

Supporting information

Empirical Correction for Resolution and Temperature-Dependent Errors such as Thermal Diffuse Scattering

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Experimental details

S1.1. Data collection

S1.1.1. Dataset 1-TXS-100K

This dataset was collected from an oil-coated shock-cooled crystal on a BRUKER TXS diffractometer with D8 goniometer and INCOATEC Helios mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) and an APEXII detector. The data were collected with omega scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 5, 6 and 7 cm at exposure times between 1 (low-order) and 60s (high-order data).

S1.1.2. Dataset 1-I μ S-100K

This dataset was collected from an oil-coated shock-cooled crystal on a BRUKER diffractometer with D8 goniometer and an INCOATEC I μ S with QUAZAR mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) and an APEXII detector. The data were collected with omega scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 5 cm at exposure times between 10 (low-order) and 45s (high-order data).

S1.1.3. Dataset 1-TSX-15K

The high-resolution data for the multipole refinement were collected from an oil-coated shock-cooled crystal on a BRUKER TXS diffractometer with D8 goniometer and INCOATEC Helios mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) equipped with an Oxford Helijet open stream liquid helium cooling device and an APEXII detector. The data were collected with omega-scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 5 cm at exposure times between 2 (low-order) and 40s (high-order data).

S1.1.4. Dataset 2-TSX-100K

This dataset was collected from an oil-coated shock-cooled crystal on a BRUKER TXS diffractometer with D8 goniometer and INCOATEC Helios mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) and an APEXII detector. Thea data were collected with omega scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 5 at exposure times between 3 (low-order) and 120s (high-order data).

S1.1.5. Dataset 2-I μ S-100K

This dataset was collected from an oil-coated shock-cooled crystal on a BRUKER diffractometer with D8 goniometer and an INCOATEC I μ S with QUAZAR mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) and an APEXII detector. Thea data were collected with omega scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 4 and 5 cm at exposure times between 20 (low-order) and 90s (high-order data).

S1.1.6. Dataset 2-TSX-15K

The high-resolution data for the multipole refinement were collected from an oil-coated shock-cooled crystal on a BRUKER TXS diffractometer with D8 goniometer and INCOATEC Helios mirror optics (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) equipped with an Oxford Helijet open stream liquid helium cooling device and an APEXII detector. The data were collected with omega-scans ($\Delta\omega = 0.3^\circ$) at fixed φ -angles with a detector distance of 5 cm at exposure times between 5 (low-order) and 90s (high-order data).

S1.2. Data reduction

All datasets were integrated with *SAINT* 8.30C (Bruker AXS Inc., 2013). The integration box was refined (IFIXSPOTSIZE=0) starting from x, y, z = 0.8°. The threshold for the spot-shape update was set to 10 I/σ . For the integration with fixed box size the option “IFIXSPOTSIZE” was set to “1” and the x, y and z dimension were set to the size in question. The rest of the integration setup was left untouched. Scaling, absorption correction and error model determination was applied with *SADABS* 2014/2.(Krause *et al.*, 2015). Afterwards the data was merged in *SADABS* and the negative intensities as well as the systematic absences were deleted.

S1.3. Structure solution and IAM refinement

The structures were solved by direct methods (*SHELXT*) (Sheldrick, 2015a) and refined by full-matrix least squares methods against F^2 .(Sheldrick, 2015b, 2008) The position and the atomic displacement parameters of the non-hydrogen atoms were refined against high order data ($d < 0.6 \text{ \AA}$). The hydrogen atoms were identified by a difference Fourier analysis using the low-order data ($d > 1 \text{ \AA}$). For compound **1** one of the two methyl groups in the asymmetric unit was found to be disordered. The

occupation factor refined to 50%. (For the treatment of this disorder during the MM refinement please see below) The independent atom model (IAM) served as the starting model for all multipole refinement including the ones with smaller fixed box sizes of compound **1**. The starting models for the refinements of compound **2** were obtained by the *INVARIOM* tool (Dittrich *et al.*, 2013).

S1.4. MM refinement

The multipole model was refined against F^2 with the full-matrix-least-squares refinement program *XDLSM* implemented in the *XD2006* (Volkov *et al.*, 2006) program package using the atom-centered multipole model by Hansen and Coppens.(Hansen & Coppens, 1978) The core and the spherical valence densities were composed of STO-HF atomic wave functions reported by Su, Coppens and Macchi (SCM bank file for compound **1**) (Su & Coppens, 1998, Macchi & Coppens, 2001) and Clementi and Roetti (CR bank file for compound **2**)(Clementi & Roetti, 1974, Clementi & Raimondi, 1963). The radial fit of these functions was described by the expansion-contraction parameters κ and κ' . For compound **1** the refinement of κ and κ' did not fully converge. Additionally the κ of Mg refined to physically unreasonable values. Thus the κ of Mg and κ' of all atoms were not refined. The expansions over the spherical harmonics were truncated at the hexadecapolar level for all non-hydrogen atoms except Mg and all multipoles ($n_l = 1$ to 4) of each atom shared the same κ' -set (KEEP KAPPA constraint). To decide whether the Mg should be refined as Mg(0) or (+II) we tested both refinements. For Mg(0) only the monopole population was refined. The refinement with Mg(0) showed much better results and thus was further used. The asphericity of the hydrogen atoms were represented by bond directed dipoles. The contraction of the non-hydrogen atoms was described by refinement of κ . For the hydrogen atoms the values were kept fixed during the refinement at $\kappa=1.1$ and $\kappa'=1.18$ (Volkov *et al.*, 2001). Moreover, the U_{iso} values of the hydrogen atoms were constrained to 1.5 U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms during the first steps of the multipole refinement. After each step the distances of the hydrogen atoms were reset to their distances from neutron diffraction experiments (Allen & Bruno, 2010). To refine the occupancy of the disordered methyl groups the mono- and dipole populations of the two parts were constrained to sum up to the poles of the not disordered one. These refined to a ratio of nearly 0.45 to 0.55 for all datasets. In a last refinement step the occupancy was set to exactly 0.45 and 0.55, respectively, and appropriate constraints for the monopole and dipole population were used.

To stabilize the refinement a maximum amount of chemical constraints and symmetry restrictions for the multipolar functions were applied for the first refinement steps. To avoid overfitting the constraints were not dismissed. The density parameters were introduced in the refinement routines in a stepwise manner but in the final cycles all refineable parameters (except κ') were refined together until convergence was reached. However, for some refinements with fixed box sizes and resolution-

dependent scaling the convergence criteria of 10^{-6} max(shift/su) was not reached. The highest observed max(shift/su) was 10^3 .

S1.5. Crystallographic details

S1.5.1. Dataset 1-TXS-100K

Table S1 Data statistics for Dataset **1-TXS-100K** with refined box size.(Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Multiplicity	$\langle I \rangle$	$\langle I \rangle / \sigma$	R _{rim}	R _{pim}
Inf - 1.83	94	94	100	34.22	106.18	187.15	0.0142	0.0025
1.83 - 1.22	222	222	100	25.05	33.89	166.53	0.0254	0.0050
1.22 - 0.97	312	312	100	26.42	19.75	191.77	0.0279	0.0055
0.97 - 0.85	309	309	100	29.2	9.51	143.33	0.0381	0.0070
0.85 - 0.77	316	316	100	26.51	5.38	106.78	0.0479	0.0093
0.77 - 0.71	344	344	100	25.57	5.5	123.44	0.0239	0.0047
0.71 - 0.67	306	306	100	24.53	6.44	121.14	0.0225	0.0046
0.67 - 0.63	381	381	100	23.2	3.84	91.91	0.0320	0.0066
0.63 - 0.61	231	231	100	22.1	3.09	76.42	0.0377	0.0080
0.61 - 0.58	420	420	100	21.23	3.26	73.63	0.0364	0.0079
0.58 - 0.56	332	332	100	20.26	2.05	54.76	0.0520	0.0115
0.56 - 0.55	178	178	100	19.39	1.84	49.08	0.0560	0.0126
0.55 - 0.53	399	399	100	17.42	1.72	44.97	0.0590	0.0140
0.53 - 0.52	223	223	100	14.1	1.52	37.8	0.0640	0.0170
0.52 - 0.50	524	524	100	13.53	1.18	30.42	0.0747	0.0202
0.50 - 0.49	264	264	100	12.73	0.93	24.73	0.0880	0.0245
0.49 - 0.48	328	328	100	12.39	0.99	25.44	0.0864	0.0245
0.48 - 0.47	330	330	100	6.92	0.92	21.71	0.0739	0.0261
0.47 - 0.46	380	380	100	4.74	0.75	17.06	0.0709	0.0324
0.46 - 0.45	353	365	96.7	4.19	0.74	15.38	0.0762	0.0357
0.55 - .45	2801	2813	99.6	10.75	1.09	27.23	0.0704	0.0199
Inf - 0.45	6246	6258	99.8	18.21	6.37	73.44	0.0270	0.0055

S1.5.2. Dataset 1-I μ S-100K

Table S2 Data statistics for Dataset **1-I μ S-100K** with refined box size. (Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R _{rim}	R _{pim}
Inf - 1.95	81	81	100.0	10.94	121.46	196.16	0.0128	0.0040

1.95 - 1.29	185	185	100.0	14.35	36.88	170.35	0.0114	0.0031
1.29 - 1.02	272	272	100.0	13.06	22.92	139.69	0.0149	0.0041
1.02 - 0.90	252	254	99.2	13.89	14.09	118.04	0.0170	0.0046
0.90 - 0.81	286	286	100.0	13.28	7.27	88.76	0.0227	0.0062
0.81 - 0.75	273	274	99.6	12.14	5.91	74.55	0.0283	0.0081
0.75 - 0.71	237	237	100.0	11.46	5.38	62.49	0.0329	0.0097
0.71 - 0.67	296	298	99.3	8.33	6.29	60.63	0.0266	0.0089
0.67 - 0.64	264	273	96.7	5.02	3.77	44.18	0.0260	0.0111
0.64 - 0.62	227	234	97.0	4.86	3.61	41.00	0.0287	0.0123
0.62 - 0.59	349	371	94.1	4.53	3.47	36.79	0.0305	0.0136
0.59 - 0.57	269	291	92.4	4.29	2.61	29.94	0.0451	0.0203
0.57 - 0.56	158	169	93.5	4.27	2.18	29.24	0.0410	0.0185
0.56 - 0.54	342	373	91.7	3.15	2.04	23.35	0.0447	0.0229
0.54 - 0.53	192	210	91.4	2.32	1.52	17.57	0.0490	0.0288
0.53 - 0.51	415	471	88.1	2.12	1.39	15.27	0.0539	0.0328
0.51 - 0.50	239	272	87.9	2.05	1.15	13.95	0.0609	0.0370
0.50 - 0.49	237	274	86.5	2.00	0.92	11.41	0.0735	0.0449
0.49 - 0.48	256	310	82.6	1.85	1.04	12.14	0.0686	0.0431
0.48 - 0.47	268	322	83.2	1.84	0.95	11.70	0.0713	0.0437
0.47 - 0.46	153	218	70.2	1.46	0.75	9.56	0.0974	0.0628
0.56 - 0.46	2102	2450	85.8	2.14	1.28	14.96	0.0562	0.0329
Inf - 0.46	5251	5675	92.5	6.05	7.63	51.72	0.0176	0.0055

S1.5.3. Dataset 1-TSX-15K

Table S3 Data statistics for Dataset **1-TXS-15K** with refined box size. (Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R _{rim}	R _{pim}
Inf - 1.82	93	94	98.9	21.91	101.31	133.95	0.0273	0.0061
1.82 - 1.22	219	219	100	26.1	37.87	122.15	0.0211	0.0042
1.22 - 0.97	309	309	100	22.1	24.5	101.14	0.0198	0.0042
0.97 - 0.84	336	336	100	22.4	12.55	81.45	0.0323	0.0068
0.84 - 0.77	280	280	100	24.45	7.33	73.04	0.0441	0.0089
0.77 - 0.71	340	340	100	22.68	8.12	70.6	0.0492	0.0103
0.71 - 0.67	295	295	100	18.38	9.94	65.38	0.0447	0.0103
0.67 - 0.63	382	382	100	13.45	6.47	55.49	0.0346	0.0094
0.63 - 0.61	229	229	100	12.71	4.77	45.77	0.042	0.0117
0.61 - 0.58	413	413	100	9.94	5.86	43.34	0.038	0.0118
0.58 - 0.56	311	311	100	6.12	4.04	31.33	0.0409	0.0165

0.56 - 0.54	367	367	100	5.85	3.65	28.46	0.0448	0.0186
0.54 - 0.53	198	198	100	5.81	2.98	25.22	0.0516	0.0213
0.53 - 0.51	456	456	100	5.51	2.96	23.4	0.054	0.0231
0.51 - 0.50	278	278	100	5.29	2.39	21.51	0.0626	0.027
0.50 - 0.49	265	265	100	5.23	2.25	19.45	0.0656	0.0286
0.49 - 0.48	312	312	100	5	2.24	19.94	0.0669	0.0298
0.48 - 0.47	341	341	100	4.84	2.1	19.1	0.0714	0.0325
0.47 - 0.46	359	359	100	4.64	1.99	17.96	0.08	0.0377
0.46 - 0.45	406	407	99.8	4.39	1.74	15.83	0.0825	0.0393
0.55 - 0.45	2814	2815	100	5.09	2.41	20.64	0.0625	0.0276
Inf - 0.45	6189	6191	100	11.55	8.38	45.85	0.0308	0.0074

S1.5.4. Dataset 2-TSX-100K

Table S4 Data statistics for Dataset 2-TXS-100K with refined box size. (Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R _{rim}	R _{pim}
Inf - 1.78	730	731	99.9	10.79	56.15	163.72	0.0133	0.0041
1.78 - 1.19	1741	1741	100	13.76	20.83	136.91	0.0163	0.0044
1.19 - 0.94	2513	2513	100	11.71	11.38	89.43	0.0228	0.0066
0.94 - 0.82	2515	2515	100	10.89	7.58	75.79	0.0302	0.0092
0.82 - 0.75	2297	2298	100	13.16	5.26	95.8	0.0324	0.0089
0.75 - 0.69	2792	2801	99.7	9.79	3.89	79.21	0.0289	0.009
0.69 - 0.65	2441	2464	99.1	8.08	3.04	65.46	0.0272	0.0095
0.65 - 0.62	2265	2295	98.7	7.67	2.7	59.52	0.0299	0.0107
0.62 - 0.59	2743	2788	98.4	7.24	2.16	50.27	0.0358	0.0131
0.59 - 0.57	2148	2190	98.1	6.7	1.84	43.84	0.0414	0.0157
0.57 - 0.55	2477	2535	97.7	3.96	1.43	35.31	0.0336	0.0163
0.55 - 0.53	2826	2900	97.4	3.63	1.11	28.66	0.038	0.0195
0.53 - 0.51	3276	3377	97	3.49	0.84	23.1	0.0448	0.0233
0.51 - 0.50	1879	1942	96.8	3.36	0.66	19.41	0.0544	0.0288
0.50 - 0.49	1985	2064	96.2	3.26	0.61	18.23	0.0551	0.0295
0.49 - 0.48	2166	2255	96.1	3.16	0.54	16.38	0.0628	0.0343
0.48 - 0.47	2319	2428	95.5	3.06	0.53	16.15	0.062	0.0342
0.47 - 0.46	2528	2652	95.3	2.93	0.5	15.25	0.0641	0.0361
0.46 - 0.45	2768	2918	94.9	2.8	0.48	14.73	0.066	0.0376
0.45 - 0.44	4228	4825	87.6	2.23	0.38	11.89	0.074	0.044
0.54 - 0.44	22608	23962	94.3	2.99	0.59	17.28	0.0558	0.0305
Inf - 0.44	48637	50232	96.8	6.08	3.9	46.47	0.0227	0.0072

S1.5.5. Dataset 2- μ S-100K

Table S5 Data statistics for Dataset 2- μ S-100K with refined box size. (Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R _{rim}	R _{pim}
Inf - 1.81	696	698	99.7	7.88	53.84	149.91	0.0134	0.005
1.81 - 1.21	1637	1643	99.6	10.1	19.81	129.71	0.0137	0.0043
1.21 - 0.96	2335	2339	99.8	12.78	11.53	122.51	0.016	0.0045
0.96 - 0.84	2318	2319	100	12.64	7.57	102.24	0.0188	0.0053
0.84 - 0.76	2469	2469	100	11.45	5.13	79.97	0.0247	0.0073
0.76 - 0.71	2131	2131	100	10.29	4.14	65.1	0.0292	0.009
0.71 - 0.67	2190	2192	99.9	6.93	3.01	49.36	0.0283	0.0106
0.67 - 0.63	2802	2807	99.8	6.02	2.74	43.73	0.0287	0.0116
0.63 - 0.60	2562	2572	99.6	5.69	2.11	35.86	0.0347	0.0144
0.60 - 0.58	2066	2077	99.5	5.45	1.92	32.01	0.0389	0.0164
0.58 - 0.56	2342	2361	99.2	5.22	1.55	27.25	0.0532	0.023
0.56 - 0.54	2684	2714	98.9	4.23	1.19	20.88	0.0538	0.0255
0.54 - 0.53	1502	1520	98.8	3.46	0.96	16.71	0.0619	0.0328
0.53 - 0.51	3324	3379	98.4	3.33	0.77	13.83	0.0713	0.0384
0.51 - 0.50	1898	1941	97.8	3.21	0.6	11.46	0.0829	0.0452
0.50 - 0.49	2019	2067	97.7	3.06	0.58	10.86	0.0907	0.0505
0.49 - 0.48	2211	2274	97.2	2.97	0.51	9.79	0.096	0.0542
0.48 - 0.47	2343	2416	97	2.85	0.5	9.54	0.0977	0.0559
0.47 - 0.46	2571	2665	96.5	2.73	0.47	8.89	0.1024	0.06
0.46 - 0.45	3658	4162	87.9	2.1	0.45	7.99	0.1054	0.0647
0.55 - 0.45	20913	21827	95.8	2.92	0.62	11.32	0.0805	0.045
Inf - 0.45	45758	46746	97.9	5.82	3.89	41.42	0.0207	0.0072

S1.5.6. Dataset 2-TSX-15K

Table S6 Data statistics for Dataset 2-TXS-15K with refined box size. (Weiss, 2001, Diederichs & Karplus, 1997)

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R _{rim}	R _{pim}
Inf - 1.85	651	652	99.8	4.81	48.99	104.21	0.0113	0.0051
1.85 - 1.23	1555	1558	99.8	4.58	19.75	57.4	0.0186	0.0086
1.23 - 0.98	2159	2159	100	3.82	12.52	33.12	0.0288	0.0147
0.98 - 0.85	2316	2316	100	4.03	8.84	38.34	0.0373	0.0186
0.85 - 0.78	1970	1971	99.9	5.04	6.55	53.45	0.0392	0.0174

0.78 - 0.72	2351	2365	99.4	4.73	5.52	45.76	0.0464	0.0212
0.72 - 0.68	2001	2048	97.7	3.98	4.17	37.3	0.0521	0.025
0.68 - 0.64	2499	2602	96	2.16	3.89	33.52	0.0283	0.0174
0.64 - 0.61	2334	2454	95.1	1.93	3.42	29.74	0.0263	0.0173
0.61 - 0.59	1799	1907	94.3	1.87	3.07	26.88	0.0285	0.0189
0.59 - 0.57	2031	2172	93.5	1.81	2.65	23.56	0.0342	0.0228
0.57 - 0.55	2315	2493	92.9	1.77	2.2	21.22	0.0382	0.0256
0.55 - 0.53	2671	2918	91.5	1.68	1.74	17.26	0.046	0.0311
0.53 - 0.52	1468	1614	91	1.65	1.47	15.08	0.0517	0.035
0.52 - 0.50	3326	3681	90.4	1.58	1.2	12.98	0.057	0.0389
0.50 - 0.49	1780	1999	89	1.52	1.03	11.51	0.0669	0.0458
0.49 - 0.48	2020	2268	89.1	1.48	0.97	10.92	0.0686	0.0471
0.48 - 0.47	2127	2425	87.7	1.42	0.95	10.76	0.0701	0.0484
0.47 - 0.46	2314	2668	86.7	1.37	0.91	10.45	0.0705	0.0486
0.46 - 0.45	2460	2873	85.6	1.31	0.88	10.15	0.0727	0.0506
0.45 - 0.44	979	1662	58.9	0.77	0.84	9.17	0.0796	0.0558
0.54 - 0.44	17851	20695	86.3	1.43	1.08	11.86	0.0616	0.0422
Inf - 0.44	43126	46805	92.1	2.38	4.63	26.4	0.0288	0.0146

S1.6. Crystallographic table

Table S7 Crystallographic data for the datasets of **1**. For each datasets four ways of data treatment are shown: Refinement against the refined box size with one scale factor / Refinement against the refined box size with 10 scale factors / against the ‘best’ integration box /corrected *.hkl file

Dataset	1-TXS-100K	1- μ S-100K	1-TXS-15K
Empirical formula	C ₃₂ H ₄₂ Mg N ₁₂	C ₃₂ H ₄₂ Mg N ₁₂	C ₃₂ H ₄₂ Mg N ₁₂
Molecular weight	691.15	691.15	691.15
Crystal size [mm]	0.26 x 0.24 x 0.13	0.16 x 0.10 x 0.06	0.26 x 0.23 x 0.18
Wavelength [Å]	0.71073	0.56086	0.6199
Crystal system	Rhombohedral	Rhombohedral	Rhombohedral
Space group	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$
<i>a</i> [Å]	10.6712(5)	10.6769(5)	10.6434(5)
<i>b</i> [Å]	10.6712(5)	10.6769(5)	10.6434(5)
<i>c</i> [Å]	24.6546(12)	24.6539(12)	24.6108(12)
α [°]	90	90	90
β [°]	90	90	90
γ [°]	120	120	120
<i>V</i> [Å ³]	2431.4(2)	2433.9(2)	2414.4(2)
<i>Z</i>	1	1	1
Temperature [K]	100(2)	100(2)	15(2)
ρ [Mgm ⁻³]	1.268	1.267	1.277
μ [mm ⁻¹]	0.098	0.098	0.099
<i>F</i> (000)	990	990	990
θ -area [°]	2.354 - 52.268	2.352 - 49.987	2.483 - 52.155
Total number of reflections	113986/113986/114801/113986	34349/34349/34622/34349	71496/71496/71532/71496
Unique reflections	5973/5973/5983/5973	5046/5046/5093/5046	6030/6030/6010/6030
Unique reflections ($I > 3\sigma$)	5457/5457/5422/5303	4524/4524/4511/4323	5457/5457/5421/5364
R_{int}	0.0267/0.0267/0.0363/0.0267	0.0167/0.0167/0.0213/0.0167	0.0299/0.0299/0.0344/0.0299
Parameters	163/172/163/163	163/172/163/163	163/172/163/163
$R\{F\}$ ($I > 3\sigma$)	0.0157/0.0137/0.0138/0.0131	0.0184/0.0171/0.0190/0.0162	0.0159/0.0150/0.0156/0.0147
$R\{F^2\}$ ($I > 3\sigma$)	0.0232/0.0163/0.0177/0.0166	0.0238/0.0216/0.0246/0.0212	0.0213/0.0198/0.0221/0.0203
$wR\{F\}$ ($I > 3\sigma$)	0.0145/0.0129/0.0193/0.0127	0.0188/0.0181/0.0244/0.0185	0.0188/0.0183/0.0192/0.0181
$wR\{F^2\}$ ($I > 3\sigma$)	0.0277/0.0244/0.0356/0.0241	0.0351/0.0335/0.0436/0.0331	0.0352/0.0341/0.0362/0.0337
GooF	3.3798/2.9880/2.0238/2.6713	3.1557/3.0147/2.7103/2.7455	2.4079/2.3310/2.1388/2.1549
Highest peak [10 ³ ·e·Å ⁻³]	0.283/0.154/0.121/0.132	0.264/0.160/0.202/0.135	0.237/0.217/0.192/0.192
Deepest hole [10 ³ ·e·Å ⁻³]	-0.152/-0.148/-0.135/-0.121	-0.188/-0.180/-0.163/-0.150	-0.195/-0.210/-0.182/-0.193

Table S8 Crystallographic data for the datasets of **2**. For each datasets four ways of data treatment are shown: Refinement against the refined box size with one scale factor / Refinement against the refined box size with 10 scale factors / against the ‘best’ integration box /corrected *.hkl file

Dataset	2-TXS-100K	2-I _{ps} -100K	2-TXS-15K
Empirical formula	C26 H19 P S	C26 H19 P S	C26 H19 P S
Molecular weight	394.44	394.44	394.44
Crystal size [mm]	0.22 x 0.19 x 0.11	0.15 x 0.10 x 0.10	0.20 x 0.15 x 0.15
Wavelength [Å]	0.71073	0.56086	0.6199
Crystal system	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> 1	<i>P</i> 1	<i>P</i> 1
<i>a</i> [Å]	10.223(2)	10.225(2)	10.213(2)
<i>b</i> [Å]	12.326(2)	12.336(3)	12.290(2)
<i>c</i> [Å]	17.357(3)	17.371(4)	17.335(3)
α [°]	101.55(2)	101.58(3)	101.62(3)
β [°]	91.23(2)	91.21(4)	91.370(2)
γ [°]	112.05(3)	111.99(4)	112.09(3)
<i>V</i> [Å ³]	1974.8(8)	1979.1(10)	1962.9(8)
<i>Z</i>	4	4	4
Temperature [K]	100(2)	100(2)	15(2)
ρ [Mgm ⁻³]	1.327	1.324	1.335
μ [mm ⁻¹]	0.254	0.253	0.255
<i>F</i> (000)	824	824	824
θ -area [°]	1.204 - 54.761	1.203 - 52.855	1.207 - 53.106
Total number of reflections	305520/305520/305404/305520	272081/272081/273150/272081	111292/111292/ /111292
Unique reflections	46690/46690/46803/46690	43292/43292/43374/43292	41237/41237/ /41237
Unique reflections ($I > 3\sigma$)	40895/40895/40673/39426	36780/36780/36617/35340	34587/34587/ /34237
R_{int}	0.0216/0.0216/0.0219/0.0216	0.0194/0.0194/0.0213/0.0194	0.0248/0.0248/ /
Parameters	720/729/720/720	720/729/720/720	720/729/ /720
$R\{F\}$ ($I > 3\sigma$)	0.0143/0.0134/0.0134/0.0125	0.0173/0.0163/0.0166/0.0150	0.0181/0.0180/ /0.0185
$R\{F^2\}$ ($I > 3\sigma$)	0.0178/0.0160/0.0167/0.0157	0.0177/0.0160/0.0174/0.0152	0.0195/0.0192/ /0.0208
$wR\{F\}$ ($I > 3\sigma$)	0.0123/0.0116/0.0116/0.0120	0.0144/0.0139/0.0166/0.0134	0.0144/0.0142/ /0.0155
$wR\{F^2\}$ ($I > 3\sigma$)	0.0239/0.0225/0.0225/0.0221	0.0271/0.0261/0.0303/0.0250	0.0280/0.0277/ /0.0302
GooF	1.8844/1.7717/1.7285/1.6139	2.0763/1.9978/2.0033/1.8588	1.2973/1.2861/ /1.2701
Highest peak [$10^3 \cdot e \cdot \text{\AA}^{-3}$]	0.285/0.225/0.0224/0.202	0.382/0.311/0.326/0.284	0.260/0.259/ /0.266
Deepest hole [$10^3 \cdot e \cdot \text{\AA}^{-3}$]	-0.269/-0.275/-0.271/-0.248	-0.186/-0.206/-0.235/-0.198	-0.228/-0.225/ /-0.292

