	50.935
Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.600	1.599
C $\alpha$ _C_O	120.522	0.920
C $\beta$ _C $\alpha$ _C	110.505	1.492
C $\beta$ _C $\gamma$ _C $\delta$	112.911	1.513
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	118.934	1.375
C $\gamma$ _C $\delta$ _O $\epsilon$ 2	118.167	1.348
N_C $\alpha$ _C	111.278	2.665
N_C $\alpha$ _C $\beta$	111.058	1.175
O $\epsilon$ 1_C $\delta$ _O $\epsilon$ 2	122.874	1.131

### 3.8 GLN

GLN mm110 n = 1114			GLN tp40 n = 3545		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-65.092	8.620	chi1	-176.823	8.781
chi2	-62.550	10.849	chi2	66.430	8.201
chi3	109.265	23.925	chi3	41.056	24.280
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.961	1.571	C $\alpha$ -C $\beta$ -C $\gamma$	113.950	1.428
C $\alpha$ -C-O	120.371	0.846	C $\alpha$ -C-O	120.428	0.793
C $\beta$ -C $\alpha$ -C	110.002	1.531	C $\beta$ -C $\alpha$ -C	110.232	1.153
C $\beta$ -C $\gamma$ -C $\delta$	112.863	1.383	C $\beta$ -C $\gamma$ -C $\delta$	112.878	1.233
C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.570	0.905	C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.588	0.835
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	120.808	0.913	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	120.793	0.875
N-C $\alpha$ -C	111.600	2.285	N-C $\alpha$ -C	111.026	1.999
N-C $\alpha$ -C $\beta$	110.721	1.056	N-C $\alpha$ -C $\beta$	110.574	1.131
O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.597	0.671	O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.598	0.643
GLN mp10 n = 1187			GLN mt0 n = 14026		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.517	9.049	chi1	-66.588	7.476
chi2	81.837	11.546	chi2	179.220	11.202
chi3	17.344	37.550	chi3	-3.560	62.388
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.250	1.346	C $\alpha$ -C $\beta$ -C $\gamma$	113.237	1.811
C $\alpha$ -C-O	120.446	0.828	C $\alpha$ -C-O	120.497	0.847
C $\beta$ -C $\alpha$ -C	109.772	1.526	C $\beta$ -C $\alpha$ -C	109.920	1.708
C $\beta$ -C $\gamma$ -C $\delta$	113.448	1.277	C $\beta$ -C $\gamma$ -C $\delta$	112.642	1.529
C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.324	0.810	C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.445	0.841
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	121.133	0.931	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	120.847	0.890
N-C $\alpha$ -C	111.602	2.349	N-C $\alpha$ -C	111.409	2.257
N-C $\alpha$ -C $\beta$	110.833	1.087	N-C $\alpha$ -C $\beta$	110.563	1.036
O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.523	0.586	O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.682	0.689
GLN tt0 n = 6749			GLN mp-120 n = 83		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-176.317	8.470	chi1	-72.531	9.919
chi2	177.556	10.840	chi2	69.333	10.790
chi3	2.032	60.613	chi3	-119.632	12.192
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.564	1.785	C $\alpha$ -C $\beta$ -C $\gamma$	114.417	1.549
C $\alpha$ -C-O	120.573	0.756	C $\alpha$ -C-O	120.541	0.847
C $\beta$ -C $\alpha$ -C	110.137	1.177	C $\beta$ -C $\alpha$ -C	109.639	1.696
C $\beta$ -C $\gamma$ -C $\delta$	112.610	1.498	C $\beta$ -C $\gamma$ -C $\delta$	113.658	1.500
C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.453	0.814	C $\gamma$ -C $\delta$ -N $\epsilon$ 2	116.593	0.649
C $\gamma$ -C $\delta$ -O $\epsilon$ 1	120.817	0.867	C $\gamma$ -C $\delta$ -O $\epsilon$ 1	120.637	1.108
N-C $\alpha$ -C	110.451	2.274	N-C $\alpha$ -C	111.532	2.739
N-C $\alpha$ -C $\beta$	110.304	1.357	N-C $\alpha$ -C $\beta$	110.709	0.977
O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.706	0.685	O $\epsilon$ 1-C $\delta$ -N $\epsilon$ 2	122.749	0.812

GLN tm-30 n = 539			GLN pp30 n = 177		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-171.950	10.161	chi1	62.991	7.823
chi2	-85.646	11.058	chi2	83.801	8.485
chi3	-29.401	20.426	chi3	29.841	20.931
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.612	1.344	C $\alpha$ _C $\beta$ _C $\gamma$	115.887	1.282
C $\alpha$ _C_O	120.536	0.819	C $\alpha$ _C_O	120.325	0.953
C $\beta$ _C $\alpha$ _C	110.941	1.307	C $\beta$ _C $\alpha$ _C	111.407	1.624
C $\beta$ _C $\gamma$ _C $\delta$	113.498	1.404	C $\beta$ _C $\gamma$ _C $\delta$	113.607	1.405
C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.468	0.706	C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.445	0.893
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.874	0.810	C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.889	0.949
N_C $\alpha$ _C	110.165	2.523	N_C $\alpha$ _C	111.018	2.559
N_C $\alpha$ _C $\beta$	110.288	1.228	N_C $\alpha$ _C $\beta$	111.503	1.154
O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.632	0.658	O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.628	0.671
GLN mm-40 n = 5810			GLN pm20 n = 482		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-63.698	8.646	chi1	69.577	9.930
chi2	-66.032	10.451	chi2	-84.394	9.331
chi3	-38.665	24.773	chi3	16.576	32.807
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.889	1.415	C $\alpha$ _C $\beta$ _C $\gamma$	115.691	1.412
C $\alpha$ _C_O	120.460	0.866	C $\alpha$ _C_O	120.313	0.930
C $\beta$ _C $\alpha$ _C	109.906	1.487	C $\beta$ _C $\alpha$ _C	110.424	1.358
C $\beta$ _C $\gamma$ _C $\delta$	112.837	1.262	C $\beta$ _C $\gamma$ _C $\delta$	113.923	1.416
C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.519	0.900	C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.267	0.854
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.852	0.903	C $\gamma$ _C $\delta$ _O $\epsilon$ 1	121.245	0.989
N_C $\alpha$ _C	111.379	2.459	N_C $\alpha$ _C	112.378	2.247
N_C $\alpha$ _C $\beta$	110.631	1.031	N_C $\alpha$ _C $\beta$	111.157	1.118
O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.607	0.768	O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.467	0.703
GLN tp-100 n = 521			GLN tm130 n = 55		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-176.963	8.590	chi1	-171.730	9.735
chi2	62.135	8.893	chi2	-75.893	10.370
chi3	-104.704	27.432	chi3	127.247	16.058
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.430	1.558	C $\alpha$ _C $\beta$ _C $\gamma$	114.897	1.440
C $\alpha$ _C_O	120.564	0.833	C $\alpha$ _C_O	120.546	0.938
C $\beta$ _C $\alpha$ _C	110.516	1.241	C $\beta$ _C $\alpha$ _C	111.262	1.629
C $\beta$ _C $\gamma$ _C $\delta$	113.019	1.281	C $\beta$ _C $\gamma$ _C $\delta$	114.423	2.701
C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.543	0.918	C $\gamma$ _C $\delta$ _N $\epsilon$ 2	117.082	1.285
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.881	0.822	C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.469	1.172
N_C $\alpha$ _C	110.370	2.300	N_C $\alpha$ _C	108.797	3.399
N_C $\alpha$ _C $\beta$	110.391	1.244	N_C $\alpha$ _C $\beta$	110.136	1.370
O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.550	0.627	O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.423	0.743



GLN pt0 n = 1835		
$\chi$	Smooth COM	StdDev
chi1	64.891	8.131
chi2	-177.468	11.198
chi3	-2.755	74.395
Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.517	1.517
C $\alpha$ _C_O	120.550	0.960
C $\beta$ _C $\alpha$ _C	110.345	1.504
C $\beta$ _C $\gamma$ _C $\delta$	112.491	1.445
C $\gamma$ _C $\delta$ _N $\epsilon$ 2	116.506	0.933
C $\gamma$ _C $\delta$ _O $\epsilon$ 1	120.837	0.965
N_C $\alpha$ _C	111.298	2.626
N_C $\alpha$ _C $\beta$	110.942	1.179
O $\epsilon$ 1_C $\delta$ _N $\epsilon$ 2	122.633	0.755

### 3.9 ASP

ASP p0 n = 11526			ASP m-30 n = 36384		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	62.914	7.500	chi1	-68.819	8.160
chi2	-2.097	31.055	chi2	-29.214	22.411
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.469	1.002	C $\alpha$ -C $\beta$ -C $\gamma$	112.902	0.936
C $\alpha$ -C-O	120.397	0.901	C $\alpha$ -C-O	120.452	0.853
C $\beta$ -C $\alpha$ -C	111.291	1.644	C $\beta$ -C $\alpha$ -C	109.347	1.666
C $\beta$ -C $\gamma$ -O $\delta$ 1	119.663	1.557	C $\beta$ -C $\gamma$ -O $\delta$ 1	119.177	1.359
C $\beta$ -C $\gamma$ -O $\delta$ 2	118.192	1.766	C $\beta$ -C $\gamma$ -O $\delta$ 2	118.245	1.700
N-C $\alpha$ -C	112.193	2.552	N-C $\alpha$ -C	111.688	2.299
N-C $\alpha$ -C $\beta$	111.140	1.255	N-C $\alpha$ -C $\beta$	110.770	1.053
O $\delta$ 1-C $\gamma$ -O $\delta$ 2	122.119	1.637	O $\delta$ 1-C $\gamma$ -O $\delta$ 2	122.552	1.551
ASP t70 n = 5865			ASP t0 n = 16717		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.210	9.216	chi1	-171.502	10.160
chi2	74.194	19.794	chi2	-1.704	23.746
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	112.426	0.823	C $\alpha$ -C $\beta$ -C $\gamma$	113.205	0.900
C $\alpha$ -C-O	120.491	0.796	C $\alpha$ -C-O	120.702	0.883
C $\beta$ -C $\alpha$ -C	110.134	1.272	C $\beta$ -C $\alpha$ -C	110.864	1.228
C $\beta$ -C $\gamma$ -O $\delta$ 1	118.489	1.107	C $\beta$ -C $\gamma$ -O $\delta$ 1	119.522	1.384
C $\beta$ -C $\gamma$ -O $\delta$ 2	118.722	1.560	C $\beta$ -C $\gamma$ -O $\delta$ 2	118.080	1.724
N-C $\alpha$ -C	110.478	2.360	N-C $\alpha$ -C	108.891	2.651
N-C $\alpha$ -C $\beta$	110.209	1.371	N-C $\alpha$ -C $\beta$	109.692	1.452
O $\delta$ 1-C $\gamma$ -O $\delta$ 2	122.750	1.535	O $\delta$ 1-C $\gamma$ -O $\delta$ 2	122.375	1.568

### 3.10 ASN

ASN p0 n = 7385			ASN t160 n = 56		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	63.756	7.814	chi1	-161.337	7.578
chi2	6.662	43.346	chi2	163.600	8.776
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.139	0.870	C $\alpha$ -C $\beta$ -C $\gamma$	114.281	1.565
C $\alpha$ -C-O	120.393	0.954	C $\alpha$ -C-O	120.446	0.868
C $\beta$ -C $\alpha$ -C	111.269	1.680	C $\beta$ -C $\alpha$ -C	111.284	1.393
C $\beta$ -C $\gamma$ -N $\delta$ 2	116.351	0.897	C $\beta$ -C $\gamma$ -N $\delta$ 2	117.039	2.119
C $\beta$ -C $\gamma$ -O $\delta$ 1	121.125	0.973	C $\beta$ -C $\gamma$ -O $\delta$ 1	120.497	2.042
N-C $\alpha$ -C	111.980	2.779	N-C $\alpha$ -C	110.082	1.999
N-C $\alpha$ -C $\beta$	111.066	1.277	N-C $\alpha$ -C $\beta$	109.206	1.421
O $\delta$ 1-C $\gamma$ -N $\delta$ 2	122.499	0.705	O $\delta$ 1-C $\gamma$ -N $\delta$ 2	122.414	0.810
ASN m-40 n = 25697			ASN t0 n = 15308		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-69.790	9.114	chi1	-171.473	10.519
chi2	-41.669	26.309	chi2	-1.493	54.722
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	112.456	0.907	C $\alpha$ -C $\beta$ -C $\gamma$	112.732	0.908
C $\alpha$ -C-O	120.432	0.865	C $\alpha$ -C-O	120.616	0.872
C $\beta$ -C $\alpha$ -C	110.002	1.725	C $\beta$ -C $\alpha$ -C	110.607	1.304
C $\beta$ -C $\gamma$ -N $\delta$ 2	116.530	0.836	C $\beta$ -C $\gamma$ -N $\delta$ 2	116.453	0.843
C $\beta$ -C $\gamma$ -O $\delta$ 1	120.778	0.885	C $\beta$ -C $\gamma$ -O $\delta$ 1	120.905	0.913
N-C $\alpha$ -C	112.235	2.548	N-C $\alpha$ -C	110.117	2.823
N-C $\alpha$ -C $\beta$	110.546	1.092	N-C $\alpha$ -C $\beta$	110.094	1.446
O $\delta$ 1-C $\gamma$ -N $\delta$ 2	122.663	0.683	O $\delta$ 1-C $\gamma$ -N $\delta$ 2	122.613	0.676
ASN m110 n = 3886					
$\chi$	Smooth COM	StdDev			
chi1	-63.571	9.679			
chi2	114.583	28.375			
Bond Angle	Mean	StdDev			
C $\alpha$ -C $\beta$ -C $\gamma$	112.713	1.132			
C $\alpha$ -C-O	120.506	0.899			
C $\beta$ -C $\alpha$ -C	109.539	1.836			
C $\beta$ -C $\gamma$ -N $\delta$ 2	116.636	1.126			
C $\beta$ -C $\gamma$ -O $\delta$ 1	120.721	1.167			
N-C $\alpha$ -C	112.034	2.790			
N-C $\alpha$ -C $\beta$	110.628	1.191			
O $\delta$ 1-C $\gamma$ -N $\delta$ 2	122.605	0.788			

### 3.11 ILE

ILE pp n = 249			ILE pt n = 8645		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	57.851	7.675	chi1	62.073	6.087
chi2	84.312	12.931	chi2	170.331	7.588
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$ 1	112.485	1.254	C $\alpha$ -C $\beta$ -C $\gamma$ 1	111.330	1.075
C $\alpha$ -C $\beta$ -C $\gamma$ 2	109.879	1.139	C $\alpha$ -C $\beta$ -C $\gamma$ 2	110.177	0.934
C $\alpha$ -C-O	120.525	0.863	C $\alpha$ -C-O	120.533	0.928
C $\beta$ -C $\alpha$ -C	111.330	1.609	C $\beta$ -C $\alpha$ -C	110.103	1.672
C $\beta$ -C $\gamma$ 1-C $\delta$ 1	114.992	1.744	C $\beta$ -C $\gamma$ 1-C $\delta$ 1	113.604	1.247
C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	110.095	1.933	C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	111.376	1.529
N-C $\alpha$ -C	112.089	2.477	N-C $\alpha$ -C	111.367	2.736
N-C $\alpha$ -C $\beta$	112.297	1.259	N-C $\alpha$ -C $\beta$	112.261	1.194
ILE mm n = 11046			ILE tt n = 4078		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-59.020	7.075	chi1	-169.614	7.781
chi2	-61.129	7.345	chi2	166.622	6.921
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$ 1	110.896	1.118	C $\alpha$ -C $\beta$ -C $\gamma$ 1	110.677	1.069
C $\alpha$ -C $\beta$ -C $\gamma$ 2	110.751	0.967	C $\alpha$ -C $\beta$ -C $\gamma$ 2	111.388	1.031
C $\alpha$ -C-O	120.511	0.804	C $\alpha$ -C-O	120.602	0.824
C $\beta$ -C $\alpha$ -C	109.830	1.601	C $\beta$ -C $\alpha$ -C	111.624	1.486
C $\beta$ -C $\gamma$ 1-C $\delta$ 1	114.774	1.211	C $\beta$ -C $\gamma$ 1-C $\delta$ 1	113.487	1.262
C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	111.274	1.468	C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	111.694	1.628
N-C $\alpha$ -C	109.450	2.459	N-C $\alpha$ -C	110.126	2.513
N-C $\alpha$ -C $\beta$	111.306	1.147	N-C $\alpha$ -C $\beta$	111.359	1.324
ILE tp n = 1847			ILE mt n = 43618		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-167.339	7.850	chi1	-62.999	6.422
chi2	65.770	7.308	chi2	169.237	7.398
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$ 1	111.100	1.136	C $\alpha$ -C $\beta$ -C $\gamma$ 1	109.978	1.076
C $\alpha$ -C $\beta$ -C $\gamma$ 2	111.430	1.023	C $\alpha$ -C $\beta$ -C $\gamma$ 2	110.616	0.917
C $\alpha$ -C-O	120.358	0.810	C $\alpha$ -C-O	120.542	0.787
C $\beta$ -C $\alpha$ -C	111.524	1.465	C $\beta$ -C $\alpha$ -C	110.356	1.578
C $\beta$ -C $\gamma$ 1-C $\delta$ 1	114.154	1.143	C $\beta$ -C $\gamma$ 1-C $\delta$ 1	113.965	1.222
C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	110.812	1.705	C $\gamma$ 1-C $\beta$ -C $\gamma$ 2	110.758	1.434
N-C $\alpha$ -C	111.583	2.335	N-C $\alpha$ -C	109.402	2.339
N-C $\alpha$ -C $\beta$	111.448	1.270	N-C $\alpha$ -C $\beta$	111.245	1.146

ILE mp n = 614		
$\chi$	Smooth COM	StdDev
chi1	-62.667	11.655
chi2	88.683	16.644
Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$ 1	111.152	1.098
C $\alpha$ _C $\beta$ _C $\gamma$ 2	110.469	1.062
C $\alpha$ _C_O	120.467	0.810
C $\beta$ _C $\alpha$ _C	110.120	1.628
C $\beta$ _C $\gamma$ 1_C $\delta$ 1	114.581	1.662
C $\gamma$ 1_C $\beta$ _C $\gamma$ 2	109.327	1.871
N_C $\alpha$ _C	108.384	2.266
N_C $\alpha$ _C $\beta$	111.945	1.274

### 3.12 LEU

LEU pp n = 512			LEU pt n = 370		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	61.357	8.260	chi1	72.738	8.428
chi2	83.113	9.544	chi2	164.797	10.811
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	119.074	2.535	C $\alpha$ -C $\beta$ -C $\gamma$	118.708	2.158
C $\alpha$ -C-O	120.599	0.824	C $\alpha$ -C-O	120.799	0.825
C $\beta$ -C $\alpha$ -C	111.509	1.361	C $\beta$ -C $\alpha$ -C	110.378	1.437
C $\beta$ -C $\gamma$ -C $\delta$ 1	111.513	1.887	C $\beta$ -C $\gamma$ -C $\delta$ 1	109.758	1.529
C $\beta$ -C $\gamma$ -C $\delta$ 2	109.775	1.660	C $\beta$ -C $\gamma$ -C $\delta$ 2	111.528	1.838
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	109.707	1.213	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.465	1.219
N-C $\alpha$ -C	110.709	2.388	N-C $\alpha$ -C	110.509	2.441
N-C $\alpha$ -C $\beta$	111.100	1.154	N-C $\alpha$ -C $\beta$	111.534	1.191
LEU mm n = 474			LEU tt n = 1543		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-82.802	10.193	chi1	-172.476	8.444
chi2	-63.907	10.043	chi2	153.401	10.545
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	117.802	2.617	C $\alpha$ -C $\beta$ -C $\gamma$	117.300	2.743
C $\alpha$ -C-O	120.327	0.897	C $\alpha$ -C-O	120.591	0.855
C $\beta$ -C $\alpha$ -C	110.079	1.585	C $\beta$ -C $\alpha$ -C	111.048	1.242
C $\beta$ -C $\gamma$ -C $\delta$ 1	110.837	1.600	C $\beta$ -C $\gamma$ -C $\delta$ 1	110.116	1.529
C $\beta$ -C $\gamma$ -C $\delta$ 2	111.869	1.704	C $\beta$ -C $\gamma$ -C $\delta$ 2	111.579	1.817
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.713	1.358	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.451	1.308
N-C $\alpha$ -C	111.122	2.643	N-C $\alpha$ -C	109.129	2.493
N-C $\alpha$ -C $\beta$	111.014	0.980	N-C $\alpha$ -C $\beta$	110.195	1.261
LEU tp n = 34062			LEU mt n = 72793		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.276	8.225	chi1	-65.787	8.163
chi2	62.594	6.962	chi2	174.346	8.051
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	116.491	2.056	C $\alpha$ -C $\beta$ -C $\gamma$	115.860	2.171
C $\alpha$ -C-O	120.525	0.785	C $\alpha$ -C-O	120.430	0.817
C $\beta$ -C $\alpha$ -C	110.188	1.203	C $\beta$ -C $\alpha$ -C	109.809	1.417
C $\beta$ -C $\gamma$ -C $\delta$ 1	111.063	1.552	C $\beta$ -C $\gamma$ -C $\delta$ 1	109.881	1.463
C $\beta$ -C $\gamma$ -C $\delta$ 2	109.781	1.492	C $\beta$ -C $\gamma$ -C $\delta$ 2	110.956	1.546
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.707	1.132	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.777	1.105
N-C $\alpha$ -C	110.160	2.381	N-C $\alpha$ -C	111.390	2.344
N-C $\alpha$ -C $\beta$	110.305	1.145	N-C $\alpha$ -C $\beta$	110.598	0.982

LEU tm n = 145			LEU mp n = 2658		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-171.753	5.870	chi1	-77.359	12.558
chi2	-75.044	6.633	chi2	71.504	15.804
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	120.433	2.351	C $\alpha$ -C $\beta$ -C $\gamma$	116.585	2.650
C $\alpha$ -C-O	120.579	0.798	C $\alpha$ -C-O	120.462	0.844
C $\beta$ -C $\alpha$ -C	111.294	1.167	C $\beta$ -C $\alpha$ -C	109.673	1.563
C $\beta$ -C $\gamma$ -C $\delta$ 1	112.234	1.906	C $\beta$ -C $\gamma$ -C $\delta$ 1	111.636	2.028
C $\beta$ -C $\gamma$ -C $\delta$ 2	111.621	1.665	C $\beta$ -C $\gamma$ -C $\delta$ 2	109.927	1.589
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	111.440	1.427	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	110.500	1.462
N-C $\alpha$ -C	108.534	2.345	N-C $\alpha$ -C	110.153	2.651
N-C $\alpha$ -C $\beta$	109.909	1.162	N-C $\alpha$ -C $\beta$	111.073	1.022

### 3.13 HIS

HIS t-170 n = 1307			HIS p90 n = 1454		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-173.314	9.678	chi1	62.492	9.688
chi2	-167.114	21.578	chi2	86.558	21.823
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.232	0.970	C $\alpha$ -C $\beta$ -C $\gamma$	114.190	1.058
C $\alpha$ -C-O	120.605	0.808	C $\alpha$ -C-O	120.637	0.942
C $\beta$ -C $\alpha$ -C	110.891	1.295	C $\beta$ -C $\alpha$ -C	110.827	1.573
C $\beta$ -C $\gamma$ -C $\delta$ 2	131.374	0.961	C $\beta$ -C $\gamma$ -C $\delta$ 2	131.002	0.858
C $\beta$ -C $\gamma$ -N $\delta$ 1	122.411	1.046	C $\beta$ -C $\gamma$ -N $\delta$ 1	122.771	0.912
C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.782	0.521	C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.819	0.565
C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.235	0.431	C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.268	0.481
C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.222	0.647	C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.202	0.647
N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.554	0.598	N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.520	0.611
N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.182	0.516	N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.169	0.512
N-C $\alpha$ -C	109.220	2.607	N-C $\alpha$ -C	111.243	2.740
N-C $\alpha$ -C $\beta$	109.641	1.518	N-C $\alpha$ -C $\beta$	111.006	1.368
HIS m90 n = 3820			HIS t-90 n = 3460		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-65.658	9.766	chi1	-173.491	10.438
chi2	88.477	17.448	chi2	-86.784	18.388
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.466	1.120	C $\alpha$ -C $\beta$ -C $\gamma$	113.699	0.994
C $\alpha$ -C-O	120.483	0.892	C $\alpha$ -C-O	120.476	0.845
C $\beta$ -C $\alpha$ -C	109.741	1.962	C $\beta$ -C $\alpha$ -C	110.435	1.218
C $\beta$ -C $\gamma$ -C $\delta$ 2	130.928	0.846	C $\beta$ -C $\gamma$ -C $\delta$ 2	130.912	0.809
C $\beta$ -C $\gamma$ -N $\delta$ 1	122.780	0.813	C $\beta$ -C $\gamma$ -N $\delta$ 1	122.783	0.726
C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.857	0.547	C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.846	0.497
C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.203	0.490	C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.194	0.449
C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.190	0.637	C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.176	0.692
N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.498	0.613	N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.506	0.592
N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.227	0.509	N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.249	0.533
N-C $\alpha$ -C	111.469	2.747	N-C $\alpha$ -C	109.906	2.468
N-C $\alpha$ -C $\beta$	110.638	1.177	N-C $\alpha$ -C $\beta$	110.072	1.459



HIS m170 n = 2642			HIS m-70 n = 9299		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-67.985	8.174	chi1	-64.458	10.010
chi2	170.975	21.700	chi2	-75.228	19.362
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.738	0.933	C $\alpha$ -C $\beta$ -C $\gamma$	113.371	1.057
C $\alpha$ -C-O	120.394	0.877	C $\alpha$ -C-O	120.409	0.870
C $\beta$ -C $\alpha$ -C	109.690	1.802	C $\beta$ -C $\alpha$ -C	109.864	1.886
C $\beta$ -C $\gamma$ -C $\delta$ 2	131.140	0.992	C $\beta$ -C $\gamma$ -C $\delta$ 2	131.054	0.813
C $\beta$ -C $\gamma$ -N $\delta$ 1	122.602	1.039	C $\beta$ -C $\gamma$ -N $\delta$ 1	122.624	0.797
C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.801	0.517	C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.862	0.504
C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.210	0.464	C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.183	0.457
C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.188	0.669	C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.185	0.614
N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.550	0.599	N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.491	0.543
N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.224	0.520	N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.255	0.518
N-C $\alpha$ -C	111.521	2.547	N-C $\alpha$ -C	111.716	2.843
N-C $\alpha$ -C $\beta$	110.748	1.158	N-C $\alpha$ -C $\beta$	110.401	1.173
HIS t70 n = 4960			HIS p-80 n = 2158		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-178.423	10.054	chi1	64.769	9.924
chi2	73.865	17.261	chi2	-80.838	16.271
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.612	1.067	C $\alpha$ -C $\beta$ -C $\gamma$	114.063	1.027
C $\alpha$ -C-O	120.572	0.826	C $\alpha$ -C-O	120.396	0.973
C $\beta$ -C $\alpha$ -C	110.128	1.340	C $\beta$ -C $\alpha$ -C	110.363	1.530
C $\beta$ -C $\gamma$ -C $\delta$ 2	131.028	0.812	C $\beta$ -C $\gamma$ -C $\delta$ 2	131.018	0.803
C $\beta$ -C $\gamma$ -N $\delta$ 1	122.666	0.789	C $\beta$ -C $\gamma$ -N $\delta$ 1	122.744	0.804
C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.856	0.515	C $\epsilon$ 1-N $\epsilon$ 2-C $\delta$ 2	108.836	0.560
C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.196	0.451	C $\gamma$ -C $\delta$ 2-N $\epsilon$ 2	107.236	0.511
C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.174	0.581	C $\gamma$ -N $\delta$ 1-C $\epsilon$ 1	109.208	0.591
N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.502	0.531	N $\delta$ 1-C $\epsilon$ 1-N $\epsilon$ 2	108.512	0.582
N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.247	0.475	N $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.185	0.505
N-C $\alpha$ -C	110.680	2.360	N-C $\alpha$ -C	112.024	2.435
N-C $\alpha$ -C $\beta$	110.179	1.485	N-C $\alpha$ -C $\beta$	111.011	1.323

### 3.14 TRP

TRP m-90 n = 934			TRP m100 n = 6204		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-67.780	12.531	chi1	-67.358	10.787
chi2	-89.279	13.865	chi2	97.262	16.987
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.832	2.468	C $\alpha$ _C $\beta$ _C $\gamma$	113.184	2.214
C $\alpha$ _C_O	120.471	0.858	C $\alpha$ _C_O	120.431	0.854
C $\beta$ _C $\alpha$ _C	109.402	2.033	C $\beta$ _C $\alpha$ _C	109.624	1.912
C $\beta$ _C $\gamma$ _C $\delta$ 1	126.715	0.715	C $\beta$ _C $\gamma$ _C $\delta$ 1	127.019	0.655
C $\beta$ _C $\gamma$ _C $\delta$ 2	126.937	0.769	C $\beta$ _C $\gamma$ _C $\delta$ 2	126.591	0.678
C $\delta$ 1_C $\gamma$ _C $\delta$ 2	106.285	0.436	C $\delta$ 1_C $\gamma$ _C $\delta$ 2	106.336	0.425
C $\delta$ 1_N $\epsilon$ 1_C $\epsilon$ 2	108.928	0.477	C $\delta$ 1_N $\epsilon$ 1_C $\epsilon$ 2	108.901	0.483
C $\delta$ 2_C $\epsilon$ 2_C $\zeta$ 2	122.432	0.343	C $\delta$ 2_C $\epsilon$ 2_C $\zeta$ 2	122.403	0.359
C $\delta$ 2_C $\epsilon$ 3_C $\zeta$ 3	118.697	0.451	C $\delta$ 2_C $\epsilon$ 3_C $\zeta$ 3	118.698	0.449
C $\epsilon$ 2_C $\delta$ 2_C $\epsilon$ 3	118.844	0.377	C $\epsilon$ 2_C $\delta$ 2_C $\epsilon$ 3	118.868	0.366
C $\epsilon$ 2_C $\delta$ 2_C $\gamma$	107.197	0.321	C $\epsilon$ 2_C $\delta$ 2_C $\gamma$	107.232	0.328
C $\epsilon$ 3_C $\zeta$ 3_C $\eta$ 2	121.019	0.456	C $\epsilon$ 3_C $\zeta$ 3_C $\eta$ 2	120.996	0.468
C $\gamma$ _C $\delta$ 1_N $\epsilon$ 1	110.119	0.494	C $\gamma$ _C $\delta$ 1_N $\epsilon$ 1	110.086	0.481
C $\gamma$ _C $\delta$ 2_C $\epsilon$ 3	133.943	0.373	C $\gamma$ _C $\delta$ 2_C $\epsilon$ 3	133.883	0.393
C $\eta$ 2_C $\zeta$ 2_C $\epsilon$ 2	117.507	0.422	C $\eta$ 2_C $\zeta$ 2_C $\epsilon$ 2	117.493	0.444
C $\zeta$ 3_C $\eta$ 2_C $\zeta$ 2	121.475	0.442	C $\zeta$ 3_C $\eta$ 2_C $\zeta$ 2	121.513	0.448
N $\epsilon$ 1_C $\epsilon$ 2_C $\delta$ 2	107.449	0.342	N $\epsilon$ 1_C $\epsilon$ 2_C $\delta$ 2	107.425	0.347
N $\epsilon$ 1_C $\epsilon$ 2_C $\zeta$ 2	130.105	0.429	N $\epsilon$ 1_C $\epsilon$ 2_C $\zeta$ 2	130.157	0.425
N_C $\alpha$ _C	110.543	2.884	N_C $\alpha$ _C	111.444	2.647
N_C $\alpha$ _C $\beta$	110.689	1.116	N_C $\alpha$ _C $\beta$	110.551	1.104

TRP p90 n = 952			TRP t60 n = 3316		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	60.293	9.995	chi1	-178.686	9.796
chi2	87.822	14.399	chi2	64.773	33.012
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.020	2.031	C $\alpha$ -C $\beta$ -C $\gamma$	114.283	2.134
C $\alpha$ -C-O	120.576	0.853	C $\alpha$ -C-O	120.656	0.800
C $\beta$ -C $\alpha$ -C	110.666	1.419	C $\beta$ -C $\alpha$ -C	110.553	1.349
C $\beta$ -C $\gamma$ -C $\delta$ 1	126.998	0.698	C $\beta$ -C $\gamma$ -C $\delta$ 1	127.132	0.782
C $\beta$ -C $\gamma$ -C $\delta$ 2	126.756	0.752	C $\beta$ -C $\gamma$ -C $\delta$ 2	126.517	0.810
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.200	0.370	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.296	0.475
C $\delta$ 1-N $\epsilon$ 1-C $\epsilon$ 2	108.930	0.600	C $\delta$ 1-N $\epsilon$ 1-C $\epsilon$ 2	108.910	0.507
C $\delta$ 2-C $\epsilon$ 2-C $\zeta$ 2	122.449	0.372	C $\delta$ 2-C $\epsilon$ 2-C $\zeta$ 2	122.392	0.364
C $\delta$ 2-C $\epsilon$ 3-C $\zeta$ 3	118.689	0.346	C $\delta$ 2-C $\epsilon$ 3-C $\zeta$ 3	118.693	0.412
C $\epsilon$ 2-C $\delta$ 2-C $\epsilon$ 3	118.831	0.360	C $\epsilon$ 2-C $\delta$ 2-C $\epsilon$ 3	118.874	0.352
C $\epsilon$ 2-C $\delta$ 2-C $\gamma$	107.258	0.317	C $\epsilon$ 2-C $\delta$ 2-C $\gamma$	107.259	0.373
C $\epsilon$ 3-C $\zeta$ 3-C $\eta$ 2	121.023	0.413	C $\epsilon$ 3-C $\zeta$ 3-C $\eta$ 2	120.990	0.446
C $\gamma$ -C $\delta$ 1-N $\epsilon$ 1	110.151	0.494	C $\gamma$ -C $\delta$ 1-N $\epsilon$ 1	110.060	0.526
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 3	133.893	0.344	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 3	133.851	0.417
C $\eta$ 2-C $\zeta$ 2-C $\epsilon$ 2	117.471	0.448	C $\eta$ 2-C $\zeta$ 2-C $\epsilon$ 2	117.488	0.451
C $\zeta$ 3-C $\eta$ 2-C $\zeta$ 2	121.508	0.461	C $\zeta$ 3-C $\eta$ 2-C $\zeta$ 2	121.536	0.454
N $\epsilon$ 1-C $\epsilon$ 2-C $\delta$ 2	107.442	0.369	N $\epsilon$ 1-C $\epsilon$ 2-C $\delta$ 2	107.453	0.377
N $\epsilon$ 1-C $\epsilon$ 2-C $\zeta$ 2	130.097	0.411	N $\epsilon$ 1-C $\epsilon$ 2-C $\zeta$ 2	130.138	0.448
N-C $\alpha$ -C	111.190	2.409	N-C $\alpha$ -C	110.124	2.157
N-C $\alpha$ -C $\beta$	111.113	1.263	N-C $\alpha$ -C $\beta$	109.963	1.422

