

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mm2

Bond precision: C-C = 0.0043 Å

Wavelength=0.71073

Cell: a=16.5928(8) b=11.8192(4) c=19.0005(8)
 alpha=90 beta=111.772(5) gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	3460.5(3)	3460.5(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	C36 H56 Fe N3 Na O Zn	C36 H56 Fe N3 Na O Zn
Sum formula	C36 H56 Fe N3 Na O Zn	C36 H56 Fe N3 Na O Zn
Mr	691.07	691.05
Dx, g cm ⁻³	1.327	1.326
Z	4	4
Mu (mm ⁻¹)	1.157	1.157
F000	1472.0	1472.0
F000'	1474.97	
h,k,lmax	21,15,25	21,15,25
Nref	8345	8165
Tmin,Tmax	0.891,0.891	0.896,1.000
Tmin'	0.891	

Correction method= MULTI-SCAN

Data completeness= 0.978

Theta(max)= 28.000

R(reflections)= 0.0464(4235)

wR2(reflections)= 0.0771(8165)

S = 0.787

Npar= 395

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

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00

Goodness of fit given = 0.787

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full Low 0.98

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.11 Ratio



Alert level G

PLAT301_ALERT_3_G Note: Main Residue Disorder	16.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	14
PLAT793_ALERT_4_G The Model has Chirality at C9 (Verify)	S
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!

0 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

3 **ALERT level C** = Check and explain

4 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 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

1 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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 31/03/2010; check.def file version of 22/03/2010