S2. Residual density

S2.1. 1-TXS-100K

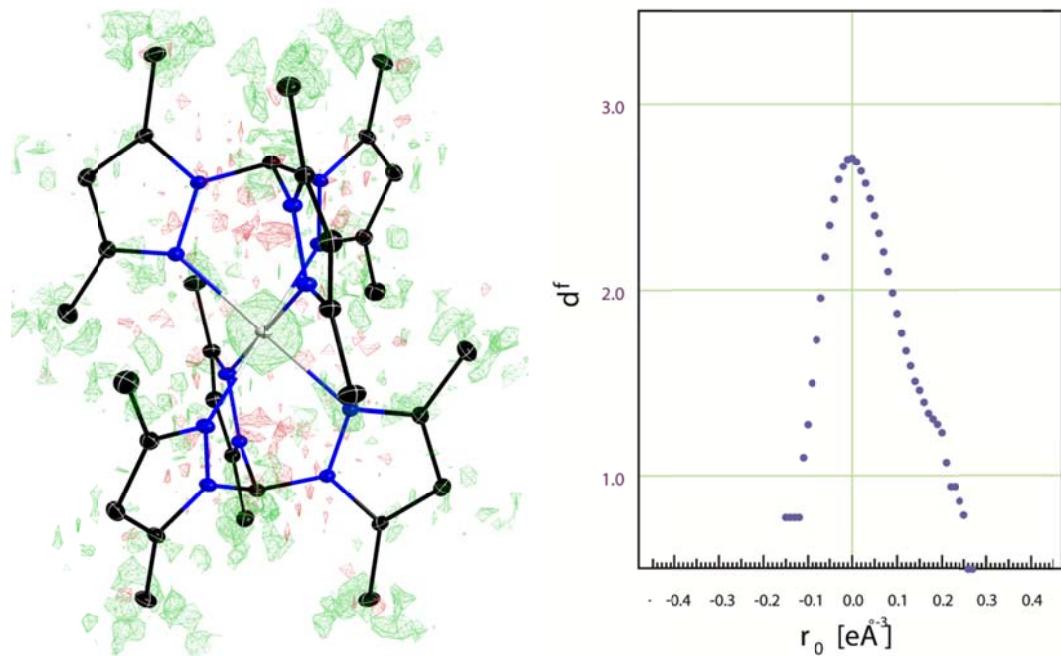


Figure S1 Residual density after MM refinement with one scale factor against data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.068 \text{ e } \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.00 Å from Mg	0.6667	0.3333	0.8333	0.28
PK(2)	is 0.06 Å from C(6)	0.667	0.333	0.7058	0.18
PK(3)	is 0.09 Å from C(5)	0.4101	0.487	0.8337	0.17
PK(4)	is 0.03 Å from C(4)	0.4468	0.353	0.6326	0.16
PK(5)	is 0.40 Å from H(4B)	0.5625	0.4568	0.608	0.16
PK(6)		0.2259	0.1089	0.9449	0.15
PK(7)		0.6668	0.3335	0.4999	0.15
PK(8)		0.2037	0.0541	0.717	0.13
PK(9)	is 0.43 Å from H(4C)	0.3333	0.3379	0.6204	0.12
PK(10)	is 0.44 Å from H(5B)	0.4592	0.6282	0.8301	0.12
HL(1)	is 0.37 Å from C(4)	0.4092	0.3294	0.6372	-0.15
HL(2)		0.1799	0.0035	0.408	-0.1
HL(3)		0.2586	0.0765	0.663	-0.1
HL(4)		0.817	0.0719	0.6638	-0.1
HL(5)		0.552	0.2034	0.71	-0.1
HL(6)		0.9598	0.0019	0.4224	-0.09
HL(7)		0.1515	0.0736	0.3347	-0.09
HL(8)		0.1541	0.0703	0.6638	-0.09
HL(9)		0.5206	0.0559	0.8272	-0.09
HL(10)		0.7157	0.4793	0.7408	0

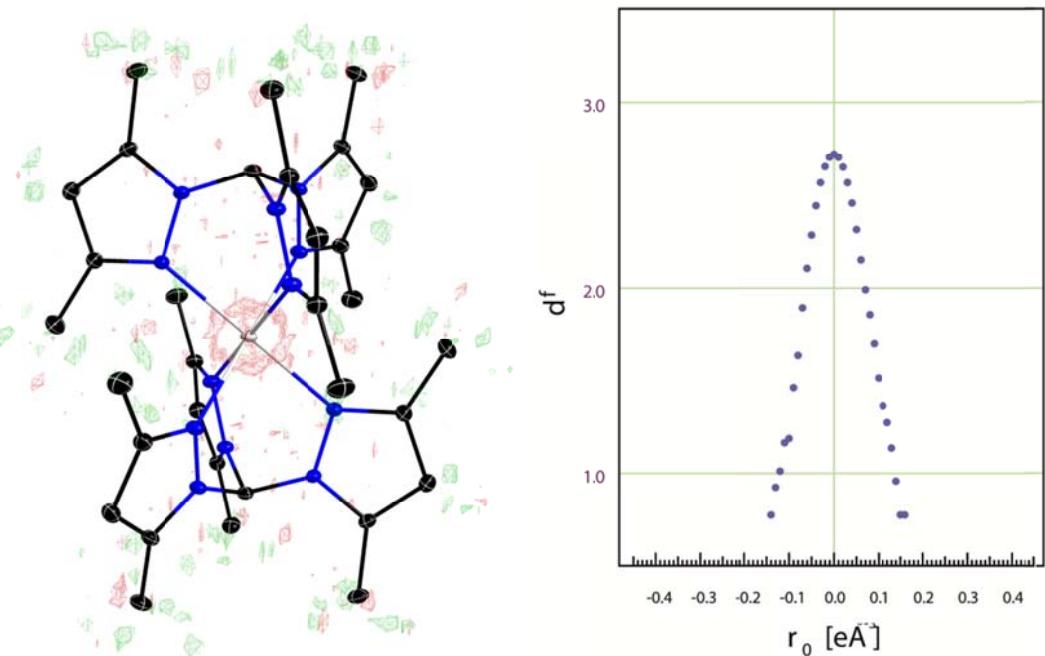


Figure S2 Residual density after MM refinement with 10 scale factors data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.068 \text{ e} \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.6665	0.3331	0.1651	0.15
PK(2)		0.2256	0.1098	0.945	0.15
PK(3)	is 0.35 Å from H(4B)	0.5586	0.4511	0.609	0.13
PK(4)	is 0.53 Å from C(4)	0.5037	0.3943	0.634	0.13
PK(5)	is 0.61 Å from C(5)	0.4585	0.4795	0.8453	0.11
PK(6)		0.5549	0.1122	0.9448	0.11
PK(7)		0.2026	0.0556	0.7174	0.11
PK(8)	is 0.76 Å from C(4)	0.4077	0.3694	0.6118	0.11
PK(9)		0.3352	0.0008	0.4991	0.1
PK(10)	is 0.47 Å from H(5B)	0.4567	0.63	0.8294	0.1
HL(1)	is 0.39 Å from C(4)	0.4074	0.3286	0.6372	-0.15
HL(2)	is 0.19 Å from H(4C)	0.3564	0.3772	0.6115	-0.1
HL(3)		0.2589	0.0757	0.6636	-0.1
HL(4)	is 0.06 Å from H(4A)	0.4085	0.2342	0.628	-0.1
HL(5)	is 0.74 Å from Mg	0.6107	0.2618	0.8439	-0.1
HL(6)		0.9086	0.0535	0.3528	-0.09
HL(7)		0.8177	0.0723	0.6641	-0.09
HL(8)	is 0.57 Å from C(3)	0.4672	0.3526	0.7098	-0.09
HL(9)	is 0.28 Å from H(4B)	0.5587	0.4197	0.6236	-0.09
HL(10)		0.5926	0.1267	0.829	-0.09

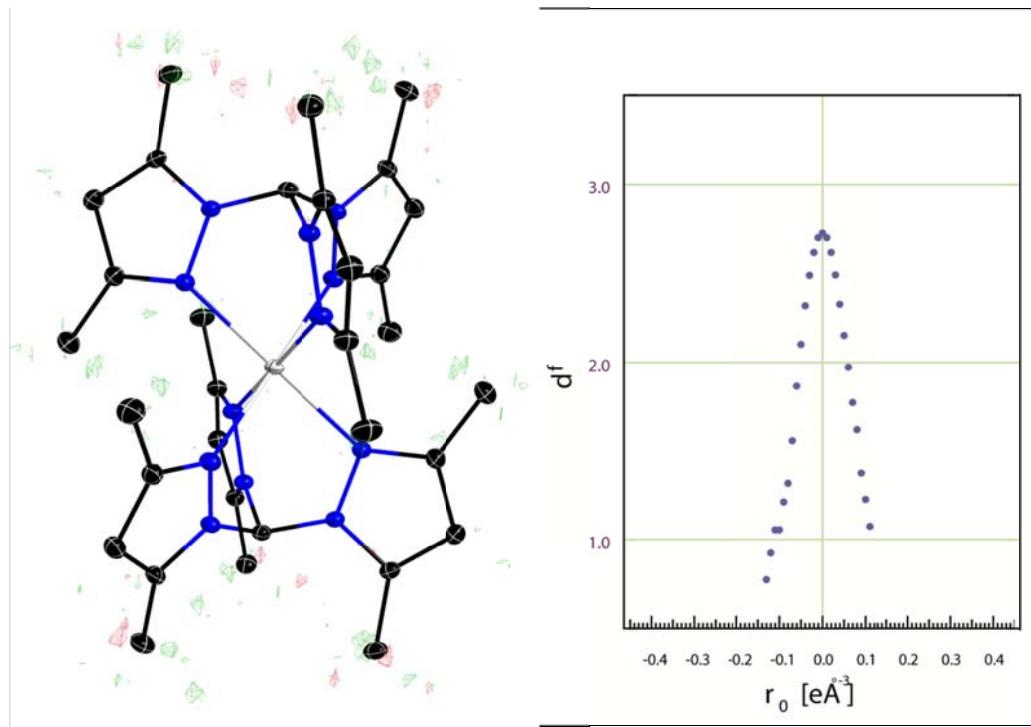


Figure S3 Residual density after MM refinement with one scale factors data integrated with ‘best’ box size ($x = 0.3$, $y = 0.45$, $z = 0.4$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.068 \text{ e } \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.55 Å from C(4)	0.5059	0.3927	0.6326	0.12
PK(2)		0.2252	0.1098	0.9455	0.11
PK(3)		0.6659	0.3325	0.1654	0.11
PK(4)	is 0.67 Å from C(5)	0.4653	0.4807	0.8452	0.1
PK(5)	is 0.42 Å from H(4B)	0.559	0.4576	0.6095	0.1
PK(6)	is 0.49 Å from H(4C)	0.331	0.3313	0.6214	0.09
PK(7)	is 0.41 Å from H(5B)	0.4583	0.626	0.8301	0.08
PK(8)	is 0.72 Å from C(5)	0.3461	0.4312	0.8233	0.08
PK(9)		0.7177	0.1864	0.6165	0.08
PK(10)	is 0.43 Å from H(2)	0.3514	0.4828	0.7083	0.08
HL(1)	is 0.40 Å from C(4)	0.4063	0.3289	0.6373	-0.13
HL(2)	is 0.20 Å from H(4C)	0.3572	0.3752	0.6103	-0.09
HL(3)	is 0.06 Å from H(4A)	0.4115	0.2348	0.6277	-0.09
HL(4)		0.2571	0.0755	0.6639	-0.09
HL(5)	is 0.53 Å from Mg	0.702	0.3513	0.8165	-0.08
HL(6)	is 0.49 Å from C(3)	0.476	0.3668	0.7086	-0.08
HL(7)	is 0.39 Å from H(5F)	0.4788	0.5106	0.8786	-0.08
HL(8)		0.9667	-0.0043	0.4156	-0.07
HL(9)		0.859	0.0176	0.3293	-0.07
HL(10)		0.9074	0.0519	0.5922	-0.07

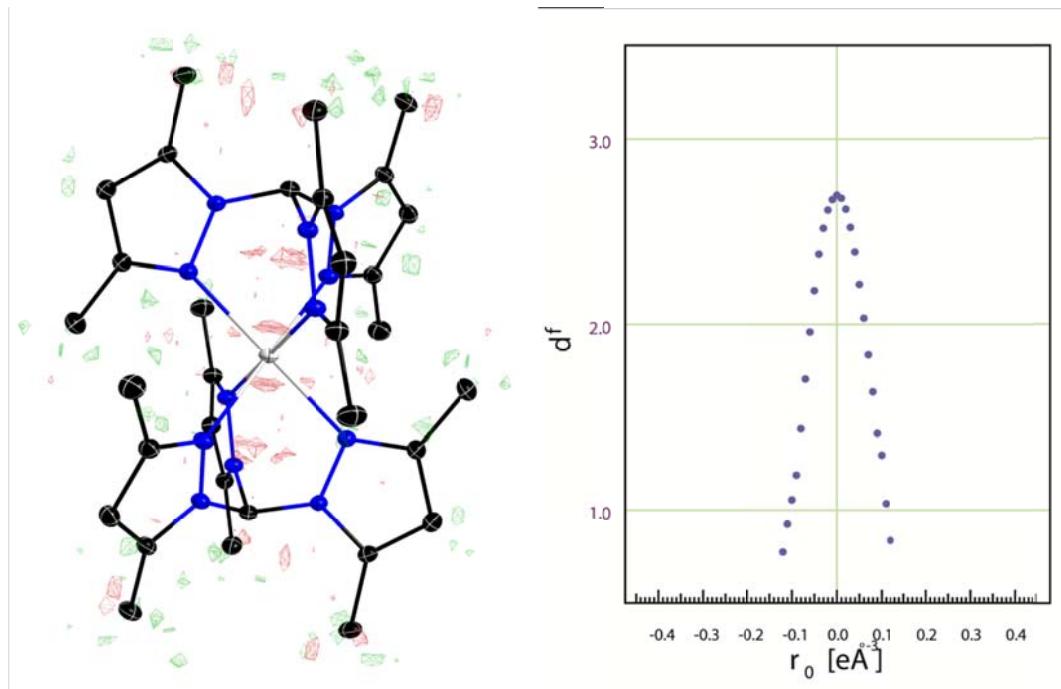


Figure S4 Residual density after MM refinement with one scale factors data with empirical TDS correction ($a = -0.15$, $b = 0.7$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.068 \text{ e Å}^{-3}$.(Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.6667	0.3329	0.1653	0.13
PK(2)		0.2243	0.1102	0.9449	0.13
PK(3)	is 0.56 Å from C(4)	0.507	0.3939	0.6328	0.12
PK(4)	is 0.76 Å from C(4)	0.4046	0.3683	0.6132	0.1
PK(5)	is 0.45 Å from H(4B)	0.5638	0.4618	0.6078	0.1
PK(6)		0.6335	0.0356	0.279	0.09
PK(7)	is 0.74 Å from C(5)	0.4501	0.4832	0.8565	0.09
PK(8)		0.2019	0.0538	0.7169	0.09
PK(9)	is 0.46 Å from H(5B)	0.4444	0.6142	0.8304	0.09
PK(10)		0.0701	0.0365	0.944	0.08
HL(1)	is 0.41 Å from C(4)	0.4056	0.3284	0.6374	-0.12
HL(2)	is 0.00 Å from Mg	0.6667	0.3333	0.8333	-0.12
HL(3)	is 0.04 Å from H(4A)	0.4088	0.2362	0.628	-0.09
HL(4)		0.9573	0	0.4227	-0.08
HL(5)	is 0.20 Å from H(4C)	0.3569	0.3763	0.611	-0.08
HL(6)		0.9089	0.0545	0.352	-0.08
HL(7)	is 0.52 Å from C(3)	0.4795	0.368	0.7099	-0.08
HL(8)		0.5543	0.1133	0.1255	-0.08
HL(9)		0.8192	0.0719	0.6639	-0.08
HL(10)		0.2597	0.0776	0.6637	-0.08

S2.2. 1- μ S-100K

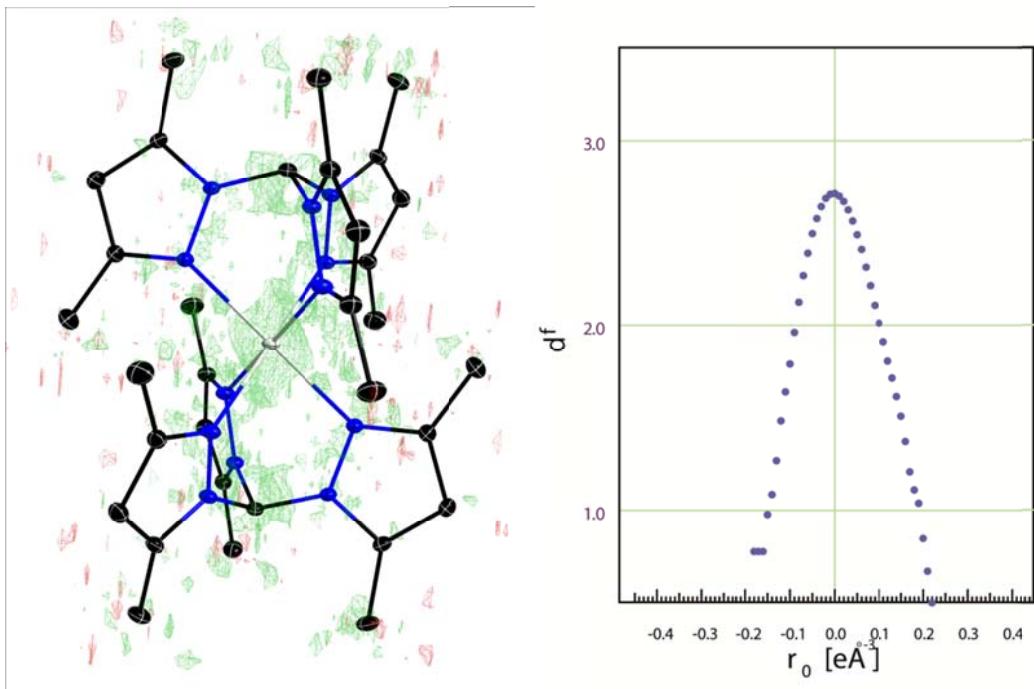


Figure S5 Residual density after MM refinement with one scale factor against data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.085 \text{ e } \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.00 Å from Mg	0.6667	0.3333	0.8333	0.26
PK(2)	is 0.04 Å from C(6)	0.6678	0.333	0.705	0.22
PK(3)	is 0.04 Å from C(4)	0.4449	0.3516	0.6351	0.2
PK(4)	is 0.09 Å from C(5)	0.4155	0.4874	0.8349	0.16
PK(5)		0.4461	0.2215	0.6953	0.16
PK(6)	is 0.19 Å from N(2)	0.5551	0.3729	0.7299	0.15
PK(7)	is 0.38 Å from H(4B)	0.5495	0.4502	0.6091	0.15
PK(8)	is 0.05 Å from N(1)	0.5519	0.4032	0.776	0.15
PK(9)		0.2231	0.1113	0.9448	0.15
PK(10)	is 1.21 Å from Mg	0.5772	0.3522	0.8103	0.14
HL(1)	is 0.38 Å from C(4)	0.408	0.3293	0.6372	-0.19
HL(2)		1.0002	0	0.0148	-0.16
HL(3)	is 0.04 Å from H(2)	0.3091	0.4576	0.7183	-0.14
HL(4)		0.5542	0.116	0.4442	-0.14
HL(5)		0.4437	0.2225	0.5539	-0.13
HL(6)		0.5151	0.1435	0.2207	-0.13
HL(7)		0.092	-0.0003	0.1171	-0.12
HL(8)		0.6658	0.3325	0.6622	-0.12
HL(9)		0.6656	0.1471	0.3126	-0.12
HL(10)		0.3386	0	0.3348	-0.12

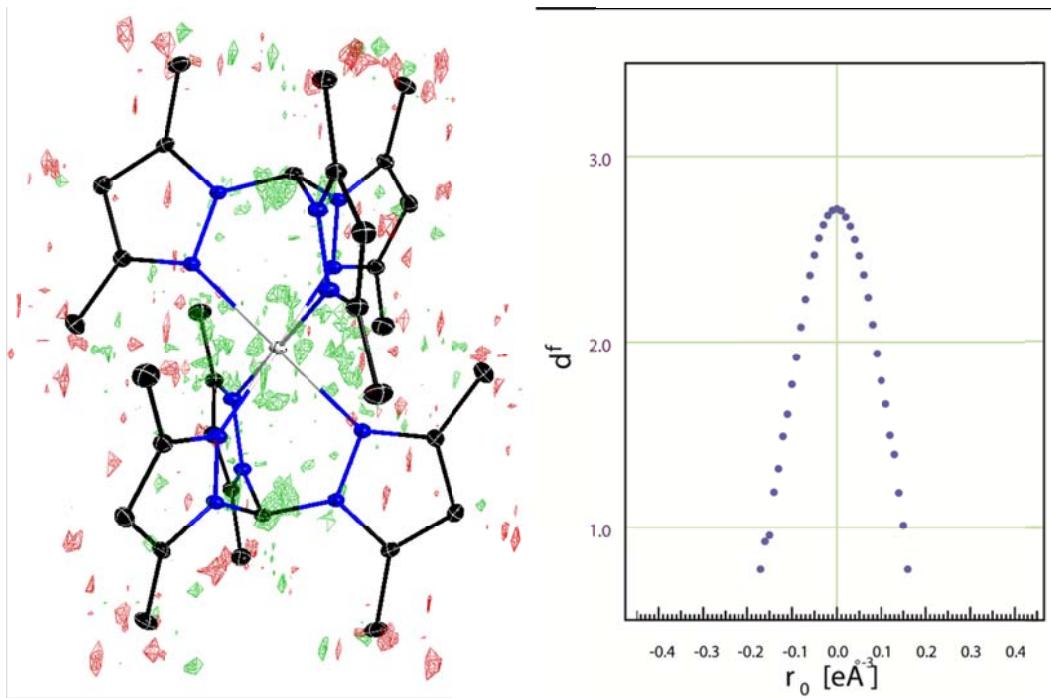


Figure S6 Residual density after MM refinement with 10 scale factors data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.085 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.4465	0.2209	0.6952	0.16
PK(2)		0.2231	0.1124	0.945	0.15
PK(3)	is 0.39 Å from H(4B)	0.5497	0.4506	0.609	0.14
PK(4)		0.9993	0.0007	0.1698	0.14
PK(5)		0.3322	0.0016	0.4995	0.14
PK(6)	is 0.09 Å from C(6)	0.6681	0.3331	0.7073	0.13
PK(7)	is 1.00 Å from Mg	0.6649	0.3378	0.793	0.12
PK(8)		0.2058	0.0676	0.7104	0.12
PK(9)		0.1667	0.0334	0.4766	0.12
PK(10)	is 1.24 Å from Mg	0.5756	0.3541	0.8099	0.12
HL(1)	is 0.39 Å from C(4)	0.4071	0.3287	0.6373	-0.18
HL(2)		0.6669	0.3327	0.32	-0.16
HL(3)	is 0.03 Å from H(2)	0.3093	0.4587	0.7181	-0.16
HL(4)	is 0.16 Å from H(4C)	0.3555	0.381	0.6165	-0.13
HL(5)		0.4442	0.2227	0.5537	-0.13
HL(6)		0.5541	0.1165	0.4445	-0.13
HL(7)	is 0.58 Å from C(5)	0.3912	0.4456	0.8485	-0.12
HL(8)	is 0.64 Å from C(4)	0.4727	0.412	0.6199	-0.12
HL(9)		0.5766	0.281	0.2183	-0.12
HL(10)		0.5157	0.1441	0.2204	-0.12

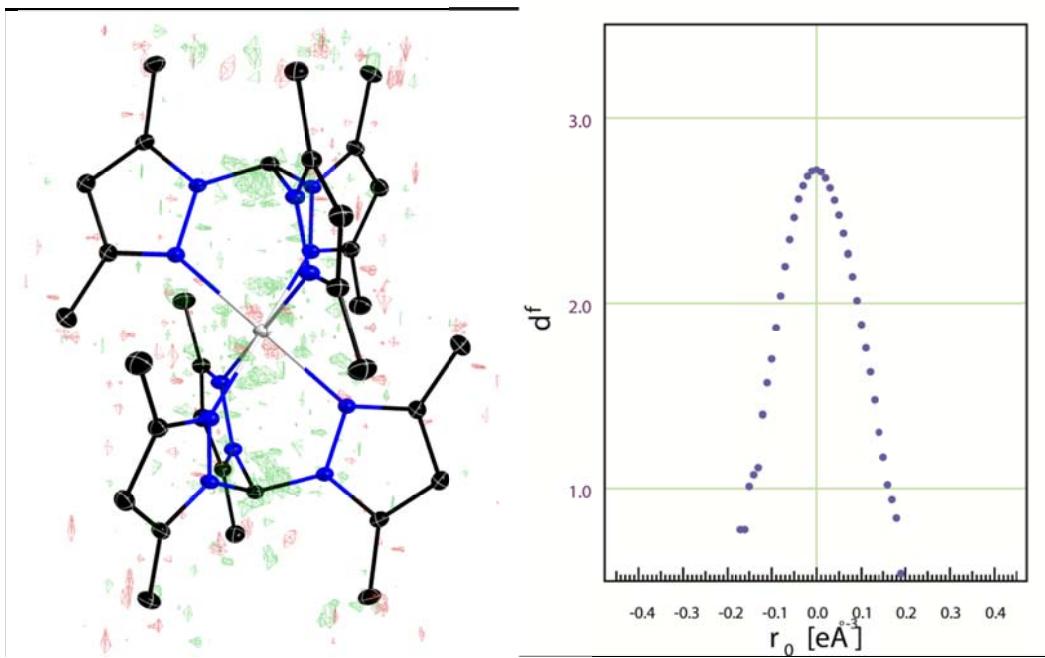


Figure S7 Residual density after MM refinement with one scale factors data integrated with ‘best’ box size ($x = 0.4$, $y = 0.4$, $z = 0.4$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.085 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.85 Å from Mg(1)	0.6678	0.3318	0.8678	0.2
PK(2)		0.6169	0.2616	0.947	0.17
PK(3)		0.6667	0.3333	0.1646	0.16
PK(4)		0.666	-0.0006	0.1659	0.15
PK(5)		0.5585	0.1099	0.9451	0.15
PK(6)		0.2024	0.0588	0.711	0.14
PK(7)		0.2959	0.0574	0.6964	0.14
PK(8)		0.2228	0.1117	0.9452	0.14
PK(9)	is 0.38 Å from N(2)	0.5335	0.3801	0.7204	0.14
PK(10)	is 0.86 Å from Mg(1)	0.749	0.3684	0.8177	0.13
HL(1)	is 0.40 Å from C(4)	0.4066	0.3276	0.6368	-0.16
HL(2)	is 0.54 Å from Mg(1)	0.7099	0.3513	0.8482	-0.14
HL(3)	is 0.61 Å from C(1)	0.4817	0.5002	0.7654	-0.12
HL(4)		0.1912	0.0288	0.889	-0.12
HL(5)		1.0022	0.0004	0.0156	-0.11
HL(6)	is 0.64 Å from C(3)	0.4279	0.3863	0.6727	-0.11
HL(7)	is 0.07 Å from H(2)	0.311	0.456	0.7197	-0.11
HL(8)	is 0.57 Å from C(5)	0.3848	0.451	0.8489	-0.11
HL(9)	is 0.65 Å from N(2)	0.5364	0.4102	0.7336	-0.11
HL(10)	is 0.19 Å from H(4A)	0.4034	0.2287	0.6344	-0.11

