

#PROGRAMM HAXIS, v0.1.0a (30/03/13)

#Options:

Path to pdb files: /Users/elfikraka/Desktop/haxisv001a8/pdb/  
Helix definition option: 3 (user defined)  
Extra analysis by using HAXIS internal definition: On

#Protein: 2GB1A (56 residues; source PDB)

#Protein sequence and Helix definition

line1: sequence  
line2: Helix definition input  
line3: Helix definition by HAXIS

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      10      20      30      40      50
MTYKLILNGKTLKGETTTEAVDAATAEKVFKQYANDNGVDGEWTYDDATKTFVTVE
      HHHHHHHHHHHHHHHH
      HHHHHHHHHHHHHHHH

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#Residue number, Residue, Cartesian coordinates of anchor point C\_alpha,  
protein backbone length s, curvature kappa, torsion tau

id	res	x	y	z	s	k	t
1	M	-13.296	0.028	3.924	0.000	0.000	0.000
2	T	-9.669	-0.447	4.998	3.955	0.670	0.000
3	Y	-7.173	-2.314	2.811	3.876	0.663	-0.072
4	K	-3.922	-3.881	4.044	3.968	0.811	-0.143
5	L	-0.651	-2.752	2.466	3.926	0.861	-0.111
6	I	2.338	-5.105	2.255	3.927	1.094	-0.094
7	L	5.682	-3.321	1.900	3.931	1.152	-0.078
8	N	8.137	-5.541	0.030	3.893	2.165	-0.017
9	G	10.920	-2.963	0.070	3.879	1.055	0.008
10	K	14.315	-4.474	-0.703	3.934	0.858	-0.112
11	T	16.093	-3.026	2.321	4.158	0.567	0.077
12	L	12.799	-2.608	4.198	4.123	0.314	0.169
13	K	9.579	-4.606	4.659	3.862	0.709	0.053
14	G	6.374	-3.757	6.521	3.854	0.446	0.096
15	E	2.583	-3.604	6.342	3.849	0.674	-0.077
16	T	-0.108	-1.143	7.430	3.848	0.553	-0.026
17	T	-3.848	-0.651	6.886	3.914	0.837	-0.132
18	T	-5.350	2.653	5.692	3.896	0.601	-0.079
19	E	-8.945	3.892	5.458	3.943	1.037	-0.147
20	A	-10.035	4.811	1.920	3.875	0.676	-0.002
21	V	-13.437	5.248	0.258	3.883	1.117	-0.075
22	D	-12.201	3.975	-3.121	4.083	0.244	0.147
23	A	-9.237	2.226	-4.777	3.926	1.003	-0.102
24	A	-7.956	5.461	-6.338	4.064	0.512	0.109
25	T	-7.460	7.449	-3.135	4.208	0.613	0.059
26	A	-6.080	4.229	-1.648	4.150	0.612	0.119
27	E	-3.260	4.204	-4.207	4.156	0.491	0.119
28	K	-2.011	7.699	-3.277	4.194	0.510	0.040
29	V	-2.843	7.366	0.433	4.131	0.540	0.137
30	F	-0.555	4.359	0.858	4.181	0.528	0.040
31	K	1.993	5.797	-1.574	4.159	0.654	0.113
32	Q	2.188	8.829	0.712	4.155	0.595	0.102
33	Y	3.147	6.462	3.535	4.184	0.446	0.087
34	A	5.735	4.444	1.604	4.178	0.631	0.088
35	N	7.291	7.781	0.621	4.171	0.606	0.102
36	D	8.013	8.481	4.295	4.197	0.669	0.099
37	N	10.155	5.328	4.045	4.219	0.628	0.093
38	G	11.601	5.491	0.523	3.957	1.329	-0.138
39	V	9.672	2.625	-1.112	3.923	1.001	0.089
40	D	8.480	3.669	-4.587	3.955	0.524	0.161
41	G	8.449	1.498	-7.716	4.005	0.253	0.291
42	E	5.817	-1.093	-8.656	4.073	0.528	0.017
43	W	2.365	-1.045	-7.038	3.870	0.824	-0.053
44	T	-0.167	-3.897	-6.929	3.873	0.673	-0.048
45	Y	-3.762	-4.276	-5.696	3.914	0.801	-0.082
46	D	-5.366	-7.437	-4.268	3.919	1.408	-0.052
47	D	-9.109	-6.810	-4.634	3.904	1.492	0.051
48	A	-9.462	-10.504	-3.768	4.120	0.532	0.121
49	T	-8.885	-9.951	-0.032	4.307	0.533	0.013
50	K	-8.673	-6.154	0.203	3.993	1.612	-0.174

51	T	-4.889	-6.162	0.598	3.882	0.831	0.038
52	F	-2.612	-3.587	-1.056	3.900	1.035	-0.072
53	T	0.960	-4.492	-1.948	3.857	0.680	-0.036
54	V	3.999	-2.641	-3.279	3.852	0.722	-0.018
55	T	7.534	-3.776	-4.109	3.851	0.598	-0.041
56	E	10.556	-1.553	-4.826	3.946	0.000	0.000

