

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DP_PDP067_ErRe3

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: DP_PDP067_ErRe3

Bond precision: C-C = 0.0165 Å

Wavelength=0.71073

Cell: a=41.1853(10) b=41.1853(10) c=7.6318(3)
 alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	11210.9(7)	11210.9(7)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	3(C30 H30 Er Re3), 0.167(C6 H6), C2	?
Sum formula	C93 H91 Er3 Re9	C93 H91 Er3 Re9
Mr	3386.33	3386.23
Dx, g cm-3	3.010	3.009
Z	6	6
Mu (mm-1)	17.882	17.882
F000	9168.0	9168.0
F000'	9119.13	
h, k, lmax	63, 63, 11	63, 63, 11
Nref	9579	9537
Tmin, Tmax	0.531, 0.699	0.380, 0.720
Tmin'	0.116	

Correction method= # Reported T Limits: Tmin=0.380 Tmax=0.720
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 33.240

R(reflections)= 0.0543(7641)

wR2(reflections)= 0.1202(9537)

S = 1.082

Npar= 328

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

PLAT971_ALERT_2_A	Check	Calcd	Resid.	Dens.	0.77A	From Re2	3.94 eA-3
PLAT971_ALERT_2_A	Check	Calcd	Resid.	Dens.	0.64A	From Re1	3.75 eA-3
PLAT971_ALERT_2_A	Check	Calcd	Resid.	Dens.	0.71A	From Re3	3.61 eA-3
PLAT972_ALERT_2_A	Check	Calcd	Resid.	Dens.	2.24A	From C31	-5.47 eA-3

Alert level B

PLAT315_ALERT_2_B	Singly Bonded Carbon Detected (H-atoms Missing).						C31 Check
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.69A	From Re2	3.44 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.65A	From Re2	3.42 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.80A	From Re3	3.41 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.78A	From Re3	3.35 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.66A	From Re2	3.34 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.67A	From Re1	3.23 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.72A	From Re2	3.17 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.71A	From Re1	3.15 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.81A	From Re3	3.14 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.64A	From Re1	3.06 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.66A	From Re2	2.98 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.67A	From Re1	2.93 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.67A	From Re1	2.89 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.72A	From Er1	2.82 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.89A	From Re1	2.78 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.71A	From Re2	2.74 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.73A	From Re2	2.70 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.71A	From Re1	2.68 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.72A	From Er1	2.66 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.66A	From Er1	2.62 eA-3
PLAT971_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.69A	From Er1	2.59 eA-3
PLAT972_ALERT_2_B	Check	Calcd	Resid.	Dens.	0.83A	From C31	-3.38 eA-3
PLAT972_ALERT_2_B	Check	Calcd	Resid.	Dens.	1.11A	From C26	-2.78 eA-3

Alert level C

PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	3.2 oblate				
PLAT213_ALERT_2_C	Atom C19	has ADP max/min Ratio	3.1 prolat				
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01647 Ang.					
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	7.479 Check					
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report					
PLAT924_ALERT_1_C	The Reported and Calculated Rho(min) Differ by .	1.70 eA-3					
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.65A	From Re3	2.44 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.10A	From C26	-2.46 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.20A	From C22	-2.45 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.66A	From C17	-2.40 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.65A	From C17	-2.40 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.28A	From C18	-2.28 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.40A	From C31	-2.00 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.69A	From C26	-1.99 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.31A	From C25	-1.99 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.48A	From C30	-1.97 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.86A	From C11	-1.90 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.92A	From C18	-1.90 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.41A	From C5	-1.87 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.08A	From C8	-1.87 eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.08A	From C8	-1.87 eA-3

PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.95A	From C8	-1.80 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.93A	From C28	-1.74 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.35A	From C19	-1.69 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.88A	From C18	-1.64 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.95A	From C4	-1.60 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.03A	From C5	-1.60 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.38A	From Re1	-1.59 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.12A	From C22	-1.58 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H3		-0.46 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H8		-0.54 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H17		-0.45 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H20		-0.39 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H22		-1.02 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H23		-1.14 eA-3

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	473.71	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C32	Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32	Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C33	Constrained at	0.3333 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	50%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.03	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.03	Ang.
	1-y,x-y,z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.03	Ang.
	1-x+y,1-x,z =	3_665	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.13	Ang.
	1/3+x-y,-1/3+x,5/3-z =	18_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.13	Ang.
	4/3-x,2/3-y,5/3-z =	16_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C32	2.13	Ang.
	1/3+y,2/3-x+y,5/3-z =	17_556	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C33	2.72	Ang.
	1/3+x-y,-1/3+x,5/3-z =	18_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C33	2.72	Ang.
	4/3-x,2/3-y,5/3-z =	16_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C33	2.72	Ang.
	1/3+y,2/3-x+y,5/3-z =	17_556	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C31	3.15	Ang.
	4/3-x,2/3-y,5/3-z =	16_656	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C32	2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C32	2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C32	2.03	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	377	Check
	C33 -C31 -C32 1.555 1.555 3.665	12.00	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	38	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	5	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

35 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
76 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
8 ALERT type 4 Improvement, methodology, query or suggestion
0 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 05/12/2020; check.def file version of 05/12/2020