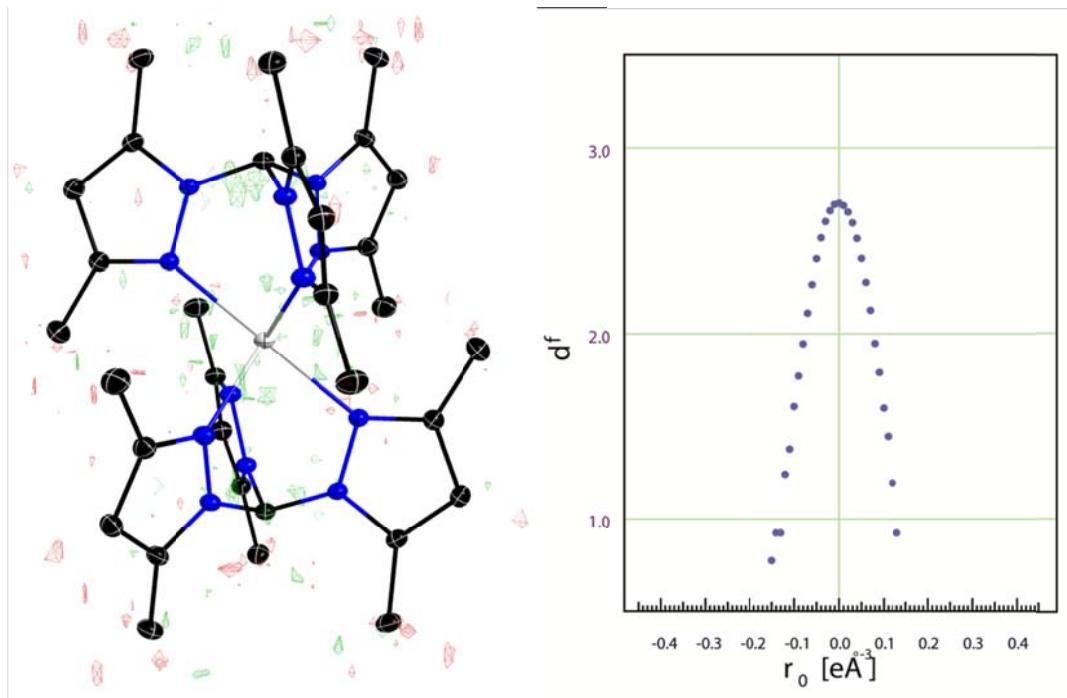


Figure S8 Residual density after MM refinement with one scale factors data with empirical TDS correction ($a = 0.0$, $b = 0.7$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.085 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.4471	0.2229	0.6946	0.14
PK(2)		0.2226	0.1132	0.9451	0.13
PK(3)	is 1.04 Å from Mg	0.667	0.3365	0.791	0.12
PK(4)	is 1.43 Å from Mg	0.8148	0.3743	0.8246	0.11
PK(5)		0.4327	0.0321	0.0314	0.11
PK(6)		0.6648	0.0009	0.1657	0.11
PK(7)		0.0659	-0.0099	0.375	0.11
PK(8)		0.6667	0.3328	0.1641	0.11
PK(9)		0.7235	0.1884	0.6243	0.11
PK(10)	is 0.39 Å from H(4B)	0.5581	0.4553	0.6118	0.11
HL(1)	is 0.40 Å from C(4)	0.4064	0.3274	0.6378	-0.15
HL(2)		1	-0.0006	0.015	-0.13
HL(3)	is 0.03 Å from H(2)	0.3123	0.4564	0.7169	-0.13
HL(4)		0.5546	0.1172	0.4444	-0.12
HL(5)	is 0.68 Å from C(4)	0.4713	0.4172	0.6207	-0.12
HL(6)		0.4455	0.2209	0.5539	-0.12
HL(7)		0.9993	-0.0007	0.3283	-0.11
HL(8)	is 0.16 Å from H(4C)	0.3615	0.3821	0.6122	-0.11
HL(9)		0.338	-0.0003	0.335	-0.1
HL(10)		0.0393	0.0231	0.0467	-0.1

S2.3. 1-TXS-15K

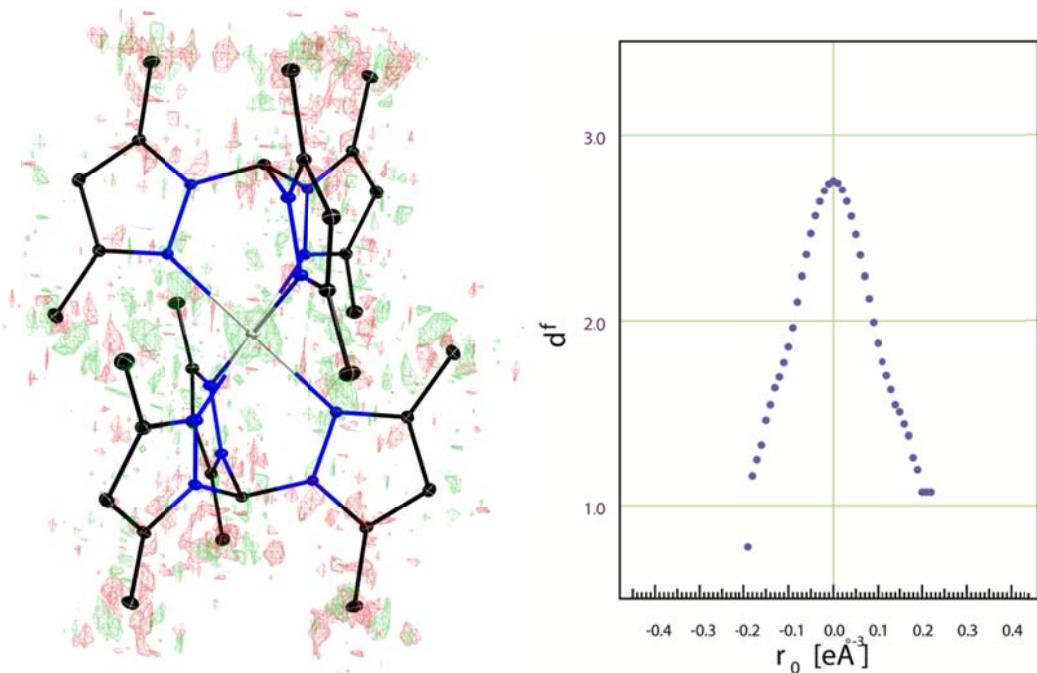


Figure S9 Residual density after MM refinement with one scale factor against data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.076 \text{ e} \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.59 Å from C(5)	0.4463	0.4811	0.8498	0.24
PK(2)	is 0.35 Å from Mg(1)	0.7003	0.3527	0.8269	0.22
PK(3)	is 0.03 Å from C(4)	0.4456	0.3537	0.633	0.18
PK(4)		0.6667	0.3333	0.1645	0.17
PK(5)	is 0.03 Å from C(6)	0.6682	0.332	0.7028	0.16
PK(6)	is 0.07 Å from N(1)	0.5574	0.4106	0.7743	0.15
PK(7)		0.2202	0.1113	0.9449	0.14
PK(8)		0.2255	0.1163	0.6104	0.13
PK(9)		0.3304	0.0026	0.1647	0.13
PK(10)		0.3521	0.0606	0.3901	0.12
HL(1)	is 0.31 Å from C(4)	0.4614	0.3716	0.6231	-0.19
HL(2)	is 0.35 Å from C(6)	0.7024	0.3528	0.7079	-0.18
HL(3)	is 0.35 Å from C(5)	0.388	0.486	0.8226	-0.17
HL(4)	is 0.06 Å from H(4A)	0.4076	0.2375	0.6253	-0.17
HL(5)	is 0.09 Å from H(4B)	0.3619	0.3811	0.6178	-0.16
HL(6)	is 0.38 Å from C(3)	0.4506	0.4086	0.7002	-0.14
HL(7)		1.0008	-0.0003	0.0161	-0.13
HL(8)	is 0.75 Å from C(1)	0.4096	0.368	0.7706	-0.13
HL(9)		0.8103	0.0729	0.3258	-0.13
HL(10)		0.6667	0.3337	0.9995	-0.13

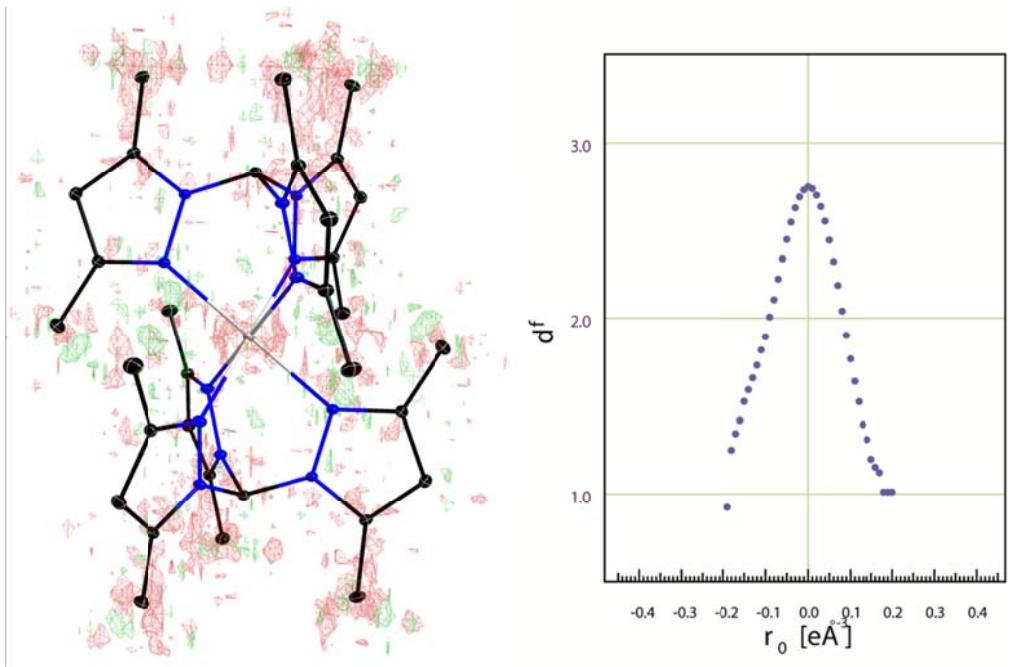


Figure S10 Residual density after MM refinement with 10 scale factors data with refined box size. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.076 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.59 Å from C(5)	0.4467	0.4806	0.8497	0.22
PK(2)		0.6663	0.3329	0.1645	0.17
PK(3)	is 0.68 Å from C(4)	0.416	0.3728	0.6136	0.13
PK(4)		0.3303	0.0024	0.1648	0.13
PK(5)		0.2252	0.1168	0.6105	0.13
PK(6)		0.2201	0.1116	0.9449	0.13
PK(7)		0.8679	0.0537	0.7189	0.12
PK(8)		0.6332	0.2644	0.6106	0.12
PK(9)	is 0.58 Å from C(4)	0.504	0.3885	0.6241	0.12
PK(10)	is 0.66 Å from C(4)	0.4469	0.2914	0.6372	0.11
HL(1)	is 0.45 Å from C(4)	0.4617	0.3907	0.6222	-0.21
HL(2)	is 0.49 Å from C(5)	0.3963	0.4436	0.8418	-0.18
HL(3)	is 0.06 Å from H(4A)	0.4066	0.2372	0.6248	-0.18
HL(4)	is 0.08 Å from H(4B)	0.3626	0.3814	0.6173	-0.17
HL(5)	is 0.37 Å from C(6)	0.7041	0.353	0.7082	-0.17
HL(6)	is 0.47 Å from C(3)	0.5088	0.4056	0.7031	-0.15
HL(7)		0.666	0.3331	0.3184	-0.14
HL(8)	is 0.71 Å from C(1)	0.4088	0.372	0.7705	-0.13
HL(9)	is 0.64 Å from Mg(1)	0.7299	0.353	0.8424	-0.13
HL(10)	is 0.48 Å from N(1)	0.5439	0.4436	0.7809	-0.13

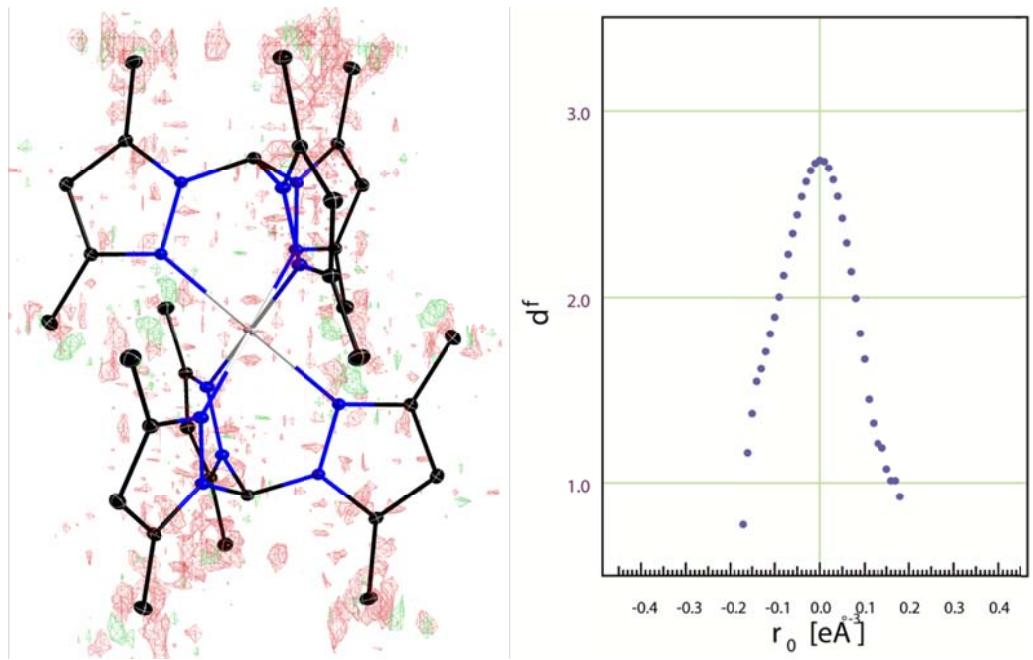


Figure S11 Residual density after MM refinement with one scale factors data integrated with ‘best’ box size ($x = 0.5$, $y = 0.6$, $z = 0.4$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.076 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.61 Å from C(5)	0.4488	0.4843	0.8508	0.19
PK(2)		0.9997	0.0008	0.166	0.12
PK(3)	is 0.60 Å from C(4)	0.5059	0.3893	0.6234	0.12
PK(4)	is 0.43 Å from H(4B)	0.3326	0.3366	0.6166	0.12
PK(5)		0.8698	0.0538	0.718	0.12
PK(6)	is 0.53 Å from N(1)	0.6045	0.4413	0.7651	0.12
PK(7)		0.6671	0.3329	0.0539	0.12
PK(8)		0.7637	0.0159	0.5693	0.11
PK(9)		0.5521	0.1023	0.9421	0.11
PK(10)	is 0.38 Å from Mg(1)	0.7016	0.3509	0.8253	0.11
HL(1)	is 0.44 Å from C(4)	0.4626	0.3907	0.6226	-0.18
HL(2)	is 0.47 Å from C(5)	0.3911	0.444	0.8399	-0.17
HL(3)	is 0.56 Å from C(3)	0.4484	0.3891	0.6712	-0.16
HL(4)	is 0.09 Å from H(4A)	0.4106	0.2363	0.624	-0.16
HL(5)	is 0.52 Å from Mg(1)	0.6662	0.3326	0.8121	-0.16
HL(6)	is 0.07 Å from H(4B)	0.3641	0.3819	0.6175	-0.15
HL(7)	is 0.39 Å from C(6)	0.6494	0.2956	0.7104	-0.14
HL(8)	is 0.54 Å from N(2)	0.5566	0.3722	0.7012	-0.13
HL(9)	is 0.71 Å from C(1)	0.4089	0.3724	0.7703	-0.13
HL(10)	is 0.50 Å from N(1)	0.5101	0.3852	0.7665	-0.13

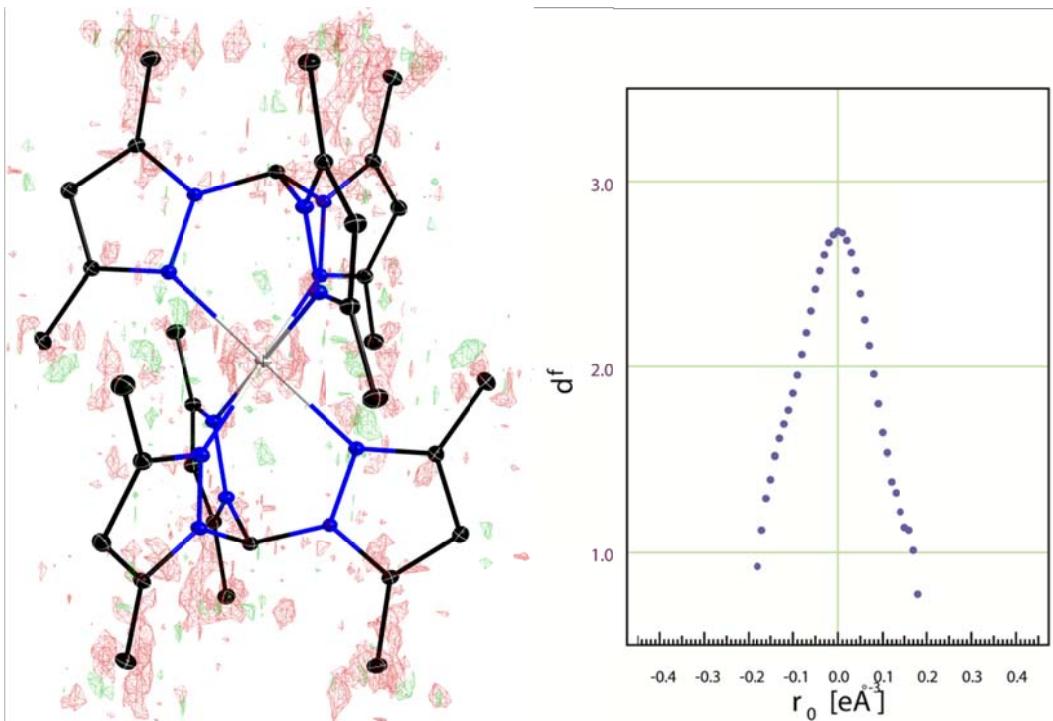


Figure S12 Residual density after MM refinement with one scale factors data with empirical TDS correction ($a = 0.0$, $b = 0.3$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.076 \text{ e } \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.61 Å from C(5)	0.4484	0.4845	0.8506	0.19
PK(2)		0.6667	0.3329	0.1648	0.16
PK(3)		0.5572	0.1063	0.9446	0.13
PK(4)		0.3369	0.0009	0.499	0.12
PK(5)	is 0.35 Å from Mg(1)	0.7006	0.3522	0.8267	0.12
PK(6)	is 0.69 Å from C(4)	0.4152	0.3728	0.6135	0.12
PK(7)		0.6319	0.2638	0.611	0.12
PK(8)		0.22	0.1121	0.9447	0.12
PK(9)	is 0.19 Å from N(1)	0.5564	0.4219	0.7729	0.11
PK(10)		0.6277	0.0357	0.2754	0.11
HL(1)	is 0.44 Å from C(4)	0.4618	0.3906	0.6223	-0.19
HL(2)	is 0.49 Å from C(5)	0.3966	0.4437	0.8418	-0.17
HL(3)	is 0.07 Å from H(4A)	0.4074	0.2371	0.6248	-0.17
HL(4)	is 0.09 Å from H(4B)	0.3631	0.3822	0.6175	-0.15
HL(5)	is 0.37 Å from C(6)	0.704	0.3535	0.7084	-0.15
HL(6)	is 0.71 Å from C(1)	0.409	0.372	0.7707	-0.14
HL(7)	is 0.45 Å from C(3)	0.5114	0.4106	0.7005	-0.14
HL(8)	is 0.74 Å from C(3)	0.4653	0.3919	0.6626	-0.12
HL(9)	is 0.51 Å from N(1)	0.5041	0.3839	0.7717	-0.12
HL(10)	is 0.66 Å from Mg(1)	0.732	0.354	0.8428	-0.12

S2.4. 2-TXS-100K

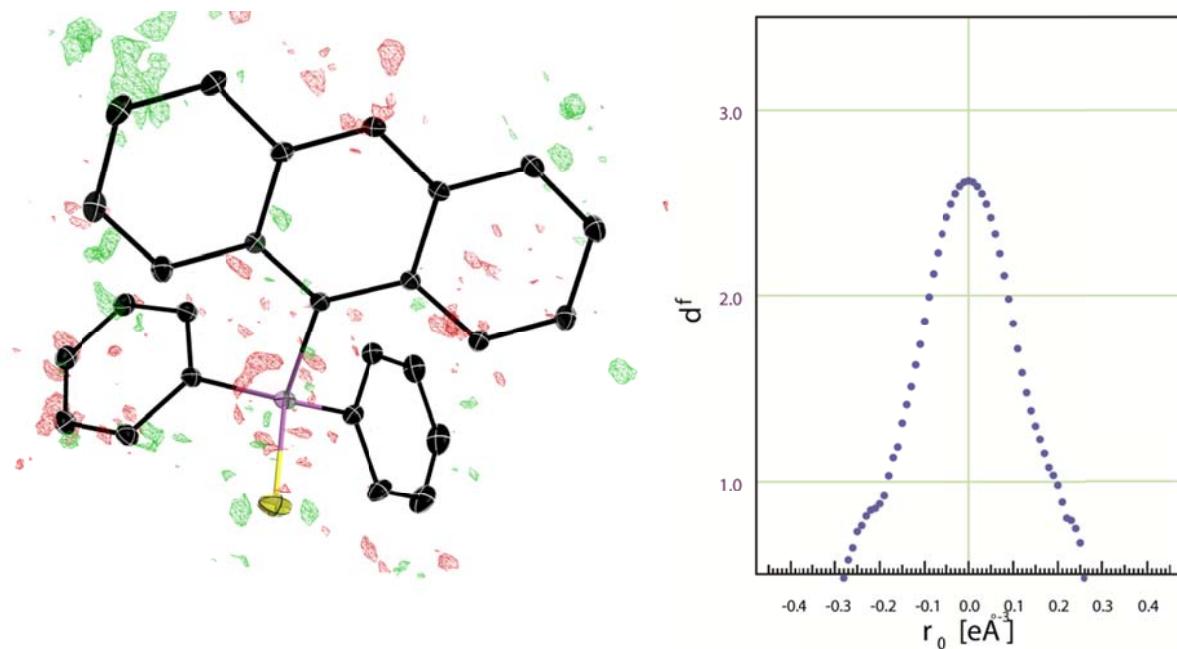


Figure S13 Residual density after MM refinement with one scale factor against data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.088 \text{ e } \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.06 Å from S(1)	0.3387	0.5513	0.7681	0.28
PK(2)		0.898	0.2737	0.069	0.23
PK(3)	is 0.03 Å from S(2)	0.79	0.5347	0.6638	0.22
PK(4)	is 0.47 Å from C(5)	-0.2585	0.356	0.9014	0.21
PK(5)	is 0.03 Å from P(1)	0.2391	0.3862	0.7848	0.21
PK(6)	is 0.48 Å from C(37)	0.6551	0.9972	0.817	0.2
PK(7)	is 0.03 Å from P(2)	0.8997	0.7021	0.6561	0.19
PK(8)		0.5236	0.2985	0.9956	0.18
PK(9)	is 0.49 Å from C(43)	0.7697	0.8778	0.5171	0.17
PK(10)	is 0.45 Å from H(32)	1.2327	1.0371	0.9845	0.16
HL(1)	is 0.46 Å from C(5)	-0.2117	0.4388	0.9184	-0.27
HL(2)	is 0.42 Å from C(23)	-0.0942	0.2546	0.6011	-0.2
HL(3)	is 0.41 Å from C(44)	0.7226	0.8327	0.4424	-0.2
HL(4)	is 0.45 Å from C(45)	0.6551	0.7143	0.4487	-0.19
HL(5)	is 0.82 Å from P(1)	0.2889	0.4429	0.8228	-0.17
HL(6)	is 0.05 Å from H(34)	1.0003	1.0789	0.9318	-0.16
HL(7)	is 0.03 Å from H(20)	0.5188	0.4386	0.7328	-0.16
HL(8)	is 0.44 Å from C(24)	-0.1964	0.1541	0.6212	-0.16
HL(9)	is 0.78 Å from P(1)	0.2702	0.3491	0.8072	-0.16
HL(10)	is 0.40 Å from C(6)	-0.1637	0.388	0.9718	-0.16

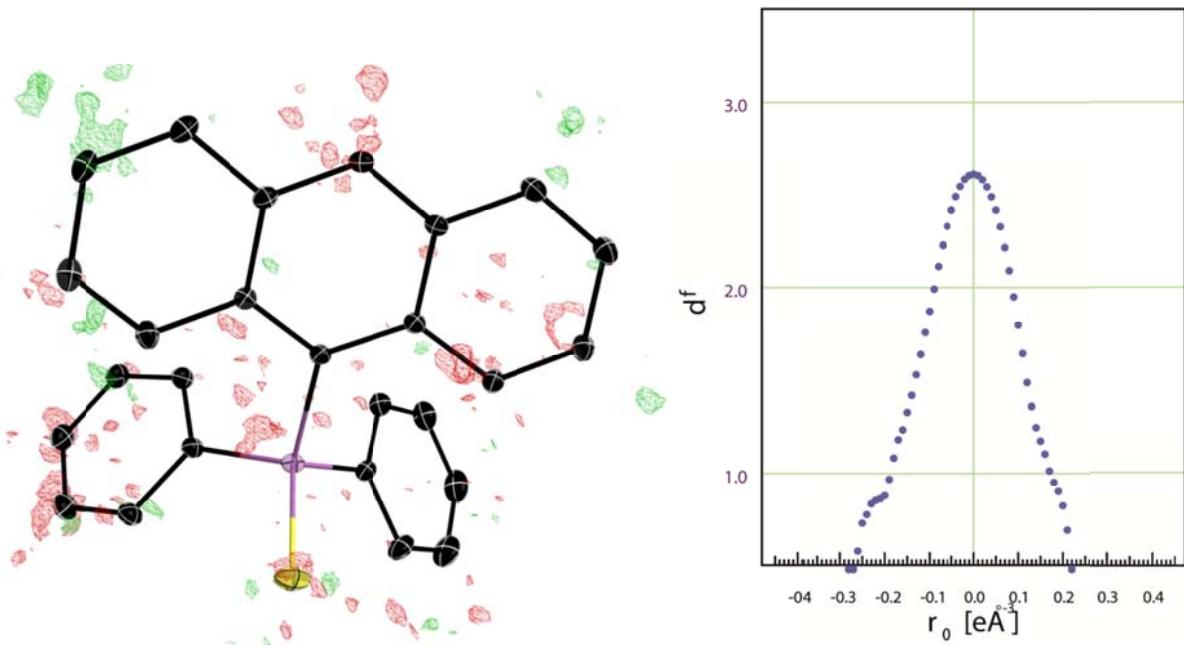


Figure S14 Residual density after MM refinement 10 scale factors data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.088 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.8975	0.2747	0.0689	0.22
PK(2)	is 0.46 Å from C(5)	-0.2579	0.3572	0.9017	0.2
PK(3)	is 0.46 Å from C(37)	0.6535	0.9959	0.8173	0.19
PK(4)		0.5247	0.2978	0.9957	0.17
PK(5)	is 0.47 Å from C(43)	0.7734	0.8774	0.5184	0.16
PK(6)	is 0.10 Å from S(1)	0.3364	0.5516	0.7657	0.16
PK(7)		0.4288	0.272	0.8996	0.15
PK(8)	is 0.43 Å from C(45)	0.6364	0.6576	0.4753	0.15
PK(9)	is 0.45 Å from H(32)	1.2246	1.038	0.9881	0.14
PK(10)	is 0.48 Å from C(16)	0.3319	0.2013	0.7971	0.14
HL(1)	is 0.44 Å from C(5)	-0.2113	0.4364	0.9205	-0.28
HL(2)	is 0.44 Å from C(23)	-0.0954	0.2541	0.6018	-0.2
HL(3)	is 0.49 Å from C(45)	0.65	0.716	0.4479	-0.19
HL(4)	is 0.43 Å from C(44)	0.7228	0.8344	0.442	-0.19
HL(5)	is 0.43 Å from S(1)	0.3329	0.5441	0.746	-0.19
HL(6)	is 0.03 Å from H(20)	0.5191	0.439	0.7335	-0.18
HL(7)	is 0.47 Å from C(24)	-0.1988	0.1535	0.6228	-0.17
HL(8)	is 0.05 Å from H(34)	1	1.0785	0.9317	-0.17
HL(9)	is 0.38 Å from P(1)	0.2304	0.3955	0.8071	-0.17
HL(10)	is 0.41 Å from C(6)	-0.1617	0.3883	0.9729	-0.16

