Computational Biology Lecture 4

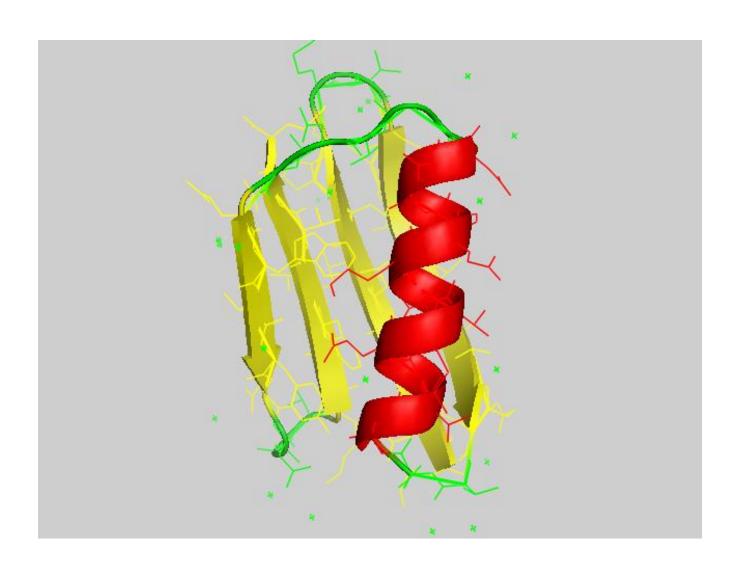
Modules in this lecture

- 1. Coordinate Systems
- 2. Potential Energy Surfaces (PES)
- 3. Molecular Representations
- 4. Molecular Surfaces
- 5. Units of length and Energy

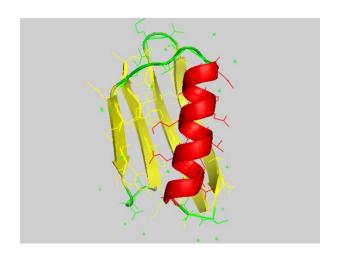
Reference text book:

