

Programming, development methods and project managements

Subject: Assignment of protein secondary structures

Objective:

Implementation of the DSSP method for the assignment of regular secondary structures (alpha helices and beta strands).

Reference:

[Wolfgang Kabsch, Christian Sander. *Dictionary of protein secondary structure: Pattern recognition of hydrogen-bonded and geometrical features*. Biopolymers, December 1983; 22\(12\): 2577-2637.](#)

Student:

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GitHub repository:

https://github.com/valentinbaloche/short_project.git

Foreword

The article of Wolfgang Kabsch and Christian Sander attempts to define a predictive algorithm for protein folding in secondary structures. This algorithm is based on the use of atomic coordinates in order to estimate the presence or absence of hydrogen bonds (H bonds).

The idea of the authors is to calculate the electrostatic interaction energy between two H-bonding groups using the equation below.

$$E = q_1 q_2 \left(\frac{1}{r(ON)} + \frac{1}{r(CH)} - \frac{1}{r(OH)} - \frac{1}{r(CN)} \right) * f$$

($q_1 = 0.42e$; $q_2 = 0.20e$; e being the unit electron charge and $r(AB)$ the interatomic distance from A to B)

It's then possible for them to define the presence or absence of an H bond using a single decision parameter. Indeed, it's possible to define an energy cutoff beyond which the formation of a H bond is impossible. In their article, they assure an H bond formation for E up to -0.5 kcal/mol.

This postulate represents the starting point of the all algorithm whose aim is then to recognize the different H-bonds patterns specific to each structure (turns, bridges, helices, beta sheets, etc.). This algorithm is now well known as the DSSP (Define Secondary Structure of Proteins) algorithm.

The objective of my project is to implement this method to assign regular secondary structures (alpha helices and beta strands) on a protein sequence. It includes several steps: 1) parsing of a Protein Data Bank (PDB) file; 2) calculation of the interaction energies between amine (NH) and carbonyl (CO) groups of the main chain; 3) the assignment of secondary structures; 4) the comparison with the prediction performed by DSSP.

Program development (see figure 1)

I- Parsing

For this first part, I have implemented the reduce program to add hydrogen coordinates in the file.pdb. From this modified fileOH.pdb, I have isolated 3 different lists: 1) the protein sequence; 2) the atoms name; 3) the atoms coordinates. To be able to iterate over them at the same time, I have added a vector harmonization step. That one creates a list of lists from the atoms name and coordinates, so that the elements of the sublists correspond to the components of each residue. I have then chosen to create a Residue class to store the different attributes of interest (name, position, coordinates of N, H, C and O from the main chain). At the same time, I have filled all these Residue objects in a list (= protein) in order to iterate over them.

II- Prediction

This part takes what is described in the article. I have used the formula presented in the previous section to calculate the interaction energies between each residue to determine which ones were most likely to form hydrogen bonds. I have then looked for the patterns associated with the helices and the beta strands. Since the attributes were protected, I have created getters and setters to use and modify them.

III- Comparison

For this last part, I have implemented the DSSP program in order to perform a comparison. From the generated file.txt, I have isolated the structural elements. I then have compared the predictions obtained for the two programs residue by residue, in order to extract a detailed comparative analysis. When running the program, a first part of the analysis is returned to the shell. It summarizes the differences between the two predictions. A second part of the analysis is sent in a file.txt. That one presents the alignment of the two predictions along the protein sequence.

