

General Comments to CheckCIF Alerts

All alerts (A,B and C) can be explained due to High Pressure setup because the crystal is inside of a Diamond anvil cell (DAC). The opening angle of the DAC limit the number of total reflections measured in the experiment. The quality of data decrease when pressure increase and the ratio about number of reflections and number of parameters to refine is lower than in normal conditions.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CuBr-Quin_000GPa

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: CuBr-Quin_000GPa

Bond precision:	C-C = 0.0077 A	Wavelength=0.71073
Cell:	a=4.1080 (2)	b=17.6594 (7) c=13.6139 (9)
	alpha=90	beta=91.496 (6) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	987.28 (9)	987.28 (9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Sum formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Mr	417.05	417.05
Dx, g cm ⁻³	2.806	2.806
Z	4	4
Mu (mm ⁻¹)	12.355	12.355
F000	784.0	784.0
F000'	784.73	
h, k, lmax	5, 24, 18	5, 23, 17
Nref	2671	1974
Tmin, Tmax	0.481, 0.690	0.290, 0.734
Tmin'	0.176	

Correction method= # Reported T Limits: Tmin=0.290 Tmax=0.734
AbsCorr = GAUSSIAN

Data completeness= 0.739 Theta(max)= 29.163

R(reflections)= 0.0386 (1629)	wR2(reflections)= 0.0699 (1974)
S = 1.138	Npar= 127

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**

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.808 Why?

 **Alert level B**

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 341 Report

 **Alert level C**

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00771 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.323 Check

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br1 --Cu1 . 18.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br1 --Cu1_a . 40.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br1 --Cu2_c . 40.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2 --Cu2 . 26.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2 --Cu2_b . 39.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2 --Cu1_f . 47.2 s.u.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 337 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.2 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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
-

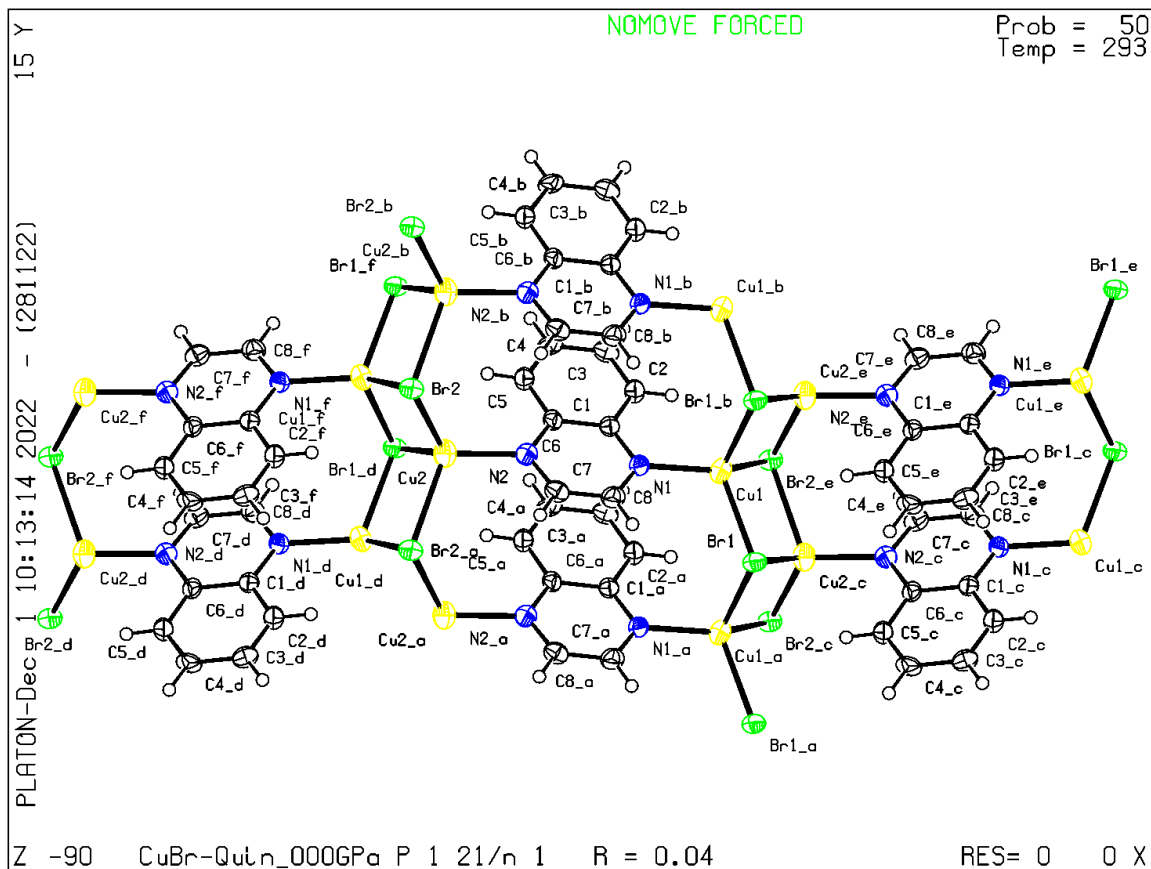
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0604( 478)      wR2(reflections)=
                                0.1688( 670)
S = 1.127                        Npar= 77
```

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.346 Why?

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.04429 Ang.

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.70 Note
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.030 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu2 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.399 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 96 Report

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.48 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 6 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 8 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.8 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 12 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 12 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

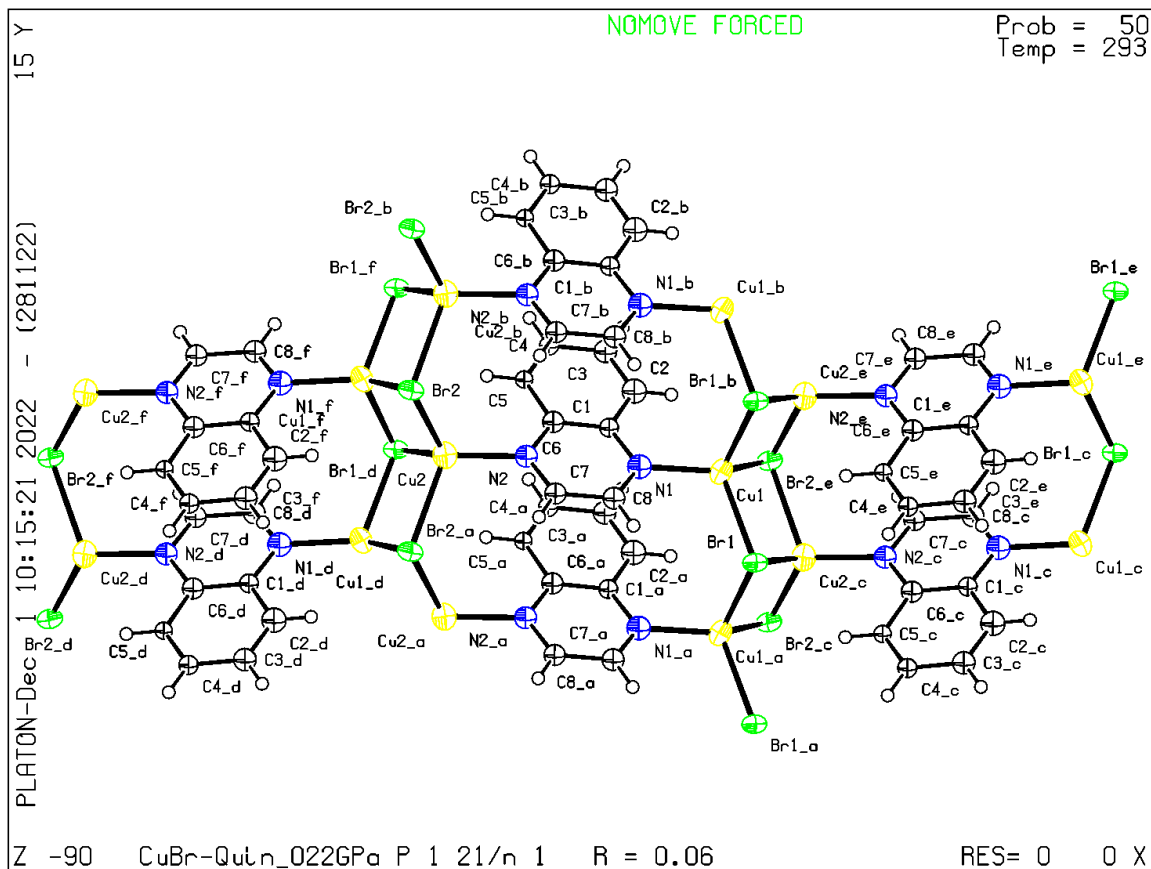
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



R(reflections)= 0.0347(530)	wR2(reflections)= 0.0824(651)
S = 1.233	Npar= 77

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**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.347 Why?

 **Alert level B**

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.02286 Ang.

 **Alert level C**

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.45 Note
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.017 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu2 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.344 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 102 Report

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br1 --Cu1_a . 5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2 --Cu1_f . 9.0 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.7 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 12 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 12 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

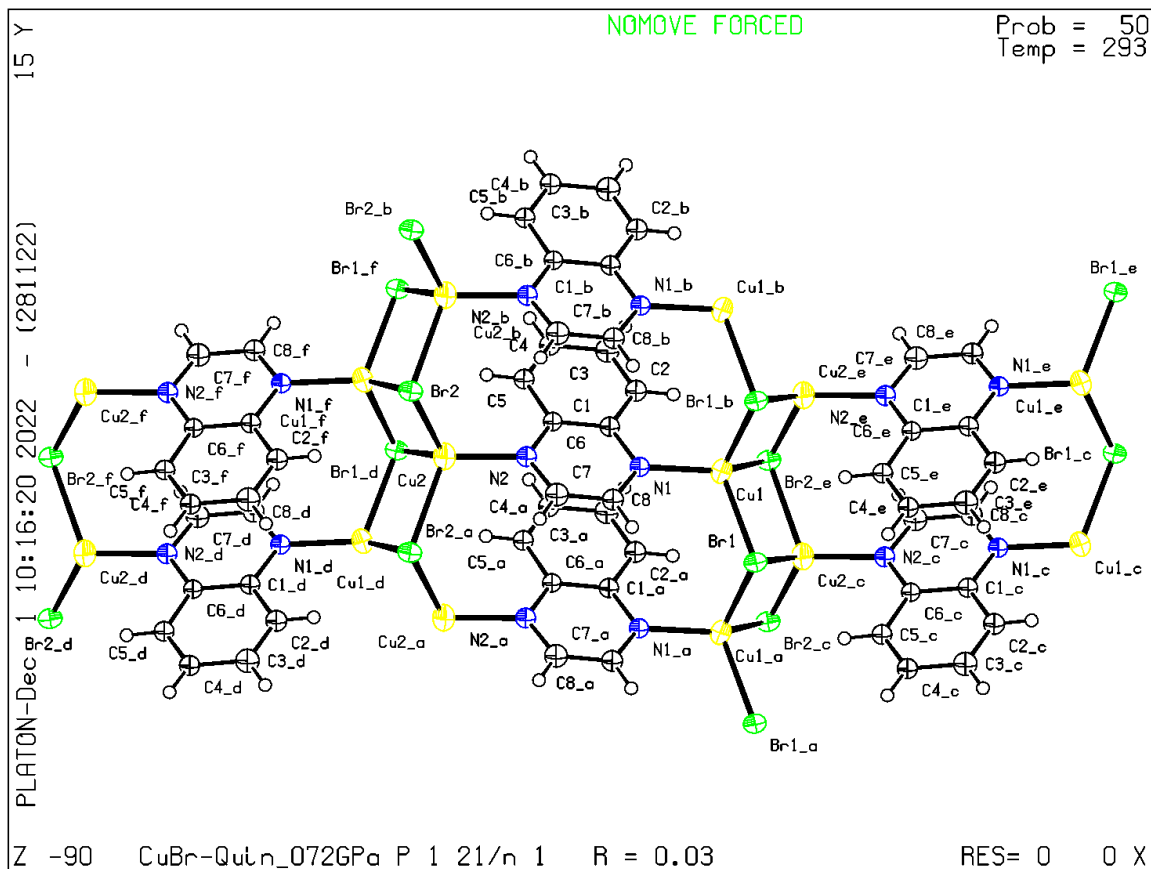
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0433( 525)      wR2(reflections)=
                                0.1070( 637)
S = 1.222                        Npar= 77
```

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.349 Why?

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.03086 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 250 Report

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.27 Note
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.020 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.574 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.95 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2 --Cu1_f . 5.2 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 17 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.1 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 11 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 11 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

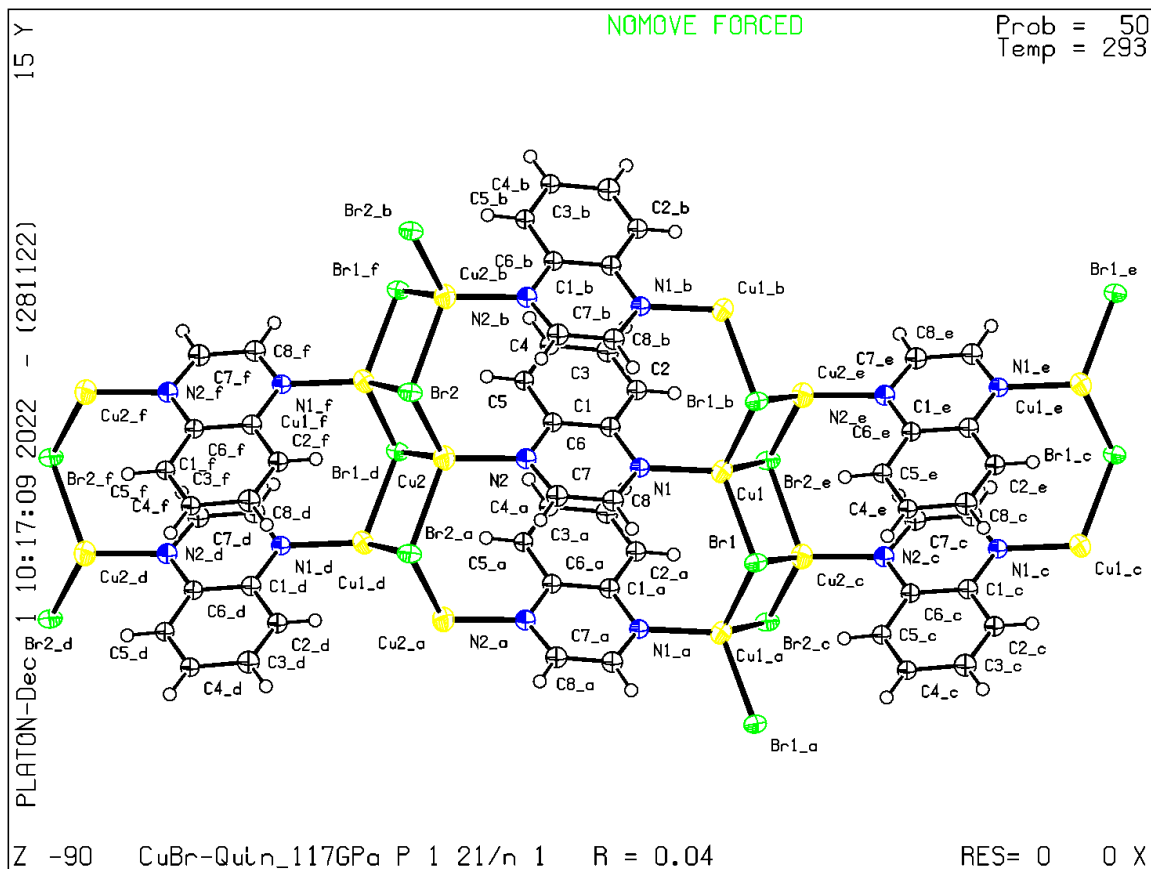
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_154GPa

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: CuBr-Quin_154GPa

Bond precision:	C-C = 0.0400 A	Wavelength=0.71073
Cell:	a=4.0491 (5)	b=17.356 (2) c=12.994 (19)
	alpha=90	beta=93.14 (3) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	911.8 (13)	911.8 (14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Sum formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Mr	417.05	417.05
Dx, g cm ⁻³	3.038	3.038
Z	4	4
Mu (mm ⁻¹)	13.378	13.377
F000	784.0	784.0
F000'	784.73	
h, k, lmax	5, 21, 16	5, 21, 5
Nref	1858	628
Tmin, Tmax	0.453, 0.626	0.254, 0.350
Tmin'	0.163	

Correction method= # Reported T Limits: Tmin=0.254 Tmax=0.350
AbsCorr = GAUSSIAN

Data completeness= 0.338 Theta(max)= 26.370

R(reflections)= 0.0489 (496)	wR2(reflections)= 0.1293 (628)
S = 1.228	Npar= 77

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.350 Why?

