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# A search for lepton-flavour violating $\tau \rightarrow 3\mu$ decays with the ATLAS detector

The ATLAS Collaboration

A search for charged lepton flavour violation in  $\tau \rightarrow 3\mu$  decays is performed in  $pp$  collisions at a centre-of-mass energy of 13 TeV using ATLAS data collected between 2016 and 2018, corresponding to an integrated luminosity of  $137 \text{ fb}^{-1}$ . The search focuses on the electroweak  $W \rightarrow \tau\nu$  production channel. Data are collected using two-muon and three-muon triggers and a multivariate analysis is used to separate the signal from the background. An unbinned likelihood fit is then performed to the resulting three-muon invariant mass spectrum and the data are found to be compatible with the background-only hypothesis. The observed (expected) limit on the branching ratio  $B(\tau \rightarrow 3\mu)$  is found to be  $8.7 \times 10^{-8}$  ( $7.5 \times 10^{-8}$ ) at 90% CL.

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## 1 Introduction

In the Standard Model (SM), flavour is not a fundamental symmetry and its violation is observed in both the neutrino [1] and quark sectors [2, 3]. It is therefore natural to question whether flavour conservation is violated for charged leptons. Although neutrino oscillations provide a route for charged Lepton Flavour Violation (cLFV) in the SM, the corresponding branching ratios ( $B$ ) are vanishingly small, of the order  $10^{-55}$  [4]. Any observation of cLFV would therefore be unambiguous evidence of physics beyond the SM (BSM). Searches for cLFV have been carried out in the decays of both muons and  $\tau$ -leptons, however, the most stringent limits on cLFV for the  $\tau$ -lepton are currently about four orders of magnitude weaker than those for the muon decay channel [5, 6]. Theoretical arguments suggest that new physics effects would be stronger for the heavier  $\tau$ -lepton [7]. Several BSM theoretical frameworks provide an enhancement to the rate of cLFV, with predicted  $\tau$ -lepton flavour violating  $B$  of the order  $10^{-9}$  [8–12], potentially detectable by current experiments.

This paper presents a new search for the cLFV process  $\tau^\pm \rightarrow \mu^\pm \mu^\mp \mu^\pm$ , henceforth referred to as  $\tau \rightarrow 3\mu$ . The most stringent limits on this process are obtained by the Belle II and LHCb experiments. The Belle-II experiment set an observed (expected) limit of  $1.9 \times 10^{-8}$  ( $1.8 \times 10^{-8}$ ) at 90% confidence level (CL) [6],<sup>1</sup> using  $424 \text{ fb}^{-1}$  of  $e^+e^-$  collision data with a centre-of-mass energy near the  $\Upsilon(4S)$  resonance. Other stringent limits were set using  $e^+e^-$  collision data by the Belle experiment with an observed limit of  $2.1 \times 10^{-8}$  [13] using  $782 \text{ fb}^{-1}$  of data, and by the BaBar experiment with an observed (expected) limit of  $3.3 \times 10^{-8}$  ( $4.0 \times 10^{-8}$ ) [14] using  $468 \text{ fb}^{-1}$  of data. Using proton–proton ( $pp$ ) collision data at the Large Hadron Collider (LHC) at  $\sqrt{s} = 13 \text{ TeV}$ , the LHCb experiment set an observed (expected) limit of  $1.9 \times 10^{-8}$  ( $2.0 \times 10^{-8}$ ) [15] using  $5.4 \text{ fb}^{-1}$  of data collected during Run 2, matching the previous most stringent observed limit. The CMS experiment set an observed (expected) limit of  $2.9 \times 10^{-8}$  ( $2.4 \times 10^{-8}$ ) [16] using  $131 \text{ fb}^{-1}$  of data collected during Run 2. The most recent analysis by the ATLAS experiment used  $20.3 \text{ fb}^{-1}$  of data collected during Run 1 at  $\sqrt{s} = 8 \text{ TeV}$  to set an observed (expected) limit of  $37.6 \times 10^{-8}$  ( $39.4 \times 10^{-8}$ ) [17].

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<sup>1</sup> All limits are reported at 90% CL in line with previous results.

The search for  $\tau \rightarrow 3\mu$  presented here uses  $137 \text{ fb}^{-1}$  of  $pp$  collision data at  $\sqrt{s} = 13 \text{ TeV}$  collected from 2016–2018 by the ATLAS experiment. This is the first ATLAS search for this process using Run 2 data, and supersedes the previous result. At the LHC,  $\tau$ -leptons are produced in large quantities either through the decays of heavy flavour hadrons, referred to as the heavy-flavour (HF) signal, or through the decays of  $W$  and  $Z$  bosons, including  $W$  bosons from top-quark decays, referred to as the electroweak (EW) signal. Although the HF signal, primarily composed of  $D_s \rightarrow \tau\nu_\tau$  decays, dominates at the LHC, the  $\tau$ -leptons produced by the EW signal have on average a larger transverse momentum and are better isolated from hadronic activity. A large fraction of the HF signal is not recorded by ATLAS due to trigger limitations, and the analysis is instead optimised for the dominant  $W \rightarrow \tau\nu_\tau$  contribution. The statistical interpretation considers both the full EW and HF  $\tau$ -lepton production mechanisms, which are henceforth referred to as the signal.

The signature of interest consists of three muons from a secondary vertex, with a three-muon invariant mass  $m_{3\mu}$  consistent with the  $\tau$ -lepton mass. The data were collected using multi-muon triggers. Candidate three-muon vertices are then reconstructed. Simulated signals and sideband data are used in a multivariate analysis (MVA) to classify events optimally in view of the small expected signal-to-background ratio. Both the signal and background are parameterised using functional forms in the  $m_{3\mu}$  spectrum. A signal-plus-background fit is performed simultaneously in all fit categories, allowing the smooth background to be estimated from the data sidebands while searching for a resonant signal close to the  $\tau$ -lepton mass.

## 2 ATLAS detector

The ATLAS experiment [18] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a near  $4\pi$  coverage in solid angle.<sup>2</sup> It consists of an inner tracking detector surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer.

