Computational Biology Lecture 4

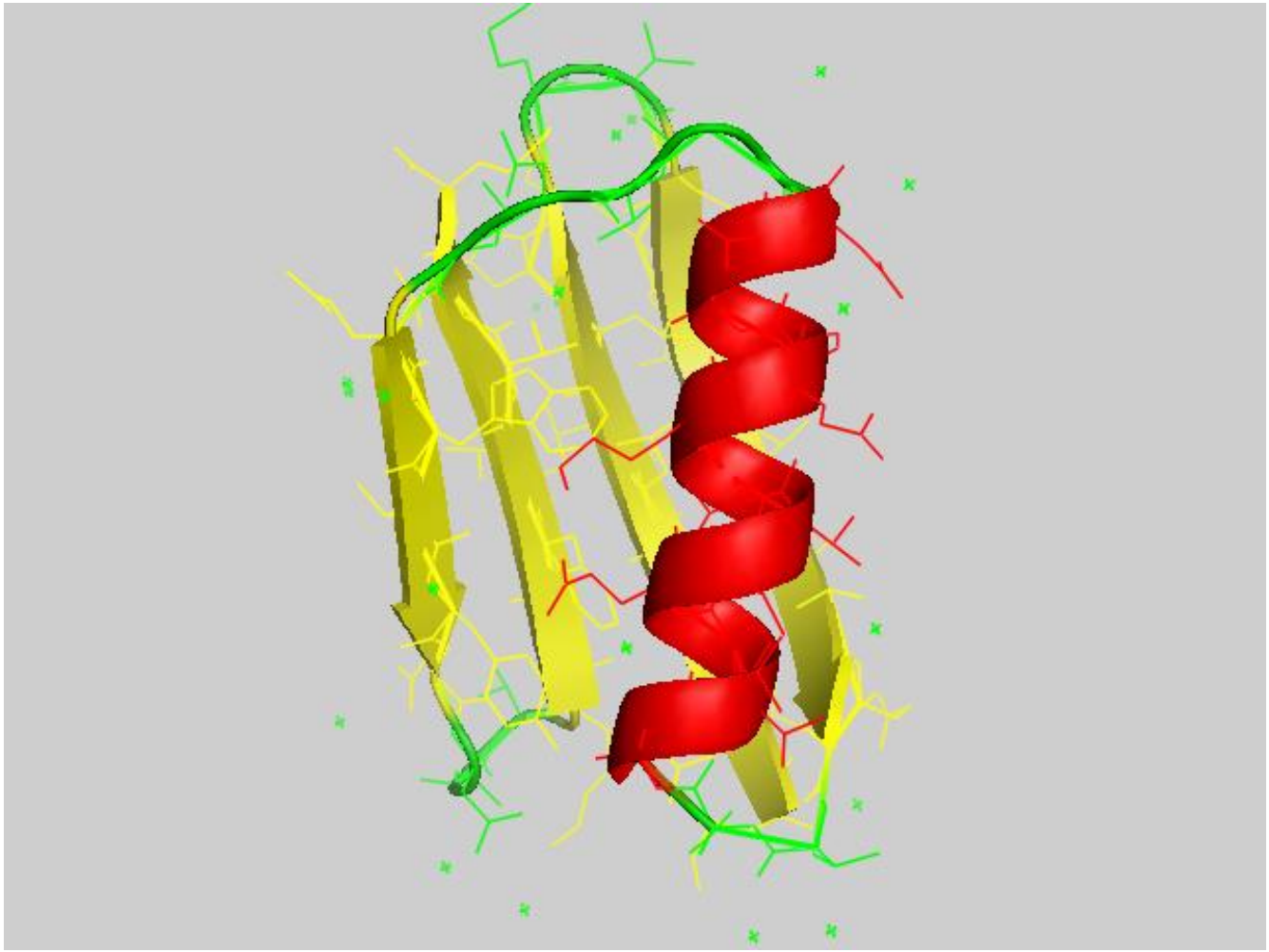
Modules in this lecture

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

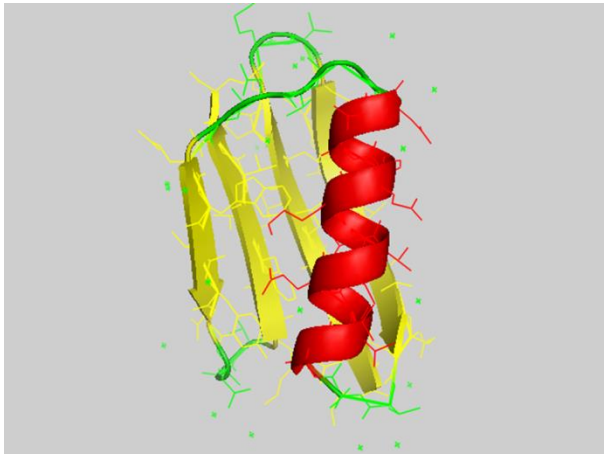
<u>Reference text book:</u>

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