Molecular Modeling; Principles and Applications, Chapter 1
By
Andrew R Leach

Protein G

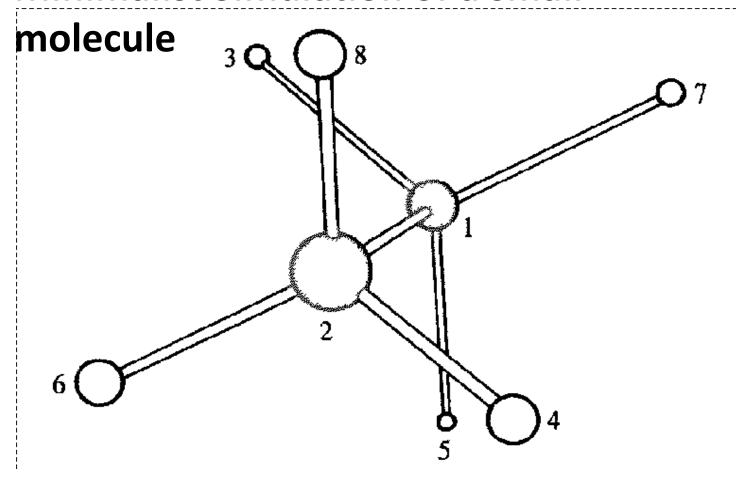


Cartesian Coordinate System

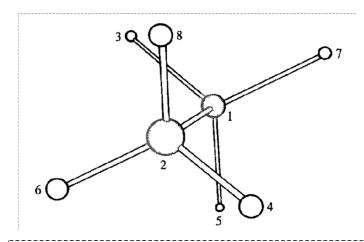


1	N	MET	Α	1	12.969	18.506	30.954	1.00 15.93	N
2	CA	MET	Α	1	13.935	18.529	29.843	1.00 17.40	С
3	С	MET	Α	1	13.138	18.692	28.517	1.00 14.65	С
4	0	MET	Α	1	12.007	18.222	28.397	1.00 13.04	0
5	СВ	MET	Α	1	14.733	17.216	29.882	1.00 20.72	С
6	CG	MET	Α	1	15.742	16.983	28.738	1.00 23.81	С
7	SD	MET	Α	1	17.378	17.025	29.359	1.00 28.11	S
8	CE	MET	A	1	17.166	16.055	30.819	1.00 27.51	С
9	N	THR	Α	2	13.719	19.413	27.573	1.00 12.63	N
10	CA	THR	Α	2	13.088	19.661	26.283	1.00 12.68	С
11	С	THR	A	2	13.561	18.631	25.300	1.00 12.02	С
12	0	THR	Α	2	14.763	18.432	25.121	1.00 13.07	0
13	CB	THR	Α	2	13.527	20.980	25.667	1.00 14.62	С
14	OG1	THR	Α	2	13.307	22.020	26.627	1.00 15.31	0
15	CG2	THR	A	2	12.704	21.284	24.409	1.00 14.47	С
	3 4 5 6 7 8 9 10 11 12 13 14	2 CA 3 C 4 O 5 CB 6 CG 7 SD 8 CE 9 N 10 CA 11 C 12 O 13 CB 14 OG1	2 CA MET 3 C MET 4 O MET 5 CB MET 6 CG MET 7 SD MET 8 CE MET 9 N THR 10 CA THR 11 C THR 12 O THR 13 CB THR 14 OG1 THR	2 CA MET A 3 C MET A 4 O MET A 5 CB MET A 6 CG MET A 7 SD MET A 8 CE MET A 9 N THR A 10 CA THR A 11 C THR A 12 O THR A 13 CB THR A 14 OG1 THR A	2 CA MET A 1 3 C MET A 1 4 O MET A 1 5 CB MET A 1 6 CG MET A 1 7 SD MET A 1 8 CE MET A 1 9 N THR A 2 10 CA THR A 2 11 C THR A 2 12 O THR A 2 13 CB THR A 2 14 OG1 THR A 2	2 CA MET A 1 13.935 3 C MET A 1 13.138 