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2OV0-Amicyanin

Residue	Δτ	Δω	C_α-C-N	C_α-C-O	O-C-N
1-D	-2.9	-0.1	112.7	120.7	126.5
2-K	4.8	-10.2	116.5	120.4	123.1
3-A	-2.3	-8.1	115.1	118.4	126.5
4-T	-0.3	-7.4	114.2	121.5	124.3
5-I	-1.2	0.1	119.7	119.5	120.8
6-P	3.9	-6.9	116.2	120	123.8
7-S	0.4	-4.2	117.3	121.1	121.6
8-E	2	-5.6	115.2	121.5	123.1
9-S	1.3	-17.7	117.7	119.6	122.2
10-P	-0.6	-1.9	115.1	121.9	122.9
11-F	-0.1	6.5	117.4	122.4	120.1
12-A	0.8	-4.6	116.7	122.2	120.8
13-A	1.3	2	118.6	120.9	120.5
14-A	3.1	2.8	118.1	121.4	120.4
15-E	2.4	5.2	118.3	119.3	122.4
16-V	1.3	4.8	115.4	122	122.5
17-A	2.8	-14.1	117	120.5	122.4
18-D	2.2	-0.8	112.3	121.1	126.6
19-G	5.4	-3.4	118.5	118.4	123.1
20-A	-1.2	-0.3	114.8	120.9	124.3
21-I	-2.8	12.1	117.7	119.4	122.8
22-V	2.2	-12.3	114.5	121.2	124.1
23-V	-1.8	-5.5	116.5	119.8	123.7
24-D	0.4	-3.5	114	121.6	124.3
25-I	-4.1	-2	115.8	120.3	123.9
26-A	-2.3	-1.3	116	120.7	123.3
27-K	2.3	-3.5	117.7	121	121.2
28-M	3.6	-0.8	116.5	119.9	123.4
29-K	0.2	-16.8	115.2	121.5	123.2
30-Y	-3.6	10.3	115.2	121.5	123.2
31-E	3.7	-9.6	116.9	120.8	122.3
32-T	-2.6	6.5	117.3	119.7	123
33-P	3.5	-3.9	118.6	119.2	122.1
34-E	-3.5	3.3	120.4	116.5	123.1
35-L	0.3	-2.8	117.1	122.6	120
36-H	-0.1	2.2	117.4	118.6	124
37-V	-0.6	-2.4	116	120.2	123.8
38-K	1.3	-7.7	115.6	121.2	123.2
39-V	0.9	0	114.7	121.8	123.6
40-G	6.2	-2	117.1	121.5	121.4
41-D	1.3	-9.6	116.7	119.7	123.5
42-T	-1	-6.8	112.8	122.7	124.6
43-V	-2.3	-0.7	118.2	120.1	123.7
44-T	-1	-7.4	115.2	120.5	124.3
45-W	-2	-3.1	115.6	120.1	124.3
46-I	-2.3	-3.6	115.5	120.3	124.3