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.04 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 254 Report

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.16 Note
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.019 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.95 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C1 -C6 0.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Br2 ..C7 . 3.34 Ang.
 2-x,1-y,2-z = 3_767 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 15 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.1 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 11 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 11 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 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
-

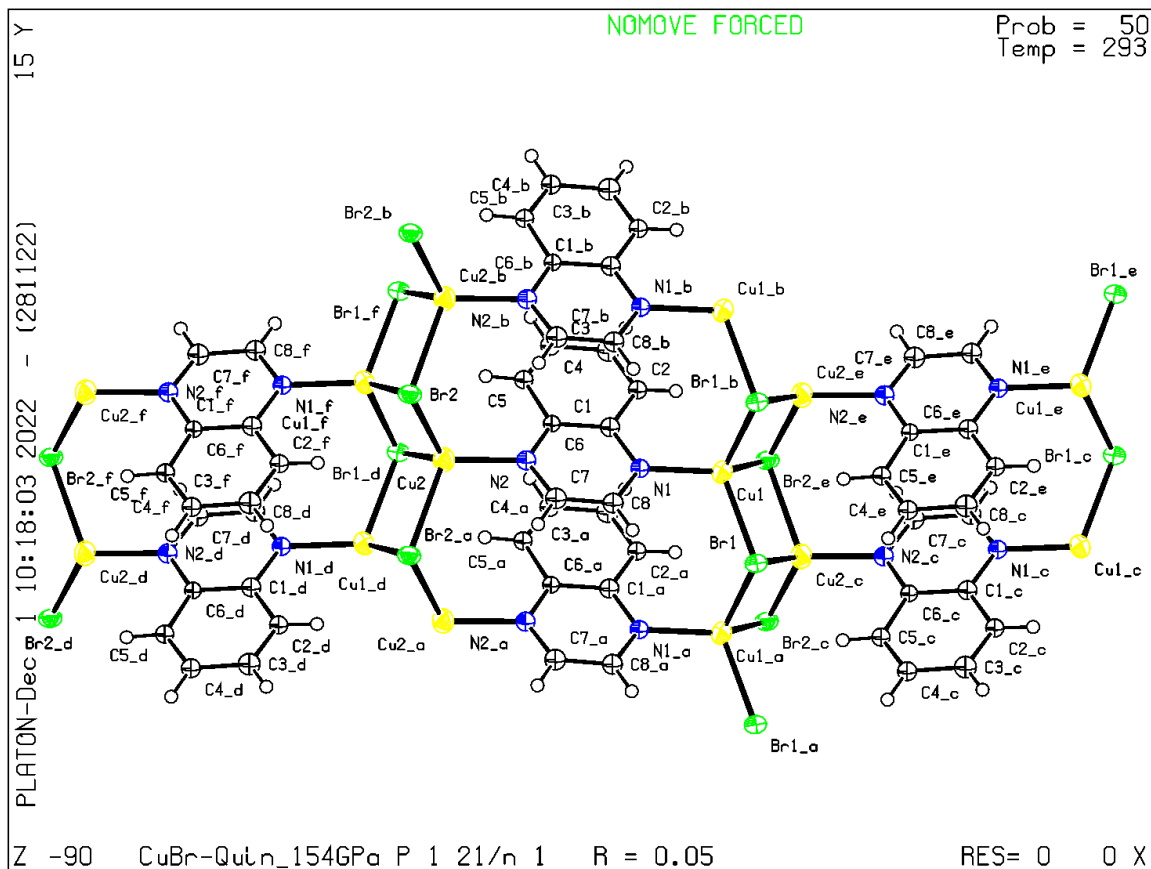
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_192GPa

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: CuBr-Quin_192GPa

Bond precision:	C-C = 0.0309 A	Wavelength=0.71073	
Cell:	a=4.0427 (4)	b=17.2708 (17)	c=12.915 (15)
	alpha=90	beta=93.24 (2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	900.3 (11)	900.3 (10)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2	
Sum formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2	
Mr	417.05	417.05	
Dx, g cm ⁻³	3.077	3.077	
Z	4	4	
Mu (mm ⁻¹)	13.549	13.549	
F000	784.0	784.0	
F000'	784.73		
h, k, lmax	5, 21, 16	5, 21, 5	
Nref	1831	623	
Tmin, Tmax	0.448, 0.622	0.248, 0.347	
Tmin'	0.159		

Correction method= # Reported T Limits: Tmin=0.248 Tmax=0.347
AbsCorr = GAUSSIAN

Data completeness= 0.340 Theta(max)= 26.349

R(reflections)= 0.0405 (510)	wR2(reflections)= 0.1173 (623)
S = 1.245	Npar= 77

```
test-name ALERT alert-type alert-level.
```

 Alert level A

 Alert level B

- Alert level C

● Alert level G

```

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 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

```

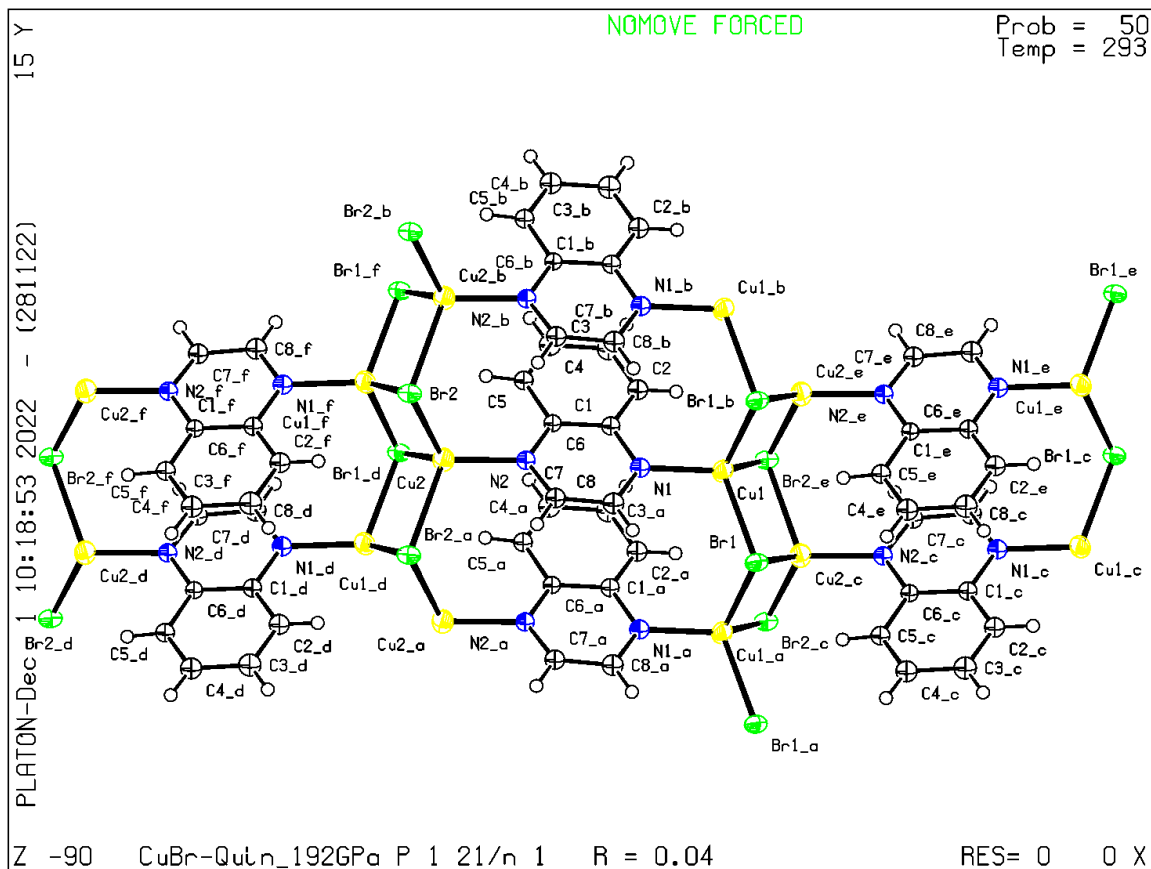
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_216GPa

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: CuBr-Quin_216GPa

Bond precision:	C-C = 0.0486 Å	Wavelength=0.71073
Cell:	a=4.0458 (4)	b=17.2700 (18) c=12.794 (14)
	alpha=90	beta=93.40 (2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	892.4 (10)	892.3 (10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Sum formula	C8 H6 Br2 Cu2 N2	C8 H6 Br2 Cu2 N2
Mr	417.05	417.05
Dx, g cm ⁻³	3.104	3.104
Z	4	4
Mu (mm ⁻¹)	13.669	13.670
F000	784.0	784.0
F000'	784.73	
h, k, lmax	5, 21, 15	5, 21, 5
Nref	1811	618
Tmin, Tmax	0.445, 0.620	0.242, 0.345
Tmin'	0.156	

Correction method= # Reported T Limits: Tmin=0.242 Tmax=0.345
AbsCorr = GAUSSIAN

Data completeness= 0.341 Theta(max)= 26.348

R(reflections)= 0.0587 (490)	wR2(reflections)= 0.1744 (618)
S = 1.209	Npar= 77

```
test-name ALERT alert-type alert-level.
```

 Alert level A

 Alert level B

- Alert level C

● Alert level G

```
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
```

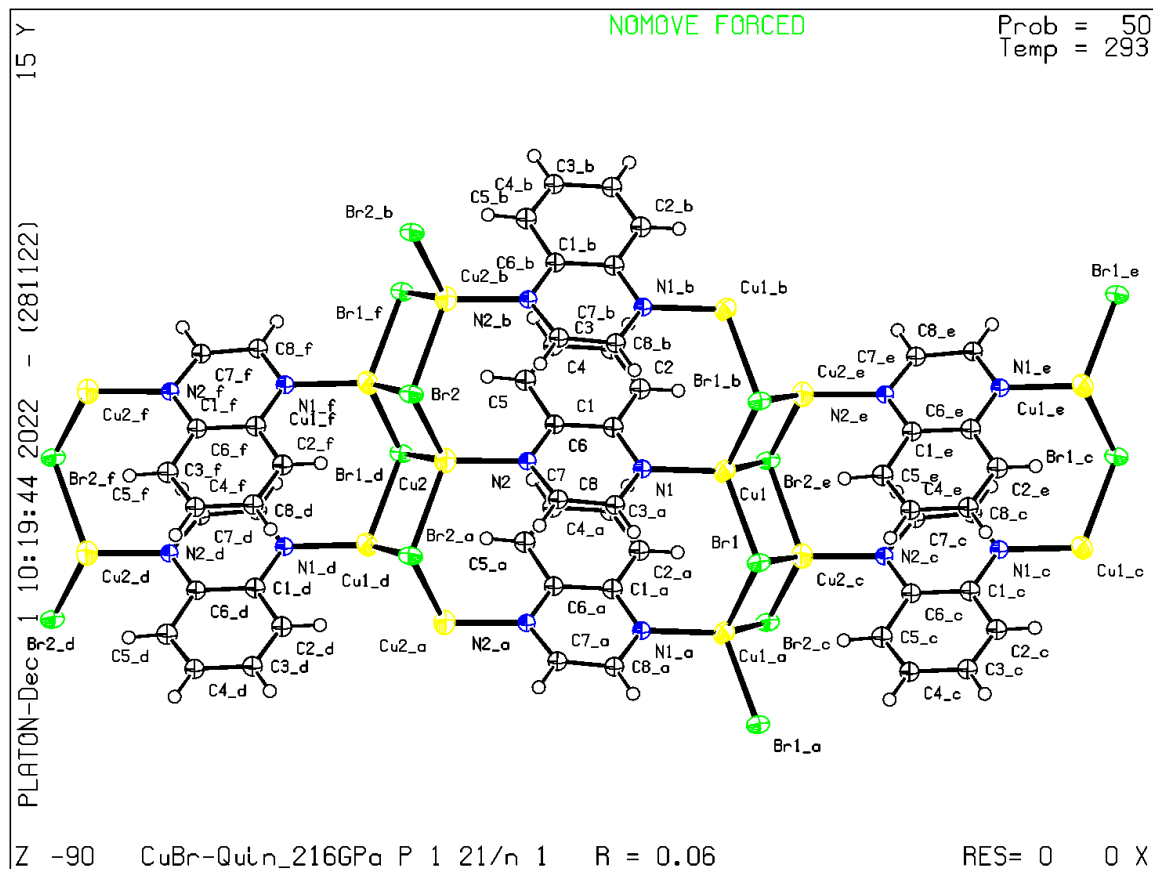
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0573( 446)      wR2(reflections)=
S = 1.151                        0.1592( 629)
Npar= 77
```

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.369 Why?

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.04571 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 360 Report

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.17 Note
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem 636 85 %Fit
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.020 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.780 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H3 . -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4 . -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8 . -0.37 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 28.49 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br1 ..C3 . 3.31 Ang.
 -1/2+x,1/2-y,1/2+z = 4_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br2 ..C7 . 3.20 Ang.
 2-x,1-y,2-z = 3_767 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 27 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 16 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.5 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 10 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 10 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

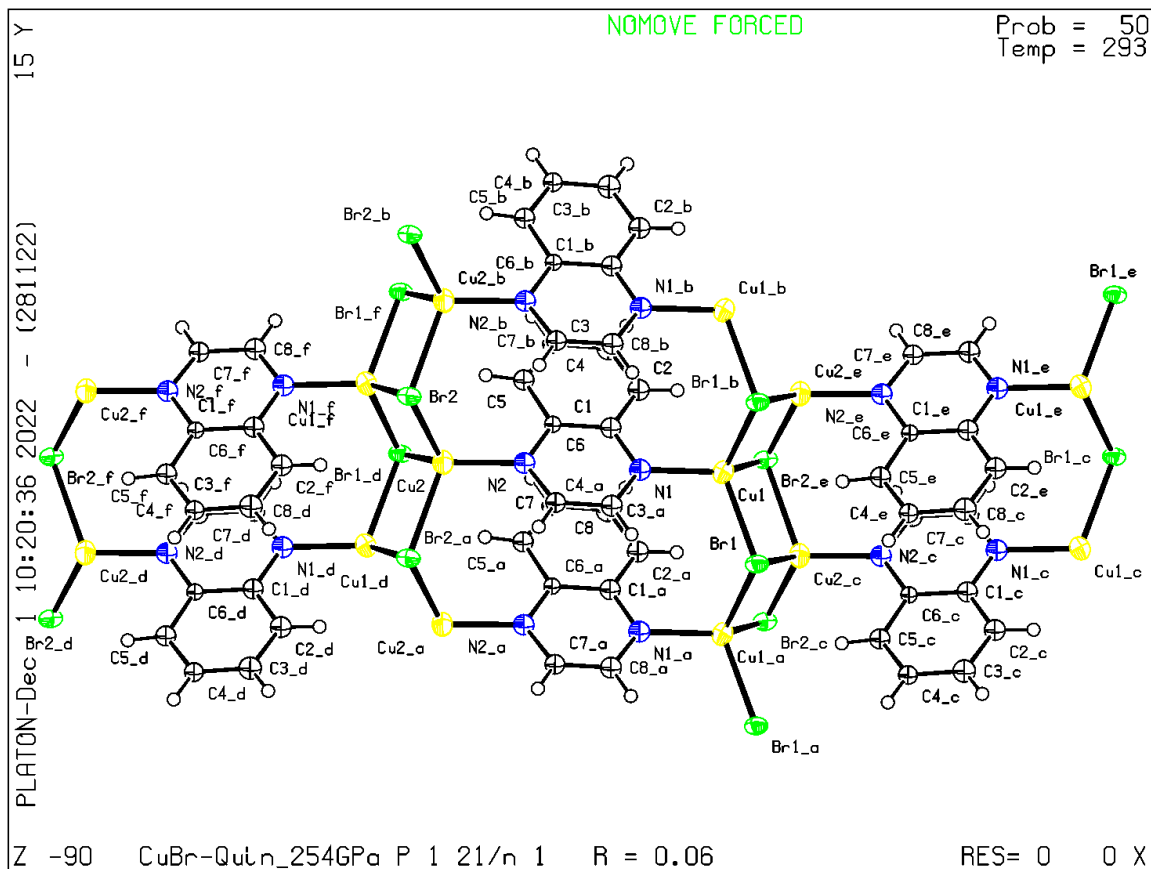
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0422( 412)      wR2(reflections)=
S = 1.193                        0.1059( 507)
Npar= 77
```