4 O MET A 1 12.007 5 CB MET A 1 14.733 6 CG MET A 1 15.742 7 SD MET A 1 17.378 8 CE MET A 1 17.166 9 N THR A 2 13.719 10 CA THR A 2 13.088 11 C THR A 2 13.561 12 O THR A 2 14.763 13 CB THR A 2 13.527 14 OG1 THR A 2 13.307	2 CA MET A 1 13.935 18.529 3 C MET A 1 13.138 18.692 4 O MET A 1 12.007 18.222 5 CB MET A 1 14.733 17.216 6 CG MET A 1 15.742 16.983 7 SD MET A 1 17.378 17.025 8 CE MET A 1 17.166 16.055 9 N THR A 2 13.719 19.413 10 CA THR A 2 13.088 19.661 11 C THR A 2 13.561 18.631 12 O THR A 2 14.763 18.432 13 CB THR A 2 13.527 20.980 14 OG1 THR A 2 13.307 22.020	2 CA MET A 1 13.935 18.529 29.843 3 C MET A 1 13.138 18.692 28.517 4 O MET A 1 12.007 18.222 28.397 5 CB MET A 1 14.733 17.216 29.882 6 CG MET A 1 15.742 16.983 28.738 7 SD MET A 1 17.378 17.025 29.359 8 CE MET A 1 17.166 16.055 30.819 9 N THR A 2 13.719 19.413 27.573 10 CA THR A 2 13.088 19.661 26.283 11 C THR A 2 13.561 18.631 25.300 12 O THR A 2 14.763 18.432 25.121 13 CB THR A 2 13.527 20.980 25.667 14 OG1 THR A 2 13.307 22.020 26.627	2 CA MET A 1 13.935 18.529 29.843 1.00 17.40 3 C MET A 1 13.138 18.692 28.517 1.00 14.65 4 O MET A 1 12.007 18.222 28.397 1.00 13.04 5 CB MET A 1 14.733 17.216 29.882 1.00 20.72 6 CG MET A 1 15.742 16.983 28.738 1.00 23.81 7 SD MET A 1 17.378 17.025 29.359 1.00 28.11 8 CE MET A 1 17.166 16.055 30.819 1.00 27.51 9 N THR A 2 13.719 19.413 27.573 1.00 12.63 10 CA THR A 2 13.088 19.661 26.283 1.00 12.68 11 C THR A 2 14.763 18.432 25.121 1.00 13.07 13 CB