#Frenet unit vector T\_i, N\_i, and B\_i (Coordinates with regard to the origin in the pdb coordinate system)

id	T_i			N_i			B_i		
	x	y	z	x	y	z	x	y	z
1	8.697e-01	-3.453e-02	4.923e-01	0.000e+00	0.000e+00	-0.000e+00	0.000e+00	0.000e+00	0.000e+00
2	8.643e-01	-3.285e-01	-3.809e-01	-4.552e-01	-1.890e-01	-8.701e-01	2.138e-01	9.254e-01	-3.128e-01
3	7.393e-01	-6.621e-01	-1.225e-01	1.355e-01	-3.192e-02	9.903e-01	-6.596e-01	-7.487e-01	6.611e-02
4	9.861e-01	1.532e-01	6.383e-02	-5.523e-02	6.656e-01	-7.443e-01	-1.565e-01	7.304e-01	6.648e-01
5	8.581e-01	-2.934e-01	-4.214e-01	-1.132e-01	-9.086e-01	4.021e-01	-5.009e-01	-2.974e-01	-8.128e-01
6	9.945e-01	-2.615e-02	1.009e-01	3.016e-02	9.988e-01	-3.837e-02	-9.982e-02	4.120e-02	9.942e-01
7	8.808e-01	-9.991e-02	-4.627e-01	-2.240e-01	-9.491e-01	-2.215e-01	-4.170e-01	2.988e-01	-8.584e-01
8	9.429e-01	4.315e-02	-3.302e-01	7.424e-02	9.394e-01	3.348e-01	3.246e-01	-3.402e-01	8.826e-01
9	9.424e-01	2.850e-01	-1.750e-01	2.026e-01	-9.028e-01	-3.793e-01	-2.661e-01	3.220e-01	-9.086e-01
10	9.328e-01	-2.197e-01	2.856e-01	-4.368e-02	7.177e-01	6.949e-01	-3.577e-01	-6.607e-01	6.599e-01
11	-2.507e-01	5.004e-01	8.287e-01	-9.667e-01	-1.741e-01	-1.873e-01	5.055e-02	-8.481e-01	5.274e-01
12	-9.226e-01	-3.598e-01	1.389e-01	2.785e-01	-8.707e-01	-4.055e-01	2.668e-01	-3.354e-01	9.035e-01
13	-8.864e-01	-1.877e-01	4.231e-01	5.020e-02	8.697e-01	4.910e-01	-4.601e-01	4.565e-01	-7.615e-01
14	-9.665e-01	1.378e-01	2.164e-01	-2.546e-01	-6.180e-01	-7.438e-01	3.128e-02	-7.740e-01	6.324e-01
15	-8.969e-01	4.335e-01	8.765e-02	4.158e-01	7.587e-01	5.015e-01	1.509e-01	4.862e-01	-8.607e-01
16	-9.119e-01	3.678e-01	1.820e-01	-4.103e-01	-8.130e-01	-4.131e-01	-3.916e-03	-4.514e-01	8.923e-01
17	-7.224e-01	5.420e-01	-4.294e-01	6.390e-01	7.606e-01	-1.149e-01	2.643e-01	-3.574e-01	-8.958e-01
18	-6.897e-01	7.224e-01	-4.988e-02	-6.763e-01	-6.181e-01	4.007e-01	2.586e-01	3.101e-01	9.149e-01
19	-7.166e-01	2.206e-01	-6.617e-01	6.906e-01	9.109e-02	-7.175e-01	-9.799e-02	-9.711e-01	-2.176e-01
20	-6.280e-01	2.421e-01	-7.396e-01	-7.699e-01	-5.470e-02	6.358e-01	1.135e-01	9.687e-01	2.207e-01
21	-5.938e-01	-8.618e-02	-8.000e-01	7.983e-01	-1.879e-01	-5.722e-01	-1.010e-01	-9.784e-01	1.804e-01
22	6.452e-01	-5.060e-01	-5.724e-01	3.014e-01	-5.198e-01	7.994e-01	-7.020e-01	-6.883e-01	-1.829e-01
23	7.411e-01	2.262e-01	-6.322e-01	-4.440e-01	8.713e-01	-2.088e-01	5.036e-01	4.354e-01	7.462e-01
24	1.425e-01	9.707e-01	1.935e-01	-8.129e-02	-1.834e-01	9.797e-01	9.865e-01	-1.553e-01	5.279e-02
25	1.727e-01	-3.171e-01	9.325e-01	9.572e-02	-9.369e-01	-3.363e-01	9.803e-01	1.474e-01	-1.315e-01
26	6.042e-01	-7.239e-01	-3.330e-01	2.879e-01	5.880e-01	-7.559e-01	7.430e-01	3.609e-01	5.636e-01
27	6.273e-01	6.595e-01	-4.141e-01	-2.238e-01	6.620e-01	7.153e-01	7.459e-01	-3.561e-01	5.629e-01
28	-1.071e-01	5.939e-01	7.974e-01	-4.963e-01	-7.268e-01	4.748e-01	8.615e-01	-3.449e-01	3.726e-01
29	9.969e-02	-6.957e-01	7.114e-01	6.713e-01	-4.807e-01	-5.641e-01	7.344e-01	5.338e-01	4.191e-01
30	7.912e-01	-3.390e-01	-5.090e-01	-2.687e-02	8.122e-01	-5.828e-01	6.110e-01	4.748e-01	6.335e-01
31	3.255e-01	9.341e-01	-1.468e-01	-4.151e-01	2.806e-01	8.654e-01	8.496e-01	-2.208e-01	4.791e-01
32	1.093e-02	1.356e-01	9.907e-01	1.644e-01	-9.775e-01	1.320e-01	9.863e-01	1.614e-01	-3.298e-02
33	4.833e-01	-8.704e-01	9.400e-02	3.107e-01	7.017e-02	-9.479e-01	8.185e-01	4.873e-01	3.044e-01
34	6.263e-01	2.803e-01	-7.274e-01	-2.300e-01	9.580e-01	1.710e-01	7.448e-01	6.020e-02	6.645e-01
35	1.940e-01	8.399e-01	5.069e-01	-1.537e-01	-4.843e-01	8.613e-01	9.689e-01	-2.450e-01	3.516e-02
36	3.450e-01	-6.060e-01	7.167e-01	2.498e-01	-6.768e-01	-6.925e-01	9.048e-01	4.179e-01	-8.210e-02
37	6.153e-01	-3.239e-01	-7.187e-01	-3.644e-02	8.991e-01	-4.363e-01	7.875e-01	2.946e-01	5.413e-01
38	-1.422e-01	-4.789e-01	-8.663e-01	-4.492e-01	-7.486e-01	4.876e-01	-8.820e-01	4.585e-01	-1.087e-01
39	-6.655e-01	-3.259e-01	-6.714e-01	7.297e-02	8.669e-01	-4.931e-01	7.428e-01	-3.772e-01	-5.532e-01
40	-2.525e-02	7.733e-02	-9.967e-01	3.069e-01	-9.483e-01	-8.135e-02	-9.514e-01	-3.079e-01	2.133e-04
41	-2.485e-01	-8.078e-01	-5.345e-01	-8.972e-01	-1.597e-02	4.413e-01	-3.651e-01	5.892e-01	-7.208e-01
42	-9.598e-01	-1.722e-01	2.215e-01	-1.681e-02	8.233e-01	5.673e-01	-2.800e-01	5.408e-01	-7.932e-01
43	-8.295e-01	-4.684e-01	3.041e-01	3.070e-01	-8.373e-01	-4.523e-01	4.665e-01	-2.818e-01	8.384e-01
44	-9.043e-01	-4.188e-01	8.278e-02	-3.812e-01	8.795e-01	2.851e-01	-1.922e-01	2.262e-01	-9.549e-01
45	-6.620e-01	-5.571e-01	5.013e-01	6.285e-01	-7.771e-01	-3.368e-02	4.083e-01	2.928e-01	8.646e-01
46	-9.206e-01	-3.577e-01	1.566e-01	-3.879e-01	8.839e-01	-2.614e-01	-4.493e-02	-3.014e-01	-9.524e-01
47	-8.813e-01	-6.412e-01	-1.694e-01	4.349e-01	-8.974e-01	7.461e-02	-1.849e-01	-7.906e-03	9.827e-01
48	2.003e-01	-4.815e-01	7.039e-01	6.088e-02	7.257e-01	6.853e-01	-9.778e-01	-9.444e-02	1.869e-01
49	-4.176e-02	8.514e-01	5.229e-01	-2.559e-01	4.968e-01	-8.293e-01	-9.658e-01	-1.684e-01	1.971e-01
50	8.071e-01	5.899e-01	2.429e-02	5.629e-01	-7.814e-01	2.693e-01	1.778e-01	-2.037e-01	-9.627e-01
51	9.178e-01	3.631e-01	-1.607e-01	-3.962e-01	8.107e-01	-4.310e-01	-2.627e-02	4.593e-01	8.879e-01
52	8.408e-01	2.594e-01	-4.752e-01	4.022e-01	-8.868e-01	2.275e-01	-3.624e-01	-3.824e-01	-8.500e-01
53	9.569e-01	1.049e-01	-2.708e-01	-1.630e-01	9.658e-01	-2.017e-01	2.404e-01	2.371e-01	9.413e-01
54	9.270e-01	1.390e-01	-3.485e-01	1.954e-01	-9.717e-01	1.323e-01	-3.202e-01	-1.908e-01	-9.279e-01
55	9.800e-01	-4.529e-02	-1.938e-01	3.477e-02	9.978e-01	-5.732e-02	1.960e-01	4.943e-02	9.794e-01
56	6.294e-01	7.595e-01	-1.643e-01	-0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00