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**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.306 Why?

 **Alert level B**

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.58 Note
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 10 Report
 N1 N2 C1 C2 C3 etc.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.03714 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 335 Report

 **Alert level C**

PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem 636 85 %Fit
PLAT234_ALERT_4_C Large Hirshfeld Difference Br2 --Cu1_f . 0.16 Ang.
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 4 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H4 . -0.42 eA-3

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.05 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br2 ..C7 . 3.23 Ang.
 2-x,1-y,2-z = 3_767 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 32 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.0 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 10 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 10 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

- 3 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
7 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
-

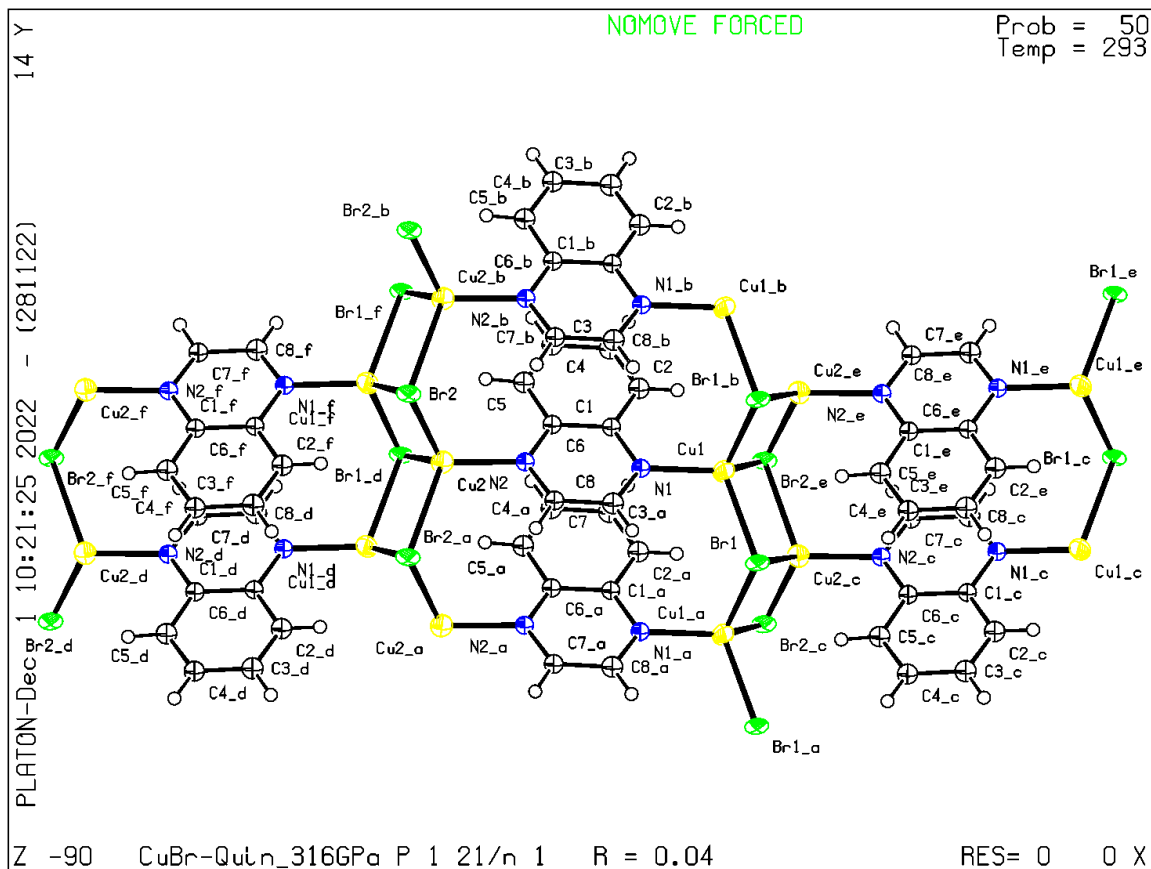
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_356GPa

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: CuBr-Quin_356GPa

Bond precision: C-C = 0.0964 Å Wavelength=0.71073

Cell: a=4.0457(9) b=17.0296(16) c=12.438(5)
 alpha=88.73(2) beta=94.39(4) gamma=87.861(13)
Temperature: 298 K

	Calculated	Reported
Volume	853.6(4)	853.6(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Sum formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Mr	834.10	417.05
Dx, g cm ⁻³	3.245	3.245
Z	2	4
Mu (mm ⁻¹)	14.290	14.291
F000	784.0	784.0
F000'	784.73	
h, k, lmax	4, 18, 13	4, 18, 6
Nref	2460	841
Tmin, Tmax	0.428, 0.565	0.254, 0.339
Tmin'	0.206	

Correction method= # Reported T Limits: Tmin=0.254 Tmax=0.339
AbsCorr = GAUSSIAN

Data completeness= 0.342 Theta(max)= 23.251

R(reflections)= 0.1375(582)	wR2(reflections)=
S = 1.120	0.3593(841)
Npar= 87	

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

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full	value Low	0.342	Why?		
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20	Report		
	N1	N2	N3	N4	C1	etc.
PLAT341_ALERT_3_A	Low Bond Precision on	C-C Bonds	0.09643	Ang.	

Alert level B

THETM01_ALERT_3_B	The value of sine(theta_max)/wavelength is less than	0.575		
	Calculated sin(theta_max)/wavelength =	0.5554		
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.36	Report
PLAT911_ALERT_3_B	Missing FCF Refl Between Thmin & STh/L=	0.555	775	Report

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings	Differ		Please Check
PLAT082_ALERT_2_C	High R1 Value	0.14	Report
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.67	Note
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85	%Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !
PLAT234_ALERT_4_C	Large Hirshfeld Difference Br1	--Cu4	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Br3	--Cu1	0.17	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		Cu1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		Cu2	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		Cu3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N3	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	4.0	Note
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C1 -C6	1.37	Ang.
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C9 -C14	1.37	Ang.
PLAT733_ALERT_1_C	Torsion Calc	-1(13), Rep	-1(3)
	C13 -C12 -C11 -C10	1_555 1_555 1_555 1_555	#	29 Check
PLAT733_ALERT_1_C	Torsion Calc	-1(13), Rep	-2(3)
	C9 -C10 -C11 -C12	1_555 1_555 1_555 1_555	#	42 Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance	...	-3.752	Report
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.039	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.28Ang From Br2	1.75	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.24Ang From Br2	1.68	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.23Ang From Cu2	1.53	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H3	.	-0.38	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11	.	-0.73	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H12	.	-0.59	eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor	...	0.500	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		273.40	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4	Report

PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1 -C6	0.21	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br1 ..C11 .	3.14	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br1 ..C12 .	3.29	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br1 ..C12 .	3.35	Ang.
	2-x,-y,-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br2 ..C7 .	3.09	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br2 ..C8 .	3.32	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br3 ..C15 .	3.15	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br4 ..C3 .	3.34	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	14	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	93%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	17	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	7	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	7	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

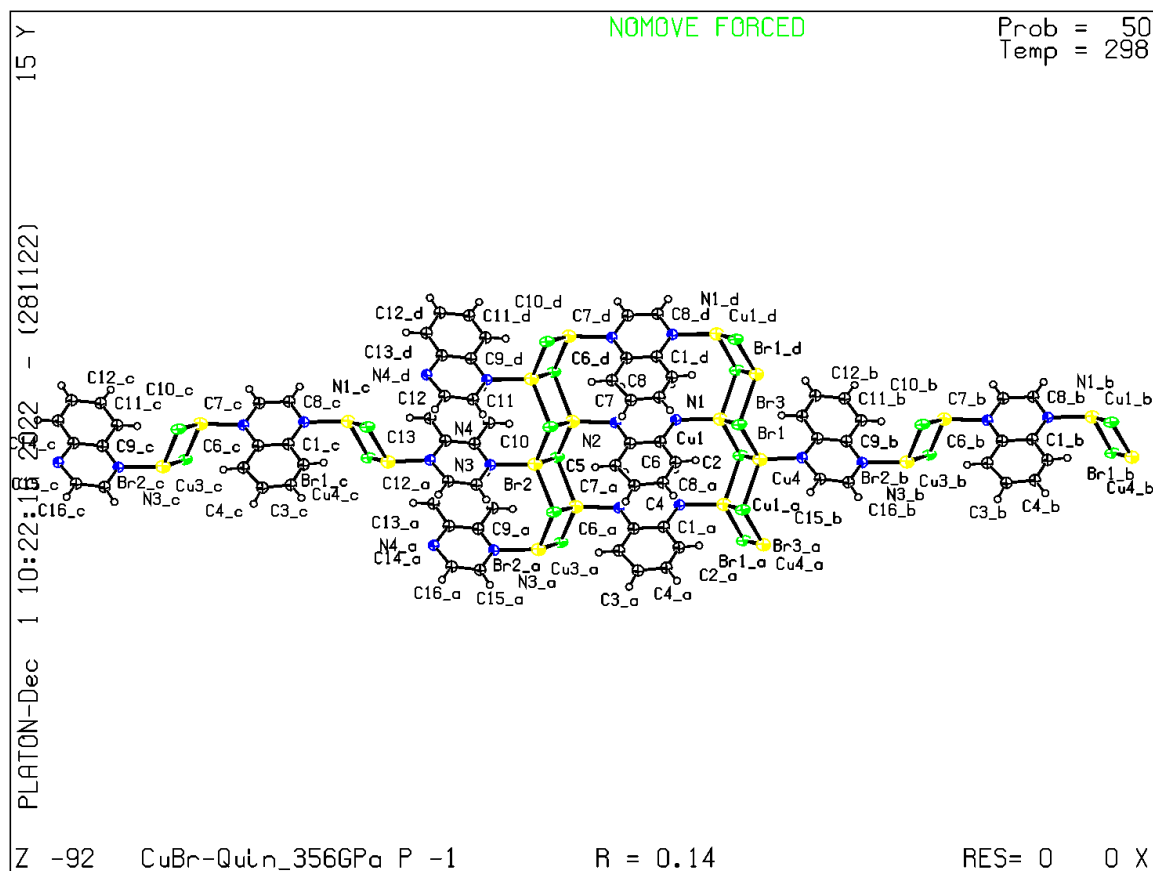
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_397GPa

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: CuBr-Quin_397GPa

Bond precision: C-C = 0.0929 Å Wavelength=0.71073

Cell: a=4.0608(10) b=16.9204(19) c=12.376(5)
 alpha=88.34(2) beta=94.54(4) gamma=86.499(15)
Temperature: 298 K

	Calculated	Reported
Volume	845.6(4)	845.7(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Sum formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Mr	834.10	417.05
Dx, g cm ⁻³	3.276	3.276
Z	2	4
Mu (mm ⁻¹)	14.425	14.424
F000	784.0	784.0
F000'	784.73	
h, k, lmax	4, 18, 13	4, 18, 6
Nref	2442	871
Tmin, Tmax	0.425, 0.562	0.247, 0.336
Tmin'	0.203	

Correction method= # Reported T Limits: Tmin=0.247 Tmax=0.336
AbsCorr = GAUSSIAN

Data completeness= 0.357 Theta(max)= 23.256

R(reflections)= 0.1372(586)	wR2(reflections)=
S = 1.170	0.3637(871)
Npar= 87	

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

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full	value Low	0.357	Why?		
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20	Report		
	N1	N2	N3	N4	C1	etc.
PLAT341_ALERT_3_A	Low Bond Precision on	C-C Bonds	0.09286	Ang.	

