

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_-143\_urac\_130k

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: UA\_-143\_urac\_130k

---

Bond precision:    C-C = 0.0040 Å                      Wavelength=1.54184

Cell:                      a=6.2352(5)              b=7.2756(6)              c=13.1328(11)  
                            alpha=90              beta=90.710(8)              gamma=90  
Temperature:              130 K

	Calculated	Reported
Volume	595.72(8)	595.72(8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.875	1.875
Z	4	4
Mu (mm-1)	1.381	1.381
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,8,16	7,8,16
Nref	1129	1122
Tmin,Tmax	0.902,0.963	0.923,1.000
Tmin'	0.902	

Correction method= # Reported T Limits: Tmin=0.923 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 0.994                      Theta(max)= 69.935

R(reflections)= 0.0550( 979)                      wR2(reflections)= 0.1776( 1122)

S = 1.123                      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

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

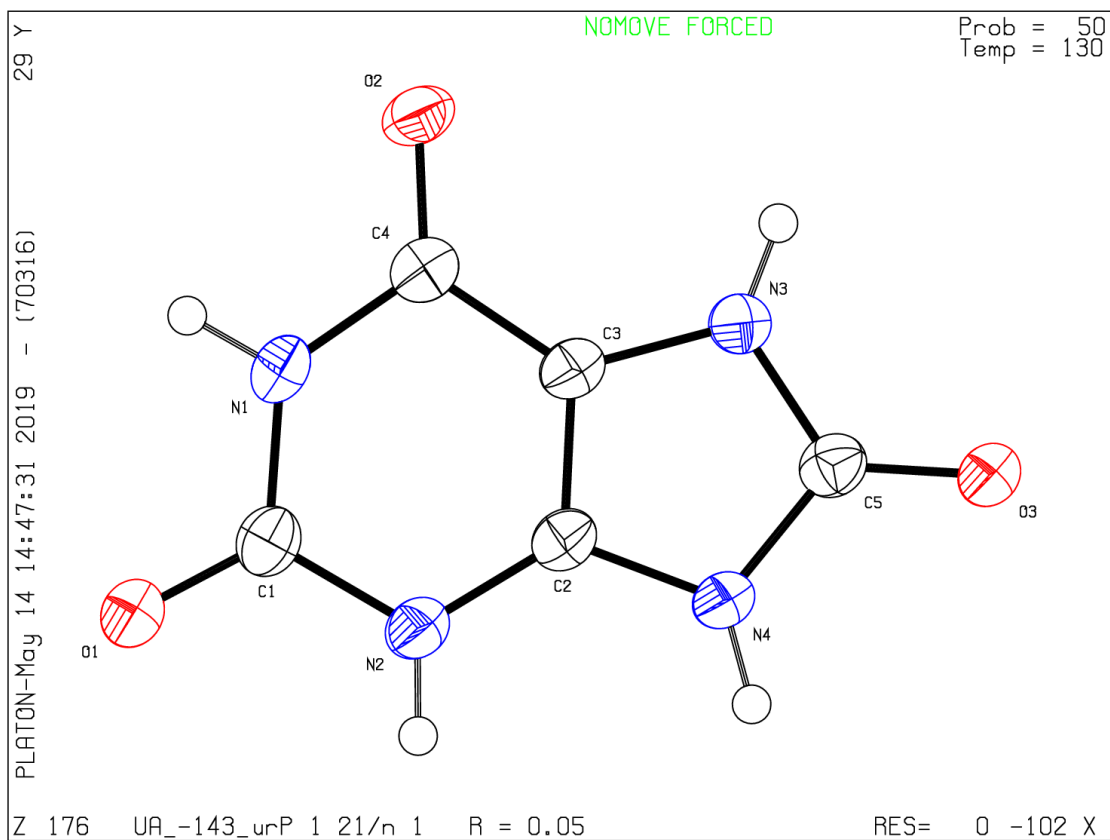
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_-100\_urac\_173k

