checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dp38_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: dp38_0m_a

Bond precision: C-C = 0.0037 A   Wavelength=0.71073

Cell: a=8.2365(3)   b=12.4920(6)   c=17.0520(7)
                   alpha=90   beta=90   gamma=90
Temperature: 105 K

	Calculated	Reported
Volume	1754.49(13)	1754.49(13)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C17 H26 O3 S2	C17 H26 O3 S2
Sum formula	C17 H26 O3 S2	C17 H26 O3 S2
Mr	342.50	342.50
Dx,g cm-3	1.297	1.297
Z	4	4
Mu (mm-1)	0.313	0.313
F000	736.0	736.0
F000'	737.28	
h,k,lmax	11,17,24	11,17,24
Nref	5136[2911]	5021
Tmin,Tmax	0.896,0.967	0.680,0.746
Tmin'	0.880	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.98   Theta(max)= 30.062

R(reflections)= 0.0577(4643)   wR2(reflections)= 0.1147(5021)

S = 1.060   Npar= 202

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 B
PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density ....   4.31 Report

Alert level C
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density   1.44 eA-3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   67 Report
               0 2 0,   4 2 0,   0 6 0,   3 6 0,   2 7 0,   1 8 0,
               1 1 1,   1 2 1,   4 2 1,   5 2 1,   0 7 1,   5 0 2,
               1 1 2,   0 2 2,   3 6 2,   1 0 3,   5 1 3,   0 2 3,
               1 2 3,   4 5 3,   0 0 4,   2 0 4,   4 0 4,   5 0 4,
               3 2 4,   3 4 4,   0 6 4,   0 7 4,   3 1 5,   0 2 5,
               4 2 5,   1 3 5,   2 5 5,   1 7 5,   3 1 6,   4 1 6,
               3 2 6,   2 3 6,   3 3 6,   1 5 6,   0 7 6,   2 0 7,
               0 1 7,   3 1 7,   0 3 7,   1 3 7,   2 3 7,   0 4 7,
               1 5 7,   2 5 7,   0 2 8,   3 2 8,   3 3 8,   0 4 8,
               1 0 9,   2 0 9,   0 2 9,   0 3 9,   1 3 9,   0 4 9,
               2 4 9,   0 1 10,   1 1 10,   0 2 10,   0 3 10,   1 3 10,
               1 0 11,
PLAT977_ALERT_2_C Check Negative Difference Density on H8   .   -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19A   .   -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22C   .   -0.45 eA-3

Alert level G
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0   0.986 Report
PLAT398_ALERT_2_G Deviating C-O-C   Angle From 120 for O7   .   109.2 Degree
PLAT795_ALERT_4_G C-Atom in CIF Coordinate List Out-of-Sequence ..   C6 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   2 Note
               0 1 1,   0 0 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   3 Note
               0 2 2,   0 2 3,   0 0 4,
PLAT930_ALERT_2_G FCF-based   Twin Law   [0 3 5] Est.d BASF   0.78 Check
PLAT930_ALERT_2_G FCF-based   Twin Law   [5 -1 -1] Est.d BASF   0.90 Check
PLAT930_ALERT_2_G FCF-based   Twin Law   [4 -2 3] Est.d BASF   0.90 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [0 3 5] Est.d BASF   0.78 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [5 -1 -1] Est.d BASF   0.90 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [4 -2 3] Est.d BASF   0.90 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [4 2 -3] Est.d BASF   0.91 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   9 Note
              -3 5 1, -1 1 2,   0 0 2,   0 0 4,   0 2 0,   0 2 2,
               0 2 3,   0 2 5,   1 1 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ....   3.72 Note
            Predicted wR2: Based on SigI**2 3.08 or SHELX Weight 11.05
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

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 0 ALERT level A = Most likely a serious problem - resolve or explain
 1 ALERT level B = A potentially serious problem, consider carefully
 6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
16 ALERT level G = General information/check it is not something unexpected

 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 5 ALERT type 5 Informative message, check
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checkCIF publication errors

 Alert level A
```
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

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 3 ALERT level A = Data missing that is essential or data in wrong format
 0 ALERT level G = General alerts. Data that may be required is missing
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Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock dp38_0m_a - ellipsoid plot