  

TRP t-100 n = 2840			TRP m-10 n = 2152		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.069	11.610	chi1	-68.163	9.051
chi2	-102.575	15.321	chi2	-7.490	21.659
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.568	2.322	C $\alpha$ -C $\beta$ -C $\gamma$	114.737	1.639
C $\alpha$ -C-O	120.572	0.865	C $\alpha$ -C-O	120.477	0.876
C $\beta$ -C $\alpha$ -C	110.328	1.328	C $\beta$ -C $\alpha$ -C	109.175	1.708
C $\beta$ -C $\gamma$ -C $\delta$ 1	126.902	0.685	C $\beta$ -C $\gamma$ -C $\delta$ 1	127.540	0.705
C $\beta$ -C $\gamma$ -C $\delta$ 2	126.743	0.706	C $\beta$ -C $\gamma$ -C $\delta$ 2	126.112	0.762
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.291	0.423	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.304	0.444
C $\delta$ 1-N $\epsilon$ 1-C $\epsilon$ 2	108.931	0.452	C $\delta$ 1-N $\epsilon$ 1-C $\epsilon$ 2	108.831	0.448
C $\delta$ 2-C $\epsilon$ 2-C $\zeta$ 2	122.409	0.358	C $\delta$ 2-C $\epsilon$ 2-C $\zeta$ 2	122.350	0.395
C $\delta$ 2-C $\epsilon$ 3-C $\zeta$ 3	118.698	0.446	C $\delta$ 2-C $\epsilon$ 3-C $\zeta$ 3	118.696	0.417
C $\epsilon$ 2-C $\delta$ 2-C $\epsilon$ 3	118.847	0.343	C $\epsilon$ 2-C $\delta$ 2-C $\epsilon$ 3	118.909	0.361
C $\epsilon$ 2-C $\delta$ 2-C $\gamma$	107.215	0.320	C $\epsilon$ 2-C $\delta$ 2-C $\gamma$	107.323	0.370
C $\epsilon$ 3-C $\zeta$ 3-C $\eta$ 2	121.007	0.474	C $\epsilon$ 3-C $\zeta$ 3-C $\eta$ 2	121.001	0.422
C $\gamma$ -C $\delta$ 1-N $\epsilon$ 1	110.106	0.474	C $\gamma$ -C $\delta$ 1-N $\epsilon$ 1	110.040	0.479
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 3	133.921	0.364	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 3	133.753	0.380
C $\eta$ 2-C $\zeta$ 2-C $\epsilon$ 2	117.509	0.445	C $\eta$ 2-C $\zeta$ 2-C $\epsilon$ 2	117.472	0.458
C $\zeta$ 3-C $\eta$ 2-C $\zeta$ 2	121.502	0.455	C $\zeta$ 3-C $\eta$ 2-C $\zeta$ 2	121.546	0.456
N $\epsilon$ 1-C $\epsilon$ 2-C $\delta$ 2	107.437	0.337	N $\epsilon$ 1-C $\epsilon$ 2-C $\delta$ 2	107.481	0.360
N $\epsilon$ 1-C $\epsilon$ 2-C $\zeta$ 2	130.138	0.435	N $\epsilon$ 1-C $\epsilon$ 2-C $\zeta$ 2	130.155	0.444
N-C $\alpha$ -C	110.520	2.428	N-C $\alpha$ -C	111.435	2.558
N-C $\alpha$ -C $\beta$	110.285	1.410	N-C $\alpha$ -C $\beta$	110.789	1.152

TRP p-90 n = 1905		
$\chi$	Smooth COM	StdDev
chi1	61.771	9.864
chi2	-89.374	12.958
Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.034	1.900
C $\alpha$ -C-O	120.452	0.925
C $\beta$ -C $\alpha$ -C	110.445	1.427
C $\beta$ -C $\gamma$ -C $\delta$ 1	126.857	0.666
C $\beta$ -C $\gamma$ -C $\delta$ 2	126.896	0.702
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	106.197	0.429
C $\delta$ 1-N $\epsilon$ 1-C $\epsilon$ 2	108.956	0.458
C $\delta$ 2-C $\epsilon$ 2-C $\zeta$ 2	122.437	0.337
C $\delta$ 2-C $\epsilon$ 3-C $\zeta$ 3	118.713	0.467
C $\epsilon$ 2-C $\delta$ 2-C $\epsilon$ 3	118.807	0.383
C $\epsilon$ 2-C $\delta$ 2-C $\gamma$	107.246	0.326
C $\epsilon$ 3-C $\zeta$ 3-C $\eta$ 2	121.030	0.455
C $\gamma$ -C $\delta$ 1-N $\epsilon$ 1	110.150	0.460
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 3	133.932	0.411
C $\eta$ 2-C $\zeta$ 2-C $\epsilon$ 2	117.525	0.442
C $\zeta$ 3-C $\eta$ 2-C $\zeta$ 2	121.461	0.459
N $\epsilon$ 1-C $\epsilon$ 2-C $\delta$ 2	107.431	0.341
N $\epsilon$ 1-C $\epsilon$ 2-C $\zeta$ 2	130.119	0.405
N-C $\alpha$ -C	112.158	2.608
N-C $\alpha$ -C $\beta$	111.097	1.241

### 3.15 TYR

TYR p90 n = 5345			TYR m-10 n = 2573		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	63.561	10.540	chi1	-68.127	9.902
chi2	-89.699	10.105	chi2	-14.743	20.163
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.844	1.858	C $\alpha$ -C $\beta$ -C $\gamma$	115.768	1.570
C $\alpha$ -C-O	120.661	0.926	C $\alpha$ -C-O	120.431	0.844
C $\beta$ -C $\alpha$ -C	110.639	1.408	C $\beta$ -C $\alpha$ -C	109.050	1.742
C $\beta$ -C $\gamma$ -C $\delta$ 1	120.990	0.643	C $\beta$ -C $\gamma$ -C $\delta$ 1	121.580	1.015
C $\beta$ -C $\gamma$ -C $\delta$ 2	120.858	0.596	C $\beta$ -C $\gamma$ -C $\delta$ 2	120.365	0.933
C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.525	0.619	C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.493	0.614
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.110	0.547	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.013	0.549
C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	120.454	0.659	C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	120.409	0.640
C $\epsilon$ 1-C $\zeta$ -OH	119.792	1.238	C $\epsilon$ 1-C $\zeta$ -OH	120.085	1.314
C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	121.160	0.575	C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	121.074	0.590
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	121.161	0.547	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	121.324	0.571
C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.559	0.620	C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.651	0.639
N-C $\alpha$ -C	111.078	2.655	N-C $\alpha$ -C	111.388	2.337
N-C $\alpha$ -C $\beta$	111.207	1.220	N-C $\alpha$ -C $\beta$	111.006	1.144
OH-C $\zeta$ -C $\epsilon$ 2	119.737	1.232	OH-C $\zeta$ -C $\epsilon$ 2	119.487	1.333
TYR m-80 n = 22199			TYR t80 n = 15992		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.760	10.454	chi1	-178.297	10.487
chi2	-80.589	16.828	chi2	75.767	16.666
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.209	2.039	C $\alpha$ -C $\beta$ -C $\gamma$	113.704	2.129
C $\alpha$ -C-O	120.440	0.872	C $\alpha$ -C-O	120.621	0.797
C $\beta$ -C $\alpha$ -C	109.628	1.926	C $\beta$ -C $\alpha$ -C	110.301	1.250
C $\beta$ -C $\gamma$ -C $\delta$ 1	120.855	0.619	C $\beta$ -C $\gamma$ -C $\delta$ 1	120.902	0.650
C $\beta$ -C $\gamma$ -C $\delta$ 2	120.850	0.609	C $\beta$ -C $\gamma$ -C $\delta$ 2	120.835	0.637
C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.504	0.901	C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.512	0.594
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.245	0.576	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.213	0.515
C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	120.505	0.729	C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	120.509	0.647
C $\epsilon$ 1-C $\zeta$ -OH	119.719	1.227	C $\epsilon$ 1-C $\zeta$ -OH	119.747	1.267
C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	121.096	0.857	C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	121.092	0.547
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	121.094	0.861	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	121.136	0.553
C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.512	0.904	C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.506	0.624
N-C $\alpha$ -C	111.427	2.768	N-C $\alpha$ -C	110.392	2.246
N-C $\alpha$ -C $\beta$	110.555	1.098	N-C $\alpha$ -C $\beta$	110.212	1.441
OH-C $\zeta$ -C $\epsilon$ 2	119.760	1.238	OH-C $\zeta$ -C $\epsilon$ 2	119.727	1.266

### 3.16 PHE

PHE p90 n = 6173			PHE m-10 n = 3795		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	63.561	9.553	chi1	-68.127	9.354
chi2	-89.699	9.392	chi2	-14.743	19.816
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.401	0.955	C $\alpha$ -C $\beta$ -C $\gamma$	114.782	0.944
C $\alpha$ -C-O	120.708	0.883	C $\alpha$ -C-O	120.421	0.867
C $\beta$ -C $\alpha$ -C	110.881	1.461	C $\beta$ -C $\alpha$ -C	108.942	1.778
C $\beta$ -C $\gamma$ -C $\delta$ 1	120.728	0.611	C $\beta$ -C $\gamma$ -C $\delta$ 1	121.533	1.211
C $\beta$ -C $\gamma$ -C $\delta$ 2	120.603	0.572	C $\beta$ -C $\gamma$ -C $\delta$ 2	119.895	1.159
C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.889	0.602	C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.896	0.603
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.623	0.527	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.528	0.558
C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	119.824	0.626	C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	119.839	0.610
C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	120.857	0.585	C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	120.779	0.593
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	120.853	0.571	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	120.990	0.611
C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.920	0.589	C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.931	0.610
N-C $\alpha$ -C	110.875	2.562	N-C $\alpha$ -C	111.046	2.423
N-C $\alpha$ -C $\beta$	111.386	1.319	N-C $\alpha$ -C $\beta$	111.198	1.109
PHE m-80 n = 26111			PHE t80 n = 18909		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.760	10.137	chi1	-178.297	9.987
chi2	-80.589	16.842	chi2	75.767	17.425
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.522	1.018	C $\alpha$ -C $\beta$ -C $\gamma$	113.789	1.068
C $\alpha$ -C-O	120.453	0.858	C $\alpha$ -C-O	120.596	0.799
C $\beta$ -C $\alpha$ -C	109.802	1.989	C $\beta$ -C $\alpha$ -C	110.333	1.299
C $\beta$ -C $\gamma$ -C $\delta$ 1	120.578	0.597	C $\beta$ -C $\gamma$ -C $\delta$ 1	120.646	0.719
C $\beta$ -C $\gamma$ -C $\delta$ 2	120.567	0.585	C $\beta$ -C $\gamma$ -C $\delta$ 2	120.535	0.679
C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.861	0.574	C $\delta$ 1-C $\epsilon$ 1-C $\zeta$	119.859	0.582
C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.802	0.520	C $\delta$ 1-C $\gamma$ -C $\delta$ 2	118.768	0.543
C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	119.894	0.601	C $\epsilon$ 1-C $\zeta$ -C $\epsilon$ 2	119.921	0.625
C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	120.766	0.555	C $\gamma$ -C $\delta$ 1-C $\epsilon$ 1	120.765	0.575
C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	120.765	0.565	C $\gamma$ -C $\delta$ 2-C $\epsilon$ 2	120.789	0.583
C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.878	0.574	C $\zeta$ -C $\epsilon$ 2-C $\delta$ 2	119.864	0.581
N-C $\alpha$ -C	111.237	2.820	N-C $\alpha$ -C	110.333	2.313
N-C $\alpha$ -C $\beta$	110.546	1.108	N-C $\alpha$ -C $\beta$	110.200	1.504

### 3.17 LYS

LYS tppt n = 262			LYS mtpt n = 1302		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-178.194	7.884	chi1	-69.197	8.112
chi2	63.490	9.400	chi2	174.242	11.443
chi3	69.535	9.208	chi3	70.524	11.862
chi4	177.447	9.222	chi4	175.197	10.265
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.808	1.236	C $\alpha$ -C $\beta$ -C $\gamma$	113.226	1.551
C $\alpha$ -C-O	120.561	0.746	C $\alpha$ -C-O	120.472	0.834
C $\beta$ -C $\alpha$ -C	110.615	1.108	C $\beta$ -C $\alpha$ -C	109.992	1.629
C $\beta$ -C $\gamma$ -C $\delta$	113.119	1.507	C $\beta$ -C $\gamma$ -C $\delta$	112.297	1.526
C $\delta$ -C $\epsilon$ -N $\zeta$	111.182	1.862	C $\delta$ -C $\epsilon$ -N $\zeta$	110.836	2.148
C $\gamma$ -C $\delta$ -C $\epsilon$	112.375	1.458	C $\gamma$ -C $\delta$ -C $\epsilon$	112.338	1.494
N-C $\alpha$ -C	110.631	2.114	N-C $\alpha$ -C	111.388	2.178
N-C $\alpha$ -C $\beta$	110.315	1.072	N-C $\alpha$ -C $\beta$	110.670	1.028
LYS mtpn n = 382			LYS mtpm n = 20		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-68.535	7.513	chi1	-70.323	7.483
chi2	176.954	10.793	chi2	174.831	16.544
chi3	70.471	10.561	chi3	90.638	14.260
chi4	67.722	10.787	chi4	-70.024	12.307
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.232	1.649	C $\alpha$ -C $\beta$ -C $\gamma$	113.518	2.044
C $\alpha$ -C-O	120.413	0.809	C $\alpha$ -C-O	120.393	0.854
C $\beta$ -C $\alpha$ -C	110.143	1.537	C $\beta$ -C $\alpha$ -C	109.711	2.119
C $\beta$ -C $\gamma$ -C $\delta$	112.417	1.436	C $\beta$ -C $\gamma$ -C $\delta$	112.286	1.595
C $\delta$ -C $\epsilon$ -N $\zeta$	112.761	2.047	C $\delta$ -C $\epsilon$ -N $\zeta$	113.304	1.836
C $\gamma$ -C $\delta$ -C $\epsilon$	112.685	1.332	C $\gamma$ -C $\delta$ -C $\epsilon$	113.039	1.525
N-C $\alpha$ -C	111.430	2.505	N-C $\alpha$ -C	111.147	2.477
N-C $\alpha$ -C $\beta$	110.479	0.982	N-C $\alpha$ -C $\beta$	110.441	1.089
LYS ttmm n = 196			LYS mmpt n = 31		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.055	8.787	chi1	-60.371	7.892
chi2	179.742	10.210	chi2	-70.556	19.909
chi3	-71.028	12.157	chi3	93.615	14.916
chi4	-67.045	11.023	chi4	175.537	10.770
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.653	1.471	C $\alpha$ -C $\beta$ -C $\gamma$	115.223	1.103
C $\alpha$ -C-O	120.540	0.817	C $\alpha$ -C-O	120.365	0.885
C $\beta$ -C $\alpha$ -C	110.229	1.299	C $\beta$ -C $\alpha$ -C	109.774	1.684
C $\beta$ -C $\gamma$ -C $\delta$	112.149	1.564	C $\beta$ -C $\gamma$ -C $\delta$	113.421	1.782
C $\delta$ -C $\epsilon$ -N $\zeta$	112.684	2.274	C $\delta$ -C $\epsilon$ -N $\zeta$	111.551	1.763
C $\gamma$ -C $\delta$ -C $\epsilon$	112.507	1.566	C $\gamma$ -C $\delta$ -C $\epsilon$	112.028	1.393
N-C $\alpha$ -C	110.163	2.445	N-C $\alpha$ -C	111.336	2.523
N-C $\alpha$ -C $\beta$	110.340	1.405	N-C $\alpha$ -C $\beta$	111.122	1.384

LYS tppt n = 1179			LYS pttm n = 262		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-178.908	9.119	chi1	64.251	6.979
chi2	69.056	9.057	chi2	-177.627	8.999
chi3	175.565	10.218	chi3	-178.897	9.880
chi4	177.246	12.012	chi4	-67.053	11.968
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.784	1.306	C $\alpha$ -C $\beta$ -C $\gamma$	114.863	1.484
C $\alpha$ -C-O	120.542	0.773	C $\alpha$ -C-O	120.416	0.959
C $\beta$ -C $\alpha$ -C	110.423	1.225	C $\beta$ -C $\alpha$ -C	110.374	1.448
C $\beta$ -C $\gamma$ -C $\delta$	112.032	1.582	C $\beta$ -C $\gamma$ -C $\delta$	110.685	2.038
C $\delta$ -C $\epsilon$ -N $\zeta$	111.094	2.255	C $\delta$ -C $\epsilon$ -N $\zeta$	112.285	2.207
C $\gamma$ -C $\delta$ -C $\epsilon$	111.035	1.468	C $\gamma$ -C $\delta$ -C $\epsilon$	111.943	1.507
N-C $\alpha$ -C	110.639	2.173	N-C $\alpha$ -C	112.006	2.537
N-C $\alpha$ -C $\beta$	110.237	1.107	N-C $\alpha$ -C $\beta$	110.949	1.132
LYS ptpt n = 149			LYS ttpm n = 4		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	64.802	8.137	chi1	-176.905	10.026
chi2	179.088	12.200	chi2	175.311	6.851
chi3	72.966	10.510	chi3	87.099	18.038
chi4	174.545	11.089	chi4	-84.400	4.171
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.757	1.637	C $\alpha$ -C $\beta$ -C $\gamma$	115.353	1.109
C $\alpha$ -C-O	120.558	0.881	C $\alpha$ -C-O	120.752	0.322
C $\beta$ -C $\alpha$ -C	110.514	1.369	C $\beta$ -C $\alpha$ -C	110.281	0.444
C $\beta$ -C $\gamma$ -C $\delta$	112.136	1.644	C $\beta$ -C $\gamma$ -C $\delta$	111.616	0.992
C $\delta$ -C $\epsilon$ -N $\zeta$	111.404	2.002	C $\delta$ -C $\epsilon$ -N $\zeta$	113.892	1.178
C $\gamma$ -C $\delta$ -C $\epsilon$	112.329	1.673	C $\gamma$ -C $\delta$ -C $\epsilon$	113.140	0.242
N-C $\alpha$ -C	111.277	2.881	N-C $\alpha$ -C	110.149	1.306
N-C $\alpha$ -C $\beta$	111.100	1.261	N-C $\alpha$ -C $\beta$	110.149	0.835
LYS mtmp n = 9			LYS mmtm n = 455		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-67.465	5.792	chi1	-61.499	8.233
chi2	-175.781	8.346	chi2	-68.646	11.677
chi3	-95.844	7.431	chi3	179.724	12.077
chi4	73.531	12.322	chi4	67.912	12.953
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.802	1.228	C $\alpha$ -C $\beta$ -C $\gamma$	114.706	1.532
C $\alpha$ -C-O	120.633	0.607	C $\alpha$ -C-O	120.424	0.926
C $\beta$ -C $\alpha$ -C	109.891	1.198	C $\beta$ -C $\alpha$ -C	109.536	1.583
C $\beta$ -C $\gamma$ -C $\delta$	111.699	1.976	C $\beta$ -C $\gamma$ -C $\delta$	112.007	1.566
C $\delta$ -C $\epsilon$ -N $\zeta$	113.681	2.374	C $\delta$ -C $\epsilon$ -N $\zeta$	112.683	2.352
C $\gamma$ -C $\delta$ -C $\epsilon$	112.703	0.792	C $\gamma$ -C $\delta$ -C $\epsilon$	111.918	1.343
N-C $\alpha$ -C	110.375	2.291	N-C $\alpha$ -C	111.132	2.592
N-C $\alpha$ -C $\beta$	110.828	0.914	N-C $\alpha$ -C $\beta$	110.696	1.055



LYS mtmt n = 1288			LYS mmtt n = 3032		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.838	6.884	chi1	-61.713	8.309
chi2	-173.335	9.861	chi2	-67.230	9.812
chi3	-73.733	11.415	chi3	-176.776	10.172
chi4	-175.371	10.611	chi4	-178.237	11.034
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.220	1.588	C $\alpha$ -C $\beta$ -C $\gamma$	114.528	1.318
C $\alpha$ -C-O	120.395	0.858	C $\alpha$ -C-O	120.437	0.909
C $\beta$ -C $\alpha$ -C	110.085	1.567	C $\beta$ -C $\alpha$ -C	109.621	1.550
C $\beta$ -C $\gamma$ -C $\delta$	112.309	1.510	C $\beta$ -C $\gamma$ -C $\delta$	111.896	1.485
C $\delta$ -C $\epsilon$ -N $\zeta$	111.022	2.203	C $\delta$ -C $\epsilon$ -N $\zeta$	111.060	2.088
C $\gamma$ -C $\delta$ -C $\epsilon$	112.110	1.439	C $\gamma$ -C $\delta$ -C $\epsilon$	111.123	1.537
N-C $\alpha$ -C	111.320	2.147	N-C $\alpha$ -C	111.460	2.474
N-C $\alpha$ -C $\beta$	110.677	0.963	N-C $\alpha$ -C $\beta$	110.685	1.006
LYS ptmt n = 180			LYS mtmm n = 413		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	66.652	8.266	chi1	-63.898	6.529
chi2	-175.856	11.695	chi2	-177.154	10.112
chi3	-71.430	11.949	chi3	-70.378	10.781
chi4	-175.836	10.280	chi4	-66.004	9.536
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.529	1.554	C $\alpha$ -C $\beta$ -C $\gamma$	113.461	1.535
C $\alpha$ -C-O	120.496	0.993	C $\alpha$ -C-O	120.496	0.839
C $\beta$ -C $\alpha$ -C	110.383	1.607	C $\beta$ -C $\alpha$ -C	109.827	1.564
C $\beta$ -C $\gamma$ -C $\delta$	112.149	1.595	C $\beta$ -C $\gamma$ -C $\delta$	112.257	1.362
C $\delta$ -C $\epsilon$ -N $\zeta$	111.502	2.102	C $\delta$ -C $\epsilon$ -N $\zeta$	112.742	2.086
C $\gamma$ -C $\delta$ -C $\epsilon$	112.382	1.893	C $\gamma$ -C $\delta$ -C $\epsilon$	112.847	1.506
N-C $\alpha$ -C	111.040	2.758	N-C $\alpha$ -C	111.498	2.399
N-C $\alpha$ -C $\beta$	111.040	1.104	N-C $\alpha$ -C $\beta$	110.576	1.050
LYS mmtm n = 701			LYS pttt n = 1348		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-60.188	8.300	chi1	65.436	7.710
chi2	-65.555	10.930	chi2	-178.083	8.719
chi3	-173.090	11.132	chi3	-179.332	9.677
chi4	-68.899	13.211	chi4	-179.680	9.677
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.535	1.395	C $\alpha$ -C $\beta$ -C $\gamma$	114.833	1.450
C $\alpha$ -C-O	120.544	0.871	C $\alpha$ -C-O	120.426	0.926
C $\beta$ -C $\alpha$ -C	109.741	1.562	C $\beta$ -C $\alpha$ -C	110.445	1.382
C $\beta$ -C $\gamma$ -C $\delta$	111.938	1.423	C $\beta$ -C $\gamma$ -C $\delta$	110.825	1.800
C $\delta$ -C $\epsilon$ -N $\zeta$	112.450	1.980	C $\delta$ -C $\epsilon$ -N $\zeta$	111.323	2.000
C $\gamma$ -C $\delta$ -C $\epsilon$	111.954	1.442	C $\gamma$ -C $\delta$ -C $\epsilon$	111.009	1.622
N-C $\alpha$ -C	111.438	2.505	N-C $\alpha$ -C	111.326	2.766
N-C $\alpha$ -C $\beta$	110.625	1.015	N-C $\alpha$ -C $\beta$	111.127	1.106

LYS pmtt n = 10			LYS pttp n = 234		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	73.156	8.365	chi1	67.562	8.321
chi2	-74.065	10.515	chi2	-179.054	10.395
chi3	-168.029	10.580	chi3	178.259	11.424
chi4	-174.606	10.738	chi4	66.699	12.404
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	116.445	1.641	C $\alpha$ -C $\beta$ -C $\gamma$	114.798	1.434
C $\alpha$ -C-O	120.801	0.552	C $\alpha$ -C-O	120.362	0.910
C $\beta$ -C $\alpha$ -C	110.351	1.279	C $\beta$ -C $\alpha$ -C	110.358	1.459
C $\beta$ -C $\gamma$ -C $\delta$	112.587	2.234	C $\beta$ -C $\gamma$ -C $\delta$	110.901	1.689
C $\delta$ -C $\epsilon$ -N $\zeta$	111.694	2.248	C $\delta$ -C $\epsilon$ -N $\zeta$	112.404	2.292
C $\gamma$ -C $\delta$ -C $\epsilon$	111.327	1.312	C $\gamma$ -C $\delta$ -C $\epsilon$	111.710	1.396
N-C $\alpha$ -C	109.953	2.378	N-C $\alpha$ -C	111.882	2.534
N-C $\alpha$ -C $\beta$	112.145	2.128	N-C $\alpha$ -C $\beta$	110.964	1.061
LYS pmmt n = 2			LYS ptpn n = 88		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	77.882	1.900	chi1	65.327	6.504
chi2	-73.692	0.100	chi2	178.405	8.210
chi3	-71.417	0.650	chi3	72.033	10.196
chi4	179.050	3.501	chi4	66.034	8.526
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	117.188	0.414	C $\alpha$ -C $\beta$ -C $\gamma$	114.593	1.165
C $\alpha$ -C-O	120.505	0.860	C $\alpha$ -C-O	120.218	0.949
C $\beta$ -C $\alpha$ -C	111.392	0.287	C $\beta$ -C $\alpha$ -C	110.015	1.295
C $\beta$ -C $\gamma$ -C $\delta$	112.478	0.183	C $\beta$ -C $\gamma$ -C $\delta$	112.236	1.244
C $\delta$ -C $\epsilon$ -N $\zeta$	112.973	1.327	C $\delta$ -C $\epsilon$ -N $\zeta$	112.492	1.705
C $\gamma$ -C $\delta$ -C $\epsilon$	114.628	0.726	C $\gamma$ -C $\delta$ -C $\epsilon$	112.732	1.316
N-C $\alpha$ -C	110.777	0.060	N-C $\alpha$ -C	111.882	2.008
N-C $\alpha$ -C $\beta$	112.732	0.611	N-C $\alpha$ -C $\beta$	110.830	1.213
LYS tmtt n = 11			LYS mptt n = 127		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-176.649	7.224	chi1	-79.911	13.329
chi2	-97.994	8.621	chi2	72.964	17.299
chi3	-178.365	12.364	chi3	176.124	12.654
chi4	65.083	6.727	chi4	175.095	11.799
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.530	1.208	C $\alpha$ -C $\beta$ -C $\gamma$	114.888	1.339
C $\alpha$ -C-O	120.750	0.371	C $\alpha$ -C-O	120.557	0.775
C $\beta$ -C $\alpha$ -C	110.380	0.684	C $\beta$ -C $\alpha$ -C	109.759	1.520
C $\beta$ -C $\gamma$ -C $\delta$	111.895	1.500	C $\beta$ -C $\gamma$ -C $\delta$	112.493	1.974
C $\delta$ -C $\epsilon$ -N $\zeta$	113.336	2.960	C $\delta$ -C $\epsilon$ -N $\zeta$	110.777	2.254
C $\gamma$ -C $\delta$ -C $\epsilon$	111.833	1.208	C $\gamma$ -C $\delta$ -C $\epsilon$	111.215	1.635
N-C $\alpha$ -C	110.290	3.100	N-C $\alpha$ -C	110.632	2.494
N-C $\alpha$ -C $\beta$	110.329	0.877	N-C $\alpha$ -C $\beta$	110.834	1.080

LYS tmmt n = 76			LYS mptp n = 24		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-172.661	8.381	chi1	-74.901	17.297
chi2	-91.117	9.791	chi2	86.563	17.226
chi3	-176.853	10.984	chi3	171.631	9.474
chi4	-178.511	10.300	chi4	65.232	12.367
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.536	1.091	C $\alpha$ -C $\beta$ -C $\gamma$	114.507	1.245
C $\alpha$ -C-O	120.767	0.570	C $\alpha$ -C-O	120.337	1.070
C $\beta$ -C $\alpha$ -C	110.874	1.034	C $\beta$ -C $\alpha$ -C	109.962	1.397
C $\beta$ -C $\gamma$ -C $\delta$	111.941	1.465	C $\beta$ -C $\gamma$ -C $\delta$	112.925	1.955
C $\delta$ -C $\epsilon$ -N $\zeta$	110.930	1.901	C $\delta$ -C $\epsilon$ -N $\zeta$	113.461	2.349
C $\gamma$ -C $\delta$ -C $\epsilon$	110.910	1.343	C $\gamma$ -C $\delta$ -C $\epsilon$	112.483	2.810
N-C $\alpha$ -C	110.141	1.880	N-C $\alpha$ -C	110.446	2.733
N-C $\alpha$ -C $\beta$	110.081	0.837	N-C $\alpha$ -C $\beta$	111.004	0.900
LYS mmtt n = 543			LYS tmmt n = 31		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-62.678	7.633	chi1	-179.225	10.299
chi2	-64.116	10.721	chi2	-93.418	11.458
chi3	-70.703	9.501	chi3	-70.433	9.062
chi4	-176.812	9.721	chi4	-179.549	10.512
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.600	1.291	C $\alpha$ -C $\beta$ -C $\gamma$	114.968	1.756
C $\alpha$ -C-O	120.386	0.970	C $\alpha$ -C-O	120.553	0.898
C $\beta$ -C $\alpha$ -C	109.614	1.454	C $\beta$ -C $\alpha$ -C	110.799	1.116
C $\beta$ -C $\gamma$ -C $\delta$	113.087	1.498	C $\beta$ -C $\gamma$ -C $\delta$	113.476	1.742
C $\delta$ -C $\epsilon$ -N $\zeta$	111.132	2.211	C $\delta$ -C $\epsilon$ -N $\zeta$	110.762	2.948
C $\gamma$ -C $\delta$ -C $\epsilon$	112.304	1.535	C $\gamma$ -C $\delta$ -C $\epsilon$	112.420	2.932
N-C $\alpha$ -C	111.744	2.329	N-C $\alpha$ -C	110.150	1.984
N-C $\alpha$ -C $\beta$	110.664	1.046	N-C $\alpha$ -C $\beta$	109.907	1.053
LYS pptt n = 25			LYS tttm n = 1121		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	64.183	7.527	chi1	-176.393	8.120
chi2	89.871	8.334	chi2	177.818	9.690
chi3	175.578	11.861	chi3	-176.243	10.410
chi4	179.092	7.380	chi4	-67.353	11.982
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	116.057	1.244	C $\alpha$ -C $\beta$ -C $\gamma$	113.869	1.587
C $\alpha$ -C-O	120.408	0.698	C $\alpha$ -C-O	120.554	0.823
C $\beta$ -C $\alpha$ -C	111.303	1.430	C $\beta$ -C $\alpha$ -C	110.236	1.118
C $\beta$ -C $\gamma$ -C $\delta$	112.212	1.704	C $\beta$ -C $\gamma$ -C $\delta$	111.025	1.728
C $\delta$ -C $\epsilon$ -N $\zeta$	111.319	1.822	C $\delta$ -C $\epsilon$ -N $\zeta$	112.289	1.930
C $\gamma$ -C $\delta$ -C $\epsilon$	110.556	1.940	C $\gamma$ -C $\delta$ -C $\epsilon$	111.816	1.408
N-C $\alpha$ -C	111.714	2.089	N-C $\alpha$ -C	110.499	2.132
N-C $\alpha$ -C $\beta$	111.577	1.190	N-C $\alpha$ -C $\beta$	110.449	1.158

LYS mppt n = 30			LYS mmmm n = 84		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-82.599	8.920	chi1	-61.396	7.210
chi2	73.518	13.474	chi2	-61.832	10.222
chi3	69.157	7.573	chi3	-66.893	10.824
chi4	177.385	5.503	chi4	-64.659	10.834
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.149	2.009	C $\alpha$ -C $\beta$ -C $\gamma$	114.697	1.362
C $\alpha$ -C-O	120.402	0.897	C $\alpha$ -C-O	120.389	1.092
C $\beta$ -C $\alpha$ -C	109.855	1.241	C $\beta$ -C $\alpha$ -C	109.559	1.464
C $\beta$ -C $\gamma$ -C $\delta$	113.706	1.587	C $\beta$ -C $\gamma$ -C $\delta$	113.177	1.448
C $\delta$ -C $\epsilon$ -N $\zeta$	111.345	1.953	C $\delta$ -C $\epsilon$ -N $\zeta$	112.615	2.804
C $\gamma$ -C $\delta$ -C $\epsilon$	112.207	1.389	C $\gamma$ -C $\delta$ -C $\epsilon$	113.211	1.913
N-C $\alpha$ -C	108.769	2.005	N-C $\alpha$ -C	111.602	2.528
N-C $\alpha$ -C $\beta$	110.866	0.910	N-C $\alpha$ -C $\beta$	110.482	1.127
LYS tmmm n = 8			LYS tttt n = 4861		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.527	11.864	chi1	-175.451	8.169
chi2	-81.761	7.499	chi2	176.592	8.767
chi3	-63.102	8.026	chi3	179.677	9.260
chi4	-64.475	4.939	chi4	-179.889	10.200
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	116.243	2.695	C $\alpha$ -C $\beta$ -C $\gamma$	113.873	1.541
C $\alpha$ -C-O	120.272	0.848	C $\alpha$ -C-O	120.582	0.775
C $\beta$ -C $\alpha$ -C	111.246	1.126	C $\beta$ -C $\alpha$ -C	110.231	1.130
C $\beta$ -C $\gamma$ -C $\delta$	114.871	1.367	C $\beta$ -C $\gamma$ -C $\delta$	111.144	1.751
C $\delta$ -C $\epsilon$ -N $\zeta$	113.141	1.476	C $\delta$ -C $\epsilon$ -N $\zeta$	111.168	1.988
C $\gamma$ -C $\delta$ -C $\epsilon$	114.998	1.617	C $\gamma$ -C $\delta$ -C $\epsilon$	111.041	1.555
N-C $\alpha$ -C	108.983	2.013	N-C $\alpha$ -C	110.548	2.283
N-C $\alpha$ -C $\beta$	109.523	1.258	N-C $\alpha$ -C $\beta$	110.335	1.208
LYS tptm n = 186			LYS tptp n = 397		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.928	7.743	chi1	-179.932	7.711
chi2	67.158	9.851	chi2	67.443	10.094
chi3	-179.368	11.634	chi3	173.601	13.627
chi4	-66.243	13.119	chi4	66.191	12.712
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.935	1.380	C $\alpha$ -C $\beta$ -C $\gamma$	114.794	1.326
C $\alpha$ -C-O	120.385	0.782	C $\alpha$ -C-O	120.523	0.836
C $\beta$ -C $\alpha$ -C	110.358	1.052	C $\beta$ -C $\alpha$ -C	110.213	1.216
C $\beta$ -C $\gamma$ -C $\delta$	111.872	1.408	C $\beta$ -C $\gamma$ -C $\delta$	112.053	1.463
C $\delta$ -C $\epsilon$ -N $\zeta$	112.546	1.999	C $\delta$ -C $\epsilon$ -N $\zeta$	112.637	1.911
C $\gamma$ -C $\delta$ -C $\epsilon$	111.915	1.346	C $\gamma$ -C $\delta$ -C $\epsilon$	112.163	1.302
N-C $\alpha$ -C	110.318	2.024	N-C $\alpha$ -C	110.295	2.083
N-C $\alpha$ -C $\beta$	110.247	1.184	N-C $\alpha$ -C $\beta$	110.322	1.121

