

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) prmnt_092721_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: prmnt_092721_0m

Bond precision: C-C = 0.0024 Å Wavelength=0.71073

Cell: a=36.3329(12) b=13.7118(5) c=19.4577(7)
 alpha=90 beta=108.999(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	9165.6(6)	9165.5(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 N32 Pr4 S32, 4(C N0.50 Na), 24(C N0.50), 15.928(Na)	C28 N14 Na4.982 Pr S8
Sum formula	C112 N56 Na19.93 Pr4 S32	C28 N14 Na4.98 Pr S8
Mr	4177.39	1044.30
Dx, g cm ⁻³	1.514	1.514
Z	2	8
Mu (mm ⁻¹)	1.513	1.513
F000	4062.4	4062.0
F000'	4070.40	
h, k, lmax	64, 24, 34	64, 24, 34
Nref	27530	27431
Tmin, Tmax	0.746, 0.860	0.677, 0.748
Tmin'	0.732	

Correction method= # Reported T Limits: Tmin=0.677 Tmax=0.748
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 39.496

R(reflections)= 0.0326(22920)

wR2(reflections)=
0.0713(27431)

S = 1.079

Npar= 599

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C64 N32 Pr4 S32, 4(C N0.50 Na), 24(C N0.50), 15.928(Na)
Rep.: C28 N14 Na4.982 Pr S8

PLAT214_ALERT_2_C Atom C01L (Anion/Solvent) ADP max/min Ratio 4.5 prolat

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C01E Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C20 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C019 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C01I Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N14 0.101 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N01G 0.128 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 2.296 Check

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note

1 1 0, 2 0 0, 3 1 0, -3 1 1, -1 1 1, 1 1 1,
-2 0 2, 0 0 2,

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report

5 1 0, -11 1 1, 0 2 1, -4 0 2, -3 1 2, -1 1 2,
2 0 2, -3 1 3, -4 0 4, -4 0 6,

PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

-8 0 4,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.33Ang From S6 1.85 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.47Ang From S6 1.61 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From S6 -2.37 eA-3



Alert level G

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 ... 0.250 Check

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.10 Why ?

PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note

PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check

Na4A Na4B N9 C17 C28 N10 N18 C01M
C22 N11 C25 C23 C26 C21 C24 N12
C18 C27

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 67% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 67% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 33% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 33% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14) 100% Note

PLAT432_ALERT_2_G Short Inter X...Y Contact N9 ..C25 . 2.99 Ang.

PLAT432_ALERT_2_G	Short Inter X...Y Contact	C17	x,y,z =	1_555	Check
			..C25	.	3.06 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C21	x,y,z =	1_555	Check
			..C23	.	3.08 Ang.
			x,-y,-1/2+z =	6_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		11	Note
	Pr01	N00G	N013	C018	C019
	C01I	C01L	C01M	C01A	C01E
					N01G
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#		7	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr01	(III)	.	3.29	Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers			5	Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		82	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			7	Note
	1 1 1, -2 0 2, -4 0 6, -4 0 4, 5 1 0, -3 1 3,				
	-11 1 1,				
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.660	Note
	Predicted wR2: Based on SigI**2	2.68	or SHELX Weight	6.61	

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

4 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
 4 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