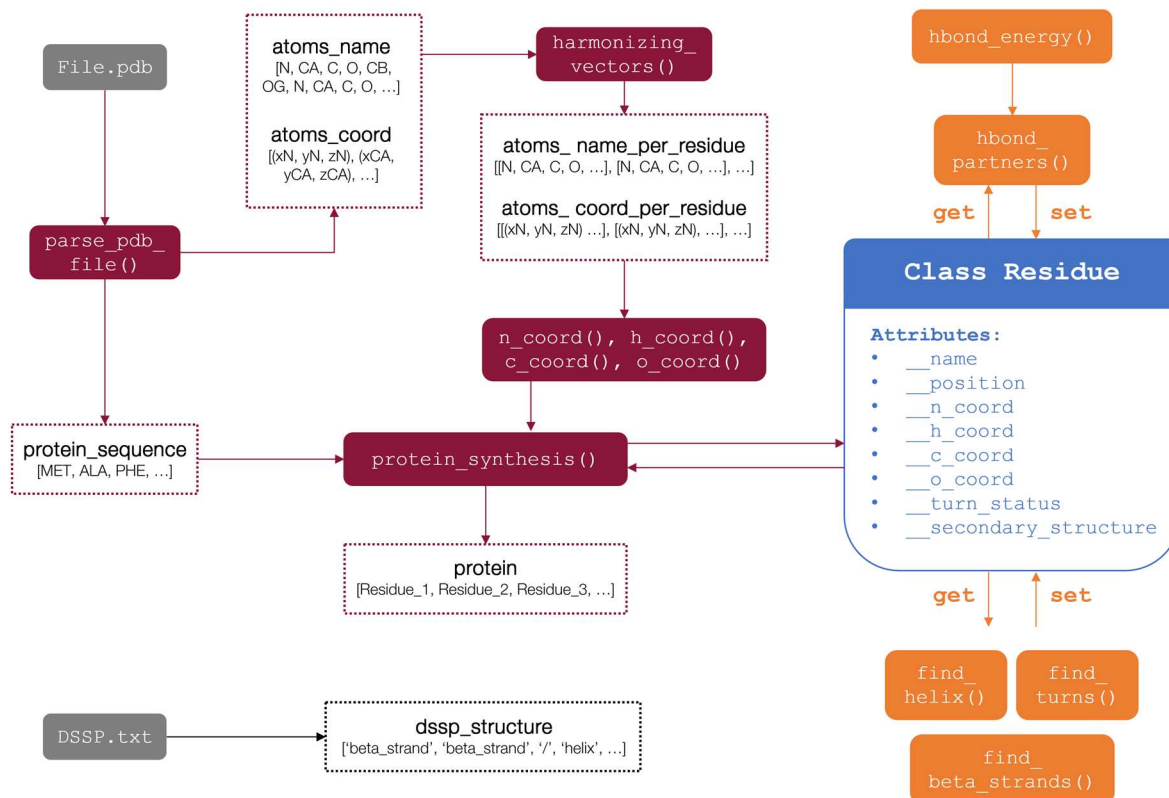


Figure 1. Workflow of the SPVB prediction program (short_project_valentin_baloche.py).

Tests

You will find below the shell outputs obtained from 3 different PDB files: 4ajv.pdb (rich in beta strands), 6drx.pdb (rich in helices) and 1bta.pdb (mix of both). The `<id>_spvb_results.txt` are in the annex.

```
$ python short_project_valentin_baloche.py 4ajv.pdb
```

```
===== ANALYSIS OF 4ajv.pdb =====
```

```
76% of the structures predicted in this program are also found in the DSSP prediction
(accuracy for each structure: helix: 0/7 ; beta strand: 69/74 ; turn : 1/11).
```

```
Comparing the regions predicted as 'unstructured' by this program and the DSSP prediction,
this program has missed 0 helix, 7 beta strand(s) and 13 turn(s).
```

```
For more details, please see the 4ajv_spvb_results.txt in your working directory.
```

```
=====
```

```
$ python short_project_valentin_baloche.py 6drx.pdb
```

```
===== ANALYSIS OF 6drx.pdb =====
```

```
90% of the structures predicted in this program are also found in the DSSP prediction  
(accuracy for each structure: helix: 293/322 ; beta strand: 0/0 ; turn : 0/2).
```

```
Comparing the regions predicted as 'unstructured' by this program and the DSSP prediction,  
this program has missed 0 helix, 0 beta strand(s) and 5 turn(s).
```

```
For more details, please see the 6drx_spvb_results.txt in your working directory.
```

```
=====
```

```
$ python short_project_valentin_baloche.py 1bta.pdb
```

```
===== ANALYSIS OF 1bta.pdb =====
```

```
78% of the structures predicted in this program are also found in the DSSP prediction  
(accuracy for each structure: helix: 37/46 ; beta strand: 14/16 ; turn : 0/3).
```

```
Comparing the regions predicted as 'unstructured' by this program and the DSSP prediction,  
this program has missed 0 helix, 1 beta strand(s) and 11 turn(s).
```

```
For more details, please see the 1bta_spvb_results.txt in your working directory.
```

```
=====
```

For the 3 files analyzed, we obtain a relatively good similarity between the predictions. Indeed, among the structures predicted by SPVB, more than 75% are also found in the DSSP prediction. The main difference revolves in the prediction of turns for which we notice different assignments.