#Local axis coordinates (projection of C alpha on axis)

#For helix, they are real axis; otherwise, they are virtual or local axis based on the generalized axis

definition by treating strands, loops, turns etc. as fragments of helices and apply the same procedure.

id	x	y	z
2	-8.228	0.151	7.753
3	-6.845	-2.391	5.211
4	-3.966	-3.347	3.447
5	-0.638	-2.649	2.421
6	2.360	-4.392	2.228
7	6.714	1.050	2.920
8	9.208	8.004	4.857
9	10.416	-0.716	1.014
10	14.313	-4.438	-0.669
11	13.843	-3.431	1.885
12	11.923	0.129	5.473
13	9.891	0.807	7.715
14	7.170	-1.826	8.845
15	2.940	-2.952	6.773
16	-1.054	-3.017	6.478
17	-2.155	1.364	6.581
18	-4.809	3.148	5.371
19	2.159	5.357	-6.079
20	2.190	5.680	-8.176
21	-9.964	4.430	-2.232
22	-12.493	4.478	-3.894
23	-10.793	5.279	-5.509
24	-8.113	5.107	-4.444
25	-7.240	5.292	-3.909
26	-5.452	5.511	-3.296
27	-3.775	5.726	-2.562
28	-3.140	6.046	-2.197
29	-1.316	6.273	-0.850
30	-0.615	6.174	-0.444
31	1.056	6.431	0.380
32	2.570	6.558	1.019
33	3.808	6.611	1.517
34	5.207	6.642	1.996
35	6.972	6.775	2.409
36	8.561	6.996	2.776
37	10.156	5.297	4.060
38	9.808	2.503	2.469
39	9.765	3.736	-1.744
40	8.494	3.627	-4.591
41	6.867	1.470	-6.938
42	5.853	-2.861	-9.874
43	4.095	-5.762	-9.586
44	0.658	-5.801	-7.546
45	-4.024	-3.952	-5.682
46	-6.593	-4.641	-5.095
47	-7.542	-10.044	-4.365
48	-9.376	-9.473	-2.795
49	-9.056	-9.619	-0.586
50	-4.468	-11.991	2.215
51	-3.866	-8.254	1.711
52	-0.530	-8.177	0.122
53	-0.688	5.270	-3.987
54	2.347	5.574	-4.398
55	7.134	-15.255	-3.450

#Parameter a<sub>i</sub> (translation per residue along axis)

2	3.852	T
3	3.509	Y
4	3.552	K
5	3.473	L
6	7.004	I
7	7.637	L
8	9.605	N
9	5.646	G
10	2.785	K
11	5.407	T
12	3.101	L
13	3.952	K
14	4.842	G