The inner detector (ID) covers the pseudorapidity range  $|\eta| < 2.5$ . It consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors, with the addition for Run 2 of an inner pixel layer known as the insertable B-layer (IBL). Lead/liquid-argon (LAr) sampling calorimeters provide electromagnetic (EM) energy measurements with high granularity within the region  $|\eta| < 3.2$ . A steel/scintillator-tile hadronic calorimeter covers the central pseudorapidity range ( $|\eta| < 1.7$ ). The endcap and forward regions are instrumented with LAr calorimeters for EM and hadronic energy measurements up to  $|\eta| = 4.9$ .

The muon spectrometer (MS) surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 Tm across most of the detector. The muon spectrometer includes a system of precision tracking chambers up to  $|\eta| = 2.7$  and fast detectors for triggering up to  $|\eta| = 2.4$ .

The luminosity is measured mainly by the LUCID-2 [19] detector that is located close to the beampipe. A two-level trigger system was used to select events [20]. The first-level trigger is implemented in hardware

<sup>2</sup> ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the  $z$ -axis along the beam pipe. The  $x$ -axis points from the IP to the centre of the LHC ring, and the  $y$ -axis points upwards. Polar coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the  $z$ -axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as  $\eta = -\ln \tan(\theta/2)$  and is equal to the rapidity  $y = \frac{1}{2} \ln \left( \frac{E+p_z}{E-p_z} \right)$  in the relativistic limit. Angular distance is measured in units of  $\Delta R \equiv \sqrt{(\Delta y)^2 + (\Delta\phi)^2}$ .

and used a subset of the detector information to accept events at a rate close to 100 kHz. This is followed by a software-based trigger that reduced the accepted rate of complete events to 1.25 kHz on average depending on the data-taking conditions.

A software suite [21] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

### 3 Data and simulated samples

The data were taken during  $pp$  collisions by ATLAS, during the years 2016–2018 of the Run 2 LHC data-taking period. This dataset corresponds to an integrated luminosity of  $137 \text{ fb}^{-1}$  [22] at  $\sqrt{s} = 13 \text{ TeV}$ . Only events recorded when LHC beams were stable and all ATLAS detector systems were operational are considered [23]. Data collected in 2015 with an additional luminosity of  $3 \text{ fb}^{-1}$  are omitted, as the dedicated triggers described in Section 5 were not yet fully operational.

For the EW signal, three sources of  $\tau$ -lepton production are modelled:  $W \rightarrow \tau\nu_\tau$ ,  $Z \rightarrow \tau\tau$  and  $t\bar{t} \rightarrow \tau X$ . The POWHEG BOX MC event generator [24–28] was used to model these signal samples at next-to-leading order (NLO) in QCD. Events are interfaced with the PYTHIA 8.245 [29] generator to model the parton shower, hadronisation, underlying event, and particle decays. The  $W \rightarrow \tau\nu_\tau$  and  $Z \rightarrow \tau\tau$  samples used the AZNLO [30] set of tuned parameters (tune) and the CT10NLO PDF set [31] for the hard-scattering processes, whereas the CTEQ6L1 PDF set [32] was used for the parton shower. Top-quark pair-production with at least one  $\tau$ -lepton in the decay ( $t\bar{t} \rightarrow \tau X$ ) used the A14 [33] tune with the NNPDF3.0NLO [34] PDF set for the hard scattering process and the NNPDF2.3LO [35] PDF set for the parton shower. These simulated samples are normalised to  $W$ ,  $Z$  and  $t\bar{t}$  production cross-sections as measured in ATLAS data for  $\sqrt{s} = 13 \text{ TeV}$  [36, 37]. Given the current stringent experimental limits on  $B(\tau \rightarrow 3\mu) < 10^{-7}$ , only one of the  $\tau$ -leptons is allowed to decay into three muons for the  $Z$  and  $t\bar{t}$  samples. At production level, the  $W$  production mode provides 83% of all  $\tau$ -leptons in the EW signal, followed by the  $Z$  production mode (16%) with only minor contributions from the  $t\bar{t}$  production mode (1%).

Three HF signal modes of  $\tau$ -lepton production are modelled:  $D_s$  mesons decaying to  $\tau$ -leptons, with the  $D_s$  either being produced directly (prompt) or through  $B$ -meson decays (non-prompt); and direct  $B$ -meson to  $\tau$ -lepton decays. The PYTHIA 8 generator was used to create these signal samples at leading-order QCD with the A14 tune and NNPDF2.3LO PDFs. Decays of heavy-flavour hadrons and  $\tau$ -leptons are performed by EVTGEN [38]. The  $D_s$  samples are normalised to the production cross-section ( $\sigma = 5000 \pm 360 \text{ (stat)} \pm 590 \text{ (syst) nb}$ ) measured by ATLAS [39] at  $\sqrt{s} = 13 \text{ TeV}$  with a branching ratio of  $B(D_s \rightarrow \tau\nu_\tau) = 5.4 \pm 0.1\%$  [40]. The prompt and non-prompt contributions to  $D_s$  production are predicted in simulation to be 80% and 20%, respectively, although the exact value for this fraction was not found to make a significant difference to the analysis. The direct  $B$ -meson sample was scaled relative to the total  $D_s$  sample using a value of 48% based on Monte Carlo simulation. Furthermore, the branching ratio  $B(B \rightarrow \tau X) = 3.4 \pm 0.4\%$  [41] is taken into account in the normalization of this sample.

The  $\tau \rightarrow 3\mu$  decays are modelled isotropically with the kinematics of the decay products determined via phase space without polarisation or spin effects taken into account, as there are multiple possible new physics scenarios with different spin correlations. This is a standard benchmark setting also used in previous analyses [6, 15, 16].

All the generated events are passed through the simulation of the ATLAS detector based on GEANT4 [42, 43] and reconstructed with the same algorithms as used for data. The effect of multiple interactions in the

same and neighbouring bunch crossings (pile-up) was modelled by overlaying the simulated hard-scattering event with inelastic  $pp$  events generated with PYTHIA 8.186 [44] using the NNPDF2.3LO PDF set [35] and the A3 tune [45]. The simulated events are weighted to reproduce the distribution of pile-up observed in the data.