Alert level B

THETM01_ALERT_3_B	The value of sine(theta_max)/wavelength is less than	0.575		
	Calculated sin(theta_max)/wavelength =	0.5555		
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.36	Report
PLAT911_ALERT_3_B	Missing FCF Refl Between Thmin & Sth/L=	0.556	739	Report

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings	Differ		Please Check
PLAT082_ALERT_2_C	High R1 Value	0.14	Report
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85	%Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.4	Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	25.024	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.863	Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H8	.	-0.39	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13	.	-0.40	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H15	.	-0.53	eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.500	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.12	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		189.62	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		1	Report
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C9	-C14	1.44	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1	-C6	0.21	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br1 ..C11	3.14	Ang.
		1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br2 ..C7	3.14	Ang.
		1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br2 ..C8	3.27	Ang.
		1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br3 ..C15	3.00	Ang.
		2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br4 ..C4	3.29	Ang.
		2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br4 ..C3	3.31	Ang.
		2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br4 ..C3	3.35	Ang.

	1-x,-y,1-z =	2_656	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	14	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	97%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	12	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.5	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	7	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	7	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

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

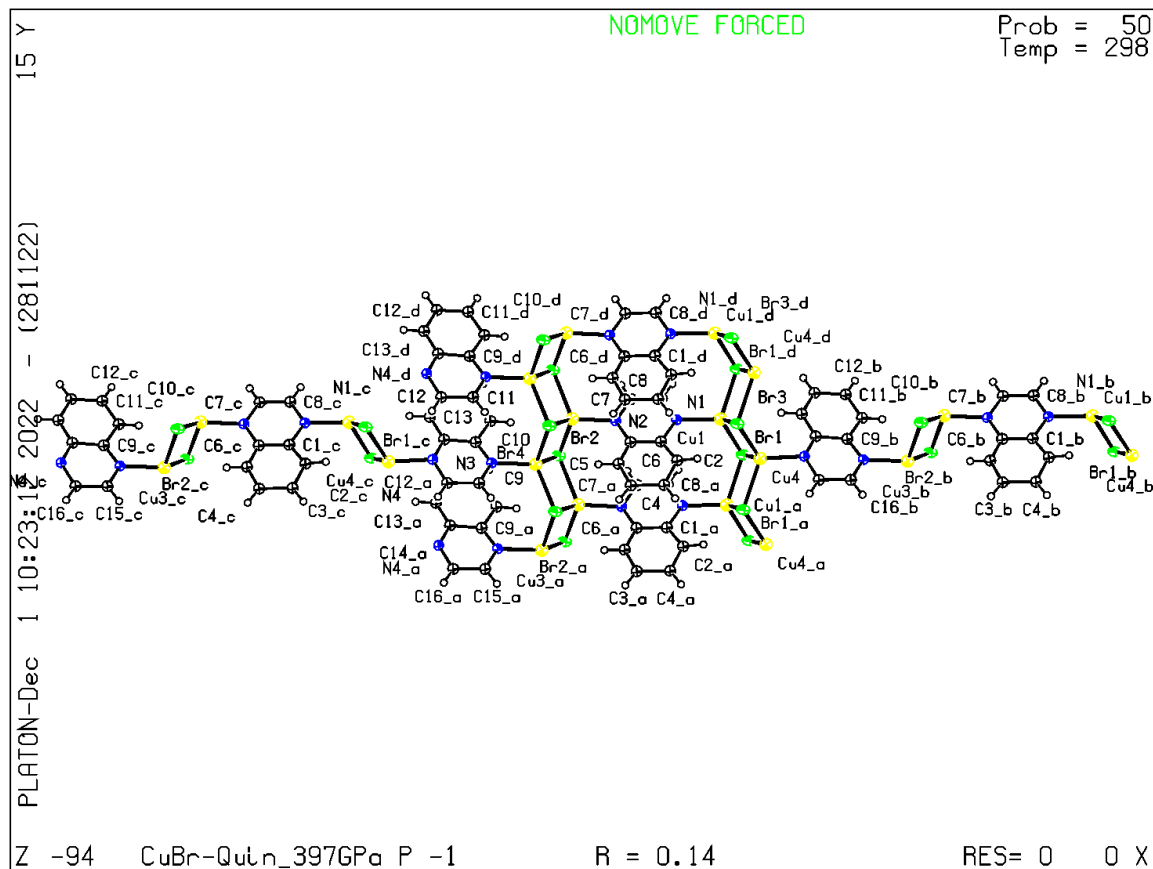
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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) CuBr-Quin_462GPa

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: CuBr-Quin_462GPa

Bond precision: C-C = 0.1093 Å Wavelength=0.71073

Cell: a=4.0605(12) b=16.839(3) c=12.287(7)
 alpha=88.48(3) beta=94.88(5) gamma=86.038(18)
Temperature: 298 K

	Calculated	Reported
Volume	834.6(6)	834.6(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Sum formula	C16 H12 Br4 Cu4 N4	C8 H6 Br2 Cu2 N2
Mr	834.10	417.05
Dx, g cm ⁻³	3.319	3.319
Z	2	4
Mu (mm ⁻¹)	14.615	14.616
F000	784.0	784.0
F000'	784.73	
h, k, lmax	4, 18, 13	4, 18, 6
Nref	2405	883
Tmin, Tmax	0.420, 0.557	0.246, 0.336
Tmin'	0.128	

Correction method= # Reported T Limits: Tmin=0.246 Tmax=0.336
AbsCorr = GAUSSIAN

Data completeness= 0.367 Theta(max)= 23.231

R(reflections)= 0.1575(558)	wR2(reflections)=
S = 1.156	0.4130(883)
Npar= 87	

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

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full	value Low	0.367	Why?		
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20	Report		
	N1	N2	N3	N4	C1	etc.
PLAT341_ALERT_3_A	Low Bond Precision on	C-C Bonds	0.10929	Ang.	

Alert level B

THETM01_ALERT_3_B	The value of sine(theta_max)/wavelength is less than 0.575										
	Calculated sin(theta_max)/wavelength =	0.5550									
PLAT082_ALERT_2_B	High R1 Value	0.16	Report							
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.41	Report							
PLAT733_ALERT_1_B	Torsion Calc	-1(13), Rep	0(2)	6.50 s.u.-R							
	C9	-C10	-C11	-C12	1_555	1_555	1_555	1_555	#	42	Check
PLAT911_ALERT_3_B	Missing FCF Refl Between Thmin & STh/L=	0.555	710	Report							

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636 85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced Please Do !
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor 3.3 Note
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C15 - C16 1.54 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance 56.986 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance 7.888 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.04Ang From Br3 1.91 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.98Ang From N3 1.59 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11	. -0.88 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H12	. -0.69 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13	. -0.34 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H15	. -0.83 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H16	. -0.37 eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	263.92 Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1	-C6 0.20 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br1 ..C11 3.06 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br2 ..C7 3.16 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br2 ..C8 3.18 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br3 ..C15 3.02 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	Br4	2-x,-y,1-z = ..C4	.	2_756 Check 3.14 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	Br4	2-x,-y,1-z = ..C3	.	2_756 Check 3.25 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	Br4	2-x,-y,1-z = ..C3	.	2_756 Check 3.32 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	Br4	1-x,-y,1-z = ..C4	.	2_656 Check 3.35 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints		1-x,-y,1-z =		2_656 Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max)				14 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)				68% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File				4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity				18 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.				2.7 Low
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.				7 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				7 Units
				0 Info

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

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

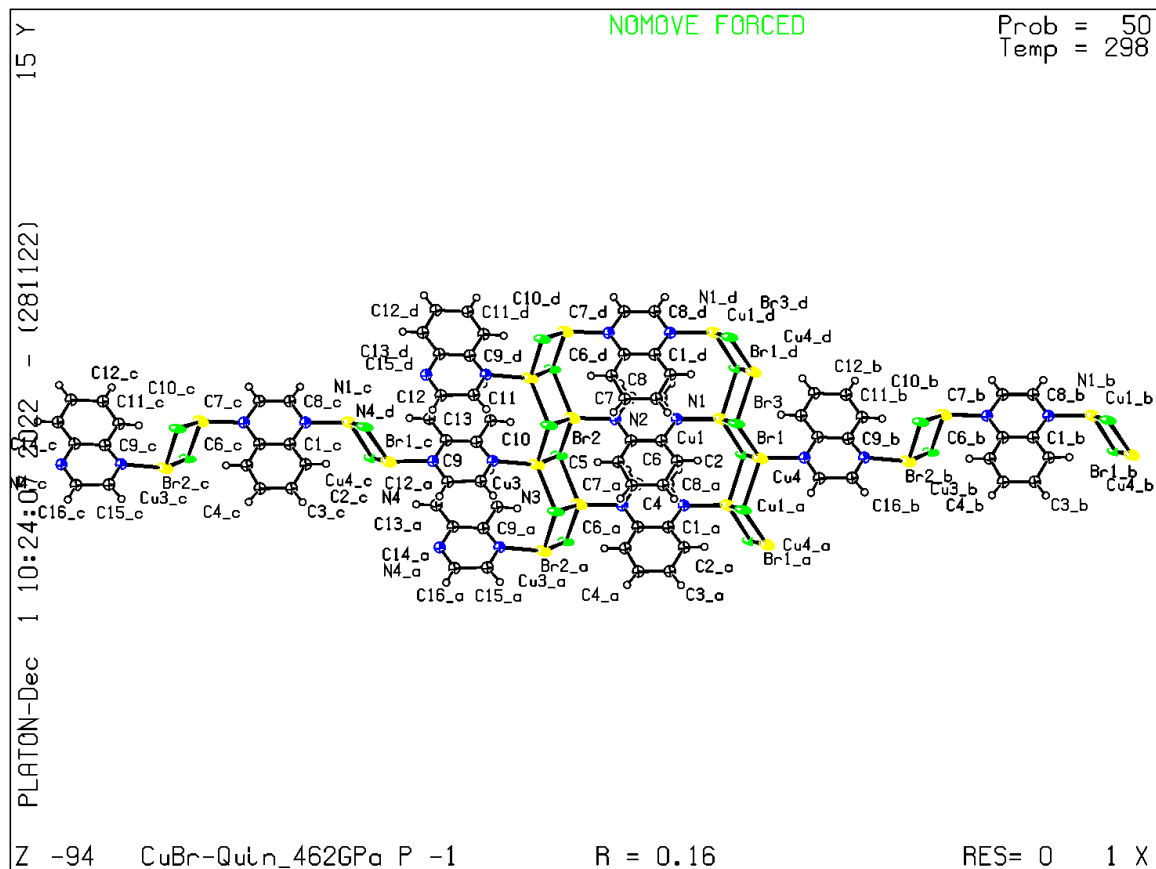
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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

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

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: CuI-Quin_000GPa

Bond precision:	C-C = 0.0096 Å	Wavelength=0.71073	
Cell:	a=4.3719(2)	b=17.7203(8)	c=13.8614(6)
	alpha=90	beta=92.886(4)	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	1072.50(8)	1072.50(8)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C8 H6 Cu2 I2 N2	C8 H6 Cu2 I2 N2	
Sum formula	C8 H6 Cu2 I2 N2	C8 H6 Cu2 I2 N2	
Mr	511.05	511.03	
Dx, g cm ⁻³	3.165	3.165	
Z	4	4	
Mu (mm ⁻¹)	9.680	9.680	
F000	928.0	928.0	
F000'	927.07		
h, k, lmax	5, 22, 17	5, 22, 17	
Nref	2197	2198	
Tmin, Tmax	0.705, 0.873	0.665, 0.905	
Tmin'	0.488		

Correction method= # Reported T Limits: Tmin=0.665 Tmax=0.905
AbsCorr = GAUSSIAN

Data completeness= 1.000 Theta(max)= 26.370

R(reflections)= 0.0376(1838)	wR2(reflections)= 0.0681(2198)
S = 1.055	Npar= 127

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

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree



Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00957 Ang.



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1 . 17.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu1_a . 29.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu2_c . 24.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I2 --Cu2 . 16.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I2 --Cu2_b . 26.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I2 --Cu1_f . 21.7 s.u.
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.8 Low

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

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

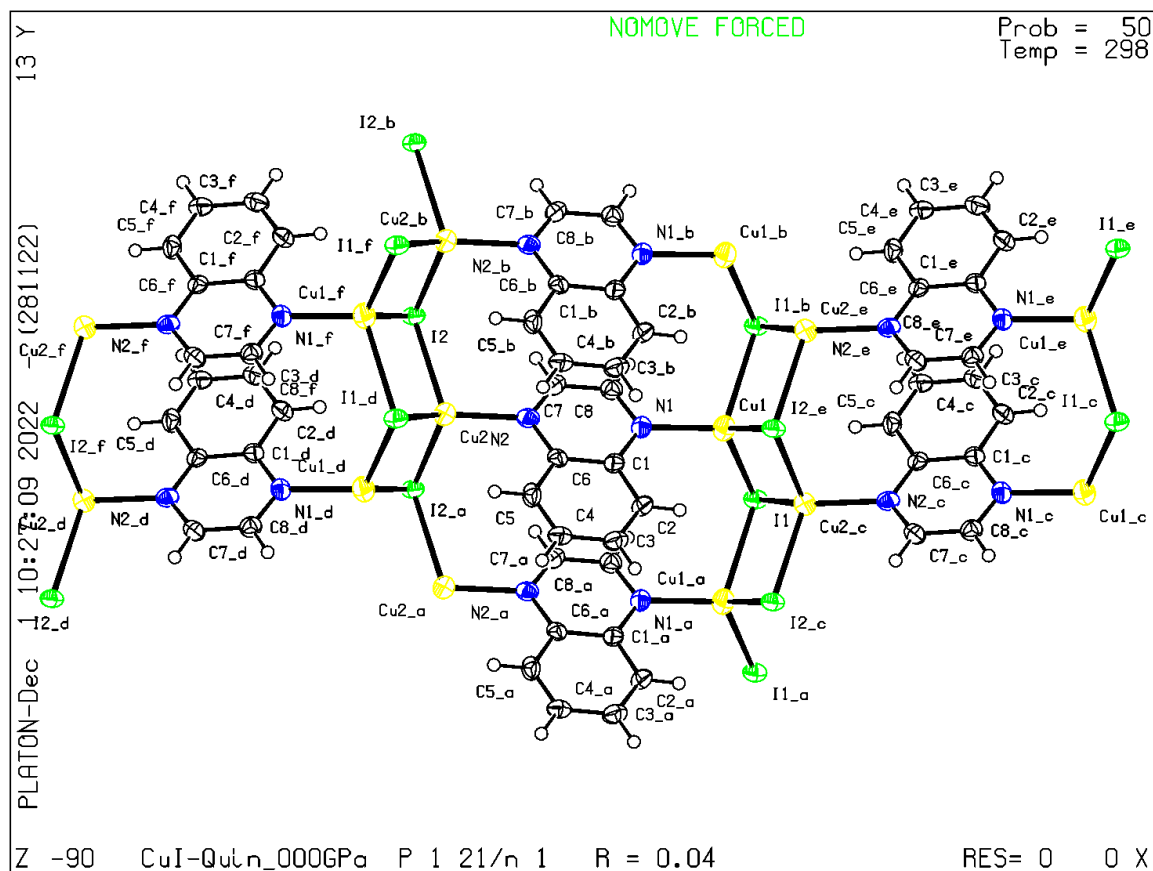
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



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**

PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.11 %
PLAT660_ALERT_1_A No Valid _diffrn_radiation_type Value Reported .	Please Do !