Minimalist Simulation of a small

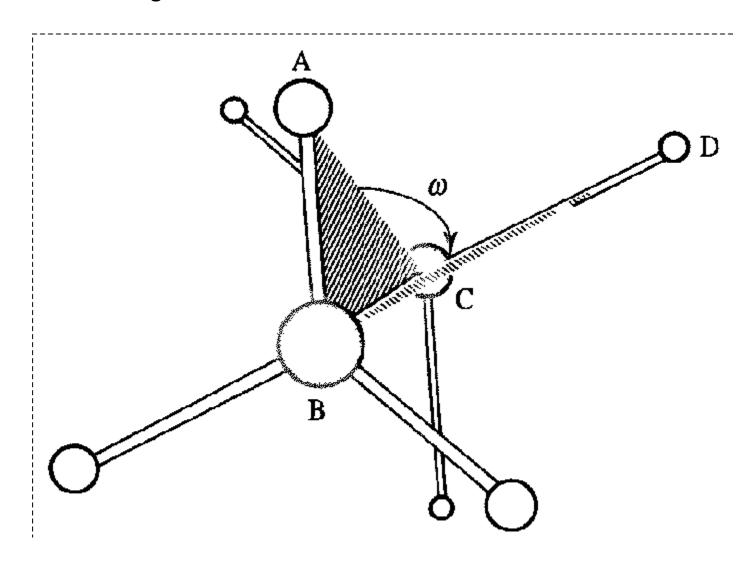


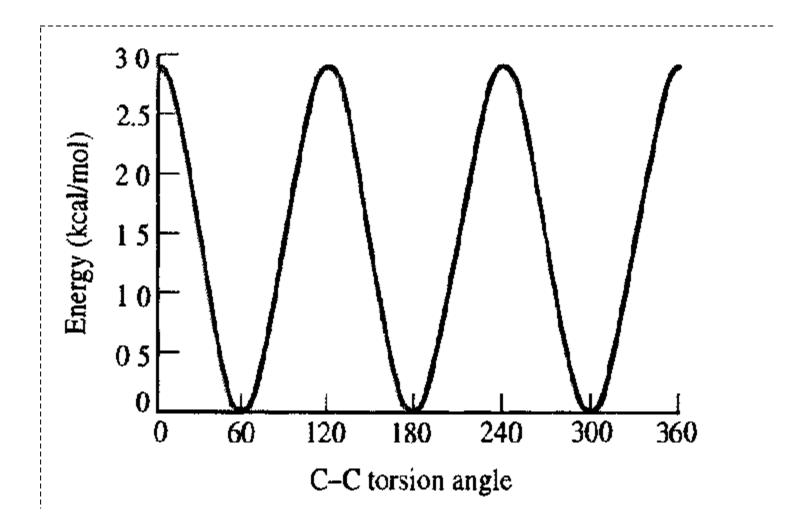
Internal Coordinate System

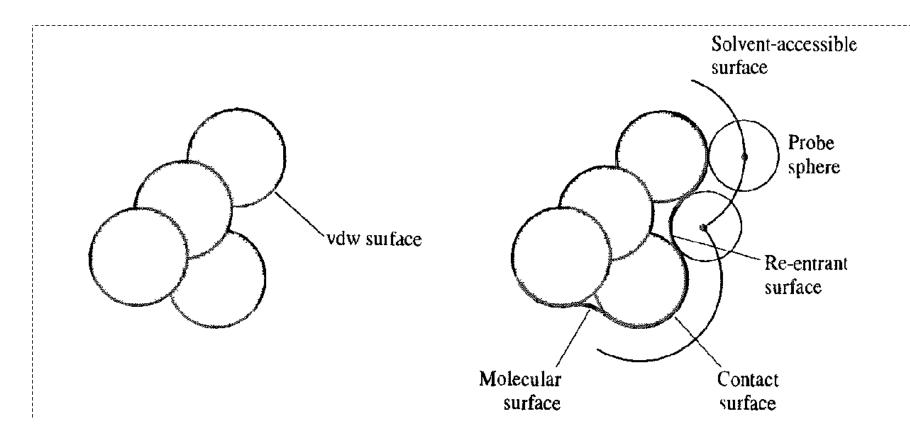


1	С						
2	C	1.54	1				
3	H	1.0	1	109.5	2		
4	H	1.0	2	109.5	1	180. 0	3
5	H	1.0	1	109.5	2	60.0	4
6	H	1.0	2	109.5	1	-60.0	5
7	H	1.0	1	109.5	2	180.0	6
8	H	1.0	2	109.5	1	60.0	7