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: UA\_-100\_urac\_173k

---

Bond precision:	C-C = 0.0040 A	Wavelength=1.54184
Cell:	a=6.2288(4)	b=7.3113(5)      c=13.1274(8)
	alpha=90	beta=90.632(6)      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	597.79(7)	597.79(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.868	1.868
Z	4	4
Mu (mm-1)	1.376	1.376
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,8,16	7,8,16
Nref	1135	1121
Tmin,Tmax	0.902,0.964	0.920,1.000
Tmin'	0.902	

Correction method= # Reported T Limits: Tmin=0.920 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.988      Theta(max)= 69.997

R(reflections)= 0.0556( 991)      wR2(reflections)= 0.1751( 1121)

S = 1.111      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

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

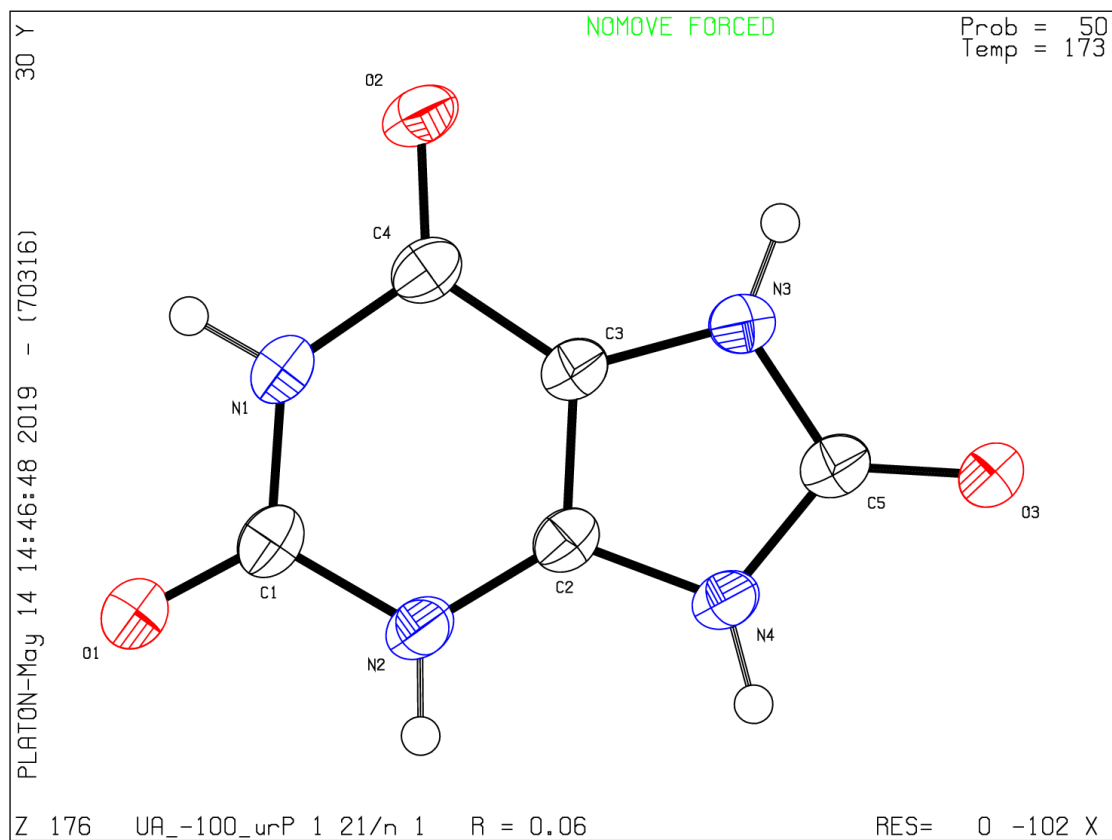
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_-60\_urac\_213k

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: UA\_-60\_urac\_213k

---

Bond precision:	C-C = 0.0040 A	Wavelength=1.54184
Cell:	a=6.2182(4)	b=7.3530(5)      c=13.1232(8)
	alpha=90	beta=90.519(6)      gamma=90
Temperature:	213 K	
	Calculated	Reported
Volume	600.00(7)	600.00(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.861	1.861
Z	4	4
Mu (mm-1)	1.371	1.371
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,8,15	7,8,15
Nref	1134	1118
Tmin,Tmax	0.902,0.964	0.954,1.000
Tmin'	0.902	

Correction method= # Reported T Limits: Tmin=0.954 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.986      Theta(max)= 69.999

R(reflections)= 0.0526( 990)      wR2(reflections)= 0.1660( 1118)

S = 1.068      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law [ 0 0 1] Est.d BASF 0.10 Check  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 5 **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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 1 ALERT type 4 Improvement, methodology, query or suggestion  
 2 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.

