

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) eumnt_030121_nbb_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: eumnt_030121_nbb_0m

Bond precision:	C-C = 0.0091 A	Wavelength=0.71073	
Cell:	a=36.199 (2)	b=13.5964 (8)	c=19.4534 (10)
	alpha=90	beta=108.732 (2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	9067.4 (9)	9067.3 (9)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C64 Eu4 N32 S32, 22 (C2 N), 2 (C3 N), 20 (Na)	C27 Eu N13.5 Na5 S8, C1.5 N0.5	
Sum formula	C114 Eu4 N56 Na20 S32	C28.50 Eu N14 Na5 S8	
Mr	4247.30	1061.82	
Dx, g cm-3	1.556	1.556	
Z	2	8	
Mu (mm-1)	1.839	1.839	
F000	4120.0	4120.0	
F000'	4128.47		
h,k,lmax	44,16,23	44,16,23	
Nref	8630	8601	
Tmin,Tmax	0.699,0.832	0.656,0.745	
Tmin'	0.685		

Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.701

R(reflections)= 0.0271 (8047)

wR2(reflections)=
0.0753 (8601)

S = 1.045

Npar= 585

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 Eu4 N32 S32, 22(C2 N), 2(C3 N), 20(Na)	
	Rep.: C27 Eu N13.5 Na5 S8, C1.5 N0.5	
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C01C Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C019 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N00X Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C01J Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C018 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C01A Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N00X	0.116 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N01G	0.181 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00912 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	9 Note
	1 1 0, 2 0 0, 3 1 0, 4 0 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	14 Report
	0 2 0, 8 2 0, 9 3 1, -10 2 2, 2 0 2, -39 1 15,	
	-38 0 16, -38 2 16, -36 0 16, -37 1 17, -37 3 17, -36 2 18,	
	-33 3 19, -28 0 20,	
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
	-42 0 10,	
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From C17	0.70 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From C01C	0.52 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From C01F	0.47 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.07Ang From C019	0.40 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.53Ang From C23	-0.60 eA-3

Alert level G

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 ...	0.250 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	35.32 Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a Note
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	4 Report
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at	0.5 Check
	C017 C0 C19 C20 N9 C17 N10 N21	
	C01I C18 C01E C21	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	67% 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 12)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 14)	100% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact N21 ..C17	2.96 Ang.
	x,y,z = 1_555 Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact C017 ..C01A	3.11 Ang.
	x,1-y,-1/2+z = 6_565 Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact C017 ..C01K	3.16 Ang.

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.