Dihedral Angle

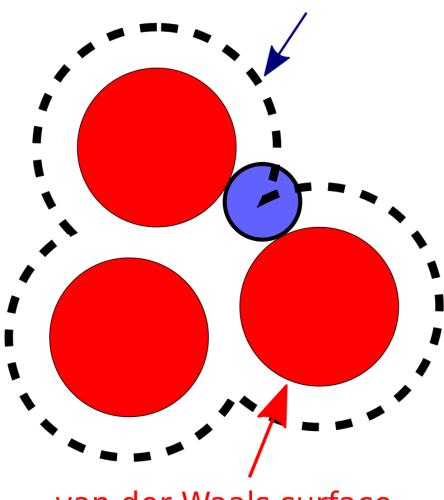






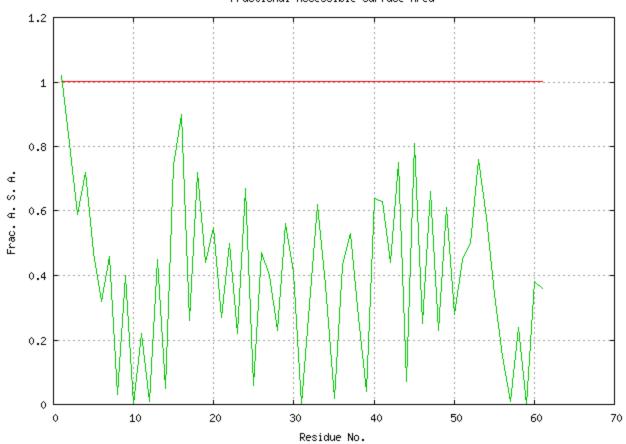
Rolling Probe Method

accessible surface



van der Waals surface

Fractional Accessible Surface Area



Tue Jan 23 07:56:12 2024

NAME	STRUC	HBOND	BTURN	ASA	ASA	VOL.	VOL.	PHI	PSI PSI	OMEGA OMEGA
n A										
	ccc c			221.9	1.02	151.2	0.92	0.0	151.9	169.7
	CBC C									-179.8
PRO	CBC C			90.0	0.59	105.7	0.91	-64.5	147.5	173.7
ALA	CBC C			88.6	0.72	87.5	0.99	-74.2	128.0	178.1
VAL	BBB B			81.4	0.47	119.9	0.88	-113.0	146.3	179.9
THR	BBB B	25A,25A		49.5	0.32	114.6	0.95	-117.4	144.1	169.7
THR	BBB B			71.9	0.46	111.7	0.93	-88.8	123.5	176.3
TYR	BBB B	23A,23A		7.1	0.03	188.9	0.97	-107.0	147.7	179.8
LYS	BBB B	57A,55A		92.8	0.40	188.1	1.11	-114.0	145.8	170.1
LEU	BBB B	21A,21A		0.0	0.00	150.7	0.92	-118.9	124.0	172.2
VAL	BBB B	59A,57A		37.7	0.22	131.3	0.96	-98.8	120.1	-175.5
ILE	BBB B	19A,19A		2.6	0.01	160.5	0.99	-113.6	117.1	175.0
ASN	BBB B	61A,59A		78.1	0.45	120.3	0.97	-113.8	70.0	-178.1
GLY	BBC B	17A		4.8	0.05	64.9	1.01	-92.8	170.3	176.6
LYS	CCC C			169.7	0.74	161.2	0.95	-66.1	-39.9	179.0
THR	CBC C			140.7	0.90	110.2	0.91	-121.8	-19.7	-179.4
LEU	CBC C	14A		54.1	0.26	163.1	0.99	-108.9	123.9	-179.1
LYS					0.72	156.9	0.93	-141.0	145.5	172.3
GLY	CCC C	12A,12A		38.7	0.44	63.3	0.98	137.6	-143.1	-176.7
GLU	BBB B			105.8	0.55	126.1	0.91	-140.4	149.8	170.8
THR	BBB B	10A,10A		42.2	0.27	115.6	0.96	-142.8	174.6	-176.1
THR	BBB B			77.3	0.50	109.2	0.91	-139.7	159.4	170.1
THR	BBB B	8A,8A		34.5	0.22	114.0	0.94	-147.6	158.1	177.1
LYS	BBB B			154.9	0.67	161.4	0.95	-111.2	136.2	178.5
ALA	BBB B	6A,6A		6.8	0.06	89.2	1.01	-155.6	161.4	176.8
VAL	BCC C			80.6	0.47	118.9	0.87	-74.0	-24.1	-177.8
	NAME A MET THR A VAL THR LYS LYS THR LYS GLU THR THR LYS GLU THR THR LYS ALA	NAME STRUC A MET CCC C THR CBC C PRO CBC C ALA CBC C VAL BBB B THR BBB B THR BBB B LEU BBB B THR CBC C THR CBC C THR CBC C LEU CBC C CTHR CBC C CGLY CCC C GLU BBB B THR BBB B	NAME STRUC HBOND A MET CCC C THR CBC C PRO CBC C ALA CBC C VAL BBB B THR BBB B 25A,25A THR BBB B 25A,55A LEU BBB B 57A,55A LEU BBB B 21A,21A VAL BBB B 59A,57A ILE BBB B 19A,19A ASN BBB B 61A,59A GLY BBC C THR CBC C THR CBC C LEU CBC C 14A LYS CBC C GLY CCC C 12A,12A GLU