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15      4.005 E
16      4.519 T
17      3.419 T
18     13.584 T
19      2.122 E
20     13.588 A
21      3.027 V
22      2.477 D
23      2.888 A
24      1.041 A
25      1.902 T
26      1.844 A
27      0.799 E
28      2.279 K
29      0.816 V
30      1.881 F
31      1.648 K
32      1.336 Q
33      1.479 Y
34      1.817 A
35      1.646 N
36      2.661 D
37      3.234 N
38      4.390 G
39      3.120 V
40      3.579 D
41      5.330 G
42      3.404 E
43      3.997 W
44      5.368 T
45      2.724 Y
46      5.534 D
47      2.481 D
48      2.237 A
49      5.875 T
50      3.818 K
51      3.696 T
52     14.062 F
53      3.077 T
54     21.392 V

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#Helices input from user defined: residue(Start) - residue(End)
# 1 : 22      36
#Helices identified by HAXIS: residue(Start) - residue(End)
# 1 : 23      36
#Currently, HAXIS look for segments showing regular geometry parameters:
#rise parameter a, radius, arc length and curvature peak (of fitted axis curve), and
#angle of neighboring local axis directions.
#Where the regular region ends are the start/ends of helix.

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#Anchor points of helix axis (projection of C_alpha position on helix axis)

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```

# 1: 22      36
  id   x       y       z
22 -12.493  4.478  -3.894
23 -10.793  5.279  -5.509
24  -8.113  5.107  -4.444
25  -7.240  5.292  -3.909
26  -5.452  5.511  -3.296
27  -3.775  5.726  -2.562
28  -3.140  6.046  -2.197
29  -1.316  6.273  -0.850
30  -0.615  6.174  -0.444
31   1.056  6.431   0.380
32   2.570  6.558   1.019
33   3.808  6.611   1.517
34   5.207  6.642   1.996
35   6.972  6.775   2.409
36   8.561  6.996   2.776

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#Polynomial fit of the helix axis: coefficients a_0 + a_1 x+a_2 x^2+...a_n x^n

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```
#2nd order: a0->a2
# 1: 22 36
x -1.194138e+01 1.554676e+00 -8.750738e-03
y 4.679109e+00 2.540311e-01 -6.858265e-03
z -5.205507e+00 5.352758e-01 4.798653e-03
#3rd order: a0->a3
# 1: 22 36
x -1.250314e+01 2.139074e+00 -1.167819e-01 5.144343e-03
y 4.641252e+00 2.934133e-01 -1.413842e-02 3.466739e-04
z -4.553786e+00 -1.427047e-01 1.301296e-01 -5.968138e-03
#5th order: a0->a5
# 1: 22 36
x -1.258294e+01 2.264990e+00 -1.426845e-01 4.144012e-03 4.556477e-04 -2.135625e-05
y 4.578922e+00 5.724760e-01 -1.795459e-01 3.422397e-02 -2.819752e-03 8.187324e-05
z -4.134046e+00 -1.294973e+00 6.599650e-01 -9.466891e-02 6.212691e-03 -1.548519e-04

#Curvature kappa and torsion tau of the helix axis presented by polynomial fits of order 2, 3, 5
```

```
Helix # 1: 22 36
```

	2nd order		3rd order		5th order	
	kappa	tau	kappa	tau	kappa	tau
22	8.912038e-03	0.000000e+00	8.050363e-02	2.462761e-03	2.138779e-01	-2.899003e-02
23	9.076882e-03	0.000000e+00	8.117445e-02	4.125639e-03	1.560586e-01	-5.735565e-02
24	9.243799e-03	0.000000e+00	7.567783e-02	7.085667e-03	8.978135e-02	-1.094208e-01
25	9.412676e-03	0.000000e+00	6.423129e-02	1.295036e-02	4.984203e-02	-1.953395e-01
26	9.583388e-03	0.000000e+00	4.828483e-02	2.726650e-02	3.813295e-02	-1.928753e-01
27	9.755794e-03	0.000000e+00	2.967510e-02	8.007067e-02	3.638132e-02	-1.916720e-01
28	9.929739e-03	0.000000e+00	1.075063e-02	6.476303e-01	3.308572e-02	-3.057252e-01
29	1.010505e-02	0.000000e+00	1.418325e-02	3.832105e-01	3.559531e-02	-2.654454e-01
30	1.028154e-02	0.000000e+00	3.437704e-02	6.501078e-02	4.225152e-02	-8.234734e-02
31	1.045900e-02	0.000000e+00	5.431003e-02	2.464042e-02	4.138111e-02	7.651240e-02
32	1.063722e-02	0.000000e+00	7.157382e-02	1.232830e-02	3.389847e-02	3.182692e-01
33	1.081594e-02	0.000000e+00	8.371374e-02	6.932030e-03	5.207478e-02	1.999722e-01
34	1.099491e-02	0.000000e+00	8.883272e-02	4.082535e-03	1.201831e-01	4.731322e-02
35	1.117386e-02	0.000000e+00	8.680696e-02	2.438595e-03	2.311081e-01	1.079763e-02
36	1.135248e-02	0.000000e+00	7.944992e-02	1.462275e-03	2.909997e-01	4.204175e-04

```
#Helix classification and global geometry parameters
```

```
#Helix (beginning and ending residue #)
#Shape: LC: weakly curved, HC: highly curved, L: linear
#Regularity: R: regular, IR: irregular, SI: strongly irregular
#C_av: average radius of curvature, C_max: maximum radius of curvature
#delta_C: Variation of radius of curvature
#delta_C/C_av
#k_av: average curvature, k_max: maximum curvature
#delta_k: Variation of radius of curvature
#delta_k/k_av
#Type: conventional type L: linear, C: curved, K: kinked
```

#	Helix	Shape	Reg.	C_av	C_max	Delta_C	Delta_C/C_av	k_av	k_max
Delta_k	Delta_k/k_av	Type							
1:	22 36	LC	IR	9.9413e+01	1.1221e+02	2.4121e+01	2.4264e-01	1.0116e-02	1.1352e-02
	2.4404e-03		C						