Protein G

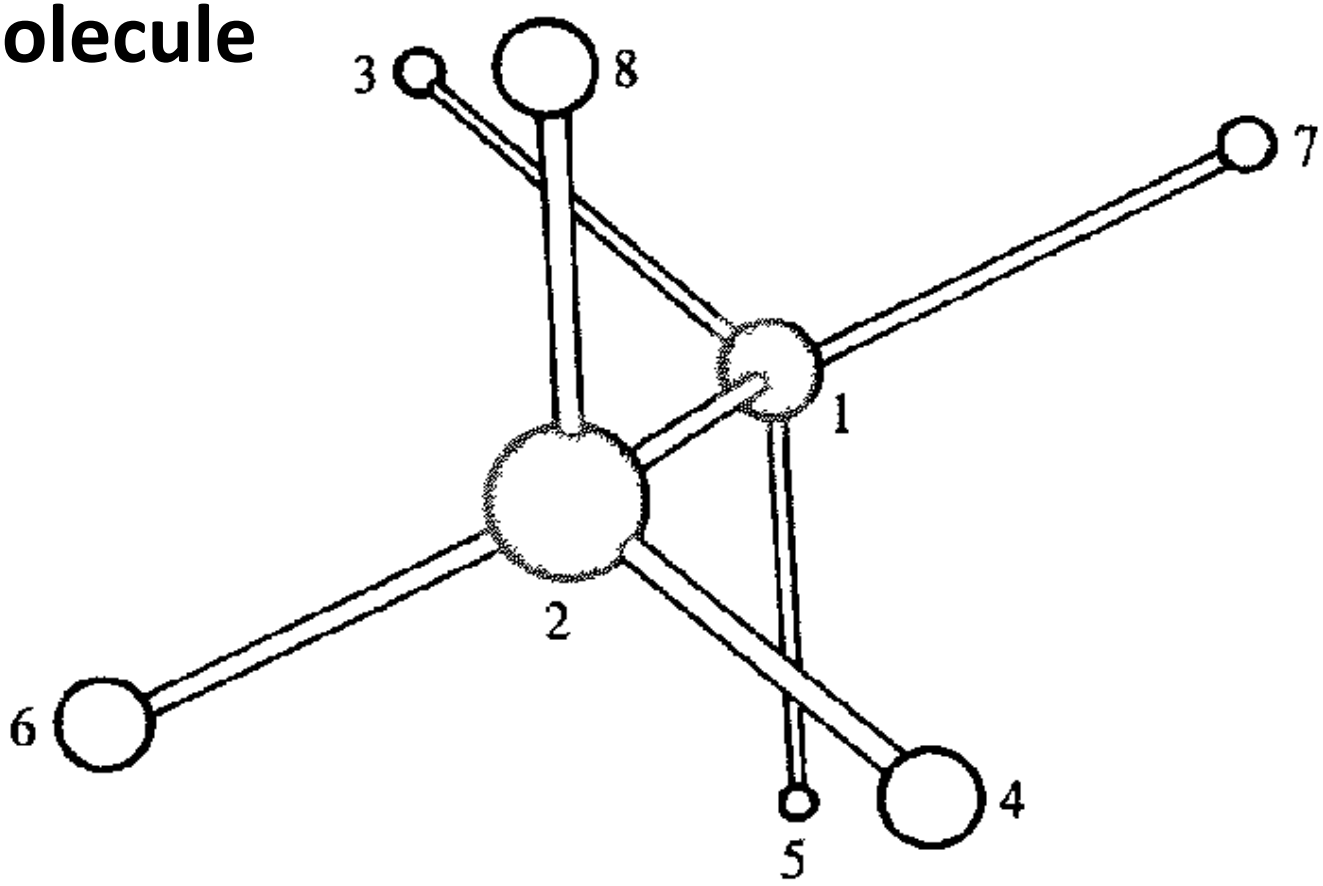


Cartesian Coordinate System

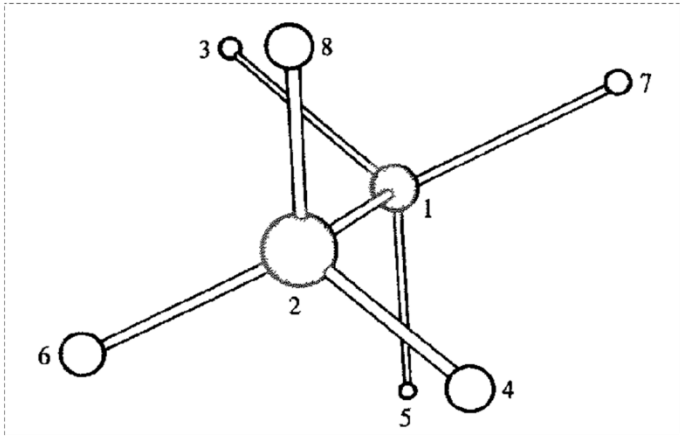


```
ATOM      1  N   MET A   1      12.969  18.506  30.954  1.00 15.93           N
