checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pvl691_sq

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: pvl691_sq

Bond precision: C-C = 0.0023 A   Wavelength=0.71073

Cell: a=23.6070(7)   b=11.3468(2)   c=26.3689(8)
                alpha=90   beta=116.055(4)   gamma=90
Temperature: 142 K

	Calculated	Reported
Volume	6345.5(4)	6345.5(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C26 H16 Cd N6 O6 S2 [+ solvent]	?
Sum formula	C26 H16 Cd N6 O6 S2 [+ solvent]	C26 H16 Cd N6 O6 S2
Mr	684.98	684.97
Dx,g cm-3	1.434	1.434
Z	8	8
Mu (mm-1)	0.866	0.866
F000	2736.0	2736.0
F000'	2732.58	
h,k,lmax	32,15,36	32,15,35
Nref	8481	7697
Tmin,Tmax	0.901,0.917	0.951,1.000
Tmin'	0.841	

Correction method= # Reported T Limits: Tmin=0.951 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.908   Theta(max)= 29.061

R(reflections)= 0.0223(7175)   wR2(reflections)= 0.0568(7697)

S = 1.027   Npar= 370

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
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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range      3.1 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C014 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....     2.3 Note
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⚪ Alert level G
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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large    8.18 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd01      --O005    .      9.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd01      --O004_d  .      8.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd01      --O006_d  .      7.0 s.u.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........      ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     57 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cd01       (II)    .     2.08 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed       ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     780 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      12 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 16/05/2021; check.def file version of 13/05/2021