checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: SQ13se_PA

Bond precision: C-C = 0.0090 AWavelength=1.54175 a=16.37064(12) b=10.00640(6) Cell: c=7.27971(3)beta=98.8213(5) alpha=90 gamma=90 293 K Temperature: Calculated Reported Volume 1178.392(12) 1178.392(12)Space group P 21/c P 21/c Hall group -P 2ybc -P 2ybc Moiety formula C22 H32 N4 O6 C22 H32 N4 O6 Sum formula C22 H32 N4 O6 C22 H32 N4 O6 448.52 448.00 Mr 1.264 0.000 Dx,g cm-3 Ζ 2 2 Mu (mm-1) 0.766 0.000 F000 480.0 0.0 F000′ 481.55 h,k,lmax 12,7,5 509 Nref Tmin,Tmax Tmin' Correction method= Not given Data completeness= 0.000 Theta(max)= R(reflections) = wR2(reflections)= S = Npar=

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 A

Alert level C REFI015_ALERT_1_A _refine_ls_shift/su_max is missing Maximum shift/s.u. ratio after final refinement cycle. The following tests will not be performed SHFSU_01

PLAT142_ALERT_4_C	su on b - A	xis Sma	all or M	lissing	ı		 0.00006	Ang.
PLAT143_ALERT_4_C	su on c - A	xis Sma	all or M	lissing	ı		 0.00003	Ang.
PLAT340_ALERT_3_C	Low Bond Pre	ecisior	n on C-	C Bond	ls		 0.0090	Ang
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C1	-	Н4	 1.14	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C1	-	Н5	 1.13	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C7	-	Н8	 1.15	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C7	-	Н9	 1.12	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C10	-	H11	 1.16	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C10	-	H12	 1.15	Ang.
PLAT351_ALERT_3_C	Long C-H	Bond ((0.96A)	C13	-	H14	 1.13	Ang.
PLAT353_ALERT_3_C	Long N-H	Bond ((0.87A)	N16	-	H17	 1.05	Ang.
PLAT390_ALERT_3_C	Deviating M	ethyl (227	Х-С-Н	Bond	Angle	 118	Deg.
PLAT390_ALERT_3_C	Deviating M	ethyl (227	Х-С-Н	Bond	Angle	 103	Deg.
PLAT411_ALERT_2_C	Short Inter	НН	Contact	. н9		H11	 2.03	Ang.
PLAT413_ALERT_2_C	Short Inter	ХНЗ	. XHn	Н29		Н30	 2.11	Ang.

Alert level G		
PLAT007_ALERT_5_G Note: Number	of Unrefined D-H Atoms	1
PLAT343_ALERT_2_G Check sp3	Angle Range in Main Residue for	C2
PLAT343_ALERT_2_G Check sp3	Angle Range in Main Residue for	C25
PLAT860_ALERT_3_G Note: Number	of Least-Squares Restraints	87
PLAT950_ALERT_5_G Reported and	Calculated Hmax Values Differ by	12
PLAT951_ALERT_5_G Reported and	Calculated Kmax Values Differ by	7
PLAT952_ALERT_5_G Reported and	Calculated Lmax Values Differ by	5
PLAT982_ALERT_1_G The C-f'=	0.017 Deviates from the IT-value	0.018
PLAT982_ALERT_1_G The N-f'=	0.029 Deviates from the IT-value	0.031
PLAT982_ALERT_1_G The O-f'=	0.047 Deviates from the IT-value	0.049
PLAT983_ALERT_1_G The C-f"=	0.009 Deviates from the IT-Value	0.009
PLAT983_ALERT_1_G The O-f"=	0.032 Deviates from the IT-Value	0.032

1 ALERT level A = Most likely a serious problem - resolve or explain 0 ALERT level B = A potentially serious problem, consider carefully 15 ALERT level C = Check. Ensure it is not caused by an omission or oversight 12 ALERT level G = General information/check it is not something unexpected 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 4 ALERT type 2 Indicator that the structure model may be wrong or deficient 12 ALERT type 3 Indicator that the structure quality may be low 2 ALERT type 4 Improvement, methodology, query or suggestion

4 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.

PLATON version of 04/07/2012; check.def file version of 28/06/2012