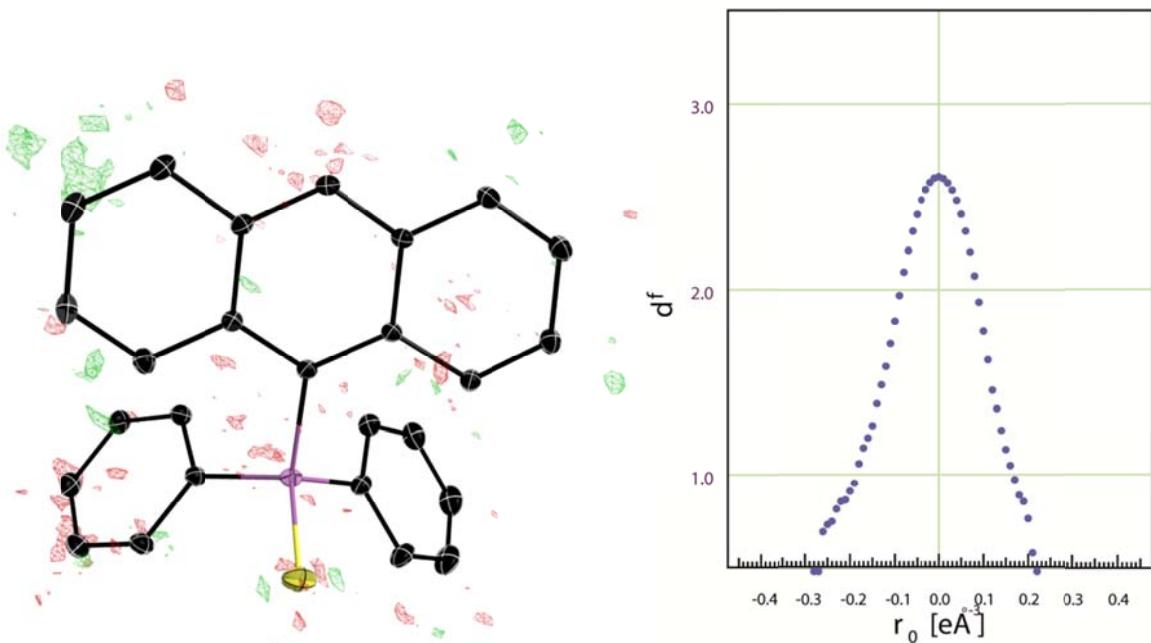


Figure S15 Residual density after MM refinement one scale factors data integrated with ‘best’ box size for molecule 2 ($x = 0.6$, $y = 0.6$, $z = 0.6$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.088 \text{ e} \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.8976	0.2737	0.0696	0.22
PK(2)	is 0.47 Å from C(5)	-0.2575	0.3561	0.9015	0.19
PK(3)	is 0.47 Å from C(37)	0.6552	0.9962	0.8169	0.18
PK(4)		0.5274	0.3004	0.9951	0.17
PK(5)	is 0.45 Å from C(45)	0.632	0.6559	0.4756	0.16
PK(6)	is 0.48 Å from C(24)	-0.1175	0.1924	0.5979	0.15
PK(7)	is 0.47 Å from C(12)	0.4414	0.2997	0.9913	0.15
PK(8)	is 0.45 Å from C(43)	0.7761	0.8739	0.5171	0.15
PK(9)	is 0.39 Å from H(16)	0.1865	0.1282	0.775	0.14
PK(10)	is 0.45 Å from C(46)	0.7486	0.677	0.5219	0.14
HL(1)	is 0.45 Å from C(5)	-0.2117	0.4385	0.9185	-0.27
HL(2)	is 0.48 Å from C(45)	0.6555	0.7159	0.4474	-0.19
HL(3)	is 0.43 Å from C(44)	0.7224	0.8335	0.4413	-0.19
HL(4)	is 0.43 Å from C(23)	-0.0941	0.2522	0.6008	-0.18
HL(5)	is 0.42 Å from S(1)	0.3314	0.5448	0.7464	-0.18
HL(6)	is 0.47 Å from C(24)	-0.198	0.153	0.6224	-0.17
HL(7)	is 0.03 Å from H(20)	0.5192	0.439	0.7335	-0.16
HL(8)	is 0.12 Å from H(34)	0.9941	1.0749	0.9285	-0.16
HL(9)	is 0.18 Å from C(25)	-0.1362	0.1279	0.6668	-0.16
HL(10)	is 0.42 Å from C(6)	-0.1585	0.3892	0.9734	-0.15

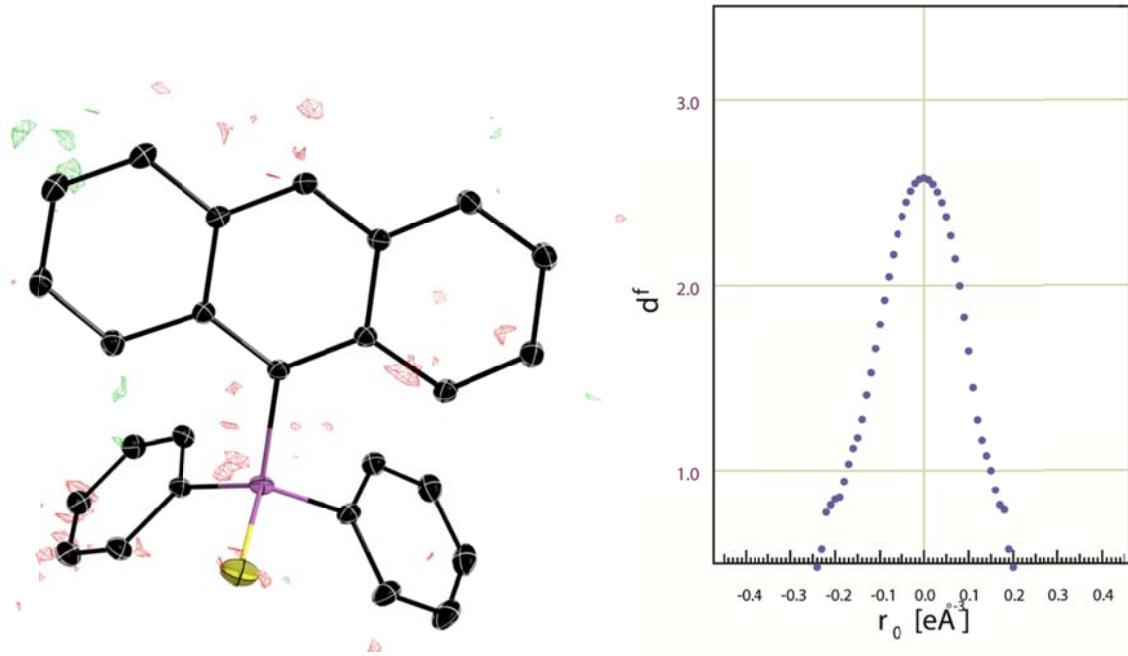


Figure S16 Residual density after MM refinement one scale factors data with empirical TDS correction for molecule 2 ($a = -0.15$, $b = 0.5$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.088 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.8979	0.2728	0.0688	0.2
PK(2)	is 0.47 Å from C(5)	-0.2588	0.3565	0.9006	0.16
PK(3)		0.5274	0.3007	0.9965	0.16
PK(4)	is 0.46 Å from C(37)	0.6529	0.9965	0.8164	0.15
PK(5)	is 0.48 Å from C(12)	0.4421	0.298	0.9922	0.14
PK(6)	is 0.47 Å from C(43)	0.7733	0.8763	0.5178	0.13
PK(7)		0.4174	0.344	0.8985	0.13
PK(8)	is 0.11 Å from S(1)	0.3364	0.5523	0.7658	0.13
PK(9)	is 0.45 Å from H(32)	1.2318	1.0365	0.9845	0.13
PK(10)		0.6233	0.2635	0.1156	0.13
HL(1)	is 0.45 Å from C(5)	-0.2115	0.4376	0.9207	-0.25
HL(2)	is 0.45 Å from C(44)	0.7208	0.8374	0.4435	-0.18
HL(3)	is 0.44 Å from S(1)	0.3331	0.5445	0.7453	-0.17
HL(4)	is 0.39 Å from P(1)	0.2293	0.3954	0.8075	-0.17
HL(5)	is 0.46 Å from C(23)	-0.0982	0.2511	0.6	-0.16
HL(6)	is 0.47 Å from C(45)	0.6553	0.7182	0.4505	-0.16
HL(7)	is 0.05 Å from H(34)	1.0007	1.0786	0.9317	-0.15
HL(8)	is 0.05 Å from H(36)	0.781	1.0837	0.9054	-0.14
HL(9)	is 0.49 Å from C(24)	-0.2037	0.1515	0.6198	-0.14
HL(10)	is 0.19 Å from C(25)	-0.1351	0.128	0.6662	-0.14

S2.5. 2- μ S-100K

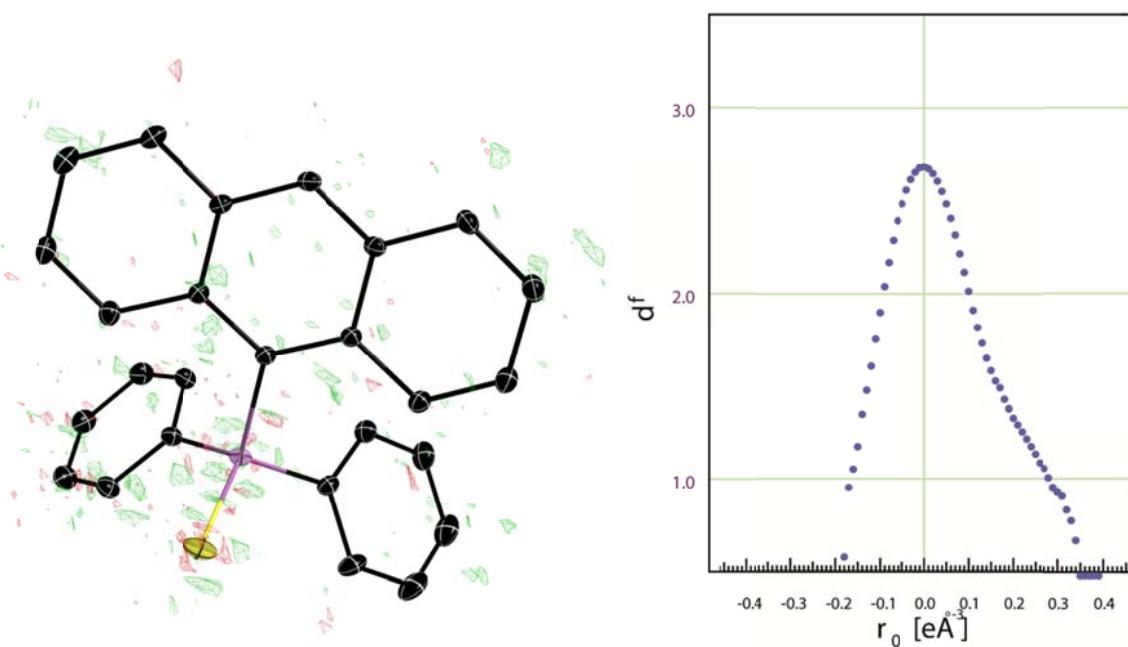


Figure S17 Residual density after MM refinement one scale factor against data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.091 \text{ e} \text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.01 Å from P(2)	0.8977	0.7028	0.6552	0.38
PK(2)	is 0.03 Å from S(2)	0.7893	0.5344	0.6629	0.38
PK(3)	is 0.05 Å from S(1)	0.3396	0.5497	0.7681	0.36
PK(4)		0.9087	0.2801	0.0722	0.32
PK(5)	is 0.52 Å from P(1)	0.25	0.3476	0.7825	0.3
PK(6)	is 0.11 Å from C(46)	0.6937	0.656	0.5236	0.26
PK(7)	is 0.18 Å from C(44)	0.6967	0.8073	0.4434	0.23
PK(8)	is 0.14 Å from C(45)	0.6409	0.6857	0.4561	0.23
PK(9)	is 0.14 Å from C(5)	-0.2319	0.4093	0.912	0.21
PK(10)	is 0.15 Å from C(24)	-0.1745	0.1675	0.6116	0.2
HL(1)	is 0.44 Å from C(5)	-0.2073	0.4364	0.9207	-0.19
HL(2)	is 0.82 Å from P(2)	0.9624	0.766	0.6765	-0.18
HL(3)	is 0.27 Å from C(45)	0.6686	0.6861	0.4721	-0.18
HL(4)	is 0.71 Å from P(2)	0.8505	0.7191	0.6344	-0.17
HL(5)	is 0.37 Å from C(46)	0.6702	0.6539	0.5363	-0.17
HL(6)	is 0.03 Å from H(10)	0.1635	0.2637	1.1208	-0.17
HL(7)	is 0.23 Å from C(37)	0.6303	0.9675	0.8066	-0.16
HL(8)	is 0.47 Å from C(23)	-0.097	0.2459	0.5994	-0.16
HL(9)	is 0.17 Å from H(44)	0.6484	0.822	0.3943	-0.16
HL(10)	is 0.81 Å from P(1)	0.2856	0.4446	0.822	-0.16

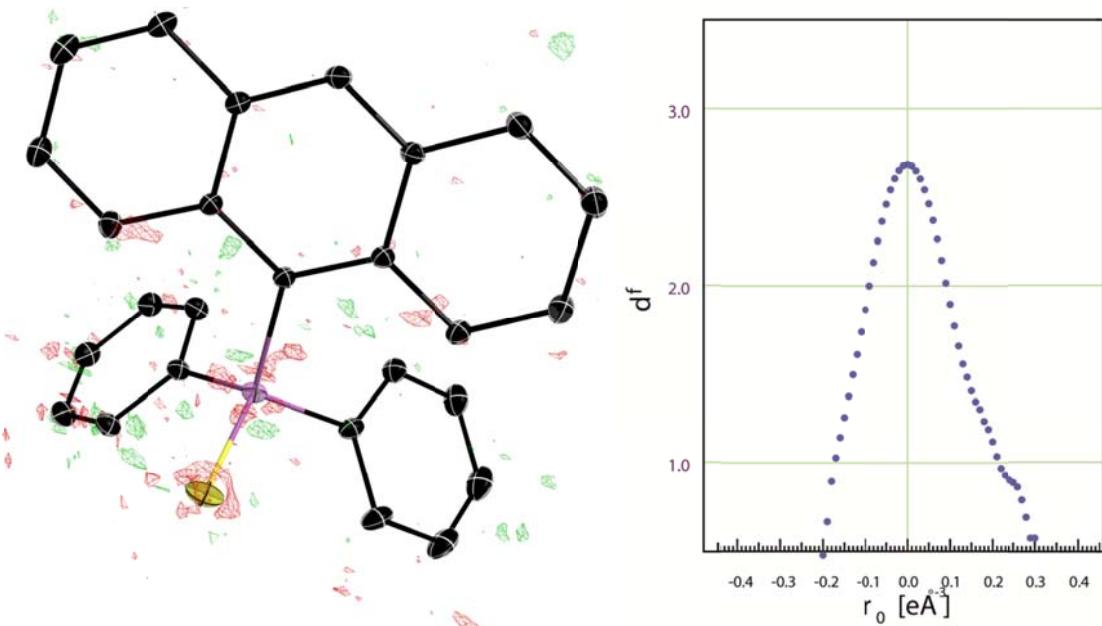


Figure S18 Residual density after MM refinement 10 scale factors data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.091 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	0.9083	0.2803	0.0718	0.31
PK(2)	is 0.01 Å from P(2)	0.8975	0.7023	0.655	0.24
PK(3)	is 0.04 Å from S(2)	0.79	0.5342	0.663	0.24
PK(4)	is 0.52 Å from P(1)	0.2506	0.3479	0.7825	0.22
PK(5)	is 0.22 Å from C(44)	0.6938	0.8058	0.441	0.21
PK(6)	is 0.10 Å from S(1)	0.3402	0.5509	0.7654	0.21
PK(7)	is 0.49 Å from C(46)	0.7514	0.6736	0.5185	0.21
PK(8)	is 0.18 Å from C(45)	0.6389	0.6865	0.4541	0.19
PK(9)	is 0.45 Å from C(12)	0.4446	0.2993	0.9958	0.19
PK(10)	is 0.46 Å from H(42)	0.9229	0.9446	0.6254	0.18
HL(1)	is 0.19 Å from C(5)	0.2311	0.3827	0.9102	-0.21
HL(2)	is 0.16 Å from C(24)	0.1464	0.1706	0.6046	-0.19
HL(3)	is 0.21 Å from C(45)	0.6643	0.6827	0.4664	-0.19
HL(4)	is 0.05 Å from H(10)	0.1592	0.2619	1.1192	-0.18
HL(5)	is 0.56 Å from P(2)	0.8596	0.7141	0.6384	-0.18
HL(6)	is 0.39 Å from S(2)	0.8216	0.5298	0.6707	-0.18
HL(7)	is 0.39 Å from P(2)	0.9288	0.6932	0.6602	-0.17
HL(8)	is 0.52 Å from C(23)	0.1013	0.2425	0.6	-0.17
HL(9)	is 0.16 Å from H(44)	0.6488	0.8216	0.3944	-0.16
HL(10)	is 0.13 Å from H(22)	0.1472	0.4173	0.6292	-0.16

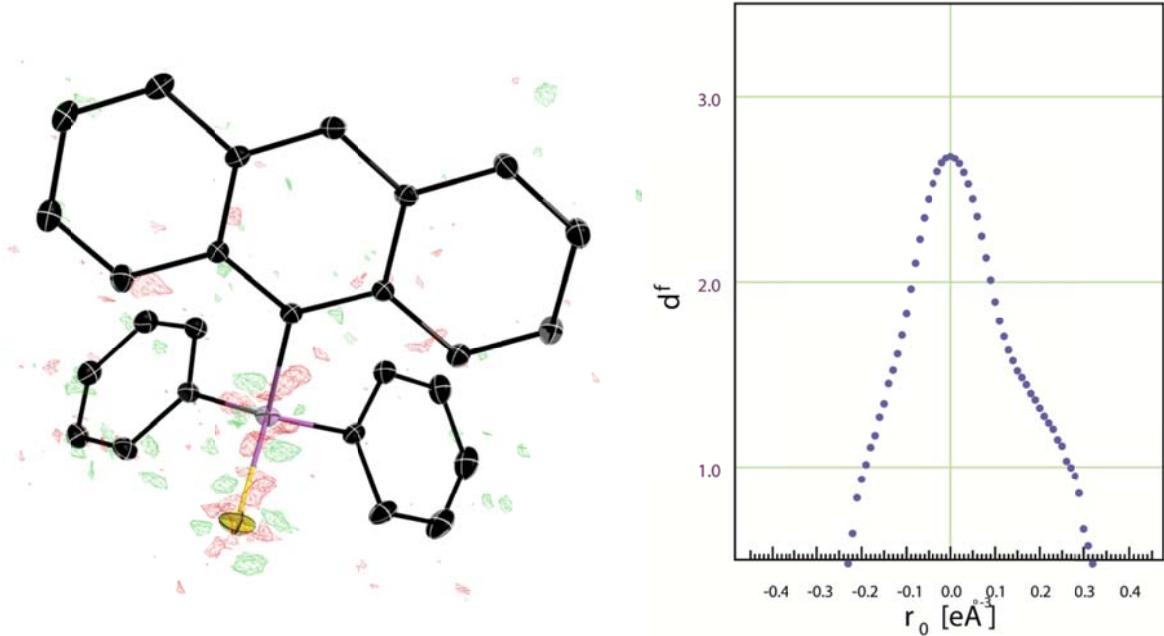


Figure S19 Residual density after MM refinement one scale factors data integrated with ‘best’ box size for molecule 2 ($x = 0.5$, $y = 0.5$, $z = 0.5$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.091 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.52 Å from P(1)	0.25	0.3475	0.7817	0.33
PK(2)		0.9087	0.2783	0.0724	0.31
PK(3)	is 0.55 Å from S(1)	0.3313	0.5928	0.7738	0.31
PK(4)	is 0.57 Å from P(2)	0.9005	0.6567	0.6504	0.29
PK(5)	is 0.58 Å from S(1)	0.352	0.5076	0.7619	0.27
PK(6)	is 0.57 Å from P(2)	0.8865	0.745	0.6623	0.25
PK(7)	is 0.04 Å from S(2)	0.7897	0.5338	0.6629	0.25
PK(8)	is 0.55 Å from P(1)	0.2257	0.4261	0.7899	0.25
PK(9)	is 0.50 Å from C(46)	0.7518	0.6744	0.5178	0.21
PK(10)	is 0.46 Å from C(12)	0.4449	0.2982	0.9961	0.19
HL(1)	is 0.48 Å from P(2)	0.8689	0.6665	0.6371	-0.24
HL(2)	is 0.45 Å from C(5)	-0.204	0.437	0.9181	-0.22
HL(3)	is 0.63 Å from P(1)	0.2869	0.4393	0.7964	-0.21
HL(4)	is 0.54 Å from P(2)	0.9264	0.7416	0.6785	-0.2
HL(5)	is 0.48 Å from S(1)	0.3045	0.5097	0.7615	-0.2
HL(6)	is 0.56 Å from P(1)	0.2072	0.3429	0.7663	-0.17
HL(7)	is 0.38 Å from S(2)	0.7776	0.5523	0.6494	-0.17
HL(8)	is 0.09 Å from H(22)	0.1479	0.4174	0.6315	-0.16
HL(9)	is 0.64 Å from C(39)	0.7114	0.7982	0.7559	-0.16
HL(10)	is 0.05 Å from H(10)	0.1599	0.2615	1.1186	-0.16

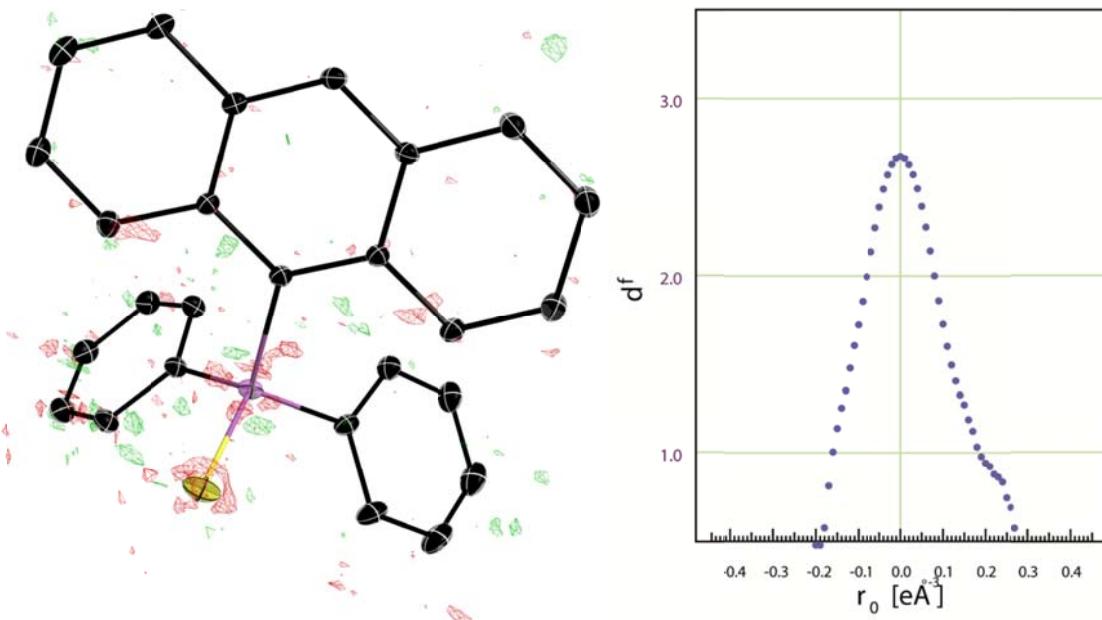


Figure S20 Residual density after MM refinement one scale factors data with empirical TDS correction for molecule 2 ($a = 0.05$, $b = 0.45$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.091 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.9066	0.2788	0.0726	0.28
PK(2)	is 0.01 Å from P(2)	0.8972	0.7017	0.6551	0.2
PK(3)	is 0.24 Å from C(44)	0.6937	0.8059	0.4401	0.19
PK(4)	is 0.44 Å from C(12)	0.4453	0.2994	0.9983	0.18
PK(5)	is 0.55 Å from S(1)	0.3313	0.5929	0.7732	0.18
PK(6)	is 0.19 Å from C(45)	0.6381	0.6871	0.4538	0.17
PK(7)	is 0.55 Å from P(1)	0.2525	0.3465	0.782	0.17
PK(8)	is 0.04 Å from S(2)	0.7896	0.5337	0.663	0.17
PK(9)	is 0.51 Å from C(46)	0.7542	0.6733	0.5198	0.17
PK(10)	is 0.53 Å from C(5)	0.2582	0.3511	0.9002	0.16
HL(1)	is 0.18 Å from C(5)	0.2322	0.3834	0.9095	-0.2
HL(2)	is 0.41 Å from P(2)	0.9302	0.6916	0.6559	-0.17
HL(3)	is 0.23 Å from C(45)	0.6654	0.686	0.4712	-0.17
HL(4)	is 0.16 Å from C(24)	0.1502	0.168	0.6023	-0.17
HL(5)	is 0.57 Å from P(1)	0.2875	0.3766	0.795	-0.16
HL(6)	is 0.03 Å from H(10)	0.1645	0.2637	1.121	-0.16
HL(7)	is 0.16 Å from C(25)	0.1296	0.1309	0.6704	-0.16
HL(8)	is 0.38 Å from S(2)	0.7786	0.5515	0.6822	-0.15
HL(9)	is 0.66 Å from C(39)	0.7126	0.7963	0.7558	-0.15
HL(10)	is 0.50 Å from C(44)	0.7244	0.8406	0.4422	-0.14

S2.6. 2-TXS-15K

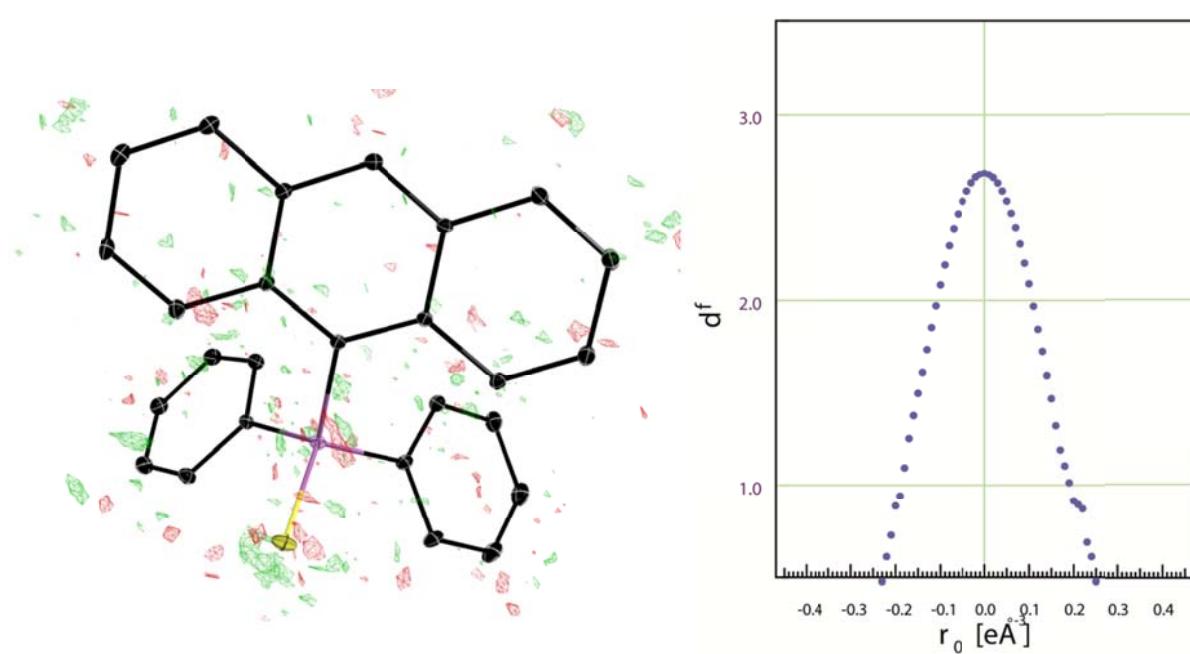


Figure S21 Residual density after MM refinement one scale factor against data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.1 \text{ e}\text{\AA}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.8991	0.2776	0.0706	0.26
PK(2)	is 0.53 Å from S(2)	0.7316	0.5267	0.6593	0.22
PK(3)	is 0.57 Å from S(1)	0.3161	0.5084	0.7837	0.2
PK(4)	is 0.35 Å from C(43)	0.7841	0.8706	0.5092	0.19
PK(5)	is 0.57 Å from S(1)	0.3784	0.5755	0.751	0.19
PK(6)	is 0.56 Å from P(1)	0.2785	0.412	0.7668	0.19
PK(7)	is 0.61 Å from P(2)	0.8317	0.688	0.655	0.19
PK(8)	is 0.58 Å from C(52)	1.2115	0.8815	0.643	0.19
PK(9)	is 0.42 Å from H(26)	0.0178	0.1545	0.7727	0.18
PK(10)	is 0.51 Å from P(2)	0.949	0.7128	0.658	0.18
HL(1)	is 0.52 Å from P(2)	0.92	0.6875	0.6753	-0.23
HL(2)	is 0.33 Å from P(1)	0.2142	0.3661	0.7729	-0.22
HL(3)	is 0.54 Å from S(1)	0.3624	0.5366	0.793	-0.21
HL(4)	is 0.05 Å from H(45)	0.5634	0.6187	0.4227	-0.2
HL(5)	is 0.12 Å from H(46)	0.6497	0.5569	0.5317	-0.2
HL(6)	is 0.51 Å from C(30)	1.2308	0.8331	0.8764	-0.2
HL(7)		0.6771	0.2197	0.9113	-0.19
HL(8)	is 0.09 Å from H(10)	0.1648	0.2698	1.127	-0.19
HL(9)	is 0.21 Å from H(5)	0.3157	0.4041	0.9101	-0.19
HL(10)	is 0.06 Å from H(34)	1.0003	1.0728	0.9327	-0.18