47-N	-0.5	0.4	116.5	119.6	123.8
48-R	2.1	-1.1	115.8	121	123.2
49-E	2.8	4.8	119.3	118.7	122
50-A	4.7	-1.5	111.8	123.7	124.4
51-M	1.4	-5.1	117.7	121.9	120.4
52-P	3.1	-1.1	120.5	117	122.4
53-H	0.4	-10.2	115.4	119.5	125.1
54-N	-1.5	-14.2	116.8	120.2	122.8
55-V	-2	7.2	114.2	121.7	124.1
56-H	-2.6	-1.9	116	120.1	123.9
57-F	-2.8	2.8	114.6	121.3	124.1
58-V	1.6	3	118.5	119.6	121.9
59-A	0.8	-1.3	115.5	122.2	122.3
60-G	3.7	7.3	113.4	122.6	123.8
61-V	0.9	-2.4	119.8	119.3	120.8
62-L	4.7	7.8	117.8	121.1	121.1
63-G	-3.1	7.6	115.7	120.6	123.7
64-E	2.8	1.5	114.5	122.3	123.3
65-A	2.2	-17	115.9	120.8	123.4
66-A	-0.8	-10.7	115.2	121.9	122.7
67-L	-2.8	-3.7	116	120.5	123.5
68-K	-4.8	3.6	115.9	120.7	123.5
69-G	1.4	-0.4	117.1	119.3	123.6
70-P	0.7	-6	115.7	121.9	122.5
71-M	0.5	-3.4	115.6	122.9	121.4
72-M	-0.3	-13.1	116.1	121.6	122.3
73-K	0.4	-1	117.7	119.5	122.9
74-K	-0.7	-0.1	116.5	122.4	121.1
75-E	4.1	-12.6	114.9	121.1	124
76-Q	0.7	11.4	116.5	119.8	123.5
77A	0	2.1	114.5	121.2	124.3
78-Y	-1.5	5.1	114.8	121.9	123.3
79-S	4	-13.2	117.3	119.4	123.2
80-L	-2.2	-3.5	114.2	122.2	123.3
81-T	-2.2	8.1	116.3	120.3	123.4
82-F	0.5	8.1	116.8	120.1	123.1
83-T	4.4	4.7	116.2	121.6	122.3
84-E	-1.5	-5.3	118.6	118.4	122.9
85-A	0.8	-4.1	116.8	119.8	123.4
86-G	-0.8	-2.8	115	121.4	123.6
87-T	-1.7	8	114.2	122.1	123.7
88-Y	0	0	115.3	119.2	125.5
89-D	0.3	0.3	115.6	120.9	123.5
90-Y	0.5	0.5	115.6	120.7	123.5
91-H	-1.1	-1.1	114.6	121.9	123.6
92-C	-1.7	-1.7	115.4	121.2	123.2
93-T	3.8	3.8	115.7	121.3	123
94-P	4	4	121.3	118.4	120.4
95-H	0.2	0.2	117.1	118.6	124.2
96-P	4.4	4.4	119.1	119.1	121.8
97-F	2.1	2.1	117.4	119.2	123.4
98-M	-0.9	-0.9	119.3	117.7	123

99-R	-0.1	-0.1	116.4	119.7	123.9
100-G	0.5	0.5	116.1	121.2	122.7
101-K	-0.5	-0.5	116.2	121	122.8
102-V	-2.8	-2.8	113.1	122	124.8
103-V	-3.6	-3.6	115.7	120.2	124.2
104-V	-2.6	-2.6	115.4	120.4	124.1
105-E	-	-	117.7	118.7	123.6

3LOE-α-defensin-1

Res. No.	Δτ	Δω	C_α-C-N	C_α-C-O	O-C-N
1-A	1	0.9	115.7	121.1	123.2
2-C	1.7	3.5	114.6	121.5	123.9
3-Y	0.6	-7.6	116.1	120.2	123.5
4-C	-0.5	6.1	116.3	121	122.6
5-R	5	-10.2	116.1	121	122.9
6*-I	-4.6	**9.3***	118.6	119.5	122
7-P	4.8	4	116.9	120.6	122.5
8-A	-1.6	-7.3	117	120.7	122.4
9-C	0.5	-5	115.3	121.5	123.2
10-I	3.7	5.9	117.6	120.2	122.1
11-A	2.5	1.5	116.4	119.8	123.8
12-G	7.1	-0.9	117.9	118.9	123.2
13-E	1.5	-8.6	116.5	121.2	122.3
14-R	-2	-2.3	114.7	121.3	124.1
15-R	3.3	-2.2	116.7	120.1	123.3
16-Y	6.3	3.4	117.1	120.1	122.8
17-G	2	10	114.7	121	124.2
18-T	1	-14.6	116.7	120.2	123.2
19-C	-0.4	-6.5	114.8	121.7	123.5
20-I	0.4	10-.3	116.1	120.4	123.3
21-Y	-0.1	3.4	115.9	120.7	123.4
22-Q	3.7	-3.2	115.9	120.3	123.8
23-G	4.8	1.4	116	121.3	122.6
24-R	2	-0.2	114.5	122	123.5
25-L	-0.1	4.5	114.8	121.2	123.9
26-W	0.5	-12.5	118	118.7	123.2
27-A	1.8	-9.5	117.1	118.9	123.9
28-F	-2.8	11.3	115.5	120.7	123.8
29-C	1.5	8.1	117.3	120	122.6
30-C	2.4	-	-	-	-