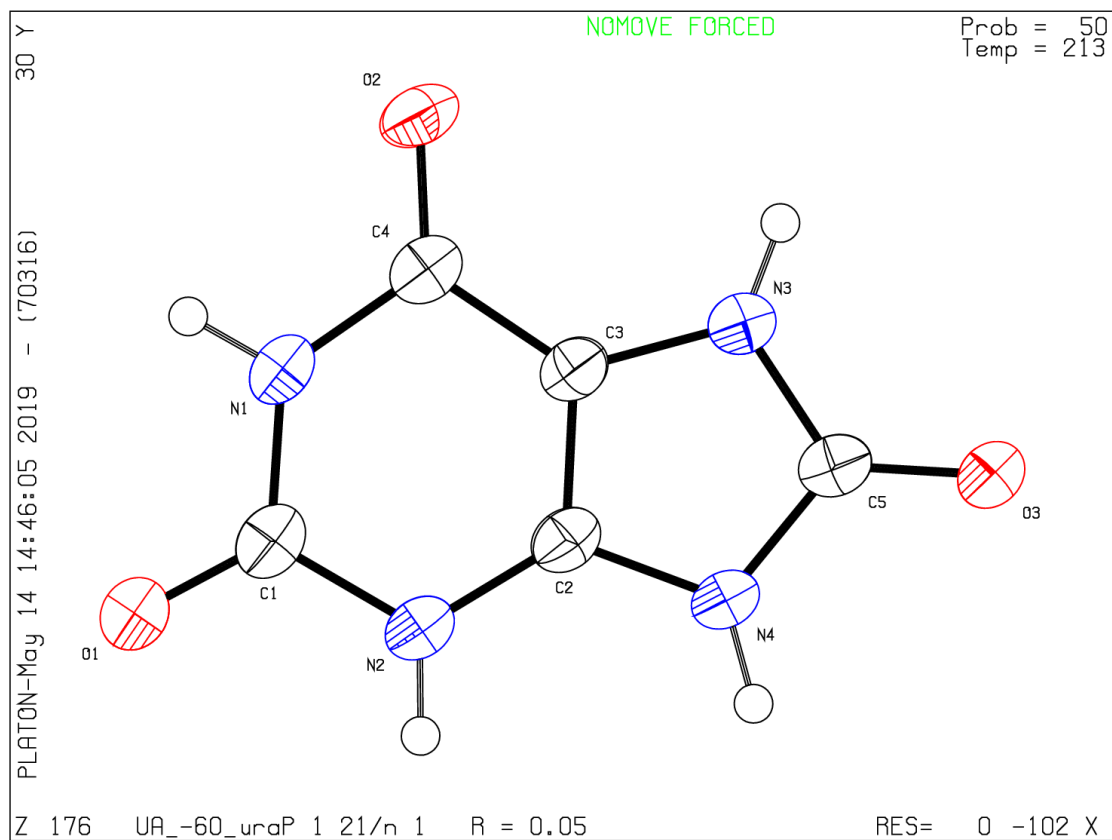
### Publication of your CIF in IUCr journals

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.





# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_-30\_urac\_243k

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: UA\_-30\_urac\_243k

---

Bond precision:	C-C = 0.0040 A	Wavelength=1.54184
Cell:	a=6.2110(4)	b=7.3857(5)      c=13.1213(8)
	alpha=90	beta=90.447(6)      gamma=90
Temperature:	243 K	
	Calculated	Reported
Volume	601.89(7)	601.89(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.855	1.855
Z	4	4
Mu (mm-1)	1.366	1.366
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,9,15	7,8,15
Nref	1137	1122
Tmin,Tmax	0.903,0.964	0.978,1.000
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.978 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.987      Theta(max)= 69.967