```
#Kinks (based on the irregularity of the rise parameter a_i)
```

#	Helix	Kinks	a_i	delt_a/a_av
1:	22 36	:	28	2.2787e+00
				3.3744e-01

```
#Kinks (based on the axis curvature kappa)
```

#pdb	kink	----	Helix	----	kinkregion	-----	k	quartet	-----		-----	rise	-----
2GB1A	25	1:	22 36	24 28	2.1182	1.9984	3.3133	3.2404					
2GB1A	28	1:	22 36	27 30	3.3133	3.2404	3.1440	3.3138	0.7987		2.2787	0.8159	

```
#END
```

```
*****
```

```
#Extra analysis by using HAXIS internal helices definition
```

```
#Helices input from HAXIS: residue(Start) - residue(End)
# 1 : 23 36
#Currently, HAXIS look for segments showing regular geometry parameters:
#rise parameter a, radius, arc length and curvature peak (of fitted axis curve), and
#angle of neighboring local axis directions.
#Where the regular region ends are the start/ends of helix.
```

```
#Anchor points of helix axis (projection of C_alpha position on helix axis)
```

```
# 1: 23 36
  id  x      y      z
 23 -10.793  5.279 -5.509
 24 -8.113  5.107 -4.444
 25 -7.240  5.292 -3.909
 26 -5.452  5.511 -3.296
 27 -3.775  5.726 -2.562
 28 -3.140  6.046 -2.197
 29 -1.316  6.273 -0.850
 30 -0.615  6.174 -0.444
 31  1.056  6.431  0.380
 32  2.570  6.558  1.019
 33  3.808  6.611  1.517
 34  5.207  6.642  1.996
 35  6.972  6.775  2.409
 36  8.561  6.996  2.776
```

```
#Polynomial fit of the helix axis: coefficients a_0 + a_1 x+a_2 x^2+...a_n x^n
```

```
#2nd order: a0->a2
```

```
# 1: 23 36
x -1.004116e+01  1.420589e+00 -1.180203e-03
y  5.055742e+00  1.977142e-01 -4.092006e-03
z -5.508480e+00  8.222862e-01 -1.321518e-02
```

```
#3rd order: a0->a3
```

```
# 1: 23 36
x -1.048785e+01  1.929242e+00 -1.027025e-01  5.206274e-03
y  5.107761e+00  1.384807e-01  7.730449e-03 -6.062798e-04
z -5.326257e+00  6.147898e-01  2.819914e-02 -2.123811e-03
```

```
#5th order: a0->a5
```

```
# 1: 23 36
x -1.068856e+01  2.522636e+00 -3.892988e-01  5.533690e-02 -3.655781e-03  9.456776e-05
y  5.263558e+00 -2.867085e-01  1.997657e-01 -3.172942e-02  2.071523e-03 -4.786623e-05
z -5.474671e+00  1.168463e+00 -2.824252e-01  6.021242e-02 -5.188572e-03  1.527719e-04
```

```
#Curvature kappa and torsion tau of the helix axis presented by polynomial fits of order 2, 3, 5
```

```
Helix # 1: 23 36
```

	2nd order		3rd order		5th order	
	kappa	tau	kappa	tau	kappa	tau
23	1.035892e-02	0.000000e+00	5.154769e-02	5.278167e-04	1.439780e-01	3.147076e-02
24	1.056020e-02	0.000000e+00	4.852195e-02	9.213785e-04	1.117869e-01	1.008524e-01
25	1.076303e-02	0.000000e+00	4.242689e-02	1.742582e-03	6.202395e-02	3.217342e-01
26	1.096711e-02	0.000000e+00	3.335810e-02	3.794867e-03	4.308569e-02	4.220308e-01
27	1.117215e-02	0.000000e+00	2.220748e-02	1.070660e-02	4.010865e-02	3.059218e-01
28	1.137781e-02	0.000000e+00	1.295422e-02	3.644561e-02	3.165484e-02	3.969179e-01
29	1.158372e-02	0.000000e+00	1.758730e-02	2.111139e-02	3.080439e-02	4.033695e-01
30	1.178950e-02	0.000000e+00	3.090146e-02	6.676884e-03	4.399245e-02	2.012598e-01
31	1.199473e-02	0.000000e+00	4.423368e-02	2.881138e-03	5.736874e-02	1.176859e-01
32	1.219896e-02	0.000000e+00	5.487294e-02	1.486711e-03	5.784672e-02	1.079956e-01
33	1.240171e-02	0.000000e+00	6.155029e-02	8.406199e-04	4.483330e-02	1.721572e-01
34	1.260249e-02	0.000000e+00	6.397519e-02	4.989729e-04	6.530241e-02	8.613725e-02
35	1.280078e-02	0.000000e+00	6.270703e-02	3.046717e-04	1.144511e-01	2.432315e-02
36	1.299601e-02	0.000000e+00	5.880650e-02	1.897211e-04	1.361687e-01	8.514018e-03