 **Alert level B**

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE.	293 Degree
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s)	10 Report
N1 N2 C1 C2 C3	etc.
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds	0.03557 Ang.

 **Alert level C**

PLAT234_ALERT_4_C Large Hirshfeld Difference I1 --Cu2_c .	0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	Cu2 Check

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0	0.993 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.12 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	1.9 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.	9 Units
PLAT984_ALERT_1_G The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

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

- 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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
-

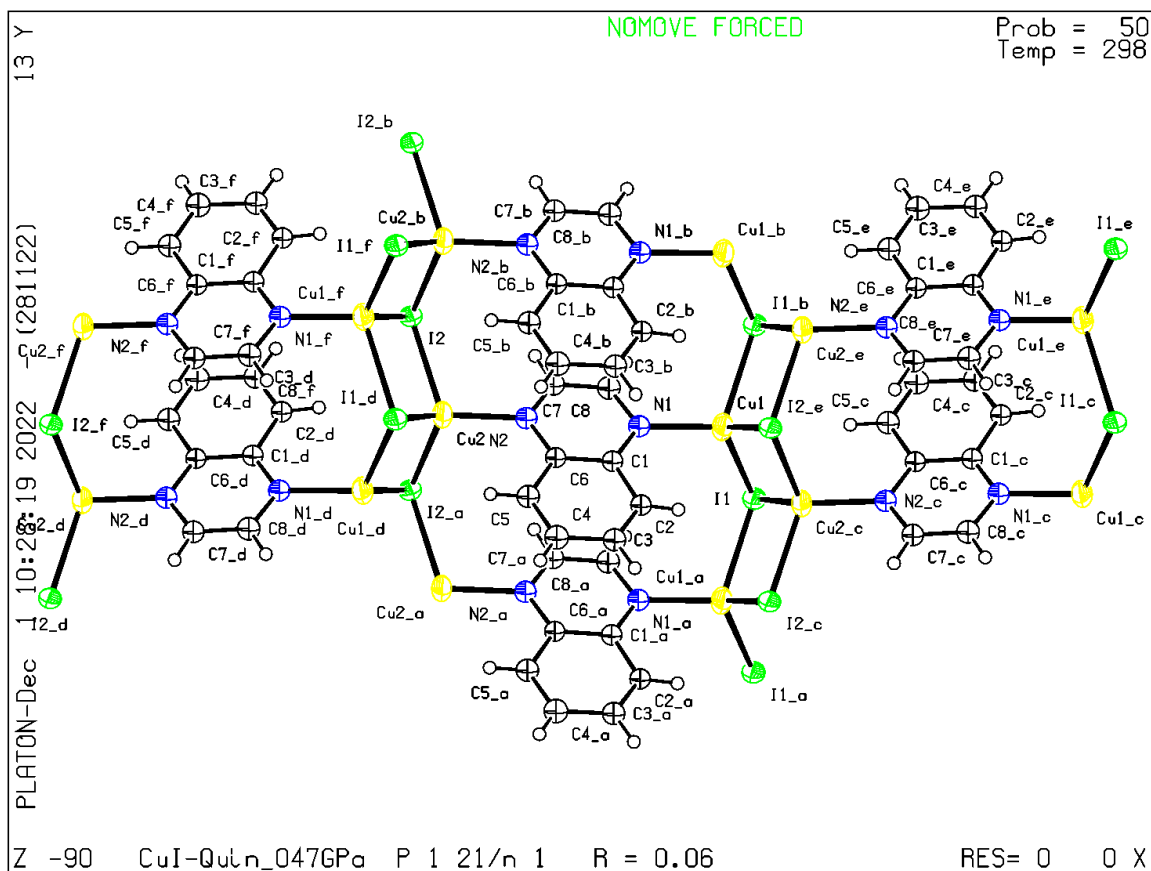
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0593( 714)      wR2(reflections)=
S = 1.034                        0.1591( 841)
Npar= 77
```

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**

PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT660_ALERT_1_A No Valid _diffrn_radiation_type Value Reported .	Please Do !

 **Alert level B**

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s)	10 Report
N1 N2 C1 C2 C3	etc.
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds	0.031 Ang.

 **Alert level C**

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	Cu2 Check
--	-----------

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0	0.993 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.11 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 --Cu2_c	7.0 s.u.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1 -C6	1.43 Ang.
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.0 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.	9 Units
PLAT984_ALERT_1_G The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

17 **ALERT level G** = General information/check it is not something unexpected

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

5 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 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

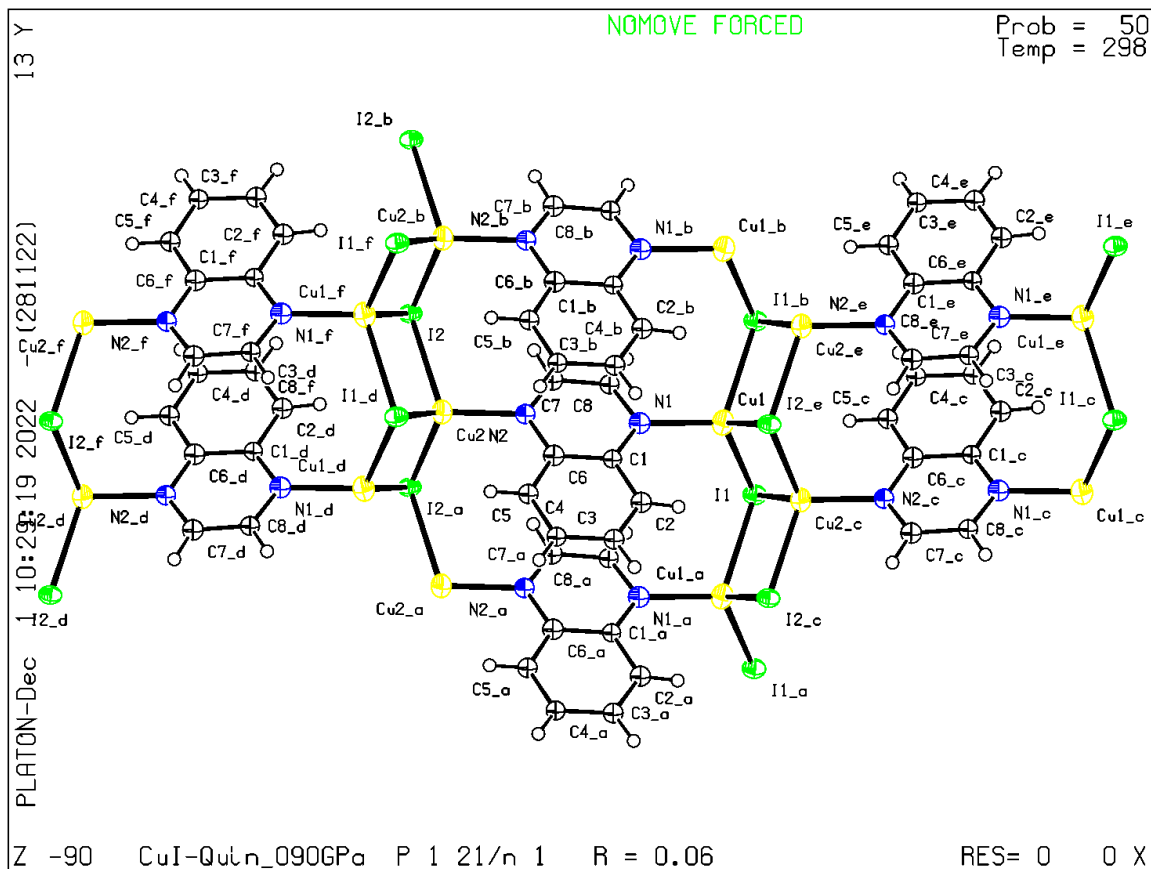
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0497( 695)      wR2(reflections)=
S = 1.087                        0.1386( 826)
Npar= 77
```

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**

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

 **Alert level B**

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	10 Report
	N1 N2 C1 C2 C3	etc.
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03029 Ang.

 **Alert level C**

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Cu1 Check
-------------------	--	-----------

 **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.988 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Cu1_f .	6.2 s.u.
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	9 Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G	The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G	The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G	The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G	The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G	The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G	The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

15 **ALERT level G** = General information/check it is not something unexpected

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

3 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 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

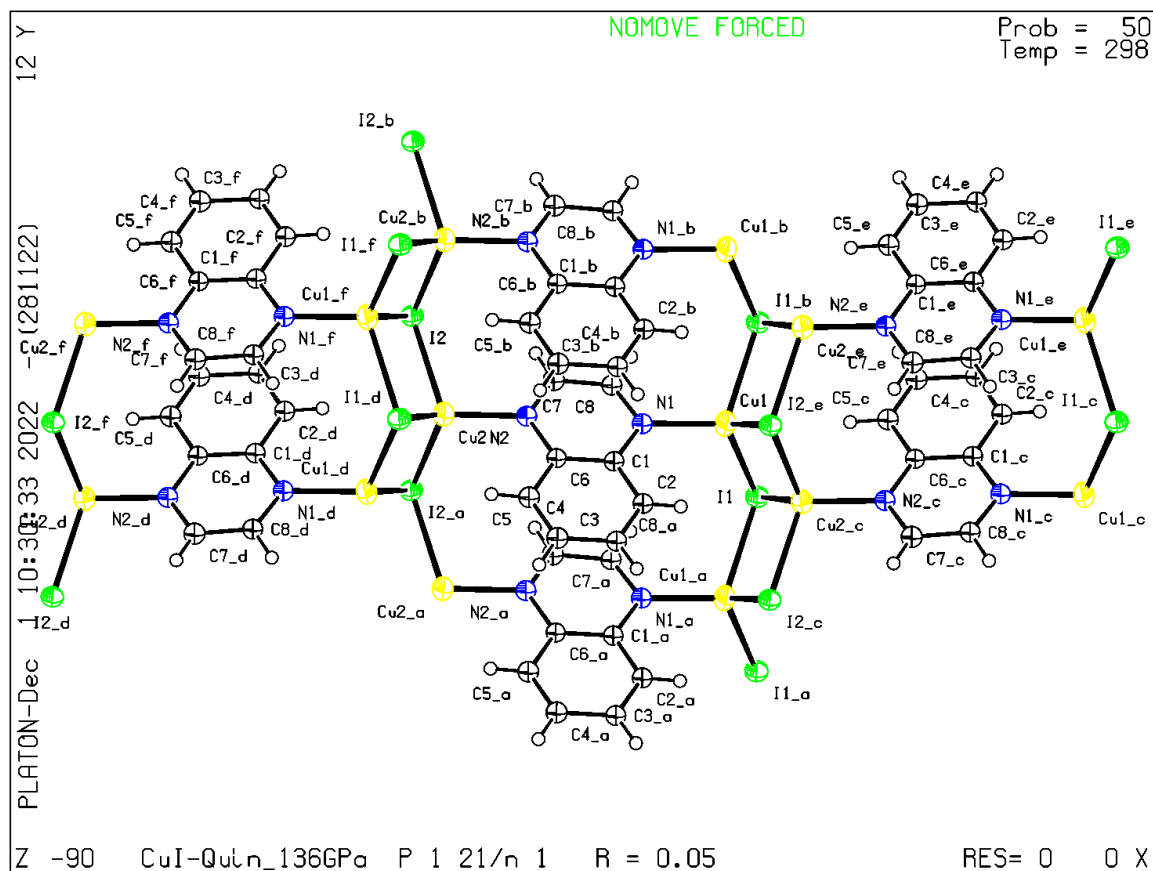
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0703( 686)      wR2(reflections)=
S = 1.043                        0.1985( 811)
Npar= 72
```

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.11 %			
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	11 Report			
I1	N1	N2	C1	C2	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !			

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03557 Ang.
-------------------	---------------------------------------	--------------

Alert level C

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5 Check
-------------------	--	----------

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub 85 %Fit
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C8 .	3.38 Ang.
	-x,1-y,-z =	3_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C4 .	3.45 Ang.
	1/2+x,3/2-y,-1/2+z =	4_675 Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	9 Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G	The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G	The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G	The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G	The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G	The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G	The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

3 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

17 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 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

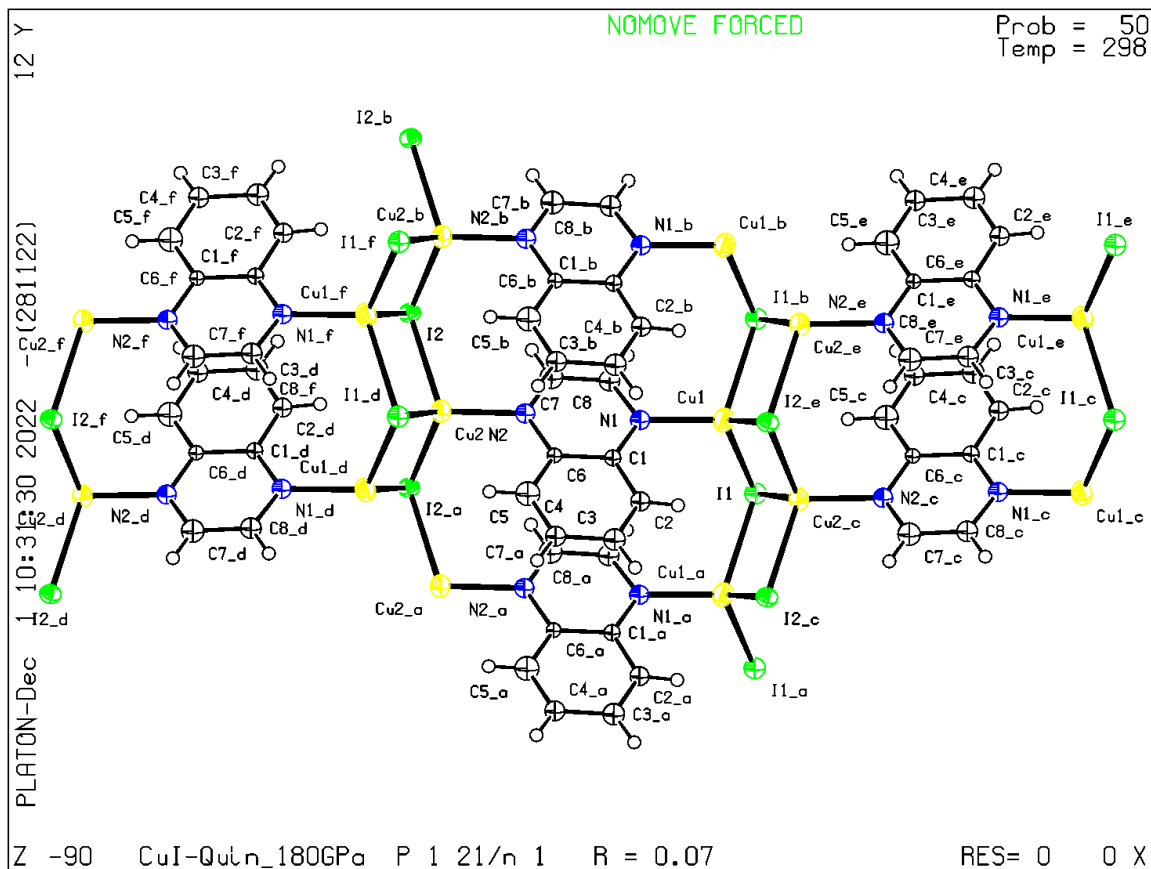
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0584( 669)      wR2(reflections)=
S = 1.078                        0.1764( 811)
Npar= 77
```

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

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full	value Low	0.412	Why?
PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF)	Ratio Differs from 1.0 by	57.12	%
PLAT660_ALERT_1_A	No Valid _diffn_radiation_type	Value Reported		Please Do !