R(reflections)= 0.0481( 1007)      wR2(reflections)= 0.1545( 1122)

S = 1.109      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law [ 0 0 1] Est.d BASF 0.09 Check  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 5 **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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 1 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

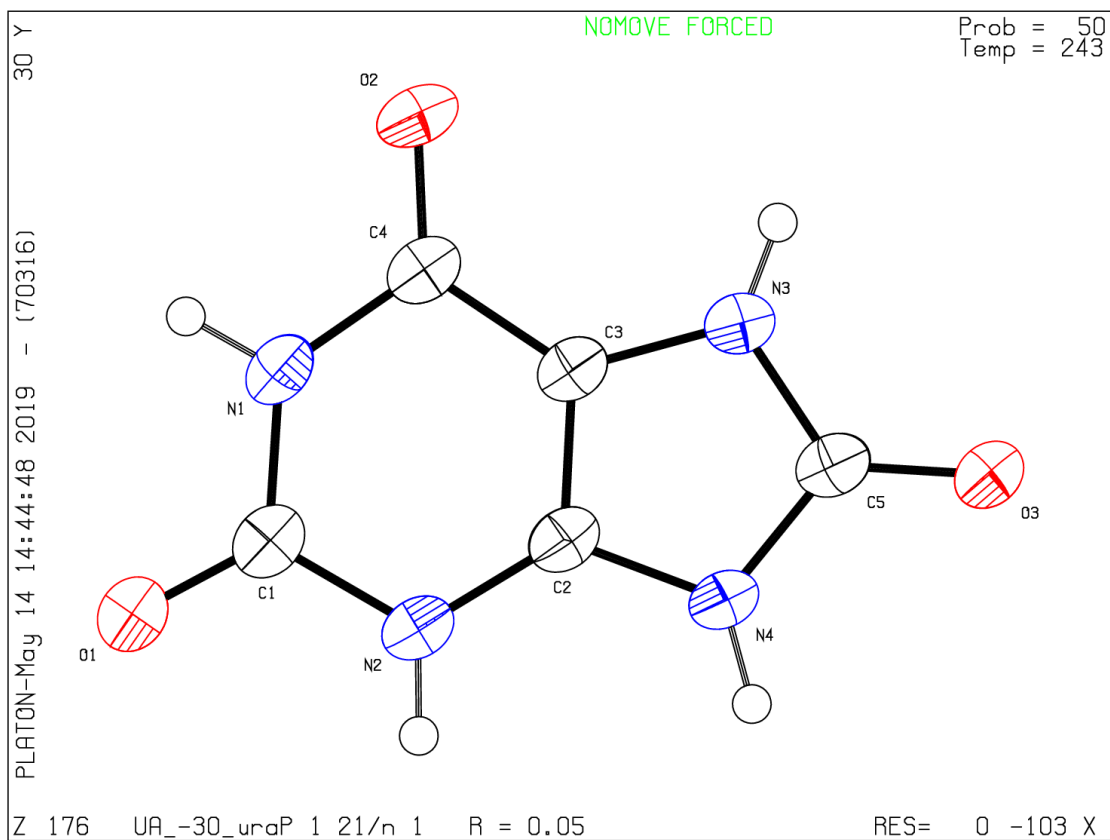
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_0\_urac\_273k

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: UA\_0\_urac\_273k

---

Bond precision:    C-C = 0.0040 Å                      Wavelength=1.54184

Cell:                      a=6.2025(4)              b=7.4163(5)              c=13.1147(8)  
                            alpha=90              beta=90.378(6)              gamma=90

Temperature:              273 K

	Calculated	Reported
Volume	603.26(7)	603.26(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.851	1.851
Z	4	4
Mu (mm-1)	1.363	1.363
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,9,15	7,8,15
Nref	1139	1120
Tmin,Tmax	0.903,0.964	0.970,1.000
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.970 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.983                      Theta(max)= 69.854

R(reflections)= 0.0462( 999)                      wR2(reflections)= 0.1409( 1120)

S = 1.093                      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 273 Check  
 PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 273 Check  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law ( 1 0 0 ) Est.d BASF 0.10 Check  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 7 **ALERT level G** = General information/check it is not something unexpected
- 3 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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 1 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