* Cis peptide bond

1IRO-Rubredoxin

Res. No.	Δτ	Δω	C_i^{α}-C_i-N	C_i^{α}–C_i-O_i	O_i-C_i-N_{i+1}	C_i-N_{i+1}-C^{α}	C_i-N_{i+1}-H	H-N_{i+1}-C^{α}_{i+1}
1-M	-1.8	6.7	116.8	119.4	123.7	-	-	-
2-K	3.5	-13.7	117.1	120	122.8	123.6	118	118.4
3-K	1.8	-3.2	115.9	119.7	124.4	123.4	118.5	118.1
4-Y	-1.1	-1.3	117.3	118.8	123.9	123.5	118	118.5
5-T	0.8	-9.8	114	122.5	123.4	120.2	120	119.8
6-C	-1	5.9	117.5	122.1	120.3	122.7	118.8	118.5
7-T	4.1	-4.8	119.4	120.2	120.3	120.1	120.1	119.8
8-V	3.2	3.7	119.2	119.6	121.1	124.8	117.5	117.7
9-C	7.3	0.2	120.5	118.6	120.9	121.7	119.2	119.1
10-G	9.4	-6.4	118	120.9	121.1	124.1	118	118
11-Y	0.9	-4.2	116.3	119.2	124.5	122.9	118.3	118.8
12-I	1.3	-11.7	117.7	122.1	120.2	123.8	117.9	118.2
13-Y	-0.6	-0.8	118.3	119.7	122	123.8	117.9	118.3
14-N	-2.7	4.1	118	119.6	122.4	124.3	117.8	117.9
15-P	3.5	-2.4	120.2	116.3	123.5	121.5	126.2	112.3
16-E	2.8	1.4	117.4	117.6	125	119.7	120.2	120.1
17-D	2.7	8.4	115.7	120.3	123.9	124.8	117.8	117.4
18-G	2.7	-7.3	113.9	123.9	122.2	119.9	120.1	120
19-D	-5.3	12.7	116	120.9	123.1	123.3	118.2	118.6
20-P	6.3	2	117.8	121.5	120.7	119.8	127.5	112.1
21-D	3.4	-4.9	115	118.3	126.7	120.9	119.6	119.5
22-N	2.4	-8.2	116.1	119.8	124.1	121.8	119.3	118.9
23-G	6.8	-0.7	118.7	117	124.2	121.3	119.4	119.3
24-V	-2.3	8.9	116.9	119.9	123.1	123.4	118.4	118.2
25-N	0.4	-12	117.2	121.8	120.9	120.5	119.7	119.9
26-P	-0.2	0.6	115.4	122.9	121.7	121.5	127.4	111.1
27-G	6.3	-2.1	119.1	119.6	121.2	121.4	119.4	119.3
28-T	1.2	-5.9	117.3	120.2	122.5	123.4	118.4	118.2
29-D	-2.1	3.1	115.4	123	121.5	120.5	119.7	119.8
30-F	4.7	1	117	121.2	121.8	119.6	120.3	120.1
31-K	2.7	1.9	117.5	118.6	123.9	120.5	119.7	119.8
32-D	5.8	-6.4	118	121.4	120.5	122.9	18.7	118.4
33-I	-1.9	-3.4	120	118	122	121.8	119	119.1
34-P	1.5	11.2	114.4	121.7	123.8	119.4	128.8	111.8
35-D	4.5	-8.9	119.9	116.4	123.6	120.2	120.2	119.6
36-D	4.8	-4.7	117.6	118.8	123.7	123.7	118	118.3
37-W	0.3	-3.1	114.9	122.4	122.6	120.5	119.7	119.8
38-V	1.1	-4.4	114.4	125	120.6	123.2	118.6	118.8
39-C	1.1	3.9	118.5	118.2	123.2	121.7	119.1	119.2
40-P	2.1	5.4	119.4	118.9	121.5	119.1	128.4	111.6
41-L	2.1	6.7	120.4	119.2	120	122	118.9	119.1
42-C	7.7	-7	120.6	119.5	119.6	124.6	117.7	117.7
43-G	7.8	-1.7	121.5	119.9	118.6	122.7	118.7	118.6
44-V	2.7	1.7	118.4	122.1	119.5	122.6	118.8	118.6
45-G	7.4	0.4	115.8	122.8	121.3	123.2	118.2	118.6
46-K	6.4	1.3	117	121	122	123.3	118.5	118.2
47-D	6.3	-5.2	119.3	119.3	121.4	121	119.4	119.6
48-Q	1.1	-3.1	119.4	117.2	123.4	121.6	119.2	119.3
49-F	1.2	-5	115.4	121.7	122.8	123.5	118.2	118.3
50-E	1.1	-3	119.2	119.3	121.3	121.3	119.3	119.4

