**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 Large K value in the Analysis of Variance ...... 2.745 Check

PLAT911\_ALERT\_3\_C Missing # FCF Refl Between THmin & STh/L= 0.600 26 Report

PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 21 Note

PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density 0 Note

**Alert level G**

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms .............. 1 Report

PLAT180\_ALERT\_4\_G Check Cell Rounding: # of Values Ending with 0 = 3 Note

PLAT194\_ALERT\_1\_G Missing \_cell\_measurement\_reflns\_used Datum .... Please Add

PLAT195\_ALERT\_1\_G Missing \_cell\_measurement\_theta\_max Datum .... Please Add

PLAT196\_ALERT\_1\_G Missing \_cell\_measurement\_theta\_min Datum .... Please Add

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O4 .. C3 .. 3.00 Ang.

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min) 4 Note

PLAT912\_ALERT\_4\_G 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