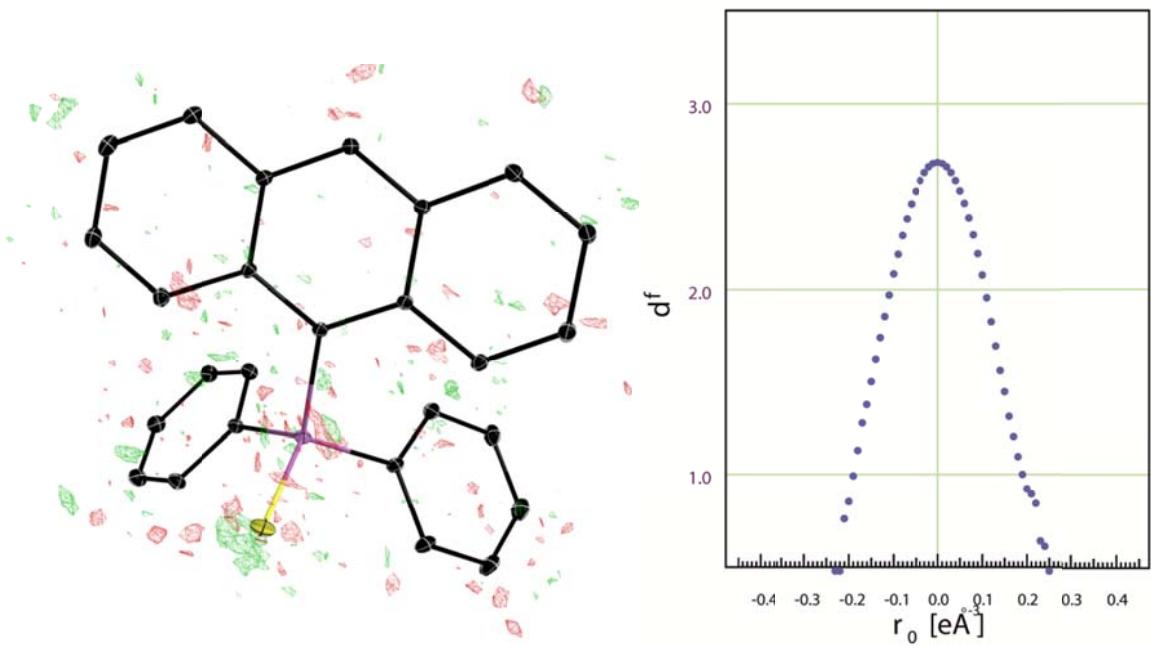


Figure S22 Residual density after MM refinement 10 scale factors against data with refined box size for molecule 2. Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.1 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)		0.8985	0.2776	0.0705	0.26
PK(2)	is 0.53 Å from S(2)	0.7323	0.5267	0.6591	0.22
PK(3)	is 0.57 Å from S(1)	0.316	0.5086	0.7835	0.21
PK(4)	is 0.48 Å from P(2)	0.9433	0.7051	0.6571	0.19
PK(5)	is 0.56 Å from S(1)	0.3777	0.5751	0.7513	0.19
PK(6)	is 0.35 Å from C(43)	0.7838	0.8707	0.5091	0.19
PK(7)	is 0.55 Å from P(1)	0.2774	0.4121	0.7672	0.19
PK(8)	is 0.60 Å from P(2)	0.832	0.6884	0.6548	0.18
PK(9)		0.9546	0.2494	0.1223	0.18
PK(10)	is 0.58 Å from C(52)	1.2117	0.8811	0.6427	0.18
HL(1)	is 0.53 Å from P(2)	0.9208	0.6869	0.6757	-0.23
HL(2)	is 0.55 Å from S(1)	0.3624	0.536	0.7938	-0.22
HL(3)	is 0.12 Å from H(46)	0.6497	0.5566	0.5316	-0.21
HL(4)	is 0.52 Å from C(30)	1.2305	0.8331	0.8768	-0.2
HL(5)	is 0.34 Å from P(1)	0.2137	0.3656	0.7727	-0.2
HL(6)	is 0.04 Å from H(45)	0.5627	0.6181	0.4227	-0.2
HL(7)	is 0.07 Å from H(20)	0.5253	0.4437	0.7352	-0.19
HL(8)	is 0.07 Å from H(10)	0.1589	0.2655	1.1249	-0.19
HL(9)	is 0.06 Å from H(34)	1.000	1.0734	0.9329	-0.18
HL(10)		0.6772	0.2198	0.9113	-0.18

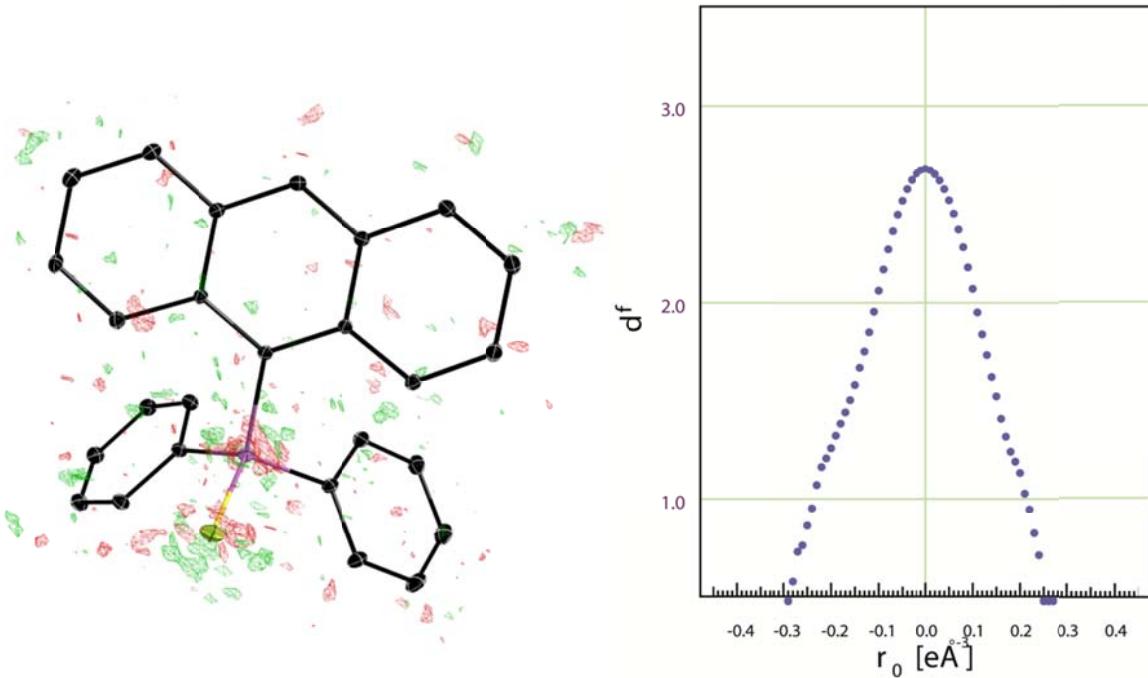


Figure S23 Residual density after MM refinement one scale factors data with TDS correction for molecule 2 ($a = 0.0$, $b = 0.1$). Atomic displacement parameters are depicted at 50 % probability level. Hydrogen atoms are omitted for clarity. Positive residual density is shown in green negative in red. Isolevels are depicted at $\pm 0.1 \text{ e Å}^{-3}$. (Meindl & Henn, 2008)

peak		x	y	z	height
PK(1)	is 0.58 Å from P(1)	0.2757	0.4143	0.7653	0.27
PK(2)	is 0.59 Å from S(1)	0.3152	0.5121	0.788	0.25
PK(3)		0.8994	0.2777	0.069	0.24
PK(4)	is 0.57 Å from S(1)	0.3687	0.5777	0.749	0.24
PK(5)	is 0.63 Å from P(2)	0.9087	0.7287	0.6273	0.23
PK(6)	is 0.53 Å from S(2)	0.7605	0.5049	0.6803	0.21
PK(7)	is 0.83 Å from S(2)	0.7298	0.5167	0.6224	0.2
PK(8)	is 0.90 Å from P(1)	0.2141	0.4408	0.8181	0.18
PK(9)	is 0.51 Å from C(8)	0.0657	0.344	1.0276	0.18
PK(10)		0.1208	0.4638	0.3664	0.18
HL(1)	is 0.48 Å from P(2)	0.919	0.6894	0.6738	-0.29
HL(2)	is 0.34 Å from P(1)	0.2659	0.4144	0.7876	-0.27
HL(3)	is 0.53 Å from S(1)	0.3637	0.5373	0.7923	-0.27
HL(4)	is 0.55 Å from S(2)	0.8193	0.5263	0.6846	-0.23
HL(5)	is 0.48 Å from S(1)	0.3112	0.5569	0.7503	-0.23
HL(6)	is 0.52 Å from C(39)	0.7045	0.8087	0.7543	-0.19
HL(7)	is 0.51 Å from C(30)	1.2308	0.8321	0.8771	-0.19
HL(8)	is 0.07 Å from H(10)	0.1584	0.267	1.1245	-0.19
HL(9)		0.6767	0.2185	0.911	-0.18
HL(10)	is 0.20 Å from H(5)	0.316	0.4053	0.9109	-0.18

S3. DRK-plots

S3.1. 1-TXS-100K

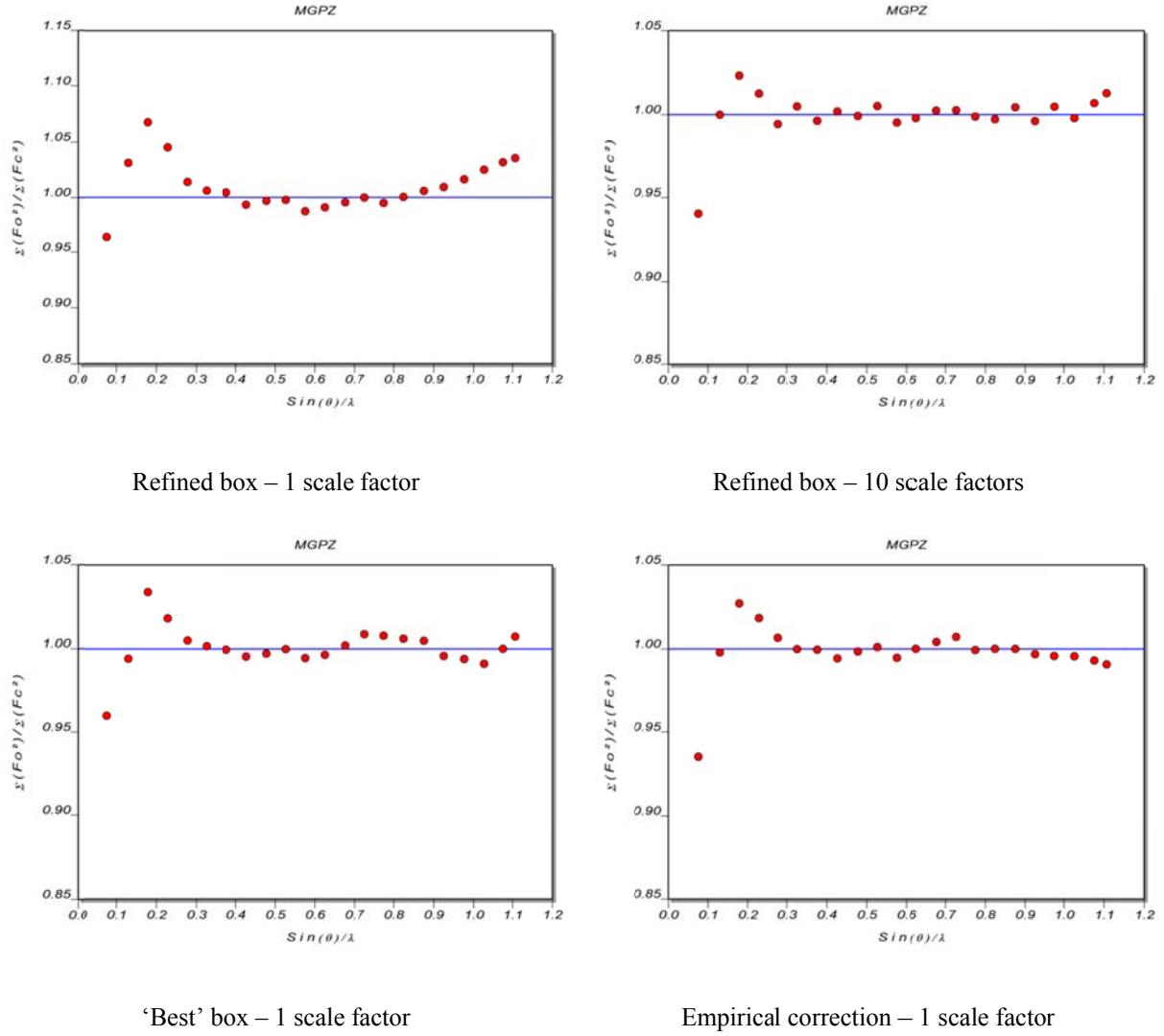


Figure S24 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for **1-TXS-100K** (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999). The too low quotient for the first bin might be explained by the small number of reflection. Only three reflections contribute to this value of which one being very close to the beam stop is determined too low.

S3.2. 1- μ S-100K

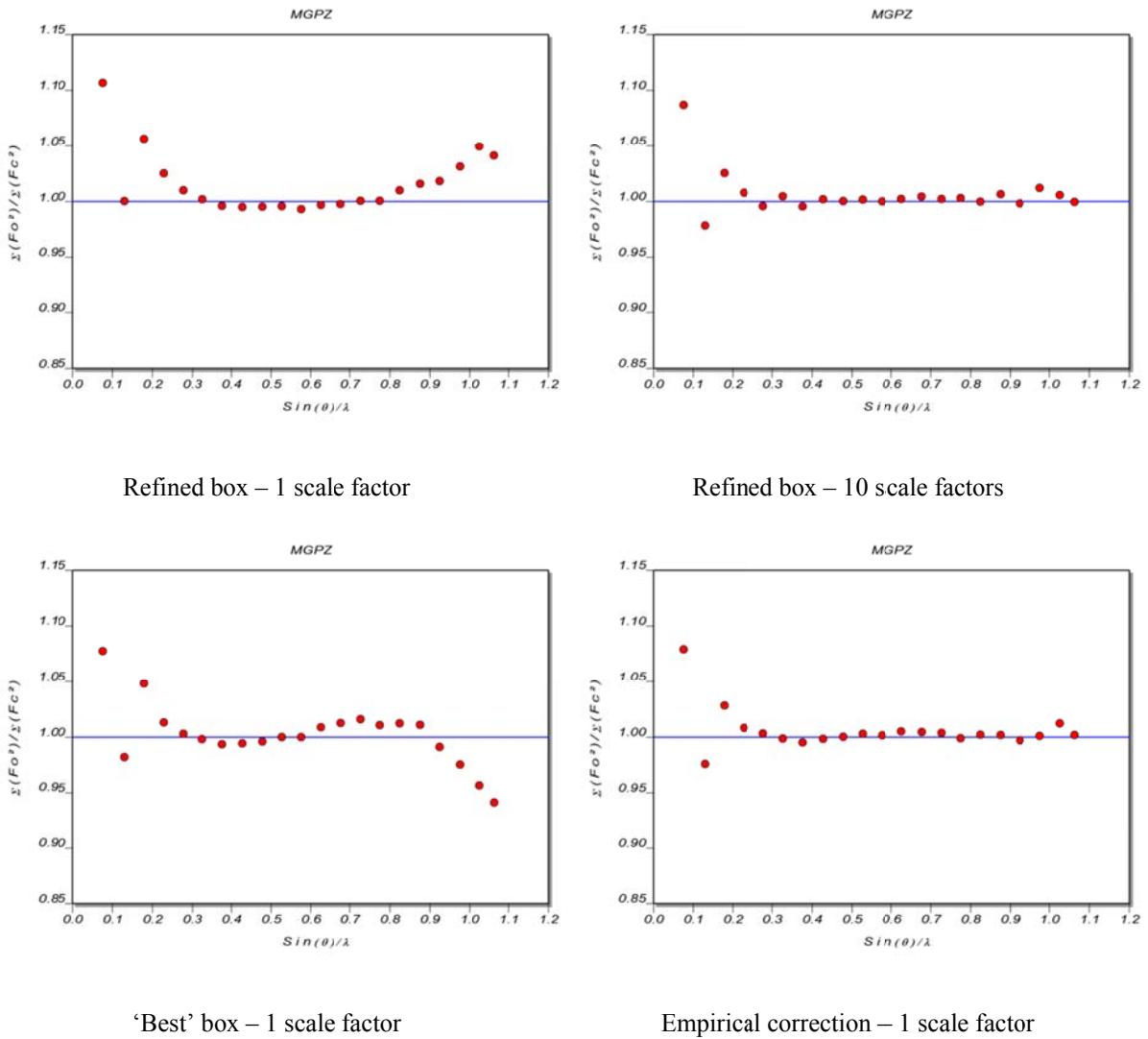


Figure S25 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for **1- μ S-100K** (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S3.3. 1-TXS-15K

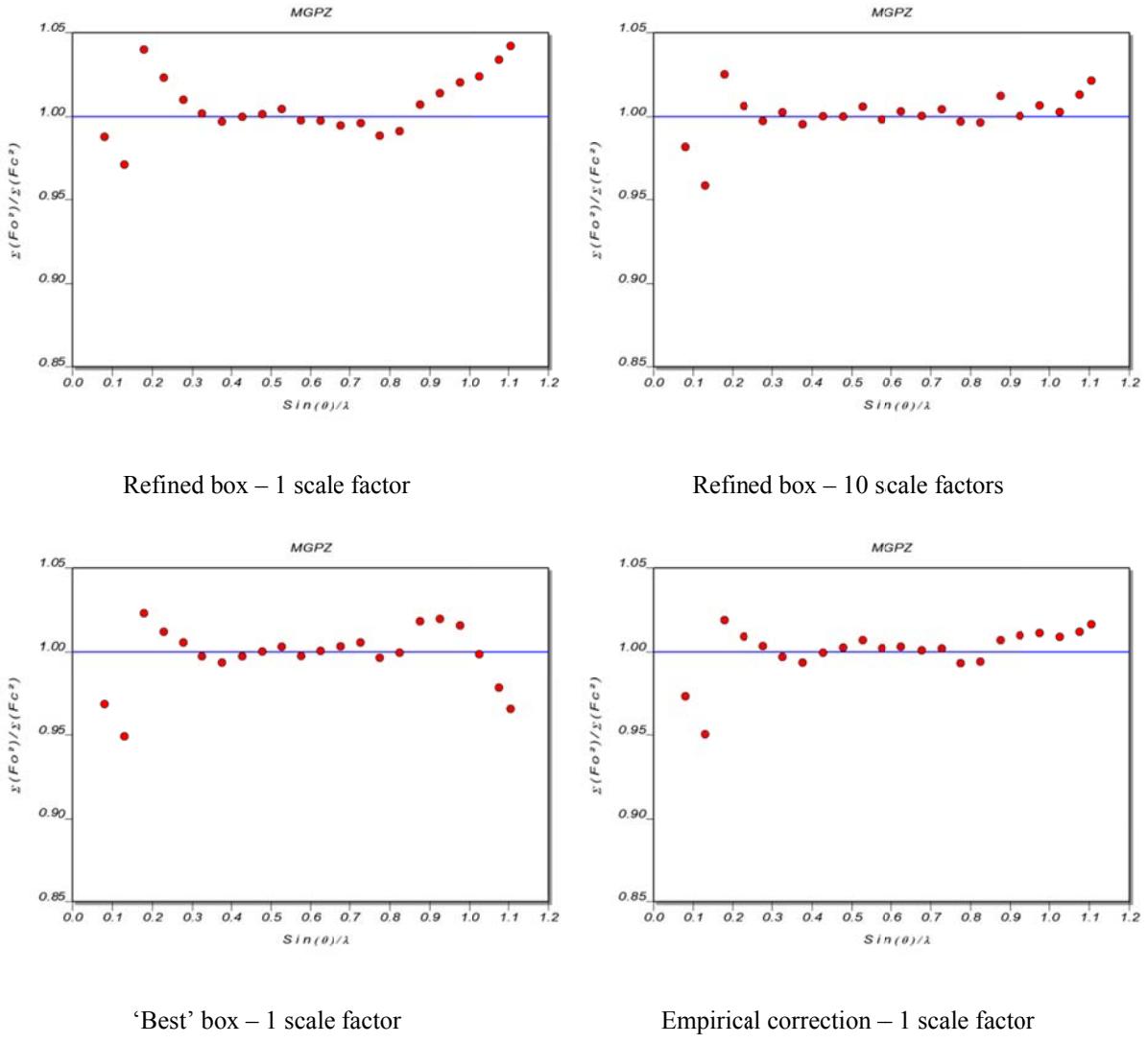


Figure S26 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for **1-TXS-15K** (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S3.4. 2-TXS-100K

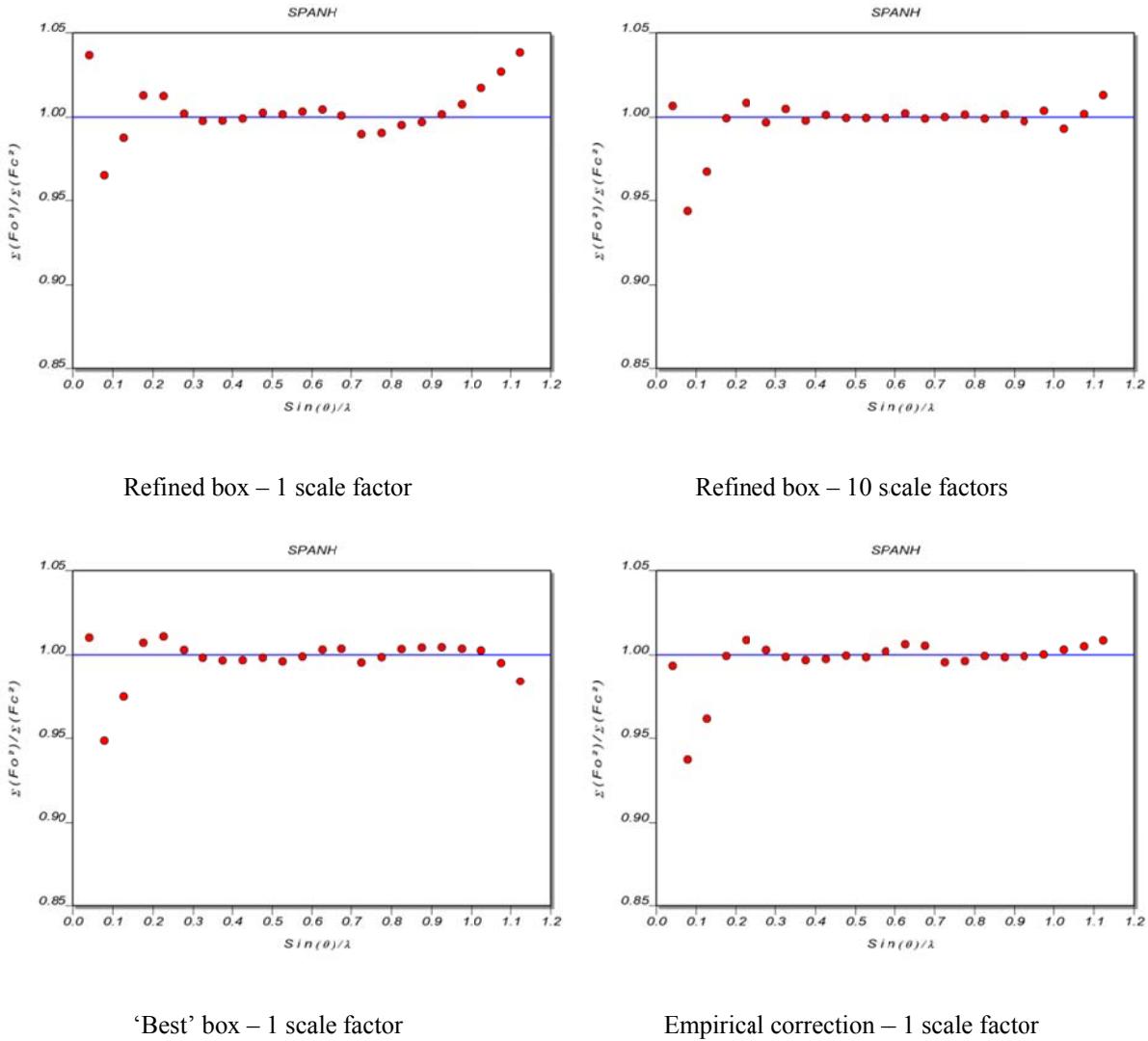


Figure S27 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for 2-TXS-100K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S3.5. 2-I μ S-100K

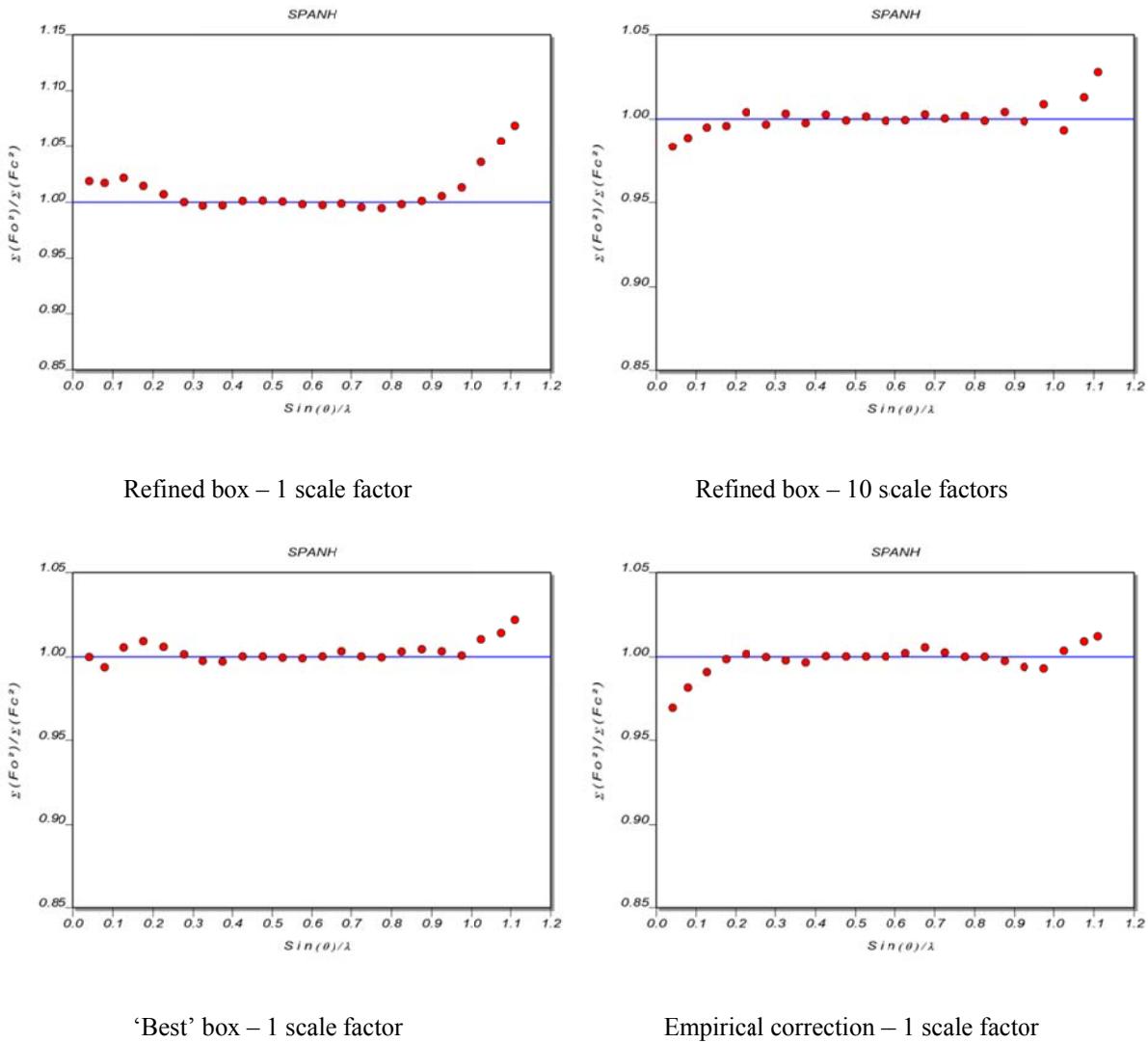


Figure S28 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for 2-I μ S-100K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S3.6. 2-TXS-15K