```
#Helix classification and global geometry parameters
```

```
#Helix (beginning and ending residue #)
#Shape: LC: weakly curved, HC: highly curved, L: linear
#Regularity: R: regular, IR: irregular, SI: strongly irregular
#C_av: average radius of curvature, C_max: maximum radius of curvature
#delta_C: Variation of radius of curvature
#delta_C/C_av
```

#k\_av: average curvature, k\_max: maximum curvature

#delta\_k: Variation of radius of curvature

#delta\_k/k\_av

#Type: conventional type L: linear, C: curved, K: kinked

#	Helix	Shape	Reg.	C_av	C_max	Delta_C	Delta_C/C_av	k_av	k_max
Delta_k	Delta_k/k_av	Type							
1:	23 36	LC IR		8.6019e+01	9.6535e+01	1.9589e+01	2.2772e-01	1.1683e-02	1.2996e-02
	2.6371e-03	2.2571e-01	C						

#Kinks (based on the irregularity of the rise parameter a\_i)

#	Helix	Kinks	a_i	delt_a/a_av
1:	23 36	:	28	2.2787e+00
				3.8585e-01

#Kinks (based on the axis curvature kappa)

#pdb	kink	----	Helix	----	kinkregion	-----	k quartet	-----		-----	rise	-----
2GB1A	28	1:	23 36	27 30	3.3133	3.2404	3.1440	3.3138		0.7987	2.2787	0.8159

#END

Description of the following pictures **P1 – P5**

**P1) Presentation of the rise parameter  $a_i$**

The rise parameter  $a_i$  ( $i$  is the residue counter) measures the difference in the positions of residues  $i$  to  $i+1$  after projection onto the helix axis. It differs for alpha (ca. 1.5 Å),  $3_{10}$  (ca. 2 Å), and pi-helices (ca. 1 Å) as described in the [HAXIS