ATOM      2  CA  MET A   1      13.935  18.529  29.843  1.00 17.40           C
ATOM      3  C   MET A   1      13.138  18.692  28.517  1.00 14.65           C
ATOM      4  O   MET A   1      12.007  18.222  28.397  1.00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

Minimalist Simulation of a small molecule

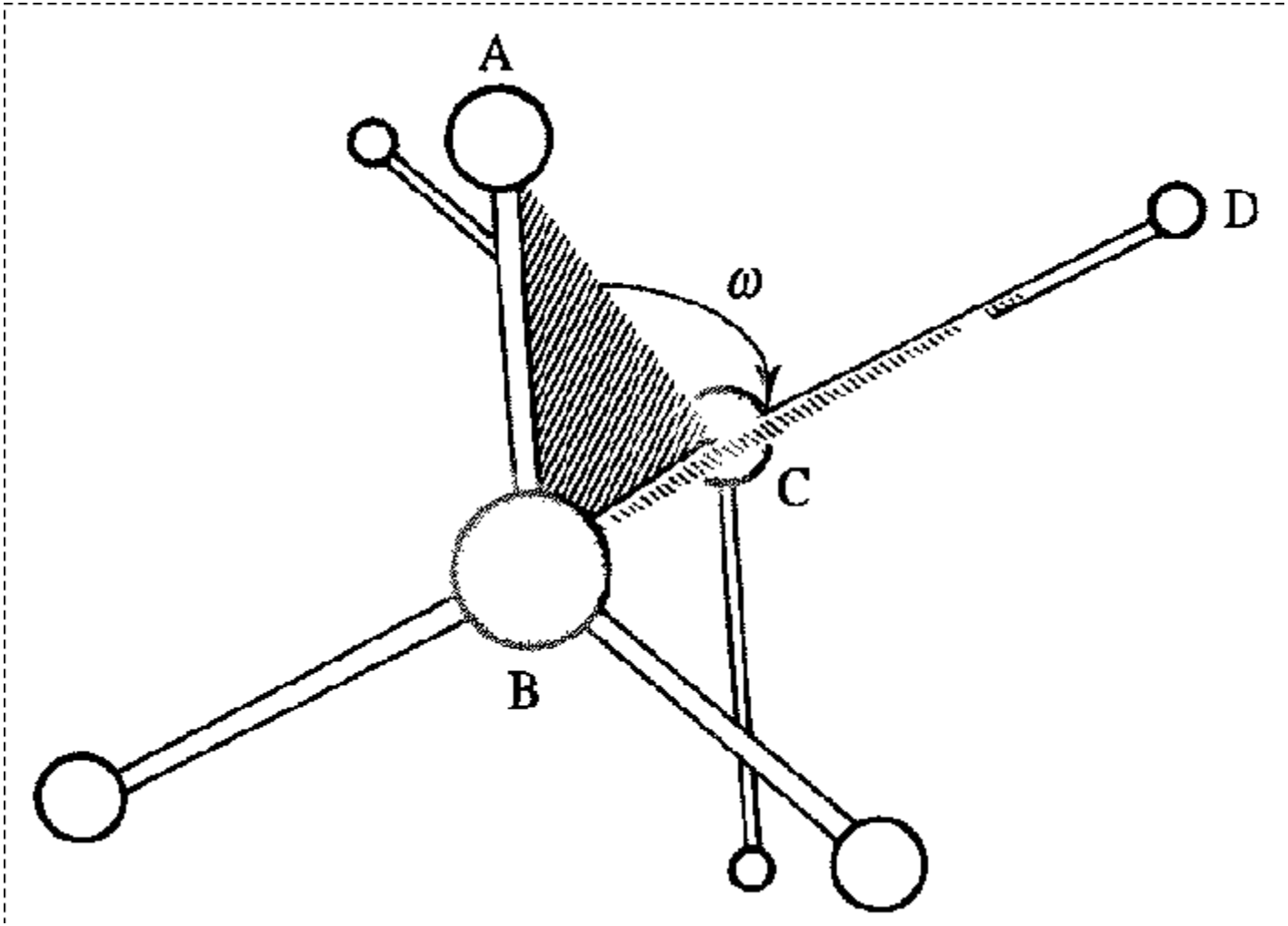


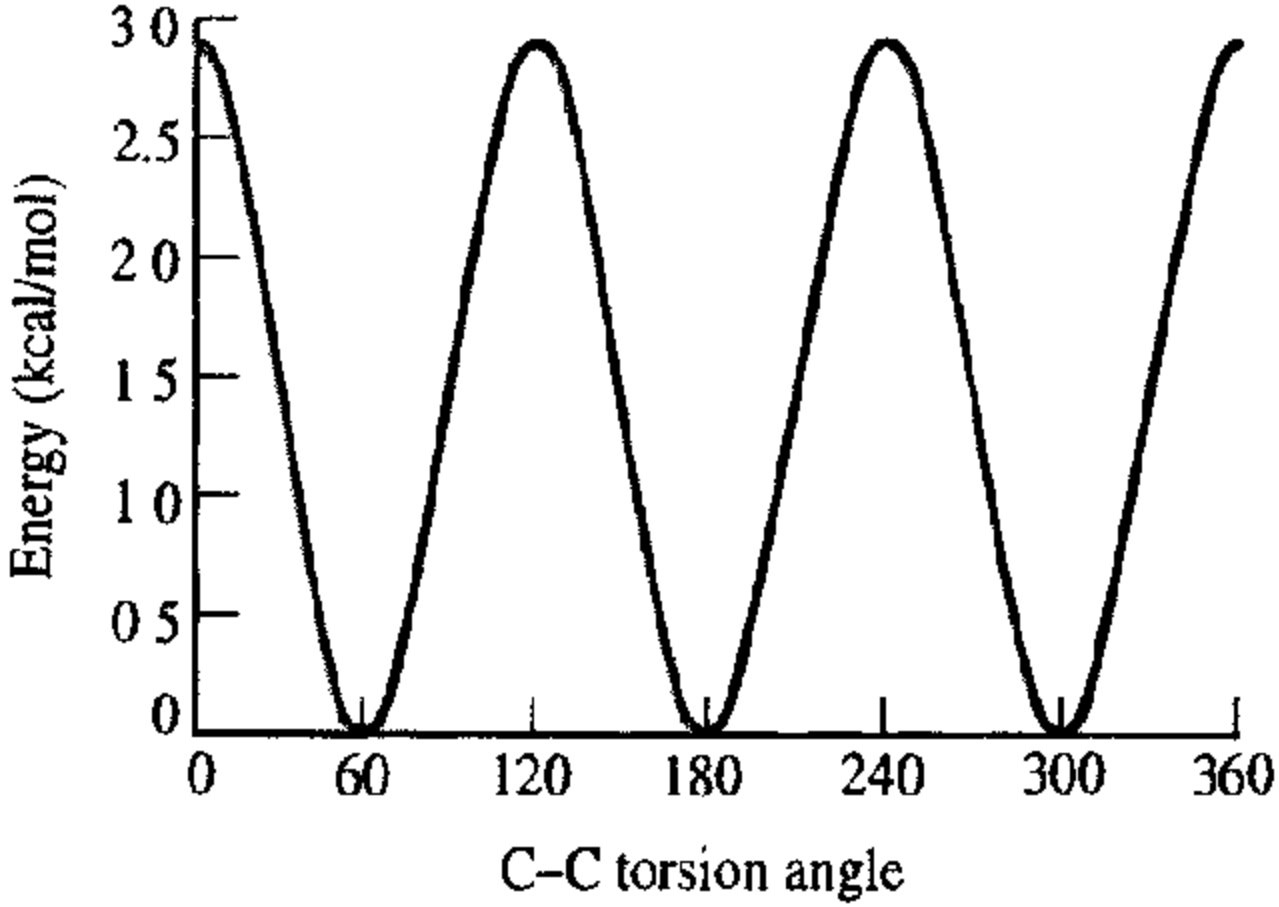
Internal Coordinate System

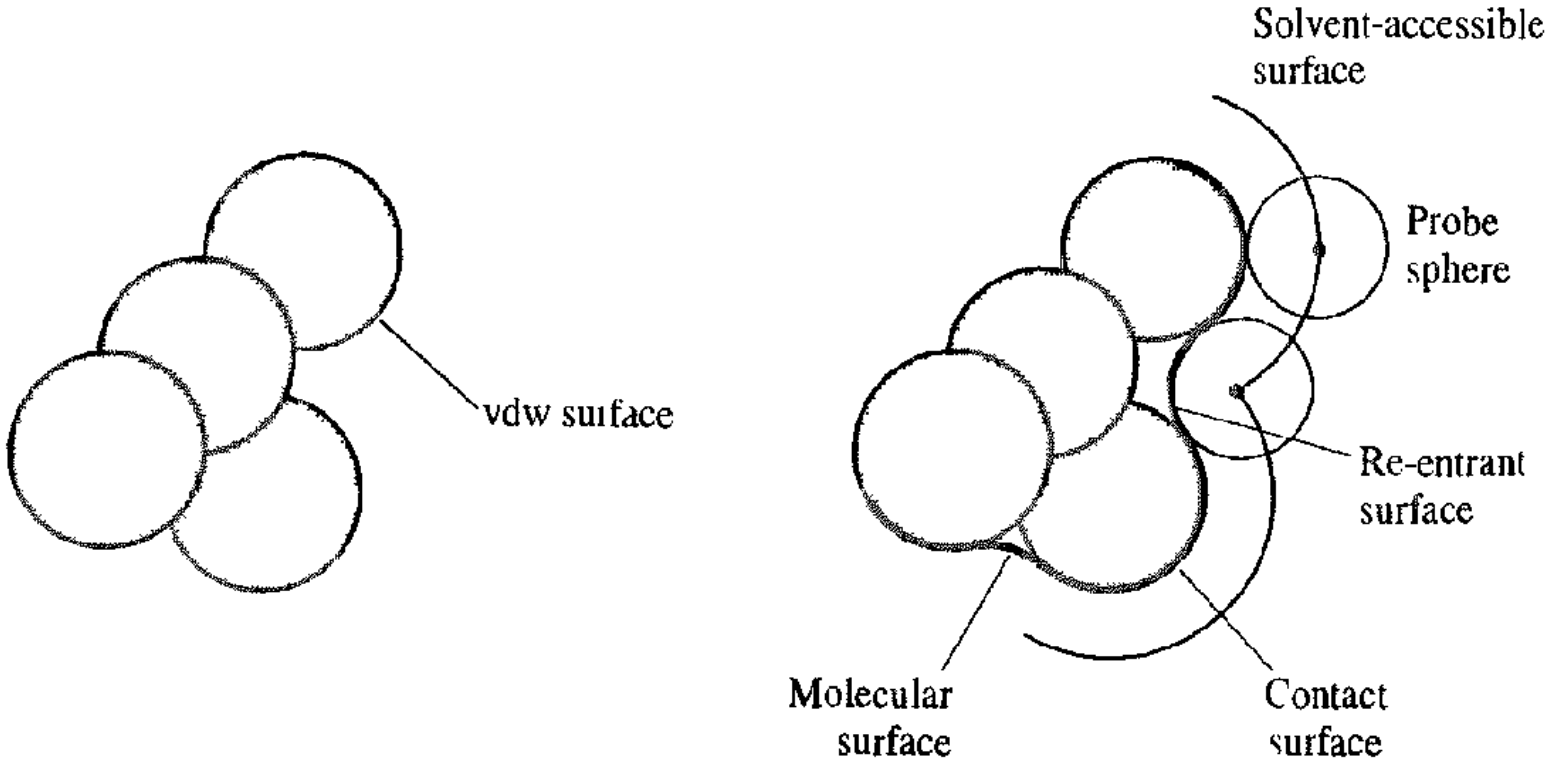


1	C						
2	C	1.54	1				
3	H	1.0	1	109.5	2		
4	H	1.0	2	109.5	1	180.0	3