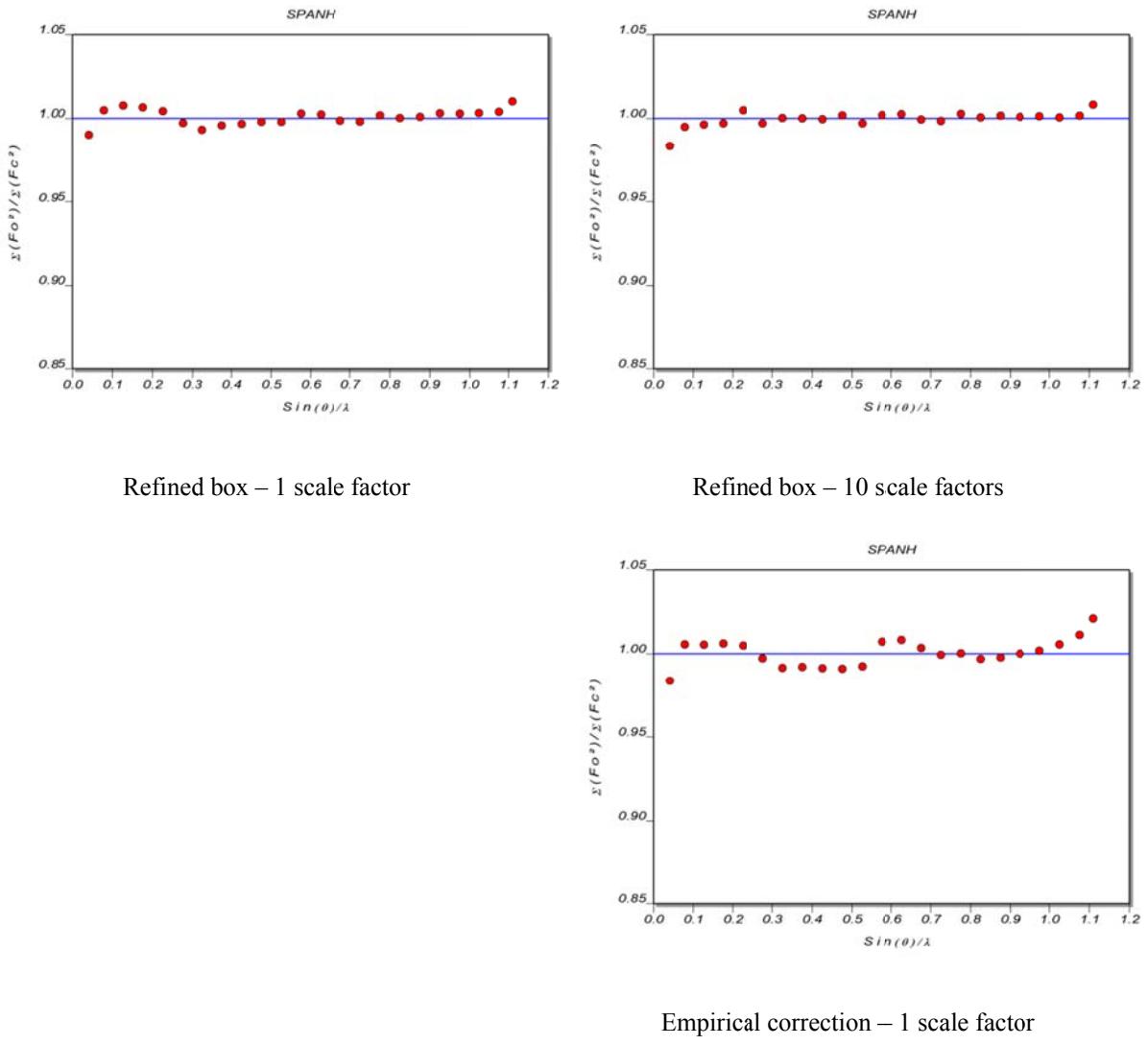


Figure S29 Plot of $\sum F_o^2 / \sum F_c^2$ vs. $\sin(\theta) / \lambda$ (DRK-plot) for 2-TXS-15K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S4. Normal probability plot

S4.1. 1-TXS-100K

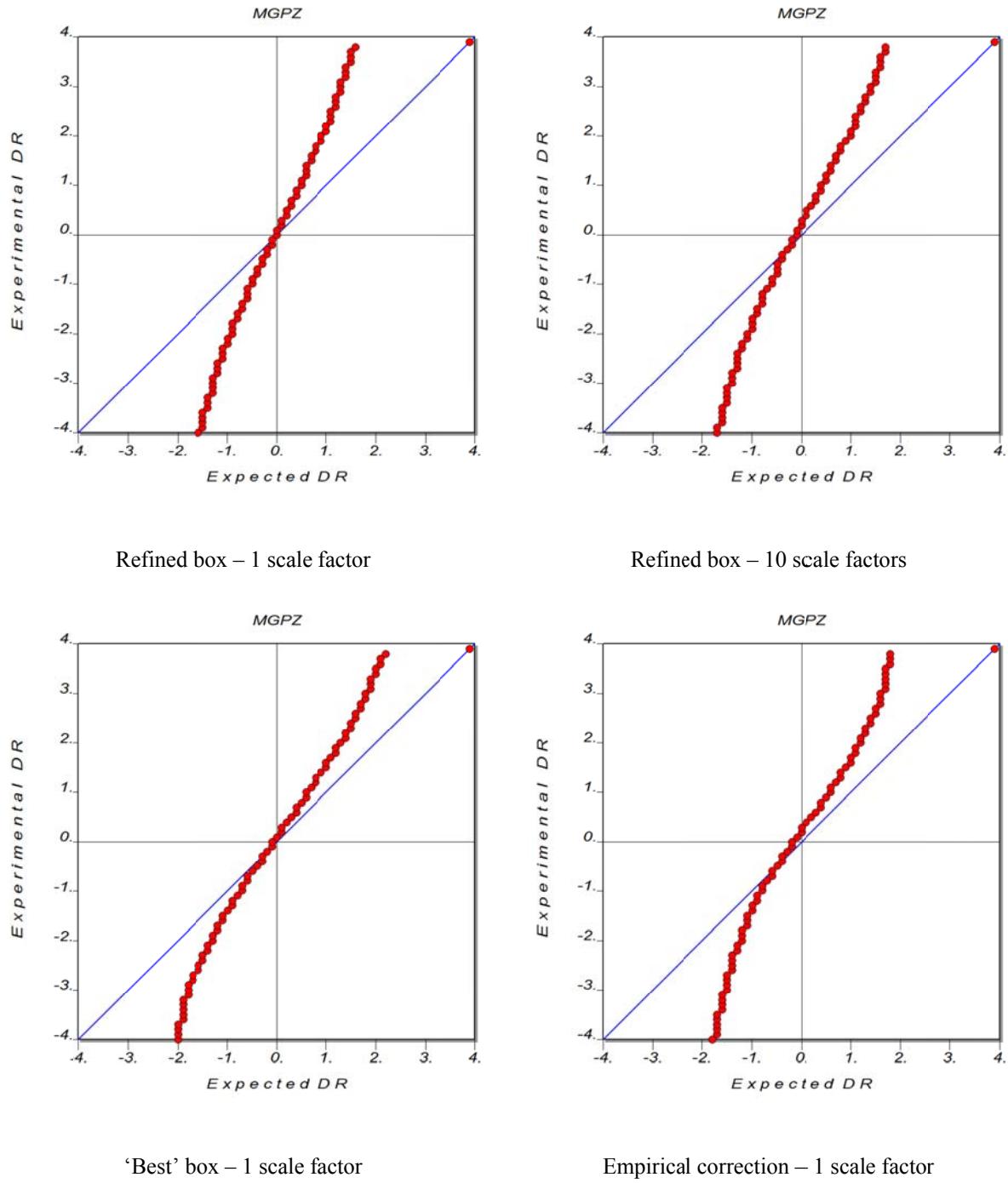


Figure S30 Normal probability plot 1-TXS-100K (Zhurov *et al.*, 2008, Zavodník *et al.*, 1999).

S4.2. 1- μ S-100K

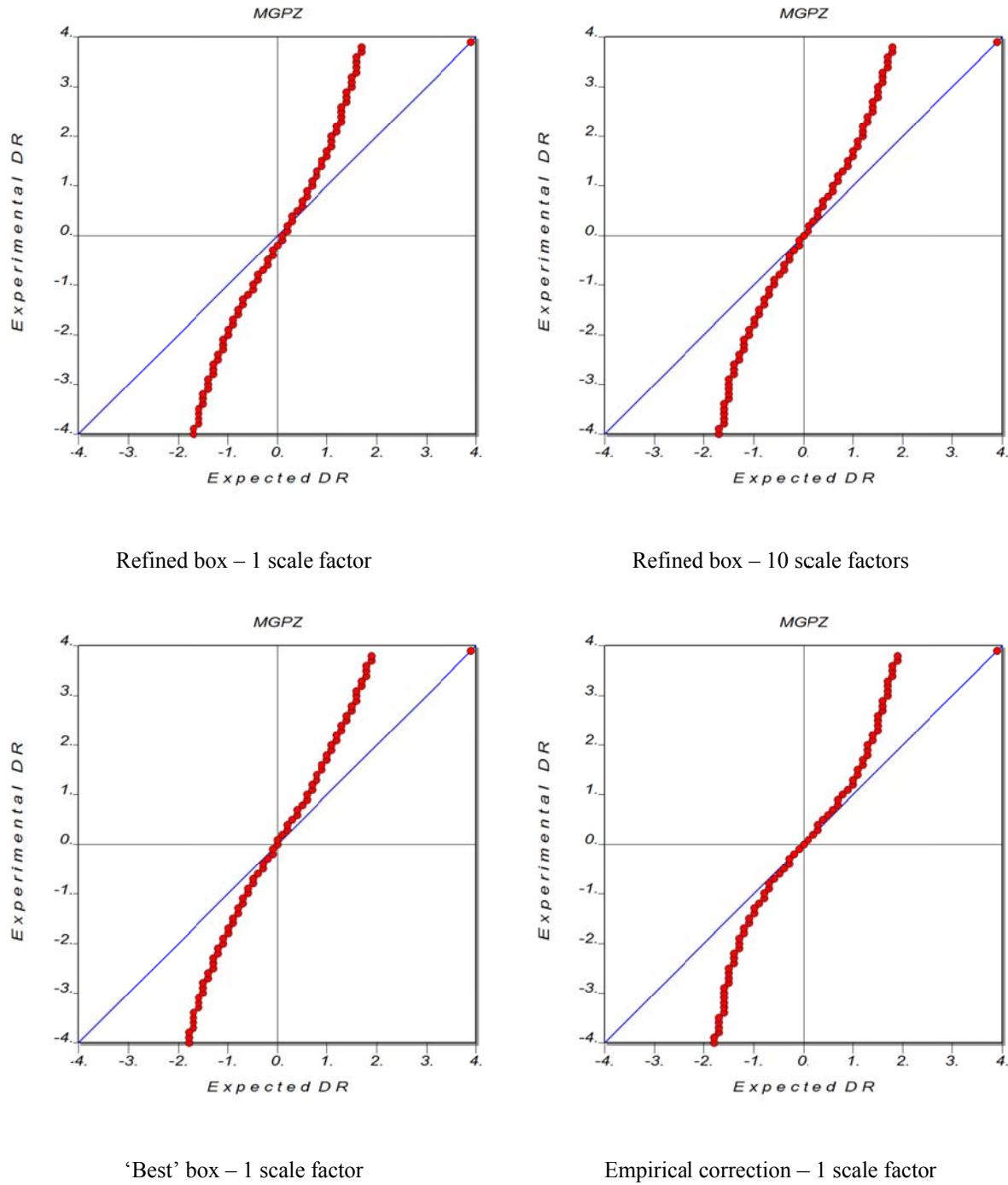


Figure S31 Normal probability plot 1- μ S-100K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S4.3. 1-TXS-15K

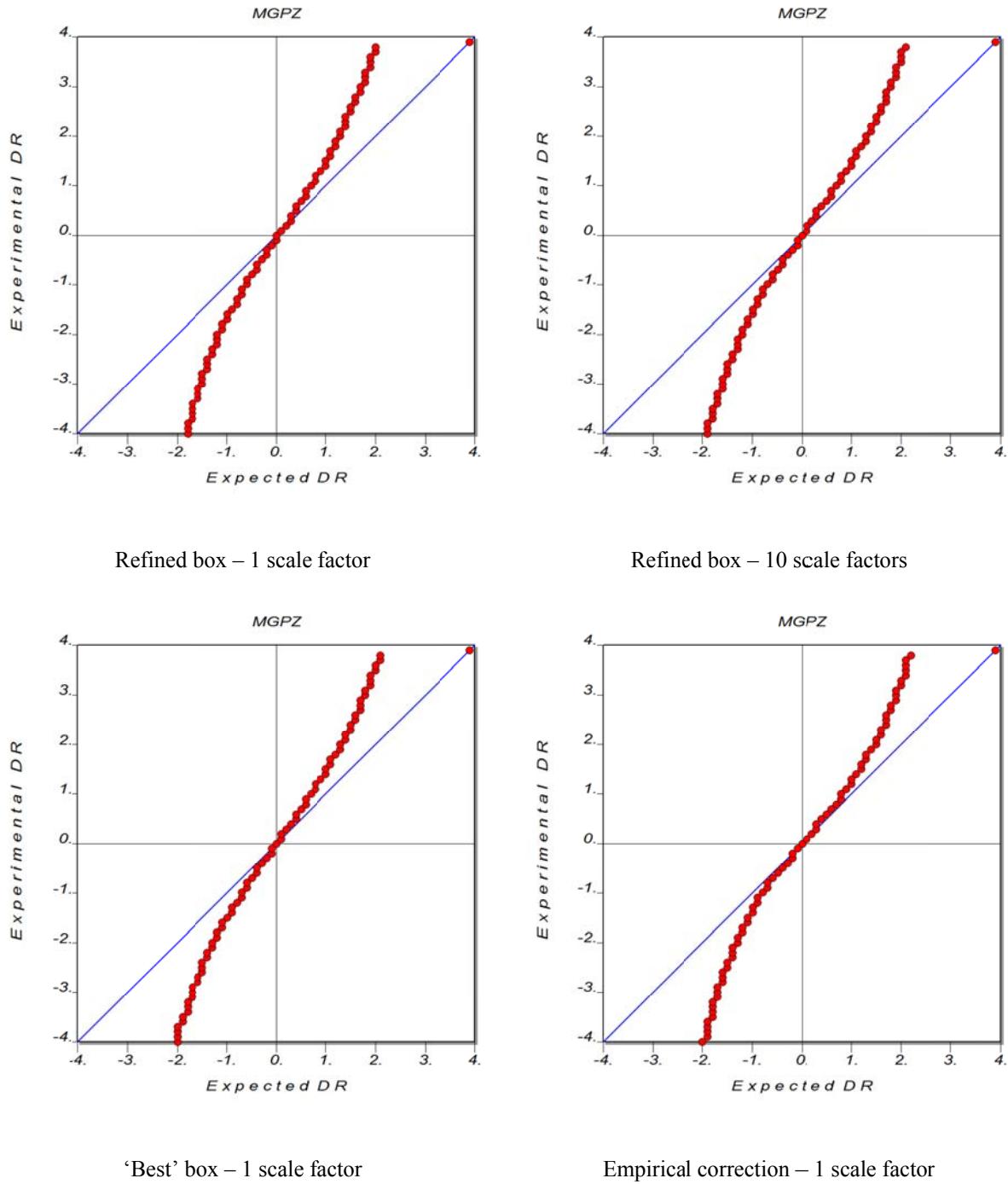


Figure S32 Normal probability plot 1-TXS-15K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S4.4. 2-TXS-100K

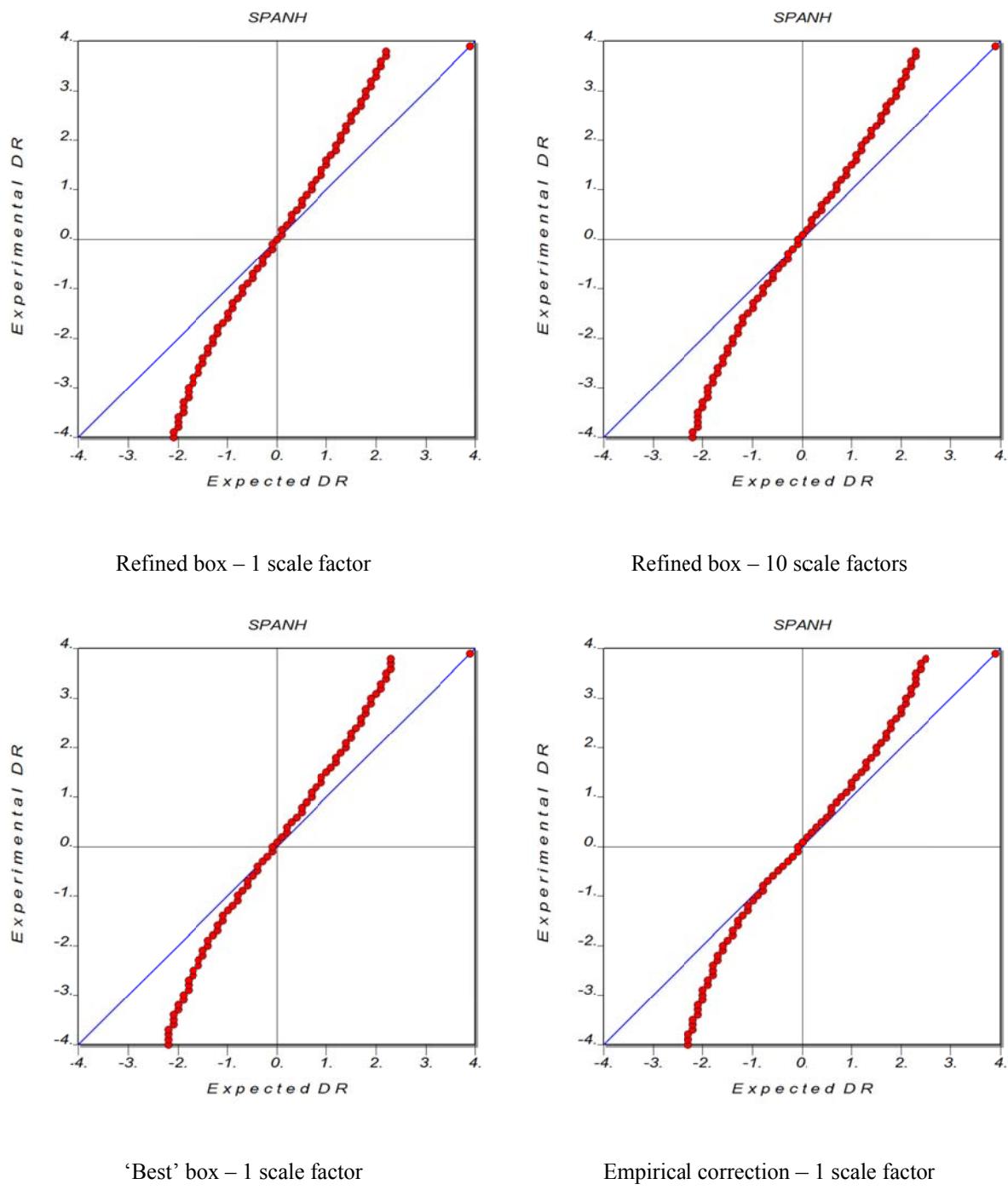


Figure S33 Normal probability plot 2-TXS-100K (Zhurov *et al.*, 2008, Zavodník *et al.*, 1999).

S4.5. 2- μ S-100K

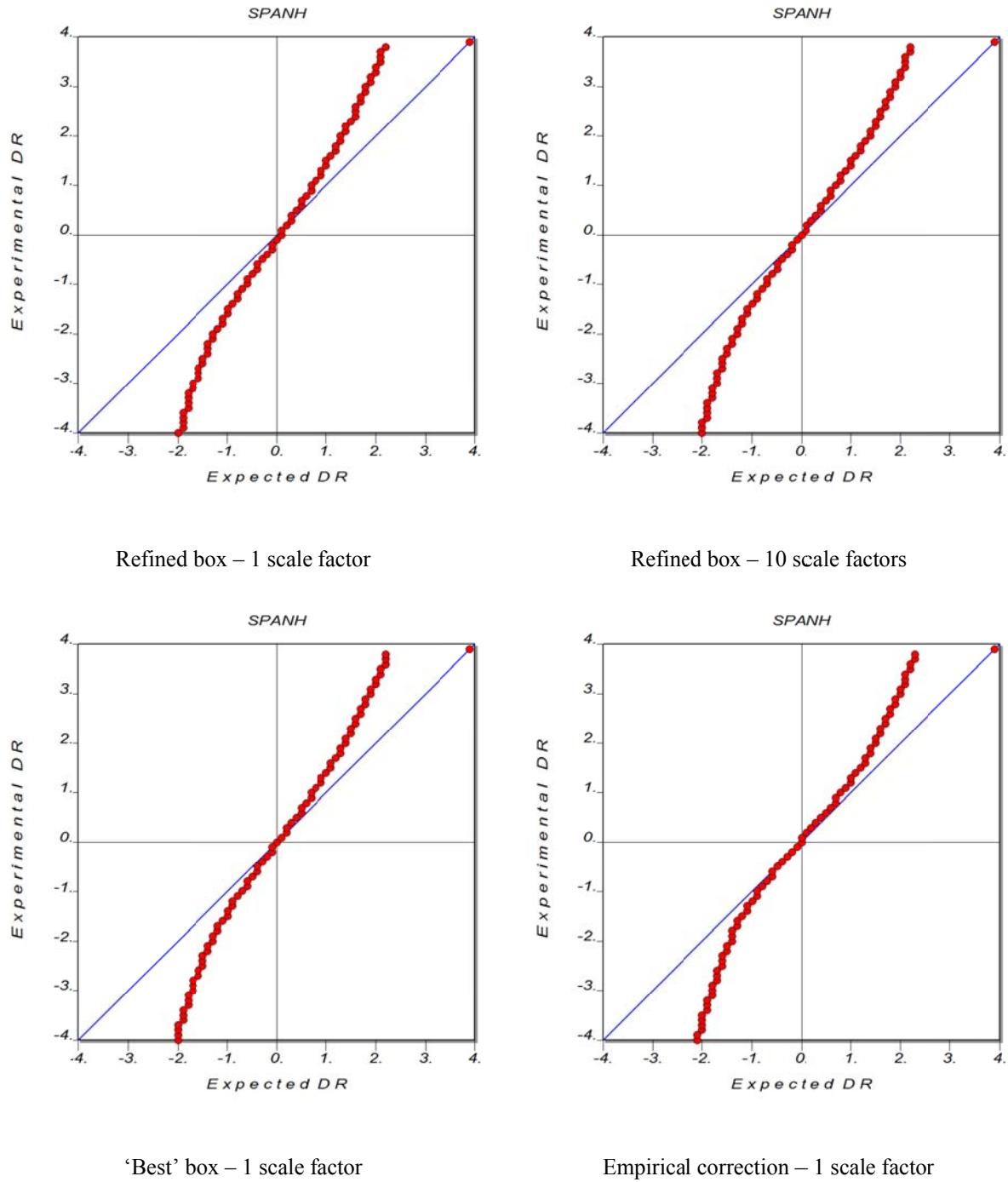


Figure S34 Normal probability plot 2- μ S-100K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S4.6. 2-TXS-15K

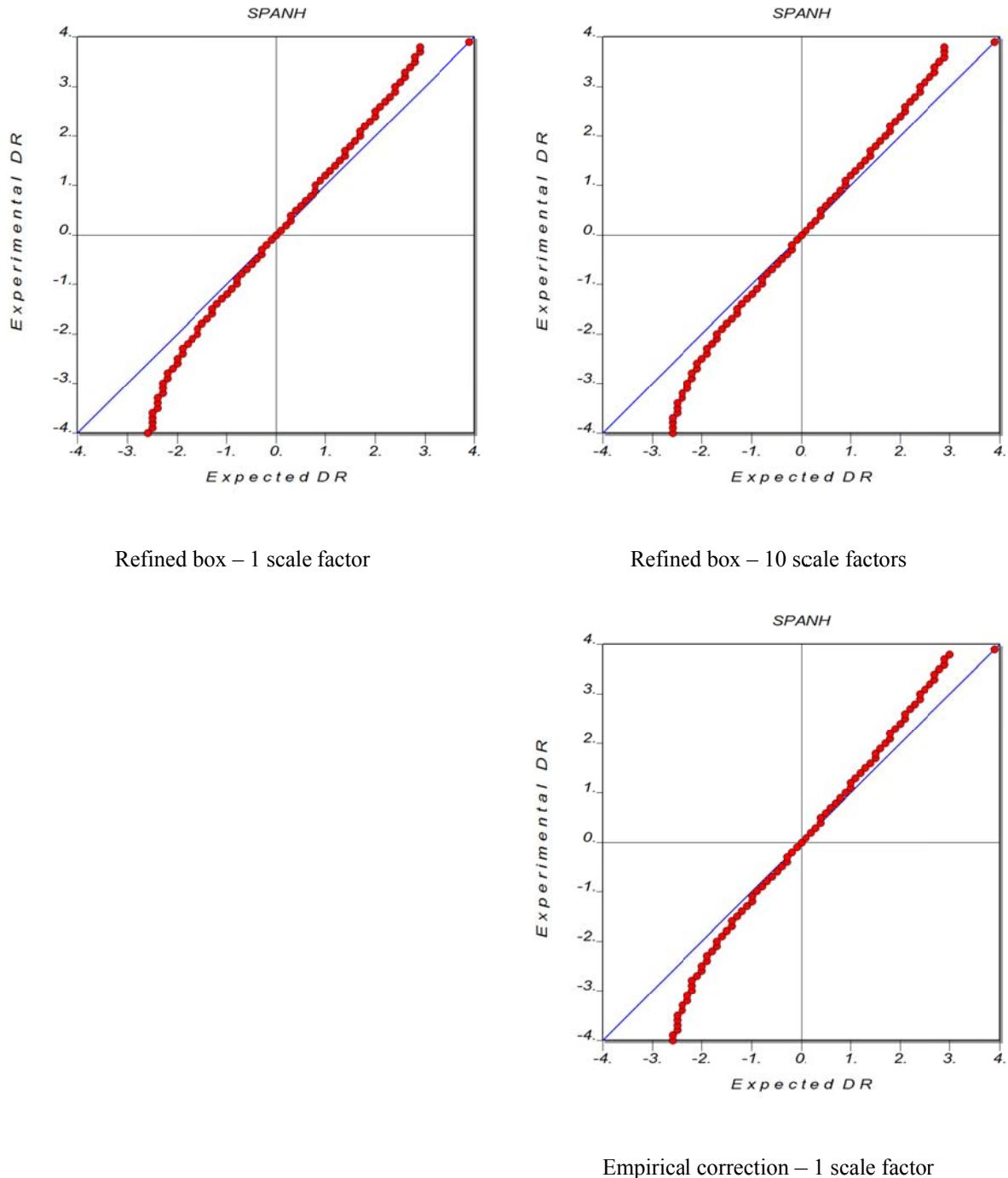


Figure S35 Normal probability plot 2-TXS-15K (Zhurov *et al.*, 2008, Zavodnik *et al.*, 1999).

