Table 1   Output of the leverage analysis for perovskite after iterative elimination of the outliers. K = overall scale factor.

hkl	$|Fo|/K$	$|Fc|$	h_i	e_i	COVRATIO	FVARATIO	Cook	DFFITS
before outliers elimination								
0 4 0	136.60	144.14	0.11	-7.54	0.40	1.16	7.46	2.88
2 14 0	8.12	7.19	0.05	0.93	1.06	1.12	0.04	0.21
1 2 1	95.92	99.90	0.05	-3.98	0.83	1.11	0.81	0.91
0 0 2	95.28	98.22	0.06	-2.93	0.94	1.12	0.51	0.71
0 4 2	83.73	86.81	0.04	-3.08	0.92	1.11	0.43	0.66
0 14 2	10.07	7.23	0.05	2.84	0.95	1.11	0.38	0.60
2 0 2	136.61	139.90	0.09	-3.29	0.94	1.16	1.11	1.04
0 0 4	88.42	92.84	0.06	-4.42	0.78	1.12	1.27	1.17
after eliminating (0 4 0) reflection								
2 14 0	8.12	7.19	0.05	0.93	1.06	1.10	0.05	0.21
1 2 1	95.86	99.89	0.05	-4.04	0.81	1.09	0.94	1.01
0 0 2	95.22	98.21	0.06	-2.99	0.93	1.11	0.59	0.78
0 4 2	83.68	86.78	0.05	-3.10	0.91	1.09	0.46	0.70
0 14 2	10.06	7.23	0.05	2.83	0.94	1.09	0.38	0.61
2 0 2	136.52	139.88	0.10	-3.36	0.93	1.15	1.30	1.14
0 0 4	88.37	92.82	0.06	-4.46	0.75	1.10	1.38	1.26
after eliminating (0 0 4) reflection								
2 14 0	8.11	7.18	0.05	0.93	1.05	1.07	0.05	0.22
1 2 1	95.81	99.89	0.06	-4.09	0.78	1.06	1.02	1.09
0 0 2	95.17	98.20	0.06	-3.03	0.92	1.08	0.64	0.83
0 4 2	83.63	86.77	0.05	-3.14	0.89	1.06	0.50	0.75
0 14 2	10.06	7.22	0.05	2.83	0.94	1.06	0.39	0.62
2 0 2	136.45	139.90	0.10	-3.45	0.91	1.12	1.49	1.25
after eliminating (2 0 2) reflection								
2 14 0	8.11	7.18	0.05	0.93	1.06	1.11	0.05	0.21
1 2 1	95.78	99.89	0.06	-4.11	0.79	1.12	1.10	1.13
0 0 2	95.15	98.20	0.07	-3.05	0.93	1.13	0.68	0.85
0 4 2	83.61	86.76	0.05	-3.15	0.90	1.11	0.52	0.76
0 14 2	10.05	7.22	0.05	2.83	0.94	1.10	0.38	0.60
after eliminating (1 2 1) reflection								
2 14 0	8.10	7.18	0.05	0.93	1.05	1.08	0.05	0.21
0 0 2	95.08	98.18	0.07	-3.10	0.91	1.10	0.76	0.93
0 4 2	83.55	86.74	0.05	-3.19	0.88	1.08	0.58	0.83
0 14 2	10.05	7.22	0.05	2.83	0.94	1.08	0.39	0.61
after eliminating (0 0 2) reflection								
2 14 0	8.10	7.18	0.05	0.92	1.06	1.08	0.04	0.21
0 4 2	83.50	86.73	0.06	-3.23	0.86	1.08	0.63	0.91
0 14 2	10.04	7.22	0.05	2.82	0.94	1.07	0.38	0.61
after eliminating (0 4 2) reflection								

hkl								
2 14 0	8.09	7.14	0.05	0.96	1.05	1.07	0.05	0.22
0 14 2	10.03	7.18	0.05	2.86	0.93	1.06	0.40	0.63
after eliminating (0 14 2) reflection								
2 14 0	8.09	7.15	0.05	0.95	1.06	1.06	0.05	0.23

Table 2 Output of the leverage analysis for loganin after iteratively elimination of the outliers. K = overall scale factor.