## 4 Object reconstruction

Muons are reconstructed from hits in both the ID and MS sub-detectors, with the track parameters determined using the combined information [46]. Muons must have a transverse momentum ( $p_T$ ) greater than 4 GeV, and  $|\eta| \leq 2.4$ . They must also satisfy the ‘‘Loose’’ identification criteria [46].

To form a three-muon decay candidate, referred to as a triplet, all events containing at least three muons with a total charge of  $Q = \pm 1$  are selected. These muons must share the same interaction origin point. Due to the relatively long lifetime of the  $\tau$ -lepton, this interaction vertex may be displaced on average from the primary vertex (PV), resulting in a secondary vertex (SV). The SV is determined using the muon track parameters and uncertainties to find the optimal intersection point of the three tracks by minimising the  $\chi^2$  of the fit [47]. If multiple SV candidates are found for the same event, the candidate is used that has the smallest impact parameter of the muon-triplet momentum with respect to the PV ( $a_0$ ). The muon-triplet momentum is calculated as the vector sum of the individual muon momenta. Tracks determined to originate from a SV are refitted with respect to this vertex and the PV is refitted excluding the tracks associated with the SV. The triplet direction is defined as the vector between the PV and SV.

Hadronic jets are reconstructed using the anti- $k_r$  algorithm [48] as implemented in FastJet [49] with a jet radius parameter  $R = 0.4$ . The inputs to this algorithm are particle flow objects [50], which combine measurements from the ATLAS inner detector and calorimeters. Only tracks matched to the PV are used to mitigate pile-up effects. The jets are calibrated to the electromagnetic scale [50], with their axis corrected to point back to the PV. Jets are corrected for pile-up contributions, energy loss in uninstrumented parts of the detector and data-to-MC differences. Any jet within  $\Delta R = 0.2$  of a muon, or matched with the inner-detector track of a muon using ghost association [51], is removed if it has fewer than three associated tracks.

The missing transverse momentum ( $\vec{p}_T^{\text{miss}}$ ) (with magnitude  $E_T^{\text{miss}}$ ) [52] is calculated as the negative vector sum of the transverse momenta for muons, jets, and additional contributions. These additional contributions may be calculated either using ID tracks associated with a vertex but not matched to a jet or muon or using unmatched clusters of energy in the calorimeter. The missing transverse momentum calculated using these contributions is referred to as  $\vec{p}_T^{\text{track-miss}}$  and  $\vec{p}_T^{\text{calo-miss}}$ , respectively.

All reconstructed simulated objects have their reconstruction and selection efficiencies and their energy/momentum scale and resolution corrected to data.

## 5 Trigger and event selection

The data were collected with several two- and three-muon triggers, with small variations between the three years of data taking. In each year, a trigger requiring one muon in the first-level trigger system with  $p_T \geq 20$  GeV and a second muon in the software-based higher-level trigger system with  $p_T \geq 6$  GeV provides the highest efficiency for signal candidates with at least one high-momentum muon. The

intermediate momentum range is covered by triggers that require two muons in the first-level trigger system with  $p_T \geq 10$  GeV for 2016 data, while in 2017 and 2018 a trigger with  $p_T \geq 11$  GeV and  $p_T \geq 6$  GeV for the leading and subleading muon provides better efficiency. Finally, a trigger requiring three muons in the first-level trigger system with  $p_T \geq 4$  GeV provides a lower threshold on muon momenta to maximize the signal acceptance for all years.

A particular challenge for the trigger system are close-by muons from the decays of high-momentum  $\tau$ -leptons that result in overlapping muon trigger regions of interest, reducing the total trigger efficiency [53]. The simulated signal trigger efficiency is corrected via a data-driven method where the multi-muon trigger efficiency is calculated as product of individual muon trigger efficiencies as a function of  $p_T$  and  $q \times \eta$  (where  $q$  is the muon charge), and correction factors as a function of  $\Delta R$ . These individual trigger efficiencies and correction factors are measured in data from  $J/\psi \rightarrow \mu\mu$  events using a tag-and-probe method [53]. The nominal results are obtained with the corrected trigger efficiencies and the full difference to the uncorrected trigger efficiencies is applied as a systematic uncertainty.

The analysis considers events in an extended three-muon mass range around the  $\tau$ -lepton mass,  $1500 \text{ MeV} < m_{3\mu} < 2000 \text{ MeV}$ , which is the region used for fits. All analysis steps are initially completed by excluding the range  $1700 \text{ MeV} < m_{3\mu} < 1850 \text{ MeV}$  that would contain 95% of the signal, which is referred to as the signal region. The sidebands are used to model the background, composed primarily of random combinations of one or two muons with additional tracks that are misidentified as belonging to muons. This approach to background modelling was used, as simulations are unreliable for modelling combinatorial background and would require an extremely large sample size.

The analysis is optimised to be sensitive to very small signal-to-background ratios. By comparing expected signal and sideband background distributions, loose preselections are applied to remove background-dominated regions while leaving plenty of events to train an MVA classifier later. To reject poor quality SVs, the SV  $\chi^2$  must be less than 40 and the transverse SV impact parameter ( $a_0^{xy}$ ) of the triplet divided by its uncertainty ( $\sigma_{a_0^{xy}}$ ) is required to be  $a_0^{xy}/\sigma_{a_0^{xy}} < 6$ . Triplet candidates with significant close-by activity in the calorimeters are removed with a selection on the sum of transverse energy ( $E_T$ ) of energy clusters within a cone of  $\Delta R = 0.2$  around the triplet four-momentum [46],  $E_T^{\text{iso}}(\Delta R = 0.2) < 20$  GeV. Similarly, triplet candidates are required to be isolated from tracks in the ID, excluding those associated with the muon triplet, by limiting the scalar sum of the  $p_T$  of ID tracks to  $p_T^{\text{iso}}/p_T^{\text{triplet}} < 1.0$ , where  $p_T^{\text{iso}}$  is calculated as a sum over tracks within  $\Delta R = \min(0.3, 10\text{GeV}/p_T^{\text{triplet}})$  of the triplet four-momentum for muons with  $p_T < 50$  GeV, and  $\Delta R = 0.2$  otherwise. Selections are also applied to the refitted di-muon invariant mass for each two-muon combination within the triplet (both same-sign and opposite-sign charge),  $m_{\mu\mu} > 325$  MeV, to reject muons produced from final state radiation photon conversions and low-mass background. After the preselection 960,000 events remain in the background sidebands.