S5. Integration with different boxes

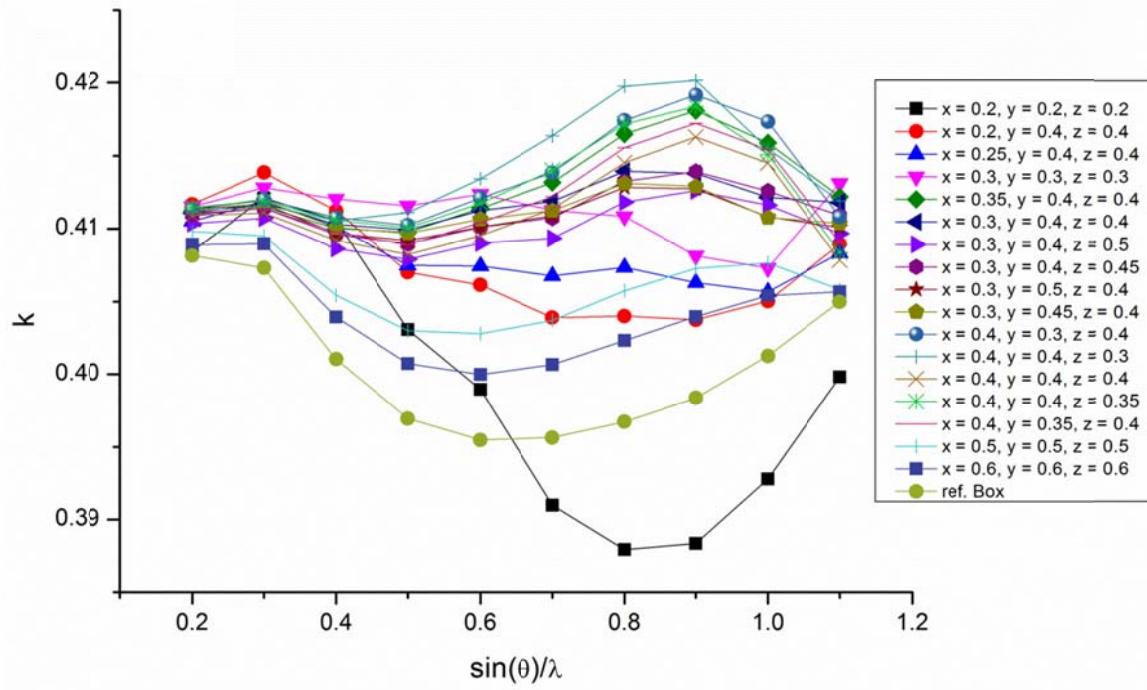


Figure S36 Resolution-dependence of the scale factors for 1-TXS-100K.

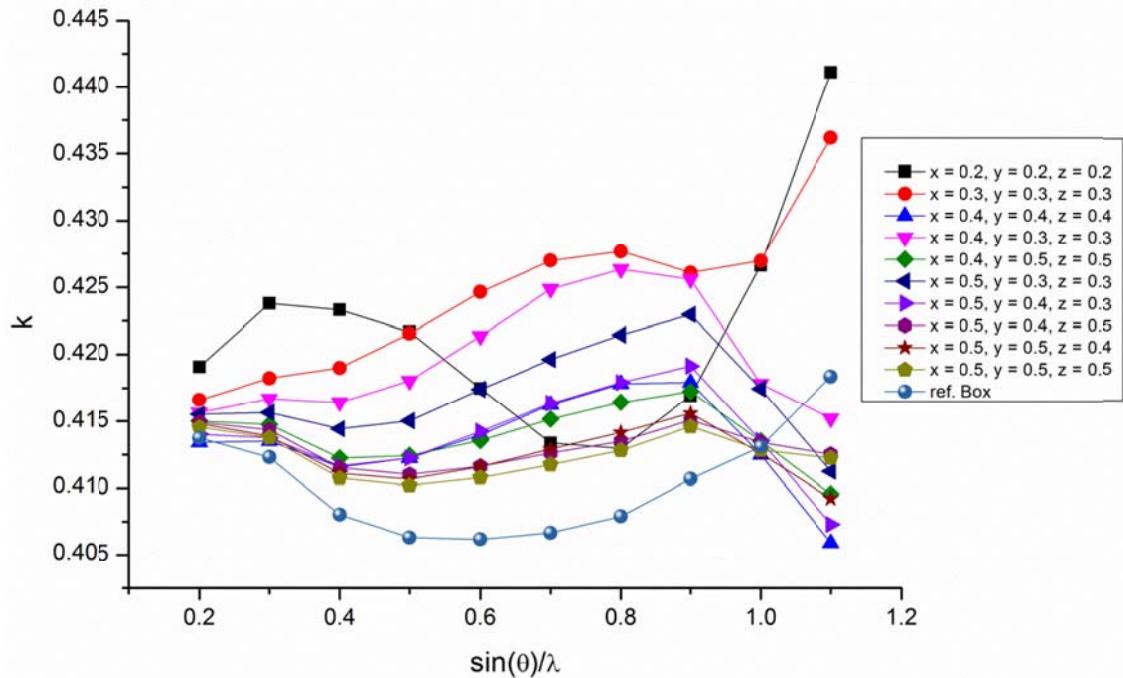


Figure S37 Resolution-dependence of the scale factors for 1-I μ S-100K.

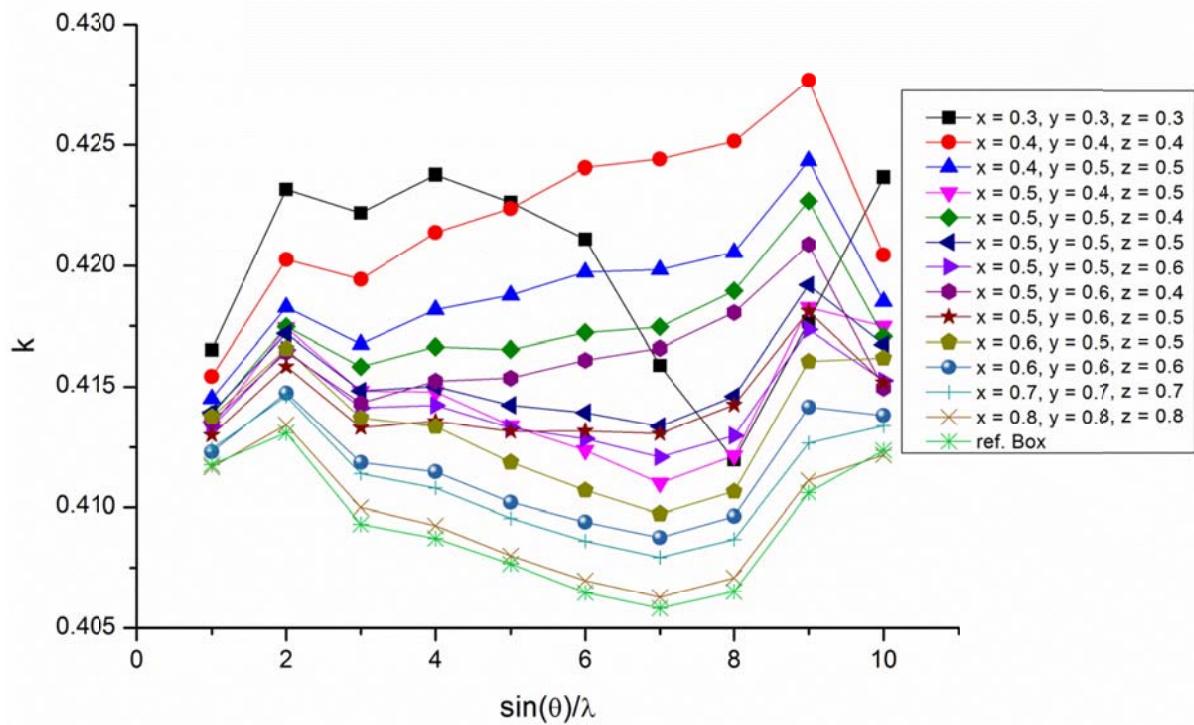


Figure S38 Resolution-dependence of the scale factors for **1-TXS-15K**.

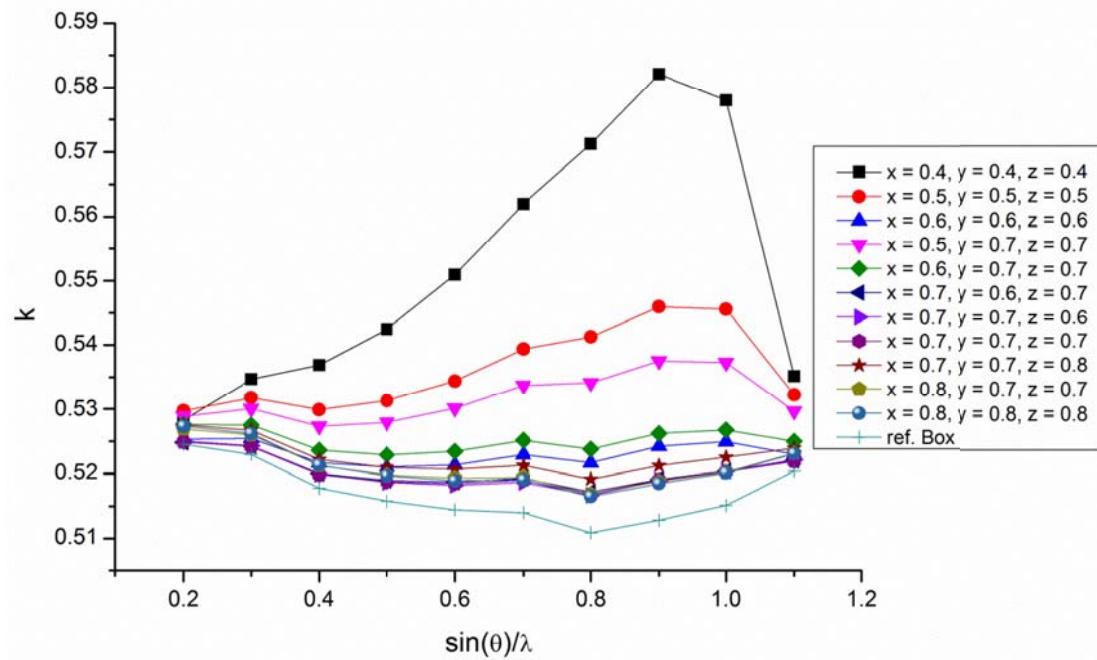


Figure S39 Resolution-dependence of the scale factors for **2-TXS-100K**.

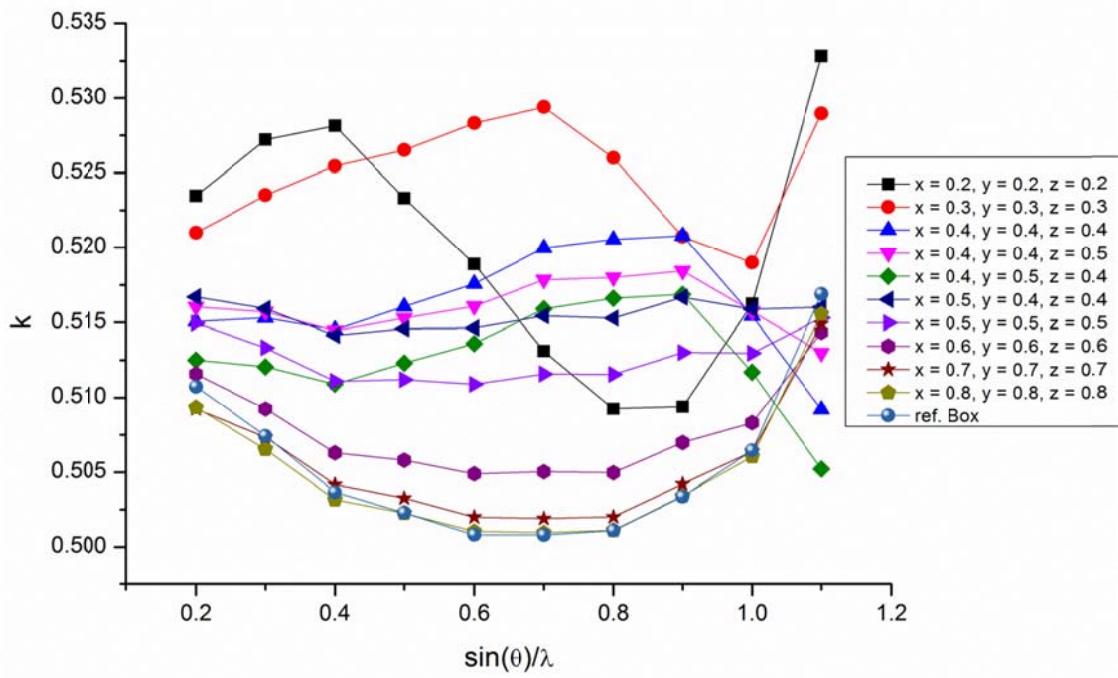


Figure S40 Resolution-dependence of the scale factors for 2-I μ S-100K

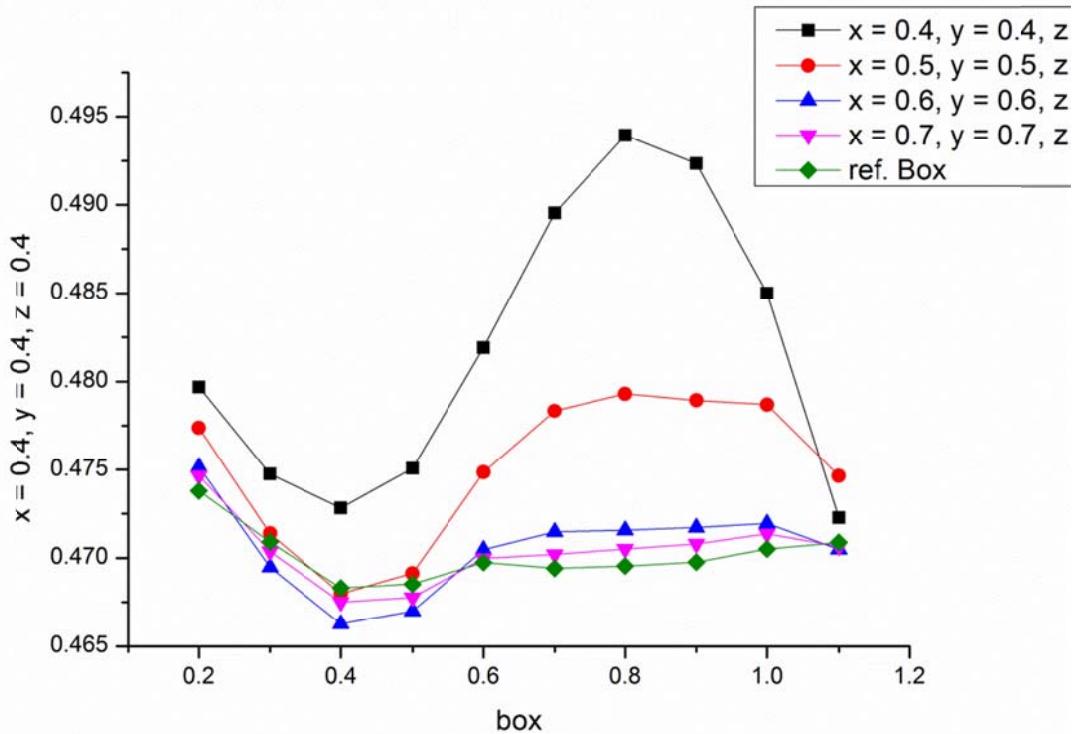


Figure S41 Resolution-dependence of the scale factors for 2-TXS-15K

Table S9 Model quality indicators for different boxes for **1-TXS-100K**.

	Net Charge Mg (1scale / 10 scale)	R ₂ (F ²) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e _{gross} (1scale / 10 scale)					
x = 0.2, y = 0.2, z = 0.2	+1.42(16)	+0.49(14)	0.0335	0.0211	0.712	0.241	-0.12	-0.113	26.6	22.0
x = 0.2, y = 0.4, z = 0.4	+1.08(13)	+0.59(13)	0.0223	0.0187	0.332	0.121	-0.098	-0.121	22.4	20.9
x = 0.25, y = 0.4, z = 0.4	+0.77(12)	+0.54(12)	0.0186	0.0172	0.151	0.125	-0.114	-0.124	20.7	20.2
x = 0.3, y = 0.3, z = 0.3	+0.50(12)	+0.54(12)	0.0185	0.018	0.124	0.125	-0.132	-0.128	20.7	20.3
x = 0.3, y = 0.4, z = 0.4	+0.55(11)	+0.54(12)	0.0176	0.017	0.113	0.114	-0.131	-0.13	20.5	20.1
x = 0.35, y = 0.4, z = 0.4	+0.53(11)	+0.50(11)	0.0184	0.0169	0.13	0.126	-0.129	-0.13	21.1	20.2
x = 0.3, y = 0.4, z = 0.5	+0.66(12)	+0.55(12)	0.018	0.0172	0.136	0.127	-0.125	-0.128	20.7	20.2
x = 0.3, y = 0.4, z = 0.45	+0.61(12)	+0.53(12)	0.0179	0.017	0.128	0.121	-0.128	-0.131	20.5	20.0
x = 0.3, y = 0.5, z = 0.4	+0.60(11)	+0.54(11)	0.0176	0.0169	0.124	0.118	-0.135	-0.138	20.7	20.3
x = 0.3, y = 0.45, z = 0.4	+0.59(11)	+0.56(12)	0.0177	0.017	0.12	0.116	-0.136	-0.137	20.6	20.3
x = 0.4, y = 0.3, z = 0.4	+0.54(12)	+0.52(12)	0.0187	0.017	0.127	0.124	-0.136	-0.129	21.8	20.6
x = 0.4, y = 0.4, z = 0.3	+0.33(11)	+0.51(11)	0.0194	0.017	0.12	0.124	-0.185	-0.142	21.4	20.0
x = 0.4, y = 0.4, z = 0.4	+0.62(11)	+0.50(11)	0.0181	0.0164	0.128	0.121	-0.126	-0.129	21.8	20.5
x = 0.4, y = 0.4, z = 0.35	+0.48(11)	+0.49(11)	0.0185	0.0166	0.122	0.12	-0.151	-0.133	21.6	20.2
x = 0.4, y = 0.35, z = 0.4	+0.59(11)	+0.50(11)	0.0183	0.0165	0.129	0.123	-0.128	-0.129	21.6	20.4
x = 0.5, y = 0.5, z = 0.5	+0.96(10)	+0.48(10)	0.0192	0.0157	0.149	0.131	-0.131	-0.139	23.3	21.7
x = 0.6, y = 0.6, z = 0.6	+1.20(10)	+0.53(9)	0.0203	0.0158	0.146	0.145	-0.138	-0.139	25.3	23.4
ref. Box	+1.57(10)	+0.66(9)	0.0232	0.0163	0.28	0.16	-0.153	-0.149	28.6	25.2
$\alpha = -0.15 (\sin(\theta)/\lambda)^2 + 0.60 (\sin(\theta)/\lambda)^3$	+0.82(8)	+0.63(8)	0.0168	0.0156	0.132	0.135	-0.125	-0.126	23.3	22.8
$\alpha = -0.15 (\sin(\theta)/\lambda)^2 + 0.70 (\sin(\theta)/\lambda)^3$	+0.78(8)	+0.64(8)	0.0166	0.0156	0.130	0.132	-0.121	-0.122	22.9	22.5

Table S10 Model quality indicators for different boxes for **1- μ S-100K**.

	Net Charge Mg (1scale / 10 scale)	R2(F2) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e_{gross} (1scale / 10 scale)					
x = 0.2, y = 0.2, z = 0.2	+1.05(19)	+0.35(19)	0.0389	0.0346	0.455	0.298	-0.219	-0.193	38.0	35.2
x = 0.3, y = 0.3, z = 0.3	+0.36(14)	+0.63(15)	0.0285	0.0276	0.19	0.193	-0.189	-0.139	33.8	33.6
x = 0.4, y = 0.4, z = 0.4	+0.52(12)	+0.61(12)	0.0246	0.0237	0.193	0.153	-0.173	-0.184	32.5	31.8
x = 0.4, y = 0.3, z = 0.3	+0.29(14)	+0.62(14)	0.0279	0.0259	0.241	0.206	-0.246	-0.153	33.4	32.8
x = 0.4, y = 0.5, z = 0.5	+0.72(10)	+0.67(10)	0.0234	0.0228	0.165	0.167	-0.179	-0.19	32.9	32.2
x = 0.5, y = 0.3, z = 0.3	+0.48(13)	+0.60(13)	0.0272	0.0261	0.226	0.185	-0.183	-0.16	34.2	33.6
x = 0.5, y = 0.4, z = 0.3	+0.57(12)	+0.64(12)	0.0251	0.0241	0.192	0.164	-0.159	-0.171	33.2	32.4
x = 0.5, y = 0.4, z = 0.5	+0.79(10)	+0.63(10)	0.0229	0.0223	0.192	0.17	-0.179	-0.184	33.1	32.3
x = 0.5, y = 0.5, z = 0.4	+0.78(9)	+0.64(9)	0.023	0.0225	0.173	0.166	-0.177	-0.185	33.5	32.6
x = 0.5, y = 0.5, z = 0.5	+0.83(9)	+0.65(9)	0.0226	0.022	0.164	0.167	-0.186	-0.189	33.5	32.6
ref. Box	+1.09(9)	+0.67(9)	0.0238	0.0216	0.23	0.161	-0.186	-0.177	35.3	32.8
$\alpha = 0.0 (\sin(\theta)/\lambda)^2 + 0.70 (\sin(\theta)/\lambda)^3$	+0.64(8)	+0.63(8)	0.212	0.0209	0.139	0.142	-0.152	-0.157	29.8	29.8

Table S11 Model quality indicators for different boxes for **1-TXS-15K**.

	Net Charge Mg (1scale / 10 scale)	R2(F2) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e_{gross} (1scale / 10 scale)					
x = 0.3, y = 0.3, z = 0.3	+0.38(16)	+0.35(16)	0.0317	0.0283	0.168	0.175	-0.22	-0.201	39.2	34.6
x = 0.4, y = 0.4, z = 0.4	+0.08(13)	+0.37(14)	0.0256	0.0232	0.158	0.178	-0.207	-0.178	32.6	29.6
x = 0.4, y = 0.5, z = 0.5	+0.33(13)	+0.43(13)	0.0233	0.022	0.18	0.19	-0.184	-0.18	31.3	29.7
x = 0.5, y = 0.4, z = 0.5	+0.86(13)	+0.45(13)	0.0234	0.0221	0.204	0.19	-0.185	-0.196	31.3	30.0
x = 0.5, y = 0.5, z = 0.4	+0.52(12)	+0.47(13)	0.0224	0.0212	0.184	0.187	-0.177	-0.176	30.5	29.2
x = 0.5, y = 0.5, z = 0.5	+0.73(12)	+0.47(13)	0.0219	0.021	0.192	0.185	-0.18	-0.187	30.5	29.6
x = 0.5, y = 0.5, z = 0.6	+0.74(12)	+0.47(12)	0.0219	0.0211	0.196	0.189	-0.179	-0.186	30.6	29.8
x = 0.5, y = 0.6, z = 0.4	+0.60(11)	+0.57(12)	0.022	0.0208	0.186	0.191	-0.175	-0.168	30.2	29.1
x = 0.5, y = 0.6, z = 0.5	+0.70(12)	+0.48(12)	0.0212	0.0204	0.194	0.189	-0.174	-0.179	30.1	29.4
x = 0.6, y = 0.5, z = 0.5	+0.95(12)	+0.50(12)	0.0219	0.0207	0.214	0.196	-0.186	-0.199	30.8	29.9
x = 0.6, y = 0.6, z = 0.6	+0.89(11)	+0.49(12)	0.021	0.02	0.222	0.207	-0.191	-0.194	30.4	29.7
x = 0.7, y = 0.7, z = 0.7	+0.96(11)	+0.52(11)	0.0208	0.0197	0.221	0.205	-0.193	-0.203	31.0	30.3
x = 0.8, y = 0.8, z = 0.8	+1.01(11)	+0.53(11)	0.0208	0.0195	0.228	0.209	-0.191	-0.203	30.7	30.0
ref. Box	+1.14(11)	+0.63(11)	0.0212	0.0198	0.231	0.205	-0.187	-0.199	31.4	30.5
$\alpha = 0.0 (\sin(\theta)/\lambda)^2 + 0.30 (\sin(\theta)/\lambda)^3$	+0.60(10)	+0.61(10)	0.0202	0.0194	0.186	0.189	-0.184	-0.185	29.0	28.1

Table S12 Model quality indicators for different boxes for **2-TXS-100K**.

	Net Charge P (1scale / 10 scale)	R2(F2) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e_{gross} (1scale / 10 scale)					
x = 0.4, y = 0.4, z = 0.4	-1.07(6)	-0.24(4)	0.0339	0.0221	0.468	0.33	-0.714	-0.329	39.9	32.0
x = 0.5, y = 0.5, z = 0.5	-0.52(3)	-0.17(3)	0.0198	0.0177	0.28	0.232	-0.342	-0.285	30.3	28.6
x = 0.6, y = 0.6, z = 0.6	-0.10(2)	-0.13(3)	0.0167	0.016	0.228	0.225	-0.288	-0.284	27.2	27.4
x = 0.5, y = 0.7, z = 0.7	-0.41(3)	-0.19(3)	0.0183	0.0171	0.227	0.224	-0.299	-0.296	28.8	28.21
x = 0.6, y = 0.7, z = 0.7	-0.13(2)	-0.14(3)	0.0167	0.016	0.227	0.225	-0.287	-0.284	27.3	27.6
x = 0.7, y = 0.6, z = 0.7	+0.02(2)	-0.13(3)	0.0165	0.0158	0.227	0.224	-0.294	-0.291	27.0	27.4
x = 0.7, y = 0.7, z = 0.6	+0.08(2)	-0.12(3)	0.0166	0.0158	0.227	0.224	-0.295	-0.291	27.0	27.3
x = 0.7, y = 0.7, z = 0.7	+0.04(2)	-0.13(3)	0.0166	0.0158	0.228	0.225	-0.295	-0.291	27.0	27.4
x = 0.7, y = 0.7, z = 0.8	+0.04(2)	-0.13(3)	0.0167	0.0159	0.227	0.224	-0.293	-0.29	27.1	27.5
x = 0.8, y = 0.7, z = 0.7	+0.10(2)	-0.13(3)	0.0169	0.0158	0.236	0.232	-0.286	-0.282	27.4	27.7
x = 0.8, y = 0.8, z = 0.8	+0.14(2)	-0.12(3)	0.0171	0.0159	0.23	0.227	-0.288	-0.284	27.3	27.7
Ref. Box	+0.27(2)	-0.11(3)	0.0178	0.016	0.267	0.228	-0.287	-0.282	27.4	27.5
$\alpha = -0.05 (\sin(\theta)/\lambda)^2 + 0.45 (\sin(\theta)/\lambda)^3$	-0.34(3)	-0.17(3)	0.0157	0.153	0.206	0.204	-0.248	-0.245	26.2	25.9

Table S13 Model quality indicators for different boxes for **2- μ S-100K**.

	Net Charge P (1scale / 10 scale)	R2(F2) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e_{gross} (1scale / 10 scale)					
x = 0.2, y = 0.2, z = 0.2	+0.76(4)	-0.16(5)	0.0389	0.0374	0.903	0.855	-0.498	-0.489	37.6	36.6
x = 0.3, y = 0.3, z = 0.3	-0.61(4)	-0.25(4)	0.0289	0.0268	0.513	0.554	-0.385	-0.364	32.8	31.6
x = 0.4, y = 0.4, z = 0.4	-0.501(4)	-0.24(4)	0.0224	0.0214	0.329	0.385	-0.372	-0.304	31.1	30.6
x = 0.4, y = 0.4, z = 0.5	-0.34(3)	-0.22(4)	0.0201	0.0197	0.394	0.417	-0.291	-0.260	26.9	26.8
x = 0.4, y = 0.5, z = 0.4	-0.48(3)	-0.25(3)	0.0207	0.0197	0.296	0.304	-0.332	-0.271	30.3	29.9
x = 0.5, y = 0.4, z = 0.4	-0.17(3)	-0.20(3)	0.0205	0.0204	0.396	0.388	-0.306	-0.307	30.3	30.4
x = 0.5, y = 0.5, z = 0.5	-0.09(3)	-0.21(3)	0.0174	0.0171	0.324	0.303	-0.238	-0.254	26.1	25.9
x = 0.6, y = 0.6, z = 0.6	+0.08(3)	-0.19(3)	0.0169	0.0163	0.326	0.296	-0.207	-0.228	26.6	26.0
x = 0.7, y = 0.7, z = 0.7	+0.14(3)	-0.22(3)	0.0171	0.0160	0.372	0.288	-0.205	-0.200	27.5	26.6
x = 0.8, y = 0.8, z = 0.8	+0.20(2)	-0.18(3)	0.0169	0.0157	0.395	0.300	-0.199	-0.194	27.5	26.3
Ref. Box	+0.29(2)	-0.15(3)	0.0176	0.0160	0.4	0.305	-0.186	-0.208	28.1	26.5
$\alpha = -0.15 (\sin(\theta)/\lambda)^2 + 0.50 (\sin(\theta)/\lambda)^3$	-0.39(3)	-0.26(3)	0.0152	0.0150	0.278	0.278	-0.204	-0.198	23.4	23.3

Table S14 Model quality indicators for different boxes for **2-TXS-15K**.