BBB B THR BBB B	NAME STRUC HBOND BTURN A MET CCC C THR CBC C PRO CBC C ALA CBC C VAL BBB B THR BBB B 25A,25A THR BBB B 25A,25A THR BBB B 57A,55A LEU BBB B 57A,55A LEU BBB B 59A,57A ILE BBB B 19A,19A ASN BBB B 61A,59A GLY BBC B 17A LYS CCC C THR CBC C LEU CBC C 14A LYS CBC C GLY CCC C 12A,12A GLU BBB B THR BBB B 10A,10A THR BBB B THR BBB B 10A,6A	MAME STRUC HBOND BTURN ASA MET CCC C 221.9 THR CBC C 126.3 PRO CBC C 90.0 ALA CBC C 88.6 VAL BBB B 81.4 THR BBB B 25A,25A 49.5 THR BBB B 71.9 TYR BBB B 23A,23A 7.1 LYS BBB B 57A,55A 92.8 LEU BBB B 21A,21A 0.0 VAL BBB B 21A,21A 0.0 VAL BBB B 59A,57A 37.7 ILE BBB B 19A,19A 2.6 ASN BBB B 61A,59A 78.1 GLY BBC B 17A 4.8 LYS CCC C 169.7 THR CBC C 14A 54.1 LYS CBC C 14A 54.1 LYS CBC C 167.1 GLY CCC C 12A,12A 38.7 GLU BBB B 10A,10A 42.2 THR BBB B 10A,10A 42.2 THR BBB B 77.3 THR BBB B 154.9 ALA BBB B 6A,6A 6.8	MET CCC C THR CBC C VAL BBB B TYR BB	MET CCC C	NAME STRUC HBOND BTURN ASA ASA VOL. VOL. A MET CCC C 221.9 1.02 151.2 0.92 THR CBC C 126.3 0.81 109.3 0.91 PRO CBC C 90.0 0.59 105.7 0.91 ALA CBC C 88.6 0.72 87.5 0.99 VAL BBB B 81.4 0.47 119.9 0.88 THR BBB B 25A,25A 49.5 0.32 114.6 0.95 THR BBB B 23A,23A 71.9 0.46 111.7 0.93 TYR BBB B 57A,55A 92.8 0.40 188.1 1.11 LEU BBB B 59A,57A 37.7 0.22 131.3 0.96 ILE BBB B 19A,19A 2.6 0.01 160.5 0.99 ASN BBB B 61A,59A 78.1 0.45 120.3 0.97 <tr< td=""><td>NAME STRUC HBOND BTURN ASA ASA VOL. VOL. PHI TA MET CCC C 221.9 1.02 151.2 0.92 0.0 THR CBC C 126.3 0.81 109.3 0.91 -83.8 PRO CBC 90.0 0.59 105.7 0.91 -64.5 ALA CBC 88.6 0.72 87.5 0.99 -74.2 VAL BBB B 81.4 0.47 119.9 0.88 -113.0 THR BBB B 71.9 0.46 111.7 0.93 -88.8 TYR BBB B 71.9 0.46 111.7 0.93 -88.8 TYR BBB B 57A,55A 92.8 0.40 188.1 1.11 -114.0 LEU BBB B 57A,55A 92.8 0.40 188.1 0.97 -107.0 LEU BBC B<</td><td>NAME STRUC HBOND BTURN ASA ASA VOL. VOL. PHI PSI THA CBC C 126.3 0.81 109.3 0.91 -83.8 150.2 PRO CBC C 90.0 0.59 105.7 0.91 -64.5 147.5 ALA CBC C 88.6 0.72 87.5 0.99 -74.2 128.0 VAL BBB B 8 81.4 0.47 119.9 0.88 -113.0 146.3 THR BBB B 71.9 0.46 111.7 0.93 -88.8 123.5 TYR BBB B 23A,23A 7.1 0.03 188.9 0.97 -107.0 147.7 LYS BBB B 57A,55A 92.8 0.40 188.1 1.11 -114.0 145.8 LEU BBB B 21A,21A 0.0 0.00 150.7 0.92 -118.9 124.0 VAL BBB B 59A,57A 37.7 0.22 131.3 0.96 -98.8 120.1 LE BBB B 19A,19A 2.6 0.01 160.5 0.99 -113.6 117.1 ASN BBB B 61A,59A 78.1 0.45 120.3 0.97 -113.8 70.0 GLY BBC B 17A 4.8 0.05 64.9 1.01 -92.8 170.3 LYS CCC C 169.7 0.74 161.2 0.95 -66.1 -39.9 THR CBC C 140.7 0.90 110.2 0.91 -121.8 -19.7 LEU CBC C 14A 54.1 0.26 163.1 0.99 -108.9 123.9 LYS CBC C 167.1 0.72 156.9 0.93 -141.0 145.5 GLY CCC C 12A,12A 38.7 0.44 63.3 0.98 137.6 -143.1 GLU BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 8 8A,8A 34.5 0.22 114.0 0.94 -147.6 158.1 LYS BBB B 8 8A,8A 34.5 0.22 114.0 0.94 -147.6 158.1 LYS BBB B 8 8A,8A 34.5 0.22 114.0 0.95 -111.2 136.2 ALA BBB B 6A,6A 6.8 0.06 89.2 1.01 -155.6 161.4</td></tr<>	NAME STRUC HBOND BTURN ASA ASA VOL. VOL. PHI TA MET CCC C 221.9 1.02 151.2 0.92 0.0 THR CBC C 126.3 0.81 109.3 0.91 -83.8 PRO CBC 90.0 0.59 105.7 0.91 -64.5 ALA CBC 88.6 0.72 87.5 0.99 -74.2 VAL BBB B 81.4 0.47 119.9 0.88 -113.0 THR BBB B 71.9 0.46 111.7 0.93 -88.8 TYR BBB B 71.9 0.46 111.7 0.93 -88.8 TYR BBB B 57A,55A 92.8 0.40 188.1 1.11 -114.0 LEU BBB B 57A,55A 92.8 0.40 188.1 0.97 -107.0 LEU BBC B<	NAME STRUC HBOND BTURN ASA ASA VOL. VOL. PHI PSI THA CBC C 126.3 0.81 109.3 0.91 -83.8 150.2 PRO CBC C 90.0 0.59 105.7 0.91 -64.5 147.5 ALA CBC C 88.6 0.72 87.5 0.99 -74.2 128.0 VAL BBB B 8 81.4 0.47 119.9 0.88 -113.0 146.3 THR BBB B 71.9 0.46 111.7 0.93 -88.8 123.5 TYR BBB B 23A,23A 7.1 0.03 188.9 0.97 -107.0 147.7 LYS BBB B 57A,55A 92.8 0.40 188.1 1.11 -114.0 145.8 LEU BBB B 21A,21A 0.0 0.00 150.7 0.92 -118.9 124.0 VAL BBB B 59A,57A 37.7 0.22 131.3 0.96 -98.8 120.1 LE BBB B 19A,19A 2.6 0.01 160.5 0.99 -113.6 117.1 ASN BBB B 61A,59A 78.1 0.45 120.3 0.97 -113.8 70.0 GLY BBC B 17A 4.8 0.05 64.9 1.01 -92.8 170.3 LYS CCC C 169.7 0.74 161.2 0.95 -66.1 -39.9 THR CBC C 140.7 0.90 110.2 0.91 -121.8 -19.7 LEU CBC C 14A 54.1 0.26 163.1 0.99 -108.9 123.9 LYS CBC C 167.1 0.72 156.9 0.93 -141.0 145.5 GLY CCC C 12A,12A 38.7 0.44 63.3 0.98 137.6 -143.1 GLU BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 10A,10A 42.2 0.27 115.6 0.91 -140.4 149.8 THR BBB B 8 8A,8A 34.5 0.22 114.0 0.94 -147.6 158.1 LYS BBB B 8 8A,8A 34.5 0.22 114.0 0.94 -147.6 158.1 LYS BBB B 8 8A,8A 34.5 0.22 114.0 0.95 -111.2 136.2 ALA BBB B 6A,6A 6.8 0.06 89.2 1.01 -155.6 161.4

