

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: MgEr

Bond precision: C-C = 0.0108 Å Wavelength=0.71073

Cell: a=12.9581(7) b=14.1259(6) c=14.2362(6)
 alpha=98.689(4) beta=107.817(4) gamma=116.987(5)
Temperature: 150 K

	Calculated	Reported
Volume	2077.6(2)	2077.64(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H90 Er2 Mg2 O22, 2(C6 H16 N)	C50 H90 Er2 Mg2 O22, 2(C6 H16 N)
Sum formula	C62 H122 Er2 Mg2 N2 O22	C62 H122 Er2 Mg2 N2 O22
Mr	1630.76	1630.75
Dx,g cm-3	1.303	1.303
Z	1	1
Mu (mm-1)	2.083	2.083
F000	844.0	844.0
F000'	843.92	
h,k,lmax	16,17,17	16,17,17
Nref	8485	8395
Tmin,Tmax	0.819,0.864	0.743,1.000
Tmin'	0.812	

Correction method= # Reported T Limits: Tmin=0.743 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.371

R(reflections)= 0.0473(7318) wR2(reflections)= 0.1113(8395)

S = 1.077 Npar= 426

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

PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 108 Ang3

Alert level C

PLAT213_ALERT_2_C Atom C3	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C Atom C5	has ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C Atom C18	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C Atom C19	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C Large Non-Solvent C	Ueq(max)/Ueq(min) Range	5.1	Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C2	-- C5 ..	0.17	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12	-- C15 ..	0.19	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12	-- C15B ..	0.19	Ang.
PLAT241_ALERT_2_C High	Ueq as Compared to Neighbors for	03	Check
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	C2	Check
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	C12	Check
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	C17	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.0108	Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		2	Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms		2	Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C12	-- C13 ..	5.7	su
PLAT230_ALERT_2_G Hirshfeld Test Diff for C12	-- C14 ..	7.1	su
PLAT230_ALERT_2_G Hirshfeld Test Diff for C12	-- C13B ..	7.0	su
PLAT230_ALERT_2_G Hirshfeld Test Diff for C12	-- C14B ..	6.6	su
PLAT300_ALERT_4_G Atom Site Occupancy of >C13	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C14	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C15	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C13B	is Constrained at	0.375	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C14B	is Constrained at	0.375	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C15B	is Constrained at	0.375	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C13_a	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C14_a	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C15_a	is Constrained at	0.625	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C13B_a	is Constrained at	0.375	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C14B_a	is Constrained at	0.375	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C15B_a	is Constrained at	0.375	Check
PLAT301_ALERT_3_G Main Residue Disorder	Percentage =	8	Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .		1.17	Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints		12	Note

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

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

13 **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

0 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

17 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*, 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.

