dockingBalanced

Cluster	Members	Representative	Weighted Score
0	62	Center	-1125.3
		Lowest Energy	-1415.7
1	60	Center	-1006.5
		Lowest Energy	-1257.9
2	56	Center	-1101.9
		Lowest Energy	-1142.6
3	55	Center	-1078.7
		Lowest Energy	-1260.3
4	48	Center	-1048.8
		Lowest Energy	-1253.2
5	40	Center	-1149.4
		Lowest Energy	-1233.0
6	38	Center	-1064.5
		Lowest Energy	-1180.9
7	38	Center	-1041.0
		Lowest Energy	-1307.4
8	35	Center	-1052.4
		Lowest Energy	-1152.6
9	33	Center	-1066.2
		Lowest Energy	-1191.2
10	33	Center	-1031.7
		Lowest Energy	-1205.5
11	29	Center	-1026.6
		Lowest Energy	-1113.4
12	29	Center	-1007.7

		Lowest Energy	-1160.9
13	29	Center	-1064.9
		Lowest Energy	-1102.2
14	29	Center	-1043.5
		Lowest Energy	-1153.6
15	27	Center	-1134.1
		Lowest Energy	-1211.8
16	24	Center	-1023.6
		Lowest Energy	-1106.1
17	24	Center	-1072.4
		Lowest Energy	-1264.8
18	24	Center	-1302.7
		Lowest Energy	-1302.7
19	20	Center	-1111.1
		Lowest Energy	-1114.6
20	19	Center	-1088.6
		Lowest Energy	-1205.9
21	19	Center	-1020.1
		Lowest Energy	-1120.2
22	18	Center	-1030.4
		Lowest Energy	-1090.4
23	18	Center	-1071.8
		Lowest Energy	-1096.1
24	17	Center	-1018.3
		Lowest Energy	-1102.9
25	13	Center	-1059.8
		Lowest Energy	-1059.8
26	12	Center	-1018.1

		Lowest Energy	-1291.8
27	11	Center	-1087.7
		Lowest Energy	-1150.8
28	11	Center	-1045.2
		Lowest Energy	-1062.8
29	10	Center	-1049.6
		Lowest Energy	-1135.1

Electrostatic-favoured

Coefficient Weights

See *Kozakov et. al.* in Papers for a description of these terms

E=0.40
E
rep
+−0.40
E
att
+1200
E
elec
+1.00
E
DARS

$$E = 0.40E_{rep} + -0.40E_{att} + 1200E_{elec} + 1.00E_{DARS}$$

Cluster Scores

We strongly encourage you to read the FAQ related to these scores before using them.

Cluster	Members	Representative	Weighted Score
0	70	Center	-1153.5
		Lowest Energy	-1440.3
1	65	Center	-1025.0
		Lowest Energy	-1267.5

2	51	Center	-1067.7
		Lowest Energy	-1261.4
3	49	Center	-1110.0
		Lowest Energy	-1190.7
4	49	Center	-1146.6
		Lowest Energy	-1291.6
5	48	Center	-1081.9
		Lowest Energy	-1303.6
6	39	Center	-1202.4
		Lowest Energy	-1312.3
7	37	Center	-1079.3
		Lowest Energy	-1207.5
8	34	Center	-1103.1
		Lowest Energy	-1258.7
9	32	Center	-1093.2
		Lowest Energy	-1131.8
10	31	Center	-1050.1
		Lowest Energy	-1197.0
11	30	Center	-1071.4
		Lowest Energy	-1186.1
12	29	Center	-1023.0
		Lowest Energy	-1140.8
13	29	Center	-1175.3
		Lowest Energy	-1175.3
14	27	Center	-1035.4
		Lowest Energy	-1239.5
15	27	Center	-1095.5
		Lowest Energy	-1152.5

16	27	Center	-1318.4
		Lowest Energy	-1318.4
17	24	Center	-1039.2
		Lowest Energy	-1144.1
18	23	Center	-1028.7
		Lowest Energy	-1114.7
19	21	Center	-1044.7
		Lowest Energy	-1261.2
20	20	Center	-1022.9
		Lowest Energy	-1142.7
21	19	Center	-1124.1
		Lowest Energy	-1124.1
22	14	Center	-1139.5
		Lowest Energy	-1140.5
23	13	Center	-1026.8
		Lowest Energy	-1089.1
24	13	Center	-1067.6
		Lowest Energy	-1067.6
25	12	Center	-1045.4
		Lowest Energy	-1116.8
26	11	Center	-1019.2
		Lowest Energy	-1292.8
27	11	Center	-1038.4
		Lowest Energy	-1098.5
28	10	Center	-1101.5
		Lowest Energy	-1101.5
29	10	Center	-1088.5
		Lowest Energy	-1153.1

Hydophobic favoured

See *Kozakov et. al.* in <u>Papers</u> for a description of these terms

E=0.40
E
rep
+−0.40
E
att
+600
E
elec
+2.00
E
DARS
$E=0.40E_{rep}+−0.40E_{att}+600E_{elec}+2.00E_{DARS}$

Cluster Scores

We strongly encourage you to read the <u>FAQ related to these scores</u> before using them.