LYS mptm n = 12			LYS ttmt n = 660		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-91.748	10.291	chi1	-174.573	9.248
chi2	61.180	11.718	chi2	-177.288	10.547
chi3	-173.655	8.343	chi3	-73.479	11.991
chi4	-60.981	12.837	chi4	-175.112	11.332
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	114.555	0.798	C $\alpha$ -C $\beta$ -C $\gamma$	113.693	1.603
C $\alpha$ -C-O	120.631	0.553	C $\alpha$ -C-O	120.605	0.861
C $\beta$ -C $\alpha$ -C	110.339	1.030	C $\beta$ -C $\alpha$ -C	110.198	1.171
C $\beta$ -C $\gamma$ -C $\delta$	112.639	0.748	C $\beta$ -C $\gamma$ -C $\delta$	112.167	1.536
C $\delta$ -C $\epsilon$ -N $\zeta$	113.329	1.651	C $\delta$ -C $\epsilon$ -N $\zeta$	110.954	2.327
C $\gamma$ -C $\delta$ -C $\epsilon$	111.743	0.606	C $\gamma$ -C $\delta$ -C $\epsilon$	112.228	1.660
N-C $\alpha$ -C	110.398	2.154	N-C $\alpha$ -C	110.305	2.344
N-C $\alpha$ -C $\beta$	110.566	0.850	N-C $\alpha$ -C $\beta$	110.345	1.237
LYS tmtm n = 18			LYS ttpt n = 1184		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-172.233	10.952	chi1	-177.650	8.175
chi2	-90.510	5.643	chi2	175.444	9.837
chi3	-172.543	12.826	chi3	173.929	10.972
chi4	-64.869	7.988	chi4	65.901	12.639
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	115.721	1.478	C $\alpha$ -C $\beta$ -C $\gamma$	113.948	1.528
C $\alpha$ -C-O	120.578	0.678	C $\alpha$ -C-O	120.577	0.751
C $\beta$ -C $\alpha$ -C	111.018	0.821	C $\beta$ -C $\alpha$ -C	110.208	1.091
C $\beta$ -C $\gamma$ -C $\delta$	112.129	1.268	C $\beta$ -C $\gamma$ -C $\delta$	111.139	1.588
C $\delta$ -C $\epsilon$ -N $\zeta$	112.795	1.744	C $\delta$ -C $\epsilon$ -N $\zeta$	112.275	2.010
C $\gamma$ -C $\delta$ -C $\epsilon$	112.083	1.552	C $\gamma$ -C $\delta$ -C $\epsilon$	111.838	1.358
N-C $\alpha$ -C	109.908	1.712	N-C $\alpha$ -C	110.677	2.233
N-C $\alpha$ -C $\beta$	109.668	0.722	N-C $\alpha$ -C $\beta$	110.404	1.146
LYS ttpt n = 858			LYS ttpp n = 217		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-178.343	8.179	chi1	-178.427	8.698
chi2	174.555	12.325	chi2	174.058	14.697
chi3	73.017	11.821	chi3	71.618	11.437
chi4	175.105	11.350	chi4	68.201	9.320
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.747	1.617	C $\alpha$ -C $\beta$ -C $\gamma$	113.616	1.605
C $\alpha$ -C-O	120.605	0.754	C $\alpha$ -C-O	120.600	0.801
C $\beta$ -C $\alpha$ -C	110.063	1.167	C $\beta$ -C $\alpha$ -C	110.087	1.255
C $\beta$ -C $\gamma$ -C $\delta$	112.132	1.476	C $\beta$ -C $\gamma$ -C $\delta$	112.162	1.668
C $\delta$ -C $\epsilon$ -N $\zeta$	111.095	2.063	C $\delta$ -C $\epsilon$ -N $\zeta$	112.803	2.394
C $\gamma$ -C $\delta$ -C $\epsilon$	112.144	1.567	C $\gamma$ -C $\delta$ -C $\epsilon$	112.733	1.464
N-C $\alpha$ -C	110.324	2.318	N-C $\alpha$ -C	110.242	2.451
N-C $\alpha$ -C $\beta$	110.250	1.312	N-C $\alpha$ -C $\beta$	110.406	1.369

LYS mttm n = 1793			LYS tppp n = 35		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.855	7.316	chi1	-177.926	12.227
chi2	-177.777	10.010	chi2	62.258	10.225
chi3	-176.656	10.804	chi3	65.517	8.325
chi4	-67.384	12.631	chi4	67.940	11.042
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.405	1.721	C $\alpha$ -C $\beta$ -C $\gamma$	115.248	1.528
C $\alpha$ -C-O	120.480	0.845	C $\alpha$ -C-O	120.677	0.833
C $\beta$ -C $\alpha$ -C	110.077	1.549	C $\beta$ -C $\alpha$ -C	110.438	0.767
C $\beta$ -C $\gamma$ -C $\delta$	111.191	1.731	C $\beta$ -C $\gamma$ -C $\delta$	113.603	1.889
C $\delta$ -C $\epsilon$ -N $\zeta$	112.202	2.051	C $\delta$ -C $\epsilon$ -N $\zeta$	113.089	1.700
C $\gamma$ -C $\delta$ -C $\epsilon$	111.733	1.461	C $\gamma$ -C $\delta$ -C $\epsilon$	113.467	1.753
N-C $\alpha$ -C	111.384	2.368	N-C $\alpha$ -C	110.994	1.841
N-C $\alpha$ -C $\beta$	110.610	0.996	N-C $\alpha$ -C $\beta$	110.242	1.136
LYS mtpp n = 1364			LYS mttt n = 8346		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-65.910	8.334	chi1	-67.654	7.115
chi2	-179.442	10.432	chi2	-178.811	9.043
chi3	176.319	10.992	chi3	-179.106	9.828
chi4	66.691	13.396	chi4	179.484	10.340
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.462	1.699	C $\alpha$ -C $\beta$ -C $\gamma$	113.450	1.626
C $\alpha$ -C-O	120.505	0.828	C $\alpha$ -C-O	120.466	0.825
C $\beta$ -C $\alpha$ -C	110.079	1.600	C $\beta$ -C $\alpha$ -C	109.994	1.554
C $\beta$ -C $\gamma$ -C $\delta$	111.245	1.729	C $\beta$ -C $\gamma$ -C $\delta$	111.139	1.844
C $\delta$ -C $\epsilon$ -N $\zeta$	112.222	1.990	C $\delta$ -C $\epsilon$ -N $\zeta$	111.114	2.090
C $\gamma$ -C $\delta$ -C $\epsilon$	111.727	1.427	C $\gamma$ -C $\delta$ -C $\epsilon$	111.046	1.587
N-C $\alpha$ -C	111.267	2.497	N-C $\alpha$ -C	111.329	2.236
N-C $\alpha$ -C $\beta$	110.596	1.017	N-C $\alpha$ -C $\beta$	110.670	0.985
LYS ttpp n = 9			LYS ptmm n = 78		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.170	3.389	chi1	66.614	8.430
chi2	-179.415	7.426	chi2	-177.929	10.052
chi3	-95.701	17.014	chi3	-69.614	9.318
chi4	76.743	24.622	chi4	-66.129	6.833
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.035	1.097	C $\alpha$ -C $\beta$ -C $\gamma$	114.440	1.310
C $\alpha$ -C-O	120.617	0.500	C $\alpha$ -C-O	120.631	1.040
C $\beta$ -C $\alpha$ -C	110.407	1.609	C $\beta$ -C $\alpha$ -C	109.920	1.510
C $\beta$ -C $\gamma$ -C $\delta$	112.734	1.712	C $\beta$ -C $\gamma$ -C $\delta$	112.368	1.441
C $\delta$ -C $\epsilon$ -N $\zeta$	114.122	1.260	C $\delta$ -C $\epsilon$ -N $\zeta$	112.964	1.788
C $\gamma$ -C $\delta$ -C $\epsilon$	112.855	0.789	C $\gamma$ -C $\delta$ -C $\epsilon$	113.025	1.147
N-C $\alpha$ -C	110.834	1.481	N-C $\alpha$ -C	110.448	2.720
N-C $\alpha$ -C $\beta$	111.415	1.053	N-C $\alpha$ -C $\beta$	110.825	1.214

### 3.18 ARG

ARG ttp-170 n = 1479			ARG pmt170 n = 40		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-175.447	9.255	chi1	73.963	11.175
chi2	179.359	13.108	chi2	-78.972	15.497
chi3	66.850	8.920	chi3	-169.420	10.046
chi4	-171.036	17.135	chi4	-169.441	15.483
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.661	1.643	C $\alpha$ -C $\beta$ -C $\gamma$	116.305	1.176
C $\alpha$ -C-O	120.599	0.749	C $\alpha$ -C-O	120.754	0.693
C $\beta$ -C $\alpha$ -C	109.991	1.239	C $\beta$ -C $\alpha$ -C	110.786	1.109
C $\beta$ -C $\gamma$ -C $\delta$	111.638	1.684	C $\beta$ -C $\gamma$ -C $\delta$	112.699	1.260
C $\delta$ -N $\epsilon$ -C $\zeta$	124.480	1.163	C $\delta$ -N $\epsilon$ -C $\zeta$	124.364	1.048
C $\gamma$ -C $\delta$ -N $\epsilon$	111.498	1.579	C $\gamma$ -C $\delta$ -N $\epsilon$	111.664	1.950
N $\epsilon$ -C $\zeta$ -N $\eta$ 1	120.443	0.880	N $\epsilon$ -C $\zeta$ -N $\eta$ 1	120.360	0.773
N $\epsilon$ -C $\zeta$ -N $\eta$ 2	119.775	0.868	N $\epsilon$ -C $\zeta$ -N $\eta$ 2	119.982	0.637
N $\eta$ 1-C $\zeta$ -N $\eta$ 2	119.763	0.690	N $\eta$ 1-C $\zeta$ -N $\eta$ 2	119.646	0.551
N-C $\alpha$ -C	110.447	2.202	N-C $\alpha$ -C	110.714	2.371
N-C $\alpha$ -C $\beta$	110.437	1.311	N-C $\alpha$ -C $\beta$	111.768	1.065
ARG mtp180 n = 2444			ARG pmm-80 n = 19		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.448	8.180	chi1	73.642	12.608
chi2	178.975	12.987	chi2	-75.958	11.183
chi3	66.423	9.105	chi3	-56.789	8.115
chi4	-171.573	16.488	chi4	-81.265	7.401
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ -C $\beta$ -C $\gamma$	113.198	1.794	C $\alpha$ -C $\beta$ -C $\gamma$	115.931	1.019
C $\alpha$ -C-O	120.477	0.832	C $\alpha$ -C-O	120.769	0.553
C $\beta$ -C $\alpha$ -C	110.045	1.655	C $\beta$ -C $\alpha$ -C	110.942	1.227
C $\beta$ -C $\gamma$ -C $\delta$	111.700	1.780	C $\beta$ -C $\gamma$ -C $\delta$	113.505	1.558
C $\delta$ -N $\epsilon$ -C $\zeta$	124.378	1.201	C $\delta$ -N $\epsilon$ -C $\zeta$	125.145	1.080
C $\gamma$ -C $\delta$ -N $\epsilon$	111.556	1.557	C $\gamma$ -C $\delta$ -N $\epsilon$	112.540	1.304
N $\epsilon$ -C $\zeta$ -N $\eta$ 1	120.430	0.998	N $\epsilon$ -C $\zeta$ -N $\eta$ 1	120.428	0.947
N $\epsilon$ -C $\zeta$ -N $\eta$ 2	119.776	0.964	N $\epsilon$ -C $\zeta$ -N $\eta$ 2	120.291	0.953
N $\eta$ 1-C $\zeta$ -N $\eta$ 2	119.778	0.767	N $\eta$ 1-C $\zeta$ -N $\eta$ 2	119.271	0.671
N-C $\alpha$ -C	111.425	2.419	N-C $\alpha$ -C	109.672	2.434
N-C $\alpha$ -C $\beta$	110.536	1.042	N-C $\alpha$ -C $\beta$	111.608	1.001

ARG ttp-110 n = 616			ARG pmt-80 n = 26		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.744	8.634	chi1	81.229	9.470
chi2	177.160	13.078	chi2	-68.144	7.677
chi3	64.599	10.834	chi3	-176.905	11.168
chi4	-113.458	9.921	chi4	-84.063	8.278
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.833	1.642	C $\alpha$ _C $\beta$ _C $\gamma$	115.724	1.165
C $\alpha$ _C_O	120.601	0.805	C $\alpha$ _C_O	120.979	0.655
C $\beta$ _C $\alpha$ _C	110.165	1.235	C $\beta$ _C $\alpha$ _C	110.263	1.032
C $\beta$ _C $\gamma$ _C $\delta$	111.993	1.747	C $\beta$ _C $\gamma$ _C $\delta$	113.303	1.809
C $\delta$ _N $\epsilon$ _C $\zeta$	125.367	1.365	C $\delta$ _N $\epsilon$ _C $\zeta$	124.962	0.996
C $\gamma$ _C $\delta$ _N $\epsilon$	111.873	2.149	C $\gamma$ _C $\delta$ _N $\epsilon$	112.046	1.732
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.080	1.283	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.047	0.855
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.472	1.155	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.621	0.610
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.427	0.892	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.312	0.539
N_C $\alpha$ _C	110.689	2.197	N_C $\alpha$ _C	110.675	2.058
N_C $\alpha$ _C $\beta$	110.301	1.286	N_C $\alpha$ _C $\beta$	111.431	1.161
ARG mpt180 n = 241			ARG mtt90 n = 2402		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-84.592	7.920	chi1	-67.677	7.490
chi2	69.331	13.033	chi2	179.859	13.521
chi3	173.629	9.225	chi3	178.901	10.618
chi4	174.437	16.865	chi4	90.605	15.171
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.784	1.415	C $\alpha$ _C $\beta$ _C $\gamma$	113.333	1.721
C $\alpha$ _C_O	120.569	0.863	C $\alpha$ _C_O	120.441	0.801
C $\beta$ _C $\alpha$ _C	109.472	1.661	C $\beta$ _C $\alpha$ _C	109.901	1.716
C $\beta$ _C $\gamma$ _C $\delta$	112.991	1.807	C $\beta$ _C $\gamma$ _C $\delta$	111.536	2.046
C $\delta$ _N $\epsilon$ _C $\zeta$	124.413	1.462	C $\delta$ _N $\epsilon$ _C $\zeta$	124.857	1.137
C $\gamma$ _C $\delta$ _N $\epsilon$	110.708	2.005	C $\gamma$ _C $\delta$ _N $\epsilon$	111.014	2.489
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.394	1.019	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.851	1.075
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.743	0.915	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.532	1.059
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.835	0.887	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.591	0.810
N_C $\alpha$ _C	110.012	2.748	N_C $\alpha$ _C	111.459	2.407
N_C $\alpha$ _C $\beta$	111.142	1.137	N_C $\alpha$ _C $\beta$	110.564	1.118



ARG ttt-90 n = 1340			ARG mpp-170 n = 61		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-176.754	9.428	chi1	-78.876	12.782
chi2	177.849	11.359	chi2	81.734	17.546
chi3	-178.261	9.828	chi3	65.059	7.321
chi4	-89.587	12.432	chi4	-166.895	17.175
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.981	1.610	C $\alpha$ _C $\beta$ _C $\gamma$	114.670	1.401
C $\alpha$ _C_O	120.539	0.783	C $\alpha$ _C_O	120.576	0.634
C $\beta$ _C $\alpha$ _C	110.257	1.264	C $\beta$ _C $\alpha$ _C	109.621	1.429
C $\beta$ _C $\gamma$ _C $\delta$	110.911	2.070	C $\beta$ _C $\gamma$ _C $\delta$	112.663	1.759
C $\delta$ _N $\epsilon$ _C $\zeta$	124.824	1.144	C $\delta$ _N $\epsilon$ _C $\zeta$	124.402	1.168
C $\gamma$ _C $\delta$ _N $\epsilon$	111.838	2.499	C $\gamma$ _C $\delta$ _N $\epsilon$	111.588	1.339
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.767	1.014	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.721	0.995
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.594	0.967	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.657	0.708
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.618	0.868	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.604	0.725
N_C $\alpha$ _C	110.395	2.306	N_C $\alpha$ _C	110.015	3.139
N_C $\alpha$ _C $\beta$	110.231	1.293	N_C $\alpha$ _C $\beta$	111.347	1.049
ARG mtm110 n = 765			ARG ptm160 n = 496		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-68.128	8.122	chi1	63.484	8.764
chi2	-177.015	9.654	chi2	-179.108	15.002
chi3	-68.916	10.457	chi3	-67.148	9.871
chi4	112.867	10.511	chi4	165.337	25.676
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.144	1.800	C $\alpha$ _C $\beta$ _C $\gamma$	114.589	1.650
C $\alpha$ _C_O	120.421	0.868	C $\alpha$ _C_O	120.504	0.981
C $\beta$ _C $\alpha$ _C	110.062	1.756	C $\beta$ _C $\alpha$ _C	110.445	1.562
C $\beta$ _C $\gamma$ _C $\delta$	112.398	1.710	C $\beta$ _C $\gamma$ _C $\delta$	111.718	1.807
C $\delta$ _N $\epsilon$ _C $\zeta$	125.289	1.468	C $\delta$ _N $\epsilon$ _C $\zeta$	124.670	1.398
C $\gamma$ _C $\delta$ _N $\epsilon$	112.093	1.877	C $\gamma$ _C $\delta$ _N $\epsilon$	111.561	2.103
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.038	1.239	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.580	1.283
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.456	1.108	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.713	1.128
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.487	0.911	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.686	1.003
N_C $\alpha$ _C	111.650	2.446	N_C $\alpha$ _C	110.911	2.561
N_C $\alpha$ _C $\beta$	110.680	1.023	N_C $\alpha$ _C $\beta$	111.010	1.279

ARG tpm-80 n = 19			ARG tpp80 n = 358		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.264	5.205	chi1	-177.765	10.202
chi2	78.524	8.110	chi2	65.211	10.766
chi3	-80.359	10.480	chi3	59.806	9.550
chi4	-79.824	9.270	chi4	84.211	9.220
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.183	1.414	C $\alpha$ _C $\beta$ _C $\gamma$	114.937	1.366
C $\alpha$ _C_O	120.634	1.078	C $\alpha$ _C_O	120.532	0.755
C $\beta$ _C $\alpha$ _C	110.271	1.141	C $\beta$ _C $\alpha$ _C	110.478	1.226
C $\beta$ _C $\gamma$ _C $\delta$	112.940	1.157	C $\beta$ _C $\gamma$ _C $\delta$	112.980	1.577
C $\delta$ _N $\epsilon$ _C $\zeta$	125.286	1.195	C $\delta$ _N $\epsilon$ _C $\zeta$	125.002	1.060
C $\gamma$ _C $\delta$ _N $\epsilon$	113.647	2.247	C $\gamma$ _C $\delta$ _N $\epsilon$	112.613	2.056
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.670	0.978	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.719	0.869
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	120.045	0.947	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.747	0.827
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.266	0.643	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.514	0.717
N_C $\alpha$ _C	110.861	1.497	N_C $\alpha$ _C	110.767	2.017
N_C $\alpha$ _C $\beta$	109.906	1.129	N_C $\alpha$ _C $\beta$	110.356	1.121
ARG ptp-170 n = 378			ARG ttt90 n = 1019		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	67.375	7.738	chi1	-176.157	9.349
chi2	-175.630	12.343	chi2	176.118	10.768
chi3	68.232	9.386	chi3	176.454	9.625
chi4	-172.286	16.066	chi4	86.745	10.698
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.529	1.454	C $\alpha$ _C $\beta$ _C $\gamma$	113.863	1.705
C $\alpha$ _C_O	120.570	0.949	C $\alpha$ _C_O	120.576	0.785
C $\beta$ _C $\alpha$ _C	110.367	1.549	C $\beta$ _C $\alpha$ _C	110.241	1.230
C $\beta$ _C $\gamma$ _C $\delta$	111.274	1.751	C $\beta$ _C $\gamma$ _C $\delta$	111.310	2.083
C $\delta$ _N $\epsilon$ _C $\zeta$	124.587	1.110	C $\delta$ _N $\epsilon$ _C $\zeta$	124.740	0.979
C $\gamma$ _C $\delta$ _N $\epsilon$	111.439	1.582	C $\gamma$ _C $\delta$ _N $\epsilon$	111.625	2.562
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.448	0.945	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.723	0.971
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.788	0.845	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.635	0.944
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.735	0.836	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.618	0.726
N_C $\alpha$ _C	111.336	2.563	N_C $\alpha$ _C	110.514	2.406
N_C $\alpha$ _C $\beta$	110.782	1.151	N_C $\alpha$ _C $\beta$	110.353	1.372

ARG ttt180 n = 2294			ARG ptt90 n = 797		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-176.225	9.089	chi1	64.935	7.664
chi2	176.468	11.199	chi2	178.802	12.133
chi3	178.543	11.535	chi3	176.614	8.716
chi4	179.245	18.737	chi4	87.625	9.730
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.469	1.751	C $\alpha$ _C $\beta$ _C $\gamma$	114.806	1.433
C $\alpha$ _C_O	120.563	0.807	C $\alpha$ _C_O	120.591	0.868
C $\beta$ _C $\alpha$ _C	110.173	1.174	C $\beta$ _C $\alpha$ _C	110.212	1.421
C $\beta$ _C $\gamma$ _C $\delta$	111.349	2.176	C $\beta$ _C $\gamma$ _C $\delta$	110.981	1.951
C $\delta$ _N $\epsilon$ _C $\zeta$	124.338	1.175	C $\delta$ _N $\epsilon$ _C $\zeta$	124.866	0.905
C $\gamma$ _C $\delta$ _N $\epsilon$	110.642	1.927	C $\gamma$ _C $\delta$ _N $\epsilon$	111.888	2.446
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.403	0.892	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.742	0.972
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.614	0.881	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.700	0.900
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.965	0.799	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.539	0.696
N_C $\alpha$ _C	110.511	2.403	N_C $\alpha$ _C	110.796	2.517
N_C $\alpha$ _C $\beta$	110.185	1.379	N_C $\alpha$ _C $\beta$	111.045	1.145
ARG tpt-90 n = 349			ARG mpt90 n = 48		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	179.343	8.509	chi1	-76.133	12.986
chi2	67.144	10.528	chi2	84.673	13.882
chi3	-179.669	8.884	chi3	170.244	9.976
chi4	-89.385	12.112	chi4	93.427	10.968
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.746	1.231	C $\alpha$ _C $\beta$ _C $\gamma$	114.551	1.718
C $\alpha$ _C_O	120.498	0.704	C $\alpha$ _C_O	120.424	0.638
C $\beta$ _C $\alpha$ _C	110.562	1.204	C $\beta$ _C $\alpha$ _C	109.252	1.448
C $\beta$ _C $\gamma$ _C $\delta$	112.329	1.639	C $\beta$ _C $\gamma$ _C $\delta$	112.595	1.663
C $\delta$ _N $\epsilon$ _C $\zeta$	124.831	1.149	C $\delta$ _N $\epsilon$ _C $\zeta$	125.017	0.927
C $\gamma$ _C $\delta$ _N $\epsilon$	111.143	2.461	C $\gamma$ _C $\delta$ _N $\epsilon$	111.068	2.089
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.708	0.996	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.075	0.893
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.670	0.955	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.387	0.679
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.598	0.674	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.518	0.577
N_C $\alpha$ _C	110.869	2.179	N_C $\alpha$ _C	110.063	2.732
N_C $\alpha$ _C $\beta$	110.210	1.209	N_C $\alpha$ _C $\beta$	111.320	1.226

ARG ppp80 n = 10			ARG pmm150 n = 12		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	62.201	5.082	chi1	75.579	3.166
chi2	86.595	6.961	chi2	-75.440	5.561
chi3	57.216	3.753	chi3	-64.975	6.260
chi4	79.687	8.472	chi4	151.999	15.442
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	116.109	0.884	C $\alpha$ _C $\beta$ _C $\gamma$	116.190	1.499
C $\alpha$ _C_O	120.837	0.551	C $\alpha$ _C_O	120.267	0.926
C $\beta$ _C $\alpha$ _C	111.013	1.509	C $\beta$ _C $\alpha$ _C	110.409	1.045
C $\beta$ _C $\gamma$ _C $\delta$	113.944	0.819	C $\beta$ _C $\gamma$ _C $\delta$	112.425	1.153
C $\delta$ _N $\epsilon$ _C $\zeta$	125.029	0.341	C $\delta$ _N $\epsilon$ _C $\zeta$	125.348	2.473
C $\gamma$ _C $\delta$ _N $\epsilon$	112.507	1.082	C $\gamma$ _C $\delta$ _N $\epsilon$	111.569	2.064
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.628	0.683	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.076	1.741
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.754	0.628	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.660	1.033
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.607	0.318	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.218	1.385
N_C $\alpha$ _C	111.134	2.176	N_C $\alpha$ _C	109.038	0.995
N_C $\alpha$ _C $\beta$	111.870	1.188	N_C $\alpha$ _C $\beta$	112.126	0.964
ARG ptm-80 n = 212			ARG ptp90 n = 219		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	65.373	8.242	chi1	65.165	9.386
chi2	-178.472	14.457	chi2	178.845	11.358
chi3	-66.034	10.268	chi3	64.039	8.608
chi4	-84.515	10.771	chi4	87.873	11.161
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.587	1.276	C $\alpha$ _C $\beta$ _C $\gamma$	114.899	1.486
C $\alpha$ _C_O	120.412	0.852	C $\alpha$ _C_O	120.463	0.961
C $\beta$ _C $\alpha$ _C	110.310	1.386	C $\beta$ _C $\alpha$ _C	110.453	1.389
C $\beta$ _C $\gamma$ _C $\delta$	111.859	1.750	C $\beta$ _C $\gamma$ _C $\delta$	111.832	1.558
C $\delta$ _N $\epsilon$ _C $\zeta$	124.958	1.447	C $\delta$ _N $\epsilon$ _C $\zeta$	124.915	1.162
C $\gamma$ _C $\delta$ _N $\epsilon$	112.317	2.278	C $\gamma$ _C $\delta$ _N $\epsilon$	112.175	2.187
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.705	1.220	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.749	1.027
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.900	1.459	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.716	0.978
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.376	0.855	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.517	0.744
N_C $\alpha$ _C	111.633	2.537	N_C $\alpha$ _C	110.908	2.837
N_C $\alpha$ _C $\beta$	110.977	1.319	N_C $\alpha$ _C $\beta$	111.117	1.191

ARG ptt-90 n = 701			ARG mtp85 n = 1815		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	66.303	7.919	chi1	-66.328	8.551
chi2	-175.118	12.042	chi2	177.775	11.141
chi3	-176.524	9.175	chi3	64.643	9.712
chi4	-87.098	11.773	chi4	87.715	10.990
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.834	1.507	C $\alpha$ _C $\beta$ _C $\gamma$	113.269	1.811
C $\alpha$ _C_O	120.480	0.932	C $\alpha$ _C_O	120.491	0.903
C $\beta$ _C $\alpha$ _C	110.425	1.553	C $\beta$ _C $\alpha$ _C	110.148	1.671
C $\beta$ _C $\gamma$ _C $\delta$	110.986	2.045	C $\beta$ _C $\gamma$ _C $\delta$	112.062	1.700
C $\delta$ _N $\epsilon$ _C $\zeta$	124.854	1.160	C $\delta$ _N $\epsilon$ _C $\zeta$	124.890	1.193
C $\gamma$ _C $\delta$ _N $\epsilon$	111.684	2.685	C $\gamma$ _C $\delta$ _N $\epsilon$	112.297	1.979
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.746	1.010	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.792	1.042
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.694	1.145	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.682	1.018
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.538	1.036	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.506	0.780
N_C $\alpha$ _C	111.689	2.532	N_C $\alpha$ _C	111.093	2.396
N_C $\alpha$ _C $\beta$	110.948	1.151	N_C $\alpha$ _C $\beta$	110.595	1.042
ARG mmm160 n = 936			ARG ptp-110 n = 76		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-61.827	9.223	chi1	67.597	8.250
chi2	-66.167	13.640	chi2	-179.670	11.943
chi3	-64.223	10.076	chi3	64.784	9.524
chi4	163.153	24.085	chi4	-108.305	9.870
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.473	1.606	C $\alpha$ _C $\beta$ _C $\gamma$	114.848	1.903
C $\alpha$ _C_O	120.402	0.877	C $\alpha$ _C_O	120.797	1.200
C $\beta$ _C $\alpha$ _C	109.777	1.549	C $\beta$ _C $\alpha$ _C	110.400	1.408
C $\beta$ _C $\gamma$ _C $\delta$	112.534	1.733	C $\beta$ _C $\gamma$ _C $\delta$	111.843	1.470
C $\delta$ _N $\epsilon$ _C $\zeta$	124.583	1.308	C $\delta$ _N $\epsilon$ _C $\zeta$	125.631	1.395
C $\gamma$ _C $\delta$ _N $\epsilon$	111.843	1.891	C $\gamma$ _C $\delta$ _N $\epsilon$	111.737	2.292
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.562	1.166	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.013	1.390
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.780	1.119	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.566	1.570
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.635	0.777	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.397	1.125
N_C $\alpha$ _C	111.413	2.408	N_C $\alpha$ _C	111.088	2.363
N_C $\alpha$ _C $\beta$	110.744	1.184	N_C $\alpha$ _C $\beta$	111.017	1.198

ARG pmt100 n = 4			ARG mmm-85 n = 992		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	70.210	7.245	chi1	-63.497	9.137
chi2	-90.541	9.055	chi2	-67.585	10.907
chi3	-174.190	5.432	chi3	-60.741	9.315
chi4	97.849	2.006	chi4	-86.156	10.015
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.830	0.421	C $\alpha$ _C $\beta$ _C $\gamma$	114.631	1.530
C $\alpha$ _C_O	120.581	0.283	C $\alpha$ _C_O	120.538	0.881
C $\beta$ _C $\alpha$ _C	110.812	0.494	C $\beta$ _C $\alpha$ _C	109.677	1.540
C $\beta$ _C $\gamma$ _C $\delta$	112.728	0.575	C $\beta$ _C $\gamma$ _C $\delta$	112.808	1.599
C $\delta$ _N $\epsilon$ _C $\zeta$	125.083	0.125	C $\delta$ _N $\epsilon$ _C $\zeta$	124.980	1.075
C $\gamma$ _C $\delta$ _N $\epsilon$	111.181	0.920	C $\gamma$ _C $\delta$ _N $\epsilon$	112.438	2.268
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.967	0.288	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.836	0.998
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.634	0.266	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.665	0.929
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.397	0.052	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.479	0.816
N_C $\alpha$ _C	110.231	1.442	N_C $\alpha$ _C	111.266	2.648
N_C $\alpha$ _C $\beta$	111.390	0.423	N_C $\alpha$ _C $\beta$	110.736	1.103
ARG mmt90 n = 556			ARG tmm-80 n = 71		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-60.697	8.901	chi1	-174.294	9.153
chi2	-68.408	12.521	chi2	-86.372	8.784
chi3	179.437	10.390	chi3	-56.434	10.717
chi4	90.018	12.897	chi4	-82.108	8.527
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.642	1.383	C $\alpha$ _C $\beta$ _C $\gamma$	115.257	1.317
C $\alpha$ _C_O	120.477	0.872	C $\alpha$ _C_O	120.621	0.778
C $\beta$ _C $\alpha$ _C	109.543	1.645	C $\beta$ _C $\alpha$ _C	111.061	1.008
C $\beta$ _C $\gamma$ _C $\delta$	112.215	1.625	C $\beta$ _C $\gamma$ _C $\delta$	113.720	2.294
C $\delta$ _N $\epsilon$ _C $\zeta$	124.963	1.175	C $\delta$ _N $\epsilon$ _C $\zeta$	124.893	1.247
C $\gamma$ _C $\delta$ _N $\epsilon$	111.520	2.338	C $\gamma$ _C $\delta$ _N $\epsilon$	112.553	1.891
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.858	1.209	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.861	1.095
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.541	1.091	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.709	0.923
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.577	0.708	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.397	0.720
N_C $\alpha$ _C	111.328	2.714	N_C $\alpha$ _C	109.672	1.698
N_C $\alpha$ _C $\beta$	110.691	1.079	N_C $\alpha$ _C $\beta$	110.067	1.009