Another minor source of background is from muon pairs produced in the decay of  $\omega(782)$  and  $\phi(1020)$  mesons combined with a third muon, or a track misidentified as belonging to a muon, to create an SV mistaken for signal. Events containing an oppositely charged muon combination with a di-muon invariant mass within 34 MeV of these meson masses [40] are removed.

The signal-to-background ratio is improved further using a gradient boosted decision tree (BDT), implemented using XGBoost [54]. After the application of the preselection, both the simulated EW signal events and aforementioned background events from the sidebands in real data are split into two equal halves (based on odd and even event numbers) and used to train two BDTs, which are then subsequently used to classify the events in the other sample. This splitting method is a version of the  $k$ -fold method with  $k = 2$  [55], and aims to reduce the bias of the BDT. The values of the BDT hyperparameters are determined to

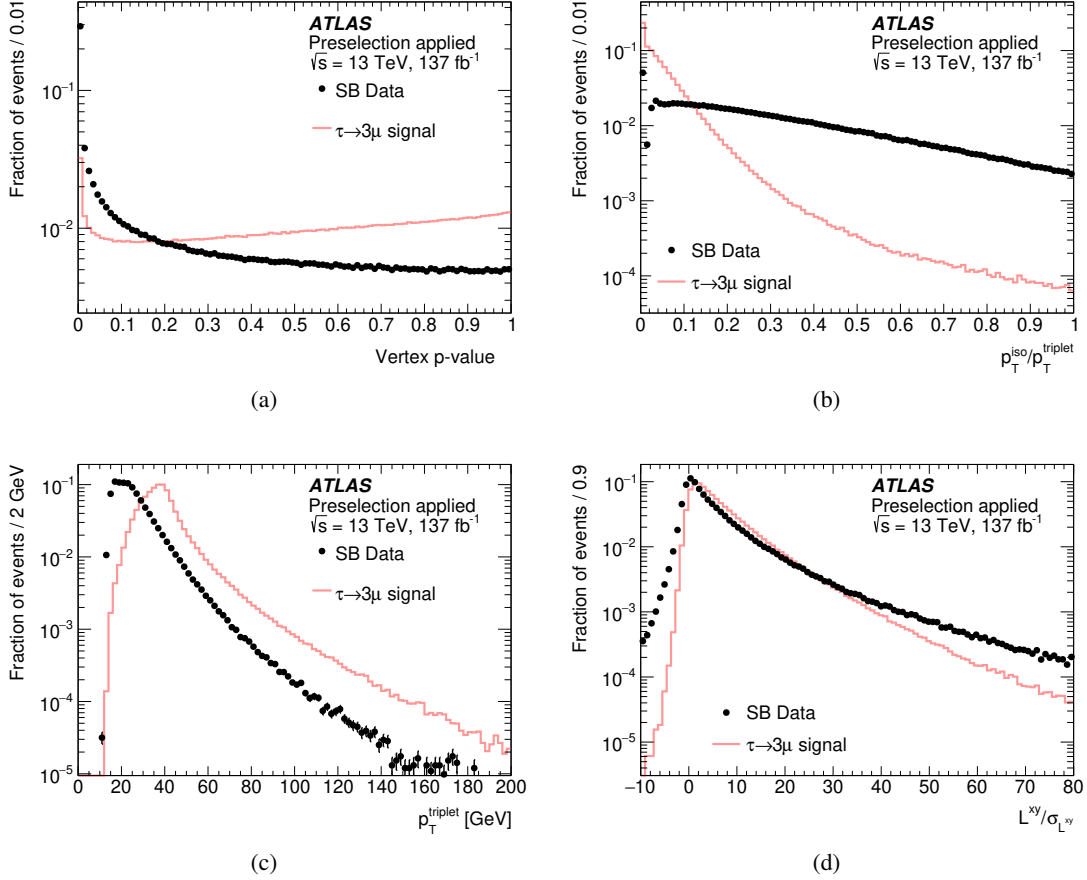


Figure 1: Distributions of representative example variables used in the BDT event classification: (a) vertex quality  $p$ -value, (b) muon isolation  $p_T^{\text{iso}}/p_T^{\text{triplet}}$ , (c) triplet  $p_T$ ,  $p_T^{\text{triplet}}$  and (d) significance of the transverse distance between the PV and SV  $L^{xy}/\sigma_{L^{xy}}$ . The plots show both the EW  $\tau \rightarrow 3\mu$  signal sample (histogram) and data from the sidebands (SB Data) (markers) after the preselection cuts. All distributions are normalised to unit area.

optimise the model accuracy: a maximum BDT depth of 8 is used; the minimum child weight, a measure of sample size at each node, is set to 3; and the hyperparameter  $\eta$ , related to the amount the tree weights are adjusted at each iteration, is set to 1. At each stage of node evaluation, 80% of the data, randomly chosen, are used, to prevent over-training. The other hyperparameters are set to their default values, and the logistic loss function [54] is used.

The BDT uses 18 input variables related to the vertex quality, muon isolation, muon triplet kinematics, and correlations between the muon triplet and  $E_T^{\text{miss}}$ . All variables are defined in Table 1, with representative examples shown in Figure 1. The variables are selected to ensure the BDT cannot reconstruct the triplet mass and sculpt the mass distribution. Certain variables, such as  $m_{3\mu}^{\text{miss}}$  and  $\Delta m_{3\mu}$ , were initially optimised for  $\tau$ -leptons from HF decays. However, as they are found to not compromise the BDT performance, they are kept. While many of the input features contribute to the discrimination power of the BDT, the most important variables are  $\Delta\phi(\text{triplet}, E_T^{\text{calo-miss}})$ ,  $a_0^{xy}/\sigma_{a_0^{xy}}$  and  $p_T^{\text{triplet}}$ .

The resulting BDT score distributions for simulated signal events and background events from the data sidebands are shown in Figure 2. Good discrimination between signal and background events is observed;

Table 1: List of input variables used in the BDT and their definitions.

