

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) polyIII_11s_sk36_pmdi12melt_0s

No syntax errors found. CIF dictionary Interpreting this report

Datablock: polyIII_11s_sk36_pmdi12melt_0s

Bond precision: C-C = 0.0052 A

Wavelength=0.71073

Cell: a=8.1128(9) b=11.0482(11) c=17.788(2)
 alpha=89.267(4) beta=79.228(4) gamma=78.377(4)
Temperature: 173 K

	Calculated	Reported
Volume	1533.7(3)	1533.7(3)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C34 H48 N2 O4	C34 H48 N2 O4
Sum formula	C34 H48 N2 O4	C34 H48 N2 O4
Mr	548.74	548.74
Dx,g cm-3	1.188	1.188
Z	2	2
Mu (mm-1)	0.077	0.077
F000	596.0	596.0
F000'	596.25	
h,k,lmax	9,13,21	9,13,21
Nref	5402	5377
Tmin,Tmax	0.992,0.995	
Tmin'	0.983	

Correction method= Not given

Data completeness= 0.995

Theta(max)= 25.000

R(reflections)= 0.0488(1928)

wR2(reflections)= 0.1359(5377)

S = 0.678

Npar= 361

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 B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low

36 Perc.



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 = 0.678
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0052 Ang
 PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 1
 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 24



Alert level G

PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00400 Deg.

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 1 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
 0 ALERT type 4 Improvement, methodology, query or suggestion
 0 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*, 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.