ARG mmp80 n = 162			ARG ppt170 n = 57		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-62.526	6.718	chi1	59.128	10.191
chi2	-75.134	12.775	chi2	87.628	12.303
chi3	74.408	11.818	chi3	173.545	12.401
chi4	77.834	6.740	chi4	173.353	17.304
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.737	1.395	C $\alpha$ _C $\beta$ _C $\gamma$	116.231	1.391
C $\alpha$ _C_O	120.409	0.955	C $\alpha$ _C_O	120.322	0.969
C $\beta$ _C $\alpha$ _C	109.778	1.494	C $\beta$ _C $\alpha$ _C	111.874	1.266
C $\beta$ _C $\gamma$ _C $\delta$	113.410	1.628	C $\beta$ _C $\gamma$ _C $\delta$	112.335	1.538
C $\delta$ _N $\epsilon$ _C $\zeta$	125.038	1.163	C $\delta$ _N $\epsilon$ _C $\zeta$	124.240	1.283
C $\gamma$ _C $\delta$ _N $\epsilon$	113.473	2.237	C $\gamma$ _C $\delta$ _N $\epsilon$	111.432	1.579
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.552	1.001	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.487	1.072
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.973	0.861	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.804	0.864
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.455	0.644	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.688	0.650
N_C $\alpha$ _C	111.404	1.837	N_C $\alpha$ _C	110.914	2.502
N_C $\alpha$ _C $\beta$	110.864	0.946	N_C $\alpha$ _C $\beta$	111.565	1.316
ARG tmt170 n = 102			ARG tpt170 n = 814		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-173.869	12.427	chi1	-178.826	9.067
chi2	-91.306	12.847	chi2	66.313	10.382
chi3	-173.542	9.387	chi3	177.963	11.762
chi4	-170.971	17.686	chi4	171.354	19.192
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.033	1.341	C $\alpha$ _C $\beta$ _C $\gamma$	114.523	1.230
C $\alpha$ _C_O	120.639	0.748	C $\alpha$ _C_O	120.503	0.727
C $\beta$ _C $\alpha$ _C	110.881	1.078	C $\beta$ _C $\alpha$ _C	110.564	1.151
C $\beta$ _C $\gamma$ _C $\delta$	112.666	1.686	C $\beta$ _C $\gamma$ _C $\delta$	112.231	1.665
C $\delta$ _N $\epsilon$ _C $\zeta$	124.504	0.916	C $\delta$ _N $\epsilon$ _C $\zeta$	124.482	1.130
C $\gamma$ _C $\delta$ _N $\epsilon$	110.691	1.634	C $\gamma$ _C $\delta$ _N $\epsilon$	110.871	1.840
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.698	1.053	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.524	0.932
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.557	0.823	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.679	0.874
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.730	0.721	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.777	0.835
N_C $\alpha$ _C	108.489	3.185	N_C $\alpha$ _C	110.740	2.001
N_C $\alpha$ _C $\beta$	109.967	1.243	N_C $\alpha$ _C $\beta$	110.226	1.193

ARG mtm180 n = 2345			ARG tpm170 n = 107		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-66.409	8.085	chi1	178.317	8.224
chi2	179.025	12.788	chi2	70.416	10.485
chi3	-67.433	8.793	chi3	-85.345	12.696
chi4	172.922	15.175	chi4	171.668	18.898
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.293	1.630	C $\alpha$ _C $\beta$ _C $\gamma$	115.673	1.247
C $\alpha$ _C_O	120.454	0.896	C $\alpha$ _C_O	120.654	0.816
C $\beta$ _C $\alpha$ _C	109.863	1.611	C $\beta$ _C $\alpha$ _C	110.589	1.350
C $\beta$ _C $\gamma$ _C $\delta$	111.616	1.670	C $\beta$ _C $\gamma$ _C $\delta$	112.743	2.166
C $\delta$ _N $\epsilon$ _C $\zeta$	124.440	1.085	C $\delta$ _N $\epsilon$ _C $\zeta$	124.733	2.270
C $\gamma$ _C $\delta$ _N $\epsilon$	111.354	1.543	C $\gamma$ _C $\delta$ _N $\epsilon$	111.912	2.110
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.429	0.902	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.506	1.047
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.767	0.885	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.754	0.922
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.787	0.769	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.724	0.725
N_C $\alpha$ _C	111.289	2.647	N_C $\alpha$ _C	111.149	1.468
N_C $\alpha$ _C $\beta$	110.530	1.055	N_C $\alpha$ _C $\beta$	109.925	1.146
ARG tpt90 n = 644			ARG ptt180 n = 795		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	178.926	8.158	chi1	65.305	8.311
chi2	65.741	7.697	chi2	-177.454	10.457
chi3	178.589	9.978	chi3	-179.814	10.366
chi4	86.350	10.341	chi4	179.152	17.477
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.738	1.264	C $\alpha$ _C $\beta$ _C $\gamma$	114.547	1.516
C $\alpha$ _C_O	120.467	0.801	C $\alpha$ _C_O	120.583	1.010
C $\beta$ _C $\alpha$ _C	110.300	1.185	C $\beta$ _C $\alpha$ _C	110.523	1.494
C $\beta$ _C $\gamma$ _C $\delta$	112.110	1.646	C $\beta$ _C $\gamma$ _C $\delta$	111.126	2.020
C $\delta$ _N $\epsilon$ _C $\zeta$	124.786	0.938	C $\delta$ _N $\epsilon$ _C $\zeta$	124.436	1.108
C $\gamma$ _C $\delta$ _N $\epsilon$	111.926	2.246	C $\gamma$ _C $\delta$ _N $\epsilon$	110.738	1.963
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.799	0.964	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.461	0.938
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.728	0.883	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.609	0.894
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.453	0.819	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.911	0.869
N_C $\alpha$ _C	111.447	2.057	N_C $\alpha$ _C	111.323	2.488
N_C $\alpha$ _C $\beta$	110.208	1.092	N_C $\alpha$ _C $\beta$	111.000	1.109



ARG ttp80 n = 1860			ARG mmt-90 n = 1392		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.383	8.106	chi1	-63.806	6.645
chi2	179.646	13.594	chi2	-68.992	8.133
chi3	62.978	9.992	chi3	-175.179	7.629
chi4	82.895	9.629	chi4	-91.022	11.173
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.688	1.494	C $\alpha$ _C $\beta$ _C $\gamma$	114.531	1.417
C $\alpha$ _C_O	120.681	0.797	C $\alpha$ _C_O	120.513	0.838
C $\beta$ _C $\alpha$ _C	110.046	1.204	C $\beta$ _C $\alpha$ _C	109.577	1.627
C $\beta$ _C $\gamma$ _C $\delta$	112.066	1.516	C $\beta$ _C $\gamma$ _C $\delta$	112.041	1.661
C $\delta$ _N $\epsilon$ _C $\zeta$	124.878	1.035	C $\delta$ _N $\epsilon$ _C $\zeta$	124.924	0.999
C $\gamma$ _C $\delta$ _N $\epsilon$	112.547	1.930	C $\gamma$ _C $\delta$ _N $\epsilon$	111.774	2.258
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.749	0.956	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.931	0.982
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.767	0.848	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.615	0.875
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.465	0.751	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.428	0.770
N_C $\alpha$ _C	110.739	2.050	N_C $\alpha$ _C	110.058	2.662
N_C $\alpha$ _C $\beta$	110.429	1.200	N_C $\alpha$ _C $\beta$	110.880	1.109
ARG mtp-110 n = 471			ARG ttm-80 n = 1462		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-65.062	8.026	chi1	-174.135	9.513
chi2	179.092	10.811	chi2	179.281	9.839
chi3	66.411	11.409	chi3	-64.732	10.594
chi4	-109.636	9.572	chi4	-84.522	9.788
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.341	1.666	C $\alpha$ _C $\beta$ _C $\gamma$	113.681	1.675
C $\alpha$ _C_O	120.363	0.920	C $\alpha$ _C_O	120.535	0.780
C $\beta$ _C $\alpha$ _C	110.083	1.683	C $\beta$ _C $\alpha$ _C	110.229	1.204
C $\beta$ _C $\gamma$ _C $\delta$	112.345	1.634	C $\beta$ _C $\gamma$ _C $\delta$	111.980	1.635
C $\delta$ _N $\epsilon$ _C $\zeta$	125.232	1.195	C $\delta$ _N $\epsilon$ _C $\zeta$	124.861	1.286
C $\gamma$ _C $\delta$ _N $\epsilon$	111.659	1.883	C $\gamma$ _C $\delta$ _N $\epsilon$	112.440	2.018
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.023	1.138	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.730	1.000
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.482	1.039	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.733	1.026
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.471	0.695	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.517	0.757
N_C $\alpha$ _C	111.125	2.599	N_C $\alpha$ _C	110.551	2.269
N_C $\alpha$ _C $\beta$	110.744	1.028	N_C $\alpha$ _C $\beta$	110.370	1.362

ARG mpt-90 n = 84			ARG mpp80 n = 52		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-78.778	13.763	chi1	-76.744	11.978
chi2	74.660	16.163	chi2	81.853	12.146
chi3	177.663	9.583	chi3	57.995	7.467
chi4	-87.847	13.189	chi4	84.630	10.212
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.931	1.316	C $\alpha$ _C $\beta$ _C $\gamma$	115.453	1.753
C $\alpha$ _C_O	120.439	0.758	C $\alpha$ _C_O	120.425	1.063
C $\beta$ _C $\alpha$ _C	109.923	1.571	C $\beta$ _C $\alpha$ _C	109.151	2.000
C $\beta$ _C $\gamma$ _C $\delta$	112.886	2.297	C $\beta$ _C $\gamma$ _C $\delta$	113.483	1.590
C $\delta$ _N $\epsilon$ _C $\zeta$	124.887	1.005	C $\delta$ _N $\epsilon$ _C $\zeta$	124.889	1.017
C $\gamma$ _C $\delta$ _N $\epsilon$	111.530	2.487	C $\gamma$ _C $\delta$ _N $\epsilon$	113.135	2.325
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.602	1.077	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.818	1.181
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.817	0.851	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.710	1.102
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.561	0.669	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.449	0.734
N_C $\alpha$ _C	110.369	2.731	N_C $\alpha$ _C	109.625	2.583
N_C $\alpha$ _C $\beta$	110.869	1.048	N_C $\alpha$ _C $\beta$	111.427	1.269
ARG ttml70 n = 1289			ARG ppp-140 n = 4		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-177.285	10.038	chi1	58.431	3.025
chi2	176.943	12.404	chi2	91.756	4.604
chi3	-67.797	9.990	chi3	62.263	10.579
chi4	171.206	17.575	chi4	-143.455	12.578
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.744	1.740	C $\alpha$ _C $\beta$ _C $\gamma$	115.223	0.896
C $\alpha$ _C_O	120.579	0.817	C $\alpha$ _C_O	120.687	0.538
C $\beta$ _C $\alpha$ _C	110.102	1.172	C $\beta$ _C $\alpha$ _C	111.973	1.456
C $\beta$ _C $\gamma$ _C $\delta$	111.466	1.806	C $\beta$ _C $\gamma$ _C $\delta$	112.231	1.497
C $\delta$ _N $\epsilon$ _C $\zeta$	124.428	1.167	C $\delta$ _N $\epsilon$ _C $\zeta$	125.872	1.184
C $\gamma$ _C $\delta$ _N $\epsilon$	111.259	1.661	C $\gamma$ _C $\delta$ _N $\epsilon$	113.783	2.259
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.512	0.950	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.992	1.242
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.740	0.927	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	120.128	1.383
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.729	0.845	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	118.855	0.611
N_C $\alpha$ _C	110.295	2.387	N_C $\alpha$ _C	113.626	2.343
N_C $\alpha$ _C $\beta$	110.260	1.339	N_C $\alpha$ _C $\beta$	111.211	1.258

ARG mmp-170 n = 118			ARG tmt90 n = 24		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-64.124	7.206	chi1	-178.402	9.046
chi2	-65.485	14.458	chi2	-93.565	8.929
chi3	85.873	9.639	chi3	-177.879	11.138
chi4	-167.047	20.100	chi4	87.027	12.177
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.481	1.279	C $\alpha$ _C $\beta$ _C $\gamma$	115.158	1.454
C $\alpha$ _C_O	120.377	0.997	C $\alpha$ _C_O	120.625	0.966
C $\beta$ _C $\alpha$ _C	109.443	1.541	C $\beta$ _C $\alpha$ _C	110.438	1.309
C $\beta$ _C $\gamma$ _C $\delta$	112.767	1.700	C $\beta$ _C $\gamma$ _C $\delta$	112.853	2.293
C $\delta$ _N $\epsilon$ _C $\zeta$	124.840	1.335	C $\delta$ _N $\epsilon$ _C $\zeta$	125.081	1.237
C $\gamma$ _C $\delta$ _N $\epsilon$	111.511	1.636	C $\gamma$ _C $\delta$ _N $\epsilon$	111.395	2.787
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.441	1.161	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.866	1.819
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.810	1.058	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.666	1.430
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.732	1.159	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.430	0.726
N_C $\alpha$ _C	110.952	2.092	N_C $\alpha$ _C	110.374	1.542
N_C $\alpha$ _C $\beta$	111.093	1.107	N_C $\alpha$ _C $\beta$	109.916	1.111
ARG ppt-90 n = 15			ARG mmt180 n = 1176		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	61.770	9.125	chi1	-61.912	9.056
chi2	90.213	11.134	chi2	-68.373	12.923
chi3	177.663	5.499	chi3	-176.971	11.436
chi4	-92.246	14.372	chi4	-176.339	17.496
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.763	1.382	C $\alpha$ _C $\beta$ _C $\gamma$	114.491	1.384
C $\alpha$ _C_O	120.637	0.931	C $\alpha$ _C_O	120.406	0.872
C $\beta$ _C $\alpha$ _C	111.235	1.747	C $\beta$ _C $\alpha$ _C	109.366	1.617
C $\beta$ _C $\gamma$ _C $\delta$	113.040	1.278	C $\beta$ _C $\gamma$ _C $\delta$	112.027	1.711
C $\delta$ _N $\epsilon$ _C $\zeta$	124.988	0.738	C $\delta$ _N $\epsilon$ _C $\zeta$	124.416	1.183
C $\gamma$ _C $\delta$ _N $\epsilon$	111.689	1.956	C $\gamma$ _C $\delta$ _N $\epsilon$	111.007	1.818
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.569	1.315	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.488	0.851
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.890	1.166	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.666	0.858
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.520	0.600	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.825	0.704
N_C $\alpha$ _C	111.578	3.116	N_C $\alpha$ _C	111.233	2.583
N_C $\alpha$ _C $\beta$	111.579	1.236	N_C $\alpha$ _C $\beta$	110.703	1.056

ARG ttm110 n = 707			ARG mtt-85 n = 2772		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-175.260	9.175	chi1	-67.013	7.854
chi2	178.639	9.448	chi2	-178.550	10.723
chi3	-64.314	10.889	chi3	-176.240	9.281
chi4	112.805	9.664	chi4	-88.795	11.696
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	113.890	1.647	C $\alpha$ _C $\beta$ _C $\gamma$	113.461	1.692
C $\alpha$ _C_O	120.595	0.792	C $\alpha$ _C_O	120.440	0.817
C $\beta$ _C $\alpha$ _C	110.255	1.210	C $\beta$ _C $\alpha$ _C	109.824	1.655
C $\beta$ _C $\gamma$ _C $\delta$	112.168	1.688	C $\beta$ _C $\gamma$ _C $\delta$	111.353	1.974
C $\delta$ _N $\epsilon$ _C $\zeta$	125.329	1.304	C $\delta$ _N $\epsilon$ _C $\zeta$	124.786	1.050
C $\gamma$ _C $\delta$ _N $\epsilon$	111.643	1.924	C $\gamma$ _C $\delta$ _N $\epsilon$	111.400	2.439
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	121.007	1.231	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.794	1.013
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.542	1.112	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.579	0.927
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.428	0.818	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.608	0.766
N_C $\alpha$ _C	110.508	2.148	N_C $\alpha$ _C	111.437	2.300
N_C $\alpha$ _C $\beta$	110.381	1.242	N_C $\alpha$ _C $\beta$	110.636	1.048
ARG tmt-80 n = 61			ARG mtm-85 n = 2772		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-174.441	10.837	chi1	-68.282	8.098
chi2	-92.932	11.397	chi2	-171.664	9.296
chi3	-177.757	10.097	chi3	-63.903	9.544
chi4	-84.998	11.511	chi4	-88.066	8.875
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.683	1.344	C $\alpha$ _C $\beta$ _C $\gamma$	113.535	1.556
C $\alpha$ _C_O	120.548	0.778	C $\alpha$ _C_O	120.470	0.805
C $\beta$ _C $\alpha$ _C	111.349	1.340	C $\beta$ _C $\alpha$ _C	110.034	1.481
C $\beta$ _C $\gamma$ _C $\delta$	112.474	1.937	C $\beta$ _C $\gamma$ _C $\delta$	111.967	1.572
C $\delta$ _N $\epsilon$ _C $\zeta$	124.697	1.123	C $\delta$ _N $\epsilon$ _C $\zeta$	124.894	1.181
C $\gamma$ _C $\delta$ _N $\epsilon$	111.276	2.098	C $\gamma$ _C $\delta$ _N $\epsilon$	112.688	1.950
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.618	0.914	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.774	1.029
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.730	0.903	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.745	0.999
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.628	0.628	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.464	0.774
N_C $\alpha$ _C	110.080	2.465	N_C $\alpha$ _C	111.345	1.977
N_C $\alpha$ _C $\beta$	110.079	1.029	N_C $\alpha$ _C $\beta$	111.057	1.027

ARG tmm160 n = 90			ARG mtt180 n = 4505		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	-172.150	10.975	chi1	-67.383	7.814
chi2	-90.073	11.030	chi2	179.853	11.048
chi3	-61.282	11.612	chi3	-179.128	10.682
chi4	163.764	18.517	chi4	177.093	17.944
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	114.778	1.273	C $\alpha$ _C $\beta$ _C $\gamma$	112.906	1.755
C $\alpha$ _C_O	120.623	0.812	C $\alpha$ _C_O	120.450	0.845
C $\beta$ _C $\alpha$ _C	111.249	1.056	C $\beta$ _C $\alpha$ _C	109.969	1.663
C $\beta$ _C $\gamma$ _C $\delta$	112.555	1.784	C $\beta$ _C $\gamma$ _C $\delta$	111.523	2.022
C $\delta$ _N $\epsilon$ _C $\zeta$	124.629	1.171	C $\delta$ _N $\epsilon$ _C $\zeta$	124.356	1.096
C $\gamma$ _C $\delta$ _N $\epsilon$	111.864	1.946	C $\gamma$ _C $\delta$ _N $\epsilon$	110.629	1.820
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.639	0.972	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.418	0.891
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.689	0.898	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.630	0.896
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.648	0.773	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.933	0.790
N_C $\alpha$ _C	109.962	2.040	N_C $\alpha$ _C	111.572	2.324
N_C $\alpha$ _C $\beta$	110.034	1.120	N_C $\alpha$ _C $\beta$	110.572	1.048
ARG ppt90 n = 18			ARG tpp-160 n = 482		
$\chi$	Smooth COM	StdDev	$\chi$	Smooth COM	StdDev
chi1	63.537	5.443	chi1	178.900	9.674
chi2	99.251	8.151	chi2	65.564	10.819
chi3	-179.890	9.880	chi3	65.339	9.793
chi4	87.261	12.365	chi4	-167.680	19.787
Bond Angle	Mean	StdDev	Bond Angle	Mean	StdDev
C $\alpha$ _C $\beta$ _C $\gamma$	115.304	1.918	C $\alpha$ _C $\beta$ _C $\gamma$	114.742	1.291
C $\alpha$ _C_O	120.718	0.836	C $\alpha$ _C_O	120.532	0.822
C $\beta$ _C $\alpha$ _C	110.703	1.689	C $\beta$ _C $\alpha$ _C	110.423	1.277
C $\beta$ _C $\gamma$ _C $\delta$	112.029	2.351	C $\beta$ _C $\gamma$ _C $\delta$	112.675	1.745
C $\delta$ _N $\epsilon$ _C $\zeta$	125.367	1.150	C $\delta$ _N $\epsilon$ _C $\zeta$	124.523	1.369
C $\gamma$ _C $\delta$ _N $\epsilon$	112.954	2.854	C $\gamma$ _C $\delta$ _N $\epsilon$	111.876	1.830
N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.972	1.007	N $\epsilon$ _C $\zeta$ _N $\eta$ 1	120.507	0.999
N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.738	0.957	N $\epsilon$ _C $\zeta$ _N $\eta$ 2	119.785	1.089
N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.258	0.808	N $\eta$ 1_C $\zeta$ _N $\eta$ 2	119.689	0.832
N_C $\alpha$ _C	111.087	2.183	N_C $\alpha$ _C	110.594	2.316
N_C $\alpha$ _C $\beta$	110.817	1.329	N_C $\alpha$ _C $\beta$	110.246	1.093

## 4 Filtered Top8000 PDB Chains and Filtered Residue Counts

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1a2p	B	73	1a2z	C	130	1a34	A	106	1a3a	A	85	1a4i	B	195
1a7d	A	88	1a7s	A	133	1a7t	B	142	1a88	A	166	1a8q	A	196
1a8s	A	165	1aba	A	56	1afb	3	66	1ag9	B	82	1aii	A	186
1ajk	B	122	1ako	A	168	1aky	A	77	1amu	B	216	1atg	A	135
1atl	B	103	1atz	B	121	1aun	A	114	1avb	A	118	1awd	A	53
1ax0	A	121	1aye	A	203	1b0b	A	79	1b1c	A	91	1b2s	F	59
1b37	B	269	1b3a	B	41	1b4f	B	36	1b5e	A	131	1b63	A	112
1b67	A	24	1b6a	A	232	1b80	A	240	1b8a	B	285	1b8d	K	86
1b8d	L	97	1b8z	A	28	1b9j	A	319	1bdo	A	53	1beh	A	118
1bg0	A	213	1bgf	A	79	1bgp	A	176	1bhp	A	21	1bj7	A	83
1bkb	A	3	1bn8	A	272	1bq8	A	44	1bqk	A	74	1brt	A	187
1bsg	A	156	1bu8	A	257	1bue	A	165	1bx1	A	145	1bx7	A	28
1bxu	A	56	1bxy	A	25	1byi	A	122	1bzs	A	96	1c02	A	93
1c0p	A	229	1c1k	A	123	1c3c	A	257	1c4q	B	49	1c75	A	1
1c7j	A	273	1c7k	A	94	1c7n	F	235	1c9s	A	38	1c9y	A	209
1cf3	A	357	1cg5	A	97	1cg5	B	92	1chd	A	116	1ci4	B	48
1cip	A	199	1cjc	A	239	1cka	A	7	1cpq	A	55	1cqm	B	62
1cru	B	305	1ctj	A	36	1cuo	A	83	1cxl	A	419	1cxy	A	42
1cyo	A	54	1cz9	A	76	1cza	N	387	1czf	A	201	1d0b	A	129
1d2n	A	115	1d2s	A	75	1d2t	A	117	1d3g	A	188	1d4o	A	115
1d4t	A	67	1d5l	B	82	1d5l	D	289	1d5t	A	279	1d7o	A	106
1dbf	A	80	1dbi	A	160	1dbw	B	61	1deu	A	158	1dgf	A	351
1di2	B	22	1djr	G	86	1dk8	A	84	1dl5	B	194	1doi	A	86
1dow	A	95	1dp7	P	51	1dpj	A	178	1dpt	A	77	1duv	H	135
1dw0	B	63	1dwk	A	98	1dxj	A	150	1dxy	A	173	1dys	B	211
1dzk	A	79	1e0c	A	153	1e0w	A	211	1e25	A	151	1e29	A	75
1e2v	A	133	1e3d	B	318	1e3d	C	154	1e4c	P	125	1e4m	M	346
1e59	A	168	1e5k	A	101	1e5m	A	221	1e6y	B	262	1e6y	C	159
1e6y	D	360	1eaj	B	87	1eao	A	80	1ear	A	50	1eb6	A	112
1edg	A	240	1edq	A	325	1eej	B	87	1efl	D	37	1eg2	A	143
1egw	B	36	1eis	A	42	1ejb	A	98	1ejd	B	207	1ekq	B	129
1elj	A	177	1elk	A	116	1elr	A	71	1elt	A	157	1elu	A	215
1elw	A	66	1eo6	B	49	1eq6	A	87	1es5	A	170	1esw	A	269
1eu3	A	156	1ex2	B	76	1exa	A	133	1exr	A	52	1ext	A	120
1eyb	A	244	1eyh	A	78	1eyl	A	82	1ez3	B	39	1f0k	B	141
1f0l	B	274	1f0y	B	166	1flu	A	239	1f2f	A	65	1f3u	G	24
1f4p	A	70	1f5j	A	136	1f5v	A	142	1f60	A	287	1f60	B	62
1f7b	C	189	1f8e	A	289	1f94	A	4	1f9z	B	65	1fd3	A	22
1fec	B	237	1fg7	A	212	1fj0	A	70	1fm4	A	85	1fn9	A	264
1fny	A	134	1fo9	A	223	1fob	A	174	1fp2	A	234	1fpo	B	94
1fqt	B	59	1fsg	A	179	1ftr	A	167	1fu0	B	49	1fur	B	248
1fw4	A	8	1fx4	A	104	1fxl	A	78	1fxo	G	170	1fy2	A	129
1fz1	B	240	1g12	A	106	1g16	A	56	1glj	A	21	1g29	2	181
1g2r	A	54	1g3p	A	123	1g4i	A	66	1g60	A	147	1g61	A	154
1g6a	A	168	1g6c	B	121	1g6h	A	99	1g6u	B	24	1g7j	A	73
1g7m	B	56	1g87	A	378	1g8a	A	136	1g8i	B	80	1g8s	A	110
1g94	A	298	1g97	A	216	1g9g	A	392	1g9k	A	249	1g9o	A	58
1ga6	A	214	1gai	A	324	1gbg	A	126	1gc0	B	160	1gcq	C	41
1gd0	A	84	1gde	B	210	1gee	E	134	1geg	G	150	1ges	B	201
1gk6	A	29	1gk7	A	20	1gk8	G	302	1gk9	A	147	1gk9	B	330

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1gkp	E	326	1gmu	C	63	1gmy	A	149	1gn0	A	52	1gnt	A	387
1gny	A	108	1go3	E	97	1go3	N	57	1goi	B	326	1gpe	A	284
1gpi	A	270	1gpp	A	136	1gpu	A	363	1gq1	A	378	1gq6	C	183
1gq8	A	208	1gql	B	490	1gt1	A	46	1gte	D	530	1gtt	A	220
1gu2	A	86	1gu7	B	225	1gud	A	186	1gui	A	115	1gut	E	39
1gv5	A	29	1gvf	A	152	1gvj	A	76	1gvn	C	62	1gvn	D	148
1gwe	A	343	1gwi	B	185	1gwu	A	209	1gx1	A	68	1gx4	A	209
1gxu	A	224	1gxv	A	153	1gxu	A	52	1gxy	A	128	1gyh	C	221
1gyo	A	63	1gyv	A	76	1gyy	B	48	1gz8	A	180	1gzw	B	78
1h03	P	34	1h0s	A	82	1h16	A	470	1h1n	A	219	1h1y	A	122
1h2b	B	180	1h2c	A	86	1h2e	A	76	1h2s	A	103	1h2s	B	14
1h32	A	150	1h4a	X	122	1h4g	A	146	1h4p	A	242	1h4r	A	184
1h5q	L	165	1h5v	A	212	1h6w	A	94	1h72	C	39	1h75	A	35
1h7e	B	131	1h80	B	220	1h8p	B	58	1h9m	A	53	1hbg	A	48
1hc9	B	44	1hd2	A	91	1hd5	A	127	1hdh	A	320	1hfo	E	72
1hfs	A	102	1hfu	A	319	1hgx	B	92	1hh8	A	103	1hjs	B	212
1hl7	B	184	1hlq	C	42	1hp1	A	335	1hq0	A	149	1ht6	A	260
1hw1	B	135	1hx1	B	18	1hxi	A	66	1hxr	B	64	1hyo	A	282
1hz6	C	40	1hzj	A	190	1hzo	A	159	1i0l	A	102	1i0v	A	53
1i12	C	94	1i19	A	314	1i1j	B	65	1i1n	A	125	1i24	A	259
1i2h	A	80	1i2m	B	166	1i2t	A	39	1i3c	B	75	1i4u	A	123
1i58	B	99	1i60	A	174	1i6m	A	144	1i88	A	258	1i8f	F	9
1i8k	B	73	1i9c	A	76	1ia6	A	230	1iap	A	57	1icp	A	204
1idr	A	34	1ie0	A	88	1ig3	A	105	1ig5	A	39	1igq	A	29
1ii5	A	119	1iir	A	203	1ijb	A	118	1ijx	C	51	1ijy	B	82
1ikp	A	317	1ikt	A	45	1inj	A	93	1inl	A	189	1io0	A	108
1iom	A	237	1ioo	B	136	1iqz	A	54	1isp	A	108	1itx	A	240
1iu8	B	121	1iue	B	64	1iuq	A	204	1iuz	A	61	1iwd	A	138
1ix1	B	108	1ix2	A	50	1ix9	A	134	1iy8	C	148	1iyb	A	136
1iyn	A	141	1izc	A	160	1ize	A	201	1j05	B	73	1j0h	B	345
1j1g	A	124	1j1y	A	67	1j24	A	77	1j2j	B	26	1j2r	A	132
1j30	B	68	1j34	A	65	1j34	B	69	1j3w	C	62	1j5x	A	178
1j71	A	193	1j75	A	10	1j77	A	95	1j7d	A	80	1j7g	A	65
1j7k	A	113	1j8e	A	31	1j8u	A	204	1j97	B	132	1j9b	A	93
1j9l	A	99	1jak	A	289	1jat	A	64	1jat	B	48	1jay	B	128
1jcd	A	24	1jcv	A	99	1jd0	B	169	1jdl	A	49	1jf8	A	84
1jfu	A	94	1jfx	A	135	1jg1	A	129	1jhd	A	250	1jhf	A	101
1ji1	A	435	1jid	A	68	1jiw	P	278	1jkg	A	79	1jkx	A	124
1jl3	D	68	1jlt	A	77	1jlt	B	76	1jml	A	1	1jnd	A	281
1jo0	A	47	1jo8	A	34	1jp4	A	202	1jpe	A	61	1jr8	A	64
1jrl	A	83	1jt2	A	139	1jub	B	157	1juh	D	215	1juv	A	11
1jv1	A	293	1jvb	A	154	1jw9	B	122	1jw9	D	23	1jwq	A	110
1jy2	N	26	1jy2	R	29	1jy3	P	36	1jya	A	48	1jyh	A	104
1jzt	A	124	1k07	A	171	1k2e	A	102	1k2x	C	96	1k33	A	27
1k38	B	139	1k3i	A	3	1k3s	A	43	1k5c	A	205	1k5n	A	198
1k66	B	81	1k6a	A	12	1k6d	B	101	1k75	B	266	1k77	A	134
1k7c	A	150	1k8w	A	142	1k92	A	244	1k94	A	95	1k9u	B	37
1ka1	A	252	1kao	A	89	1kb0	A	410	1kcq	A	63	1kcz	B	241
1keq	B	136	1kfr	A	88	1kfw	A	245	1kgd	A	100	1kgs	A	146
1khi	A	79	1kj9	A	217	1kfv	A	166	1kl9	A	50	1klx	A	60
1km9	A	70	1kms	A	106	1kmt	A	91	1kng	A	78	1koe	A	100
1kpt	A	60	1kpu	B	69	1kq1	B	30	1kq3	A	245	1kqf	A	657

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1kqr	A	101	1krh	A	209	1krn	A	49	1ks8	A	267	1ku1	A	102
1kug	A	143	1kvd	C	32	1kve	D	46	1kw4	A	35	1kw6	B	179
1kwg	A	374	1ky3	A	90	1kzq	A	125	1l1d	B	80	1l2p	A	21
1l2t	B	89	1l3i	E	33	1l3k	A	88	1l5o	A	181	1l5w	B	422
1l6r	A	143	1l6w	B	112	1l7l	A	88	1l9x	A	171	1lc3	A	170
1lc5	A	220	1le6	A	62	1les	B	31	1lfk	A	176	1lj5	A	209
1lj8	A	326	1lk5	B	125	1lkd	A	142	1lke	A	62	1llf	B	371
1lml	A	237	1lo6	A	100	1lq9	A	74	1lqa	A	225	1lqv	A	96
1lqx	A	40	1lr0	A	69	1lr7	A	44	1lrh	A	119	1lri	A	61
1lrk	A	166	1ls6	A	151	1ls9	A	50	1lua	C	160	1lv7	A	143
1lvw	B	173	1lw6	E	188	1lw6	I	48	1lwd	B	242	1ly2	A	75
1m0d	C	12	1m0s	B	120	1m0u	A	115	1m0z	A	162	1m1f	A	72
1m1r	A	47	1m22	B	246	1m2t	B	62	1m2x	D	120	1m33	A	137
1m3u	C	152	1m48	A	61	1m4i	A	122	1m4j	A	61	1m5t	A	83
1m65	A	133	1m66	A	167	1m6i	A	245	1m6j	B	150	1m6s	A	196
1m70	D	101	1m7a	B	116	1m7g	A	137	1m7j	A	335	1m7s	D	338
1m7y	A	219	1m8s	A	60	1m93	B	94	1mb4	A	216	1mc2	A	83
1md6	A	91	1mdo	A	179	1me8	A	148	1meo	A	123	1mex	H	121
1mex	L	140	1mg4	A	64	1mg7	B	208	1mgq	C	40	1mgr	A	55
1mgt	A	108	1mhn	A	38	1mhx	A	27	1mi3	B	233	1mjf	B	159
1mjh	B	76	1mk0	A	65	1mkk	A	61	1mky	A	213	1mlw	A	150
1mn8	B	59	1mo0	B	129	1mo1	A	46	1moq	A	203	1mpl	A	238
1mpx	B	408	1mvf	A	54	1mvf	D	9	1mvo	A	75	1mw9	X	272
1mwq	A	58	1mxg	A	272	1mxr	A	242	1my6	B	118	1mz4	A	70
1mzb	A	39	1n08	B	87	1n0q	B	56	1n0w	A	109	1n12	A	73
1n13	G	29	1n1j	A	51	1n1j	B	58	1n2x	A	140	1n3y	A	104
1n40	A	256	1n45	B	104	1n71	C	78	1n7e	A	40	1n7h	B	219
1n7s	A	26	1n7s	B	35	1n7s	C	44	1n7s	D	31	1n83	A	156
1n8f	B	218	1n8k	A	254	1n93	X	208	1n9l	A	44	1n9p	A	107
1na5	A	112	1naa	A	389	1nb9	A	79	1nbu	D	44	1nc7	D	70
1ncw	H	149	1ndb	B	311	1ndd	A	41	1ne7	C	155	1nep	A	97
1nf8	A	129	1nff	B	115	1nfv	N	77	1nh2	A	97	1nh2	B	10
1nh2	D	50	1nhc	E	215	1nhk	L	85	1nki	B	79	1nlf	A	110
1nli	A	170	1nls	A	155	1nn5	A	131	1nnf	A	196	1nnh	A	215
1nnl	A	98	1nns	A	187	1nnw	B	104	1noa	A	62	1nof	A	246
1nox	A	113	1npy	B	163	1nq6	A	211	1nq7	A	145	1nqu	B	97
1nr0	A	361	1nr4	G	27	1nrj	A	36	1nrj	B	114	1nrv	B	55
1nrw	A	154	1ns5	B	87	1nte	A	61	1nth	A	277	1ntv	A	71
1nu0	A	67	1nul	A	64	1nut	A	109	1nvm	C	215	1nvm	F	164
1nw2	H	58	1nwa	A	119	1nwp	A	75	1nww	A	96	1nxc	A	339
1nxj	A	97	1nxm	A	129	1nxo	A	62	1ny1	B	142	1nyk	B	89
1nyt	C	172	1nz0	A	64	1nza	A	47	1nzi	A	86	1nzj	A	186
1o04	E	358	1o0e	B	115	1o0y	B	105	1o13	A	53	1o1x	A	98
1o1y	A	153	1o1z	A	153	1o26	C	102	1o2d	A	229	1o3u	A	65
1o4s	A	196	1o4t	A	49	1o4v	A	85	1o4w	A	2	1o50	A	55
1o54	A	144	1o58	D	159	1o5k	B	154	1o5u	A	17	1o5x	A	161
1o66	B	113	1o69	B	196	1o6a	A	54	1o75	A	114	1o7e	B	167
1o7i	A	76	1o82	A	35	1o8b	B	133	1o8s	A	88	1o8v	A	83
1o8x	A	99	1o91	C	83	1o97	D	185	1o98	A	287	1o9g	A	124
1o9r	E	115	1oa0	B	374	1oa2	C	154	1oai	A	39	1oal	A	84
1oao	A	411	1oaq	H	78	1oaq	L	71	1ob3	A	139	1ob8	A	64
1obb	A	227	1obf	O	235	1obo	A	102	1oc2	B	214	1oc7	A	251