51-E	0.4	-12.7	120.2	121.3	118.3	123.3	118.5	118.2
52-V	-2.2	-1.5	116.8	121.3	121.7	129.3	115.6	115.1
53-E	-	-	-	-	-	122	119.1	118.9

4K7T-Bacitracin A

Res. No.	Δτ	Δω	C_i^{α}-C_i- N_{i+1}	C_i^{α}–C_i-O_i	O_i-C_i-N_{i+1}	C_i-N_{i+1}- C^{α}_{i+1}	C_i-N_{i+1}-H $_{i+1}$	H-N_{i+1}-C^{α}_{i+1}
1-I	0.9	-4	116.1	119.3	122.6	-	-	-
2-C	2.2	-6	117.8	119.8	112.4	120.6	124.9	114.5
3-L	2.4	0.3	117.3	119.5	123.2	121	124.9	114.1
4-E	4.8	3.7	116.9	120.7	122.3	121.3	124.3	114.2
5-I	0.7	-3.7	115.8	121.1	123.1	120	125.1	114.8
6-K	0.8	-3.4	116.5	120.2	123.3	122.2	124.1	113.7
7-X	3.7	-1.4	117.4	119.9	122.7	123	123.6	113.4
8-I	-2.7	4.3	115.2	121.6	123.1	121.8	124	114.2
9-F	1.7	5.1	117.8	119.3	122.8	122.3	124.1	113.6
10-H	5.1	0.2	119.9	118.2	121.9	118.4	126.1	115.5
11-D	7.6	0.5	117	120	123	119.3	125.5	115.2
12-N	3.1	-	-	-	-	118.3	121.1	120.6

N(rch)5-Peptoid

Res. No.	Δτ	Δω	C_i^{α}-C_i- N_{i+1}	C_i^{α}–C_i-O_i	O_i-C_i-N_{i+1}	C_i-N_{i+1}- C^{α}_{i+1}	C_i-N_{i+1}-C	C-N_{i+1}-C^{α}_{i+1}
1	-0.7	-0.1	117.3	119.3	123.4	-	-	-
2	4	-3.5	120.1	118.2	121.4	123.1	119.7	117
3	2.5	3	117.8	118.6	123.5	122	120.6	117.2
4	3.4	0.2	116.4	119.6	124	123.4	116.8	119.1
5	4.7	-	115.5	122.1	122.4	123.1	118.9	118.0

1CWA-Cyclosporine-A

Res. No.	Δτ	Δω	C_i^{α}-C_i- N_{i+1}	C_i^{α}–C_i-O_i	O_i-C_i-N_{i+1}	C_i-N_{i+1}- C^{α}_{i+1}	C_i-N_{i+1}-C_M	C_m--N_{i+1}-C^{α}_{i+1}
1-DAL	-1.3	-0.5	120.2	118	121.8	119.2	-	-
2-MLE	2	2.8	118.1	120	121.9	117.6	125.1	117.2
3-MLE	2	-5.7	117.4	119.7	122.9	116	123.8	120
4-MVA	-0.1	2.5	116.8	119.5	123.6	116	127.7	116
5-BMT	3.5	1.6	116.8	123.2	121	114.5	125.8	119
6-ABA	2.6	0.9	123.2	119.3	117.5	121.5	-	-
7-SAR	1.6	-6.5	121.8	117.1	121	119.5	121	119.4
8-MLE	-1.8	2.7	120.7	120.4	118.9	121.3	120.1	118.6
9-Val	-2	3.6	119.2	119.6	121.2	120.8	-	-
10-MLE	1.1	-3	114.6	121.9	123.4	115.4	124.8	119.5
11-Ala	2.6	-6.4	116.1	121.9	122	122	-	-

Table S1 Deviation in bond angle, **N-C_{α}-C (Δτ)** &bond angles around carbonyl carbons together with the deviation in peptide bond torsion angle, **ω in degrees,** for the PDB structures, **2OV0, 3LOE , 1IRO**, **4K7T& 1CWA.**