Alert level B

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	10	Report		
	N1	N2	C1	C2	C3	etc.
PLAT342_ALERT_3_B	Low Bond Precision on	C-C Bonds	0.03571	Ang.	

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info		
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check		
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT	Unusually Large	0.13	Report	
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In	Ka	0.31850	Ang.	
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	85	%Fit	
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1	-C6	1.43	Ang.	
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1	-C6	0.18	Ang.	
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1	..C8	3.38	Ang.	
		-x,1-y,-z =	3_565	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2	..C4	3.48	Ang.	
		1/2+x,3/2-y,-1/2+z =	4_675	Check	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0	Low	
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		9	Units	
PLAT984_ALERT_1_G	The C-f' =	0.0033	Deviates from the B&C-Value	-0.0008	Check
PLAT984_ALERT_1_G	The Cu-f' =	0.3201	Deviates from the B&C-Value	0.1660	Check
PLAT984_ALERT_1_G	The I-f' =	-0.4742	Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The N-f' =	0.0061	Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The C-f" =	0.0016	Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The Cu-f" =	1.2651	Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The I-f" =	1.8119	Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The N-f" =	0.0033	Deviates from the B&C-Value	0.0005	Check

3 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

19 **ALERT level G** = General information/check it is not something unexpected

11 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

3 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

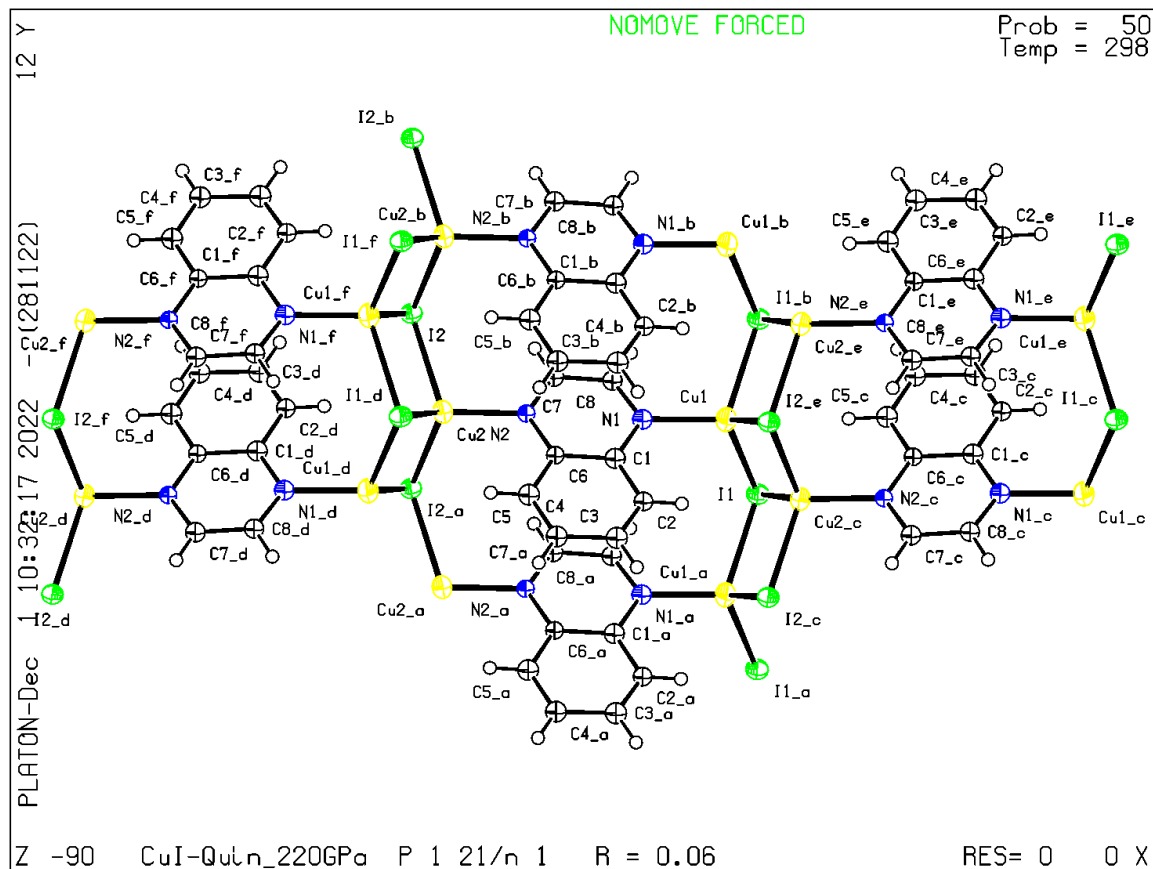
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



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**

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

 **Alert level B**

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	10 Report
	N1 N2 C1 C2 C3	etc.
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03229 Ang.

 **Alert level C**

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Cu2 Check
-------------------	--	-----------

 **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.993 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem sub	85 %Fit
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C8 .	3.32 Ang.
	-x,1-y,-z =	3_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C4 .	3.44 Ang.
	1/2+x,3/2-y,-1/2+z =	4_675 Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	8 Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G	The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G	The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G	The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G	The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G	The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G	The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

17 **ALERT level G** = General information/check it is not something unexpected

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

5 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 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

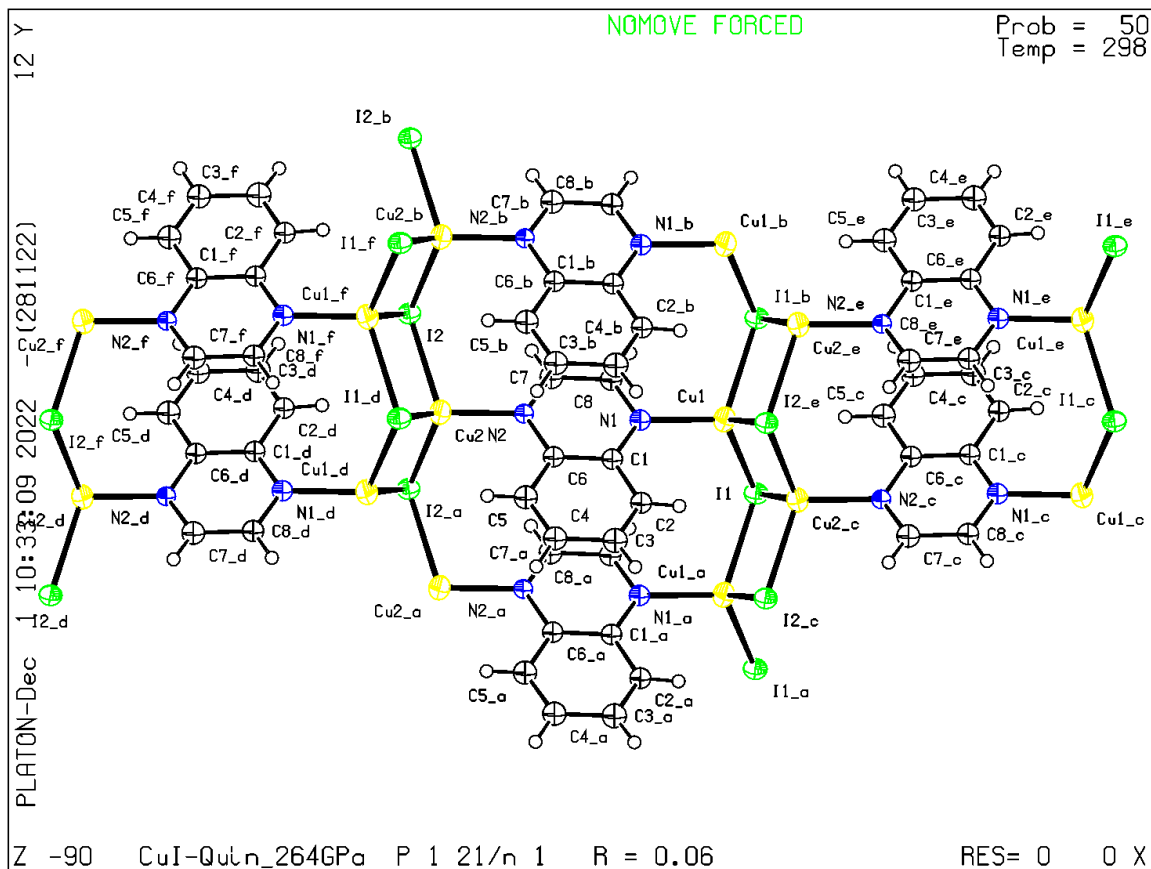
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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

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

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: CuI-Quin_325GPa

Bond precision: C-C = 0.0629 Å Wavelength=0.31850

Cell: a=4.3090(2) b=17.0807(9) c=12.645(2)
 alpha=88.916(11) beta=95.228(11) gamma=92.637(4)
Temperature: 298 K

	Calculated	Reported
Volume	925.73(16)	925.71(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Cu4 I4 N4	0.5(C16 H12 Cu4 I4 N4)
Sum formula	C16 H12 Cu4 I4 N4	C8 H6 Cu2 I2 N2
Mr	1022.10	511.03
Dx, g cm ⁻³	3.667	3.667
Z	2	4
Mu (mm ⁻¹)	4.809	11.215
F000	928.0	928.0
F000'	922.57	
h, k, lmax	5, 21, 16	5, 21, 7
Nref	4106	1242
Tmin, Tmax	0.692, 0.855	0.057, 1.000
Tmin'	0.420	

Correction method= # Reported T Limits: Tmin=0.057 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.302 Theta(max)= 11.779

R(reflections)= 0.0976(796)	wR2(reflections)=
S = 1.057	0.3065(1242)
Npar= 99	

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j) Tensor	5.3 Note
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.06286 Ang.

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31 Report
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem 636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !
PLAT234_ALERT_4_C	Large Hirshfeld Difference I2 --Cu3 .	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference I4 --Cu2 .	0.17 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Cu1 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Cu2 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Cu3 Check

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.974 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	4 Report
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1 -C6 .	1.42 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1 -C6	0.21 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14	0.21 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.40 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .	3.28 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .	3.48 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.19 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .	3.48 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.28 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.46 Ang.
	1-x,-y,1-z =	2_656 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12 Note

PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.3	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	9	Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008	Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660	Check
PLAT984_ALERT_1_G	The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The C-f" = 0.0016 Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The I-f" = 1.8119 Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The N-f" = 0.0033 Deviates from the B&C-Value	0.0005	Check

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

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 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
 6 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

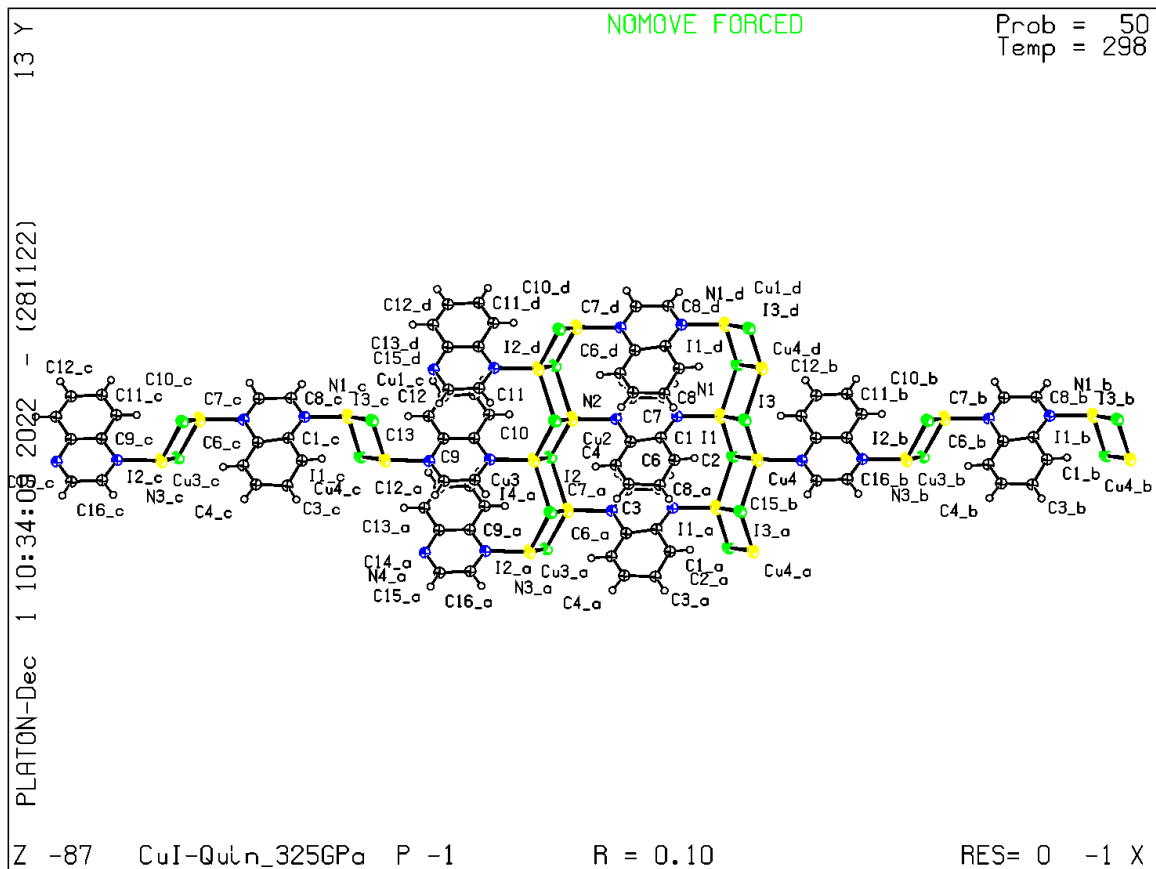
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock CuI-Quin_325GPa - ellipsoid plot



checkCIF/PLATON report

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

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: CuI-Quin_369GPa

Bond precision: C-C = 0.0456 Å Wavelength=0.31850

Cell: a=4.3058 (2) b=17.0097 (8) c=12.575 (2)
 alpha=87.899 (9) beta=95.572 (9) gamma=93.641 (4)
Temperature: 298 K