Continued on next page



PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1oc8	A	91	1ocy	A	138	1od6	A	76	1odk	A	120	1odm	A	246
1odo	A	220	1odv	A	67	1odz	A	273	1oew	A	203	1of1	A	128
1of8	B	231	1ofc	X	122	1off	A	57	1off	A	301	1ofs	C	110
1ofz	A	202	1ogm	X	433	1oh0	A	74	1oh4	A	100	1oh9	A	124
1oi0	C	54	1oi2	A	215	1oi6	B	138	1oi7	A	151	1oih	D	102
1ojh	F	27	1ojk	A	302	1ojx	C	145	1ok0	A	37	1oki	B	124
1okt	A	93	1om0	A	144	1on3	A	267	1ong	A	135	1oni	C	72
1onj	A	41	1onr	A	146	1ooe	A	154	1oot	A	29	1oq1	B	120
1oqj	A	64	1orn	A	72	1orr	A	169	1oru	B	100	1os6	A	32
1osy	B	82	1ou8	B	64	1ouw	C	96	1ow1	A	90	1ow3	A	131
1owf	A	13	1ox0	A	275	1oxs	C	190	1oyg	A	341	1oyw	A	253
1oz9	A	86	1p0f	B	199	1p0h	A	162	1p0k	A	89	1p1j	A	317
1p1m	A	236	1p1x	B	149	1p28	B	83	1p2f	A	109	1p31	B	255
1p3c	A	145	1p5g	X	289	1p5z	B	152	1p6o	B	106	1p6z	N	36
1p71	A	44	1p99	A	124	1p9h	A	77	1pa2	A	79	1pbj	A	66
1pcf	C	36	1pdo	A	57	1pe9	B	208	1pfb	A	39	1pfz	A	121
1pg4	B	368	1pg6	A	83	1pgv	A	87	1phn	A	104	1pj5	A	546
1pk3	B	34	1pkh	A	108	1pko	A	57	1pl2	B	149	1pl3	A	118
1plc	A	55	1pmh	X	103	1pn0	B	441	1pn2	C	162	1pnc	A	63
1pp0	C	96	1pqh	B	61	1psr	A	64	1pt6	A	107	1pu7	A	139
1puc	A	43	1puf	B	11	1puo	B	97	1pvb	A	65	1pvm	A	95
1pvx	A	127	1pwa	A	78	1px5	B	179	1pxv	B	114	1pyf	A	186
1pyl	A	62	1pyo	B	56	1pzg	A	205	1pzs	A	106	1q08	B	52
1q0p	A	80	1q0q	A	247	1q0r	A	182	1q11	A	180	1q1r	B	220
1q1y	A	114	1q2o	B	235	1q35	A	216	1q40	A	65	1q40	B	72
1q44	A	129	1q4r	A	64	1q4u	B	67	1q5m	B	222	1q5z	A	90
1q6h	A	140	1q6o	A	138	1q74	C	165	1q7e	A	246	1q7l	A	151
1q7l	B	67	1q7r	A	42	1q8b	A	53	1q8d	A	58	1q8f	A	211
1q9u	A	67	1qad	A	74	1qb5	E	46	1qb7	A	126	1qba	A	487
1qcs	A	100	1qd9	C	80	1qfo	B	50	1qg6	C	135	1qg8	A	163
1qgj	A	180	1qgu	A	316	1qgu	D	381	1qh5	B	169	1qho	A	487
1qhq	A	71	1qhv	A	123	1qjw	B	198	1qkr	A	80	1ql0	B	161
1qlw	A	212	1qmv	H	99	1qmy	C	95	1qnn	C	112	1qnx	A	116
1qou	B	110	1qoz	B	124	1qq7	B	118	1qrp	E	158	1qsa	A	420
1qt9	A	68	1qu1	D	50	1qu9	A	84	1qul	A	187	1qus	A	172
1qv9	C	122	1qve	B	79	1qvz	B	116	1qw9	B	334	1qwd	A	102
1qwg	A	159	1qwk	A	177	1qwm	B	333	1qwo	A	314	1qwr	A	161
1qwx	B	81	1qwy	A	160	1qwz	A	136	1qxy	A	168	1qy6	A	114
1qyb	A	98	1qyz	A	63	1qz9	A	237	1qzr	A	230	1r0d	G	64
1r0k	A	101	1r0m	B	246	1r0u	A	84	1r12	A	159	1r17	A	224
1r26	A	80	1r29	A	78	1r2m	A	46	1r2r	B	162	1r3d	A	127
1r3q	A	179	1r45	B	135	1r4v	A	74	1r4x	A	201	1r55	A	96
1r5l	A	143	1r5m	A	213	1r62	A	77	1r6d	A	180	1r6w	A	204
1r6x	A	235	1r77	B	65	1r7a	B	304	1r7j	A	50	1r89	A	220
1r8h	D	34	1r8s	A	101	1r9c	A	66	1r9d	A	412	1r9f	A	51
1r9h	A	69	1r9w	A	79	1ra0	A	296	1rc9	A	143	1rdg	A	34
1rdo	2	67	1rdq	E	235	1rff	B	270	1rfs	A	72	1rfy	B	54
1rg8	B	91	1rgx	C	46	1rgz	A	204	1rh6	B	29	1rh9	A	241
1rhc	A	163	1rhf	B	41	1rie	A	81	1rjc	A	60	1rk8	A	50
1rk8	B	44	1rkd	A	147	1rki	A	47	1rkq	A	187	1rku	A	136
1rkx	C	148	1rky	A	343	1rl0	A	169	1rlh	A	70	1rli	A	69
1rlk	A	65	1rm6	A	451	1rm6	B	178	1rm6	C	105	1roc	A	104

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1rp0	B	168	1rq2	B	107	1rqb	A	231	1rro	A	74	1rtt	A	103
1ru4	A	264	1rut	X	95	1rw9	A	501	1rwi	A	166	1rwj	A	35
1rwr	A	170	1rwz	A	124	1rx0	C	213	1rxq	C	103	1rxy	A	155
1ry9	C	82	1ryi	B	181	1ryl	A	80	1ryo	A	196	1ryq	A	35
1rz3	A	88	1rzh	H	132	1rzh	L	150	1rzh	M	135	1rzl	A	48
1s0a	B	234	1s0i	A	423	1s1d	B	203	1s1f	A	197	1s2o	A	154
1s2w	A	150	1s4k	B	62	1s57	B	69	1s5a	B	72	1s5d	A	139
1s5u	D	63	1s69	A	64	1s7k	A	81	1s99	A	97	1s9u	A	137
1sa3	A	144	1sau	A	67	1sbp	A	182	1sbx	A	64	1sby	A	166
1sd5	A	97	1sdi	A	127	1sds	A	43	1se8	A	95	1seg	A	39
1seh	A	73	1sf9	A	59	1sff	C	226	1sfs	A	100	1sfx	B	67
1sg4	C	149	1sg6	A	150	1sgv	B	136	1sgw	A	134	1sh7	B	183
1sh8	B	69	1shk	A	38	1shu	X	113	1sk4	A	97	1skz	A	63
1sl9	A	125	1smb	A	68	1smo	A	80	1smx	B	40	1sn2	B	62
1sng	A	199	1snn	A	115	1sny	A	67	1so7	A	199	1soi	A	69
1spj	A	153	1sqn	B	154	1sqs	B	129	1ss4	B	69	1suu	A	169
1svd	M	73	1sw5	B	181	1swy	A	100	1sxq	B	229	1sxr	A	101
1sxv	A	103	1sy7	B	391	1syy	A	175	1szd	A	128	1szh	A	77
1szn	A	280	1szo	K	171	1t00	A	67	1t06	A	120	1t07	A	38
1t0a	A	97	1t0b	D	164	1t0f	B	106	1t0f	C	18	1t0h	A	53
1t0p	B	41	1t1j	B	75	1t1v	B	63	1t2a	B	198	1t2d	A	221
1t2h	B	72	1t2w	C	56	1t3i	B	217	1t3q	A	91	1t3q	B	415
1t3y	A	81	1t4b	B	218	1t61	C	130	1t61	E	128	1t6c	A	200
1t6g	A	207	1t6g	D	132	1t6t	1	62	1t6u	L	84	1t6v	N	75
1t7r	A	165	1t82	C	68	1t8h	A	141	1t8t	B	147	1t8z	C	29
1t92	B	65	1t95	A	14	1t9m	B	94	1ta8	A	173	1taw	B	20
1taz	A	191	1tbf	A	213	1tc5	B	104	1tca	A	222	1tcv	C	171
1tcz	C	50	1td4	A	54	1te2	A	131	1tez	B	221	1tf4	A	285
1tg0	A	32	1tg7	A	602	1tgr	A	26	1tgx	B	18	1th7	H	46
1thg	A	290	1thq	A	69	1thx	A	60	1tjy	A	215	1tke	A	142
1tmx	A	176	1to4	A	88	1toa	B	140	1top	A	77	1tov	A	55
1tp6	A	77	1tp9	B	110	1tq4	A	210	1tqh	A	127	1tqj	B	138
1tr0	J	83	1tsf	A	40	1tu1	B	78	1tu7	B	153	1tu9	A	79
1tua	A	97	1tuh	A	48	1tuk	A	37	1tvn	B	194	1tw9	C	102
1twd	A	118	1twy	D	120	1tx2	A	154	1txg	B	218	1txo	B	104
1ty0	B	122	1tz0	B	53	1tzj	B	78	1tzp	A	182	1tzw	A	76
1tzy	C	14	1tzy	F	14	1u02	A	127	1u07	A	45	1u0a	D	150
1u0f	A	373	1u0k	B	173	1u11	A	91	1u1s	D	33	1u1w	B	172
1u2b	A	80	1u2h	A	62	1u2p	A	75	1u2w	B	33	1u36	A	47
1u3i	A	120	1u53	A	104	1u55	A	70	1u5d	B	73	1u5f	A	3
1u60	B	206	1u69	D	95	1u6e	A	185	1u6r	B	277	1u6t	A	69
1u6z	B	331	1u7i	A	88	1u7l	A	189	1u7p	A	90	1u84	A	42
1u8f	Q	204	1u8v	C	341	1u8y	B	106	1u94	A	135	1u9c	A	151
1u9k	A	67	1u9p	A	40	1ua4	A	223	1uai	A	147	1ual	A	139
1uar	A	142	1uas	A	221	1uay	B	117	1ub3	A	119	1uc4	A	339
1uc4	G	75	1udr	B	60	1ueb	A	108	1uec	A	75	1ued	A	202
1ueh	A	106	1uek	A	145	1uf5	A	186	1ufi	B	28	1ufy	A	78
1ug6	A	280	1ugi	E	33	1ugp	A	136	1ugp	B	153	1ugx	A	88
1uha	A	51	1uhe	A	47	1uhg	D	179	1uhk	B	127	1ui0	A	127
1uix	A	29	1uj0	A	30	1uj2	A	104	1uj6	A	115	1uj8	A	43
1ujn	A	126	1ujp	A	140	1uk7	A	179	1ukf	A	116	1ukk	A	48
1ukm	A	77	1ukm	B	66	1uku	A	71	1ukz	A	94	1ulr	A	52

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1umd	C	185	1umd	D	200	1umg	A	193	1umk	A	186	1umz	A	129
1uow	A	95	1uoy	A	41	1uoz	A	177	1ups	B	284	1upt	D	27
1upt	E	100	1uqx	A	72	1uqz	A	227	1ur5	A	156	1urn	C	55
1urr	A	41	1urs	A	195	1urx	A	191	1us5	A	151	1use	A	19
1usf	B	99	1usg	A	200	1uso	A	42	1usp	B	59	1usq	B	79
1ut7	B	78	1uti	A	33	1uu3	A	194	1uu4	A	162	1uuf	A	191
1uuj	A	44	1uuq	A	279	1uuy	A	99	1uv4	A	196	1uvq	A	116
1uvq	B	110	1uw4	C	56	1uw4	D	183	1uwc	A	179	1uwf	A	102
1uwk	B	348	1uws	B	238	1uww	A	135	1uwz	A	70	1uxo	A	132
1uxx	X	77	1uy1	A	86	1uyx	A	88	1uz3	A	75	1uzn	B	88
1v05	A	62	1v08	B	322	1v0a	A	107	1v0w	A	322	1v0z	B	275
1v2b	B	112	1v2z	A	66	1v37	A	97	1v3y	B	97	1v4p	C	111
1v4v	A	133	1v58	B	99	1v5f	A	312	1v5i	B	46	1v5v	B	263
1v5y	A	128	1v6s	A	224	1v6t	A	129	1v70	A	51	1v7p	C	99
1v7r	A	109	1v7w	A	498	1v84	A	132	1v8c	C	81	1v8f	A	128
1v8h	A	55	1v8y	A	82	1v96	B	68	1v98	A	39	1v9y	B	53
1va0	A	48	1vbi	A	168	1vbk	B	158	1vbu	A	208	1vbw	A	35
1vc4	B	127	1vcd	A	56	1vch	C	32	1vd1	A	97	1vd6	A	115
1vdk	B	169	1vdw	A	130	1vel	A	159	1vef	B	217	1vfl	A	139
1vfy	A	54	1vg8	C	100	1vgg	A	107	1vgy	B	158	1vh4	B	254
1vh5	A	83	1vhc	F	115	1vhe	A	199	1vhf	A	62	1vhn	A	169
1vhq	A	122	1vhs	A	57	1vht	B	137	1vhu	A	114	1vhv	A	132
1vhw	A	147	1vi3	A	98	1vi4	A	99	1vi6	B	94	1via	B	85
1vic	B	106	1vim	A	128	1vio	A	126	1vje	A	100	1vjk	A	63
1vjo	A	226	1vk1	A	147	1vk2	A	109	1vkc	A	66	1vke	F	64
1vkf	C	92	1vkh	A	154	1vki	A	123	1vkk	A	98	1vkm	C	152
1vkn	A	147	1vl1	A	154	1vl2	B	240	1vl4	A	201	1vl5	B	114
1vl7	A	73	1vla	C	65	1vlc	A	119	1vlj	A	68	1vlp	C	285
1vlr	A	199	1vly	A	185	1vm0	A	59	1vm9	A	71	1vma	A	143
1vmb	A	70	1vme	B	203	1vmf	C	100	1vmg	A	49	1vmh	A	91
1vmj	A	95	1vp2	A	110	1vp6	C	62	1vp8	A	119	1vpb	A	98
1vpd	A	173	1vph	E	92	1vpm	B	68	1vpr	A	169	1vps	A	168
1vq3	B	51	1vqs	D	76	1vqu	A	66	1vqz	A	147	1vr5	B	330
1vr6	C	1	1vr8	A	81	1vrm	A	192	1vsr	A	79	1vyf	A	60
1vyk	A	84	1vzi	B	77	1vzm	B	18	1vzy	B	102	1w0d	A	168
1w0h	A	153	1w0n	A	72	1w0p	A	412	1w0u	A	34	1w1d	A	111
1w1q	A	315	1w2i	B	55	1w2y	A	108	1w3h	A	162	1w3i	A	193
1w3w	A	205	1w3y	A	450	1w4r	F	94	1w4s	A	97	1w4t	A	154
1w4v	B	74	1w4x	A	312	1w5r	B	178	1w66	A	143	1w6s	C	426
1w6s	D	34	1w70	A	38	1w7x	L	33	1w8u	A	93	1w96	B	276
1w99	A	293	1w9a	B	91	1w9i	A	450	1w9p	A	276	1w9s	A	93
1wa0	X	225	1wa3	A	108	1wb0	A	203	1wb6	B	201	1wba	A	104
1wbe	A	117	1wbh	B	119	1wbj	A	158	1wbj	B	243	1wc1	C	60
1wc2	A	120	1wc9	A	91	1wcg	B	349	1wck	A	90	1wcu	A	99
1wd3	A	307	1wdd	S	63	1wdr	A	333	1wdv	B	94	1wei	A	115
1whz	A	44	1wj9	A	93	1wka	A	68	1wko	A	120	1wkq	B	100
1wkr	A	251	1wku	B	150	1wkx	A	33	1wky	A	260	1wl4	A	240
1wl8	A	124	1wlg	B	171	1wlj	A	90	1wly	A	190	1wlz	C	58
1wm2	A	45	1wma	A	179	1wmd	A	260	1wmh	A	50	1wmw	A	188
1wmz	D	99	1wn2	A	51	1wna	A	40	1wo8	D	74	1wog	E	169
1woq	B	109	1wor	A	173	1wov	B	150	1wp5	A	195	1wpa	A	69
1wpu	B	123	1wpu	A	62	1wq8	A	63	1wqj	B	45	1wqj	I	32

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1wr8	B	123	1wrd	A	58	1wri	A	51	1wrm	A	72	1ws0	A	87
1ws8	A	66	1wsd	A	174	1wst	A	210	1wt6	A	40	1wte	A	175
1wtj	A	171	1wto	A	38	1wu9	B	47	1wur	B	115	1wv3	A	110
1wve	D	45	1wvf	A	341	1wwi	A	77	1wwz	B	90	1wx1	B	104
1wxc	B	49	1wxi	A	144	1wxx	A	193	1wy1	A	64	1wy2	B	180
1wz3	A	50	1wz8	A	120	1wzn	B	129	1wzo	B	113	1wzz	A	180
1x0c	A	347	1x0l	A	164	1x13	B	181	1x1i	A	425	1x1n	A	327
1x1o	B	125	1x1t	A	131	1x2i	A	41	1x2t	C	73	1x38	A	298
1x3o	A	40	1x3s	A	101	1x3x	B	41	1x46	A	97	1x54	A	284
1x6i	A	68	1x6o	A	77	1x7d	A	210	1x82	A	100	1x8d	C	62
1x91	A	93	1x9d	A	338	1x9i	A	189	1x9u	A	63	1xa4	A	252
1xbb	A	162	1xbu	A	163	1xcr	A	147	1xd3	C	138	1xdn	A	196
1xdw	A	30	1xdz	A	150	1xe0	J	52	1xe7	C	93	1xeo	A	101
1xes	B	208	1xfi	A	185	1xfk	A	161	1xfz	A	72	1xg2	A	208
1xg2	B	106	1xg4	A	153	1xg5	A	155	1xg7	B	125	1xgk	A	175
1xgs	A	140	1xhd	A	109	1xhk	B	79	1xhn	A	116	1xiw	A	40
1xiw	C	57	1xiw	H	66	1xiy	A	86	1xk4	H	60	1xk4	I	57
1xki	A	58	1xkp	B	66	1xkp	C	49	1xky	B	197	1xkz	B	161
1xlq	C	59	1xm3	A	108	1xm8	A	162	1xmk	A	45	1xmp	B	108
1xmt	A	59	1xnf	A	154	1xnk	A	122	1xo7	B	106	1xoc	A	289
1xod	A	55	1xov	A	144	1xph	A	100	1xpm	D	227	1xpp	C	49
1xqa	A	58	1xqd	A	224	1xql	A	170	1xqo	A	165	1xre	A	124
1xrf	A	203	1xrk	B	82	1xru	B	156	1xs5	A	125	1xsq	A	84
1xt5	A	79	1xtp	A	140	1xtt	C	108	1xu1	D	81	1xu1	T	24
1xv5	A	232	1xvg	C	234	1xvg	E	104	1xvq	A	80	1xvw	B	82
1xvx	A	201	1xw6	A	87	1xwt	A	282	1xwv	A	59	1xww	A	105
1xx1	C	148	1xxq	D	100	1xy7	B	50	1y07	C	69	1y08	A	168
1y0b	D	126	1y0h	A	67	1y0k	A	113	1y0m	A	43	1y0u	A	56
1y0y	A	165	1y12	A	94	1y1p	A	205	1y1x	A	83	1y20	A	168
1y2b	B	246	1y2m	C	440	1y2t	B	110	1y37	A	189	1y3n	A	280
1y42	X	194	1y4j	B	140	1y4w	A	361	1y51	A	52	1y55	Y	86
1y5e	A	87	1y5h	A	58	1y5i	B	344	1y60	E	70	1y63	A	91
1y66	C	23	1y6x	A	57	1y71	A	57	1y7p	B	105	1y7r	B	78
1y7t	B	158	1y7w	A	157	1y8a	A	193	1y9i	A	75	1y9l	A	58
1y9q	A	95	1y9w	B	67	1y9z	B	291	1yac	B	128	1yal	A	128
1yar	D	77	1yar	N	104	1yar	S	124	1yb0	B	99	1yb1	A	126
1yb5	A	172	1ybi	B	236	1ybk	D	39	1yc5	A	168	1yc7	B	78
1yc9	A	210	1yd3	A	67	1ydy	A	165	1ye8	A	126	1yfn	C	54
1yfu	A	70	1yg9	A	201	1yif	A	314	1yj7	A	108	1ykd	A	237
1yki	B	163	1yle	A	198	1ylm	B	98	1ylx	B	50	1ym3	A	107
1ymd	A	123	1ymt	A	125	1yn3	B	59	1yn8	E	40	1yn9	A	117
1ynb	C	71	1ynh	B	226	1ynp	B	184	1yo3	A	51	1yoa	A	99
1yoc	B	86	1yoe	A	203	1yon	A	117	1yp1	A	80	1yph	D	87
1yph	E	66	1yq2	C	668	1yqd	A	202	1yqe	A	133	1yqh	A	72
1yqw	B	153	1yqw	Q	347	1yqz	A	281	1yrk	A	91	1ys1	X	225
1ysl	B	195	1ysq	A	111	1ysr	B	26	1yt3	A	208	1yt8	A	310
1ytq	A	127	1yu4	B	232	1yu6	B	173	1yuc	A	97	1yv1	A	103
1yvr	A	220	1yw5	A	115	1yx1	A	140	1yxj	B	80	1yxm	B	121
1yxy	A	146	1yya	A	156	1yzf	A	123	1yzz	A	87	1z0n	B	60
1z0s	C	139	1z1l	A	204	1z1s	A	78	1z21	A	68	1z2n	X	216
1z3e	A	83	1z3e	B	42	1z3q	A	140	1z3x	A	155	1z40	E	98
1z41	B	214	1z47	A	132	1z4j	A	134	1z4r	A	83	1z67	A	68

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
1z6m	A	104	1z6n	A	92	1z6o	D	96	1z6o	M	102	1z70	X	180
1z72	A	117	1z76	B	84	1z7a	D	198	1z7g	B	80	1z7x	W	240
1z84	A	207	1z8g	A	226	1z8o	A	216	1z96	A	19	1z9l	A	65
1z9t	A	138	1zar	A	161	1zb9	A	76	1zbf	A	81	1zc0	A	133
1zce	A	91	1zch	A	153	1zcz	A	50	1zd7	B	98	1zd8	A	142
1zd9	A	101	1zdy	A	167	1zel	B	155	1zem	A	130	1zgd	B	185
1zgz	D	69	1zh5	B	123	1zhh	A	156	1zhh	B	49	1zhq	A	75
1zhv	A	69	1zhx	A	253	1zi9	A	135	1zja	A	364	1zjc	A	273
1zjj	B	148	1zk4	A	138	1zk5	A	106	1zk7	A	264	1zkc	A	119
1zke	B	59	1zki	B	67	1zkk	B	113	1zkl	A	218	1zko	B	78
1zkp	B	161	1zl0	B	177	1zle	A	26	1zlh	B	47	1zlm	A	37
1zm8	A	70	1zma	A	55	1zn6	A	107	1zn8	A	107	1zo2	A	76
1zos	C	136	1zp3	C	143	1zpd	F	369	1zps	B	61	1zpv	A	40
1zpw	X	48	1zq9	B	184	1zr0	D	30	1zr3	B	65	1zr6	A	271
1zru	A	189	1zs4	D	49	1zs9	A	144	1zsw	A	151	1zsy	A	186
1zt5	A	49	1zu3	A	45	1zuo	A	73	1zuw	C	131	1zuy	A	26
1zv1	A	32	1zv9	A	113	1zvt	A	144	1zwh	A	119	1zwx	A	166
1zwy	C	91	1zwz	A	83	1zx6	A	38	1zx8	C	56	1zxt	B	37
1zxx	A	100	1zy7	A	251	1zz0	A	236	1zzg	B	205	1zzk	A	36
1zzo	A	66	1zzw	A	94	256b	B	66	2a07	K	53	2a0m	A	188
2a0n	A	150	2a13	A	100	2a14	A	187	2a15	A	76	2a26	C	30
2a2m	B	127	2a2n	C	65	2a2r	B	121	2a33	A	81	2a35	A	113
2a3n	A	218	2a3t	A	210	2a40	E	162	2a47	A	91	2a4a	A	143
2a4v	A	105	2a53	C	39	2a5d	A	95	2a5j	A	118	2a5l	A	96
2a5s	A	169	2a61	C	80	2a6c	B	37	2a6s	B	47	2a6v	A	157
2a70	A	174	2a7l	B	51	2a84	A	146	2a8n	A	62	2a8y	C	136
2a9i	A	68	2a9s	A	97	2aan	A	73	2aax	A	164	2ab0	A	114
2aba	A	224	2abs	A	170	2abw	B	130	2acf	D	109	2ad6	A	330
2ad6	D	40	2ae2	A	142	2aee	B	113	2aen	E	125	2aex	A	170
2ag4	B	104	2ag5	B	145	2agd	B	181	2agk	A	149	2ah4	X	148
2ah5	A	143	2ah6	B	75	2ahe	A	133	2ahf	A	228	2ahn	A	143
2ahu	A	272	2aie	P	97	2aj6	A	47	2aj7	A	90	2akz	B	238
2amj	B	86	2aml	B	259	2anv	A	86	2any	A	157	2ao9	D	76
2ap1	A	154	2ap3	A	116	2apg	A	324	2apj	C	152	2apo	A	110
2apr	A	209	2apx	A	76	2aq5	A	275	2aqm	A	93	2aqp	A	88
2aqv	B	161	2ar1	A	91	2arc	B	96	2arr	A	216	2as0	A	187
2as9	B	106	2asc	A	37	2asd	A	211	2asf	A	86	2ash	B	192
2asu	B	106	2at8	X	87	2atv	A	26	2au7	A	102	2avd	B	138
2avk	A	81	2axc	A	144	2axq	A	252	2axy	A	41	2ayd	A	58
2azw	A	76	2b06	A	103	2b0a	A	80	2b0t	A	308	2b0v	A	97
2b1k	A	62	2b1v	A	126	2b1y	A	41	2b3f	D	269	2b3g	A	63
2b3m	A	76	2b49	A	157	2b4v	A	263	2b4y	A	147	2b4z	A	51
2b58	A	102	2b5a	A	45	2b5h	A	126	2b5w	A	212	2b61	A	242
2b69	A	219	2b6e	H	53	2b6n	A	187	2b7k	A	86	2b7r	A	397
2b82	A	160	2b8m	A	69	2b94	A	124	2b9e	A	187	2b9h	A	237
2b9w	A	179	2ba2	C	34	2bay	E	47	2bba	A	124	2bbe	A	69
2bbr	A	123	2bcg	G	293	2bcg	Y	119	2bcm	B	85	2bcr	A	128
2bdr	A	93	2bei	B	66	2bek	D	110	2bem	A	122	2beq	D	8
2ber	A	392	2bez	C	37	2bf6	A	327	2bff	A	207	2bff	B	220
2bfw	A	107	2bg1	A	216	2bgs	A	200	2bh4	X	66	2bh8	B	38
2bhz	A	311	2bi0	A	190	2big	B	230	2bii	B	266	2bik	B	151
2biv	B	123	2bjf	A	233	2bji	A	174	2bjv	A	136	2bk9	A	103

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2bka	A	141	2bkf	A	9	2bkm	B	77	2bko	A	72	2bkr	A	151
2bkx	A	165	2bky	B	55	2bky	Y	51	2bl0	A	32	2bl0	B	100
2bl8	B	55	2blf	A	252	2blf	B	52	2bln	B	198	2bm3	A	89
2bmo	A	244	2bmo	B	123	2bnm	B	95	2bo1	A	71	2bo4	F	266
2bog	X	169	2boo	A	134	2boy	C	140	2bpq	A	175	2bqx	A	94
2br9	A	133	2brf	A	61	2brj	A	115	2bry	B	279	2bsj	A	69
2bt6	A	79	2bt9	A	58	2bu3	B	135	2buu	A	111	2buw	B	155
2bv2	B	57	2bv4	A	68	2bw0	A	191	2bw4	A	183	2bw8	A	128
2bwf	A	57	2bwl	A	67	2bwq	A	72	2bwr	B	267	2bz1	A	91
2bz6	H	155	2bzg	A	152	2bzl	A	180	2bzv	A	90	2c07	A	133
2c0c	A	224	2c0d	B	111	2c0g	B	52	2c0h	A	252	2c0n	A	116
2c0r	B	211	2c0z	A	119	2c15	A	182	2c1d	A	159	2c1d	D	72
2c1i	A	246	2c1s	A	77	2c1z	A	252	2c29	F	161	2c2i	B	95
2c2n	A	201	2c2p	A	104	2c2u	A	114	2c3b	B	6	2c3n	C	148
2c3v	A	58	2c41	F	106	2c42	B	643	2c43	A	164	2c46	C	131
2c4e	A	150	2c4f	T	55	2c4j	D	160	2c4n	A	126	2c53	A	152
2c5a	B	249	2c5q	E	167	2c60	A	58	2c61	A	287	2c6q	B	190
2c6u	A	85	2c6z	A	171	2c71	A	139	2c78	A	247	2c82	B	159
2c8h	D	124	2c8m	A	102	2c92	D	88	2c95	B	120	2c9i	D	124
2c9j	F	116	2c9q	A	52	2c9w	A	32	2cay	A	93	2cb2	E	147
2cb8	A	49	2cb9	A	122	2cbz	A	170	2cc0	B	119	2cc6	A	44
2ccj	B	91	2ccq	A	62	2ccw	A	57	2cdn	A	112	2cdp	C	78
2cdu	B	256	2cf7	C	106	2cfe	A	109	2cft	A	147	2cfu	A	359
2cg1	A	415	2cg7	A	37	2cgh	A	119	2cgq	A	48	2ch5	B	220
2chc	B	81	2ci0	A	218	2cia	A	55	2cio	A	116	2cir	A	197
2ciu	A	71	2ciw	A	220	2cj4	A	97	2cjj	A	39	2cjl	B	138
2cjp	A	177	2cjs	C	34	2cjt	A	89	2cjz	A	183	2ckf	D	124
2ckk	A	85	2cks	A	190	2cm4	A	83	2cm5	A	67	2cmj	B	192
2cmt	A	86	2cn0	H	155	2cn3	B	475	2cnq	A	154	2cnz	A	74
2cov	I	63	2cs7	A	38	2cu5	A	76	2cul	A	119	2cvd	D	137
2cve	A	103	2cvi	B	59	2cvl	C	65	2cvz	D	148	2cw5	B	94
2cw9	A	72	2cwa	A	69	2cwd	A	71	2cwi	B	72	2cwq	B	60
2cwr	A	57	2cws	A	150	2cwy	A	53	2cwz	D	72	2cx1	A	103
2cx7	A	60	2cxa	A	129	2cxh	A	87	2cxi	B	199	2cxk	E	48
2cxx	B	109	2cxy	A	62	2cye	C	71	2cyg	A	207	2cyy	A	78
2cz2	A	139	2cz4	A	39	2cz9	A	204	2czd	A	131	2czl	A	159
2czq	B	129	2d0i	B	165	2d16	A	95	2d1c	A	247	2d1l	B	78
2d1s	A	368	2d1x	A	25	2d1y	C	119	2d29	A	171	2d2e	A	97
2d2r	B	101	2d37	A	109	2d3d	A	65	2d3n	A	294	2d4k	A	61
2d4n	A	66	2d4p	A	79	2d4v	C	275	2d52	B	264	2d5b	A	248
2d5c	A	98	2d5k	C	98	2d5m	A	119	2d5z	B	98	2d68	B	54
2d69	A	235	2d6m	A	97	2d73	A	459	2d7t	H	80	2d7t	L	70
2d7v	A	68	2d8d	B	49	2d8l	A	214	2db7	A	33	2dbn	A	221
2dby	A	190	2dc3	A	99	2dc4	B	93	2dd7	A	115	2ddb	C	136
2ddr	A	177	2ddx	A	224	2de3	A	222	2de6	A	205	2de6	F	56
2deb	B	427	2dep	A	235	2dfa	A	48	2dfb	A	128	2dfd	C	186
2dg1	C	203	2dg5	C	190	2dga	A	300	2dge	B	68	2dgk	A	251
2dho	A	152	2dka	A	232	2dkh	A	276	2dkj	A	238	2dko	A	60
2dlb	A	50	2dlf	H	71	2dm9	B	84	2dok	A	91	2dp6	A	137
2dp9	A	53	2dpf	D	61	2dpl	A	173	2dqa	A	85	2dqd	L	66
2dql	A	75	2dr1	B	172	2dri	A	139	2drm	B	37	2ds2	D	19
2ds5	A	32	2dsj	B	208	2dsn	B	249	2dsy	C	47	2dt4	A	95

