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Supporting information for article:

Robustness test of the *spacegroupMining* model for determining space groups from atomic pair distribution function data

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Table S1 Top-6 accuracy and top-1 accuracy when r_{\max} is chosen from 10 Å to 30 Å.

r_{\max} (Å)	10	12	14	16	18	20	22	24	26	28	30
Top-6 accuracy	0.648	0.717	0.747	0.778	0.820	0.871	0.882	0.890	0.901	0.901	0.902
Top-1 accuracy	0.285	0.367	0.433	0.449	0.511	0.552	0.600	0.617	0.652	0.671	0.677

Table S2 Top-6 accuracy and top-1 accuracy when Q_{\max} is chosen from 12 Å⁻¹ to 30 Å⁻¹.

Q_{\max} (Å ⁻¹)	12	15	18	21	23	24	27	30
Top-6 accuracy	0.777	0.795	0.811	0.822	0.902	0.900	0.805	0.84
Top-1 accuracy	0.516	0.591	0.597	0.604	0.677	0.663	0.598	0.610

Table S3 Top-6 accuracy and top-1 accuracy when Q_{damp} is chosen from 0 to 0.15 Å⁻¹.

Q_{damp} (Å ⁻¹)	0	0.03	0.04	0.06	0.09	0.12	0.15
Top-6 accuracy	0.861	0.897	0.902	0.879	0.741	0.648	0.578
Top-1 accuracy	0.602	0.659	0.677	0.579	0.390	0.294	0.234

Table S4 Top-6 accuracy and top-1 accuracy when ADP is chosen from 0.005 Å² to 0.01 Å².

adp (Å ²)	0.005	0.006	0.007	0.008	0.009	0.01
Top-6 accuracy	0.873	0.895	0.904	0.902	0.900	0.900
Top-1 accuracy	0.618	0.649	0.664	0.677	0.666	0.641