publication; see http://smu.edu/catco/publications/2009-present.html](http://smu.edu/catco/publications/2009-present.html), [paper 342](#). Formally one can calculate also an axis for  $\beta$ -strands, loops, coils, and turns by applying the same approach. Only in the latter cases, the rise parameters are significantly larger than 2 Å and irregular. In the figure **P1** the rise parameters are given for all residues of the proteins. Those of the helix can easily be identified: A23 – N35. Systematic study of the rise parameters for  $\beta$ -strands, loops, etc. can lead to new a description of these secondary structural units.

**P2) Presentation of the curvature  $k$  as a function of the arc length  $s$  of the helix axis (given for each helix in the protein)**

The curvature of the helix axis (calculated by HAXIS and fitted by a fifth order polynomial; see [HAXIS publication; see http://smu.edu/catco/publications/2009-present.html](http://smu.edu/catco/publications/2009-present.html), [paper 342](#)) is given as a function of the arc length  $s$  and the positions of the anchor-points ( $C\alpha$ ) of the residues forming the helix are given by dots and the appropriate residue symbol. As an example, the helix from A23 to N35 is shown. The helix axis is strongly bent toward its center (E27 – F30) as indicated by 4 curvature peaks. It is almost linear toward its end (small curvature peaks).

**P3) Presentation of the spline-fitted axis of the entire protein**

As mentioned for **P1**, a local axis can be calculated not only for helices but also for  $\beta$ -strands, coils, loops, or turns. These local axes are connected in the 3-dimensional perspective representation (in  $x, y, z$ -space) with the help of cubic spline-fits to a smooth line representing no longer the backbone line of the protein but the axis line of the secondary structural units. The only helix (A23 – N35) is easily recognized because its axis corresponds to the regularly bent (almost horizontal) line in the upper part of the diagram.

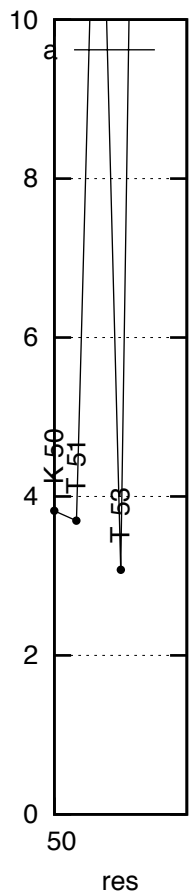
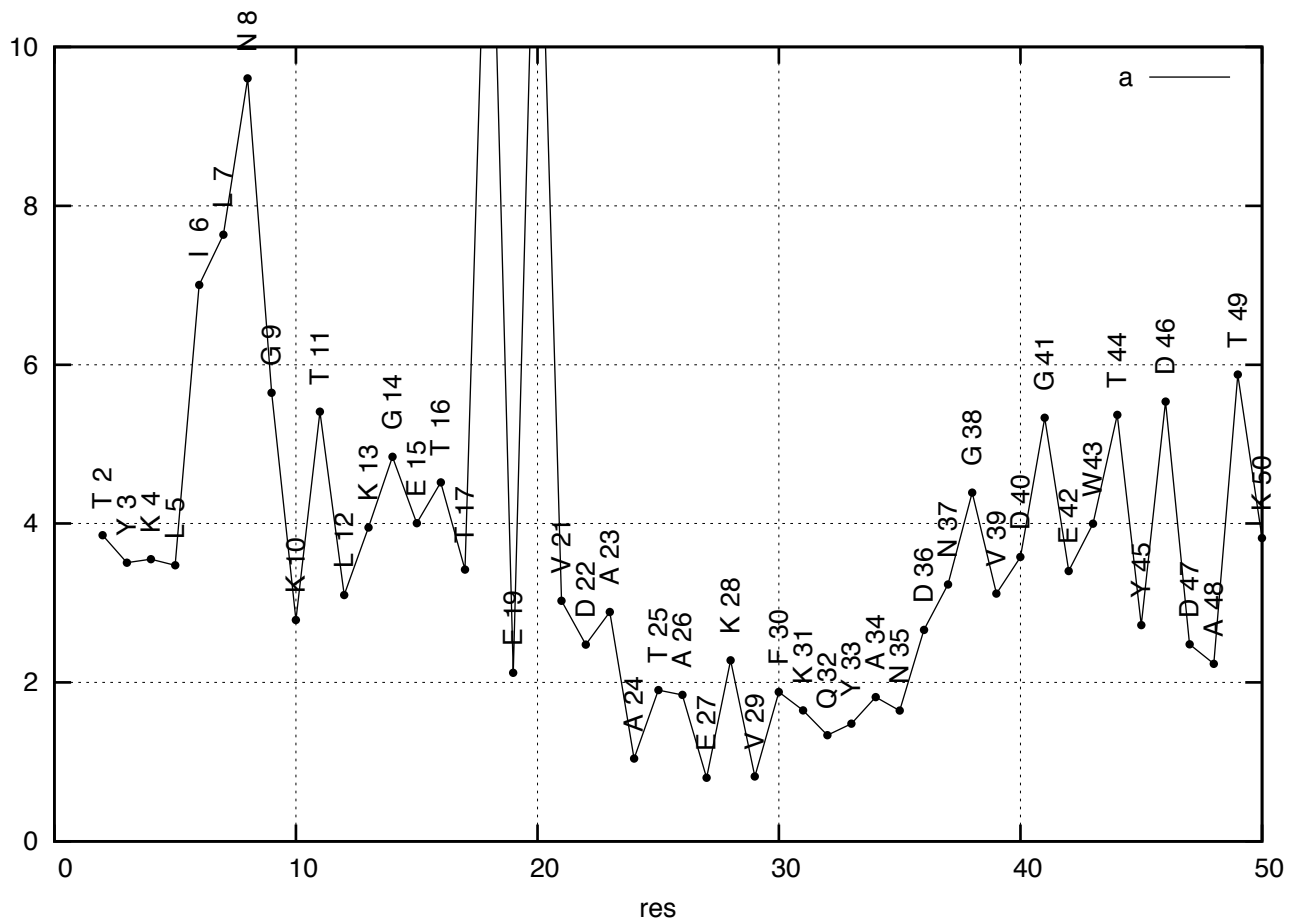
**P4) Presentation of the position of the helix axis with regard to the protein backbone line (given for each helix in the protein)**

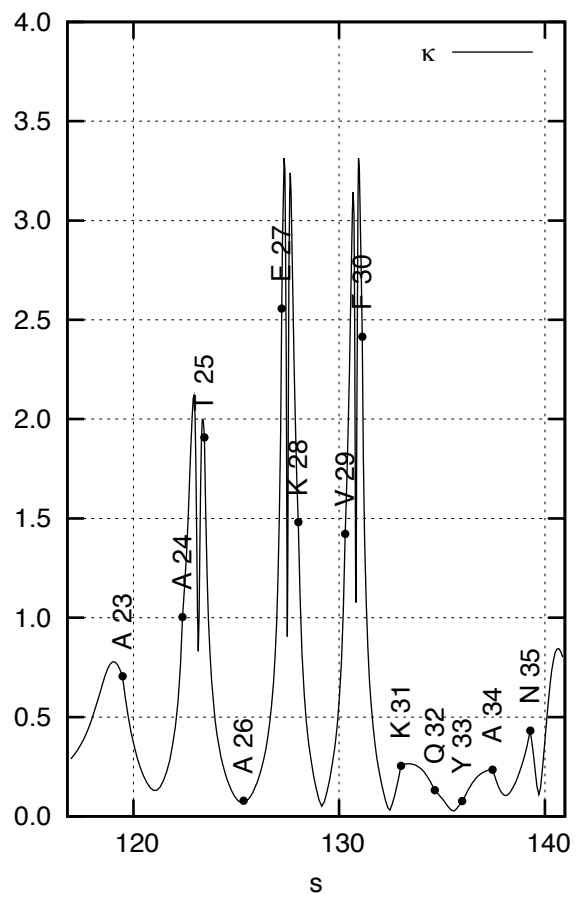
A simple backbone line is generated by connecting the  $C\alpha$  anchor points of the residues. The helix axis is indicated by red dots, which correspond to the positions of the helix residues projected onto the helix axis.

**P5) Enlargement of P4 showing just the helix (given for each helix in the protein)**

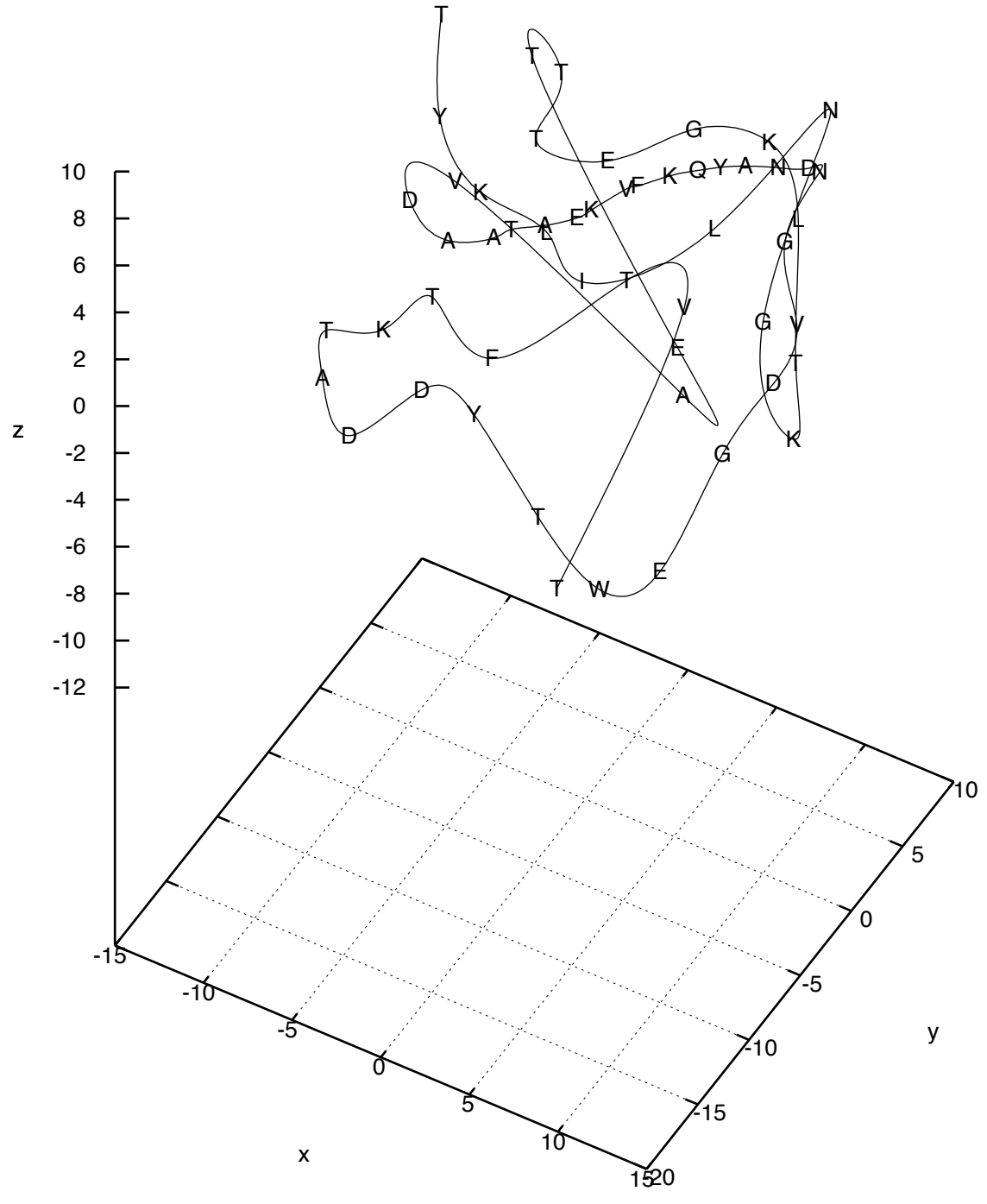
Backbone line and helix axis (given by red dots) are shown exclusively. This plot is generated in the same way as **P4**, however only the helix in question is shown.



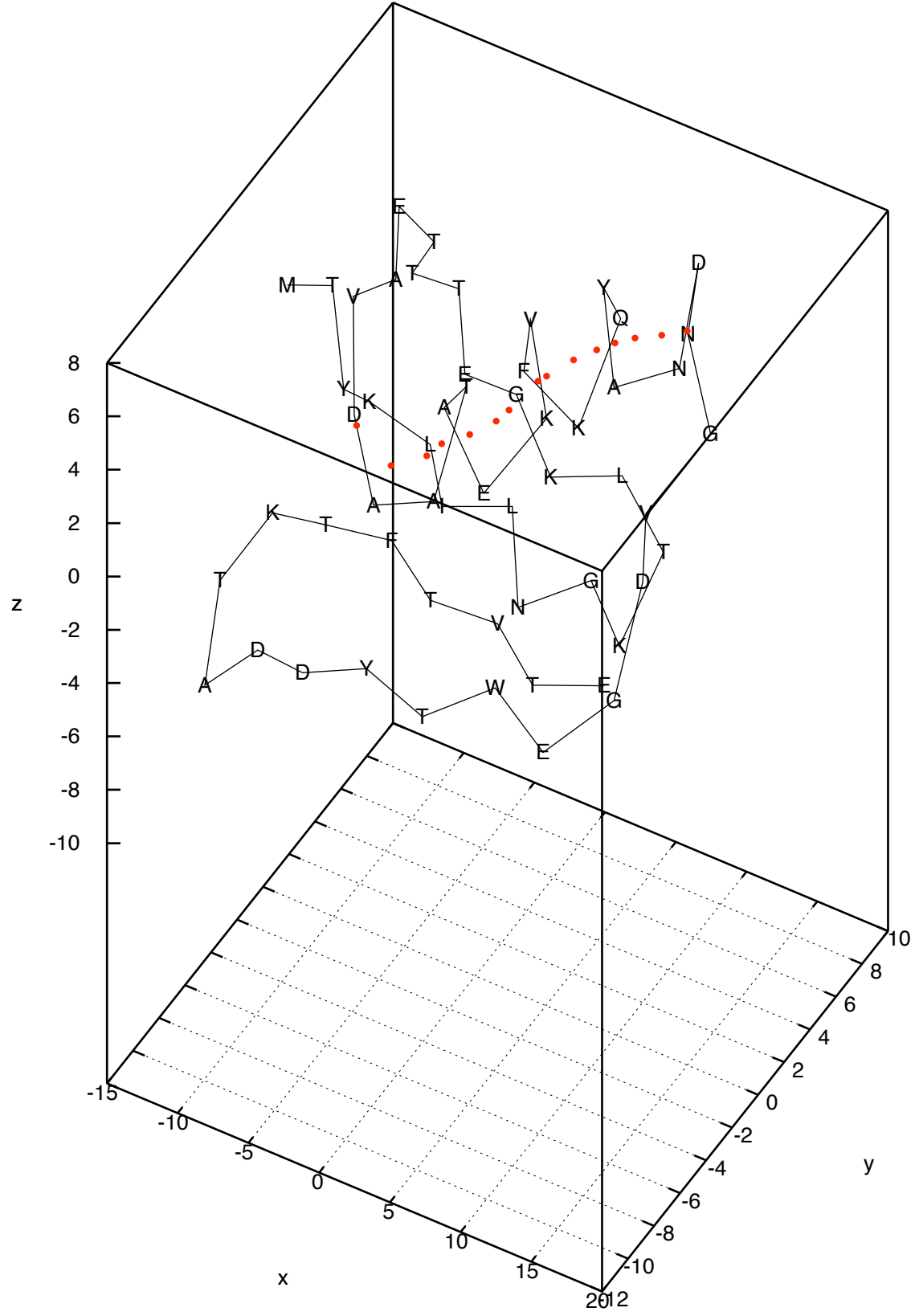




r(s) ———



r(s) ———



r(s) ———