Overall, the SPVB program seems to work on sequences of various sizes and for the prediction of both helices and beta strands.

Annex

4ajv_spvb_results.txt

	RESIDUE	SPVB-PREDICTION	DSSP-PREDICTION
0	1-THR	beta strand	/
1	2-PHE	beta strand	beta strand
2	3-ASN	beta strand	beta strand
3	4-MET	beta strand	beta strand
4	5-GLU	beta strand	beta strand
5	6-LEU	beta strand	beta strand
6	7-TYR	beta strand	beta strand
7	8-ASN	/	/
8	9-THR	turn	/
9	10-ASP	/	turn
10	11-LEU	/	turn
11	12-PHE	/	/
12	13-LEU	/	/
13	14-VAL	turn	/
14	15-PRO	/	/
15	16-SER	/	/
16	17-PRO	/	/
17	18-GLY	/	/
18	19-VAL	/	/
19	20-PHE	beta strand	beta strand
20	21-SER	beta strand	beta strand
21	22-VAL	beta strand	beta strand
22	23-ALA	turn	/
23	24-GLU	/	turn
24	25-ASN	/	turn
25	26-GLU	beta strand	/
26	27-HIS	beta strand	beta strand
27	28-VAL	beta strand	beta strand
28	29-TYR	beta strand	beta strand
29	30-VAL	beta strand	beta strand
30	31-GLU	beta strand	beta strand
31	32-VAL	beta strand	beta strand
32	33-SER	beta strand	beta strand
33	34-VAL	beta strand	beta strand
34	35-THR	beta strand	beta strand
35	36-LYS	beta strand	beta strand
36	37-ALA	/	/
37	38-ASP	/	/
38	39-GLN	/	/
39	40-ASP	beta strand	/
40	41-LEU	beta strand	beta strand
41	42-GLY	beta strand	beta strand
42	43-PHE	beta strand	beta strand
43	44-ALA	beta strand	beta strand
44	45-ILE	/	beta strand
45	46-GLN	turn	beta strand
46	47-THR	beta strand	beta strand
47	48-CYS	beta strand	beta strand
48	49-PHE	beta strand	beta strand
49	50-ILE	beta strand	beta strand
50	51-SER	beta strand	beta strand
51	52-PRO	/	/
52	53-TYR	/	/

53	54-SER	/	/
54	55-ASN	/	/
55	56-PRO	/	/
56	57-ASP	/	/
57	58-ARG	/	/
58	59-MET	/	/
59	60-SER	/	/
60	61-ASP	/	/
61	62-TYR	turn	/
62	63-THR	/	beta strand
63	64-ILE	beta strand	beta strand
64	65-ILE	beta strand	beta strand
65	66-GLU	beta strand	beta strand
66	67-ASN	/	turn
67	68-ILE	/	turn
68	69-CYS	turn	beta strand
69	70-PRO	/	beta strand
70	71-LYS	/	/
71	72-ASP	turn	/
72	73-ASP	/	turn
73	74-SER	/	turn
74	75-VAL	/	/
75	76-LYS	beta strand	beta strand
76	77-PHE	beta strand	beta strand
77	78-TYR	beta strand	beta strand
78	79-SER	/	beta strand
79	80-SER	/	beta strand
80	81-LYS	beta strand	beta strand
81	82-ARG	beta strand	beta strand
82	83-VAL	beta strand	beta strand
83	84-HIS	beta strand	beta strand
84	85-PHE	beta strand	beta strand
85	86-PRO	turn	turn
86	87-ILE	/	turn
87	88-PRO	/	turn
88	89-HIS	/	turn
89	90-ALA	beta strand	beta strand
90	91-GLU	beta strand	beta strand
91	92-VAL	beta strand	beta strand
92	93-ASP	beta strand	beta strand
93	94-LYS	beta strand	beta strand
94	95-LYS	beta strand	beta strand
95	96-ARG	beta strand	beta strand
96	97-PHE	beta strand	beta strand
97	98-SER	beta strand	beta strand
98	99-PHE	beta strand	beta strand
99	100-VAL	/	beta strand
100	101-PHE	turn	/
101	102-LYS	/	/
102	103-SER	/	/
103	104-VAL	/	/
104	105-PHE	/	/
105	106-ASN	/	/
106	107-THR	/	/
107	108-SER	beta strand	/
108	109-LEU	beta strand	beta strand
109	110-LEU	beta strand	beta strand
110	111-PHE	beta strand	beta strand
111	112-LEU	beta strand	beta strand
112	113-HIS	beta strand	beta strand
113	114-CYS	beta strand	beta strand

