checkCIF/PLATON report (full structural check)

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

CIF dictionary
Interpreting this report

Datablock: PIYA

Bond precision: C-C = 0.0118 A Wavelength=0.71073

Cell: a=9.0686(4) b=10.1876(4) c=27.0683(13)
alpha=90 beta=90 gamma=90

	Calculated	Reported
Volume	2500.77(19)	2500.8(2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C13 H7 Br Cr O3	C13 H7 Br Cr O3
Sum formula	C13 H7 Br Cr O3	C13 H7 Br Cr O3
Mr	343.09	343.10
Dx,g cm-3	1.822	1.823
Z	8	8
Mu (mm-1)	4.105	4.110
F000	1344.0	1344.0
F000'	1344.87	
h,k,lmax	11,13,34	11,13,34
Nref	3116(5476)	5466
Tmin,Tmax	0.416,0.848	0.471,0.850
Tmin'	0.377	

Correction method= AbsCorr=NUMERICAL
Data completeness= 1.75(1.00) Theta(max)= 27.000
R(reflections)= 0.0250(3407) wR2(reflections)= wR= 0.0270(3407)
S = 1.880 Npar= 368

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

PLAT432_ALERT_2_B Short Inter X...Y Contact Br1B .. C3B .. 3.23 Ang.

Alert level C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 10 for a non-centrosymmetric structure, where ZMAX > 18
sine(theta)/lambda 0.6388
Proportion of unique data used 0.6233
Ratio reflections to parameters 9.2582
PLAT164_ALERT_4_C Nr. of Refined C-H H-Atoms in Heavy-At Struct... 14
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ... 12
PLAT350_ALERT_3_C Short C-H Bond (0.96A) C4A - H4A ... 0.80 Ang.
PLAT350_ALERT_3_C Short C-H Bond (0.96A) C5A - H5A ... 0.81 Ang.
PLAT350_ALERT_3_C Short C-H Bond (0.96A) C9A - H9A ... 0.82 Ang.

Alert level G

ABSTM02_ALERT_3_G The ratio of expected to reported Tmax/Tmin(RR) is > 1.10
Tmin and Tmax reported: 0.471 0.850
Tmin and Tmax expected: 0.422 0.848
RR = 1.115
Please check that your absorption correction is appropriate.
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 27.00
From the CIF: _reflns_number_total 5466
Count of symmetry unique reflns 3116
Completeness (_total/calc) 175.42%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2350
Fraction of Friedel pairs measured 0.754
Are heavy atom types Z>Si present yes

0 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
6 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

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

Publication of your CIF

A full structural check has been run on your CIF. This includes checks on:

- CIF syntax and construction
- Cell and geometry details
- Space-group symmetry
- Anisotropic displacement parameters

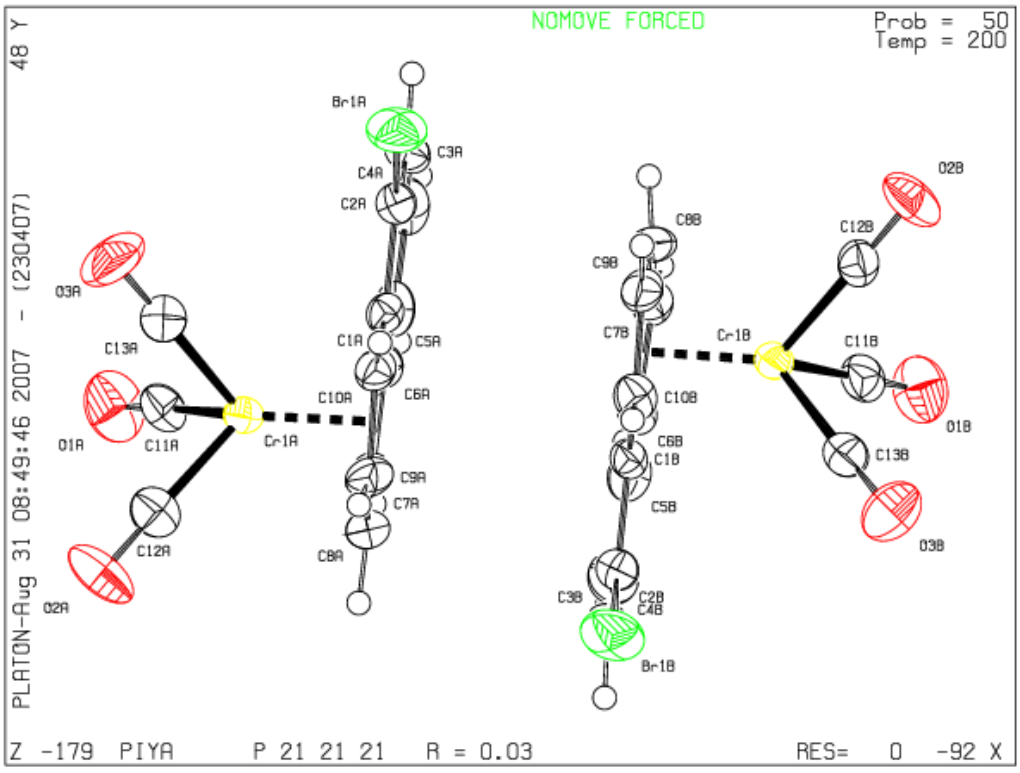
These full checks give an indication of potential problems with your CIF. Please note that if you intend to submit your CIF for publication in Acta Crystallographica Section C or E, you must make sure that full publication checks are run on the final version of the CIF prior to submission.

If you intend to submit to another section of Acta Crystallographica, Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least basic structural checks are run on the final version of your CIF prior to submission.

To submit your CIF for publication in an IUCr journal click here.

PLATON version of 23/04/2007; check.def file version of 23/04/2007

Datablock PIYA - ellipsoid plot



Download CIF editor (enCIFer) from the CCDC

Test a new CIF entry