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2dt8	A	153	2dtc	B	58	2dtj	A	95	2dtx	A	160	2dur	A	178
2duy	A	31	2dvm	B	240	2dvx	B	206	2dwc	A	178	2dwu	A	145
2dx6	A	65	2dxa	A	90	2dxe	B	97	2dxq	A	98	2dy0	A	106
2dy1	A	299	2dyj	B	40	2dyk	A	67	2dyu	A	197	2e01	A	258
2e0a	A	186	2e0q	A	77	2e0t	A	95	2e10	B	122	2e1n	B	31
2e1v	B	261	2e1z	A	191	2e27	L	47	2e2o	A	143	2e2r	A	147
2e3a	A	239	2e3h	A	45	2e3p	B	156	2e3z	B	287	2e42	A	11
2e4t	A	353	2e5f	A	198	2e5y	B	59	2e6u	X	90	2e7u	A	217
2e7z	A	329	2e85	A	74	2e8e	A	73	2e8v	B	140	2e9m	A	289
2e9y	B	147	2ea3	A	95	2eab	A	602	2eb4	B	167	2ebb	A	62
2ecs	A	41	2ecu	A	92	2een	B	76	2eeo	B	51	2eey	A	69
2efr	B	33	2efv	A	41	2eg1	A	54	2eg3	A	141	2egd	B	56
2egj	A	85	2egu	A	112	2egv	A	112	2egx	A	74	2egz	A	132
2eh3	A	122	2eh6	A	150	2ehg	A	69	2ehp	A	67	2ehq	A	354
2eht	A	51	2ehz	A	188	2ei5	B	38	2eiq	B	69	2eix	A	155
2eiy	B	180	2ej8	A	74	2eja	B	202	2ejn	B	102	2eju	A	171
2ejw	A	154	2ejx	A	75	2ekg	A	138	2ekp	A	134	2eky	C	66
2elc	B	165	2elf	A	193	2eo4	A	65	2eo5	A	220	2epj	A	238
2epl	X	392	2eq6	B	232	2eqa	A	175	2erf	A	131	2erw	A	27
2erx	A	93	2ery	B	102	2es4	D	66	2esk	A	88	2esl	A	102
2esr	B	62	2ess	A	70	2et1	A	136	2etb	A	164	2etj	A	98
2etv	A	188	2etx	A	129	2eu7	X	82	2eut	A	224	2ev0	B	57
2ev1	A	96	2evb	A	30	2eve	A	86	2evf	A	193	2evr	A	128
2ew0	A	96	2ewh	A	41	2ewt	A	42	2ewu	A	69	2ex0	B	237
2ex2	A	257	2ex4	A	140	2exh	D	276	2exr	A	277	2exv	A	9
2ez9	A	398	2f01	B	64	2f02	B	139	2f0c	A	98	2f1k	B	166
2f22	B	92	2f23	B	67	2f2b	A	146	2f2e	B	44	2f46	A	77
2f4p	B	28	2f51	A	59	2f5g	B	58	2f5t	X	159	2f5v	A	419
2f5x	A	184	2f60	K	33	2f64	B	103	2f68	X	129	2f6e	A	83
2f6q	B	32	2f6r	A	85	2f6u	A	127	2f71	A	196	2f7b	A	152
2f7v	A	177	2f8a	A	125	2f91	A	162	2f99	C	78	2f9i	C	117
2f9i	D	90	2f9n	B	131	2f9s	B	76	2f9w	B	117	2fa8	A	54
2fad	A	46	2faf	A	379	2fao	B	155	2fb5	A	126	2fb6	A	67
2fba	A	364	2fbd	A	74	2fbn	A	108	2fbq	A	112	2fc3	A	63
2fcf	A	1	2fcl	A	99	2fco	B	92	2fct	A	12	2fcw	A	66
2fcw	B	51	2fd5	A	81	2fd7	A	29	2fds	A	182	2fdv	A	291
2fe3	A	90	2fe5	A	61	2fe8	A	178	2fef	B	152	2fex	A	106
2ff4	A	237	2ffc	A	178	2ffu	A	310	2fg1	A	80	2fgb	A	203
2fgo	A	46	2fgr	A	203	2fhf	A	543	2fhp	A	120	2fhx	B	23
2fhz	A	69	2fhz	B	62	2fi1	A	152	2fi9	A	47	2fim	A	103
2fj8	A	90	2fjz	A	46	2fk9	A	91	2fkk	A	34	2fl7	A	106
2flh	B	98	2flu	X	172	2fn6	A	174	2fmm	C	47	2fmp	A	207
2fn0	A	182	2fn3	A	286	2fn4	A	55	2fn9	B	190	2fne	A	3
2fnu	A	245	2fo3	A	55	2foj	A	94	2fom	A	25	2fom	B	79
2fos	A	170	2foz	A	199	2fp2	B	114	2fp7	A	19	2fp7	B	84
2fpe	A	30	2fpq	A	259	2fpx	B	123	2fq3	A	54	2fq4	A	90
2fq6	B	246	2fqp	C	65	2fqw	A	144	2fr2	A	102	2fr5	C	65
2fre	A	129	2frg	P	64	2fs6	A	87	2fsj	A	187	2fsq	A	135
2fsr	A	88	2fss	C	144	2fsx	A	85	2ft0	A	136	2ft6	A	85
2ftr	B	63	2ftx	A	49	2ftx	B	40	2ftz	A	101	2fu0	A	108
2fu4	A	51	2fue	A	151	2ful	A	105	2fup	A	57	2fur	B	94
2fvh	A	43	2fvv	A	51	2fwh	A	55	2fww	A	101	2fyf	A	237

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2fyg	A	77	2fym	D	251	2fyq	A	110	2fyx	A	1	2fzp	A	85
2fzv	B	128	2fzw	B	228	2g0c	A	20	2g0i	B	67	2g0w	A	160
2g1u	A	80	2g2c	A	92	2g2n	C	80	2g30	A	49	2g3a	A	65
2g3d	A	44	2g40	A	94	2g50	A	332	2g5c	D	133	2g5r	A	62
2g5x	A	154	2g64	A	80	2g6y	C	121	2g76	A	160	2g7s	A	102
2g81	I	36	2g82	P	219	2g84	A	113	2g8o	B	194	2g8s	B	212
2g9f	A	34	2g9w	A	69	2ga4	A	201	2ga4	D	50	2ga8	A	165
2gag	A	488	2gag	B	181	2gag	C	88	2gai	B	350	2gas	A	151
2gau	A	120	2gax	A	71	2gb7	D	165	2gbt	A	69	2gbw	E	212
2gc4	B	80	2gc4	L	45	2gc6	A	236	2gco	A	115	2gcu	C	179
2gd2	A	203	2gdq	B	225	2gdz	A	157	2gec	A	81	2gen	A	87
2gey	D	90	2gf3	B	228	2gf6	D	82	2gff	A	55	2gfh	A	11
2gfn	B	92	2gfq	B	180	2gg2	A	181	2gg6	A	292	2gh0	B	64
2gh0	D	34	2gh9	A	190	2gha	A	263	2ghs	A	191	2gi3	A	253
2gia	B	80	2gib	B	60	2gig	A	124	2gim	A	69	2giy	A	51
2gj3	A	79	2gj8	A	92	2gjd	C	86	2gjs	B	42	2gke	A	199
2gkp	A	100	2gkr	I	35	2glz	B	80	2gm6	A	41	2gmq	A	38
2gmy	E	101	2gn4	B	103	2gnc	A	27	2gok	A	181	2gom	A	42
2gou	A	242	2gpc	B	132	2gpe	B	24	2gpi	A	60	2gq1	A	174
2gqp	B	111	2gqt	A	149	2gqw	A	237	2grc	A	82	2grr	B	94
2gs5	A	119	2gs8	A	179	2gsd	A	249	2gso	B	242	2gsv	B	32
2gte	A	88	2gtr	A	137	2gu2	B	171	2gu3	A	71	2gud	B	70
2guh	A	80	2gui	A	111	2guv	C	44	2guy	A	323	2gvk	A	180
2gw3	B	106	2gw4	D	68	2gwg	B	171	2gwm	A	125	2gwn	A	260
2gx5	D	91	2gxg	A	81	2gxu	A	108	2gyq	B	87	2gz1	B	227
2gz4	A	126	2gz5	A	177	2gze	A	55	2gze	B	85	2gzg	B	100
2gzv	A	48	2h0u	A	127	2h12	A	246	2h1c	A	63	2h1r	A	132
2h1t	B	123	2h1v	A	190	2h26	A	127	2h2b	A	60	2h2r	B	82
2h2z	A	170	2h30	A	99	2h3h	A	215	2h3l	A	71	2h4p	A	227
2h4v	B	185	2h54	B	63	2h62	A	55	2h64	B	10	2h6e	A	148
2h6f	A	218	2h6f	B	263	2h6n	A	215	2h88	A	332	2h88	B	158
2h88	D	19	2h88	P	40	2h8e	A	63	2h8g	B	116	2h8o	A	141
2h9b	A	144	2h9d	B	34	2h9h	A	133	2ha8	B	99	2hax	B	36
2haz	A	59	2hba	A	11	2hbo	A	26	2hbv	A	151	2hc1	A	128
2hc8	A	63	2hc9	A	279	2hcf	A	142	2hd9	A	91	2hda	A	29
2hdo	A	118	2he0	A	99	2he2	A	63	2he4	A	49	2hei	B	107
2hek	B	99	2heu	B	226	2hew	F	80	2hf1	B	21	2hf2	B	89
2hf9	A	134	2hfk	A	128	2hhc	A	159	2hhg	A	83	2hhj	A	168
2hhv	A	361	2hi0	A	158	2hin	B	31	2hiy	A	127	2hjh	A	183
2hjb	A	68	2hke	B	163	2hkv	A	27	2hl7	A	32	2hlc	A	136
2hjr	A	45	2hls	A	104	2hly	A	121	2hmc	A	147	2hmq	D	82
2hng	A	48	2hos	B	8	2hox	A	271	2hpg	B	176	2hps	A	128
2hpn	A	160	2hq1	A	103	2hq2	A	212	2hq4	A	78	2hq6	A	84
2hq9	B	71	2hqh	C	44	2hqk	A	107	2hqs	D	284	2hqs	H	61
2hqr	A	161	2hra	A	90	2hrz	A	197	2hsa	A	230	2hsb	A	3
2hsj	D	141	2hsz	B	132	2ht9	B	48	2hta	A	185	2htd	A	69
2hu9	A	55	2huc	A	142	2huh	A	92	2huj	A	68	2hur	B	88
2hv8	A	114	2hv8	E	35	2hvm	A	162	2hvw	C	93	2hw4	A	46
2hwn	D	13	2hx5	A	81	2hxi	B	100	2hxm	A	168	2hxp	A	78
2hxt	A	269	2hxx	A	167	2hxx	A	139	2hy5	A	63	2hy5	B	69
2hy7	A	244	2hyk	A	123	2hyt	A	102	2hyv	A	199	2hyx	D	180
2hze	B	52	2hzi	B	219	2i02	A	60	2i0q	A	204	2i0z	A	161

Continued on next page



PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2i13	B	15	2i1n	A	52	2i24	N	81	2i2o	A	129	2i2q	A	68
2i33	B	142	2i3d	A	133	2i3f	A	135	2i49	A	258	2i4a	A	68
2i51	A	111	2i5c	C	11	2i5d	A	105	2i5r	B	57	2i5u	A	38
2i5v	O	185	2i61	A	38	2i62	D	160	2i6c	A	91	2i6d	A	130
2i6g	B	104	2i6h	A	111	2i6v	A	62	2i71	B	247	2i7a	A	43
2i7c	C	205	2i7d	A	152	2i7f	B	60	2i7g	B	152	2i8d	B	80
2i8g	A	82	2i9a	D	78	2i9i	A	137	2i9x	A	48	2ia1	A	68
2ia7	A	70	2iai	A	108	2iay	A	77	2ib5	A	130	2ib8	A	237
2ibd	A	123	2ibj	A	52	2ibl	A	78	2ibn	A	144	2ibp	B	245
2ic0	A	220	2ic2	B	60	2ic5	A	88	2ic6	A	47	2ic7	B	128
2icg	A	84	2ici	A	151	2icr	A	148	2ict	A	49	2icu	A	143
2icx	A	296	2id3	B	103	2id4	A	316	2id6	A	85	2id8	A	175
2idl	B	65	2ie6	A	2	2iel	A	78	2ieq	A	58	2ifc	C	239
2ifq	C	62	2ig6	A	32	2ig8	A	77	2igi	A	119	2igp	A	82
2igv	A	106	2igx	A	161	2ih3	C	45	2ih5	A	266	2ihd	A	78
2ihy	B	118	2iil	D	151	2ii2	A	212	2iia	A	48	2ij2	A	325
2ijh	A	33	2ijq	A	87	2ijx	D	16	2ikb	B	93	2iks	A	164
2im9	A	193	2imf	A	119	2imh	B	133	2imi	B	158	2imj	C	96
2iml	C	117	2imq	X	164	2imr	A	192	2ims	A	98	2imz	B	72
2in3	A	1	2in8	A	74	2inc	A	94	2inc	B	113	2inw	B	67
2ion	A	85	2ior	A	111	2ioy	B	145	2ip1	A	241	2ip2	B	146
2ip6	A	51	2ipr	B	95	2ipx	A	131	2iq7	A	212	2iru	B	165
2is8	A	81	2is9	A	142	2isa	H	347	2isb	A	88	2ist	A	152
2it1	A	127	2it9	C	36	2ite	A	88	2iu5	A	128	2ium	A	143
2iuw	A	132	2ivf	A	526	2ivf	B	205	2ivn	A	197	2ivx	A	165
2ivy	A	60	2iw0	A	137	2iw1	A	260	2iw2	B	319	2iwn	A	52
2iwo	B	44	2iwr	A	86	2iwz	A	210	2ix4	B	252	2ixc	A	142
2ixd	B	105	2ixk	A	123	2ixm	A	209	2iy9	A	176	2iya	A	249
2iyf	A	234	2iyv	A	95	2iz6	B	66	2izu	A	181	2izz	B	158
2j05	A	40	2j0i	A	177	2j0v	C	77	2j13	A	98	2j1a	A	92
2j1p	B	151	2j1s	A	101	2j23	A	81	2j27	A	167	2j2j	F	131
2j3x	A	287	2j41	D	103	2j43	B	145	2j5g	A	189	2j5i	F	148
2j5y	A	29	2j5z	C	101	2j6a	A	92	2j6b	A	70	2j6f	A	23
2j6g	A	173	2j6l	F	335	2j6v	B	161	2j6y	D	66	2j73	B	71
2j78	B	299	2j7p	E	98	2j7q	C	149	2j7u	A	228	2j7y	A	20
2j80	A	79	2j8b	A	54	2j8g	A	224	2j8k	A	110	2j8m	A	92
2j91	A	237	2j97	A	57	2j9a	A	290	2j9b	B	68	2j9o	B	163
2j9w	A	78	2ja2	A	209	2jae	B	342	2jah	A	136	2jam	A	171
2jay	A	80	2jb0	A	41	2jb7	B	103	2jb8	A	167	2jba	B	67
2jc4	A	176	2jc5	A	160	2jc9	A	299	2jcb	A	106	2jcc	A	100
2jda	A	97	2jdd	A	96	2jdf	A	95	2jdi	A	246	2jdi	D	277
2jdk	D	78	2je3	A	82	2je8	B	574	2jek	A	97	2jep	B	254
2jer	F	262	2jfg	A	276	2jft	A	135	2jg2	A	254	2jg6	A	134
2jgn	B	74	2jgs	C	63	2jh1	A	136	2jhn	B	177	2jhg	A	149
2ji7	A	363	2jig	B	122	2jik	A	62	2jil	A	47	2jis	A	321
2jjb	A	308	2jjc	A	137	2jjf	A	266	2jjn	A	213	2jjq	A	206
2jjs	C	86	2jju	B	79	2jk9	A	111	2jkb	A	457	2jkg	A	92
2jkh	A	133	2jko	A	151	2jl1	A	148	2jlp	A	85	2jll	A	258
2lis	A	94	2mnr	A	228	2nl9	A	75	2nli	A	212	2nlo	A	171
2nlr	A	4	2nlv	B	68	2nm0	B	78	2nml	A	51	2nmu	A	84
2nmx	A	156	2nn5	A	107	2nn8	A	96	2nnr	A	11	2nnu	A	137
2no4	A	123	2noo	A	310	2np5	B	84	2npn	A	120	2npt	C	51

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2npt	D	46	2nq3	A	60	2nq9	A	166	2nql	B	217	2nqt	B	205
2nqw	A	57	2nr5	C	33	2nr7	A	143	2nrk	A	96	2nrr	A	36
2ns1	A	167	2ns1	B	5	2nsa	A	56	2nsf	A	132	2nsq	A	59
2nt4	A	65	2ntp	A	215	2nug	B	101	2nuh	A	49	2nuk	A	97
2nuw	A	182	2nv0	B	67	2nva	B	252	2nw2	B	175	2nw8	B	164
2nwh	A	138	2nwv	A	59	2nx0	A	78	2nx4	C	113	2nxb	B	96
2nxf	A	208	2nxv	A	173	2nxw	A	312	2nyb	A	108	2nyi	B	92
2nyn	C	202	2nyu	A	73	2nz7	A	59	2nzc	A	23	2nzh	A	71
2o07	B	193	2o08	A	58	2o0a	A	150	2o0b	A	252	2o0m	A	148
2o11	A	159	2o16	A	82	2o1c	B	92	2o1q	B	76	2o20	F	176
2o23	B	137	2o28	A	102	2o2c	C	366	2o2g	A	113	2o2k	A	212
2o2p	D	319	2o2x	A	130	2o30	A	48	2o36	A	341	2o37	A	43
2o38	A	32	2o3f	B	25	2o3h	A	158	2o4a	A	23	2o4d	A	77
2o4v	B	262	2o57	C	170	2o5f	B	56	2o5u	A	92	2o62	A	164
2o66	A	61	2o6f	A	85	2o6l	A	66	2o6p	A	83	2o6s	A	138
2o6x	A	196	2o6y	G	318	2o74	F	121	2o7i	A	415	2o7r	A	210
2o8p	A	150	2o8q	A	58	2o90	A	63	2o9c	A	175	2o9s	A	39
2oa2	A	83	2oaa	B	157	2ob0	A	21	2ob3	B	231	2ob5	A	87
2obi	A	120	2obl	A	174	2obp	A	38	2oc3	A	175	2oc5	A	129
2oc6	A	61	2ocg	A	154	2ocs	A	51	2ocz	A	27	2od0	B	52
2od4	A	63	2od5	A	25	2od6	C	51	2oda	B	130	2ode	D	61
2odf	E	133	2odi	B	148	2odk	C	31	2odl	A	227	2oe3	A	73
2oeb	A	96	2oem	A	210	2ofk	A	107	2ofz	A	74	2og1	A	163
2og5	A	217	2og9	B	137	2ogf	B	77	2ogi	A	75	2ogx	A	139
2oh1	D	87	2oh5	A	187	2ohw	B	94	2oik	D	90	2oix	A	80
2oiz	B	262	2oiz	D	72	2oj6	C	115	2ojh	A	110	2okf	B	73
2okm	A	95	2okq	A	53	2oku	A	74	2ol1	B	78	2oln	A	246
2olp	A	94	2olr	A	352	2omk	A	130	2oml	A	122	2omo	G	66
2omy	B	59	2omz	A	328	2on5	A	141	2onf	B	85	2oo0	A	258
2oo1	B	65	2ooa	A	25	2ooc	B	46	2ooj	B	47	2ook	A	31
2ooq	A	128	2op6	A	89	2opc	A	70	2opg	B	57	2opj	A	142
2opl	B	113	2opw	A	139	2oqa	B	151	2oqb	A	68	2oqe	B	456
2oqg	B	45	2oqh	D	199	2oqk	A	55	2oqm	D	83	2oqx	A	227
2oqz	A	111	2or7	A	62	2ord	B	261	2orw	A	115	2os0	A	116
2os5	A	85	2os9	B	97	2osa	A	25	2oso	A	90	2osv	B	155
2osx	A	283	2ot9	A	85	2otm	B	90	2otu	E	68	2ou3	A	88
2ou5	B	107	2ou6	A	113	2oua	A	113	2oui	A	215	2ous	A	229
2ouw	A	10	2ov0	A	70	2ov9	C	77	2ovj	A	131	2ow9	B	118
2ows	A	200	2ox0	A	159	2ox4	H	249	2ox6	B	112	2ox7	B	80
2oxc	A	142	2oxg	A	70	2oxg	Y	63	2oxl	B	30	2oxn	A	204
2oxw	A	106	2oy7	A	200	2oy9	B	53	2oya	B	57	2oyh	A	80
2oyo	A	136	2oyp	A	68	2oze	A	184	2ozf	A	53	2ozh	A	87
2ozl	A	189	2ozn	A	87	2ozn	B	86	2ozt	A	205	2p02	A	255
2p09	A	51	2p0a	B	197	2p0f	A	59	2p0n	A	91	2p0s	A	70
2p0u	A	225	2p0w	B	221	2p12	A	93	2p13	A	19	2p14	A	130
2p17	A	151	2p18	A	171	2p1g	B	156	2p1h	A	12	2p1m	B	390
2p1t	A	148	2p25	A	69	2p2d	C	188	2p2r	A	35	2p2s	A	213
2p2v	A	116	2p2w	A	213	2p35	B	125	2p39	A	90	2p3e	A	236
2p3h	A	43	2p3p	B	138	2p3w	A	67	2p49	B	73	2p4d	A	91
2p4e	P	62	2p4h	X	187	2p4k	A	137	2p4o	A	35	2p51	A	148
2p54	A	141	2p58	A	26	2p58	C	61	2p5y	A	170	2p65	A	113
2p67	A	136	2p68	A	158	2p6h	B	72	2p6w	A	155	2p6x	A	99

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2p6y	A	72	2p6z	A	80	2p7i	B	108	2p8b	A	191	2p8e	B	177
2p8g	A	118	2p8i	D	70	2p8t	A	104	2p92	B	41	2p97	B	102
2p9b	A	205	2p9w	A	201	2p9x	D	47	2pa1	A	45	2pa5	A	202
2pa6	B	236	2pa7	B	74	2pag	A	70	2pb2	B	234	2pbc	C	53
2pbd	P	90	2pbi	C	80	2pbi	D	171	2pbk	B	137	2pbl	A	155
2pbp	A	144	2pbq	B	85	2pc1	A	93	2pc8	A	271	2pcj	B	122
2pcn	A	66	2pcu	A	200	2pd1	B	51	2pdr	B	72	2peb	B	50
2pef	A	227	2pet	A	136	2pey	B	98	2pf5	A	45	2pfe	B	100
2pfi	A	78	2pfz	A	180	2pg0	B	226	2pge	A	179	2pgf	A	224
2pgo	A	377	2pgw	F	191	2pgz	A	146	2ph0	B	75	2ph3	A	108
2phn	A	127	2phx	B	128	2pi6	A	218	2pie	A	88	2pij	A	25
2piy	B	199	2pjs	B	59	2pjz	A	137	2pk3	A	179	2pk8	A	59
2pke	A	87	2pkf	A	215	2pkh	H	73	2pko	A	47	2pkt	A	65
2pky	X	178	2pl1	A	72	2pli	A	50	2plj	A	247	2pln	A	66
2plr	A	119	2plw	A	113	2pma	A	62	2pmb	C	143	2pmk	A	113
2pmq	A	213	2pmr	A	49	2pn0	B	75	2pn2	A	4	2pn6	A	90
2pn8	B	135	2pnd	A	85	2pne	A	28	2pnw	A	221	2pnx	A	37
2pny	A	151	2poc	A	198	2poi	A	43	2pok	B	255	2por	A	119
2pos	D	70	2poy	A	111	2ppp	A	51	2ppt	B	62	2pq7	A	87
2pqm	B	180	2pqr	B	79	2pqr	D	20	2pqv	A	108	2pqx	A	125
2pr5	A	97	2pr7	B	71	2prb	A	126	2prv	A	92	2prz	D	138
2ps2	A	196	2psd	A	216	2psp	B	50	2pst	X	43	2pt0	B	209
2ptt	B	77	2ptv	A	70	2ptz	A	209	2pu3	A	121	2pu9	A	56
2pu9	B	49	2pur	A	169	2pv2	A	57	2pv4	A	18	2pvq	A	103
2pw0	A	241	2pwy	A	168	2py4	A	94	2py5	A	305	2pyq	B	44
2pyt	A	69	2pyw	A	304	2pyx	A	342	2pz0	B	148	2pze	B	117
2pzh	B	86	2q03	A	44	2q0l	A	212	2q0t	C	159	2q0u	A	238
2q0y	A	88	2q12	A	86	2q16	B	94	2q1u	B	204	2q20	B	60
2q24	A	69	2q28	A	355	2q2a	D	156	2q2f	A	22	2q2g	A	104
2q2h	A	89	2q2v	B	143	2q30	E	42	2q35	A	153	2q3b	A	187
2q3g	A	54	2q3h	A	1	2q3x	B	78	2q5c	A	102	2q5x	A	82
2q62	G	149	2q66	A	288	2q6k	A	158	2q73	C	55	2q79	A	36
2q7d	A	193	2q7e	A	8	2q7w	A	199	2q86	A	86	2q86	B	121
2q87	A	53	2q88	A	132	2q8g	A	206	2q8k	A	205	2q8n	C	36
2q8p	A	131	2q8r	G	52	2q8x	B	163	2q9k	A	82	2q9o	B	395
2q9u	A	291	2qa1	A	27	2qa9	E	112	2qac	A	68	2qap	A	192
2qc5	A	167	2qck	A	46	2qcv	A	140	2qd6	A	58	2qde	F	210
2qdx	A	183	2qe8	A	232	2qe9	A	38	2qec	A	7	2qed	A	124
2qee	F	268	2qeu	C	73	2qev	A	2	2qf4	B	111	2qf9	A	84
2qfa	A	86	2qfa	B	42	2qfa	C	26	2qfe	A	92	2qff	A	37
2qfs	A	286	2qg1	A	48	2qg3	A	68	2qg6	A	113	2qgu	A	122
2qgy	B	249	2qh9	A	98	2qhk	A	74	2qhl	B	58	2qho	B	39
2qhp	A	156	2qhq	B	80	2qhs	A	144	2qia	A	167	2qib	A	139
2qif	A	34	2qih	B	81	2qik	A	173	2qim	A	80	2qip	A	111
2qiw	A	122	2qiy	B	77	2qjj	D	235	2qjv	B	67	2qjw	B	98
2qjx	A	66	2qk1	A	147	2qkf	C	135	2qkh	A	39	2qkp	C	85
2ql8	B	97	2qlt	A	153	2qlw	B	72	2qm0	B	124	2qm8	A	189
2qmc	A	214	2qmc	D	122	2qmj	A	521	2qml	A	105	2qmm	A	125
2qmo	A	147	2qmq	A	186	2qn0	A	266	2qng	A	98	2qnk	A	194
2qnl	A	100	2qnt	A	67	2qnw	A	48	2qo4	A	94	2qod	A	157
2qor	A	126	2qos	C	85	2qpn	B	158	2qpw	A	94	2qpx	A	232
2qq4	B	53	2qq5	A	74	2qqi	A	164	2qqj	A	184	2qr3	A	75

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2qr6	A	141	2qrl	A	242	2qrr	B	41	2qru	A	165	2qrw	I	72
2qs9	A	124	2qsa	A	58	2qsb	A	35	2qsi	A	60	2qsk	A	56
2qsq	B	33	2qsw	A	41	2qsx	A	116	2qt7	B	51	2qt8	A	180
2qtd	A	54	2qtq	A	76	2qtz	A	255	2qub	I	398	2qud	A	63
2qul	C	176	2quy	H	238	2qv5	A	117	2qvb	A	209	2qvg	A	67
2qvk	A	86	2qvo	A	43	2qvu	B	161	2qw5	B	210	2qwl	A	252
2qwo	B	53	2qwu	A	109	2qx0	A	60	2qx2	A	93	2qx8	B	151
2qxf	A	269	2qxi	A	126	2qxy	B	50	2qy1	B	204	2qy9	A	160
2qyc	B	47	2qzc	A	130	2qzq	A	115	2qzt	B	58	2r01	A	115
2r0b	A	91	2r0c	A	142	2r0h	C	77	2r0x	A	88	2r0y	A	132
2r11	A	169	2r14	A	21	2r16	A	102	2r1b	B	122	2r1i	A	66
2r1j	R	43	2r2a	A	106	2r2c	B	67	2r2d	A	150	2r2y	A	67
2r2z	A	43	2r31	A	113	2r37	A	114	2r3b	B	160	2r47	A	86
2r48	A	50	2r4g	A	143	2r4i	D	83	2r4q	A	50	2r4v	A	105
2r5o	B	103	2r5t	A	105	2r5u	D	38	2r6j	B	195	2r6n	A	118
2r6o	B	123	2r6u	B	61	2r6v	A	106	2r6z	B	113	2r75	1	190
2r77	A	123	2r78	A	75	2r7h	A	34	2r80	C	92	2r84	B	165
2r8e	E	125	2r8q	A	208	2r8w	B	174	2r99	A	122	2r9f	A	210
2ra2	C	31	2ra3	B	147	2ra4	A	36	2ra6	B	82	2ra9	A	97
2raf	C	122	2ras	A	20	2rau	A	187	2rb7	B	204	2rbb	A	70
2rbc	A	166	2rbd	A	90	2rbg	B	95	2rbk	A	161	2rc3	A	95
2rc8	B	177	2rcc	B	187	2rci	A	131	2rcq	A	108	2rcv	E	125
2rcz	B	47	2rdc	B	58	2rdh	C	124	2rdm	A	36	2rdq	A	174
2rdu	A	234	2rdz	A	284	2re2	A	67	2ree	A	107	2reg	A	168
2rek	A	51	2rem	B	65	2rer	A	54	2rff	A	72	2rfg	A	197
2rfi	B	157	2rfm	B	90	2rfq	B	239	2rfr	A	80	2rfv	A	209
2rgi	A	54	2rh0	B	58	2rhf	A	50	2rhi	A	207	2rhk	C	12
2rhm	B	100	2ri0	B	150	2ri7	A	118	2ri9	A	313	2rij	A	198
2rik	A	188	2ril	A	44	2ris	A	134	2rji	A	55	2rjw	A	51
2rk3	A	103	2rk5	A	53	2rk9	B	67	2rkl	A	25	2rkq	A	108
2rku	A	49	2rkv	A	285	2rky	C	54	2rld	D	71	2tnf	B	81
2uur	A	96	2uuu	C	293	2uuy	B	32	2uvj	A	216	2uvk	A	175
2uvo	B	106	2uw1	A	199	2uxq	A	252	2uxw	A	351	2uxy	A	225
2uy2	A	173	2uyq	A	143	2uyt	A	303	2uyw	A	65	2uyz	A	103
2uyz	B	41	2uz0	A	167	2uz1	D	347	2uzc	C	56	2uzj	B	169
2v03	A	182	2v05	A	208	2v09	A	265	2v0c	A	513	2v0h	A	307
2v0p	A	67	2v0s	A	155	2v0u	A	100	2v1o	B	87	2v1q	A	41
2v1w	B	43	2v25	A	90	2v27	A	154	2v2f	F	199	2v2g	C	155
2v2k	B	74	2v2p	A	116	2v33	B	42	2v36	D	119	2v3f	B	339
2v3g	A	181	2v3s	A	62	2v40	A	237	2v4n	A	163	2v4v	A	90
2v4x	A	90	2v57	C	74	2v5i	A	388	2v5j	A	163	2v5z	A	352
2v62	A	99	2v6a	O	96	2v6h	A	66	2v6k	B	137	2v6u	A	66
2v6v	B	98	2v6x	A	56	2v6x	B	17	2v76	A	62	2v7b	A	265
2v7f	A	77	2v7k	A	187	2v7s	A	89	2v7w	C	156	2v84	A	157
2v87	B	51	2v8c	A	83	2v8i	A	306	2v8u	A	189	2v94	A	38
2v9m	A	160	2v9t	B	136	2vac	A	87	2vag	A	178	2vap	A	150
2vba	D	255	2vbf	A	355	2vbk	A	326	2vc3	A	189	2vc8	A	32
2vch	A	307	2vck	D	150	2vd8	A	239	2vdx	A	3	2ve8	E	6
2veb	A	15	2vec	A	77	2vef	A	162	2vep	A	133	2vfk	A	137
2vfq	A	371	2vfr	A	268	2vfx	C	127	2vgl	B	122	2vg3	C	187
2vgp	B	184	2vgp	D	12	2vgx	A	70	2vh3	A	65	2vha	B	168
2vi3	A	124	2vi8	A	266	2vid	A	117	2vif	A	77	2vig	A	164