114	115-GLU	beta strand	beta strand
115	116-LEU	beta strand	beta strand
116	117-THR	beta strand	beta strand
117	118-LEU	beta strand	beta strand
118	119-CYS	beta strand	beta strand
119	120-SER	turn	beta strand
120	121-ARG	/	/
121	122-ASN	/	/
122	123-LYS	/	/
123	124-GLY	/	/
124	125-SER	/	/
125	126-GLN	/	turn
126	127-LYS	/	turn
127	128-LEU	/	/
128	129-PRO	turn	/
129	130-LYS	/	/
130	131-CYS	/	/
131	132-VAL	/	/
132	133-THR	helix	/
133	134-PRO	helix	turn
134	135-ASP	helix	turn
135	136-ASP	helix	turn
136	137-ALA	helix	turn
137	138-CYS	helix	turn
138	139-THR	helix	/
139	140-THR	/	/
140	141-PHE	beta strand	/
141	142-THR	beta strand	beta strand
142	143-LYS	beta strand	beta strand
143	144-PRO	beta strand	beta strand
144	145-LEU	beta strand	beta strand
145	146-ALA	beta strand	beta strand
146	147-VAL	beta strand	beta strand
147	148-VAL	beta strand	beta strand
148	149-LEU	beta strand	beta strand
149	150-GLN	beta strand	beta strand
150	151-VAL	/	beta strand
151	152-ASP	/	/

6drx_spvb_results.txt

	RESIDUE	SPVB-PREDICTION	DSSP-PREDICTION
0	1-VAL	/	/
1	2-GLU	/	/
2	3-GLU	/	/
3	4-GLN	/	/
4	5-GLY	/	/
5	6-ASN	/	/
6	7-LYS	helix	/
7	8-LEU	helix	helix
8	9-HIS	helix	helix
9	10-TRP	helix	helix
10	11-ALA	helix	helix
11	12-ALA	helix	helix
12	13-LEU	helix	helix
13	14-LEU	helix	helix
14	15-ILE	helix	helix
15	16-LEU	helix	helix
16	17-MET	helix	helix

17	18-VAL	helix	helix
18	19-ILE	helix	helix
19	20-ILE	helix	helix
20	21-PRO	helix	helix
21	22-THR	helix	helix
22	23-ILE	helix	helix
23	24-GLY	helix	helix
24	25-GLY	helix	helix
25	26-ASN	helix	helix
26	27-THR	helix	helix
27	28-LEU	helix	helix
28	29-VAL	helix	helix
29	30-ILE	helix	helix
30	31-LEU	helix	helix
31	32-ALA	helix	helix
32	33-VAL	helix	helix
33	34-SER	helix	helix
34	35-LEU	helix	helix
35	36-GLU	helix	/
36	37-LYS	helix	helix
37	38-LYS	helix	helix
38	39-LEU	helix	helix
39	40-GLN	helix	/
40	41-TYR	helix	/
41	42-ALA	helix	turn
42	43-THR	helix	turn
43	44-ASN	helix	helix
44	45-TYR	helix	helix
45	46-PHE	helix	helix
46	47-LEU	helix	helix
47	48-MET	helix	helix
48	49-SER	helix	helix
49	50-LEU	helix	helix
50	51-ALA	helix	helix
51	52-VAL	helix	helix
52	53-ALA	helix	helix
53	54-ASP	helix	helix
54	55-LEU	helix	helix
55	56-LEU	helix	helix
56	57-VAL	helix	helix
57	58-GLY	helix	helix
58	59-LEU	helix	helix
59	60-PHE	helix	helix
60	61-VAL	helix	helix
61	62-MET	helix	helix
62	63-PRO	helix	helix
63	64-ILE	helix	helix
64	65-ALA	helix	helix
65	66-LEU	helix	helix
66	67-LEU	helix	helix
67	68-THR	helix	helix
68	69-ILE	helix	helix
69	70-MET	helix	helix
70	71-PHE	helix	/
71	72-GLU	/	/
72	73-ALA	/	/
73	74-MET	/	/
74	75-TRP	/	/
75	76-PRO	/	/
76	77-LEU	/	/
77	78-PRO	helix	/

