



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx_

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: shelx_

Bond precision:	C-C = 0.0154 Å	Wavelength=0.71073
Cell:	a=11.820 (2) alpha=90	b=19.070 (4) beta=106.80 (3) c=19.350 (4) gamma=90
Temperature:	297 K	
	Calculated	Reported
Volume	4175.5 (16)	4175.5 (16)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H17 F18 N4 O7 Sm	?
Sum formula	C33 H17 F18 N4 O7 Sm	C33 H17 F18 N4 O7 Sm
Mr	1073.87	1073.85
Dx, g cm ⁻³	1.708	1.708
Z	4	4
Mu (mm ⁻¹)	1.535	1.535
F000	2092.0	2092.0
F000'	2093.10	
h, k, lmax	15, 24, 25	15, 24, 25
Nref	9606	9567
Tmin, Tmax	0.732, 0.770	0.730, 0.780
Tmin'	0.717	

Correction method= # Reported T Limits: Tmin=0.730 Tmax=0.780
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 27.497

R(reflections)= 0.0584(4086)

wR2(reflections)=
0.1793(9567)

S = 0.984

Npar= 577

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

PLAT234_ALERT_4_B	Large	Hirshfeld Difference F10	--C28	.	0.28 Ang.
PLAT234_ALERT_4_B	Large	Hirshfeld Difference F17B	--C33	.	0.26 Ang.
PLAT241_ALERT_2_B	High	MainResAtom Ueq as Compared to Neighbours			F13 Check
PLAT241_ALERT_2_B	High	MainResAtom Ueq as Compared to Neighbours			F18 Check



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.124

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 43% Check

PLAT201_ALERT_2_C Isotropic non-H Atoms in Main Residue(s) Occ>0.5 4 Report

F13	F18	C23	C29														
PLAT213_ALERT_2_C	Atom F1	has ADP max/min Ratio	3.3 prolat														
PLAT213_ALERT_2_C	Atom F3	has ADP max/min Ratio	3.9 prolat														
PLAT213_ALERT_2_C	Atom F12	has ADP max/min Ratio	3.3 prolat														
PLAT213_ALERT_2_C	Atom F14B	has ADP max/min Ratio	3.1 prolat														
PLAT213_ALERT_2_C	Atom F17	has ADP max/min Ratio	3.1 prolat														
PLAT234_ALERT_4_C	Large	Hirshfeld Difference C8	--C9 . 0.18 Ang.														
PLAT234_ALERT_4_C	Large	Hirshfeld Difference C25	--C26 . 0.19 Ang.														
PLAT234_ALERT_4_C	Large	Hirshfeld Difference C32	--C33 . 0.25 Ang.														
PLAT241_ALERT_2_C	High	MainResAtom Ueq as Compared to Neighbours	O2 Check														
PLAT241_ALERT_2_C	High	MainResAtom Ueq as Compared to Neighbours	C17 Check														
PLAT241_ALERT_2_C	High	MainResAtom Ueq as Compared to Neighbours	C21 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	Sm1 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C13 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C20 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C22 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C25 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C27 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C30 Check														
PLAT242_ALERT_2_C	Low	MainResAtom Ueq as Compared to Neighbours	C32 Check														
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	Sm1 0.129 Check														
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds	0.01541 Ang.														
PLAT767_ALERT_4_C	INS	Embedded LIST 6 Instruction Should be LIST 4	Please Do														
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	35 Report														
2	0	0,	4	0	0,	6	0	0,	2	1	0,	3	1	0,	4	1	0,
5	1	0,	6	1	0,	7	1	0,	0	2	0,	3	2	0,	4	2	0,
5	2	0,	6	2	0,	-9	0	1,	-7	0	1,	-5	0	1,	-3	0	1,

-9 1 1, -8 1 1, -7 1 1, -6 1 1, -5 1 1, -4 1 1,
 -3 1 1, -8 8 1, -10 0 2, -8 0 2, -6 0 2, -4 0 2,
 (5 More NOT listed: see .ckf listing file)

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
	H3A		
PLAT020_ALERT_3_G	The Reported Value of Rint is Greater Than 0.12	0.124	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	4	Note
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F17 --C33 .	6.5	s.u.
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C19	Check
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C23	Check
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C24	Check
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C28	Check
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C29	Check
PLAT242_ALERT_2_G	Low MainResAtom Ueq as Compared to Neighbours	C33	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
	H00S		
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	43.90	Deg.
	C29 -F13 -F15 1_555 1_555 1_555 #	40	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Sm1 (III) .	3.55	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min)[Deg]=	2.11	Note
	1 1 0, -1 0 1, 0 1 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	55.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.616	Note
	Predicted wR2: Based on SigI**2 3.88 or SHELX Weight 18.22	Note	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 26 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 29 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
 4 ALERT type 5 Informative message, check
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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

Datablock shelx_ - ellipsoid plot

