

Amino Acid	Atom Name	Atom Type	Number of Shifts	Minimum Shift	Maximum Shift	Average Shift	Standard Deviation
ALA	H	H	1920	3.97	11.35	8.17	0.61
ALA	HA	H	1849	1.92	6.16	4.26	0.43
ALA	HB	H	1688	-0.56	3.70	1.38	0.28
ALA	C	C	403	171.00	182.20	177.72	2.19
ALA	CA	C	672	47.15	63.50	53.05	2.16
ALA	CB	C	533	14.50	25.70	18.87	1.73
ALA	N	N	906	99.44	137.20	122.97	3.88
ARG	H	H	1236	5.02	11.15	8.27	0.59
ARG	HA	H	1175	2.12	5.94	4.28	0.43
ARG	HB2	H	997	-0.38	3.29	1.76	0.30
ARG	HB3	H	991	0.17	3.29	1.79	0.26
ARG	HG2	H	804	-0.64	2.54	1.58	0.25
ARG	HG3	H	799	-0.22	2.54	1.58	0.24
ARG	HD2	H	811	1.81	3.85	3.13	0.20
ARG	HD3	H	805	1.81	3.70	3.14	0.19
ARG	HE	H	539	3.25	11.82	7.33	0.54
ARG	HH11	H	86	5.88	7.49	6.71	0.21
ARG	HH12	H	78	6.26	7.49	6.72	0.20
ARG	HH21	H	79	6.26	7.49	6.72	0.20
ARG	HH22	H	79	6.26	7.49	6.72	0.20
ARG	C	C	251	168.67	181.50	176.33	2.33
ARG	CA	C	397	50.50	65.13	56.93	2.48
ARG	CB	C	272	26.44	37.60	30.68	1.76
ARG	CG	C	175	23.70	31.90	27.15	1.12
ARG	CD	C	194	40.70	45.20	43.10	0.75
ARG	CZ	C	32	157.70	160.60	159.20	0.79
ARG	N	N	487	103.60	130.90	120.37	3.96
ARG	NE	N	60	80.80	114.90	85.60	5.52
ARG	NH1	N	6	70.10	72.90	72.30	1.08
ARG	NH2	N	5	72.60	72.90	72.74	0.12
ASN	H	H	1201	5.32	11.26	8.36	0.64
ASN	HA	H	1133	3.20	6.25	4.69	0.39
ASN	HB2	H	988	0.57	4.25	2.77	0.35
ASN	HB3	H	980	0.26	3.83	2.81	0.33
ASN	HD21	H	629	5.11	9.36	7.19	0.50
ASN	HD22	H	629	3.14	9.40	7.24	0.56
ASN	C	C	259	170.00	179.70	175.25	1.67
ASN	CA	C	398	47.65	58.70	53.54	1.99
ASN	CB	C	287	32.00	44.50	38.60	1.68
ASN	CG	C	52	173.50	179.50	175.78	1.43
ASN	N	N	505	106.30	132.70	118.80	4.51
ASN	ND2	N	165	104.70	120.22	112.79	2.54

ASP	H	H	1387	6.39	11.54	8.35	0.57
ASP	HA	H	1320	2.59	6.33	4.62	0.31
ASP	HB2	H	1164	1.33	6.60	2.74	0.30
ASP	HB3	H	1157	1.14	3.83	2.75	0.28
ASP	C	C	327	171.40	181.80	176.56	1.65
ASP	CA	C	492	46.10	59.00	54.41	2.03
ASP	CB	C	383	32.60	45.10	40.50	1.62
ASP	CG	C	32	173.49	180.60	177.84	1.89
ASP	N	N	635	109.90	133.80	120.31	4.13
CYS	H	H	1088	6.49	10.71	8.43	0.66
CYS	HA	H	1108	1.70	6.16	4.72	0.58
CYS	HB2	H	1055	0.42	4.65	2.94	0.43
CYS	HB3	H	1054	0.14	4.65	3.01	0.43
CYS	C	C	93	169.97	178.20	173.93	1.98
CYS	CA	C	138	50.30	65.60	57.13	3.49
CYS	CB	C	107	23.80	64.70	36.16	7.97
CYS	N	N	184	111.10	132.39	118.83	3.98
GLN	H	H	1023	5.93	11.94	8.22	0.61
GLN	HA	H	960	2.66	6.00	4.28	0.44
GLN	HB2	H	801	0.10	2.62	2.03	0.26
GLN	HB3	H	798	0.19	4.04	2.06	0.27
GLN	HG2	H	682	0.26	3.28	2.31	0.30
GLN	HG3	H	679	0.26	3.28	2.32	0.27
GLN	HE21	H	475	5.45	9.14	7.11	0.48
GLN	HE22	H	475	5.08	9.02	7.12	0.45
