



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi002

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: rudi002

Bond precision: C-C = 0.0109 Å

Wavelength=1.54178

Cell: a=14.1859(5) b=14.2782(5) c=21.3407(8)
 alpha=89.739(2) beta=72.199(2) gamma=74.792(2)
Temperature: 100 K

	Calculated	Reported
Volume	3958.0(3)	3958.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	3(C H B11 Cl11), Gd H16 O8, 3(C6 H4 F2)	Gd H16 O8, 3(C H B11 Cl11), 3(C6 H4 F2)
Sum formula	C21 H31 B33 Cl33 F6 Gd O8	C21 H31 B33 Cl33 F6 Gd O8
Mr	2209.29	2209.29
Dx, g cm ⁻³	1.854	1.854
Z	2	2
Mu (mm ⁻¹)	16.150	16.151
F000	2130.0	2130.0
F000'	2140.39	
h, k, lmax	17, 17, 26	17, 17, 26
Nref	16222	15871
Tmin, Tmax	0.064, 0.072	0.493, 0.754
Tmin'	0.006	

Correction method= # Reported T Limits: Tmin=0.493 Tmax=0.754
AbsCorr = MULTISCAN

Data completeness= 0.978

Theta(max)= 74.628

R(reflections)= 0.0497(15348)

wR2(reflections)=
0.1168(15871)

S = 1.028

Npar= 927

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.



Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc.: 3(C H B11 Cl11), Gd H16 O8, 3(C6 H4 F2)	
	Rep.: Gd H16 O8, 3(C H B11 Cl11), 3(C6 H4 F2)	
PLAT213_ALERT_2_C	Atom Cl1 has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom Cl2 has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C	Atom Cl3 has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C	Atom Cl4 has ADP max/min Ratio	3.8 prolat
PLAT213_ALERT_2_C	Atom Cl7 has ADP max/min Ratio	3.5 prolat
PLAT214_ALERT_2_C	Atom O3 (Anion/Solvent) ADP max/min Ratio	4.2 prolat
PLAT214_ALERT_2_C	Atom O8 (Anion/Solvent) ADP max/min Ratio	4.1 prolat
PLAT244_ALERT_4_C	Low MinorResAtom Ueq as Compared to Neighbours	Gd1 Check
PLAT244_ALERT_4_C	Low MinorResAtom Ueq as Compared to Neighbours	C4 Check
PLAT244_ALERT_4_C	Low MinorResAtom Ueq as Compared to Neighbours	C5 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	4.0 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	2.2 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4)	2.2 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 6)	2.1 Note
PLAT314_ALERT_2_C	Small Angle for H2O: Metal-O4 -H4A .	90.25 Degree
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C4 -C9 .	1.37 Ang.
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C10 -C15 .	1.36 Ang.
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C16 -C21 .	1.37 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01089 Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C1 - H1 .	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C2 - H2 .	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C3 - H3 .	1.12 Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	56 Report
	-1 16 0, 0 16 0, 1-16 1, 2 -4 1, 1 -1 1, -1 0 1,	
	-1 16 1, 0 16 1, -1 -4 2, 0 16 2, -15 -5 3, 0 16 3,	
	-15 -6 4, 16 2 4, -3 14 5, -1-16 6, 10-10 6, -14 -5 6,	
	-14 -4 6, 0 2 6, -14 -6 7, -14 -5 7, 16 -1 10, 16 2 10,	
	15 -3 11, 16 0 11, 16 1 11, 16 4 11, 5 15 11, 15 -2 12,	
	(26 More NOT listed: see .ckf listing file)	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.35Ang From O6	1.56 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.86Ang From Gd1	-1.96 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.81Ang From O7 .	1.17 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.09Ang From O6 .	1.00 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.88Ang From O4 .	0.84 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.79Ang From O4 .	-1.08 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.49Ang From O7 .	-0.82 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.99Ang From O8 .	-0.73 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H1A .	-0.42 eA-3

PLAT977_ALERT_2_C	Check Negative Difference Density on H1B	.	-0.64 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H2A	.	-0.32 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4B	.	-0.35 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H5B	.	-0.31 eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		3	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms		1	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		16	Report
	H1A H1B H2A H2B H3A H3B H4A H4B			
	H5A H5B H6A H6B H7A H7B H8A H8B			
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		29.11	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002	Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT303_ALERT_2_G	Full Occupancy Atom H4A with # Connections		2.00	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C2	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C3	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl2 ..Cl3	.	3.30	Ang.
	-x,1-y,2-z =		2_567	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl14 ..Cl30	.	3.32	Ang.
	-1+x,y,z =		1_455	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl17 ..Cl25	.	3.15	Ang.
	x,y,z =		1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl22 ..Cl27	.	3.39	Ang.
	x,-1+y,z =		1_545	Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H1B ..CL13	.	2.93	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H6B ..CL18	.	2.91	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #		3	Note
	C H B11 Cl11			
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd1 (III)	.	3.43	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		7	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=		3.22	Note
	0 0 1,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		294	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
	0 2 6,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		5	Note
	-1 -4 2, -1 0 1, 0 2 6, 1 -1 1, 2 -4 1,			
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		3.504	Note
	Predicted wR2: Based on SigI**2 3.33 or SHELX Weight 11.35			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..		!	Note

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
38 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
27 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
41 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
10 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

Datablock rudi002 - ellipsoid plot

