checkCIF/PLATON report (full structural check)

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

CIF dictionary
Interpreting this report

Datablock: I

Bond precision: C-C = 0.0118 A Wavelength=0.71073
Cell: a=9.3231(17) b=26.611(6) c=18.218(4)
alpha=90 beta=91.596(7) gamma=90

	Calculated	Reported
Volume	4518.1(16)	4518.0(16)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C42 H50 O6 P2 Rh, C H Cl3, B F4	C42 H50 O6 P2 Rh +, B F4 -, C H CL3
Sum formula	C43 H51 B Cl3 F4 O6 P2 Rh	C43 H51 B Cl3 F4 O6 P2 Rh
Mr	1021.85	1021.85
Dx,g cm-3	1.502	1.502
Z	4	4
Mu (mm-1)	0.689	0.689
F000	2096.0	2096.0
F000'	2095.05	
h,k,lmax	11,33,22	10,33,22
Nref	9501(18583)	15833
Tmin,Tmax	0.726,0.973	0.785,0.973
Tmin'	0.543	

Correction method= AbsCorr=MULTI-SCAN
Data completeness= 1.67(0.85) Theta(max)= 26.420
R(reflections)= 0.0635(13832) wR2(reflections)= 0.1502(15833)
S = 1.070 Npar= 645

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 Low	0.87
PLAT035_ALERT_1_A	No _chemical_absolute_configuration info given .	?
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	88

Alert level B

PLAT063_ALERT_3_B	Crystal Probably too Large for Beam Size	0.90 mm
PLAT222_ALERT_3_B	Large Non-Solvent H Ueq(max)/Ueq(min) ...	4.17 Ratio
PLAT431_ALERT_2_B	Short Inter HL..A Contact Cl8A .. O33 ..	2.93 Ang.

Alert level C

PLAT042_ALERT_1_C	Calc. and Rep. MoietyFormula Strings Differ	?
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	1
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) ...	3.33 Ratio
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) ...	3.12 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Ueq(max)/Ueq(min) ...	3.92 Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Rh1 - P2 ..	6.03 su
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors for	C7
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors for	C8
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors for	B1
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors for	B2
PLAT302_ALERT_4_C	Anion/Solvent Disorder	10.00 Perc.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang ...	12
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	72.00 A**3

Alert level G

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 26.42
From the CIF: _reflns_number_total 15833
Count of symmetry unique reflns 9501
Completeness (_total/calc) 166.65%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 6332
Fraction of Friedel pairs measured 0.666
Are heavy atom types Z>Si present yes

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PLAT791_ALERT_1_G Confirm the Absolute Configuration of C21    ...          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C22    ...          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C23    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C24    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C25    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C26    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C31    ...          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C32    ...          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C33    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C34    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C35    ...          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C36    ...          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .....          1
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  3 ALERT level A = In general: serious problem
  3 ALERT level B = Potentially serious problem
 13 ALERT level C = Check and explain
 14 ALERT level G = General alerts; check

 14 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
  7 ALERT type 3 Indicator that the structure quality may be low
  6 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

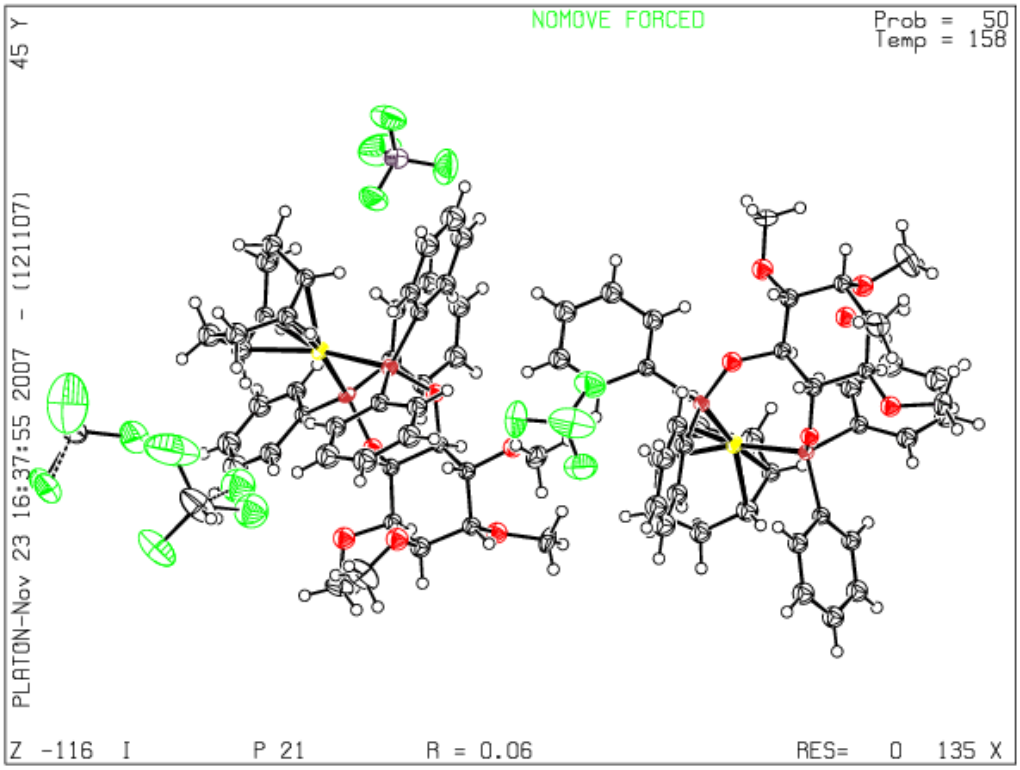
These full checks give an indication of potential problems with your CIF. Please note that if you intend to submit your CIF for publication in Acta Crystallographica Section C or E, you must make sure that full publication checks are run on the final version of the CIF prior to submission.

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 12/11/2007; check.def file version of 29/10/2007

Datablock I - ellipsoid plot



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