

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cm_mnt_2_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: cm_mnt_2_0m

Bond precision:	C-C = 0.0050 A	Wavelength=0.71073
Cell:	a=36.2631 (14) alpha=90	b=13.4983 (5) beta=108.573 (2) c=19.4223 (8) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	9011.9 (6)	9011.9 (6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 Cm4 N32 S32, C3 N1.50, 16(C2 N), 2(C N1.33), 4(C1.15 N0.40)	C27.25 Cm N13.792 Na5 S8
Sum formula	C109 Cm4 N55.17 Na20 S32	C27.25 Cm N13.79 Na5 S8
Mr	4543.93	1135.92
Dx, g cm-3	1.675	1.674
Z	2	8
Mu (mm-1)	2.265	2.265
F000	4312.3	4312.0
F000'	4263.42	
h, k, lmax	60, 22, 32	60, 22, 32
Nref	21984	21956
Tmin, Tmax	0.642, 0.797	0.646, 0.747
Tmin'	0.629	

Correction method= # Reported T Limits: Tmin=0.646 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta (max)= 36.400

R(reflections)= 0.0322(18441)

wR2(reflections)=
0.0783(21956)

S = 1.036

Npar= 591

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 Cm4 N32 S32, C3 N1.50, 16(C2 N), 2(C N1.33), 4(C1.15 N0.
Rep.: C27.25 Cm N13.792 Na5 S8

PLAT214_ALERT_2_C Atom C24 (Anion/Solvent) ADP max/min Ratio 4.2 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 N013 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C017 Check

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

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N10 0.117 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N013 0.160 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N00Q 0.104 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N014 0.148 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C19 0.133 Check

PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for C21 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

-3 1 1, 1 1 1, -8 0 2, -2 0 2, 0 0 2, -3 1 3,
-4 0 4,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.62Ang From Cm01 2.44 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From Na4A 1.77 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From Cm01 1.69 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Na5 1.53 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.30Ang From Na4A -1.76 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Na4A 1.49 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Cm01 1.24 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Na5 1.06 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From C27 . 1.05 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From C19 . 1.03 eA-3



Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 4 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 ... 0.250 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 31.56 Why ?

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

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check

C18 C22 C23 C25 N01F N01G C01A C01B

C19 Na4A Na4B

PLAT300_ALERT_4_G Atom Site Occupancy of N10 Constrained at 0.75 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C21 Constrained at 0.75 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C24 Constrained at 0.375 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of N17	Constrained at	0.6666	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N33	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N9	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N11	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20	Constrained at	0.35	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1B	Constrained at	0.25	Check
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)		67%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 8)		100%	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 11)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 14)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 15)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 17)		100%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact N17 ..C19	.	2.48	Ang.
	x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact N17 ..C19	.	2.48	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C019 ..C18	.	2.81	Ang.
	x,1-y,-1/2+z =		6_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C01D ..C18	.	2.75	Ang.
	x,1-y,-1/2+z =		6_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C01E ..C19	.	1.90	Ang.
	x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C01E ..C19	.	1.90	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..N33	.	1.73	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..N11	.	2.56	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..C20	.	2.71	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..N33	.	3.01	Ang.
	x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C25 ..C26	.	2.98	Ang.
	x,1-y,1/2+z =		6_566	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C27 ..C20	.	1.81	Ang.
	x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C27 ..N11	.	2.96	Ang.
	x,y,z =		1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		13	Note
	Cm01 N00Q N013 N014 C017 C018 C019 C01A			
	C01D C01E N01F N01G C01B			
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C01E --C19		1.90	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C01E --C19		1.90	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C27 --C20		1.80	Ang.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		6	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		5	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		24	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
	1 1 0, 2 0 0,			

PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	19	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		4	Note
	1 1 1, -4 0 4, -8 0 2, -3 1 3,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.3	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		1.910	Note
	Predicted wR2: Based on SigI**2	4.11 or SHELX Weight	7.56	
PLAT983_ALERT_1_G	The Cm-f"=	4.8980 Deviates from IT-Value =	4.6980	Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
35 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
36 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.

