Supplementary Table 2. Hydrogen bonds for the LT-polymorph of alunogen [Å, °]. (D: donor, A: acceptor). Interactions with H…A distances up to 2.6 Å have been considered.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O13-H131...O2#1	0.861(18)	1.905(19)	2.702(4)	153(3)
O13-H132...O1#2	0.847(18)	1.828(19)	2.667(4)	171(4)
O14-H141...O3	0.843(17)	1.825(19)	2.667(4)	176(3)
O14-H142...O12	0.852(18)	1.75(2)	2.577(4)	162(4)
O15-H151...Ow4	0.886(18)	1.700(19)	2.555(4)	161(3)
O15-H152...O12#3	0.853(18)	1.81(2)	2.640(4)	162(4)
O16-H161...O1#1	0.860(17)	1.789(17)	2.645(3)	174(3)
O16-H162...O5#4	0.849(18)	1.85(2)	2.676(4)	165(4)
O17-H171...O4	0.865(18)	1.781(17)	2.644(3)	174(3)
O17-H172...O7#5	0.838(18)	1.91(2)	2.692(4)	154(4)
O18-H181...Ow2	0.838(17)	1.792(17)	2.618(4)	168(4)
O18-H182...O3#3	0.834(18)	1.88(2)	2.684(4)	160(4)
O19-H191...O11	0.815(18)	1.86(2)	2.657(4)	166(4)
O19-H192...Ow3#2	0.823(17)	1.747(19)	2.564(4)	172(4)
O20-H201...O4#6	0.830(17)	1.821(18)	2.649(4)	175(3)
O20-H202...O8#2	0.845(18)	1.872(19)	2.715(3)	175(3)
O21-H212...O8#7	0.832(18)	1.873(18)	2.693(4)	169(4)
O21-H211...O7#2	0.837(17)	1.851(19)	2.675(4)	167(4)
O22-H221...O5#8	0.840(18)	1.86(2)	2.671(4)	160(4)
O22-H222...O2#9	0.817(18)	1.85(2)	2.640(4)	163(4)
O23-H232...O6	0.851(18)	1.834(18)	2.671(4)	168(3)
O23-H231...Ow1#8	0.866(18)	1.806(18)	2.668(4)	173(4)
O24-H241...O6#8	0.827(18)	1.880(18)	2.703(3)	174(4)
O24-H242...O10#8	0.818(18)	1.787(19)	2.601(4)	173(4)
Ow1-Hw11...O8	0.862(18)	2.17(2)	2.944(4)	149(3)
Ow1-Hw12...O9	0.871(18)	1.93(2)	2.783(5)	167(4)
Ow2-Hw22...O9	0.874(18)	1.85(2)	2.715(4)	170(4)
Ow2-Hw21...O11#3	0.879(18)	1.92(2)	2.795(4)	171(4)
Ow3-Hw31...Ow1#8	0.859(19)	2.59(2)	2.899(5)	103(4)
Ow3-Hw32...Ow5	0.846(19)	2.40(5)	2.879(8)	116(4)
Ow4-Hw41...O10	0.827(19)	2.20(3)	2.881(5)	139(4)
Ow4-Hw42...Ow2#2	0.843(18)	2.01(3)	2.826(4)	162(5)
Ow5-Hw51...O9	0.866(14)	2.04(6)	2.798(7)	145(9)

Ow5-Hw52...Ow4#10	0.87(7)	2.44(8)	3.278(8)	162(8)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z-1 #2 x-1,y,z #3 x,y,z-1 #4 -x+1,y-1/2,-z

#5 -x+1,y-1/2,-z+1 #6 -x+1,y+1/2,-z+1 #7 x-1,y,z+1

#8 x,y,z+1 #9 -x+1,y+1/2,-z+2 #10 x+1,y,z