Supporting information

Table S1 Analysis of variance statistics for refinement of **IIc**.

Fc/*Fc*(max)	0.000	0.008	0.011	0.016	0.021	0.027	0.036	0.049	0.070	0.118	1.000
# in group		534	359	518	396	422	419	441	438	436	443
Goof		1.212	0.948	0.965	1.074	1.123	1.069	1.009	1.106	1.133	0.984
K		3.916	1.634	1.132	1.030	0.973	0.959	0.964	1.013	1.003	1.023

Res. (Å)	0.70	0.77	0.80	0.85	0.90	0.96	1.05	1.17	1.36	1.74	∞
# in group		448	433	445	436	443	437	442	440	444	438
Goof		1.177	1.034	1.031	0.993	1.072	1.068	1.011	0.989	0.991	1.279
K		0.888	1.027	1.047	1.035	1.081	1.051	1.030	1.006	1.013	1.021
R_1		0.304	0.240	0.186	0.134	0.135	0.079	0.052	0.040	0.030	0.025

K = Mean[Fo^2] / Mean[Fc^2] for group

Table S2 Analysis of variance statistics for refinement of **IId**.

Fc/*Fc*(max)	0.000	0.005	0.009	0.014	0.019	0.025	0.033	0.044	0.062	0.104	1.000
# in group		340	306	332	283	305	289	301	301	299	308
Goof		1.492	1.286	0.940	0.915	1.040	0.990	1.083	1.120	1.048	0.982
K		13.631	2.717	1.427	1.076	0.984	0.975	0.948	1.006	0.998	1.018

Res. (Å)	0.70	0.76	0.79	0.83	0.87	0.92	1.00	1.09	1.25	1.57	∞
# in group		318	298	314	300	308	303	306	302	306	309
Goof		1.215	1.057	1.050	1.056	1.059	1.137	1.061	0.934	1.057	1.384
K		0.903	0.980	1.021	1.041	1.059	1.072	1.035	1.014	0.994	1.018
R_1		0.356	0.281	0.213	0.166	0.125	0.111	0.063	0.042	0.036	0.027

K = Mean[Fo^2] / Mean[Fc^2] for group