GLN	C	C	229	170.70	180.40	176.39	1.90
GLN	CA	C	362	50.70	61.70	56.58	2.24
GLN	CB	C	271	23.20	40.39	29.16	1.96
GLN	CG	C	178	27.98	38.00	33.70	0.98
GLN	CD	C	35	172.80	182.60	179.14	1.66
GLN	N	N	478	110.20	133.20	119.71	3.96
GLN	NE2	N	161	105.60	122.30	111.80	2.26
GLU	H	H	1727	6.15	11.04	8.31	0.61
GLU	HA	H	1631	2.54	6.29	4.26	0.42
GLU	HB2	H	1361	0.48	2.91	2.04	0.22
GLU	HB3	H	1355	0.50	2.92	2.05	0.21
GLU	HG2	H	1147	0.85	3.20	2.32	0.22
GLU	HG3	H	1140	0.66	3.14	2.33	0.21
GLU	C	C	405	169.10	180.60	177.11	1.98
GLU	CA	C	660	50.95	62.40	57.42	2.15
GLU	CB	C	495	25.70	36.50	29.98	1.69
GLU	CG	C	374	28.10	42.20	35.94	1.34
GLU	CD	C	26	177.76	183.60	181.16	1.52
GLU	N	N	845	111.26	134.50	120.68	3.55
GLY	H	H	1969	4.45	12.22	8.35	0.74
GLY	HA2	H	1842	0.34	6.17	3.90	0.43
GLY	HA3	H	1803	1.27	6.01	3.98	0.39
GLY	C	C	376	168.20	182.40	173.87	1.88
GLY	CA	C	682	41.50	55.41	45.25	1.48
GLY	N	N	826	88.30	130.80	109.20	4.12

HIS	H	H	554	5.53	10.80	8.26	0.75
HIS	HA	H	559	2.46	8.90	4.62	0.52
HIS	HB2	H	500	0.37	8.70	3.10	0.49
HIS	HB3	H	498	0.81	8.70	3.13	0.51
HIS	HD1	H	48	6.46	17.20	11.56	3.76
HIS	HD2	H	587	4.30	8.82	7.10	0.53
HIS	HE1	H	621	3.21	9.60	8.11	0.54
HIS	HE2	H	35	6.87	16.53	10.99	3.37
HIS	C	C	96	170.50	179.31	174.97	2.17
HIS	CA	C	184	50.90	63.70	55.99	2.60
HIS	CB	C	160	23.40	36.00	29.67	2.22
HIS	CG	C	39	122.67	136.80	130.59	3.41
HIS	CD2	C	54	115.90	127.65	119.64	2.27
HIS	CE1	C	43	127.60	138.60	136.09	1.74
HIS	N	N	217	105.00	133.70	118.70	4.41
HIS	ND1	N	23	168.20	248.00	192.74	17.24
HIS	NE2	N	23	166.70	231.50	180.95	15.19
ILE	H	H	1163	6.07	10.47	8.25	0.66
ILE	HA	H	1114	1.03	5.99	4.20	0.56
ILE	HB	H	1010	-1.12	2.78	1.79	0.34
ILE	HG12	H	820	-1.79	2.44	1.25	0.40
ILE	HG13	H	810	-2.04	2.88	1.27	0.42
ILE	HG2	H	940	-2.07	1.77	0.79	0.32
ILE	HD1	H	256	-1.20	1.26	0.70	0.33
ILE	C	C	283	169.40	180.90	175.99	1.94
ILE	CA	C	425	54.94	67.09	61.81	2.86
ILE	CB	C	316	26.80	43.30	38.50	2.01
ILE	CG1	C	201	20.66	38.25	27.79	2.04
ILE	CG2	C	232	12.26	22.60	17.25	1.46
ILE	CD1	C	192	8.00	18.10	13.41	1.62
ILE	N	N	569	99.00	133.70	121.75	4.61
LEU	H	H	2068	5.94	10.53	8.22	0.61
LEU	HA	H	1984	1.95	5.96	4.31	0.45
LEU	HB2	H	1693	0.00	2.57	1.63	0.32
LEU	HB3	H	1680	-1.21	2.68	1.61	0.34
LEU	HG	H	1536	-1.06	3.90	1.53	0.31
LEU	HD1	H	1669	-0.83	2.15	0.76	0.26
LEU	HD2	H	1660	-1.03	2.78	0.77	0.28
LEU	C	C	438	169.30	189.78	177.21	2.02
LEU	CA	C	720	50.40	65.10	55.63	2.23
LEU	CB	C	549	36.30	53.70	42.40	1.94
LEU	CG	C	384	21.90	36.83	26.76	1.40
LEU	CD1	C	477	16.91	29.60	24.67	1.70