Variable	Description
<b>Vertex quality</b>	
Track $p$ -value product $\chi^2_{4\text{-track}}$	Product of the three muons refitted ID track $p$ -values from the track fit. $\chi^2$ -value of the SV with 4 ID tracks instead of the usual 3. This variable helps identify events where the triplet contains muons from independent vertices with further charged particles.
Vertex $p$ -value	The $p$ -value associated with the triplet vertex from the SV fit.
<b>Muon isolation</b>	
$E_T^{\text{iso}}(\Delta R = 0.2)$	Muon calorimeter isolation with $\Delta R = 0.2$ .
$E_T^{\text{iso}}(\Delta R = 0.4)$	Muon calorimeter isolation with $\Delta R = 0.4$ .
$p_T^{\text{iso}}/p_T^{\text{triplet}}$	Muon track isolation with $\Delta R = 0.2$ divided by the triplet $p_T$ .
<b>Triplet related quantities</b>	
$a_0^{xy}/\sigma_{a_0^{xy}}$	Triplet transverse SV IP significance.
$L^{xy}/\sigma_{L^{xy}}$	Significance of the distance in the transverse plane from the PV to the SV projected onto the direction of the vertex candidate's transverse momentum.
$\Delta\phi(\text{triplet}, \vec{p}_T^{\text{track-miss}})$	Azimuthal angle between the triplet and the track-based $E_T^{\text{miss}}$ calculation.
$\Delta\phi(\text{triplet}, \vec{p}_T^{\text{calo-miss}})$	Azimuthal angle between the triplet and the calorimeter-based $E_T^{\text{miss}}$ calculation.
$p_T^{\text{triplet}}$	Transverse momentum of the vector sum of the refitted muon momenta
$\eta_{\text{triplet}}$	$\eta$ of the refitted SV of the triplet.
$m_{\text{coll-jet}}$	Invariant mass of the closest jet reconstructed within $\Delta R \leq 0.4$ to the muon triplet.
$ \vec{p}_T^{\text{triplet}} - \vec{p}_T^{\text{jet}} $	Momentum balance between the triplet candidate and the leading $p_T$ hadronic jet, if a jet is reconstructed.
$ \sum_{\text{PV}} \vec{p}_T^{\text{track}} $	Modulus of the vector sum of the $p_T$ of all tracks with $p_T > 1$ GeV associated with the PV of the triplet.
$m_T^{\text{track}}$	The transverse mass of the triplet, calculated using the triplet $p_T$ and the track-based $E_T^{\text{miss}}$ : $m_T^{\text{track}} = \sqrt{2E_T^{\text{track-miss}} p_T^{\text{triplet}} (1 - \cos(\Delta\phi(\text{triplet}, E_T^{\text{track-miss}})))}$
$m_{3\mu}^{\text{miss}}$	A measure of the missing energy at the point of the initially decaying particle $m_{3\mu}^{\text{miss}} = \sqrt{m_1^2 + m_{3\mu}^2 - 2E_1 E_{\text{triplet}} + 2p_1 p_{\text{triplet}} \cos(\Delta\alpha_{S-P})}$ . This variable was optimised for the HF signal from a $D_s$ decay, so it uses $m_1 = m_{3\mu} + m_{D_s} - m_\tau$ , where $E_1$ is the total energy at the PV, $\vec{p}_I = \frac{m_1}{m_{3\mu}} p_{\text{triplet}} \hat{S}$ is the scaled momentum of the initially decaying particle with magnitude $p_I$ , $p_{\text{triplet}}$ is the total momentum of the muons triplet, $\hat{S}$ is the unit vector pointing from the PV to SV, and $\Delta\alpha_{S-P}$ is the angle between $p_{\text{triplet}}$ and $\hat{S}$ .
$\Delta m_{3\mu}$	A measure of the maximum possible missing energy at the point of the initially decaying particle, effectively the invariant mass of the initially decaying particle, minus the mass of the triplet: $\Delta m_{3\mu} = \sqrt{2(p_T^{\text{triplet}} \sin(\Delta\alpha_{S-P}))^2 + m_{3\mu}^2} - m_{3\mu}$ .

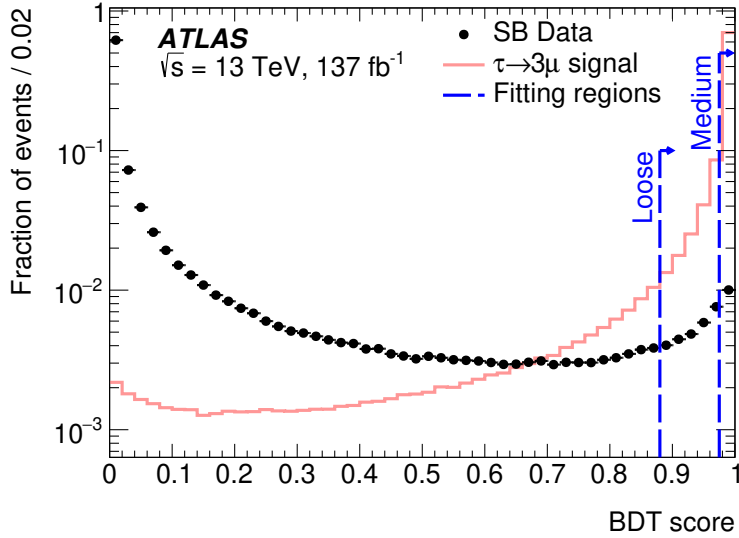


Figure 2: BDT score distribution for the EW  $\tau \rightarrow 3\mu$  signal sample (histogram), and background from sideband data (SB Data) (markers). All distributions are normalised to unit area, and the error bars are too small to be visible. The vertical lines mark the boundaries of the loose ( $0.88 < \text{BDT} \leq 0.975$ ) and medium ( $0.975 < \text{BDT} \leq 0.998$ ) BDT bins used for the event categorisation. The tight boundary ( $0.998 < \text{BDT}$ ) is not shown as it is indistinguishable from the vertical axis.