hkl	$|Fo|/K$	$|Fc|$	h_i	e_i	COVRATIO	FVARATIO	Cook	DFFITS
before outliers elimination								
2 0 0	95.72	104.69	0.37	-8.97	1e-5	1.89	64.21	7.53
0 4 0	83.86	92.19	0.40	-8.33	1e-5	1.98	65.64	7.60
2 13 1	25.96	19.59	0.08	6.36	0.04	1.31	3.39	1.69
0 0 2	79.99	79.45	0.28	0.54	1.51	1.69	0.13	0.33
-7 1 2	24.15	17.48	0.12	6.67	0.02	1.36	5.43	2.27
0 3 2	78.43	77.93	0.30	0.50	1.56	1.74	0.13	0.32
0 0 4	153.16	152.78	0.43	0.38	1.90	2.11	0.15	0.35
0 7 5	2.82	2.22	0.24	0.60	1.40	1.59	0.12	0.31
after eliminating (0 4 0) reflection								
2 0 0	95.64	105.08	0.38	-9.44	1e-5	1.68	79.85	8.70
4 1 0	24.98	27.78	0.33	-2.80	0.55	1.62	5.23	2.23
2 13 1	25.93	19.59	0.08	6.34	0.02	1.18	3.74	1.87
0 0 2	79.92	79.34	0.29	0.58	1.49	1.53	0.18	0.40
-7 1 2	24.13	17.45	0.12	6.69	0.01	1.22	6.08	2.55
0 0 4	153.04	152.64	0.43	0.40	1.89	1.90	0.19	0.42
1 0 5	35.04	34.61	0.32	0.43	1.58	1.60	0.11	0.32
after eliminating (2 0 0) reflection								
4 1 0	24.96	27.81	0.33	-2.85	0.51	1.59	5.50	2.31
4 4 0	2.23	1.67	0.26	0.55	1.45	1.45	0.14	0.36
2 13 1	25.92	19.58	0.08	6.34	0.02	1.16	3.81	1.91
0 0 2	79.87	79.30	0.29	0.57	1.50	1.51	0.17	0.40
-7 1 2	24.12	17.43	0.12	6.69	0.01	1.19	6.20	2.61
0 0 4	152.93	152.59	0.43	0.34	1.91	1.88	0.14	0.36
after eliminating (4 1 0) reflection								
4 4 0	2.23	1.72	0.26	0.50	1.45	1.42	0.11	0.33
2 13 1	25.91	19.52	0.09	6.39	0.01	1.13	3.99	1.98
0 0 2	79.85	79.39	0.29	0.47	1.52	1.48	0.12	0.34
-7 1 2	24.11	17.42	0.12	6.69	0.01	1.17	6.35	2.68
0 0 4	152.91	152.58	0.43	0.33	1.90	1.83	0.13	0.36
1 0 5	35.01	34.58	0.32	0.43	1.58	1.53	0.12	0.34
after eliminating (-7 1 2) reflection								
2 13 1	25.92	19.52	0.09	6.39	0.01	1.09	4.13	2.05

Table 3   Output of the leverage analysis for oxalic acid after iterative elimination of the outliers. K = overall scale factor. Note that after elimination of the (3 0 -3) reflection no outliers have been indicated by the analysis.

hkl	$|F_o|/K$	$|F_c|$	h_i	e_i	COVRATIO	FVARATIO	Cook	DFFITS
before outliers elimination								
0 0 8	18.35	17.83	0.17	0.53	1.234	1.290	0.06	0.24
1 0 1	27.95	27.50	0.21	0.45	1.309	1.365	0.07	0.25
1 0 3	26.67	28.95	0.29	-2.28	1.138	1.501	2.75	1.63
1 0 -5	39.04	41.24	0.29	-2.20	1.149	1.500	2.55	1.59
2 0 0	23.64	25.45	0.27	-1.81	1.206	1.467	1.54	1.27
3 0 -3	18.86	19.62	0.28	-0.76	1.411	1.498	0.29	0.53
1 1 -3	18.87	20.42	0.22	-1.55	1.186	1.369	0.79	0.91
2 1 0	23.41	22.91	0.19	0.50	1.268	1.324	0.07	0.25
3 1 -5	22.16	21.51	0.12	0.65	1.158	1.216	0.06	0.24
after eliminating (1 0 3) reflection								
0 0 8	18.43	17.88	0.19	0.55	1.267	1.333	0.08	0.28
1 0 1	28.07	27.61	0.23	0.46	1.330	1.394	0.07	0.26
1 0 -5	39.20	41.04	0.29	-1.84	1.233	1.527	1.87	1.40
2 0 0	23.74	25.03	0.30	-1.29	1.355	1.541	0.95	1.02
3 0 -3	18.94	19.43	0.30	-0.49	1.461	1.536	0.14	0.36
1 1 -3	18.95	20.26	0.22	-1.31	1.224	1.379	0.57	0.78
2 1 0	23.50	22.91	0.20	0.60	1.273	1.343	0.10	0.31
3 1 0	12.23	11.67	0.15	0.57	1.200	1.262	0.06	0.24
3 1 -5	22.25	21.58	0.12	0.68	1.161	1.228	0.07	0.25
after eliminating (1 0 -5) reflection								
0 0 8	18.38	17.87	0.18	0.51	1.258	1.252	0.07	0.26
1 0 1	28.00	27.59	0.23	0.41	1.337	1.325	0.06	0.25
2 0 0	23.68	25.01	0.31	-1.33	1.345	1.480	1.14	1.17
3 0 -3	18.89	19.42	0.30	-0.53	1.471	1.468	0.17	0.41
1 1 -3	18.91	20.14	0.23	-1.23	1.239	1.320	0.56	0.80
2 1 0	23.44	22.88	0.20	0.56	1.278	1.276	0.10	0.31
3 1 0	12.20	11.64	0.15	0.56	1.204	1.200	0.06	0.25
3 1 -5	22.20	21.46	0.12	0.73	1.155	1.162	0.08	0.29
after eliminating (2 0 0) reflection								
0 0 8	18.31	17.80	0.17	0.50	1.243	1.261	0.06	0.25
1 0 1	27.88	27.43	0.21	0.45	1.305	1.321	0.07	0.25
3 0 -3	18.81	19.45	0.29	-0.63	1.428	1.462	0.22	0.47
1 1 -3	18.83	20.15	0.22	-1.32	1.208	1.332	0.60	0.84
2 1 0	23.35	22.85	0.19	0.49	1.272	1.290	0.07	0.26
3 1 -5	22.11	21.46	0.13	0.64	1.172	1.196	0.07	0.26
after eliminating (1 1 -3) reflection								
0 0 8	18.26	17.81	0.18	0.45	1.248	1.242	0.05	0.23
3 0 -3	18.76	19.47	0.28	-0.71	1.414	1.432	0.27	0.53