	Calculated	Reported
Volume	914.36 (16)	914.40 (16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Cu4 I4 N4	0.5 (C16 H12 Cu4 I4 N4)
Sum formula	C16 H12 Cu4 I4 N4	C8 H6 Cu2 I2 N2
Mr	1022.10	511.03
Dx, g cm ⁻³	3.712	3.712
Z	2	4
Mu (mm ⁻¹)	4.869	11.354
F000	928.0	928.0
F000'	922.57	
h, k, lmax	5, 21, 16	5, 21, 7
Nref	4052	1232
Tmin, Tmax	0.688, 0.853	0.165, 1.000
Tmin'	0.416	

Correction method= # Reported T Limits: Tmin=0.165 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.304 Theta (max)= 11.778

R(reflections)= 0.0815 (812)	wR2(reflections)=
S = 1.047	0.2599 (1232)
Npar= 75	

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.11 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.04564 Ang.
-------------------	---------------------------------------	--------------

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.26 Report
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem 636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !
PLAT368_ALERT_2_C	Short C(sp2)-C(sp2) Bond C12 - C13 .	1.17 Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.977 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.16 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4 Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1 -C6	0.23 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14	0.26 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.39 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .	3.25 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .	3.42 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.29 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .	3.41 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.33 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.3 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	9 Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660 Check
PLAT984_ALERT_1_G	The I-f' = -0.4742 Deviates from the B&C-Value	-0.8576 Check
PLAT984_ALERT_1_G	The N-f' = 0.0061 Deviates from the B&C-Value	-0.0009 Check
PLAT985_ALERT_1_G	The C-f" = 0.0016 Deviates from the B&C-Value	0.0003 Check
PLAT985_ALERT_1_G	The Cu-f" = 1.2651 Deviates from the B&C-Value	0.2861 Check
PLAT985_ALERT_1_G	The I-f" = 1.8119 Deviates from the B&C-Value	2.7116 Check
PLAT985_ALERT_1_G	The N-f" = 0.0033 Deviates from the B&C-Value	0.0005 Check

3 **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
25 **ALERT level G** = General information/check it is not something unexpected

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 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.

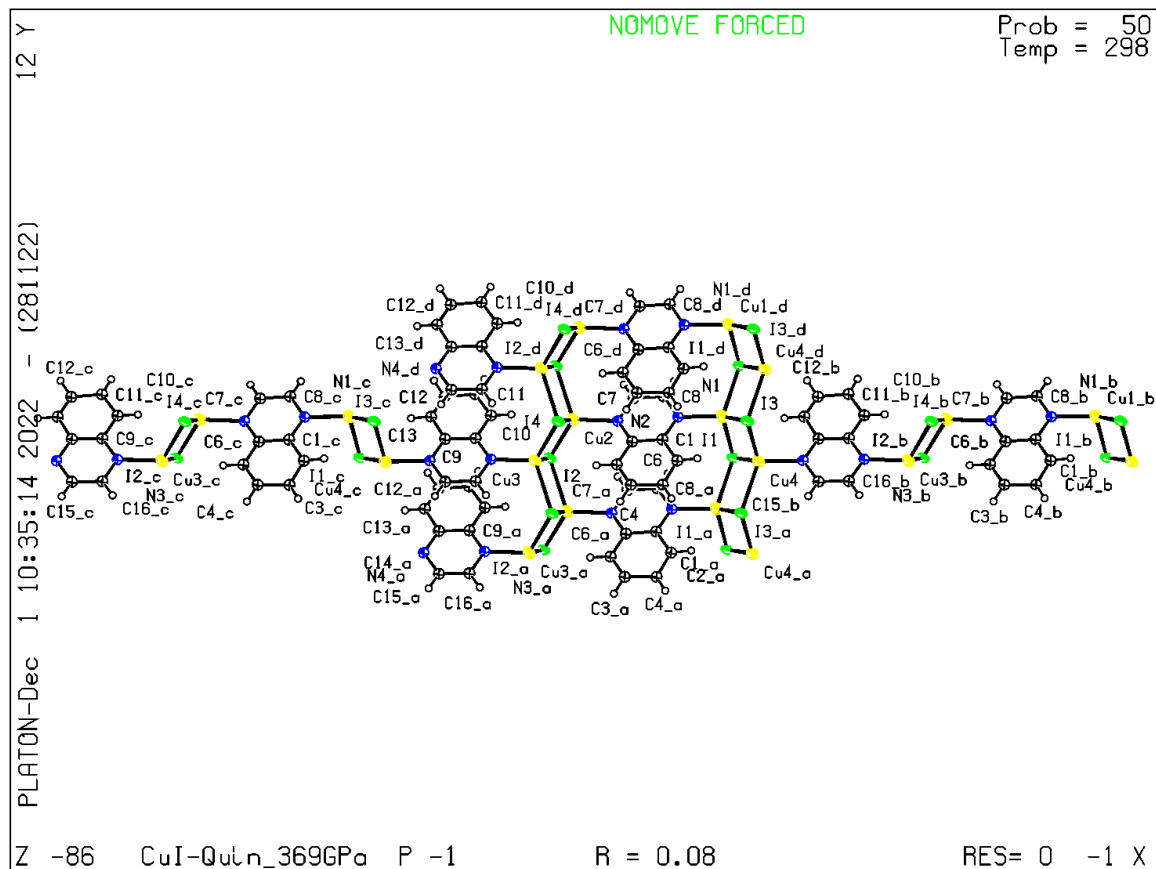
Publication of your CIF in IUCr journals

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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022



checkCIF/PLATON report

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

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: CuI-Quin_420GPa

Bond precision: C-C = 0.0460 Å Wavelength=0.31850

Cell: a=4.2967(2) b=16.9316(9) c=12.4932(16)
 alpha=87.23(1) beta=95.864(10) gamma=94.214(5)
Temperature: 298 K

	Calculated	Reported
Volume	900.92(13)	900.93(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Cu4 I4 N4	0.5(C16 H12 Cu4 I4 N4)
Sum formula	C16 H12 Cu4 I4 N4	C8 H6 Cu2 I2 N2
Mr	1022.10	511.03
Dx, g cm ⁻³	3.768	3.768
Z	2	4
Mu (mm ⁻¹)	4.942	11.524
F000	928.0	928.0
F000'	922.57	
h, k, lmax	5, 21, 15	5, 21, 7
Nref	4001	1222
Tmin, Tmax	0.684, 0.851	0.228, 1.000
Tmin'	0.411	

Correction method= # Reported T Limits: Tmin=0.228 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.305 Theta(max)= 11.781

R(reflections)= 0.0871(798)	wR2(reflections)=
S = 1.022	0.2657(1222)
Npar= 75	

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.046 Ang.
-------------------	---------------------------------------	------------

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27 Report
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem b/2	85 %Fit
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem 636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.977 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.18 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem sub	85 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4 Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.32 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C12 .	3.42 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.45 Ang.
	2-x,-y,-z =	2_755 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .	3.22 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .	3.34 Ang.
	1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.27 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .	3.42 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.36 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C4 .	3.38 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C4 .	3.43 Ang.
	1-x,-y,1-z =	2_656 Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.3 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	8 Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008 Check

PLAT984_ALERT_1_G	The Cu-f' =	0.3201	Deviates from the B&C-Value	0.1660	Check
PLAT984_ALERT_1_G	The I-f' =	-0.4742	Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The N-f' =	0.0061	Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The C-f" =	0.0016	Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The Cu-f" =	1.2651	Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The I-f" =	1.8119	Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The N-f" =	0.0033	Deviates from the B&C-Value	0.0005	Check

3 **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
 28 **ALERT level G** = General information/check it is not something unexpected

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

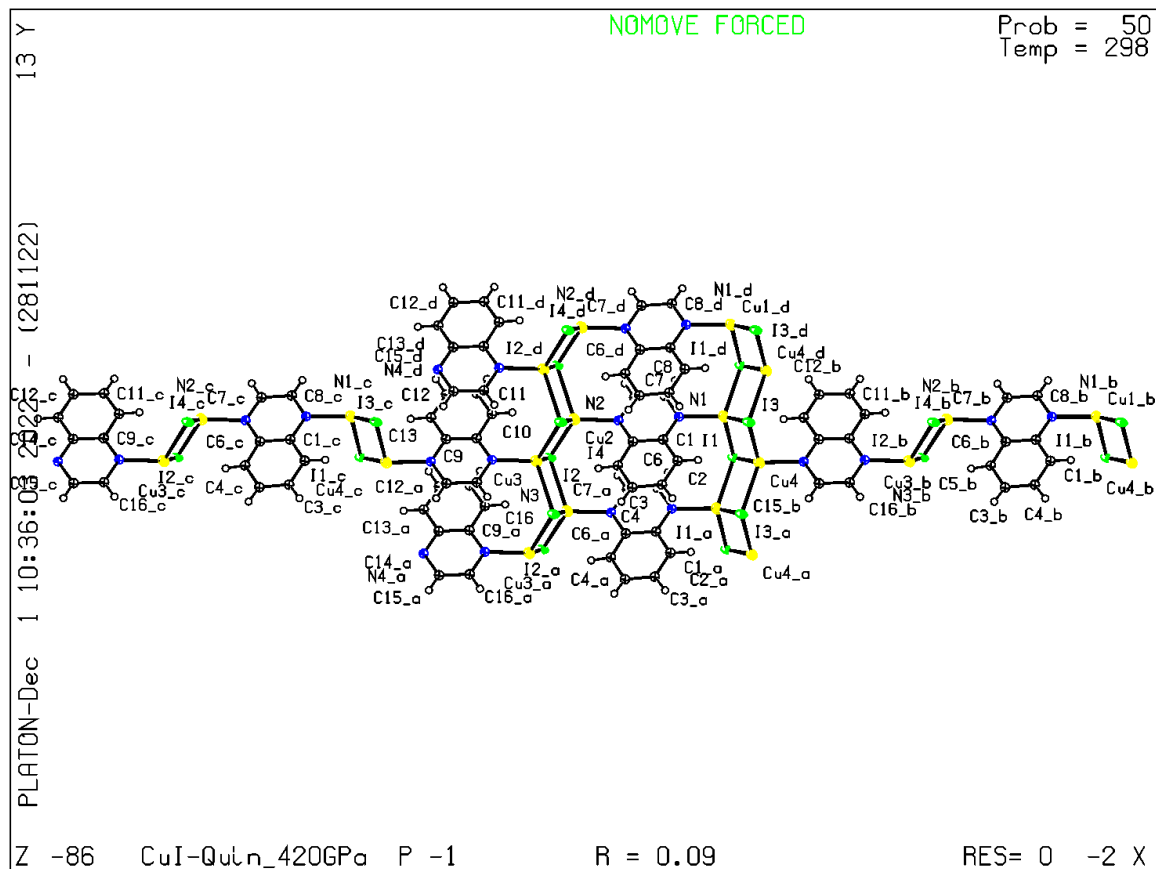
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0728( 780)      wR2(reflections)=
S = 1.070                        0.2302( 1165)
Npar= 75
```

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.11 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03757 Ang.
-------------------	---------------------------------------	--------------

Alert level C

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	b/2	85 %Fit
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		3.0 Note
PLAT702_ALERT_1_C	Angle Calc 107.4(5), Rep 108(3), Dev..		1.20 Sigma
	N4 -CU4 -I3 1_545 1_555 1_455 #		49 Check

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0		0.973 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.14 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.31850 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	85 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4 Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9	-C14	0.19 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1	..C11 .	3.37 Ang.
		1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1	..C11 .	3.44 Ang.
		2-x,-y,-z =	2_755 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1	..C12 .	3.47 Ang.
		1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2	..C7 .	3.22 Ang.
		1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2	..C8 .	3.33 Ang.
		1-x,-y,-z =	2_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3	..C15 .	3.19 Ang.
		2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3	..C16 .	3.29 Ang.
		2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4	..C3 .	3.29 Ang.
		2-x,-y,1-z =	2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4	..C4 .	3.40 Ang.
		2-x,-y,1-z =	2_756 Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.3 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		8 Units

PLAT984_ALERT_1_G	The	C-f' =	0.0033	Deviates from the B&C-Value	-0.0008	Check
PLAT984_ALERT_1_G	The	Cu-f' =	0.3201	Deviates from the B&C-Value	0.1660	Check
PLAT984_ALERT_1_G	The	I-f' =	-0.4742	Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The	N-f' =	0.0061	Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The	C-f" =	0.0016	Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The	Cu-f" =	1.2651	Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The	I-f" =	1.8119	Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The	N-f" =	0.0033	Deviates from the B&C-Value	0.0005	Check

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

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

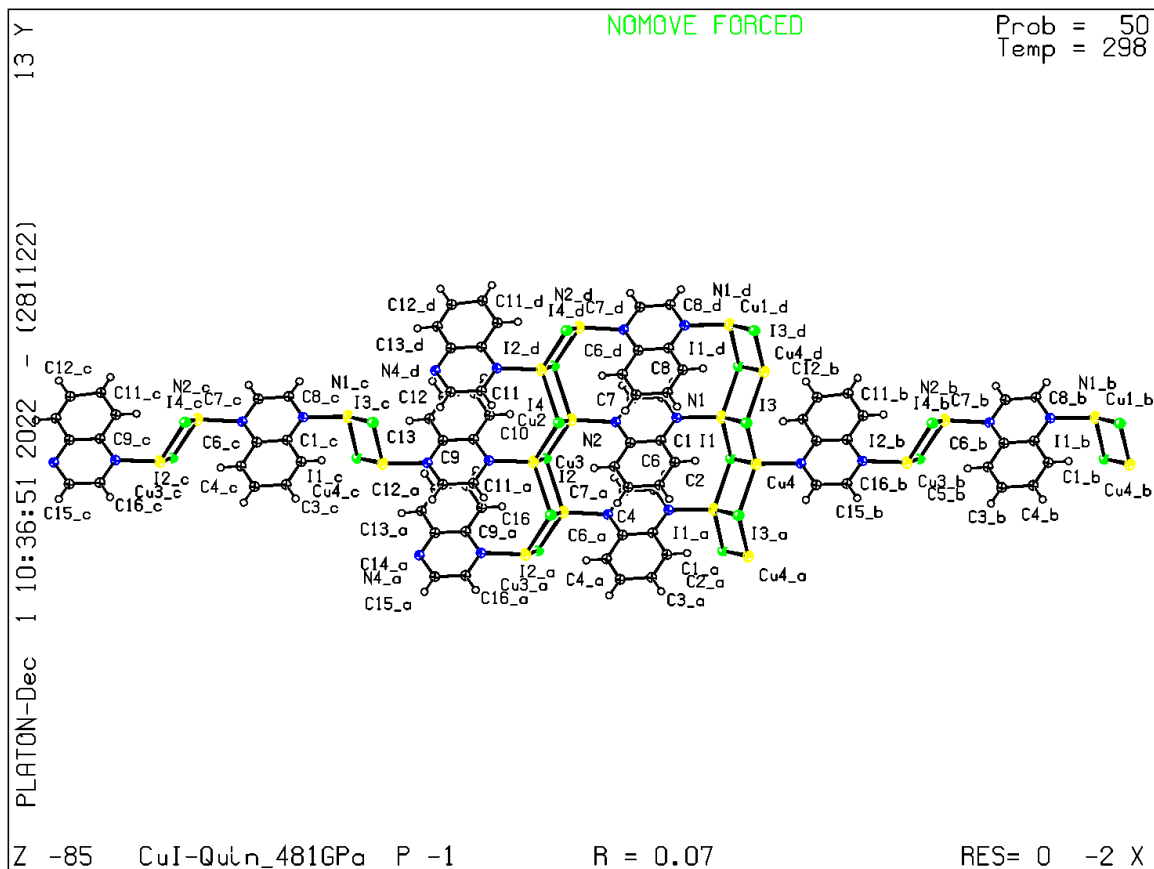
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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

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

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: CuI-Quin_543GPa

Bond precision: C-C = 0.0392 Å Wavelength=0.31850

Cell: a=4.2732 (2) b=16.7757 (8) c=12.3479 (15)
 alpha=86.492 (9) beta=96.410 (9) gamma=94.934 (4)
Temperature: 298 K

	Calculated	Reported
Volume	875.19 (12)	875.19 (12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Cu4 I4 N4	0.5 (C16 H12 Cu4 I4 N4)
Sum formula	C16 H12 Cu4 I4 N4	C8 H6 Cu2 I2 N2
Mr	1022.10	511.03
Dx, g cm ⁻³	3.879	3.878
Z	2	4
Mu (mm ⁻¹)	5.087	11.863
F000	928.0	928.0
F000'	922.57	
h, k, lmax	5, 21, 15	5, 21, 7
Nref	3874	1188
Tmin, Tmax	0.675, 0.847	0.352, 1.000
Tmin'	0.401	

Correction method= # Reported T Limits: Tmin=0.352 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.307 Theta (max)= 11.778

R(reflections)= 0.0706 (779)	wR2(reflections)= 0.2245 (1188)
S = 1.088	Npar= 75

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j) Tensor	4.7 Note
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03921 Ang.

Alert level C

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	b/2	85 %Fit
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.974	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850	Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	85 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Cu1 .	5.3	s.u.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.37	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C12 .	3.40	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.46	Ang.
	2-x,-y,-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .	3.20	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .	3.31	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.22	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .	3.31	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.36	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C4 .	3.38	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.3	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported lmax Differ.	8	Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008	Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660	Check

PLAT984_ALERT_1_G	The	I-f' =	-0.4742	Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The	N-f' =	0.0061	Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The	C-f" =	0.0016	Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The	Cu-f" =	1.2651	Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The	I-f" =	1.8119	Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The	N-f" =	0.0033	Deviates from the B&C-Value	0.0005	Check

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

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

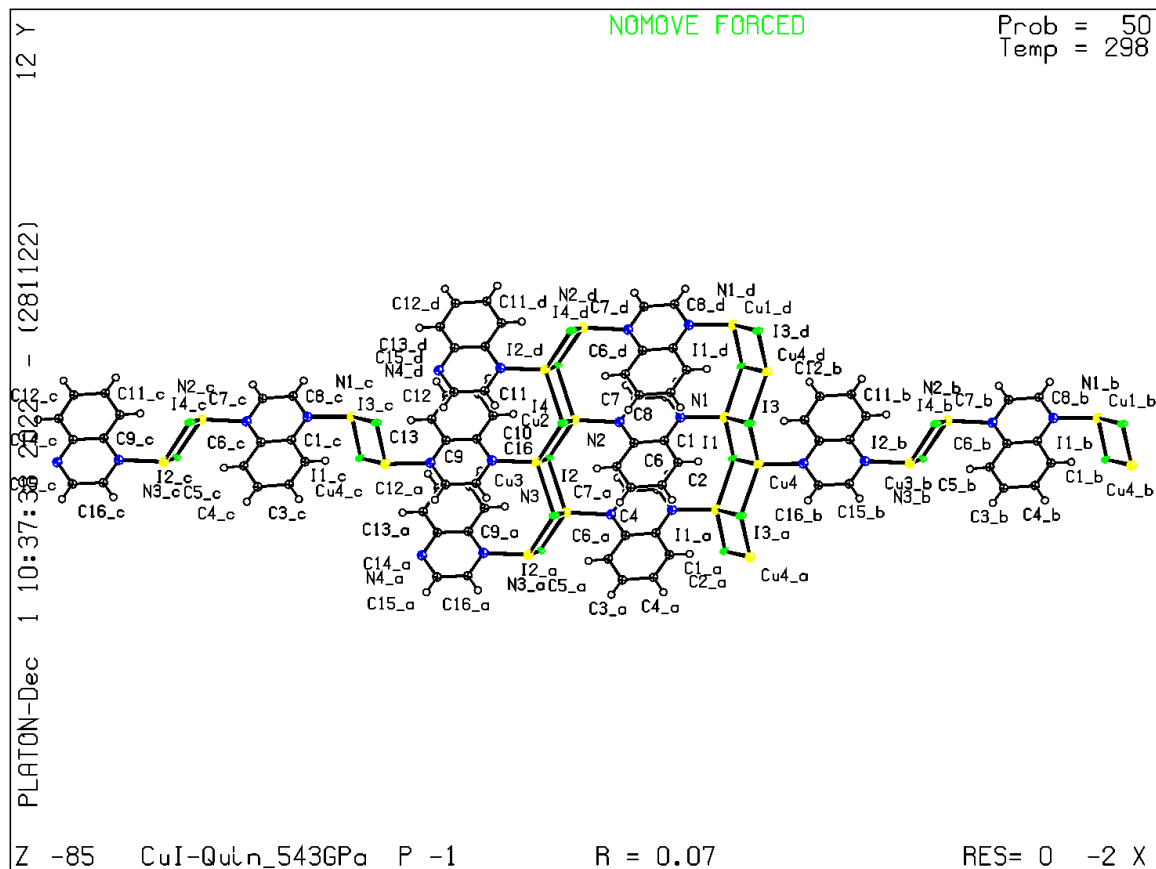
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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