Table 2: Number of events in each fit category. The top two lines (EW and HF signal) correspond to the expected signal for  $B(\tau \rightarrow 3\mu) = 1 \times 10^{-7}$ , while in the lower two lines the fitted background contributions and the observed data events in the signal region ( $1700 \text{ MeV} < m_{3\mu} < 1850 \text{ MeV}$ ) are listed.

Source	BDT category	Events in fit category					
		Loose		Medium		Tight	
		Barrel	Endcap	Barrel	Endcap	Barrel	Endcap
EW signal		1.0	2.0	3.2	5.8	2.5	5.3
HF signal		1.0	2.4	0.6	1.4	0.1	0.2
Background in signal region		191.9	275.8	88.0	135.6	3.4	6.4
Signal region data		209	291	86	141	5	5

additionally no significant over-training was found.

Events are split into different categories to optimise the sensitivity based on the BDT output score and different  $m_{3\mu}$  detector resolutions. Events in the barrel, defined as  $|\eta_{\text{triplet}}| < 1.2$ , are found to have a signal mass resolution of approximately 25 MeV, significantly better than the resolution, about 34 MeV, for the remainder of the events that are assigned to the endcap category. Therefore, barrel and endcap events are separated. To find the optimal BDT categories, the expected limit on  $B(\tau \rightarrow 3\mu)$  is determined for a range of different BDT categories by performing a simultaneous unbinned maximum-likelihood fit on the  $m_{3\mu}$  distribution in all fit categories. The optimal limit is achieved using three BDT categories, referred to as loose, medium and tight, as indicated on Figure 2. Table 2 shows the expected and observed signal and background yields in all six categories.

The simulated signals are parameterised separately in each category with a double sided Crystal Ball (DSCB) function [56, 57], which models the signal  $m_{3\mu}$  distribution well. The background  $m_{3\mu}$  shape is

Table 3: Signal normalisation uncertainties from different systematic variations for the six fit categories. Only effects with a magnitude of at least 1% in at least one category are reported. The effect of each systematic variation is treated as correlated between categories. Systematic effects shown with different signs refer to migration effects that lead to anti-correlations between the yields of different categories. Further global signal normalisation effects are discussed in the text.

Systematic uncertainty	Systematic signal uncertainty [%]						
	BDT category	Loose		Medium		Tight	
		Barrel	Endcap	Barrel	Endcap	Barrel	Endcap
Trigger efficiency	$\pm 26.7$	$\pm 10.1$	$\pm 20.9$	$\pm 9.1$	$\pm 16.2$	$\pm 11.4$	
Muon reconstruction efficiency	$\pm 3.7$	$\pm 3.5$	$\pm 3.4$	$\pm 3.2$	$\pm 2.9$	$\pm 3.0$	
$E_T^{\text{miss}}$ track resolution	$\pm 1.9$	$\pm 1.1$	$\pm 0.8$	$\pm 1.2$	$\mp 2.4$	$\mp 2.3$	
Jet energy scale	$\pm 5.0$	$\pm 3.3$	$\pm 0.9$	$\pm 0.4$	$\mp 5.1$	$\mp 3.2$	
Pile-up	$\pm 1.5$	$\pm 1.5$	$< 0.1$	$< 0.1$	$\mp 1.8$	$\mp 1.4$	

parameterised by a smooth function, chosen as an exponential, with the exponent allowed to be positive or negative. This is determined to be a suitable model in two ways. First, it is tested if the background model is able to describe the data sidebands. Second, signal-plus-background fits are performed to signal-depleted regions of low BDT score, defined as the point below which less than 10% of the signal would be retained. The measured signal yield in this region, known as the spurious signal [58], is found to be suitable following the criteria in Ref.[59] for the chosen functional form.

## 6 Systematic uncertainties

The analysis is found to be limited by the statistical uncertainty of the dataset. Experimental systematic uncertainties apply to the simulated signal, as the background is determined directly from the data. Further cross-checks on the impact of the choice of background parameterisation are reported at the end of this Section, including a dedicated systematic uncertainty.

The main source of systematic uncertainty is from the trigger efficiency, determined as described in Section 5. Additional uncertainties are also considered for: the muon reconstruction efficiency as determined in  $J/\psi \rightarrow \mu\mu$  and  $Z \rightarrow \mu\mu$  events using a tag-and-probe method [46]; the jet energy scale [60]; the resolution of the  $E_T^{\text{miss}}$  [52]; and the level of pile-up [61]. These effects vary in size between the fit categories and correlations are considered. The effect on the signal normalisation for each category is shown in Table 3. Other systematic variations are found to have an effect of less than 1% and are neglected.

Further sources of systematic uncertainties have a global effect on the normalisation. The uncertainty in the integrated luminosity is 0.84% [22], obtained using the LUCID-2 detector [19] for the primary luminosity measurements, complemented by measurements using the inner detector and calorimeters. The uncertainty on the EW signal cross-section is conservatively taken as the maximum fractional uncertainty in the  $W \rightarrow \ell\nu$ ,  $Z \rightarrow \ell\ell$  and  $t\bar{t}$  cross-section measurements [36, 37], which is 3.0%. For the HF signal, the uncertainty in the  $D_s$  inclusive production cross-section [39] of 14% is used along with a 1.9% uncertainty in the  $B(D_s \rightarrow \tau\nu\tau)$  [40] and a 12% uncertainty in the  $B(B \rightarrow \tau X)$  [41]. The impact of further simulation modelling uncertainties are expected to be negligible and are not considered.

The effect of the systematic uncertainties in the signal shape is also considered, with the muon momentum calibration [62] being the only variation having an effect. The muon momentum scale uncertainty has

a maximum effect on the mean of the signal DSCB of 0.1% in the barrel and 0.3% in the endcap. The momentum resolution has a maximum effect on the width of the signal DSCB of 3.2% (0.8%) in the barrel and 1.6% (3.3%) in the endcap for the ID (MS) contribution.