LEU	CD2	C	473	16.91	29.20	24.27	1.75
LEU	N	N	975	109.76	134.60	121.71	4.17

LYS	H	H	2052	5.36	11.53	8.21	0.65
LYS	HA	H	1894	2.54	5.95	4.26	0.42
LYS	HB2	H	1623	0.16	3.94	1.77	0.26
LYS	HB3	H	1614	-0.37	3.94	1.79	0.26
LYS	HG2	H	1196	-0.05	2.99	1.36	0.27
LYS	HG3	H	1188	-0.29	2.99	1.37	0.28
LYS	HD2	H	1048	0.46	3.18	1.61	0.24
LYS	HD3	H	1057	0.28	3.18	1.61	0.24
LYS	HE2	H	1047	1.63	3.93	2.92	0.20
LYS	HE3	H	1055	1.78	3.93	2.92	0.19
LYS	HZ	H	229	6.78	9.26	7.52	0.21
LYS	C	C	380	170.20	181.50	176.65	2.04
LYS	CA	C	684	49.50	62.60	56.77	2.19
LYS	CB	C	504	24.50	39.16	32.78	1.83
LYS	CG	C	329	22.10	30.80	24.88	1.02
LYS	CD	C	313	22.00	34.70	28.92	1.10
LYS	CE	C	309	36.31	44.90	41.65	0.92
LYS	N	N	942	109.60	132.60	121.01	3.94
LYS	NZ	N	2	33.70	34.10	33.90	0.28
MET	H	H	466	5.88	9.70	8.29	0.59
MET	HA	H	468	2.91	6.00	4.41	0.42
MET	HB2	H	375	-0.97	2.84	2.01	0.40
MET	HB3	H	373	-0.97	2.90	2.01	0.41
MET	HG2	H	308	0.55	3.80	2.47	0.34
MET	HG3	H	307	0.55	3.80	2.46	0.31
MET	HE	H	263	-0.19	3.30	1.84	0.56
MET	C	C	135	169.80	180.30	176.71	2.09
MET	CA	C	207	50.80	61.40	56.08	2.26
MET	CB	C	161	28.40	39.80	32.86	2.42
MET	CG	C	114	27.30	36.50	32.13	1.16
MET	CE	C	91	12.90	40.00	17.43	4.61
MET	N	N	251	109.60	131.30	120.22	4.02
PHE	H	H	929	5.72	11.46	8.43	0.73
PHE	HA	H	921	3.10	6.30	4.63	0.57
PHE	HB2	H	836	1.39	4.14	2.96	0.35
PHE	HB3	H	831	1.48	3.79	3.01	0.34
PHE	HD1	H	1022	2.02	7.94	6.80	1.02
PHE	HD2	H	1016	2.02	7.94	6.80	1.03
PHE	HE1	H	993	2.95	8.80	6.85	1.02
PHE	HE2	H	989	2.95	8.80	6.85	1.02
PHE	HZ	H	854	3.04	9.50	6.84	0.94
PHE	C	C	235	169.75	180.64	175.59	2.17
PHE	CA	C	360	51.93	64.20	58.27	2.69
PHE	CB	C	291	34.10	46.40	39.78	1.86
PHE	CG	C	21	136.20	140.40	138.35	1.12
PHE	CD1	C	150	122.30	134.00	131.35	1.21
PHE	CD2	C	134	122.30	134.00	131.34	1.26
PHE	CE1	C	139	127.10	133.00	130.50	0.96
PHE	CE2	C	125	127.10	132.57	130.53	0.92
PHE	CZ	C	117	118.70	132.90	129.03	1.55
PHE	N	N	449	110.49	131.80	120.59	4.21

PRO	HA	H	928	1.63	5.75	4.41	0.36
PRO	HB2	H	797	0.07	3.69	2.01	0.40
PRO	HB3	H	794	0.14	3.79	2.09	0.42
PRO	HG2	H	710	-0.19	4.92	1.91	0.39
PRO	HG3	H	709	-0.19	4.92	1.94	0.37
PRO	HD2	H	769	1.34	4.62	3.61	0.38
PRO	HD3	H	767	0.39	5.16	3.65	0.42
PRO	C	C	197	172.90	180.71	176.71	1.71
PRO	CA	C	325	56.90	67.10	63.21	1.60
PRO	CB	C	237	28.50	35.10	31.79	1.10
PRO	CG	C	166	22.79	31.10	27.07	1.15
PRO	CD	C	187	47.68	52.20	50.20	0.92
PRO	N	N	20	106.00	138.77	130.53	8.81
SER	H	H	1578	6.08	10.36	8.30	0.59
SER	HA	H	1542	1.91	6.14	4.51	0.43
SER	HB2	H	1346	1.42	5.03	3.84	0.31
SER	HB3	H	1333	1.50	4.78	3.85	0.32