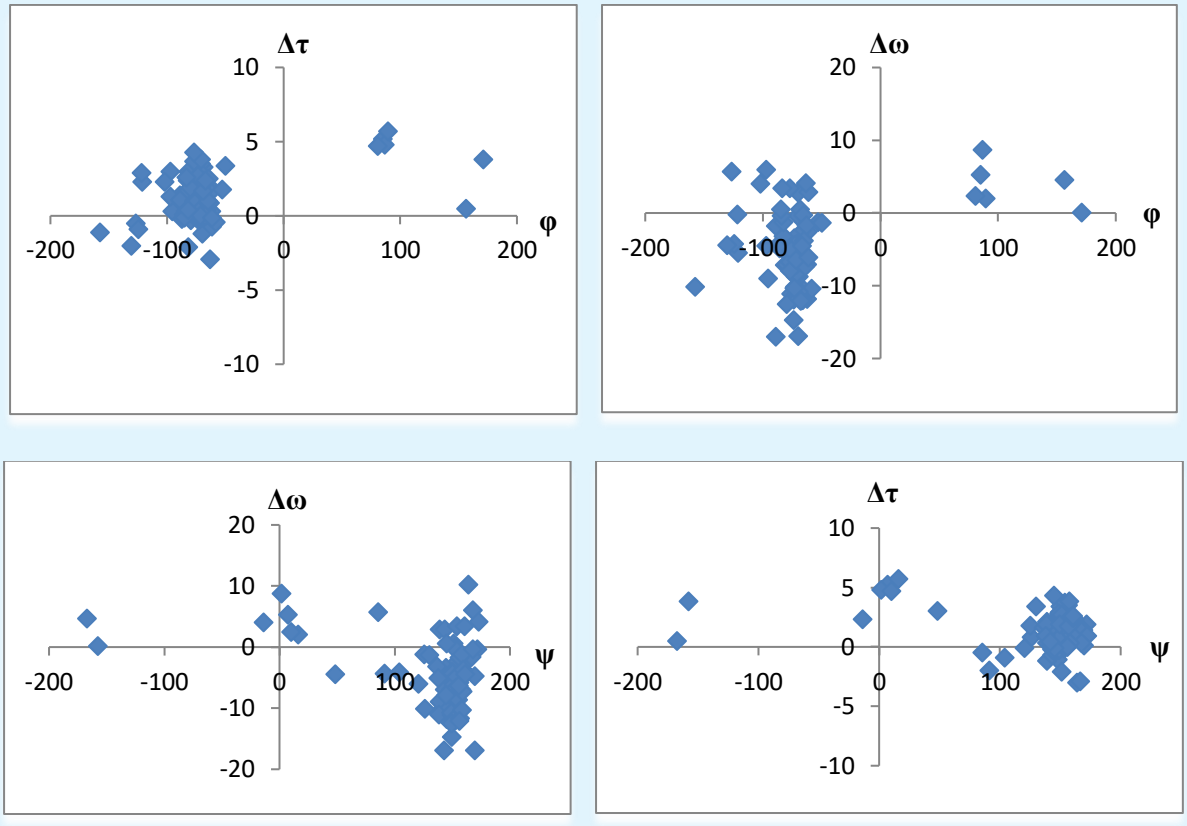
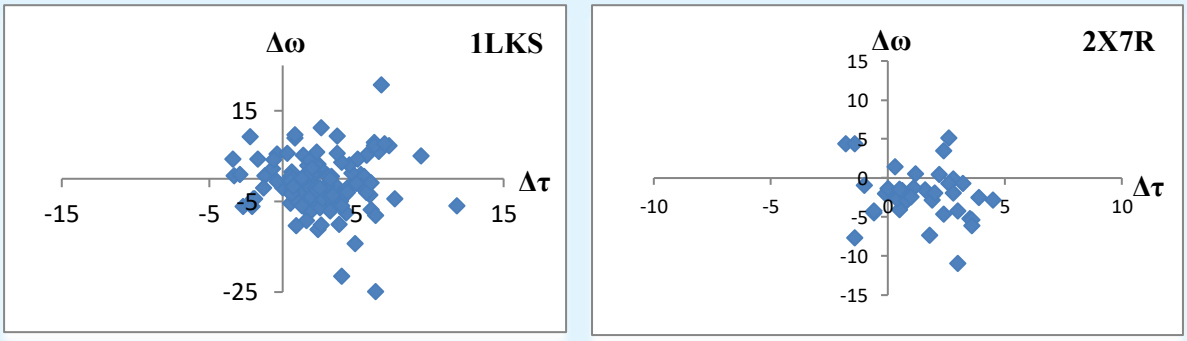


Figure S1: Plot of Δτvs φ & Δωvs φ and Δτvs ψ & Δωvs ψ for 2PNE showing the similarities of Δτ/Δω vs φ and ψ.