The impact of a different choice of background parameterisation on the number of background events has been investigated by replacing the nominal exponential function by a second-order polynomial or a power law. The different functions resulted in a maximum 5% change in the number of extracted background events, well within the statistical uncertainty on the background extraction. Constraining the background to be constant or falling with increasing  $m_{3\mu}$  results in no systematic change in the number of background events. Although the magnitude of the spurious signal uncertainty is found to be suitable following the criteria in Ref. [59] for the chosen functional form, a systematic uncertainty to account for possible residual mismodelling effects is applied. The spurious signal yield, in the signal-depleted region mentioned previously, is scaled for each of the fit categories and treated as an uncorrelated systematic uncertainty. This background parameterisation uncertainty only has a small impact on the final results.

## 7 Results

To find evidence for the decay of  $\tau \rightarrow 3\mu$  or to set a limit on the branching ratio, a simultaneous unbinned maximum-likelihood fit is performed on the  $m_{3\mu}$  distribution in all six fit categories. The sum of EW and HF signals are parameterised in each category separately with a DSCB, while the background is parameterised with an exponential function. The systematic uncertainties as discussed in Section 6 are implemented as nuisance parameters in the fit. For these fits,  $B(\tau \rightarrow 3\mu)$  is varied as the parameter of interest, and the profile likelihood test statistic in the asymptotic approximation [63] is used. Injection tests with signals in the range of  $B(\tau \rightarrow 3\mu) = 10^{-8}$ – $10^{-6}$  are performed to verify that the fit is unbiased.

Figure 3 shows the background-only fit and the expected signal, for  $B(\tau \rightarrow 3\mu) = 1 \times 10^{-6}$ , in the unblinded  $m_{3\mu}$  spectra. No significant signal is observed and the best-fit signal strength value is  $B(\tau \rightarrow 3\mu) = (1.5 \pm 4.0) \times 10^{-8}$ . An upper limit is set using the  $CL_s$  method [64]. The observed (expected) upper limit is found to be  $B(\tau \rightarrow 3\mu) < 8.7 \times 10^{-8}$  ( $7.5 \times 10^{-8}$ ) at 90% CL. The upper limit is also calculated at 95% CL, resulting in an observed (expected) upper limit of  $10.6 \times 10^{-8}$  ( $9.3 \times 10^{-8}$ ). The  $CL_s$  limit scan is shown in Figure 4. The small difference between the observed and expected limits is due to upward data fluctuations in four out of six categories, as shown in Table 2.

Using pseudo experiments to calculate the limit instead of the asymptotic approximation is found to have a negligible impact on the limits obtained: the observed limit improves by 1%, while the expected limit worsens by 3%. Excluding all systematic uncertainties results in an improvement to the expected limit by 4.4%, with the trigger efficiency systematic uncertainty having the largest contribution of 2.1%, followed by the spurious signal systematic uncertainty contribution of 1.8%.

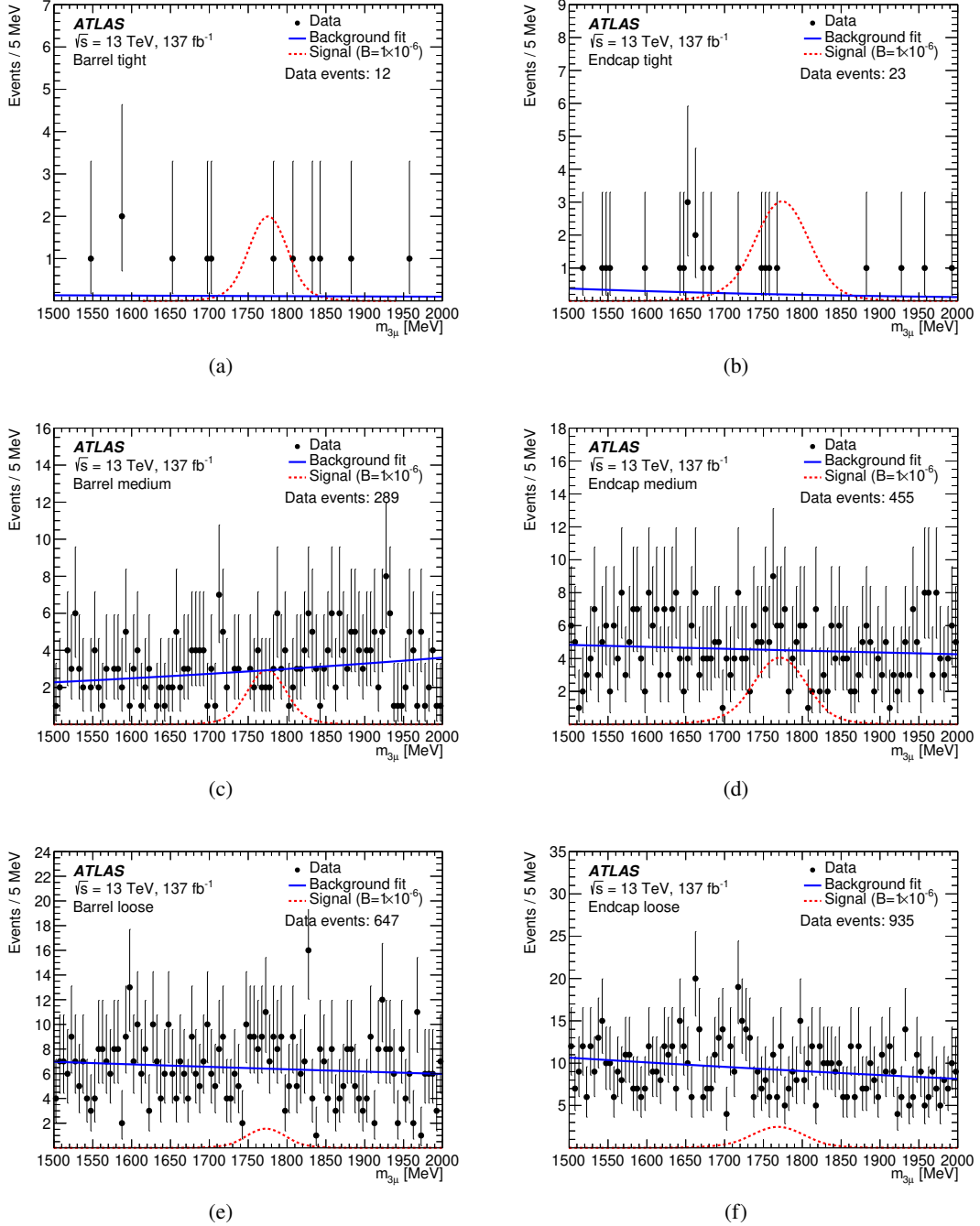


Figure 3: The  $m_{3\mu}$  in data (markers), background-only fit (solid line) and expected EW plus HF signal, for  $B(\tau \rightarrow 3\mu) = 1 \times 10^{-6}$  as an illustration (dotted line) in the (a,c,e) barrel and (b,d,f) endcap categories for the (a,b) tight, (c,d) medium and (e,f) loose BDT categories.