78	79-LEU	helix	turn
79	80-VAL	helix	turn
80	81-LEU	helix	helix
81	82-CYS	helix	helix
82	83-PRO	helix	helix
83	84-ALA	helix	helix
84	85-TRP	helix	helix
85	86-LEU	helix	helix
86	87-PHE	helix	helix
87	88-LEU	helix	helix
88	89-ASP	helix	helix
89	90-VAL	helix	helix
90	91-LEU	helix	helix
91	92-PHE	helix	helix
92	93-SER	helix	helix
93	94-THR	helix	helix
94	95-ALA	helix	helix
95	96-SER	helix	helix
96	97-ILE	helix	helix
97	98-TRP	helix	helix
98	99-HIS	helix	helix
99	100-LEU	helix	helix
100	101-CYS	helix	helix
101	102-ALA	helix	helix
102	103-ILE	helix	helix
103	104-SER	helix	helix
104	105-VAL	helix	helix
105	106-ASP	helix	helix
106	107-ARG	helix	helix
107	108-TYR	helix	helix
108	109-ILE	helix	helix
109	110-ALA	helix	helix
110	111-ILE	helix	helix
111	112-LYS	helix	helix
112	113-LYS	helix	/
113	114-PRO	/	/
114	115-ILE	/	/
115	116-GLN	/	/
116	117-ALA	/	/
117	118-ASN	helix	/
118	119-GLN	helix	helix
119	120-TYR	helix	helix
120	121-ASN	helix	helix
121	122-SER	helix	helix
122	123-ARG	helix	helix
123	124-ALA	helix	helix
124	125-THR	helix	helix
125	126-ALA	helix	helix
126	127-PHE	helix	helix
127	128-ILE	helix	helix
128	129-LYS	helix	helix
129	130-ILE	helix	helix
130	131-THR	helix	helix
131	132-VAL	helix	helix
132	133-VAL	helix	helix
133	134-TRP	helix	helix
134	135-LEU	helix	helix
135	136-ILE	helix	helix
136	137-SER	helix	helix
137	138-ILE	helix	helix
138	139-GLY	helix	helix

139	140-ILE	helix	helix
140	141-ALA	helix	helix
141	142-ILE	helix	turn
142	143-PRO	helix	helix
143	144-VAL	helix	helix
144	145-PRO	helix	helix
145	146-ILE	helix	helix
146	147-LYS	helix	helix
147	148-GLY	helix	/
148	149-ILE	/	/
149	150-GLU	/	/
150	151-THR	/	/
151	152-ASN	/	/
152	153-PRO	/	/
153	154-ASN	/	/
154	155-ASN	/	/
155	156-ILE	turn	/
156	157-THR	/	/
157	158-CYS	/	/
158	159-VAL	/	/
159	160-LEU	/	/
160	161-THR	turn	/
161	162-LYS	/	turn
162	163-GLU	/	turn
163	164-ARG	/	turn
164	165-PHE	helix	/
165	166-GLY	helix	helix
166	167-ASP	helix	helix
167	168-PHE	helix	helix
168	169-MET	helix	helix
169	170-LEU	helix	helix
170	171-PHE	helix	helix
171	172-GLY	helix	helix
172	173-SER	helix	helix
173	174-LEU	helix	helix
174	175-ALA	helix	helix
175	176-ALA	helix	helix
176	177-PHE	helix	helix
177	178-PHE	helix	helix
178	179-THR	helix	helix
179	180-PRO	helix	helix
180	181-LEU	helix	helix
181	182-ALA	helix	helix
182	183-ILE	helix	helix
183	184-MET	helix	helix
184	185-ILE	helix	helix
185	186-VAL	helix	helix
186	187-THR	helix	helix
187	188-TYR	helix	helix
188	189-PHE	helix	helix
189	190-LEU	helix	helix
190	191-THR	helix	helix
191	192-ILE	helix	helix
192	193-HIS	helix	helix
193	194-ALA	helix	helix
194	195-LEU	helix	helix
195	196-GLN	helix	helix
196	197-LYS	helix	helix
197	198-LYS	helix	helix
198	199-ALA	helix	helix
199	200-ALA	helix	helix