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2vj0	A	177	2vjp	B	266	2vjv	B	66	2vk2	A	205	2vk8	C	346
2vkj	A	65	2vkl	A	41	2vkp	B	56	2kv	A	71	2vla	A	179
2vlf	B	285	2vlg	B	58	2vli	B	98	2vlu	A	56	2vm2	C	19
2vm5	A	67	2vmb	A	60	2vmc	A	189	2vmi	A	103	2vn6	A	112
2vn6	B	43	2vng	A	116	2vnk	C	170	2vnl	A	53	2vnz	X	163
2vo4	A	115	2vo8	A	83	2vo9	B	88	2voa	A	167	2voc	A	45
2vof	A	72	2vov	A	177	2voz	A	201	2vpa	A	118	2vpg	A	44
2vph	B	36	2vpj	A	122	2vpn	A	184	2vpt	A	138	2vq2	A	143
2vq4	A	69	2vq8	A	76	2vqg	D	41	2vqp	A	159	2vqq	B	223
2vqr	A	358	2vqx	A	210	2vre	A	95	2vri	A	96	2vro	B	309
2vrs	C	134	2vrw	B	231	2vs0	A	45	2vsm	A	267	2vsm	B	83
2vsv	A	58	2vte	B	164	2vtf	B	414	2vuj	A	125	2vun	B	226
2vuo	A	117	2vuv	A	71	2vuw	A	181	2vv6	D	66	2vve	A	157
2vvm	A	310	2vvp	B	99	2vvt	B	184	2vvw	A	82	2vw8	A	193
2vwf	A	41	2vwr	A	56	2vws	C	175	2vx5	A	260	2vxg	B	71
2vxk	A	101	2vxn	A	157	2vxq	A	36	2vxr	A	313	2vxt	H	116
2vxt	I	79	2vxt	L	134	2vxy	A	124	2vxz	A	92	2vy8	A	80
2vyo	A	122	2vyq	A	216	2vyw	A	101	2vyx	C	44	2vz5	A	42
2vzc	A	61	2vzm	A	221	2vzp	B	75	2w0i	A	64	2w0p	B	46
2w15	A	143	2w1j	B	129	2w1p	A	156	2w1r	A	70	2w1s	A	98
2w1v	A	189	2w1z	B	161	2w20	A	311	2w2b	B	127	2w2k	A	243
2w2r	A	95	2w31	B	104	2w39	A	200	2w3g	A	86	2w3j	A	76
2w3p	B	374	2w3q	A	135	2w3v	A	89	2w3x	A	51	2w3z	A	170
2w40	A	320	2w43	A	126	2w47	A	87	2w4c	A	66	2w4f	A	47
2w4i	F	152	2w50	B	66	2w56	B	41	2w59	A	67	2w5a	A	136
2w5w	B	190	2w61	A	318	2w6a	B	32	2w70	A	312	2w79	B	124
2w7a	B	61	2w7n	A	38	2w7s	B	126	2w7w	B	125	2w7z	A	141
2w83	C	34	2w86	A	70	2w87	A	83	2w8x	A	42	2w91	A	450
2w9h	A	89	2w9k	B	67	2w9r	A	64	2w9y	A	81	2wa2	B	153
2waa	A	210	2wan	A	514	2wao	A	211	2waw	A	91	2wb6	A	42
2wbf	X	135	2wbn	B	106	2wbp	A	171	2wbs	A	44	2wbw	A	143
2wc8	B	58	2wci	A	67	2wcj	A	82	2wco	A	380	2wcr	A	95
2wcu	A	69	2wcv	C	67	2wcw	B	51	2wdc	A	331	2wds	A	59
2wdu	B	119	2we2	A	147	2we5	C	149	2wee	B	98	2wei	A	187
2wel	A	188	2weu	A	333	2wf6	A	153	2wfc	C	92	2wfh	B	5
2wfj	A	118	2wfo	A	111	2wfw	B	66	2wfs	A	320	2wge	A	202
2wgp	B	108	2wgy	A	243	2wh7	A	106	2whg	B	117	2whl	A	187
2wi8	A	173	2wiy	A	277	2wj5	A	51	2wj9	B	94	2wje	A	158
2wji	B	42	2wjn	H	127	2wjn	C	169	2wjn	L	129	2wjn	M	161
2wjr	A	122	2wk0	A	168	2wk1	A	163	2wkk	C	101	2wkx	A	176
2wl1	A	93	2wl9	B	182	2wlr	A	269	2wlu	A	109	2wm3	A	186
2wm5	A	278	2wmf	A	432	2wmi	B	393	2wml	A	169	2wn3	C	199
2wn4	A	277	2wnh	A	236	2wnp	F	131	2wns	A	112	2wnv	A	80
2wnv	E	73	2wnv	F	91	2wnx	A	87	2wny	B	44	2wo1	A	84
2woe	C	159	2wol	A	383	2wot	A	203	2woy	A	231	2wp3	O	37
2wp7	A	74	2wpg	A	361	2wpq	C	66	2wpv	D	34	2wpv	E	172
2wq4	C	77	2wq9	A	107	2wqi	D	23	2wqk	A	127	2wr8	A	42
2wra	A	69	2wry	A	98	2wsb	C	126	2wsd	A	349	2wsh	B	48
2wsi	A	149	2wso	A	138	2wt1	A	101	2wt4	A	185	2wta	A	123
2wte	B	86	2wtg	A	105	2wtm	C	174	2wto	A	53	2wu6	A	231
2wu9	A	228	2wue	A	141	2wuh	A	87	2wuk	A	39	2wuq	B	162
2wut	A	73	2wuu	A	242	2wux	A	108	2wv3	A	31	2wvf	A	62

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2wvv	A	272	2wvx	C	484	2ww2	B	476	2ww5	A	307	2wwe	A	85
2wwf	C	128	2wwk	T	63	2wwx	A	120	2wwx	B	143	2wxu	A	178
2wy3	A	67	2wy3	B	81	2wy4	A	90	2wy7	Q	39	2wy8	A	192
2wyc	A	98	2wye	B	279	2wyh	B	623	2wyk	A	193	2wyu	B	31
2wz1	A	119	2wz8	A	81	2wz9	A	70	2wzb	A	270	2wzi	B	327
2wzm	A	169	2wzw	B	111	2wzx	A	232	2x0k	A	205	2x0q	A	350
2x18	E	76	2x1b	A	55	2x1d	D	204	2x1p	C	72	2x1q	B	69
2x23	B	174	2x26	B	151	2x2o	A	76	2x32	A	111	2x3c	A	133
2x3e	B	163	2x3f	A	158	2x3g	A	67	2x3h	C	328	2x3m	A	94
2x3n	A	198	2x45	A	93	2x47	A	160	2x49	A	197	2x4j	A	48
2x4k	B	40	2x4l	A	183	2x55	A	98	2x5c	B	20	2x5f	B	228
2x5h	B	41	2x5p	A	56	2x5x	A	217	2x5y	A	122	2x61	A	129
2x6u	A	68	2x6w	A	395	2x7b	A	86	2x7m	A	58	2x8h	A	406
2x8j	C	156	2x8r	A	128	2x8s	A	206	2x8x	X	2	2x96	A	218
2x98	B	248	2x9x	A	234	2xau	A	378	2xb1	C	52	2xb4	A	111
2xba	A	151	2xbk	A	178	2xbl	A	124	2xc2	A	61	2xc3	A	268
2xcb	A	59	2xce	F	73	2xcj	A	48	2xcz	A	71	2xda	A	83
2xde	A	77	2xdg	A	36	2xdj	F	31	2xdp	A	61	2xdw	A	514
2xed	A	141	2xeg	A	400	2xeh	A	44	2xet	B	67	2xeu	A	34
2xev	A	74	2xex	A	73	2xf2	A	451	2xf7	A	25	2xfe	A	74
2xfr	A	313	2xfv	A	61	2xgy	A	48	2xh2	C	242	2xhd	A	164
2xhi	A	183	2xhn	A	359	2xi9	B	152	2xij	A	358	2xio	A	187
2xiv	A	123	2xj3	A	45	2xjq	A	149	2xkg	A	63	2xkr	A	264
2xl8	A	55	2xla	A	155	2xlk	A	81	2xmj	A	37	2mxm	A	170
2xn4	A	151	2xn6	A	221	2xnq	A	52	2xoc	B	140	2xon	L	87
2xov	A	91	2xpp	A	91	2xq0	A	200	2xqo	A	133	2xqu	A	32
2xs4	A	113	2xst	A	74	2xsu	A	212	2xtp	A	131	2xw9	A	134
2xwc	A	128	2xws	A	86	2xwt	C	152	2xxj	D	135	2xxl	B	215
2xxz	A	152	2xy2	A	70	2xz2	A	34	2xzi	A	272	2xzv	A	117
2y1q	A	63	2y27	B	271	2y3z	A	148	2y44	A	86	2y5s	B	117
2y69	A	300	2y69	D	10	2y69	E	7	2y69	P	30	2y7b	A	69
2y88	A	126	2y8k	A	317	2y8m	A	86	2yay	A	40	2yb1	A	161
2yqc	A	275	2yqu	B	290	2yqz	A	134	2yr5	B	473	2yrx	A	150
2ysk	A	84	2yv1	A	134	2yv5	A	159	2yv7	A	90	2yv9	B	104
2yva	B	98	2yve	A	111	2yvi	A	56	2yvo	A	125	2yvt	A	163
2yw2	A	6	2ywd	A	101	2ywi	B	106	2ywj	A	110	2ywk	A	55
2ywl	A	95	2ywn	A	92	2ywo	A	108	2yxm	A	52	2yxn	A	185
2yxo	B	141	2yxw	A	173	2yxz	A	104	2yyh	C	26	2yyk	A	265
2yyv	B	97	2yz1	B	80	2yzc	D	165	2yzh	C	98	2yzk	B	77
2yzt	A	37	2yzu	A	42	2yzv	A	142	2yzy	A	88	2z0a	B	42
2z0e	A	115	2z0j	E	144	2z0m	A	178	2z0q	A	165	2z0t	C	63
2z0x	A	92	2z10	A	108	2z14	A	77	2z1a	A	283	2z1f	A	120
2z1n	A	137	2z1y	A	215	2z26	A	233	2z2f	A	85	2z2o	A	151
2z2y	A	204	2z38	A	169	2z3g	D	83	2z3v	A	76	2z48	A	289
2z4u	A	184	2z62	A	181	2z68	A	143	2z6i	A	163	2z6n	A	57
2z6o	A	99	2z6r	A	159	2z6w	A	101	2z72	A	204	2z7b	A	103
2z7f	E	139	2z7f	I	36	2z84	A	108	2z8a	A	96	2z8f	A	258
2z8l	A	121	2z8q	A	36	2z8u	B	52	2z8x	A	412	2z9b	A	130
2z9v	B	253	2za0	A	135	2zad	D	214	2zb7	A	208	2zbc	E	55
2zbl	A	298	2zbo	A	62	2zbt	B	134	2zbx	A	263	2zc8	A	191
2zca	A	76	2zcn	A	79	2zco	A	166	2zcn	A	85	2zd1	A	172
2zdh	A	173	2zdo	B	73	2zdr	A	212	2zed	A	228	2zex	A	108

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
2zez	B	64	2zf9	A	97	2zfd	A	133	2zfd	B	77	2zfg	A	191
2zfn	A	195	2zfy	A	126	2zfd	D	45	2zgd	A	46	2zfq	A	96
2zhj	A	190	2zhn	A	111	2zfh	C	98	2zib	A	82	2zjd	C	83
2zkg	A	119	2zkm	X	526	2zlg	B	203	2zm0	A	259	2zmu	A	113
2znd	A	121	2znr	A	130	2zo6	A	136	2zod	A	112	2zoo	A	256
2zos	A	117	2zou	B	88	2zpd	A	97	2zpm	A	44	2zpo	A	65
2zpu	A	166	2zqe	A	52	2zqm	A	61	2zqn	B	96	2zs0	A	86
2zs0	D	81	2zs1	B	65	2zs1	C	79	2zsc	B	61	2zsg	B	194
2zsh	B	22	2zsi	A	207	2zsj	D	137	2zu1	B	121	2zu2	A	146
2zut	C	494	2zux	B	391	2zuy	A	380	2zvp	X	210	2zw2	A	50
2zwa	B	329	2zwd	A	197	2zuj	A	109	2zwn	A	226	2zwu	A	214
2zx2	A	148	2zxj	B	6	2zxy	A	41	2zya	B	306	2zyh	B	291
2zyo	A	226	2zxd	C	158	2zxd	E	115	2zxd	J	85	2zzj	A	156
2zys	O	44	2zzv	B	204	3a02	A	34	3a03	A	36	3a04	A	110
3a07	A	88	3a0u	A	80	3a0y	B	101	3a1c	A	67	3a1u	A	132
3a21	A	426	3a2q	A	170	3a2v	I	152	3a2z	A	104	3a3d	B	274
3a3v	A	266	3a40	X	199	3a4u	A	156	3a4u	B	40	3a4w	B	216
3a55	A	180	3a57	A	114	3a5f	B	205	3a5p	D	70	3a5r	A	223
3a6r	B	73	3a6s	B	57	3a71	A	266	3a74	B	279	3a77	A	124
3a7i	A	140	3a7l	A	76	3a7n	A	129	3a8g	A	129	3a8g	B	140
3a8k	A	212	3a8u	X	294	3a9b	A	264	3a9f	A	58	3a9i	A	185
3a9l	B	127	3a9q	N	115	3a9s	B	353	3a9z	A	250	3aa0	A	159
3aa6	B	147	3aaf	B	15	3aal	A	188	3aam	A	139	3aar	A	220
3aay	B	159	3ab6	A	68	3ab8	A	134	3aba	A	262	3abd	B	110
3abf	E	21	3acd	A	88	3aci	A	136	3act	B	568	3acz	C	243
3adg	A	47	3ado	A	188	3adr	A	134	3aey	A	165	3afm	A	143
3afv	A	310	3ag7	A	67	3agn	A	80	3agx	B	49	3ah2	A	222
3ahc	A	570	3ahn	A	376	3ahx	D	280	3ahy	A	309	3ahz	A	349
3ai3	C	157	3aia	A	149	3aia	A	212	3aj7	A	462	3ajd	A	172
3ajo	A	117	3ajx	C	114	3ak2	B	155	3ak8	H	115	3akb	A	97
3akh	A	317	3alf	A	260	3alu	A	107	3amn	B	164	3anp	C	76
3ans	B	161	3ap9	A	106	3apa	A	91	3aq2	B	119	3b2t	B	193
3b2y	A	72	3b34	A	566	3b3t	A	187	3b42	A	60	3b49	A	137
3b4n	A	199	3b4q	B	41	3b4u	B	196	3b4w	A	249	3b4y	B	166
3b51	X	395	3b5e	B	107	3b5g	B	63	3b5l	B	136	3b5m	B	112
3b5o	A	109	3b64	A	78	3b6e	A	101	3b6h	A	294	3b6i	A	107
3b76	A	60	3b79	A	62	3b7c	A	60	3b7e	A	293	3b7l	A	119
3b7n	A	184	3b7o	A	175	3b7s	A	442	3b84	A	44	3b8b	A	138
3b8f	C	92	3b8i	E	157	3b8z	B	145	3b9c	C	84	3b9d	A	353
3b9q	A	175	3b9t	A	279	3b9y	A	216	3ba1	A	199	3ba3	A	87
3bal	B	92	3bb0	A	395	3bb7	A	191	3bb9	B	61	3bbb	D	96
3bby	A	123	3bc1	B	28	3bc1	E	120	3bc9	A	406	3bcb	A	280
3bcw	A	72	3bcy	A	105	3bd1	A	37	3bd2	A	76	3bde	A	69
3bdf	A	258	3bdi	A	114	3bdu	E	27	3bdv	A	105	3be4	A	116
3be6	C	181	3bec	A	209	3bed	B	65	3bei	A	17	3bem	A	110
3ber	A	139	3beu	B	129	3bex	A	166	3bf5	A	39	3bf7	B	147
3bfg	B	114	3bfm	A	93	3bfo	B	41	3bfq	G	74	3bfv	A	170
3bg8	A	145	3bge	A	82	3bgo	P	36	3bgu	B	48	3bgy	B	99
3bh4	A	280	3bh7	A	97	3bh7	B	181	3bhd	B	118	3bhg	A	213
3bhn	A	127	3bhq	A	106	3bhw	B	83	3bhy	A	171	3bio	A	180
3bit	A	248	3bix	A	299	3biy	A	4	3bj1	C	54	3bj1	D	78
3bjd	B	185	3bje	A	210	3bjh	A	1	3bjk	B	62	3bjn	A	82

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3bkj	H	154	3bkp	A	114	3bkr	A	89	3bkt	A	47	3bkw	B	104
3bkx	A	156	3bl6	A	127	3bld	A	210	3blz	B	79	3bm3	B	151
3bm7	A	56	3bmb	B	52	3bmw	A	526	3bmx	B	415	3bmz	B	111
3bn6	A	89	3bn7	A	65	3bnj	A	282	3bo5	A	156	3bo6	B	125
3bod	A	112	3boe	A	133	3bof	B	268	3bom	C	95	3bom	D	82
3bon	A	300	3bor	A	121	3bos	B	130	3bov	A	56	3bp1	B	147
3bp3	A	37	3bp5	A	70	3bpk	B	112	3bpt	A	228	3bpu	A	45
3bpv	A	68	3bpw	A	222	3bpz	D	137	3bq9	B	228	3bqp	B	43
3bqy	A	92	3br8	A	54	3brb	A	39	3brc	B	79	3bs1	A	81
3bs2	A	104	3bs3	A	37	3bs4	A	160	3bs6	A	150	3bs9	B	23
3bsn	A	245	3bsy	B	123	3bt5	A	76	3but	A	48	3buu	A	140
3buv	B	214	3bv6	D	220	3bv8	A	49	3bvk	F	123	3bwh	A	181
3bwl	B	74	3bws	B	250	3bwu	C	103	3bwu	D	51	3bwu	F	55
3bwv	B	100	3bwx	A	173	3bx4	A	82	3bx4	B	80	3bxu	B	157
3bxp	B	139	3by4	A	89	3by9	A	160	3byb	B	39	3byp	A	50
3byq	C	111	3bzh	A	54	3bzq	A	71	3bzw	A	148	3bzz	B	52
3c05	A	39	3c05	D	34	3c0c	A	10	3c0f	B	56	3c0i	A	123
3c18	A	104	3c1d	A	64	3c1o	A	145	3c1v	B	64	3c24	B	133
3c2u	A	392	3c37	B	108	3c3j	F	238	3c3m	A	72	3c3p	C	68
3c3y	B	68	3c4b	A	137	3c4s	A	31	3c4z	A	147	3c58	A	185
3c5a	A	175	3c5e	A	300	3c5j	A	104	3c5j	B	93	3c5k	A	72
3c5n	A	88	3c5y	L	91	3c61	D	189	3c65	A	75	3c68	B	404
3c6a	A	80	3c6c	A	172	3c6k	A	207	3c6v	B	92	3c6w	A	33
3c7f	A	318	3c7t	A	142	3c7x	A	110	3c85	C	57	3c8c	B	129
3c8e	A	193	3c8i	A	62	3c8l	B	57	3c8m	A	201	3c8o	A	88
3c8p	A	34	3c8u	A	94	3c8x	A	58	3c8z	A	253	3c97	A	58
3c9a	B	135	3c9f	B	217	3c9h	B	174	3c9p	A	82	3c9q	A	133
3c9u	B	158	3c9x	A	205	3c9z	A	150	3ca7	A	31	3cai	A	230
3can	A	98	3cb0	D	106	3cb6	A	257	3cbl	A	85	3cbn	A	81
3cbt	A	123	3cbw	B	239	3cbx	A	48	3cc6	A	145	3cc8	A	101
3ccd	B	53	3ccf	A	63	3ccg	A	95	3cck	A	73	3ccz	B	228
3ce1	A	91	3ce6	A	295	3ce7	A	66	3cec	A	41	3cet	B	171
3cfz	A	159	3cg1	A	186	3cg4	A	69	3cg6	A	46	3cgh	A	333
3cgi	C	57	3cgx	A	105	3ch0	A	180	3chk	A	181	3chm	A	89
3chv	A	148	3ci6	B	95	3ci7	A	30	3cij	A	181	3cim	C	47
3cin	A	162	3cit	B	77	3civ	A	184	3ciw	A	209	3cj1	A	258
3cj8	B	111	3cjd	A	94	3cje	A	73	3cjm	A	173	3cjm	A	75
3cjp	B	135	3cjs	A	38	3cjs	B	39	3cjj	A	133	3ck1	A	69
3ck6	B	127	3ckc	B	318	3ckf	A	150	3ckj	A	150	3ckk	A	119
3ckm	A	182	3cl5	A	245	3clm	A	225	3cls	C	137	3clv	A	112
3cm0	A	67	3cmb	D	154	3cmc	Q	175	3cmg	A	410	3cmj	A	306
3cn4	B	69	3cne	C	96	3cnh	A	73	3cnk	B	60	3cnr	B	30
3cnu	A	69	3cny	A	191	3co8	A	231	3cou	A	108	3cox	A	318
3cp0	A	31	3cp5	A	63	3cp7	B	134	3cpq	A	138	3cpq	B	50
3cps	B	193	3cpt	A	61	3cq0	A	200	3cq2	A	22	3cq5	B	228
3cqb	B	54	3cql	A	160	3cqt	A	39	3cqy	A	102	3crm	A	68
3crn	B	51	3cry	A	106	3csk	A	73	3css	A	173	3ct1	A	123
3ctg	A	72	3ctk	A	173	3ctp	B	164	3ctz	A	385	3cu0	A	119
3cu2	B	128	3cu4	A	42	3cu9	A	205	3cui	A	228	3cux	A	276
3cv1	A	396	3cvb	A	69	3cve	A	38	3cvo	C	85	3cwr	B	90
3cwv	A	126	3cww	A	545	3cx5	E	42	3cx5	F	3	3cx5	G	36
3cx5	I	7	3cx5	O	100	3cxk	A	77	3cxm	A	156	3cxn	B	133

Continued on next page



PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3cy4	A	100	3cyi	A	68	3cyp	B	74	3czf	B	70	3czt	X	57
3czx	B	116	3czz	B	74	3d00	A	20	3d01	D	91	3d03	B	178
3d06	A	108	3d0c	B	108	3d0f	A	56	3d0j	A	71	3d0k	A	149
3d0n	A	167	3d0o	A	187	3d1b	C	75	3d1g	A	153	3d1k	A	98
3d1p	A	63	3d1r	A	154	3d22	A	81	3d2l	B	89	3d2q	A	50
3d2w	A	51	3d30	A	85	3d32	A	78	3d33	B	55	3d34	A	116
3d3b	A	70	3d3r	A	32	3d3s	D	52	3d3y	A	169	3d3z	A	140
3d40	A	153	3d43	B	138	3d47	A	243	3d4e	A	94	3d4i	A	143
3d4u	A	192	3d59	A	187	3d5p	A	74	3d6i	B	75	3d6r	A	65
3d79	A	114	3d7a	B	60	3d7i	B	45	3d7j	D	78	3d85	C	39
3d8t	A	116	3d9n	B	95	3d9t	A	64	3d9x	C	65	3d9y	A	66
3da0	C	93	3da8	A	132	3dac	A	48	3dai	A	69	3dal	A	108
3dan	A	260	3dao	A	153	3daq	A	221	3das	A	182	3dau	A	95
3db7	A	80	3dbk	A	178	3dbo	B	63	3dc5	C	129	3dc8	B	318
3dcd	B	207	3dcn	A	108	3dcy	A	136	3dcz	A	98	3dd6	A	117
3dd7	C	68	3ddj	A	147	3ddl	B	52	3ddq	B	183	3dds	B	487
3def	A	120	3del	B	141	3deo	A	100	3dew	A	88	3df7	A	161
3df8	A	61	3dff	A	152	3dfg	A	81	3dfq	A	183	3dg3	A	217
3dgb	A	208	3dgp	A	41	3dgp	B	43	3dgt	A	188	3dha	A	155
3dhf	B	320	3dhi	B	203	3dhi	C	44	3dho	C	146	3dhp	A	352
3di4	B	181	3die	A	55	3dj9	A	59	3dje	B	267	3djl	A	308
3djo	A	85	3dk9	A	275	3dkc	A	197	3dkm	A	51	3dkr	A	158
3dl0	A	139	3dlc	A	138	3dlm	A	126	3dlq	I	66	3dlq	R	91
3dlv	A	32	3dm8	A	78	3dmc	A	88	3dme	B	194	3dmg	A	224
3dmi	A	54	3dmo	A	83	3dms	A	255	3dn7	B	77	3dnf	B	119
3dnh	B	36	3dnp	A	144	3dnu	A	215	3do8	A	81	3dou	A	95
3dpg	B	136	3dpk	A	84	3dqg	A	87	3dqp	A	148	3dqy	A	60
3dr0	C	47	3dr4	B	137	3dr6	B	101	3dra	A	206	3dra	B	223
3drw	B	225	3drz	B	42	3ds4	B	54	3ds8	A	160	3dsb	B	108
3dsk	A	315	3dso	A	31	3dt5	A	24	3dt9	A	130	3dtb	A	393
3dtt	A	129	3dtz	C	131	3dup	A	160	3dur	B	73	3duw	A	112
3dv9	A	132	3dvw	A	134	3dwg	A	197	3dwg	C	51	3dwv	B	91
3dxl	A	204	3dxs	X	38	3dxt	A	203	3dxz	A	128	3dy0	A	156
3dyj	A	153	3dz1	A	152	3dz4	B	43	3dza	A	101	3dzw	A	69
3dzz	A	215	3e02	A	110	3e03	A	150	3e05	B	65	3e0e	A	49
3e0h	A	55	3e0i	A	172	3e0x	A	171	3e0z	A	64	3e11	B	72
3e13	X	225	3e17	B	49	3e18	B	152	3e23	A	105	3e2d	A	341
3e2v	B	256	3e39	B	112	3e3m	D	189	3e3u	A	122	3e48	A	141
3e49	A	134	3e4g	A	116	3e4v	A	118	3e4w	B	143	3e55	A	106
3e57	A	88	3e58	A	142	3e5h	A	104	3e5u	A	108	3e6j	A	149
3e6q	G	70	3e6s	F	88	3e6z	X	48	3e7d	A	99	3e7h	A	67
3e7r	L	23	3e8o	B	67	3e8t	A	128	3e96	B	188	3e97	A	106
3e99	A	73	3e9a	A	157	3e9f	A	57	3e9k	A	285	3e9t	B	73
3e9v	A	66	3ea3	B	184	3ea6	A	99	3eau	A	164	3eaz	A	74
3ebb	B	144	3ebh	A	611	3ebl	A	180	3ebt	A	85	3ebv	A	188
3eby	A	85	3ec0	B	63	3ec3	B	117	3ec4	B	109	3ec6	A	70
3ec9	B	70	3ecd	A	235	3ecf	B	74	3ech	A	80	3ecy	B	14
3ed4	B	243	3ed5	A	111	3ed7	A	111	3edf	A	390	3edg	A	133
3edn	A	184	3edo	B	104	3eds	A	80	3edv	A	184	3ee4	A	172
3eea	B	92	3eeh	A	56	3ees	A	32	3eet	A	66	3ef2	B	205
3ef4	A	70	3ef6	A	188	3ef8	A	96	3efy	A	112	3eg4	A	156
3ega	A	136	3egg	A	176	3egg	D	32	3ego	B	105	3egw	C	117

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3eh1	A	400	3ehe	B	125	3ehg	A	77	3ehw	B	85	3ei9	B	294
3eif	A	471	3ein	A	139	3eix	A	189	3eiz	A	106	3ej9	B	33
3ej9	C	38	3eja	A	145	3ejf	A	125	3ejg	A	114	3ejk	A	83
3eju	A	742	3ejv	A	89	3ek2	A	161	3ek3	A	109	3eki	A	222
3eko	B	142	3elf	A	183	3elg	B	63	3elj	A	213	3elk	A	39
3els	A	75	3elw	A	159	3elx	A	76	3em1	A	96	3emi	A	70
3emr	A	140	3emw	A	108	3en0	C	159	3en8	A	72	3enk	B	125
3enu	A	70	3eo7	A	276	3eo8	F	158	3eod	A	4	3eof	A	131
3eoi	A	73	3eoj	A	187	3epr	A	192	3epx	A	212	3eqn	B	494
3eqx	A	214	3er6	A	87	3era	B	34	3erb	A	119	3erj	A	56
3erp	B	160	3erx	B	79	3es1	A	106	3es4	A	65	3esg	B	107
3esl	B	123	3esm	A	69	3ess	A	143	3etf	C	253	3etn	A	115
3etv	A	190	3eu9	C	102	3eua	D	204	3euf	D	153	3eul	A	64
3eun	A	45	3eup	B	115	3eur	A	76	3evf	A	144	3evk	D	70
3evy	B	8	3ew0	A	55	3ew1	D	85	3ew8	A	187	3ewh	A	213
3ewi	A	62	3ewj	A	145	3ewn	A	112	3ewy	A	163	3exe	D	224
3exn	A	88	3exr	A	152	3ey6	A	81	3ey8	B	68	3eye	A	91
3eyg	A	152	3eyi	A	44	3eyp	B	11	3eyt	D	86	3ezi	B	47
3f09	A	42	3f0d	F	82	3f0h	A	218	3f0i	A	82	3f0n	B	181
3f0y	C	149	3f1p	B	1	3f2e	A	42	3f2k	A	123	3f2u	A	25
3f2z	A	107	3f3e	A	164	3f3k	B	197	3f3q	A	67	3f3x	A	62
3f3z	A	155	3f40	A	55	3f42	B	35	3f43	A	69	3f44	A	120
3f47	A	171	3f4m	A	66	3f4s	A	101	3f52	A	42	3f5h	B	20
3f5l	B	342	3f5o	G	65	3f5v	B	137	3f67	A	130	3f6c	B	70
3f6d	B	125	3f6o	A	56	3f6q	A	116	3f6q	B	47	3f6v	A	58
3f6w	C	27	3f6y	A	164	3f74	B	121	3f75	A	131	3f75	P	46
3f7e	A	81	3f7l	A	95	3f7q	A	112	3f7w	A	133	3f7x	A	69
3f8d	B	182	3f8k	A	61	3f8m	B	103	3f8t	A	224	3f8x	D	78
3f95	B	94	3f9b	A	197	3f9r	A	136	3f9s	B	80	3faj	A	49
3fan	A	103	3fau	A	41	3fb9	A	52	3fbg	A	197	3fbl	A	49
3fbu	B	96	3fc0	B	58	3fcd	B	56	3fcp	D	137	3fcx	B	178
3fd3	A	112	3fd7	B	77	3fdb	A	26	3fde	B	131	3fdh	A	265
3fdj	A	155	3fdl	A	98	3fdq	A	71	3fdr	A	56	3fdx	A	73
3fe0	A	86	3fe4	B	141	3fe7	A	59	3fed	A	433	3fes	A	72
3fev	A	43	3ff0	B	74	3ff1	B	297	3ff2	A	49	3ff5	B	35
3ff7	C	69	3ff9	B	54	3ffr	A	218	3fg0	F	309	3fg1	D	386
3fg8	A	56	3fg9	E	106	3fgd	A	207	3fge	A	99	3fgr	A	100
3fgv	A	54	3fgy	B	71	3fh1	A	58	3fh2	A	85	3fh9	A	105
3fhd	A	261	3fhf	A	108	3fhg	A	78	3fh1	C	120	3fhw	B	48
3fi9	B	89	3fia	A	56	3fid	A	185	3fil	B	36	3fiq	A	102
3fiu	D	135	3fj1	A	197	3fj2	A	99	3fjs	C	50	3fju	B	55
3fjv	A	98	3fk8	A	76	3fka	A	67	3fkb	E	97	3fkc	A	64
3fkr	B	160	3fl2	A	59	3flb	A	105	3flg	A	82	3fm0	A	212
3fm2	A	75	3fmb	B	58	3fmc	A	222	3fmk	A	239	3fmu	A	1
3fmy	A	36	3fn2	B	36	3fn5	A	101	3fn8	B	25	3fnc	A	97
3fo3	A	384	3fo8	D	152	3fob	B	170	3foj	A	57	3fot	A	321
3fp2	A	175	3fp5	A	67	3fpc	A	223	3fpf	A	179	3fpk	B	145
3fpq	B	144	3fpr	D	38	3fpu	B	35	3fpw	A	77	3fpz	B	192
3fq3	C	118	3fq4	A	68	3fqm	A	58	3fr7	A	299	3frh	A	154
3frq	A	112	3frr	A	94	3fs2	B	120	3fs5	A	79	3fs7	A	57
3fsd	A	60	3fse	A	52	3fss	A	127	3fsy	A	129	3ft1	C	57
3ftd	A	132	3ftt	A	123	3fu1	A	72	3fuc	C	147	3fut	A	159