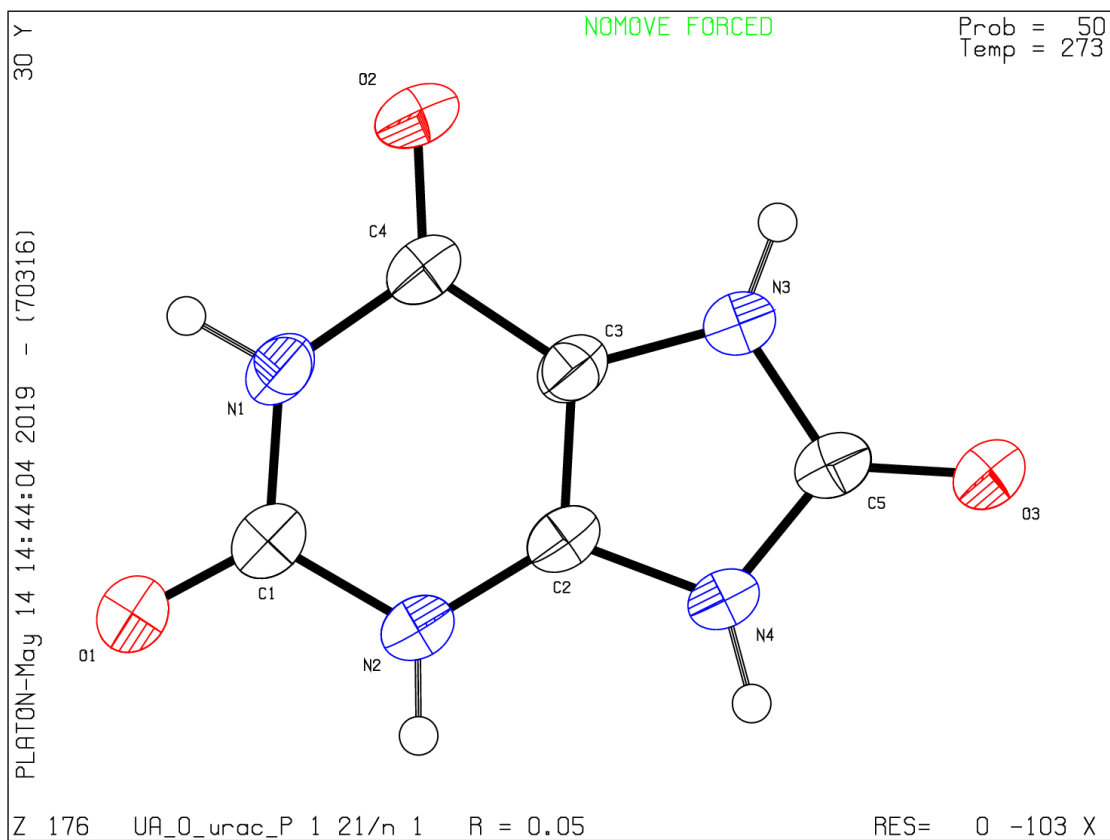
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_30\_urac\_303k

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: UA\_30\_urac\_303k

---

Bond precision:	C-C = 0.0030 A	Wavelength=1.54184
Cell:	a=6.1963(3)	b=7.4512(4)      c=13.1114(7)
	alpha=90	beta=90.282(5)      gamma=90
Temperature:	303 K	
	Calculated	Reported
Volume	605.34(5)	605.34(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.845	1.845
Z	4	4
Mu (mm-1)	1.359	1.359
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,9,15	7,9,15
Nref	1143	1125
Tmin,Tmax	0.903,0.964	0.974,1.000
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.974 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.984      Theta(max)= 69.957

R(reflections)= 0.0420( 1025)      wR2(reflections)= 0.1153( 1125)

S = 1.061      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report



### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note  
 PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law [ 0 0 1] Est.d BASF 0.11 Check  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 6 **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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 2 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

