**S9 Table.** Check-Cif report for TABA

|  |  |  |
| --- | --- | --- |
| Bond precision: | C-C = 0.0022 Å | |
| Wavelength | 0.71073 | |
| Temperature | 298 K | |
| Cell dimensions | a = 8.3990(11) **Å**  b = 8.4870(8) **Å**  c = 9.8050(11) **Å**  alpha = 87.999(7)**˚**  beta = 82.508(6)**˚**  gamma = 88.714(7)**˚** | |
| Data completeness | 0.987 | |
| Theta(max) | 26.740 | |
| R(reflections)= | 0.0479( 2291) | |
| wR2(reflections)= | 0.1416( 2915) | |
|  | **Calculated** | **Reported** |
| Volume | 692.42(14) | 692.42(14) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C13 H12 O8 | C13 H12 O8 |
| Sum formula | C13 H12 O8 | C13 H12 O8 |
| Mr | 296.23 | 296.23 |
| Dx,g cm-3 | 1.421 | 1.421 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.120 | 0.120 |
| F000 | 308.0 | 308.0 |

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level**.

Click on the hyperlinks for more details of the test.

**Alert level C**

[PLAT906\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT906.html%22)) Large K value in the Analysis of Variance ...... 2.745 Check

[PLAT911\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT911.html%22)) Missing # FCF Refl Between THmin & STh/L= 0.600 26 Report

[PLAT913\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT913.html%22)) Missing # of Very Strong Reflections in FCF .... 21 Note

[PLAT978\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT978.html%22)) Number C-C Bonds with Positive Residual Density 0 Note

**Alert level G**

[PLAT007\_ALERT\_5\_G](javascript:makeHelpWindow(%22PLAT007.html%22)) Number of Unrefined Donor-H Atoms .............. 1 Report

[PLAT180\_ALERT\_4\_G](javascript:makeHelpWindow(%22PLAT180.html%22)) Check Cell Rounding: # of Values Ending with 0 = 3 Note

[PLAT194\_ALERT\_1\_G](javascript:makeHelpWindow(%22PLAT194.html%22)) Missing \_cell\_measurement\_reflns\_used Datum .... Please Add

[PLAT195\_ALERT\_1\_G](javascript:makeHelpWindow(%22PLAT195.html%22)) Missing \_cell\_measurement\_theta\_max Datum .... Please Add

[PLAT196\_ALERT\_1\_G](javascript:makeHelpWindow(%22PLAT196.html%22)) Missing \_cell\_measurement\_theta\_min Datum .... Please Add

[PLAT432\_ALERT\_2\_G](javascript:makeHelpWindow(%22PLAT432.html%22)) Short Inter X...Y Contact O4 .. C3 .. 3.00 Ang.

[PLAT910\_ALERT\_3\_G](javascript:makeHelpWindow(%22PLAT910.html%22)) Missing # of FCF Reflection(s) Below Theta(Min) 4 Note

[PLAT912\_ALERT\_4\_G](javascript:makeHelpWindow(%22PLAT912.html%22)) Missing # of FCF Reflections Above STh/L= 0.600 9 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **ALERT level G** = General information/check it is not something unexpected