	Net Charge P (1scale / 10 scale)	R2(F2) (1scale / 10 scale)	Highest Peak (1scale / 10 scale)	Deepest Hole (1scale / 10 scale)	e_{gross} (1scale / 10 scale)					
x = 0.4, y = 0.4, z = 0.4	-0.80(7)	-0.22(6)	0.0348	0.027	0.497	0.341	-0.727	-0.458	36.9	33.7
x = 0.5, y = 0.5, z = 0.5	-0.67(6)	-0.24(5)	0.0261	0.023	0.342	0.277	-0.524	-0.448	33.2	31.7
x = 0.6, y = 0.6, z = 0.6	-0.58(5)	-0.29(4)	0.0219	0.0202	0.243	0.25	-0.384	-0.362	31.6	30.8
x = 0.7, y = 0.7, z = 0.7	-0.45(4)	-0.28(4)	0.0199	0.0191	0.254	0.255	-0.305	-0.295	31.2	30.8
Ref. Box	-0.32(4)	-0.22(4)	0.0195	0.0192	0.252	0.251	-0.236	-0.239	31.8	31.6
$\alpha = 0.0 (\sin(\theta)/\lambda)^2 + 0.10 (\sin(\theta)/\lambda)^3$	-0.69(5)	-0.26(5)	0.0208	0.0200	0.264	0.255	-0.289	-0.297	31.0	30.7

S6. Model parameters

Table S15 Selected model parameters for **1-TXS-100K**, **1- μ S-100K** and **1-TXS-15K**. For each datasets three ways of data treatments are shown: Refinement against the refined box size (Ref. Box), against the manual chosen fixed integration box (Best Box**) and against a corrected *.hkl file. The correction factors were obtained by the above described procedure. In the first line of each dataset values for one scale factor refinement in the second values with resolution-dependent scaling were shown.

	parameter	1-TXS-100K			1- μ S-100K			1-TXS-15K		
		Ref. Box	Best Box	α cor.	Ref. Box	Best Box	α cor.	Ref. Box	Best Box	α cor.
1 scale	scale factor	0.39573(16)	0.41138(17)	0.41082(15)	0.40721(21)	0.41358(23)	0.41604(20)	0.40764(16)	0.41518(16)	0.41491(16)
1 scale 10scale	Net charge	1.57(10)	0.59(11)	0.78(8)	1.09(9)	0.52(12)	0.64(8)	1.12(11)	0.58(11)	0.59(10)
	Mg	0.66(9)	0.56(12)	0.64(8)	0.67(9)	0.61(12)	0.63(8)	0.61(11)	0.55(12)	0.61(10)
1 scale 10scale	Net charge	-0.332(17)	-0.154(15)	-0.120(14)	-0.240(16)	-0.134(17)	-0.152(16)	-0.176(14)	-0.112(14)	-0.107(13)
	N(1)	-0.119(16)	-0.154(16)	-0.098(15)	-0.162(15)	-0.147(17)	-0.152(16)	-0.113(14)	-0.110(14)	-0.108(13)
1 scale 10scale	Net charge	-0.236(18)	-0.043(16)	-0.046(15)	-0.107(18)	-0.050(19)	-0.055(18)	-0.071(15)	-0.017(15)	-0.015(15)
	N(2)	-0.048(16)	-0.049(16)	-0.035(15)	-0.061(17)	-0.068(19)	-0.059(18)	-0.017(15)	-0.017(15)	-0.016(15)
1 scale 10scale	U_{eq} Mg	0.0103	0.0129	0.0135	0.0107	0.0124	0.0141	0.0063	0.0073	0.0082
		0.0105	0.0129	0.0136	0.0108	0.0124	0.0141	0.0064	0.0074	0.0082
1 scale 10scale	U_{eq} N(1)	0.0120	0.0145	0.0151	0.0123	0.0140	0.0158	0.0074	0.0083	0.0092
		0.0121	0.0145	0.0152	0.0124	0.0141	0.0158	0.0074	0.0084	0.0092
1 scale 10scale	U_{eq} N(1)	0.0109	0.0134	0.0140	0.0112	0.0128	0.0146	0.0067	0.0076	0.0085
		0.0110	0.0134	0.0141	0.0113	0.0129	0.0146	0.0067	0.0077	0.0085
1 scale 10scale	κ Mg*	3.19(6)	0.90(2)	0.95(2)	1.14(4)	0.90(2)	0.886(16)	0.84(2)	0.856(16)	0.842(14)
		0.86(2)	0.823(19)	0.864(19)	0.853(18)	0.832(19)	0.848(16)	0.822(16)	0.825(16)	0.819(14)
1 scale 10scale	κ N(1) / N(2)	0.9972(8)	0.9904(8)	0.9915(7)	0.9878(9)	0.9911(10)	0.9942(10)	0.9956(8)	0.9936(8)	0.9965(8)
		0.9949(9)	0.9955(10)	0.9961(8)	0.9955(10)	0.9965(12)	0.9968(11)	0.99670(9)	0.9963(10)	0.9975(9)

* This parameter was not refined in the final refinement protocol.

** Best box **1-TXS-100K** x = 0.3, y = 0.45, z = 0.4, **1- μ S-100K** x = 0.4, y = 0.4, z = 0.4 and **1-TXS-15K** x = 0.5, y = 0.6, z = 0.4. Correction factor α **1-TXS-100K** $a = -0.15$, $b = 0.7$, **1- μ S-100K** $a = 0.0$, $b = 0.7$ and **1-TXS-15K** $a = 0.0$, $b = 0.3$.

Table S16 Selected model parameters for **2-TXS-100K**, **2-I μ S-100K** and **2-TXS-15K**. For each datasets three ways of data treatments are shown: Refinement against the refined box size (Ref. Box), against the manual chosen fixed integration box (Best Box**) and against a corrected *.hkl file. The correction factors were obtained by the above described procedure. In the first line of each dataset values for one scale factor refinement in the second values with resolution-dependent scaling were shown.

	parameter	2-TXS-100K			2-I μ S-100K			2-TXS-15K		
		Ref. Box	Best Box	α cor.	Ref. Box	Best Box	α cor.	Ref. Box	Best Box	α cor.
1 scale	scale factor	0.51547(8)	0.52153(7)	0.52848(7)	0.50081(9)	0.51059(10)	0.51428(9)	0.46950(9)	-	0.47324(10)
1 scale 10scale	Net charge S	-0.203(18)	-0.238(17)	-0.209(17)	-0.188(18)	-0.21(2)	-0.195(18)	-0.09(2)	-	-0.09(3)
		-0.205(18)	-0.216(17)	-0.217(17)	-0.186(19)	-0.21(2)	-0.185(18)	-0.07(3)	-	-0.08(3)
1 scale 10scale	Net charge P	+0.27(2)	-0.10(2)	-0.33(3)	+0.30(2)	-0.08(3)	-0.38(3)	-0.32(4)	-	-0.69(4)
		-0.11(3)	-0.13(3)	-0.17(3)	-0.15(3)	-0.20(3)	-0.26(3)	-0.22(4)	-	-0.26(5)
1 scale 10scale	κ S	1.0290(10)	1.0000(10)	0.9798(9)	1.0236(12)	0.9949(13)	0.9753(11)	1.0022(16)	-	0.9795(16)
		0.9916(13)	0.9887(12)	0.9835(17)	0.9892(14)	0.9851(16)	0.9811(14)	0.995(2)	-	0.993(2)
1 scale 10scale	κ P	1.0467(17)	0.9914(15)	0.9512(14)	1.0384(19)	0.980(2)	0.9419(16)	0.973(2)	-	0.932(2)
		0.976(2)	0.972(2)	0.963(2)	0.969(2)	0.962(3)	0.953(2)	0.968(3)	-	0.963(3)
1 scale 10scale	U_{eq} S(1)	0.0148	0.0152	0.0172	0.0150	0.0158	0.0170	0.0092	-	0.0100
		0.0148	0.0153	0.0172	0.0151	0.0159	0.0171	0.0091	-	0.0100
1 scale 10scale	U_{eq} P(1)	0.0094	0.0098	0.0118	0.0094	0.0103	0.0116	0.0058	-	0.0066
		0.0093	0.0098	0.0117	0.0096	0.0104	0.0116	0.0058	-	0.0067

** Best box **2-TXS-100K** x = 0.6, y = 0.6, z = 0.6, **2-I μ S-100K** x = 0.5, y = 0.5, z = 0.5. Correction factor α **2-TXS-100K** $a = -0.15$, $b = 0.5$, **2-I μ S-100K** $a = 0.05$, $b = 0.45$ and **2-TXS-15K** $a = 0.0$, $b = 0.1$.

S7. ‘Automatic’ correction

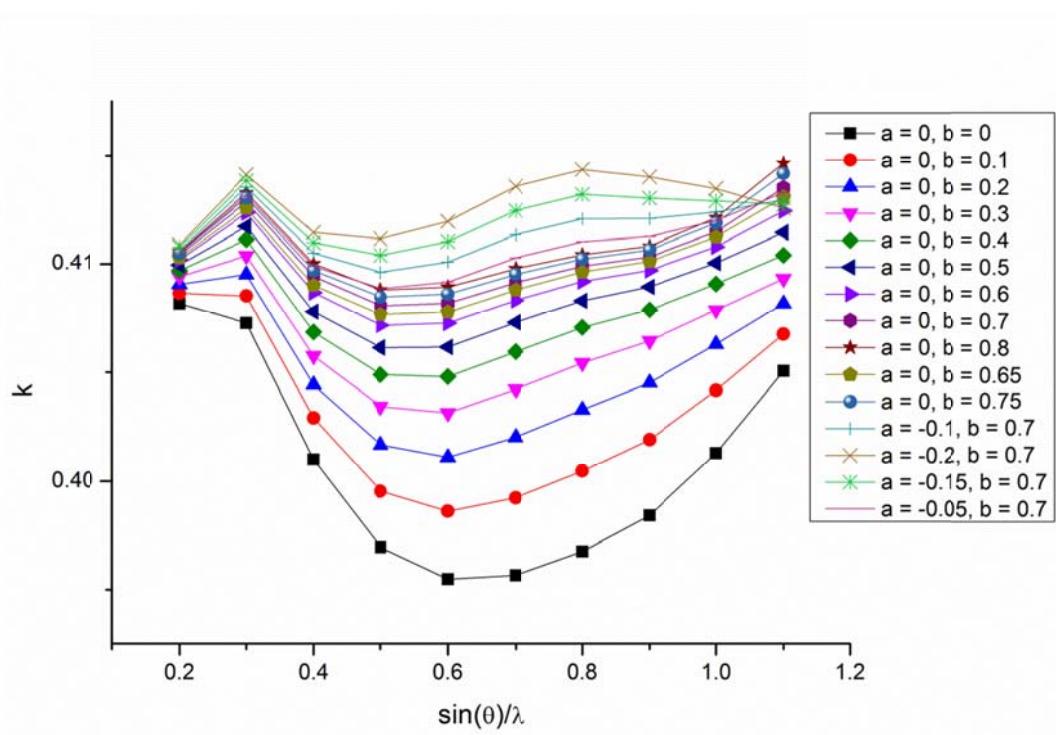


Figure S42 Resolution-dependence of the scale factors with different correction factors for **1-TXS-100K**

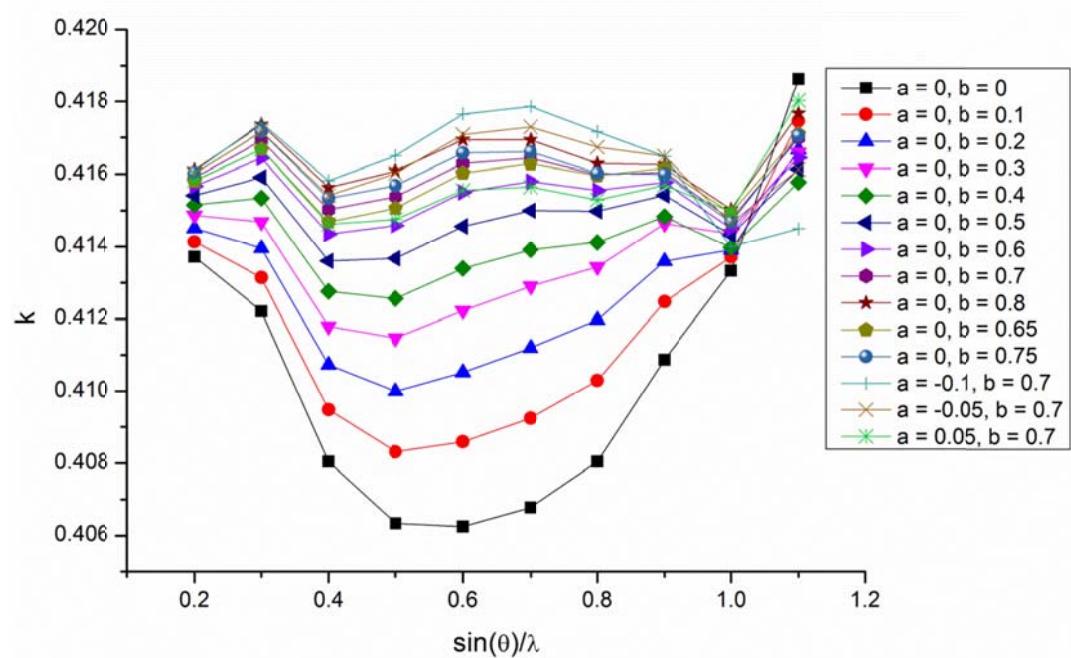


Figure S43 Resolution-dependence of the scale factors with different correction factors for **1-IuS-100K**

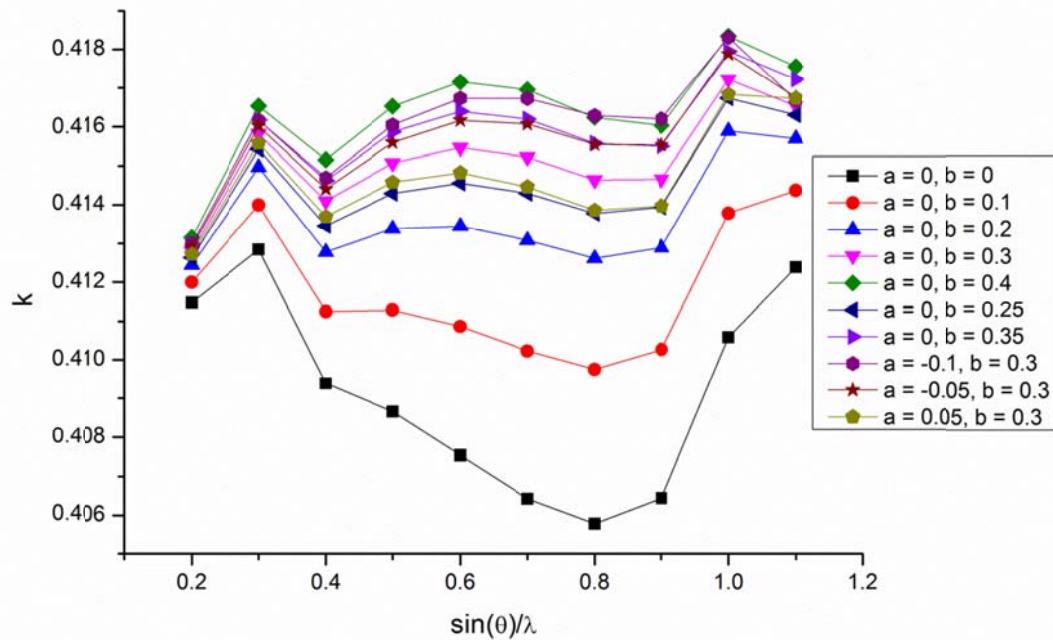


Figure S44 Resolution-dependence of the scale factors with different correction factors for **1-TXS-15K**

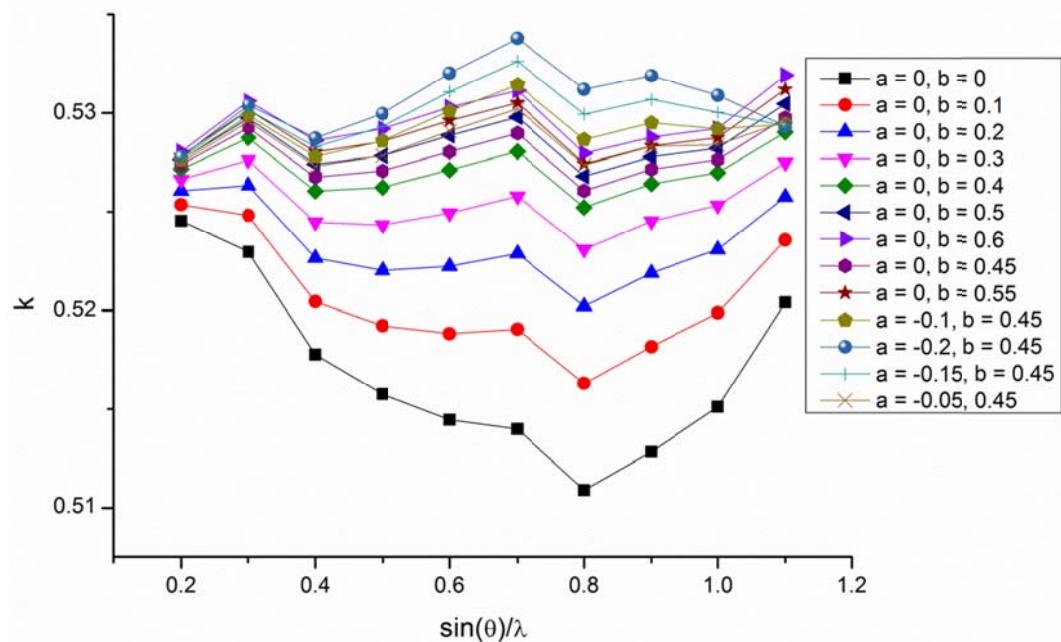


Figure S45 Resolution-dependence of the scale factors with different correction factors for **2-TXS-100K**

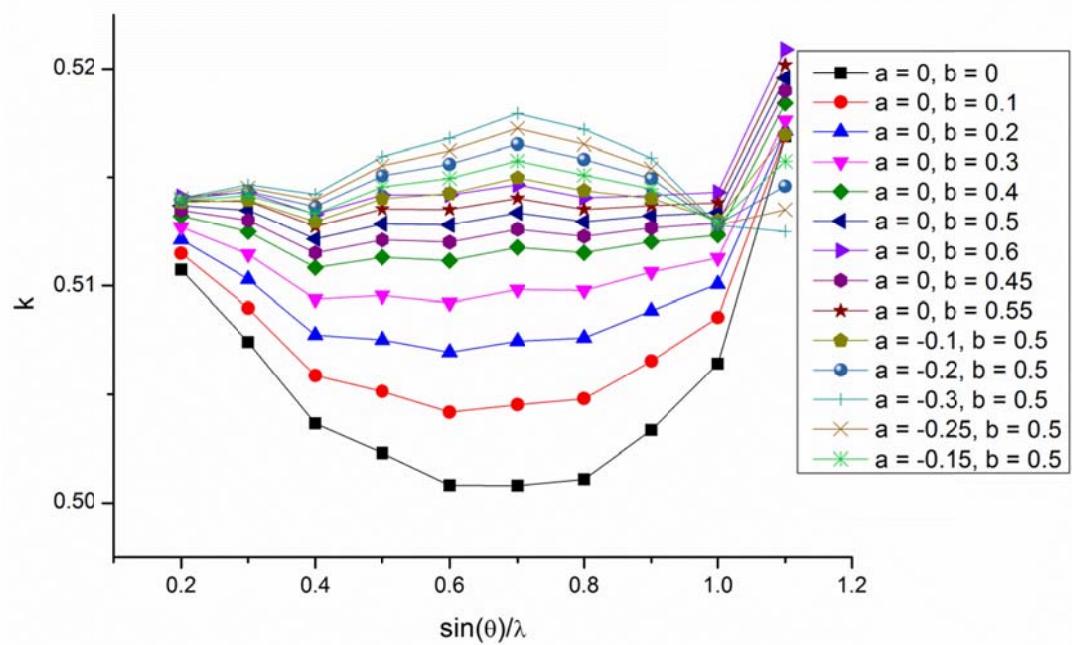


Figure S46 Resolution-dependence of the scale factors with different correction factors for **2-1 μ S-100K**

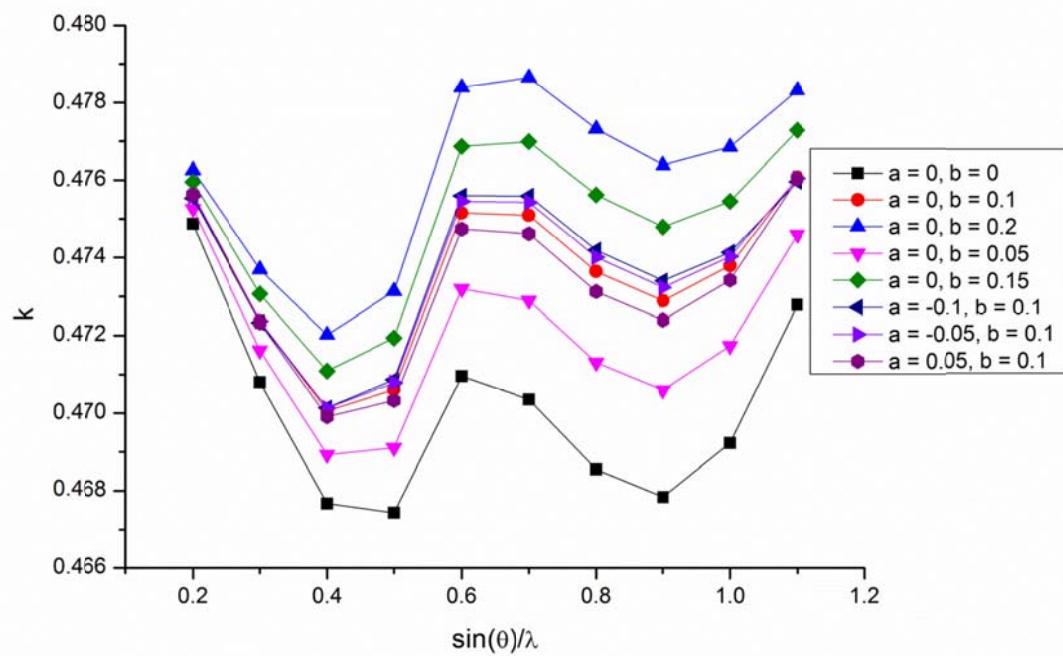


Figure S47 Resolution-dependence of the scale factors with different correction factors for **2-TXS-15K**

Table S17 Standard deviation for a constant line of the resolution-dependent scale factor for different correction factors.

1-TXS-100K			1-I μ S-100K			1-TXS-15K		
Cor. factor	deviation	$R_2(F^2)$	Cor. factor	deviation	$R_2(F^2)$	Cor. factor	deviation	$R_2(F^2)$
a = 0, b = 0	4.53E-03	0.0163	a = 0, b = 0	3.86E-03	0.0215	a = 0, b = 0	2.46E-03	0.0196
a = 0, b = 0.1	3.62E-03	0.016	a = 0, b = 0.1	2.83E-03	0.0213	a = 0, b = 0.1	1.61E-03	0.0194
a = 0, b = 0.2	2.95E-03	0.0158	a = 0, b = 0.2	2.04E-03	0.0211	a = 0, b = 0.2	1.23E-03	0.0192
a = 0, b = 0.3	2.47E-03	0.0157	a = 0, b = 0.3	1.53E-03	0.021	a = 0, b = 0.3	1.18E-03	0.0191
a = 0, b = 0.4	2.13E-03	0.0156	a = 0, b = 0.4	1.03E-03	0.0209	a = 0, b = 0.4	1.35E-03	0.0191
a = 0, b = 0.5	1.90E-03	0.0155	a = 0, b = 0.5	8.21E-04	0.0208	a = 0, b = 0.25	1.21E-03	0.0192
a = 0, b = 0.6	1.77E-03	0.0155	a = 0, b = 0.6	7.14E-04	0.0208	a = 0, b = 0.35	1.29E-03	0.0196
a = 0, b = 0.7	1.73E-03	0.0154	a = 0, b = 0.7	7.07E-04	0.0207	a = -0.1, b = 0.3	1.33E-03	0.0192
a = 0, b = 0.8	1.78E-03	0.0154	a = 0, b = 0.8	7.59E-04	0.0207	a = -0.05, b = 0.3	1.26E-03	0.0191
a = 0, b = 0.65	1.75E-03	0.0154	a = 0, b = 0.65	7.34E-04	0.0208	a = 0.05, b = 0.3	1.25E-03	0.0192
a = 0, b = 0.75	1.76E-03	0.0154	a = 0, b = 0.75	7.30E-04	0.0207			
a = -0.1, b = 0.7	1.23E-03	0.0155	a = -0.1, b = 0.7	1.23E-03	0.0207			
a = -0.2, b = 0.7	1.25E-03	0.0156	a = -0.05, b = 0.7	7.90E-04	0.0207			
a = -0.15, b = 0.7	1.15E-03	0.0155	a = 0.05, b = 0.7	9.56E-04	0.0207			
a = -0.05, b = 0.7	1.44E-03	0.0155						

Table S18 Standard deviation for a constant line of the resolution-dependent scale factor for different correction factors.

2-TXS-100K			2-I μ S-100K			2-TXS-15K		
Cor. factor	deviation	$R_2(F^2)$	Cor. factor	deviation	$R_2(F^2)$	Cor. factor	deviation	$R_2(F^2)$
a = 0, b = 0	4.23E-03	0.016	a = 0, b = 0	4.93E-03	0.016	a = 0, b = 0	2.29E-03	0.0204
a = 0, b = 0.1	2.85E-03	0.0158	a = 0, b = 0.1	3.79E-03	0.0156	a = 0, b = 0.1	1.96E-03	0.02
a = 0, b = 0.2	1.94E-03	0.0156	a = 0, b = 0.2	2.96E-03	0.0153	a = 0, b = 0.2	2.24E-03	0.0197
a = 0, b = 0.3	1.39E-03	0.0154	a = 0, b = 0.3	2.40E-03	0.0151	a = 0, b = 0.05	2.00E-03	0.0202
a = 0, b = 0.4	1.15E-03	0.0153	a = 0, b = 0.4	2.08E-03	0.0149	a = 0, b = 0.15	2.06E-03	0.0199
a = 0, b = 0.5	1.15E-03	0.0152	a = 0, b = 0.5	1.99E-03	0.0147	a = -0.1, b = 0.1	1.97E-03	0.0204
a = 0, b = 0.6	1.28E-03	0.0152	a = 0, b = 0.6	2.05E-03	0.0146	a = -0.05, b = 0.1	1.96E-03	0.0199
a = 0, b = 0.45	1.12E-03	0.0153	a = 0, b = 0.45	2.01E-03	0.0148	a = 0.05, b = 0.1	1.97E-03	0.0202
a = 0, b = 0.55	1.20E-03	0.0152	a = 0, b = 0.55	2.00E-03	0.0147			
a = -0.1, b = 0.45	1.07E-03	0.0153	a = -0.1, b = 0.5	1.07E-03	0.0149			
a = -0.2, b = 0.45	1.67E-03	0.0154	a = -0.2, b = 0.5	1.04E-03	0.0151			
a = -0.15, b = 0.45	1.33E-03	0.0153	a = -0.3, b = 0.5	1.76E-03	0.0153			
a = -0.05, 0.45	9.90E-04	0.0153	a = -0.25, b = 0.5	1.37E-03	0.0152			
			a = -0.15, b = 0.5	9.03E-04	0.0150			

S8. Artificial TDS contaminated datasets – Influence of parameters *a* and *b*

Table S19 Influence on the model parameter with $a = 0.3$, $b = 0.0$ ordered by the significance of the change (Diff/su). For the sake of clarity only the first three atomic displacement parameters are shown.

Parameter	Value without contamination	Value with contamination	Diff / su
H(4A) U11	0.02862(2)	0.02621	100.3
H(2) U11	0.02073(2)	0.01880	96.1
Mg(1) U11	0.01522(18)	0.013625	88.6
:	:	:	:
C(4) KS	0.9575(15)	0.9516	3.8
C(1) KS	1.0014(11)	0.9974	3.7
C(4) M1	4.218(16)	4.258	2.4

Table S20 Influence on the model parameter with $a = 0.0$, $b = 0.5$ ordered by the significance of the change (Diff/su). For the sake of clarity only the first three atomic displacement parameters are shown.

Parameter	Value without contamination	Value with contamination	Diff / su
H(4A) U11	0.02862(2)	0.02427	181.2
H(2) U11	0.02073(2)	0.01724	174.5
Mg(1) U11	0.01522(18)	0.012281	163.3
:	:	:	:
C(1) KS	1.0014(11)	1.0149	12.6
N(1) M1	5.155(9)	5.268	12.4
N(2) M1	5.04(10)	5.14	9.8

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