5	H	1.0	1	109.5	2	60.0	4
6	H	1.0	2	109.5	1	−60.0	5
7	H	1.0	1	109.5	2	180.0	6
8	H	1.0	2	109.5	1	60.0	7

Dihedral Angle




3 0
2.5
2 0
1 5
1 0
0 5
0
Energy (kcal/mol)
0
60
120
180
240
300
360
C–C torsion angle


vdw surface
Solvent-accessible surface
Probe sphere
Re-entrant surface
Molecular surface
Contact surface

Rolling Probe Method

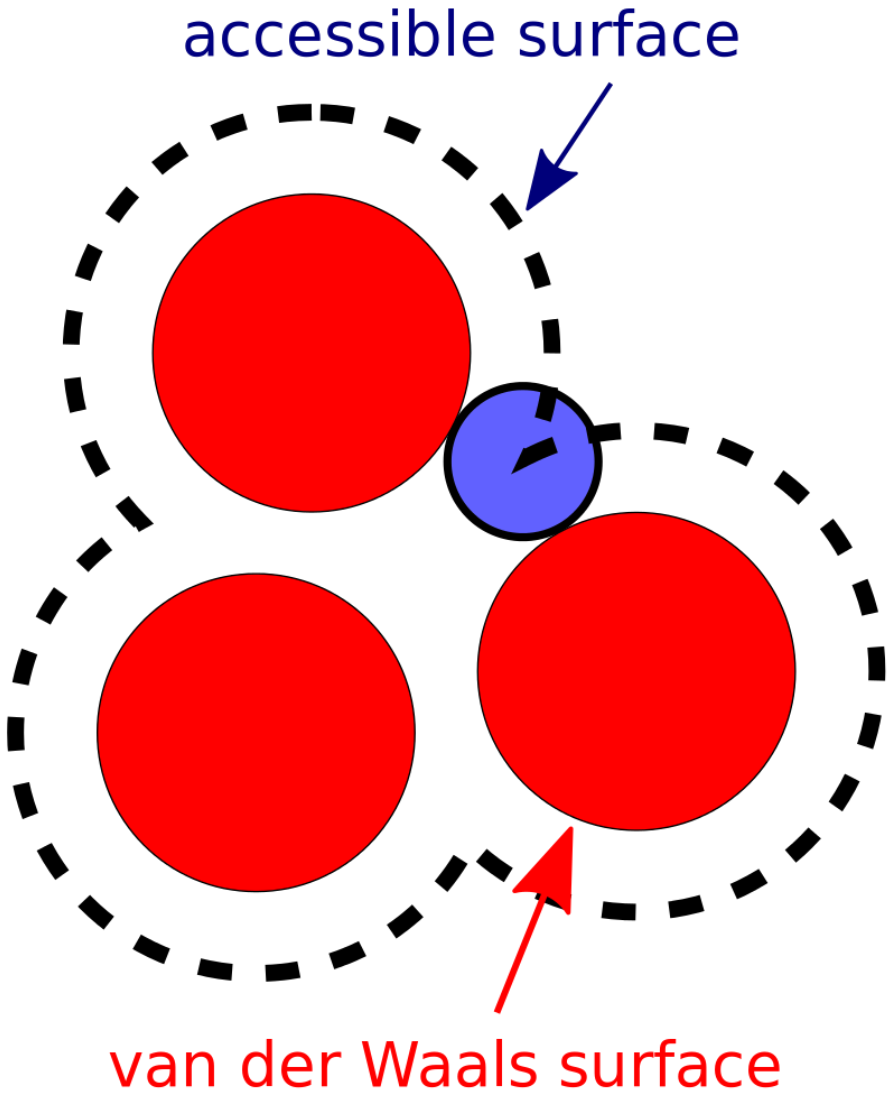
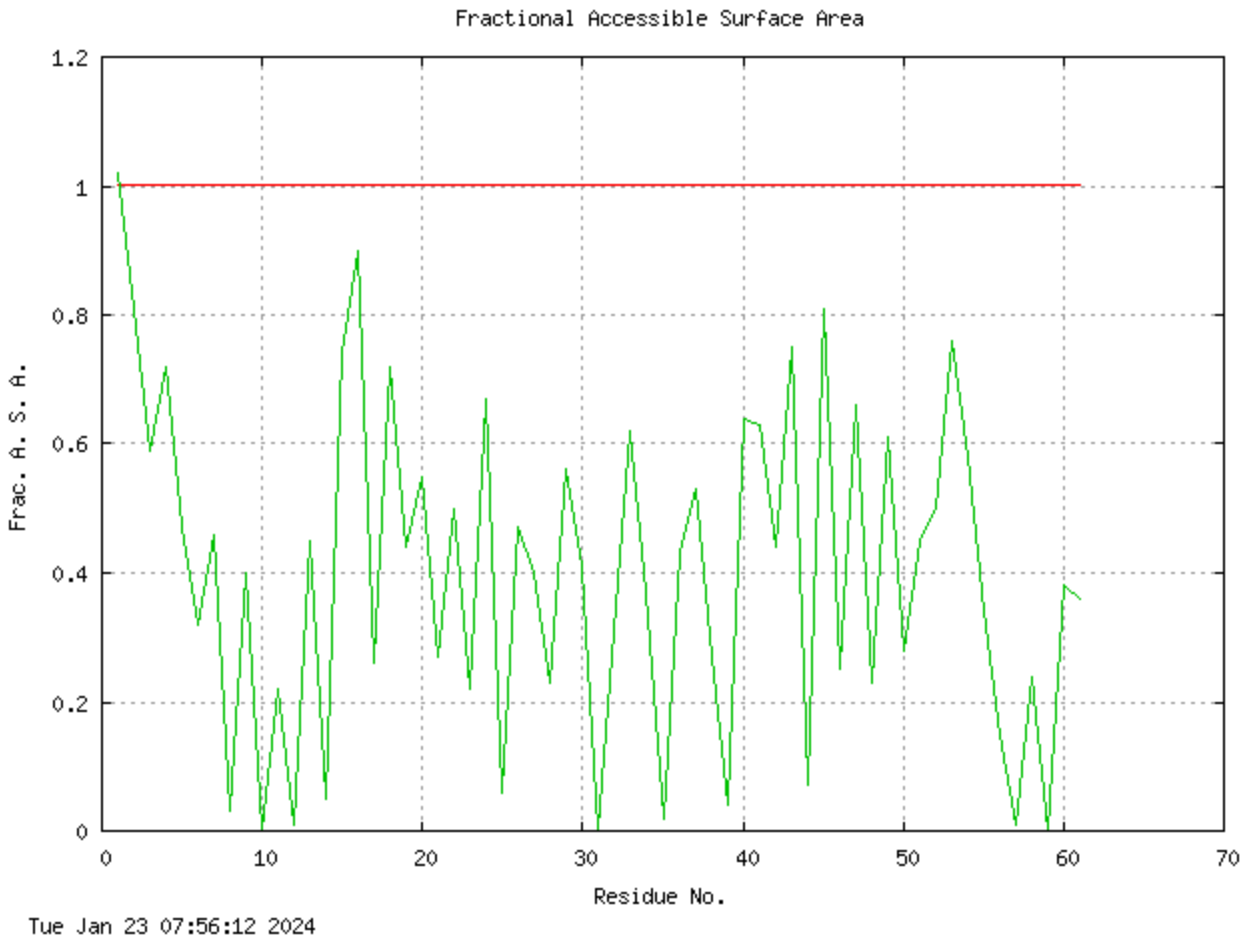


Image Courtesy: Wiki


Fractional Accessible Surface Area
Frac. A. S. A.
Residue No.
1.2
1
0.8
0.6
0.4
0.2
0
0
10
20
30
40
50
60
70
Tue Jan 23 07:56:12 2024

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

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

Units

All SI Units

Except

Angstrom = 0.1 nm
kcal = 4.184 kJ