Table 4. Matrix of the DOT solutions that satisfied the 10 Å Cα and 7 Å heavy atom distance constraint filters clustered according to similarity.

Rank	Energy	1	2	3	5	8	9	10	13	4	7	11	12	6	14	15
Energy		−14.7	−12.2	−12.0	−11.8	−11.7	−11.6	−11.4	−11.0	−12.0	−11.7	−11.4	−11.1	−11.8	−10.9	−10.9
1	−14.7	0	1.7	1.4	3.3	4	2.4	7.6	9.2	17.2	16.5	30.1	31.3	32.5	37.7	302
2	−12.2	8.4	0	1	2	3.3	1	6.4	9.1	16.9	15.9	29.6	30.9	32.3	37.4	29.7
3	−12.0	8.1	10.1	0	2.2	4.2	2	7.3	9.9	16.6	15.8	29.7	30.9	32.1	37.5	30.2
5	−11.8	7.4	6.0	7.4	0	4.4	2.2	6.1	9.9	15.2	14.1	27.9	29.2	30.6	35.8	28.7
8	−11.7	10.5	12.0	8.9	6.0	0	2.4	4.2	6	18.6	17.2	30.0	31.4	33.6	37.3	28.4
9	−11.6	7.4	6.0	7.4	0	6.0	0	5.5	8.4	17.2	16.1	29.5	30.9	32.6	37.2	29.3
10	−11.4	19.8	16.2	19.2	13.1	12.3	13.1	0	6.5	76.1	15.8	27.6	29.3	32.3	34.5	25.4
13	−12.0	36.0	41.1	33.9	35.2	29.3	35.2	35.5	0	21.7	20.1	30.8	32.4	35.6	36.8	26.0
4	−12.0	70.5	65.2	72.3	71.2	77.1	71.2	76.1	106	0	3.2	15.3	15.8	15.6	24.2	23.7
7	−11.7	62.8	56.6	64.4	62.5	68.4	62.5	66.0	97.6	12.2	0	14.8	15.7	16.9	23.9	22.0
11	−11.4	118	112	120	117	123	117	119	152	49.8	55.4	0	2.4	10.2	10.0	16.2
12	−11.1	120	114	122	120	16	120	122	155	50.5	57.7	8.1	0	8.1	9.6	17.9
6	−11.8	118	114	121	120	126	112	125	154	49.6	59.8	26.8	19.2	0	15.8	25.3
14	−10.9	157	152	160	158	164	158	162	167	87.6	96.8	46.7	41.0	38.8	0	15.3
15	−10.9	170	165	173	171	177	171	175	154	10	110	58.7	53.7	52.7	14.7	0

The data in the table to the upper right of the diagonal is the distance between the center of mass of each of the solutions. The lower left triangle shows the smallest angle that would allow overlap of the different structures when the centers of coordinates are superimposed. Solutions 1, 2, 3, 5, 8, and 9 formed a large cluster of highly similar structures. Solutions 10 and 13 were somewhat more divergent but were still close to the overall orientation of this first cluster. Solutions 4, 7, 11, 12, 6, 14, and 15 had angles of rotation that were substantially different.