

Cambridge Structural Database
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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	148,710	12.7	12.7
0.0301-0.0400	249,813	21.3	33.9
0.0401-0.0500	260,436	22.2	56.1
0.0501-0.0700	305,485	26	82.1
0.0701-0.0900	117,321	10	92
0.0901-0.1000	27,777	2.4	94.4
0.1001-0.1500	38,233	3.3	97.7
0.1501-	7,767	0.7	98.3
Not reported	19,729	1.7	100