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3fv3	G	230	3fv5	A	99	3fv9	G	226	3fvb	B	110	3fvh	A	148
3fvu	B	296	3fvy	A	465	3fw2	B	80	3fw3	A	165	3fwa	A	310
3fwh	A	190	3fwy	A	172	3fwz	B	81	3fx4	A	191	3fx7	A	58
3fxg	F	225	3fxh	A	41	3fxq	A	170	3fxz	A	163	3fy1	B	250
3fy3	A	43	3fyb	A	56	3fym	A	56	3fyn	A	75	3fyq	A	74
3fz4	A	66	3fza	A	80	3fze	A	77	3g00	A	175	3g02	B	256
3g08	A	159	3g0e	A	227	3g0k	A	85	3g0m	A	71	3g0o	A	141
3g0t	B	304	3g14	A	102	3g16	A	102	3g1j	B	45	3g1l	A	113
3g1v	A	133	3g1z	A	175	3g20	B	81	3g23	A	163	3g25	A	277
3g26	A	49	3g2b	A	51	3g2s	B	84	3g36	C	33	3g39	A	104
3g3s	B	110	3g3t	A	146	3g48	A	74	3g51	A	140	3g5j	B	86
3g5p	D	117	3g5r	A	226	3g5t	A	5	3g5w	C	215	3g66	A	109
3g68	A	232	3g6k	F	213	3g6m	A	258	3g7d	A	207	3g7g	E	72
3g7n	B	166	3g7r	B	110	3g7u	A	137	3g7w	A	245	3g85	A	132
3g89	B	121	3g8h	A	86	3g8y	A	232	3g8z	A	69	3g98	B	43
3g9a	B	77	3g9k	L	138	3g9m	B	24	3ga3	A	91	3ga4	A	78
3ga7	A	153	3gad	F	83	3gag	B	124	3gah	A	120	3gas	E	132
3gay	B	128	3gaz	B	153	3gba	D	174	3gbe	A	355	3gbs	A	104
3gbw	A	101	3gbz	A	121	3gc6	A	144	3gcz	A	162	3gd6	A	169
3gd8	A	122	3gdc	A	191	3gdl	B	155	3gdp	B	334	3ge3	A	324
3ge3	E	58	3ge5	B	115	3ge6	A	122	3ged	A	114	3gef	A	67
3gem	C	127	3geu	D	59	3gf3	A	362	3gf6	B	144	3gfa	A	111
3gfu	A	83	3gfv	A	132	3gg2	D	229	3gg7	A	158	3gg9	B	83
3ggw	B	133	3ggw	C	175	3gh5	A	358	3gh6	A	147	3ghd	A	40
3ghj	A	55	3gi7	B	44	3gip	A	269	3gir	A	207	3giu	A	130
3giw	A	164	3gj0	B	116	3giu	A	293	3gjy	A	167	3gk6	A	45
3gk7	B	287	3gkb	C	160	3gkj	A	140	3gkm	A	89	3gkr	A	231
3gkt	A	72	3gkv	B	83	3gl0	A	159	3gl1	B	234	3gl9	C	78
3glr	A	143	3glv	B	63	3gmf	A	84	3gmg	A	82	3gmi	A	202
3gms	A	188	3gmv	X	87	3gmx	B	94	3gn6	B	167	3gne	A	145
3gnl	B	148	3gnr	A	322	3gnz	P	120	3go2	A	265	3go5	A	182
3go6	A	150	3go9	A	304	3goa	B	214	3goc	B	115	3goh	A	142
3gon	A	178	3gox	B	125	3gp3	D	145	3gp4	B	78	3gp7	A	155
3pgp	B	99	3gpi	A	162	3gpk	B	54	3gpu	A	157	3gqh	A	73
3gqj	A	149	3gqq	A	91	3gqv	A	201	3gr3	B	140	3grd	B	71
3grh	A	248	3grn	A	57	3gru	A	43	3gs2	A	57	3gs9	A	180
3gsh	A	50	3gt2	A	56	3gt5	A	243	3gt9	B	52	3gue	A	267
3gux	B	144	3guy	B	110	3gv6	A	33	3gve	A	214	3gvq	B	158
3gvl	A	464	3gvo	A	210	3gw9	C	246	3gwa	A	207	3gwb	A	148
3gwc	D	143	3gwh	B	49	3gwi	A	118	3gwk	E	64	3gwm	A	2
3gwn	A	73	3gwo	A	24	3gwz	A	191	3gx8	A	55	3gxb	A	85
3gxh	B	82	3gxr	B	108	3gy1	A	253	3gy9	A	85	3gyb	A	153
3gyc	B	218	3gyd	B	90	3gyk	B	97	3gyl	B	160	3gza	A	287
3gzb	A	100	3gzg	A	119	3gzh	A	275	3gzk	A	321	3gzs	B	92
3gzs	A	283	3gzx	B	126	3h04	A	164	3h05	A	104	3h08	A	71
3h09	B	610	3h0n	A	120	3h0o	A	158	3h0u	C	176	3h11	A	76
3h12	B	252	3h14	A	171	3h1d	A	166	3h1g	A	92	3h1n	A	137
3h1s	B	138	3h1w	A	239	3h20	A	38	3h2d	B	70	3h2g	A	218
3h2s	B	117	3h2z	A	210	3h34	A	40	3h36	A	32	3h3h	B	57
3h3l	B	94	3h3n	X	156	3h41	A	202	3h49	B	132	3h4i	A	244
3h4n	A	32	3h4o	A	125	3h4x	A	187	3h50	A	72	3h51	B	71
3h55	B	205	3h5i	A	41	3h5j	B	91	3h5l	B	268	3h5n	D	198

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3h5q	A	240	3h62	B	213	3h6p	B	36	3h6p	C	30	3h6x	C	69
3h70	A	196	3h74	A	182	3h78	A	185	3h7a	A	97	3h7c	X	225
3h7f	B	288	3h7h	A	73	3h7h	B	71	3h7i	A	194	3h7o	B	124
3h7r	A	196	3h7u	A	215	3h81	C	149	3h87	B	5	3h87	D	32
3h8g	C	274	3h8u	B	57	3h8x	A	104	3h8z	A	46	3h91	A	32
3h93	A	90	3h95	A	87	3h9c	A	379	3h9e	O	220	3h9m	A	255
3h9u	C	280	3h9w	A	46	3ha2	A	101	3ha9	A	97	3hap	A	130
3hbd	A	118	3hbg	A	205	3hbn	A	199	3hbv	P	224	3hbw	B	58
3hc1	A	122	3hc3	L	142	3hcj	A	101	3hcn	B	177	3hcz	A	88
3hd4	A	57	3hdc	A	98	3hdf	B	60	3hdj	B	168	3hdl	A	156
3hdo	B	195	3hdx	A	315	3he8	B	90	3hef	B	56	3hfo	A	45
3hfq	A	215	3hft	A	108	3hfw	A	212	3hg3	B	245	3hgb	A	74
3hgl	A	37	3hgm	A	54	3hgu	A	120	3hh1	A	59	3hh7	A	47
3hh8	A	172	3hhi	B	188	3hhp	D	174	3hhs	A	468	3hhs	B	450
3hht	A	156	3hht	B	159	3hi7	B	506	3hid	A	260	3his	A	174
3hj4	B	233	3hjb	A	334	3hje	A	477	3hjr	A	377	3hjs	A	135
3hjb	B	150	3hjb	A	213	3hk1	A	94	3hk4	C	36	3hko	A	169
3hkw	A	363	3hcx	A	10	3hl0	B	166	3hl1	A	104	3hl5	B	57
3hlx	A	164	3hlz	B	173	3hm4	B	92	3hmc	A	116	3hms	A	40
3hmz	A	124	3hn0	A	141	3hn3	B	262	3hn5	B	133	3hn7	A	277
3hnb	M	90	3hnt	H	142	3hnx	A	68	3ho6	A	136	3hog	A	54
3hoi	A	92	3hol	A	283	3hp4	A	114	3hp7	A	162	3hpc	X	87
3hpw	A	65	3hq1	B	356	3hq9	B	190	3hqc	A	65	3hqx	A	76
3hr0	A	160	3hr7	A	88	3hra	A	125	3hrl	A	60	3hrp	A	246
3hrq	B	147	3hrv	A	67	3hrx	A	126	3hs3	A	164	3hsa	A	67
3hsh	A	32	3hsr	D	62	3hss	B	155	3hsv	A	88	3ht1	A	94
3ht5	A	210	3htl	X	254	3htn	C	86	3htw	A	125	3hty	O	26
3hu5	A	113	3huh	A	73	3huu	B	89	3hv2	B	85	3hvi	A	139
3hvu	C	77	3hvv	A	97	3hvw	A	81	3hwu	A	82	3hx3	A	118
3hx8	D	69	3hx9	A	49	3hxa	F	49	3hxd	A	72	3hxf	B	179
3hxi	A	127	3hxl	A	166	3hxs	B	30	3hxt	A	103	3hxx	A	255
3hyn	A	123	3hyq	A	64	3hz2	A	49	3hz6	A	290	3hzb	E	53
3hzb	A	57	3i06	A	132	3i09	A	3	3i0w	A	181	3i0y	A	74
3i0z	B	252	3i10	A	182	3i11	A	129	3i1a	A	157	3i1j	A	144
3i1u	A	219	3i24	A	88	3i26	D	291	3i2n	A	42	3i2v	A	83
3i2z	A	44	3i31	A	19	3i33	A	247	3i35	A	36	3i36	A	153
3i3f	B	85	3i3g	A	70	3i45	A	243	3i47	A	186	3i48	B	159
3i4g	A	342	3i4j	D	150	3i4o	B	36	3i4q	A	97	3i4s	A	81
3i4z	B	61	3i57	B	110	3i5c	B	42	3i5r	A	47	3i5x	A	322
3i6c	A	74	3i6i	A	181	3i6t	B	226	3i6y	A	154	3i7m	A	82
3i7u	B	61	3i83	B	119	3i8s	C	128	3i95	A	149	3i96	A	66
3ia1	B	80	3ia2	F	170	3ia4	D	104	3ia7	B	162	3ia8	B	78
3ian	A	208	3iar	A	245	3iav	A	239	3ib0	A	208	3ib5	A	195
3ib7	A	199	3ibo	A	77	3ibw	A	41	3ibz	A	94	3ic3	B	53
3ic4	A	55	3icc	B	150	3ich	A	126	3icj	A	64	3ics	A	151
3idl	A	41	3id7	A	241	3ida	A	378	3idu	A	50	3idw	A	1
3ie4	A	59	3ie5	A	79	3ie7	A	135	3iee	A	144	3iei	C	191
3iev	A	164	3ifd	A	2	3ife	A	238	3ig9	C	25	3igh	X	106
3igs	A	128	3igx	B	175	3igz	B	324	3ihs	A	46	3iht	A	107
3ihu	A	105	3ihv	A	384	3ihz	B	81	3ii7	A	182	3ii9	A	219
3iib	A	262	3iii	A	392	3iij	A	116	3iiu	M	81	3ij3	A	263
3ijl	A	216	3ijw	A	134	3ik7	D	84	3ikb	B	132	3ikw	A	220

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3il9	B	190	3ilo	A	84	3ilw	A	256	3im1	A	172	3im6	A	77
3im9	A	206	3imf	B	96	3imh	A	230	3imk	A	97	3imo	B	24
3ing	A	165	3io3	A	120	3iof	A	145	3ioh	A	191	3ioq	A	120
3iox	A	265	3ioy	B	12	3ip4	A	267	3ip8	A	146	3ipc	A	211
3ipf	A	21	3ipi	A	107	3ipw	A	173	3iq0	A	134	3iq1	D	101
3iq2	B	95	3iq3	A	7	3iqi	X	197	3iql	A	40	3iqt	A	85
3ir3	B	45	3ir4	A	136	3ir8	A	141	3irb	A	70	3irp	X	303
3irv	A	143	3is6	A	138	3isa	B	121	3isg	A	135	3iso	A	150
3isq	A	265	3isr	A	173	3ist	B	139	3isu	A	47	3isx	A	187
3it3	B	210	3it4	B	135	3it4	C	107	3itd	A	163	3itf	B	70
3itq	A	129	3iu0	A	189	3iu1	A	263	3iu4	H	117	3iu5	A	77
3iu6	A	99	3iu7	A	203	3iuj	A	309	3iuk	A	343	3iuo	B	69
3iup	A	205	3ius	B	133	3iuw	A	36	3iux	A	59	3iuz	A	190
3iv0	A	266	3iv4	A	48	3ive	A	325	3iwf	B	65	3iwl	A	39
3iuv	B	66	3ix3	B	95	3ixc	A	95	3ixq	D	122	3ixr	A	100
3jpb	B	137	3jq0	A	320	3jq1	B	328	3jqd	A	129	3jqj	C	49
3jql	A	83	3jqu	A	55	3jqy	C	126	3jr2	C	138	3jrr	B	100
3jrv	A	92	3js4	B	138	3js5	A	113	3js8	A	322	3jsc	A	63
3jst	B	206	3jsr	A	52	3jsy	B	107	3jsz	A	323	3jte	A	34
3jtx	B	265	3jtz	A	51	3ju2	A	57	3ju3	A	62	3ju5	D	217
3ju8	B	140	3jub	A	106	3jun	A	77	3juu	A	182	3jva	F	182
3jve	A	65	3jvm	A	74	3jwg	A	86	3jx9	B	80	3jxg	B	136
3jxo	A	47	3jxs	A	109	3jxy	A	172	3jyg	A	105	3jzl	A	221
3k01	A	253	3k0b	A	249	3k0z	A	88	3k11	A	258	3k12	F	75
3k1h	A	70	3k1t	A	270	3k1u	A	199	3k1w	B	174	3k1z	A	151
3k21	A	80	3k26	A	250	3k2a	A	39	3k2c	B	112	3k2o	A	167
3k2v	B	69	3k2w	E	120	3k2z	A	129	3k31	A	156	3k3c	D	60
3k3k	A	43	3k3t	A	85	3k3v	A	56	3k40	B	219	3k4i	A	120
3k4w	H	150	3k59	A	403	3k5j	A	127	3k62	A	206	3k69	A	91
3k6f	A	69	3k6g	C	34	3k6i	A	65	3k6m	A	299	3k6q	B	79
3k6v	A	204	3k6y	A	148	3k7f	B	334	3k7p	B	94	3k89	A	172
3k8d	A	112	3k8g	A	126	3k8u	A	75	3k8w	A	174	3k9o	A	127
3k9r	B	33	3k9w	A	102	3ka4	A	118	3ka5	A	25	3ka7	A	234
3kao	A	209	3kax	A	190	3kbb	A	110	3kbf	A	90	3kbg	A	94
3kbr	A	76	3kby	A	105	3kc2	B	219	3kcc	A	79	3kcg	H	124
3kci	A	208	3kcp	A	136	3kd3	A	156	3kd6	B	134	3kda	A	198
3kde	C	38	3kdf	A	42	3kdf	D	34	3kdw	A	125	3ke4	A	88
3ke7	B	75	3keb	B	115	3kef	B	141	3keo	B	133	3kep	B	77
3kev	A	49	3kez	B	288	3kfa	A	209	3kfi	A	87	3kfo	A	116
3kfq	C	40	3kg0	C	63	3kg4	A	69	3kg9	B	143	3kgd	B	141
3kgk	A	56	3kgw	B	244	3kgy	B	120	3kgz	B	83	3kh1	A	120
3kh7	A	105	3khe	A	90	3khf	B	65	3khi	A	105	3khy	A	163
3ki8	A	172	3kij	C	106	3kiz	A	233	3kjd	B	226	3kjq	A	109
3kji	A	67	3kk4	B	76	3kkb	A	59	3kkf	A	67	3kkg	A	90
3kki	A	234	3kkq	A	138	3kky	A	97	3kkz	A	138	3kl0	B	282
3kl6	B	36	3klb	A	85	3klk	A	553	3klq	A	48	3klr	A	50
3km5	B	120	3kmi	A	74	3kmt	C	66	3kmu	A	157	3kmv	D	93
3knv	A	40	3ko8	A	148	3kog	A	125	3kol	A	78	3kom	A	393
3kop	D	96	3kor	D	66	3kos	A	111	3kp8	A	55	3kpb	D	69
3kpe	A	28	3kq0	A	83	3kqf	D	129	3kqi	A	47	3kqr	A	139
3kre	A	177	3krr	A	187	3kru	A	240	3ks6	B	145	3ks9	A	101
3ksh	A	91	3ksm	B	163	3ksv	A	60	3ksx	A	124	3kt7	A	369

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3kt9	A	64	3kta	B	88	3kta	C	84	3ktc	B	188	3kto	B	47
3ktz	A	135	3ku3	B	75	3kus	B	46	3kuu	C	98	3kuv	A	79
3kv0	A	69	3kv1	A	85	3kvc	A	299	3kvh	A	118	3kwe	A	92
3kwk	A	101	3kwl	A	332	3kwo	C	74	3kwr	A	50	3kws	A	171
3kwu	A	77	3kxq	B	150	3kxt	A	18	3kxw	A	336	3kya	A	312
3kyj	A	68	3kyj	B	51	3kyz	A	66	3kz5	A	28	3kz7	A	57
3kzd	A	53	3kzj	A	74	3kzn	A	192	3kzu	B	258	3kzx	A	134
3l00	A	90	3l07	B	177	3l0l	B	158	3l0q	B	289	3l12	A	174
3l18	A	124	3l1e	A	67	3l1n	A	89	3l1v	B	55	3l1w	F	145
3l23	A	154	3l29	A	76	3l2c	A	55	3l2h	D	104	3l32	A	33
3l39	A	136	3l3b	A	73	3l3f	X	204	3l41	A	153	3l4a	A	75
3l4e	A	94	3l4h	A	62	3l4n	A	69	3l4p	A	536	3l4r	A	104
3l51	A	86	3l51	B	78	3l52	A	162	3l55	B	205	3l5a	A	235
3l5e	B	265	3l5i	A	132	3l6b	A	197	3l6d	B	125	3l6g	A	150
3l6n	A	135	3l6t	A	53	3l77	A	139	3l7h	B	42	3l7o	A	135
3l7t	B	51	3l7x	A	80	3l80	A	99	3l81	A	122	3l84	A	423
3l8a	B	253	3l8d	A	92	3l8h	B	113	3l9a	X	47	3l9c	B	125
3l9f	D	98	3l9q	A	94	3l9s	A	123	3l9u	A	125	3l9w	B	156
3l9y	B	75	3la7	B	57	3laa	A	100	3lab	A	101	3lae	A	32
3lag	A	62	3las	B	114	3lat	A	129	3lb2	A	53	3lb5	A	83
3lbe	D	78	3lbf	C	30	3lbl	A	59	3lbm	B	194	3lc0	A	155
3lcc	A	143	3ld3	A	112	3ld7	B	53	3ldc	A	53	3ldg	A	175
3ldu	A	143	3ldv	B	128	3le0	A	88	3le3	A	57	3le4	A	35
3lec	A	140	3led	A	230	3leq	A	40	3let	A	119	3lew	A	311
3lez	A	144	3lf3	A	123	3lf5	B	53	3lf6	B	22	3lfh	F	39
3lfj	B	101	3lfk	C	60	3lfr	A	76	3lft	A	176	3lg3	A	232
3lg5	A	208	3lgb	B	112	3lgi	A	122	3lgn	A	77	3lh4	A	68
3lhe	A	63	3lhi	A	127	3lhn	A	65	3lho	A	146	3lhq	A	120
3lhr	B	53	3lhx	B	145	3li5	A	183	3li9	A	155	3lid	B	170
3lij	A	109	3liy	A	47	3ljq	A	162	3lju	X	244	3ljw	B	81
3lk5	A	132	3lk7	A	273	3lke	A	112	3lkm	A	155	3lkt	B	124
3lkt	Q	170	3ll5	B	108	3ll7	A	219	3llb	A	53	3llc	A	132
3llo	A	81	3llp	B	281	3llv	A	76	3llx	A	199	3lm2	B	111
3lm3	A	265	3lm4	D	172	3lm7	B	172	3lma	B	130	3lmd	A	105
3lmp	A	126	3lmz	A	154	3ln3	A	199	3lnc	B	90	3lny	A	39
3lo8	A	6	3log	C	185	3lop	A	195	3lot	C	192	3lou	C	156
3lp6	C	87	3lpc	A	217	3lpe	B	20	3lpe	G	13	3lpw	B	125
3lpz	A	153	3lq4	B	293	3lqb	A	135	3lqs	A	186	3lqw	A	75
3lqx	A	22	3lr2	A	58	3lr4	A	62	3lrt	A	161	3lru	B	76
3ls0	A	63	3ls6	A	126	3ls9	A	293	3lsn	A	139	3lss	A	102
3lsu	B	121	3lsz	D	99	3lt6	F	32	3ltj	A	77	3luc	A	83
3luf	B	136	3lui	B	71	3lul	A	167	3lum	D	190	3lur	B	93
3lus	B	69	3luu	A	42	3lv0	A	114	3lv8	A	105	3lvf	P	127
3lvu	D	134	3lvz	A	170	3lw0	B	187	3lw6	A	138	3lwa	A	87
3lwc	A	40	3lwd	A	125	3lwg	B	81	3lwk	A	99	3lwx	A	106
3lwz	A	71	3lx3	A	99	3lx4	B	196	3lx5	A	167	3lxl	A	177
3lxp	A	183	3lxq	B	208	3lxr	A	128	3lxr	F	126	3lxs	A	152
3lxy	A	181	3lxz	A	137	3ly0	B	220	3ly1	C	220	3ly7	A	212
3lyd	A	86	3lyf	D	119	3lyg	A	78	3lyh	A	57	3lyl	B	92
3lyp	B	125	3lyy	A	55	3lz5	A	205	3lza	B	90	3lzk	C	59
3lzo	B	67	3lzw	A	186	3m07	A	327	3m0f	A	124	3m0j	A	160
3m0m	B	272	3m0r	A	10	3m0s	A	29	3m19	A	143	3m1h	B	112

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3m1t	A	128	3m1u	A	247	3m21	D	23	3m2o	A	80	3m2r	D	360
3m2r	E	269	3m31	A	89	3m32	C	167	3m3h	A	96	3m3m	A	141
3m3p	A	173	3m4a	A	184	3m4d	A	140	3m4i	A	49	3m58	A	158
3m5k	B	99	3m5m	B	115	3m5q	A	229	3m5v	A	158	3m66	A	133
3m6b	A	182	3m6j	A	77	3m6u	A	240	3m6z	A	175	3m70	A	89
3m73	A	200	3m7a	A	87	3m7k	A	31	3m7o	A	53	3m7q	B	40
3m84	A	173	3m86	B	56	3m8j	A	64	3m8o	H	119	3m8u	A	329
3m97	X	68	3m9l	A	114	3m9q	B	59	3mab	A	51	3man	A	185
3mao	A	65	3maz	A	54	3mb4	B	44	3mb5	A	174	3mbg	B	62
3mbk	B	178	3mbx	H	135	3mc1	A	103	3mc4	B	143	3mcb	B	3
3mcq	A	147	3mcw	B	117	3mcx	A	321	3mcz	B	198	3md1	A	51
3md7	A	190	3md9	A	149	3mdm	A	273	3mdo	B	192	3mdp	A	62
3mdq	A	177	3mdu	A	264	3mdx	A	83	3me5	A	7	3me7	B	107
3mea	A	115	3meb	B	290	3mf7	A	74	3mfd	A	177	3mfi	A	346
3mg1	B	144	3mgd	A	75	3mgi	B	115	3mgn	B	22	3mgw	A	103
3mh9	A	99	3mhg	C	209	3mhr	A	135	3mhs	A	195	3mhs	B	9
3mhw	U	167	3mhy	C	61	3mhz	A	291	3mil	A	163	3mio	A	115
3miy	B	148	3mjd	A	112	3mjf	A	239	3mjo	B	200	3mjv	B	253
3mk1	A	288	3mk6	C	162	3mkc	A	197	3mkh	B	198	3mkk	B	439
3mm6	A	159	3mm6	B	210	3mmg	A	152	3mmh	B	91	3mmw	D	155
3mmy	D	21	3mmy	E	208	3mmz	C	93	3mn1	C	84	3mn2	B	37
3nmn	B	50	3mno	A	141	3mo4	A	204	3mo8	A	77	3mol	B	71
3mos	A	362	3moy	A	162	3mpb	B	151	3mpc	A	63	3mpm	A	161
3mpr	D	155	3mpz	B	76	3mq0	B	100	3mq2	B	119	3mqd	A	272
3mqh	D	135	3mqq	A	53	3mqw	F	81	3mqz	A	99	3mr5	A	188
3ms5	A	253	3mst	A	117	3msu	B	210	3msw	A	43	3msx	B	60
3mt0	A	129	3mt6	D	119	3mte	A	94	3mti	A	71	3mtq	B	81
3mtr	B	114	3mtw	A	240	3mu7	A	181	3mu9	A	109	3muj	B	76
3mux	B	165	3muz	3	581	3mvc	B	69	3mvk	G	86	3mvn	A	65
3mvp	A	89	3mvr	A	280	3mvs	A	147	3mvu	A	69	3mw8	A	110
3mwc	A	64	3mwf	A	173	3mwx	A	215	3mx6	B	189	3mxn	A	113
3mxn	B	66	3mxo	B	118	3mxt	A	112	3mxu	A	80	3mxz	A	58
3myb	A	168	3myf	C	44	3myu	B	133	3myv	B	292	3myx	A	145
3mz0	A	208	3mz2	A	172	3mzo	A	96	3mzv	B	68	3n07	B	104
3n08	A	100	3n0l	B	157	3n0r	A	131	3n0w	A	193	3n0x	A	207
3n10	B	112	3n11	A	222	3n1e	B	69	3n1f	A	99	3n1f	D	53
3n1s	M	70	3n1u	A	73	3n29	B	227	3n2a	A	172	3n2b	A	151
3n2n	E	126	3n2s	D	123	3n37	A	192	3n3s	A	438	3n4f	C	222
3n4i	B	106	3n4k	B	98	3n5a	A	79	3n5b	A	37	3n5b	B	28
3n5l	B	147	3n5o	B	153	3n5w	B	221	3n6y	B	68	3n6z	A	182
3n72	B	83	3n79	A	85	3n7o	A	137	3n8b	A	41	3n8u	A	216
3n98	A	309	3n9b	B	73	3n9g	H	148	3n9i	B	168	3n9r	A	167
3n9u	B	120	3n9u	C	50	3na5	A	308	3naq	B	148	3nbm	A	62
3nci	A	570	3nda	A	225	3ndd	A	202	3ndh	B	114	3ndj	A	261
3ndn	D	76	3ndo	A	137	3ne8	A	129	3nec	B	90	3nep	X	131
3neu	A	40	3nf5	B	58	3nfi	B	55	3nfq	A	84	3nft	A	151
3nfu	A	56	3nfw	B	138	3ng7	X	239	3ngf	A	173	3ngg	B	38
3ngh	A	52	3ngj	A	152	3nhe	A	229	3nhe	B	56	3nht	A	210
3ni0	A	53	3ni2	A	292	3niw	A	136	3nj2	A	96	3njc	B	63
3njd	B	189	3nje	B	96	3njg	A	61	3nke	B	119	3nkl	A	40
3nkq	A	375	3nl9	A	86	3nm4	B	118	3nn1	A	97	3nnb	A	250
3no0	A	154	3no2	A	156	3no3	A	163	3no5	B	87	3no6	C	148

Continued on next page

PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3no7	A	39	3nof	B	60	3noh	A	50	3noj	A	77	3nok	A	139
3nol	A	168	3noo	B	130	3npd	A	70	3npf	B	191	3npk	A	182
3nqi	A	108	3nqn	B	35	3nqp	A	312	3nqx	A	193	3nr1	A	89
3nr5	A	68	3nr6	B	9	3nre	C	184	3nrf	A	54	3nrh	B	76
3nrl	B	36	3nrr	B	334	3nrw	A	46	3nrx	A	52	3ns2	A	71
3ns6	B	56	3nsl	F	56	3nsz	A	237	3nt1	B	373	3nt3	B	149
3ntc	L	112	3ntk	A	71	3nu8	B	204	3nua	A	136	3nuf	A	66
3nul	A	72	3nuq	A	162	3nv1	A	89	3nvb	A	253	3nvt	B	148
3nvw	J	111	3nwc	B	58	3nwo	A	198	3nwp	B	118	3nwr	A	235
3nx3	A	202	3nx4	A	85	3nxb	B	54	3nxg	E	179	3nxl	A	216
3nxq	A	330	3ny3	A	41	3ny5	B	30	3ny7	A	71	3nye	A	232
3nyh	A	318	3nyi	A	102	3nyk	A	75	3nym	B	61	3nyq	A	259
3nyv	A	143	3nyy	A	140	3nze	B	138	3nzn	B	70	3nzz	A	167
3o03	A	143	3o04	A	193	3o07	A	152	3o0a	B	126	3o0d	C	207
3o0f	A	143	3o0g	D	61	3o0h	A	261	3o0k	B	166	3o0l	A	27
3o0m	B	82	3o0p	A	9	3o0q	A	273	3o0w	A	154	3o0y	A	410
3o10	B	85	3o12	A	103	3o14	B	135	3o18	B	88	3o1k	B	19
3o1n	A	155	3o1p	A	142	3o22	A	65	3o26	A	126	3o2j	A	146
3o2r	D	78	3o2t	A	193	3o35	B	92	3o38	D	107	3o3m	C	195
3o3m	D	181	3o3t	A	158	3o3u	N	353	3o41	A	119	3o4h	A	151
3o4r	B	112	3o4v	B	129	3o5v	B	57	3o66	A	153	3o6d	A	95
3o6n	A	196	3o6p	A	111	3o70	A	23	3o72	C	199	3o79	A	52
3o7b	A	148	3o7i	A	101	3o7m	D	69	3o83	B	284	3o85	B	36
3o8m	A	323	3o8q	A	131	3o91	C	132	3o9z	A	191	3oa2	C	159
3oa3	B	159	3oaj	A	195	3oam	A	130	3obe	B	160	3obh	A	8
3obi	C	168	3obl	B	62	3obx	A	82	3oc7	A	157	3oc9	A	223
3ocj	A	167	3ocm	A	72	3ocr	A	105	3ocu	A	165	3od1	A	101
3od5	B	158	3od9	A	78	3odg	A	173	3odt	A	191	3odv	A	20
3oe3	B	36	3oec	C	166	3oep	A	275	3of4	C	100	3of5	A	111
3of7	A	242	3ofg	B	28	3ofk	C	74	3og9	B	133	3oga	A	59
3ogg	A	289	3ogh	B	90	3ogn	B	80	3ogr	A	672	3ohe	B	81
3ohg	A	184	3ohr	A	165	3oi8	A	42	3oid	C	166	3oig	A	165
3oin	A	30	3oio	A	49	3oir	B	72	3oiu	A	101	3oiz	A	43
3oj0	A	66	3oj6	B	83	3oj7	A	76	3ojc	D	93	3ojg	A	167
3ojs	A	135	3oks	B	283	3okx	B	97	3ol0	A	30	3ol3	A	50
3olq	A	127	3om0	A	175	3omc	B	121	3omd	B	82	3oms	A	45
3omt	A	53	3on1	A	44	3on2	A	85	3on4	E	109	3ono	A	99
3onp	A	41	3onr	I	31	3oo8	A	271	3ooi	A	126	3oon	A	38
3ooo	B	91	3oop	A	48	3oos	A	166	3oou	A	70	3oow	C	84
3oox	A	179	3op4	A	125	3op7	A	167	3op8	A	33	3op9	A	29
3opk	A	60	3oq2	A	40	3oqi	B	135	3oqp	A	120	3oqv	A	69
3oqy	B	64	3or3	A	89	3or5	A	87	3oro	A	138	3oru	A	148
3orv	B	192	3orv	D	154	3os4	A	190	3os7	A	229	3osd	A	149
3ose	A	69	3osm	A	68	3osu	B	98	3ot1	A	114	3ot2	B	1
3ot3	A	138	3ot9	B	263	3oti	B	212	3otl	A	82	3otn	B	286
3ou2	A	118	3ouf	B	60	3oug	I	68	3oui	A	117	3out	B	183
3ouz	B	174	3ovc	A	83	3ovp	B	112	3ovx	A	146	3owa	B	111
3owc	B	42	3owr	C	80	3owv	A	107	3oxp	A	106	3oyy	B	83
3oz2	A	171	3ozh	A	197	3p02	A	173	3p09	B	90	3p0b	A	291
3p0q	C	120	3p0r	A	117	3p0t	A	79	3p1a	A	176	3p1f	A	87
3p1g	A	72	3p1v	A	184	3p1w	A	197	3p1x	A	16	3p24	C	175
3p2c	B	284	3p2n	A	233	3p2t	A	125	3p2u	B	143	3p2y	A	189

Continued on next page



PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N	PDB	Cn	N
3p32	A	88	3p3c	A	188	3p3e	A	190	3p3g	A	117	3p3o	A	184
3p3v	B	98	3p48	A	69	3p4h	A	31	3p4l	A	130	3p4t	A	231
3p5h	A	75	3p5p	A	412	3p5u	A	141	3p6l	A	142	3p73	A	168
3p73	B	64	3p94	D	108	3p97	C	181	3p9c	A	196	3p9p	A	500
3p9x	A	59	3pa6	A	55	3pas	B	91	3pb6	X	202	3pbf	A	59
3pbo	A	210	3pc3	A	336	3pct	B	122	3pcv	A	55	3pd2	B	75
3pde	A	34	3pdn	A	256	3pdw	A	152	3pe4	A	358	3pe6	A	173
3pe7	A	254	3pe8	A	139	3pea	B	123	3pel	B	93	3pes	A	55
3pew	A	250	3pf2	A	203	3pf6	A	37	3pfo	A	205	3pfs	A	80
3pg6	C	74	3pgx	A	171	3phs	A	156	3phx	B	53	3pi7	A	148
3pim	A	114	3pj0	B	228	3pj3	A	130	3pjp	B	128	3pju	D	47
3pjy	B	78	3pk0	A	150	3pkv	A	128	3pl0	B	101	3pl2	B	148
3plf	D	174	3plw	A	67	3plx	B	55	3pmc	B	84	3pmd	A	83
3pmm	A	161	3pms	A	217	3pmt	A	28	3pn8	A	88	3pna	A	56
3pnn	A	100	3pnx	A	6	3po0	A	42	3po8	A	62	3poh	A	250
3poz	A	117	3pp9	A	91	3ppl	B	259	3pqa	B	309	3pro	D	76
3prp	A	95	3psm	A	37	3pt1	A	245	3pu9	A	113	3pua	A	116
3pve	A	86	3pvi	B	103	3px2	A	136	3pxl	A	340	3pzf	A	135
3pzj	B	59	3pzs	B	138	3pzw	A	509	3pzy	A	81	3q0h	A	58
3q0i	A	135	3q12	C	176	3q1c	A	197	3q1n	A	186	3q20	B	37
3q23	B	625	3q2e	A	59	3q34	A	102	3q3u	A	203	3q3w	B	80
3q4s	A	136	3q4t	A	124	3q4u	A	149	3q58	A	100	3q5y	A	143
3q60	A	165	3q62	B	92	3q64	A	109	3q6d	B	175	3q6j	A	306
3q7c	A	127	3q7m	A	174	3q90	A	63	3q93	B	24	3qan	C	199
3qao	A	48	3qat	B	196	3qbm	B	101	3qbp	A	278	3qc7	A	109
3qd5	B	92	3qds	B	98	3qe1	A	63	3qee	A	196	3qh4	A	199
3qhx	A	238	3qhz	M	93	3qi7	B	152	3qit	A	159	3qk3	A	83
3qk8	C	166	3qki	B	335	3qle	A	108	3qlj	D	155	3qm3	E	221
3qmd	A	7	3qmn	P	58	3qn1	A	124	3qn1	B	167	3qnm	A	145
3qoj	A	61	3qom	A	335	3qoo	A	81	3qp4	A	95	3qqi	B	117
3qry	A	304	3qu1	B	110	3qug	A	31	3quv	B	146	3qxb	B	181
3qxf	A	206	3qxz	B	161	3qy1	B	103	3qy3	A	63	3qyf	A	148
3qyj	A	184	3qyq	C	83	3qz6	A	143	3qzb	A	85	3r0p	B	39
3r1i	A	153	3r1w	C	120	3r3r	A	122	3r3s	C	189	3r6f	A	77
4dmr	A	520	4rhn	A	65	4ubp	A	71	4ubp	B	74	4ubp	C	345
6cel	A	297	6fdr	A	70	6rxn	A	33	7rsa	A	83			