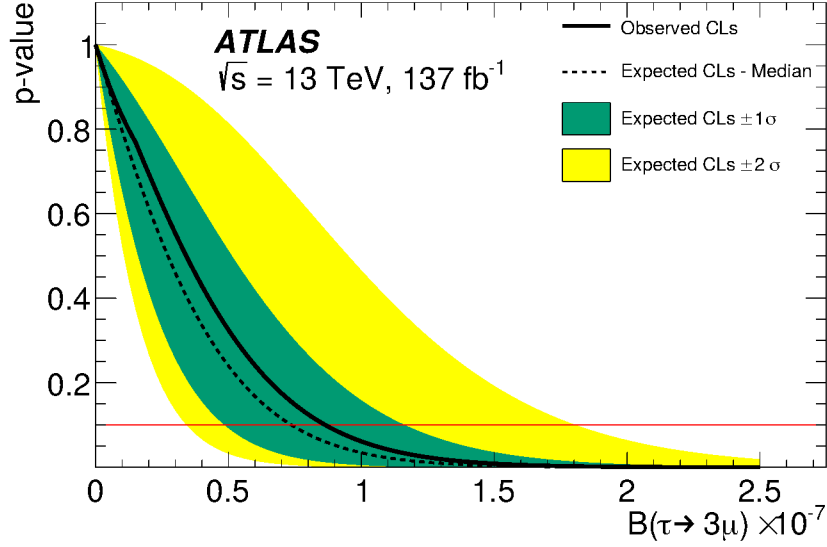


Figure 4:  $B(\tau \rightarrow 3\mu)$  limit scan showing the expected limit (dotted line),  $\pm 1(2)\sigma$  error bands (green and yellow), and the observed limit using the  $CL_s$  method (solid line). A  $p$ -value of 0.1 (90% CL) is shown by the horizontal line.

## 8 Conclusion

This paper presents a search for the cLFV process  $\tau \rightarrow 3\mu$ , using  $137 \text{ fb}^{-1}$  of  $pp$  collision data collected by the ATLAS experiment during Run 2 of the Large Hadron Collider at  $\sqrt{s} = 13 \text{ TeV}$ . The analysis is optimised using MVA analysis techniques for electroweak sources, but also considers  $\tau$ -lepton production from heavy-flavour sources. No evidence for  $\tau \rightarrow 3\mu$  decays is found and observed (expected) limits are set on  $B(\tau \rightarrow 3\mu) < 8.7 \times 10^{-8}$  ( $7.5 \times 10^{-8}$ ) at 90% CL. This result improves upon the previous ATLAS Run 1 limit by a factor of 5, where a factor of 3 is expected solely from the larger production cross-sections at the increased centre-of-mass energy and larger integrated luminosity. The additional improvement is attributed to detector improvements such as the new IBL detector, improved machine learning methods, and more efficient triggers. The analysis is limited by statistical uncertainties and thus improvements in sensitivity are expected with the analysis of additional data.

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F. Costanza [ID4](#), D. Costanzo [ID143](#), J. Couthures [ID4](#), G. Cowan [ID95](#), K. Cranmer [ID173](#), L. Cremer [ID48](#),  
D. Cremonini [ID24b,24a](#), S. Crépe-Renaudin [ID59](#), F. Crescioli [ID129](#), T. Cresta [ID72a,72b](#), M. Cristinziani [ID145](#),  
M. Cristoforetti [ID77a,77b](#), T.M. Critchley [ID55](#), E. Critelli [ID96](#), A. Cueto [ID99](#), H. Cui [ID96](#), Z. Cui [ID7](#),  
B.M. Cunnett [ID150](#), W.R. Cunningham [ID58](#), E. Cuppini [ID110](#), F. Curcio [ID166](#), J.R. Curran [ID51](#),  
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W. Dabrowski [ID85a](#), T. Dado [ID37](#), S. Dahbi [ID152](#), T. Dai [ID106](#), D. Dal Santo [ID20](#), C. Dallapiccola [ID103](#),  
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F. Dattola [ID47](#), S. D'Auria [ID70a,70b](#), A. D'Avanzo [ID71a,71b](#), T. Davidek [ID135](#), J. Davidson [ID170](#),  
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N. De Groot [ID115](#), P. de Jong [ID116](#), H. De la Torre [ID117](#), A. De Maria [ID112a](#), S. De Miranda Rimes [ID81d](#),  
A. De Salvo [ID74a](#), U. De Sanctis [ID75a,75b](#), F. De Santis [ID69a,69b](#), A. De Santo [ID150](#),  
J.B. De Vivie De Regie [ID59](#), K.G. De Vries [ID116](#), J. Debevc [ID93](#), D.V. Dedovich [ID38](#), J. Degens [ID92](#),  
A.M. Deiana [ID44](#), J. Del Peso [ID99](#), L. Delagrangé [ID27](#), F. Deliot [ID137](#), C.M. Delitzsch [ID48](#),  
M. Della Pietra [ID71a,71b](#), D. Della Volpe [ID55](#), A. Dell'Acqua [ID37](#), L. Dell'Asta [ID70a,70b](#), M. Delmastro [ID4](#),  
C.C. Delogu [ID56b,56a](#), P.A. Delsart [ID59](#), S. Demers [ID175](#), M. Demichev [ID38](#), H. Denizli [ID22a,1](#),  
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V. Fadeyev [ID138](#), D. Fakoudis [ID100](#), S. Falciano [ID74a](#), L.F. Falda Ulhoa Coelho [ID27](#), F. Fallavollita [ID110](#),

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