

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) npmnt_0m

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: npmnt_0m

Bond precision: C-C = 0.0069 Å Wavelength=0.71073

Cell: a=14.0465(4) b=18.5992(5) c=18.0751(5)
 alpha=90 beta=91.711(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4720.1(2)	4720.1(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 N16 Np2 S16, 2(C0.96 K N0.48), 11.044(C2 N), 8(K)	C28 K5 N14 Np S8
Sum formula	C56 K10 N28 Np2 S16	C28 K5 N14 Np S8
Mr	2442.90	1221.40
Dx, g cm ⁻³	1.719	1.719
Z	2	4
Mu (mm ⁻¹)	3.034	3.034
F000	2328.0	2328.0
F000'	2290.34	
h,k,lmax	23,31,30	23,30,30
Nref	22904	22697
Tmin,Tmax	0.515,0.579	0.651,0.810
Tmin'	0.494	

Correction method= # Reported T Limits: Tmin=0.651 Tmax=0.810
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 36.339

R(reflections)= 0.0425(17936)

wR2(reflections)=
0.1144(22697)

S = 1.065

Npar= 533

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
bluish

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C32 N16 Np2 S16, 2(C0.96 K N0.48), 11.044(C2 N), 8(K)
Rep.: C28 K5 N14 Np S8

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C010 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C01F Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N9 0.145 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N21 0.172 Check
PLAT723_ALERT_1_C Torsion Calc -119.00, Rep -121(21) Dev... 2.00 Sigma
C0 -C017-C01B-N01B 1_555 1_555 1_555 1_555 # 98 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.279 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 22 Report
0 2 0, 1 2 0, 1 0 1, -1 1 1, 1 1 1, 2 1 1,
0 2 1, 1 2 1, -1 3 1, 0 0 2, 2 0 2, -3 1 2,
0 1 2, -1 2 2, 3 3 2, -3 2 3, 1 3 3, -2 0 4,
2 1 4, -1 2 5, -1 1 6, -1 0 7,

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
0 2 2,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From K4 1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.23Ang From N019 1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.63Ang From K4 -2.43 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.29Ang From K4 -1.93 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.61Ang From K2 -1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.67Ang From K1 -1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.54Ang From K2 -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.44Ang From K2 -1.61 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From N9 . 0.98 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From N00K . 0.54 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 9 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.63 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 59% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 17 Note
Np01 N00K N00R C010 C015 C017 C018 N019
C01A N01B C01C C01D C01E C01F C01B C0

N01C

PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #	3	Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers	1	Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints	63	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
-1 0 1, 0 1 1,		
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	183	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	2	Note
-2 0 4, 2 1 4,		
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	15	Note
0 2 0, 0 0 2, -1 1 1, 0 2 1, -1 2 5, 2 1 1,		
-3 1 2, 3 3 2, -1 2 2, -1 3 1, 1 3 3, -3 2 3,		
-1 0 7, 2 0 2, -1 1 6,		
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.8	Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	3.652	Note
Predicted wR2: Based on SigI**2 3.13 or SHELX Weight 10.74		

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
2 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* 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.

