

$d_c = 1.4 \text{ \AA}$

ID*	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	173	2.74	42.7
2	388	8.37	37.9
3	366	6.11	21.9
4	85	9.53	9.7
5	130	12.09	8.6

$d_c = 2.0 \text{ \AA}$

ID	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	268	3.30	29.1
2	127	9.43	24.6
3	90	6.79	20.3
4	650	7.14	12.1
5	184	6.73	8.0
6	28	4.96	4.9

$d_c = 1.1 \text{ \AA}$

ID	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	147	2.68	12.2
2	298	8.31	11.5
3	134	5.42	8.9
4	43	11.82	3.6
5	28	9.79	3.6

$d_c = 1.5 \text{ \AA}$

ID	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	149	2.82	11.8
2	96	9.35	10.5
3	54	6.67	7.6
4	31	5.97	6.5
5	68	5.48	5.3
6	37	7.88	4.9
7	76	7.96	4.7
8	25	6.81	3.1

$d_c = 0.9 \text{ \AA}$

ID	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	74	2.63	4.4
2	102	7.99	4.0
3	39	5.30	2.7
4	23	8.08	2.4

$d_c = 1.4 \text{ \AA}$

ID	$n^\dagger$	$\langle \text{rmsd} \rangle^\ddagger$	$\langle k \rangle^\S$
1	106	2.60	10.8
2	58	9.31	10.7
3	33	6.43	6.6
4	32	6.77	5.4
5	47	5.42	4.4
6	28	9.70	4.1
7	22	7.96	4.1
8	61	7.89	3.9

\*Cluster ID sorted by  $\langle k \rangle$ .

$^\dagger$ Number of structures in a cluster.

$^\ddagger$ Average rmsd of structures from the experimental structure.

$^\S$ Average connectivity of structures.

(A)

(B)