4416	N	PHE	A1116	108.052	79.091	-11.109	1.00 11.57
4417	CA	PHE	A1116	108.691	79.424	-9.827	1.00 11.89
4418	C	PHE	A1116	109.486	80.728	-9.898	1.00 9.97
4419	0	PHE	A1116	109.575	81.454	-8.905	1.00 10.78
4420	CB	PHE	A1116	109.613	78.293	-9.343	1.00 11.49
4421	CG	PHE	A1116	108.887	77.145	-8.708	1.00 14.69
4422	CD1	PHE	A1116	108.175	77.326	-7.518	1.00 12.55
4423	CD2	PHE	A1116	108.947	75.866	-9.275	1.00 13.15
4424	CE1	PHE	A1116	107.494	76.248	-6.919	1.00 14.21
4425	CE2	PHE	A1116	108.274	74.772	-8.673	1.00 8.56
4426	CZ	PHE	A1116	107.552	74.970	-7.505	1.00 10.32
4427	H	PHE	A1116	108.335	78.251	-11.595	1.00 0.00
4428	HA	PHE	A1116	107.933	79.481	-9.046	1.00 0.00
4429	HB2	PHE	A1116	110.172	77.891	-10.188	1.00 0.00
4430	HB3	PHE	A1116	110.309	78.683	-8.600	1.00 0.00
4431	HD1	PHE	A1116	108.143	78.299	-7.050	1.00 0.00
4432	HD2	PHE	A1116	109.511	75.703	-10.181	1.00 0.00
4433	HE1	PHE	A1116	106.929	76.404	-6.012	1.00 0.00
4434	HE2	PHE	A1116	108.325	73.792	-9.125	1.00 0.00
4435	HZ	PHE	A1116	107.034	74.142	-7.045	1.00 0.00
	4417 4418 4419 4420 4421 4422 4423 4424 4425 4426 4427 4428 4429 4430 4431 4432 4433 4434	4417 CA 4418 C 4419 O 4420 CB 4421 CG 4422 CD1 4423 CD2 4424 CE1 4425 CE2 4426 CZ 4427 H 4428 HA 4429 HB2 4430 HB3 4431 HD1 4432 HD2 4433 HE1 4434 HE2	4417 CA PHE 4418 C PHE 4419 O PHE 4420 CB PHE 4421 CG PHE 4422 CD1 PHE 4423 CD2 PHE 4424 CE1 PHE 4425 CE2 PHE 4426 CZ PHE 4427 H PHE 4428 HA PHE 4429 HB2 PHE 4430 HB3 PHE 4431 HD1 PHE 4431 HD1 PHE 4432 HD2 PHE 4433 HE1 PHE 4434 HE2 PHE	4417 CA PHE A1116 4418 C PHE A1116 4419 O PHE A1116 4420 CB PHE A1116 4421 CG PHE A1116 4422 CD1 PHE A1116 4423 CD2 PHE A1116 4424 CE1 PHE A1116 4425 CE2 PHE A1116 4426 CZ PHE A1116 4427 H PHE A1116 4428 HA PHE A1116 4429 HB2 PHE A1116 4430 HB3 PHE A1116 4431 HD1 PHE A1116 4431 HD1 PHE A1116 4432 HD2 PHE A1116 4433 HE1 PHE A1116	4417 CA PHE A1116 108.691 4418 C PHE A1116 109.486 4419 O PHE A1116 109.575 4420 CB PHE A1116 109.613 4421 CG PHE A1116 108.887 4422 CD1 PHE A1116 108.175 4423 CD2 PHE A1116 108.947 4424 CE1 PHE A1116 107.494 4425 CE2 PHE A1116 108.274 4426 CZ PHE A1116 107.552 4427 H PHE A1116 108.335 4428 HA PHE A1116 107.933 4429 HB2 PHE A1116 107.933 4429 HB2 PHE A1116 110.172 4430 HB3 PHE A1116 110.309 4431 HD1 PHE A1116 108.143 4432 HD2 PHE A1116 109.511 4433 HE1 PHE A1116 106.929 4434 HE2 PHE A1116 108.325	4417 CA PHE A1116 108.691 79.424 4418 C PHE A1116 109.486 80.728 4419 O PHE A1116 109.575 81.454 4420 CB PHE A1116 109.613 78.293 4421 CG PHE A1116 108.887 77.145 4422 CD1 PHE A1116 108.175 77.326 4423 CD2 PHE A1116 108.947 75.866 4424 CE1 PHE A1116 107.494 76.248 4425 CE2 PHE A1116 107.494 76.248 4426 CZ PHE A1116 107.552 74.970 4427 H PHE A1116 107.552 74.970 4427 H PHE A1116 107.933 79.481 4429 HB2 PHE A1116 107.933 79.481 4429 HB2 PHE A1116 107.933 79.481 4430 HB3 PHE A1116 100.172 77.891 4430 HB3 PHE A1116 100.172 77.891 4431 HD1 PHE A1116 109.511 75.703 4433 HE1 PHE A1116 109.511 75.703 4434 HE2 PHE A1116 108.325 73.792	4417 CA PHE A1116 108.691 79.424 -9.827 4418 C PHE A1116 109.486 80.728 -9.898 4419 O PHE A1116 109.575 81.454 -8.905 4420 CB PHE A1116 109.613 78.293 -9.343 4421 CG PHE A1116 108.887 77.145 -8.708 4422 CD1 PHE A1116 108.175 77.326 -7.518 4423 CD2 PHE A1116 108.947 75.866 -9.275 4424 CE1 PHE A1116 107.494 76.248 -6.919 4425 CE2 PHE A1116 108.274 74.772 -8.673 4426 CZ PHE A1116 107.552 74.970 -7.505 4427 H PHE A1116 108.335 78.251 -11.595 4428 HA PHE A1116 107.933 79.481 -9.046 4429 HB2 PHE A1116 107.933 79.481 -9.046 4429 HB2 PHE A1116 100.172 77.891 -10.188 4430 HB3 PHE A1116 100.309 78.683 -8.600 4431 HD1 PHE A1116 108.143 78.299 -7.050 4432 HD2 PHE A1116 109.511 75.703 -10.181 4433 HE1 PHE A1116 106.929 76.404 -6.012 4434 HE2 PHE A1116 108.325 73.792 -9.125

zunouuuuuttttttt

Units

All SI Units

Except

Angstrom = 0.1 nm

kcal = 4.184 kJ