200	201-ASP	helix	helix
201	202-LEU	helix	helix
202	203-GLU	helix	helix
203	204-ASP	helix	helix
204	205-ASN	helix	helix
205	206-TRP	helix	helix
206	207-GLU	helix	helix
207	208-THR	helix	helix
208	209-LEU	helix	turn
209	210-ASN	helix	turn
210	211-ASP	helix	helix
211	212-ASN	helix	helix
212	213-LEU	helix	helix
213	214-LYS	helix	helix
214	215-VAL	helix	helix
215	216-ILE	helix	helix
216	217-GLU	helix	helix
217	218-LYS	helix	/
218	219-ALA	/	/
219	220-ASP	/	/
220	221-ASN	helix	/
221	222-ALA	helix	helix
222	223-ALA	helix	helix
223	224-GLN	helix	helix
224	225-VAL	helix	helix
225	226-LYS	helix	helix
226	227-ASP	helix	helix
227	228-ALA	helix	helix
228	229-LEU	helix	helix
229	230-THR	helix	helix
230	231-LYS	helix	helix
231	232-MET	helix	helix
232	233-ARG	helix	/
233	234-ALA	/	/
234	235-ALA	/	/
235	236-PHE	helix	/
236	237-ARG	helix	helix
237	238-HIS	helix	helix
238	239-GLY	helix	helix
239	240-PHE	helix	turn
240	241-ASP	helix	helix
241	242-ILE	helix	helix
242	243-LEU	helix	helix
243	244-VAL	helix	helix
244	245-GLY	helix	helix
245	246-GLN	helix	helix
246	247-ILE	helix	helix
247	248-ASP	helix	helix
248	249-ASP	helix	helix
249	250-ALA	helix	helix
250	251-LEU	helix	helix
251	252-LYS	helix	helix
252	253-LEU	helix	helix
253	254-ALA	helix	helix
254	255-ASN	helix	helix
255	256-GLU	helix	helix
256	257-GLY	/	turn
257	258-LYS	/	/
258	259-VAL	helix	/
259	260-LYS	helix	helix
260	261-GLU	helix	helix

261	262-ALA	helix	helix
262	263-GLN	helix	helix
263	264-ALA	helix	helix
264	265-ALA	helix	helix
265	266-ALA	helix	helix
266	267-GLU	helix	helix
267	268-GLN	helix	helix
268	269-LEU	helix	helix
269	270-LYS	helix	helix
270	271-THR	helix	helix
271	272-THR	helix	helix
272	273-ARG	helix	helix
273	274-ASN	helix	helix
274	275-ALA	helix	helix
275	276-TYR	helix	helix
276	277-ILE	helix	helix
277	278-GLN	helix	helix
278	279-LYS	helix	helix
279	280-TYR	helix	helix
280	281-LEU	helix	helix
281	282-GLN	helix	helix
282	283-THR	helix	helix
283	284-ILE	helix	helix
284	285-SER	helix	helix
285	286-ASN	helix	helix
286	287-GLU	helix	helix
287	288-GLN	helix	helix
288	289-ARG	helix	helix
289	290-ALA	helix	helix
290	291-SER	helix	helix
291	292-LYS	helix	helix
292	293-VAL	helix	helix
293	294-LEU	helix	helix
294	295-GLY	helix	helix
295	296-ILE	helix	helix
296	297-VAL	helix	helix
297	298-PHE	helix	helix
298	299-PHE	helix	helix
299	300-LEU	helix	helix
300	301-PHE	helix	helix
301	302-LEU	helix	helix
302	303-LEU	helix	helix
303	304-MET	helix	helix
304	305-TRP	helix	helix
305	306-CYS	helix	helix
306	307-PRO	helix	helix
307	308-PHE	helix	helix
308	309-PHE	helix	helix
309	310-ILE	helix	helix
310	311-THR	helix	helix
311	312-ASN	helix	helix
312	313-ILE	helix	helix
313	314-THR	helix	helix
314	315-LEU	helix	helix
315	316-VAL	helix	helix
316	317-LEU	helix	helix
317	318-CYS	helix	/
318	319-ASP	/	/
319	320-SER	/	/
320	321-CYS	/	/
321	322-ASN	/	/