```
R(reflections)= 0.0657( 794)      wR2(reflections)=
S = 1.087                        0.2177( 1173)
Npar= 75
```

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03736 Ang.
-------------------	---------------------------------------	--------------

Alert level C

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	b/2	85 %Fit
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0	0.968	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.31850	Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	85 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.36	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C12 .	3.37	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .	3.48	Ang.
	2-x,-y,-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .	3.18	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .	3.28	Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.17	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .	3.23	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .	3.47	Ang.
	1-x,-y,1-z =	2_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .	3.29	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C4 .	3.40	Ang.
	2-x,-y,1-z =	2_756	Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.3	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	8	Units
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	-0.0008	Check
PLAT984_ALERT_1_G	The Cu-f' = 0.3201 Deviates from the B&C-Value	0.1660	Check

PLAT984_ALERT_1_G	The	I-f' =	-0.4742	Deviates from the B&C-Value	-0.8576	Check
PLAT984_ALERT_1_G	The	N-f' =	0.0061	Deviates from the B&C-Value	-0.0009	Check
PLAT985_ALERT_1_G	The	C-f" =	0.0016	Deviates from the B&C-Value	0.0003	Check
PLAT985_ALERT_1_G	The	Cu-f" =	1.2651	Deviates from the B&C-Value	0.2861	Check
PLAT985_ALERT_1_G	The	I-f" =	1.8119	Deviates from the B&C-Value	2.7116	Check
PLAT985_ALERT_1_G	The	N-f" =	0.0033	Deviates from the B&C-Value	0.0005	Check

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

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

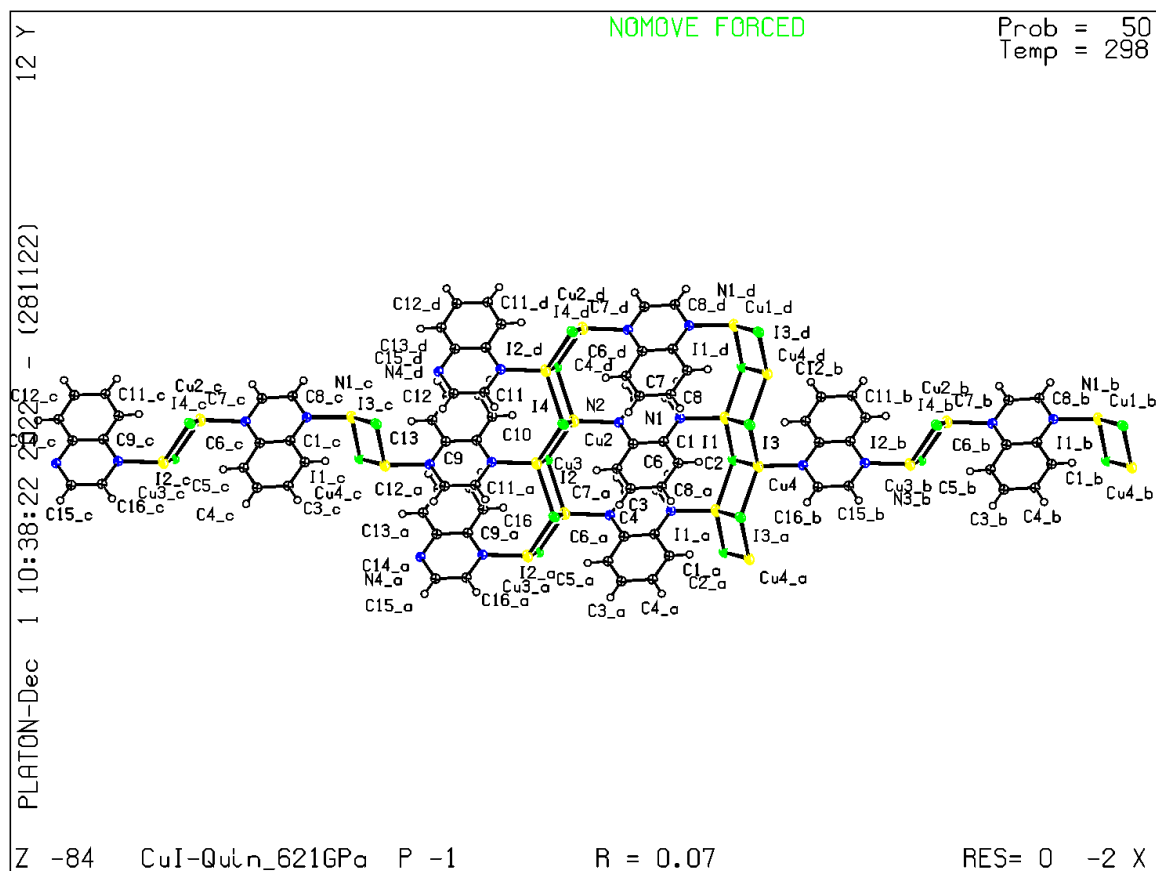
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious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

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

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: CuI-Quin_700GPa

Bond precision: C-C = 0.0381 Å Wavelength=0.31850

Cell: a=4.2434(3) b=16.6059(13) c=12.2104(19)
 alpha=86.177(15) beta=96.911(15) gamma=95.458(7)
Temperature: 298 K

	Calculated	Reported
Volume	848.96(16)	848.96(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Cu4 I4 N4	0.5(C16 H12 Cu4 I4 N4)
Sum formula	C16 H12 Cu4 I4 N4	C8 H6 Cu2 I2 N2
Mr	1022.10	511.03
Dx, g cm ⁻³	3.998	3.998
Z	2	4
Mu (mm ⁻¹)	5.244	12.229
F000	928.0	928.0
F000'	922.57	
h, k, lmax	5, 21, 15	5, 21, 7
Nref	3748	1123
Tmin, Tmax	0.666, 0.843	0.589, 1.000
Tmin'	0.390	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.300 Theta(max)= 11.774

R(reflections)= 0.0667(671)	wR2(reflections)= 0.2242(1123)
S = 1.061	Npar= 75

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

PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	57.12 %
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	20 Report
	N1 N2 N3 N4 C1	etc.
PLAT660_ALERT_1_A	No Valid _diffrn_radiation_type Value Reported .	Please Do !

Alert level B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03814 Ang.
-------------------	---------------------------------------	--------------

Alert level C

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	b/2	85 %Fit
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	636	85 %Fit
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced		Please Do !
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		3.4 Note
PLAT368_ALERT_2_C	Short C(sp2)-C(sp2) Bond C4 - C5 .		1.21 Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0		0.957 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.500 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.13 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.31850 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	85 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4 Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1 -C6		0.25 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14		0.16 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .		3.30 Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C12 .		3.34 Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I1 ..C11 .		3.40 Ang.
	2-x,-y,-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C7 .		3.14 Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .		3.22 Ang.
	1-x,-y,-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I2 ..C8 .		3.48 Ang.
	2-x,-y,-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .		3.19 Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C16 .		3.24 Ang.
	2-x,-y,1-z =	2_756	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3 ..C15 .		3.48 Ang.
	1-x,-y,1-z =	2_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact I4 ..C3 .		3.32 Ang.
	2-x,-y,1-z =	2_756	Check

```

PLAT432_ALERT_2_G Short Inter X...Y Contact I4 ..C4 . 3.40 Ang.
2-x,-y,1-z = 2_756 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.3 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 8 Units
PLAT984_ALERT_1_G The C-f' = 0.0033 Deviates from the B&C-Value -0.0008 Check
PLAT984_ALERT_1_G The Cu-f' = 0.3201 Deviates from the B&C-Value 0.1660 Check
PLAT984_ALERT_1_G The I-f' = -0.4742 Deviates from the B&C-Value -0.8576 Check
PLAT984_ALERT_1_G The N-f' = 0.0061 Deviates from the B&C-Value -0.0009 Check
PLAT985_ALERT_1_G The C-f" = 0.0016 Deviates from the B&C-Value 0.0003 Check
PLAT985_ALERT_1_G The Cu-f" = 1.2651 Deviates from the B&C-Value 0.2861 Check
PLAT985_ALERT_1_G The I-f" = 1.8119 Deviates from the B&C-Value 2.7116 Check
PLAT985_ALERT_1_G The N-f" = 0.0033 Deviates from the B&C-Value 0.0005 Check

```

```

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

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
20 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock CuI-Quin_700GPa - ellipsoid plot