SER	HG	H	25	2.08	8.97	5.19	1.15
SER	C	C	312	170.20	181.40	174.62	1.66
SER	CA	C	521	52.40	66.91	58.49	2.20
SER	CB	C	411	57.22	70.80	63.77	1.55
SER	N	N	611	103.00	133.00	116.31	3.82
THR	H	H	1486	6.33	11.01	8.25	0.65
THR	HA	H	1441	0.87	6.28	4.49	0.51
THR	HB	H	1286	0.92	5.90	4.18	0.38
THR	HG1	H	71	0.32	8.21	4.17	1.75
THR	HG2	H	1274	-0.45	4.07	1.16	0.30
THR	C	C	331	170.60	180.60	174.69	1.63
THR	CA	C	530	52.90	69.50	61.96	2.83
THR	CB	C	377	58.60	78.30	69.52	2.01
THR	CG2	C	286	17.00	25.50	21.41	1.13
THR	N	N	657	97.70	130.44	115.10	5.35
TRP	H	H	311	5.49	10.76	8.37	0.83
TRP	HA	H	293	2.87	6.75	4.72	0.58
TRP	HB2	H	268	1.82	4.54	3.19	0.35
TRP	HB3	H	265	1.82	4.49	3.23	0.33
TRP	HD1	H	350	5.81	8.93	7.16	0.36
TRP	HE1	H	311	6.79	11.90	10.11	0.57
TRP	HE3	H	362	1.85	8.98	7.04	1.28
TRP	HZ2	H	378	2.63	8.50	7.01	1.10
TRP	HZ3	H	376	0.76	8.20	6.53	1.24
TRP	HH2	H	375	2.84	8.28	6.70	1.13
TRP	C	C	49	172.50	180.20	176.19	1.82
TRP	CA	C	90	52.00	63.44	57.49	2.82
TRP	CB	C	67	25.15	35.20	30.05	1.88
TRP	CG	C	82	107.50	114.60	110.37	1.55
TRP	CD1	C	72	119.50	129.75	125.51	1.79
TRP	CD2	C	65	126.20	130.10	127.56	0.96
TRP	CE2	C	51	135.51	139.20	137.76	0.97
TRP	CE3	C	37	115.10	127.30	119.92	2.00
TRP	CZ2	C	41	111.40	119.20	114.01	1.39
TRP	CZ3	C	39	117.50	124.80	121.40	1.55
TRP	CH2	C	40	120.21	124.80	123.18	1.14
TRP	N	N	110	101.75	131.00	120.25	4.47
TRP	NE1	N	52	121.68	132.40	129.30	2.13

TYR	H	H	907	5.64	10.89	8.38	0.75
TYR	HA	H	918	2.63	6.70	4.65	0.54
TYR	HB2	H	841	0.70	4.70	2.89	0.35
TYR	HB3	H	838	0.75	4.70	2.96	0.33
TYR	HD1	H	1104	2.77	8.00	6.82	0.80
TYR	HD2	H	1097	2.77	8.50	6.82	0.81
TYR	HE1	H	1107	2.61	7.68	6.58	0.72
TYR	HE2	H	1100	2.61	8.50	6.59	0.73
TYR	HH	H	17	5.99	10.16	9.08	1.08
TYR	C	C	154	170.50	178.97	175.35	1.87
TYR	CA	C	279	52.40	64.21	57.68	2.55
TYR	CB	C	209	33.75	45.25	39.12	2.10
TYR	CG	C	52	125.70	131.10	129.29	1.21
TYR	CD1	C	130	130.50	135.00	132.38	0.97
TYR	CD2	C	121	118.15	135.00	132.08	2.08
TYR	CE1	C	137	112.70	119.70	117.29	0.99
TYR	CE2	C	126	115.00	119.50	117.32	0.89
TYR	CZ	C	50	153.54	162.70	156.37	2.49
TYR	N	N	320	110.00	133.20	120.44	4.90
VAL	H	H	1592	4.88	10.46	8.26	0.70
VAL	HA	H	1539	1.73	6.09	4.15	0.56
VAL	HB	H	1393	-0.29	3.42	1.97	0.34
VAL	HG1	H	1382	-0.57	5.98	0.82	0.32
VAL	HG2	H	1375	-2.32	6.06	0.83	0.34
VAL	C	C	315	169.90	181.60	175.75	1.98
VAL	CA	C	537	55.90	70.39	62.26	2.99
VAL	CB	C	394	27.70	40.40	32.77	1.83
VAL	CG1	C	320	15.30	24.70	21.11	1.54
VAL	CG2	C	314	15.50	26.30	21.31	1.58
VAL	N	N	714	96.29	136.80	121.05	5.42