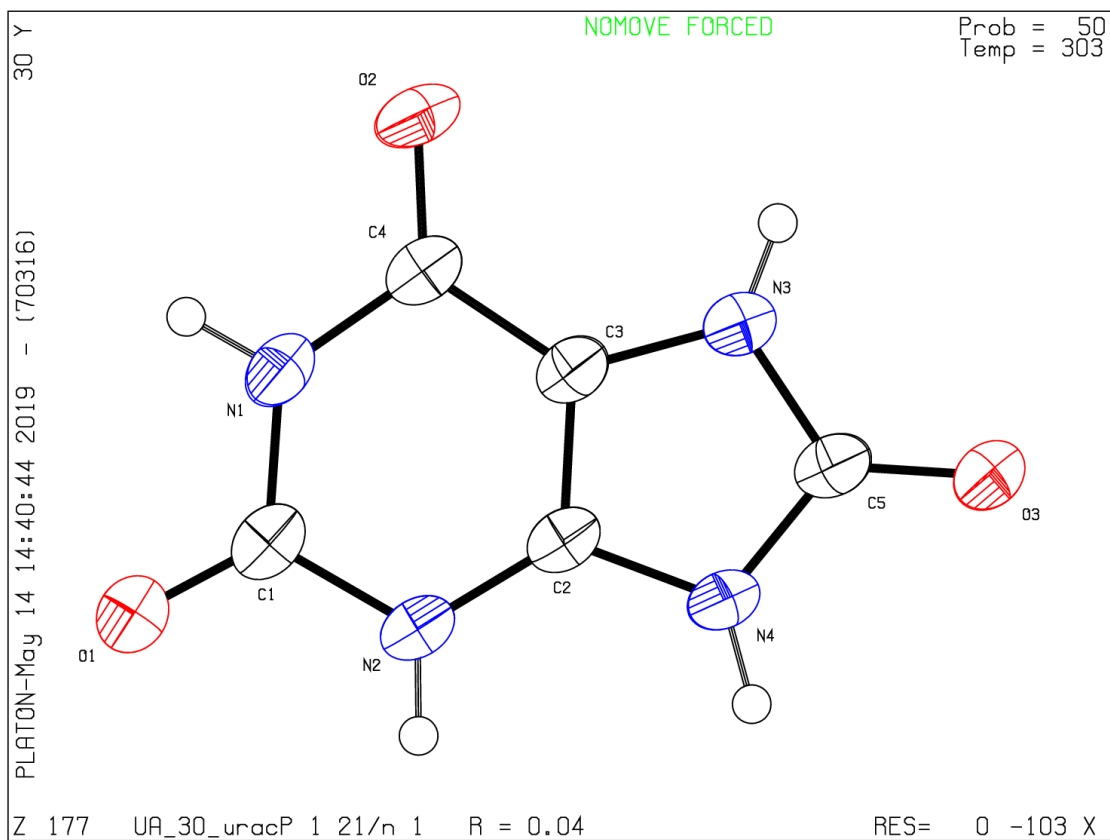
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UA\_60\_urac\_333k

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: UA\_60\_urac\_333k

---

Bond precision:	C-C = 0.0030 A	Wavelength=1.54184
Cell:	a=6.1898(3)	b=7.4857(4)      c=13.1103(5)
	alpha=90	beta=90.217(4)      gamma=90
Temperature:	333 K	
	Calculated	Reported
Volume	607.46(5)	607.46(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C5 H4 N4 O3	C5 H4 N4 O3
Sum formula	C5 H4 N4 O3	C5 H4 N4 O3
Mr	168.12	168.12
Dx,g cm-3	1.838	1.838
Z	4	4
Mu (mm-1)	1.354	1.354
F000	344.0	344.0
F000'	345.34	
h,k,lmax	7,9,15	7,9,15
Nref	1151	1131
Tmin,Tmax	0.903,0.964	0.988,1.000
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.988 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.983      Theta(max)= 69.945

R(reflections)= 0.0365( 1020)      wR2(reflections)= 0.0989( 1131)

S = 1.066      Npar= 111

---

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 16 Report



## Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
 PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed .. ! Info  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note  
 PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law [ 0 0 1] Est.d BASF 0.11 Check  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 6 **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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 2 ALERT type 4 Improvement, methodology, query or suggestion  
 2 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.