322	323-GLN	helix	/
323	324-THR	helix	helix
324	325-THR	helix	helix
325	326-LEU	helix	helix
326	327-GLN	helix	helix
327	328-MET	helix	helix
328	329-LEU	helix	helix
329	330-LEU	helix	helix
330	331-GLU	helix	helix
331	332-ILE	helix	helix
332	333-PHE	helix	helix
333	334-VAL	helix	helix
334	335-TRP	helix	helix
335	336-ILE	helix	helix
336	337-GLY	helix	helix
337	338-TYR	helix	helix
338	339-VAL	helix	helix
339	340-SER	helix	helix
340	341-SER	helix	helix
341	342-GLY	helix	helix
342	343-VAL	helix	helix
343	344-ASN	helix	helix
344	345-PRO	helix	helix
345	346-LEU	helix	helix
346	347-VAL	helix	helix
347	348-TYR	helix	helix
348	349-THR	helix	helix
349	350-LEU	helix	turn
350	351-PHE	helix	turn
351	352-ASN	helix	/
352	353-LYS	helix	helix
353	354-THR	helix	helix
354	355-PHE	helix	helix
355	356-ARG	helix	helix
356	357-ASP	helix	helix
357	358-ALA	helix	helix
358	359-PHE	helix	helix
359	360-GLY	helix	helix
360	361-ARG	helix	helix
361	362-TYR	helix	helix
362	363-ILE	helix	helix
363	364-THR	helix	turn
364	365-CYS	/	turn
365	366-ASN	/	/
366	367-TYR	/	/
367	368-ARG	/	/

1bta_spvb_results.txt

	RESIDUE	SPVB-PREDICTION	DSSP-PREDICTION
0	1-LYS	beta strand	/
1	2-LYS	beta strand	beta strand
2	3-ALA	beta strand	beta strand
3	4-VAL	beta strand	beta strand
4	5-ILE	beta strand	beta strand
5	6-ASN	turn	beta strand
6	7-GLY	/	turn
7	8-GLU	/	turn
8	9-GLN	/	turn
9	10-ILE	/	/

10	11-ARG	/	/
11	12-SER	helix	/
12	13-ILE	helix	helix
13	14-SER	helix	helix
14	15-ASP	helix	helix
15	16-LEU	helix	helix
16	17-HIS	helix	helix
17	18-GLN	helix	helix
18	19-THR	helix	helix
19	20-LEU	helix	helix
20	21-LYS	helix	helix
21	22-LYS	helix	helix
22	23-GLU	helix	helix
23	24-LEU	helix	helix
24	25-ALA	/	turn
25	26-LEU	/	/
26	27-PRO	turn	/
27	28-GLU	/	turn
28	29-TYR	/	turn
29	30-TYR	/	/
30	31-GLY	/	/
31	32-GLU	/	/
32	33-ASN	helix	/
33	34-LEU	helix	helix
34	35-ASP	helix	helix
35	36-ALA	helix	helix
36	37-LEU	helix	helix
37	38-TRP	helix	helix
38	39-ASP	helix	helix
39	40-CYS	helix	helix
40	41-LEU	helix	helix
41	42-THR	helix	turn
42	43-GLY	/	turn
43	44-TRP	/	turn
44	45-VAL	/	/
45	46-GLU	/	/
46	47-TYR	/	/
47	48-PRO	/	/
48	49-LEU	beta strand	beta strand
49	50-VAL	beta strand	beta strand
50	51-LEU	beta strand	beta strand
51	52-GLU	beta strand	beta strand
52	53-TRP	beta strand	beta strand
53	54-ARG	beta strand	beta strand
54	55-GLN	helix	/
55	56-PHE	helix	turn
56	57-GLU	helix	turn
57	58-GLN	helix	helix
58	59-SER	helix	helix
59	60-LYS	helix	helix
60	61-GLN	helix	helix
61	62-LEU	helix	turn
62	63-THR	/	turn
63	64-GLU	/	turn
64	65-ASN	/	/
65	66-GLY	helix	/
66	67-ALA	helix	helix
67	68-GLU	helix	helix
68	69-SER	helix	helix
69	70-VAL	helix	helix
70	71-LEU	helix	helix

71	72-GLN	helix	helix
72	73-VAL	helix	helix
73	74-PHE	helix	helix
74	75-ARG	helix	helix
75	76-GLU	helix	helix
76	77-ALA	helix	helix
77	78-LYS	helix	helix
78	79-ALA	helix	helix
79	80-GLU	helix	turn
80	81-GLY	/	turn
81	82-CYS	/	/
82	83-ASP	beta strand	/
83	84-ILE	beta strand	beta strand
84	85-THR	beta strand	beta strand
85	86-ILE	beta strand	beta strand
86	87-ILE	beta strand	beta strand
87	88-LEU	/	beta strand
88	89-SER	turn	/