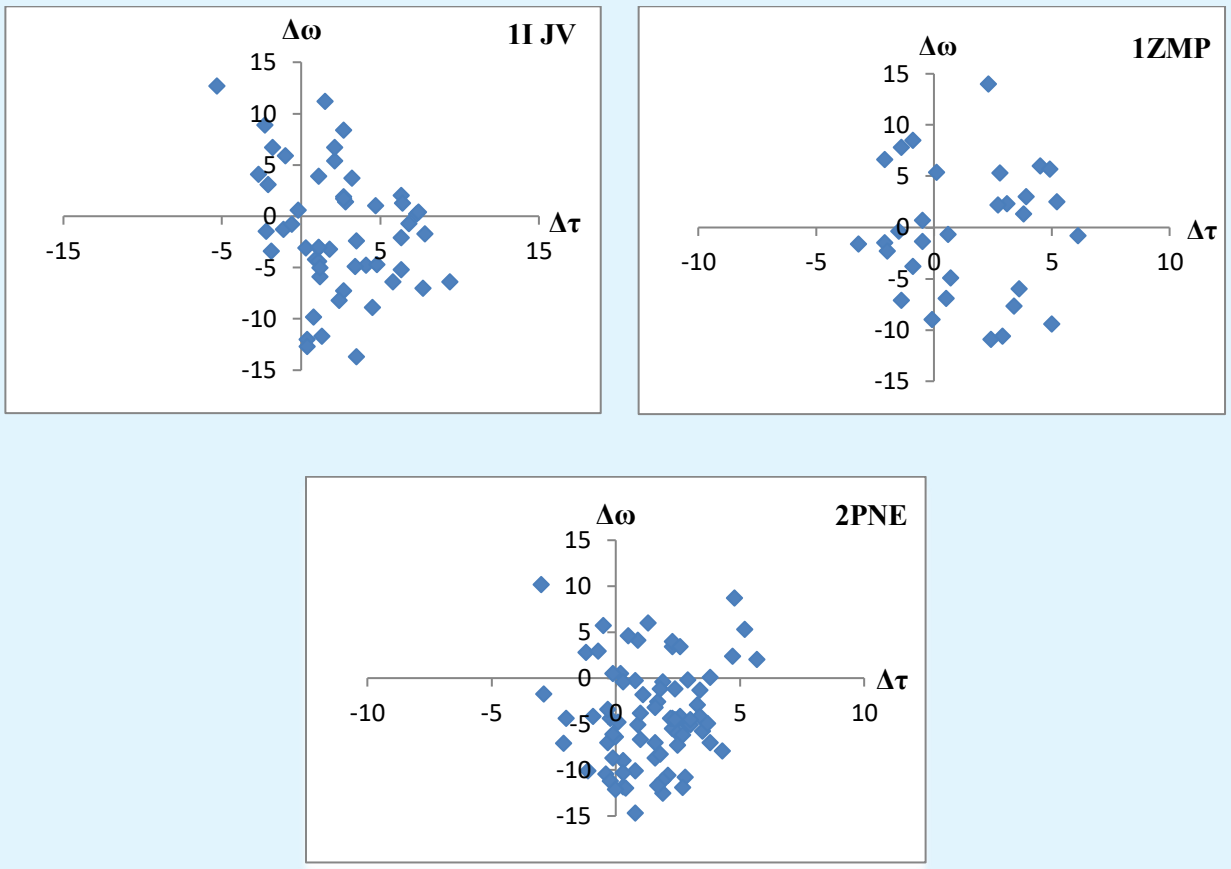


Figure S2: Plot between Δτ and Δω (in degrees) for PDB structure, 1LKS, 2X7R, 1I JV, 1ZMP and 2PNE showing the relationship between the two which depends on the secondary structure element and compactness of the structure.