checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: mrmn-b

Bond precision: C-C = 0.0046 A   Wavelength=1.54184

Cell:	a=39.4563(3)	b=16.35832(15)	c=90
	alpha=100.1751(8)	beta=90	gamma=
Temperature:	285 K		

	Calculated	Reported
Volume	9018.64(13)	9018.64(13)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C30 H47 O P2 S), C9 H5 F6 O4 S2, C7 H5 O S2, C6 H6, 6(F), 3(O	2(C9 H5 F6 O4 S2), 2(C30 H47 O P2 S), C6 H6
Sum formula	C84 H110 F12 O10 P4 S6	C84 H110 F12 O10 P4 S6
Mr	1824.02	1823.95
Dx,g cm-3	1.343	1.343
Z	4	4
Mu (mm-1)	2.749	2.749
F000	3832.0	3832.0
F000'	3855.99	
h,k,lmax	17,49,20	17,48,20
Nref	18304	17960
Tmin,Tmax		0.745,1.000
Tmin'		

Correction method= MULTI-SCAN

Data completeness= 0.981   Theta(max)= 73.916

R(reflections)= 0.0549(15661)   wR2(reflections)= 0.1531(17960)

S = 1.068   Npar= Npar =1221

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
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...   Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...   Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...   Please Check
PLAT242_ALERT_2_C Low   Ueq as Compared to Neighbors for .....   C96 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0046 Ang.

_____

⚪ **Alert level G**
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   14.07 Why ?
PLAT142_ALERT_4_G su on b - Axis Small or Missing ....   0.00030 Ang.
PLAT143_ALERT_4_G su on c - Axis Small or Missing ....   0.00015 Ang.
PLAT242_ALERT_2_G Low   Ueq as Compared to Neighbors for .....   C216 Check
PLAT242_ALERT_2_G Low   Ueq as Compared to Neighbors for .....   C237 Check
PLAT301_ALERT_3_G Main Residue Disorder .... Percentage =   3 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder .... Percentage =   65 Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O1 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O5 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O24 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O14 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O19 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   62 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .   1.20 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   291 Note

_____

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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check

_____

_____

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*, 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 05/02/2014; check.def file version of 05/02/2014

NOMOVE FORCED

Prob = 50
Temp = 285

65 Y

PLATON-Mar 5 02:36:45 2014 — (100912)

Z 156   mrmn-b   P 1 21/n 1   R = 0.05

RES= 0   -21 X