5 cycles isotropic LS, no reflection weighting, no H atoms
wR2 = 0.1286, GooF = 0.910, R1 = 0.0453 for all 1784 data

Q1	1	0.4508	-0.1260	0.5224	1.00000	0.05	1.00	0.82 O2
Q2	1	0.0523	0.2104	-0.0154	1.00000	0.05	0.97	0.79 O1
Q3	1	0.0974	0.3471	0.5818	1.00000	0.05	0.75	0.76 O6
Q4	1	0.6007	0.2344	0.0857	1.00000	0.05	0.65	0.78 O4
Q5	1	0.4343	0.6818	0.0821	1.00000	0.05	0.62	0.79 O5
Q6	1	0.7154	0.1179	0.2184	1.00000	0.05	0.60	0.86 O4
Q7	1	0.1544	0.4643	0.2957	1.00000	0.05	0.59	0.68 O3
Q8	1	0.0678	0.4047	0.4197	1.00000	0.05	0.57	0.82 O3
Q9	1	0.2160	0.4631	0.7249	1.00000	0.05	0.53	0.93 O6
Q10	1	0.0616	0.0233	-0.0188	1.00000	0.05	0.52	0.47 O1
Q11	1	0.4293	0.0608	0.5230	1.00000	0.05	0.51	0.42 O2
Q12	1	0.3480	0.6193	0.2087	1.00000	0.05	0.47	0.70 O5

6 cycles anisotropic LS, no reflection weighting, no H atoms
wR2 = 0.1232, GooF = 0.882, R1 = 0.0436 for all 1784 data

Q1	1	0.4420	-0.1306	0.5173	1.00000	0.05	0.98	0.82 O2
Q2	1	0.0523	0.2100	-0.0174	1.00000	0.05	0.95	0.79 O1
Q3	1	0.0957	0.3500	0.5819	1.00000	0.05	0.74	0.76 O6
Q4	1	0.6015	0.2311	0.0831	1.00000	0.05	0.65	0.80 O4
Q5	1	0.4354	0.6854	0.0811	1.00000	0.05	0.61	0.80 O5
,Q6	1	0.1590	0.4695	0.2939	1.00000	0.05	0.59	0.72 O3
Q7	1	0.7121	0.1193	0.2185	1.00000	0.05	0.58	0.85 O4
Q8	1	0.0621	0.3991	0.4214	1.00000	0.05	0.57	0.82 O3
Q9	1	0.2151	0.4595	0.7245	1.00000	0.05	0.53	0.91 O6
Q10	1	0.3497	0.6132	0.2116	1.00000	0.05	0.49	0.71 O5
Q11	1	0.3562	0.0262	0.6031	1.00000	0.05	0.35	0.62 O2
Q12	1	0.1400	0.0571	-0.1111	1.00000	0.05	0.35	0.67 O1

7 cycles anisotropic LS with reflection weighting, no H atoms
wR2 = 0.0996, GooF = 1.102, R1 = 0.0434 for all 1784 data

Q1	1	0.4410	-0.1314	0.5173	1.00000	0.05	0.98	0.82 O2
Q2	1	0.0452	0.2099	-0.0170	1.00000	0.05	0.95	0.81 O1
Q3	1	0.0946	0.3508	0.5817	1.00000	0.05	0.74	0.77 O6
Q4	1	0.6010	0.2301	0.0827	1.00000	0.05	0.66	0.80 O4
Q5	1	0.4363	0.6832	0.0815	1.00000	0.05	0.61	0.79 O5
Q6	1	0.1601	0.4734	0.2951	1.00000	0.05	0.59	0.73 O3
Q7	1	0.0611	0.3991	0.4205	1.00000	0.05	0.58	0.82 O3
Q8	1	0.7109	0.1195	0.2186	1.00000	0.05	0.57	0.84 O4
Q9	1	0.2137	0.4593	0.7239	1.00000	0.05	0.52	0.90 O6
Q10	1	0.3519	0.6091	0.2102	1.00000	0.05	0.48	0.72 O5
Q11	1	0.3570	0.0252	0.6041	1.00000	0.05	0.35	0.62 O2
Q12	1	0.1413	0.0579	-0.1103	1.00000	0.05	0.34	0.66 O1

FIGURE S1. Output from a SHELX.LST file for three stages of refinement of the $P2_1$ structure before H atoms are included in the model. Highlighted in yellow are peaks in unmodelled residual electron density that correspond to H atoms. The header of each block of entries gives some details of the stage of refinement and associated agreement indices. All 10 H atoms of the $P2_1$ structure appear in the difference-Fourier map after only 5 cycles of isotropic least-squares refinement. The penultimate column gives values of the electron density ($e/Å^3$), which closely approximate to the number of electrons at this site. The last column gives the distance to and identity of the first-nearest-neighbor atom. The first two rows of each block correspond to the two fully occupied H sites of the two zig-zag chains. The remaining eight highlighted peaks correspond to the half-occupied crankshaft H sites. See text for further explanation.