

Approximate Lattice Similarity

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A common problem is the accumulation of a list of unit cells in differing presentations. For instance, some may be primitive, some centered, or some not reduced, even though they are all measured from the same crystal form. The data below is Protein Data Bank data close to phospholipase A2 as examined by [Le Trong and Stenkamp, 2007]. In the tables, after the first table (which is the original data) in each table the unit cells are adjusted to be as similar as possible to the cell in the first line.

Table 1. Unit cells of phospholipase A2 from the Protein Data Bank

1DPY R 57.98 57.98 57.98 92.02 92.02 92.02 REFERENCE
1G0Z H 80.36 80.36 99.44 90 90 120
1G2X C 80.95 80.57 57.1 90 90.35 90
1U4J H 80.36 80.36 99.44 90 90 120
2OSN R 57.1 57.1 57.1 89.75 89.75 89.75

Table 2. The data of Table 1 matching the rhombohedral reference

1DPY R 57.98 57.98 57.98 92.02 92.02 92.02 REFERENCE
1G0Z H 57.02 57.02 57.02 90.39 90.39 89.61
1G2X C 57.11 57.11 57.1 89.75 90.25 90.27
1U4J H 57.02 57.02 57.02 90.39 90.39 89.61
2OSN R 57.1 57.1 57.1 90.25 90.25 89.75

Table 3. The data of Table 1 matching the monoclinic reference

1G2X C 80.95 80.57 57.1 90 90.35 90 REFERENCE
1DPY R 83.43 80.54 57.98 87.09 90 90
1G0Z H 80.91 80.36 57.02 90 90.56 90
1U4J H 80.91 80.36 57.02 90 90.56 90
2OSN R 80.93 80.58 57.1 90 90.35 90

Table 4. The data of Table 1 matching the hexagonal reference

1U4J H 80.36 80.36 99.44 90 90 120 REFERENCE
1DPY R 83.43 80.54 101.6 91.66 90 121.19
1G0Z H 80.36 80.36 99.44 90 90 120
1G2X C 80.58 80.58 99.35 90.01 89.99 120.01
2OSN R 80.58 80.58 99.33 90 90 120

References

[Le Trong and Stenkamp, 2007] Le Trong, I. and Stenkamp, R. E. (2007). An alternate description of two crystal structures of phospholipase A2 from *Bungarus caeruleus*. *Acta Cryst.* D63:548 – 549.