

Datablock: q

Bond precision:	C-C = 0.0057 A	Wavelength=0.71073
Cell:	a=13.3891(7) b=13.5291(7) c=16.1602(7)	
	alpha=86.016(2) beta=66.320(2) gamma=62.099(2)	
Temperature	110 K	
:		
	Calculated	Reported
Volume	2343.7(2)	2343.7(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H48 F18 Gd2 N12 O16, 2(C4 H8 O2) [+ solvent]	C52 H48 F18 Gd2 N12 O16, 2(C4 H8 O2)
Sum formula	C60 H64 F18 Gd2 N12 O20 [+ solvent]	C60 H64 F18 Gd2 N12 O20
Mr	1929.73	1929.73
Dx,g cm-3	1.367	1.367
Z	1	1
Mu (mm-1)	1.499	1.499
F000	958.0	958.0
F000'	958.29	
h,k,lmax	18,18,22	18,18,22
Nref	12452	12294
Tmin,Tmax	0.819,0.842	0.584,0.650
Tmin'	0.819	
Correction method=	# Reported T Limits: Tmin=0.584	
Tmax=0.650 AbsCorr =	MULTI-SCAN	
Data completeness=	0.987	Theta(max)= 29.000
R(reflections)=	0.0446(10312)	wR2(reflections)= 0.0974(12294)
S =	0.990	Npar= 511

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

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	42	Report
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Gd01	1.28	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.00Ang From O2S	.	0.58	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H19	.	-0.46	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		3	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		2	Report
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
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C1	Check

And 2 other PLAT242 Alerts

PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C9	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C17	Check

PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1S	.	108.8	Degree
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		11	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C4 H8 O2			
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd01 (III)	.	3.47	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	116	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		15	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.9	Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
5 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. 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

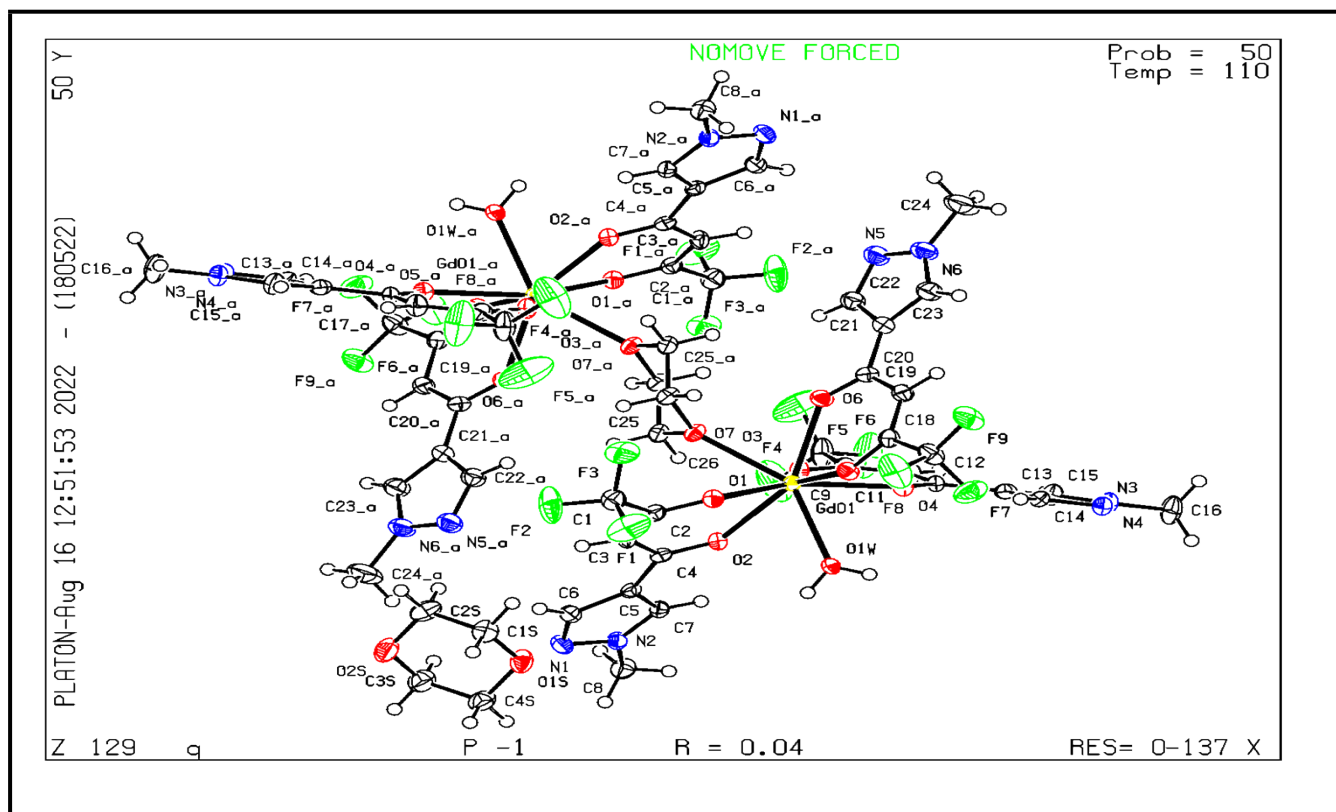
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/05/2022; check.def file version of 17/05/2022

Datablock q - ellipsoid plot



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