No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: shelx

Bond precision: Ag-Ag = 0.0030 A Wavelength=0.71073
Cell: a=4.6066(19) b=16.031(7) c=18.594(8)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1373.1(10)	1373.1(10)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C 2c 2
Moiety formula	Ag6 Nd4 Te10, 2(Rb)	?
Sum formula	Ag6 Nd4 Rb2 Te10	Ag3 Nd2 Rb Te5
Mr	2671.12	1335.56
Dx,g cm-3	6.461	6.461
Z	2	4
Mu (mm-1)	25.513	25.513
F000	2232.0	2232.0
F000'	2206.58	
h,k,lmax	5,19,22	5,19,22
Nref	761	762
Tmin,Tmax	0.097,0.078	0.121,0.746
Tmin'	0.062	

Correction method= # Reported T Limits: Tmin=0.121
Tmax=0.746 AbsCorr = MULTI-SCAN
Data completeness= 1.001 Theta(max)= 25.666
R(reflections)= 0.0662(716) wR2(reflections)= 0.1576(762)
S = 1.148 Npar= 37

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

PLAT213_ALERT_2_A Atom Nd1 has ADP max/min Ratio ..... 5.4 oblate

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -6.839
Test value = -6.000
PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -6.84 eA-3

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT213_ALERT_2_C Atom Te3 has ADP max/min Ratio ..... 3.2 oblate
PLAT213_ALERT_2_C Atom Te4 has ADP max/min Ratio ..... 4.0 oblate
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.15 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Nd1 (III) . 2.83 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

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

```
5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
3 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

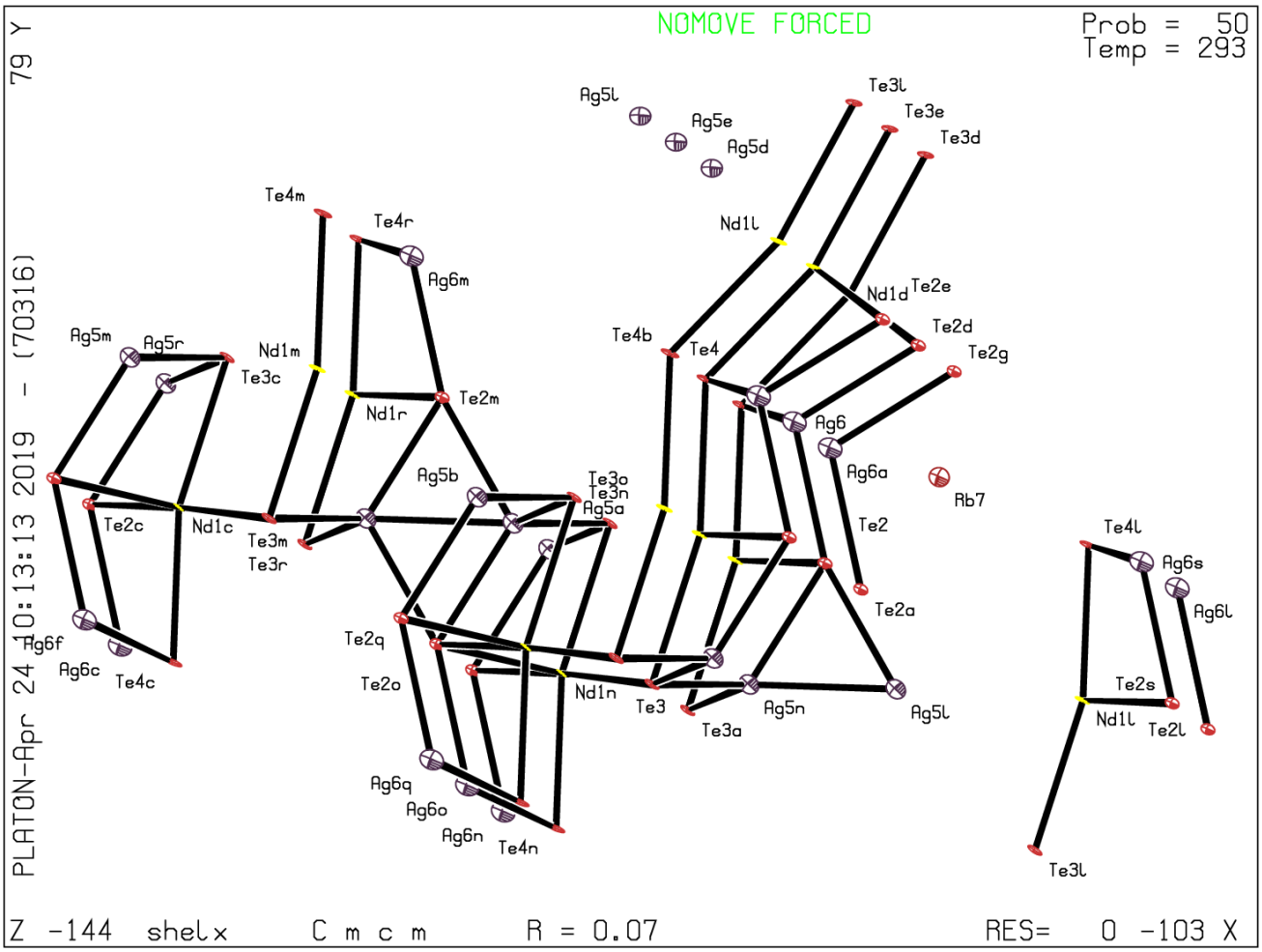
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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.

PLATON version of 17/03/2019; check.def file version of 04/03/2019

Datablock shelx - ellipsoid plot



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