Cambridge Structural Database
1 January 2023

CSD R-factor Statistics

The precision of crystal structure determinations is often assessed using the crystallographic R-factor, a measure of how well the structure factors computed using the refined structural model agree with structure factors given by the experimentally observed diffraction intensities. CSD structures with unreported R-factors often arise from short communications, and most frequently from the earlier literature.

R-factor range	No. in range	% CSD	Cumulative %
0.0100-0.0300	157,726	12.8	12.8
0.0301-0.0400	262,805	21.2	34
0.0401-0.0500	273,040	22.1	56.1
0.0501-0.0700	319,937	25.9	82.1
0.0701-0.0900	123,441	10	92
0.0901-0.1000	29,424	2.4	94.4
0.1001-0.1500	40,668	3.3	97.7
0.1501-	8,332	0.7	98.4
Not reported	19,859	1.6	100