Cluster	Members	Representative	Weighted Score
0	124	Center	-1846.8
		Lowest Energy	-2302.5
1	113	Center	-1764.3
		Lowest Energy	-2200.7
2	65	Center	-1775.4
		Lowest Energy	-1935.4
3	53	Center	-1843.3
		Lowest Energy	-1843.3
4	52	Center	-1773.1
		Lowest Energy	-1942.3

5	51	Center	-1659.7
		Lowest Energy	-1975.9
6	47	Center	-1738.6
		Lowest Energy	-1850.1
7	41	Center	-1754.1
		Lowest Energy	-2141.0
8	36	Center	-1711.0
		Lowest Energy	-1841.5
9	32	Center	-1780.1
		Lowest Energy	-2101.7
10	29	Center	-1774.0
		Lowest Energy	-1813.3
11	25	Center	-1796.1
		Lowest Energy	-1961.6
12	22	Center	-1852.5
		Lowest Energy	-1852.5
13	21	Center	-1689.5
		Lowest Energy	-1830.8
14	20	Center	-1705.0
		Lowest Energy	-1815.4
15	20	Center	-1779.0
		Lowest Energy	-1784.8
16	18	Center	-1679.9
		Lowest Energy	-1782.7
17	17	Center	-1753.3
		Lowest Energy	-1870.4
18	16	Center	-1825.1
		Lowest Energy	-1825.1

19	16	Center	-1748.3
		Lowest Energy	-1797.2
20	14	Center	-1669.1
		Lowest Energy	-1742.0
21	13	Center	-1734.5
		Lowest Energy	-1734.5
22	13	Center	-1659.7
		Lowest Energy	-1808.3
23	12	Center	-1678.0
		Lowest Energy	-1796.7
24	12	Center	-1762.6
		Lowest Energy	-1762.6
25	12	Center	-1744.2
		Lowest Energy	-1789.7
26	11	Center	-1900.9
		Lowest Energy	-1900.9
27	11	Center	-1819.3
		Lowest Energy	-1819.3
28	10	Center	-1748.3
		Lowest Energy	-1823.4
29	10	Center	-1654.4
		Lowest Energy	-1745.8

Vanderwall Favoured

Coefficient Weights

See *Kozakov et. al.* in Papers for a description of these terms

$E = 0.40$
E_{rep}

+−0.10

E
att

+600

E
elec

+0.00

E
DARS

$E = 0.40E_{rep} + -0.10E_{att} + 600E_{elec} + 0.00E_{DARS}$

Cluster Scores

We strongly encourage you to read the <u>FAQ related to these scores</u> before using them.

Cluster	Members	Representative	Weighted Score
0	94	Center	-175.4
		Lowest Energy	-194.1
1	64	Center	-178.1
		Lowest Energy	-210.0
2	63	Center	-168.8
		Lowest Energy	-196.3
3	59	Center	-152.8
		Lowest Energy	-181.0
4	48	Center	-154.8
		Lowest Energy	-194.0
5	45	Center	-159.1
		Lowest Energy	-177.7
6	39	Center	-169.2
		Lowest Energy	-203.0
7	36	Center	-151.9
		Lowest Energy	-200.2
8	32	Center	-156.4

		Lowest Energy	-187.4
9	31	Center	-158.6
		Lowest Energy	-174.5
10	30	Center	-152.9
		Lowest Energy	-192.4
11	29	Center	-167.2
		Lowest Energy	-179.4
12	28	Center	-175.5
		Lowest Energy	-189.7
13	20	Center	-153.7
		Lowest Energy	-187.4
14	18	Center	-174.8
		Lowest Energy	-174.8
15	18	Center	-150.7
		Lowest Energy	-163.5
16	17	Center	-176.5
		Lowest Energy	-176.5
17	15	Center	-151.7
		Lowest Energy	-169.3
18	15	Center	-161.2
		Lowest Energy	-186.5
19	15	Center	-159.3
		Lowest Energy	-162.7
20	14	Center	-159.4
		Lowest Energy	-177.0
21	13	Center	-168.3
		Lowest Energy	-168.3
22	13	Center	-158.3

		Lowest Energy	-175.0
23	12	Center	-164.2
		Lowest Energy	-168.6
24	11	Center	-152.0
		Lowest Energy	-180.7
25	11	Center	-153.0
		Lowest Energy	-170.3
26	10	Center	-190.2
		Lowest Energy	-190.2
27	10	Center	-172.4
		Lowest Energy	-172.4
28	9	Center	-159.4
		Lowest Energy	-161.3
29	9	Center	-152.5
		Lowest Energy	-169.7