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Search for single production of vector-like T quarks decaying into Ht or Zt in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector



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ABSTRACT: This paper describes a search for the single production of an up-type vector-like quark (T) decaying as $T \rightarrow Ht$ or $T \rightarrow Zt$. The search utilises a dataset of pp collisions at $\sqrt{s} = 13$ TeV collected with the ATLAS detector during the 2015–2018 data-taking period of the Large Hadron Collider, corresponding to an integrated luminosity of 139 fb^{-1} . Data are analysed in final states containing a single lepton with multiple jets and b -jets. The presence of boosted heavy resonances in the event is exploited to discriminate the signal from the Standard Model background. No significant excess above the Standard Model expectation is observed, and 95% CL upper limits are set on the production cross section of T quarks in different decay channels. The results are interpreted in several benchmark scenarios to set limits on the mass and universal coupling strength (κ) of the vector-like quark. For singlet T quarks, κ values above 0.53 are excluded for all masses below 2.3 TeV. At a mass of 1.6 TeV, κ values as low as 0.35 are excluded. For T quarks in the doublet scenario, where the production cross section is much lower, κ values above 0.72 are excluded for all masses below 1.7 TeV, and this exclusion is extended to κ above 0.55 for low masses around 1.0 TeV.

KEYWORDS: Hadron-Hadron Scattering , Vector-Like Quarks

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1 Introduction

The discovery of a new particle consistent with the Standard Model (SM) Higgs boson by the ATLAS [1] and CMS [2] experiments at the Large Hadron Collider (LHC) represents a milestone in high-energy physics. A comprehensive programme of measurements of the Higgs boson’s properties to unravel its nature is underway at the LHC, so far yielding results compatible with the SM predictions. However, a pressing question remains as to why the electroweak mass scale (and the Higgs boson mass along with it) is so small compared to the Planck scale, a situation known as the hierarchy problem. Naturalness arguments [3] require that quadratic divergences that arise from radiative corrections to the Higgs boson

mass are cancelled out by some new mechanism in order to avoid fine-tuning. To that effect, several explanations have been proposed in theories beyond the SM (BSM theories).

One such solution involves the existence of a new strongly interacting sector, in which the Higgs boson would be a pseudo Nambu-Goldstone boson (pNGB) [4] of a spontaneously broken global symmetry. The Composite Higgs [5–7] model is a particular realisation of this scenario, which also addresses additional open questions in the SM, including the hierarchy in the mass spectrum of the SM particles. A key prediction is the existence of new fermionic resonances referred to as vector-like quarks (VLQs), which are also common in many other BSM scenarios [8–11]. Vector-like quarks are defined as colour-triplet spin-1/2 fermions whose left- and right-handed chiral components have the same transformation properties under the weak-isospin SU(2) gauge group [12, 13]. Assuming an unchanged scalar sector with respect to the Standard Model, theoretical constraints on renormalisability and gauge completeness restrict the SU(2) representation of the vector-like quarks to seven possible multiplets: singlets ($T^{2/3}$) or ($B^{-1/3}$), doublets ($X^{5/3} T^{2/3}$) or ($T^{2/3} B^{-1/3}$), or triplets ($X^{5/3} T^{2/3} B^{-1/3}$) or ($T^{2/3} B^{-1/3} Y^{-4/3}$).¹ The vector-like quarks in these models are expected to couple preferentially to third-generation quarks and can have flavour-changing neutral-current decays in addition to the charged-current decays characteristic of chiral quarks [12, 14]. Thus, the up-type T quark can decay into a W boson and a b -quark, and also into a top quark and a Z or Higgs boson. The relative couplings to the massive bosons of the Standard Model are determined by the gauge representation of the vector-like quarks. The relative couplings to the W , Z and Higgs bosons can be expressed in terms of the ξ_W , ξ_Z and ξ_H parameters, respectively [15]. In the asymptotic limit of large VLQ mass, these ξ parameters correspond to the branching ratios of the T quark into their respective decay modes. The asymptotic limit holds to a very good approximation for VLQ masses above 1 TeV. For a T singlet, $\xi_W = 0.5$ and $\xi_Z = \xi_H = 0.25$. For T quarks that are in an ($X T$) doublet, or in a ($T B$) doublet with mixing only to up-type SM singlets [14, 15], $\xi_W = 0$, and $\xi_Z = \xi_H = 0.5$.

At the LHC, vector-like quarks with masses below ~ 1 TeV would be produced mostly in pairs via the strong interaction. For higher masses, however, single production, mediated by the electroweak interaction, may dominate depending on the coupling strength of the interaction between the vector-like quark and the SM quarks [13]. The single-production channel for vector-like quarks provides a unique opportunity to probe the universal coupling strength (κ) in addition to the relative couplings and branching ratios that can be probed in pair production searches. The universal coupling strength controls both the production cross section and the resonance width of the VLQ. For a VLQ with mass m_T , the resonance width Γ_T scales as $\Gamma_T \propto \kappa^2 m_T^3$ [15]. Thus, the relative width (Γ_T/m_T) of the VLQ resonance scales quadratically with both κ and m_T , and is independent of the multiplet representation.

The dominant channel for resonant production of a single T quark is t -channel production mediated by a gauge boson (figure 1a). The final state is characterised by the presence

¹The indices in superscript indicate the electric charges of the vector-like quarks. These indices are omitted in the notation for the rest of the paper.

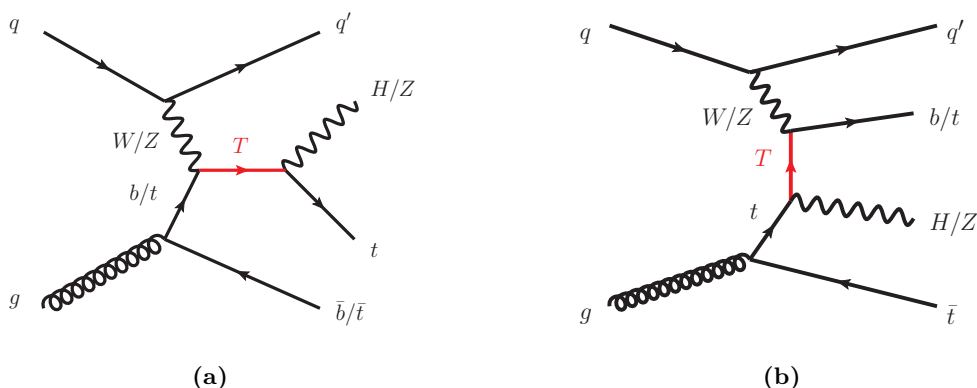


Figure 1. Example of leading-order Feynman diagrams of single vector-like T production in association with a b -quark or t -quark and subsequent decay into either Ht or Zt in the (a) resonant and (b) non-resonant modes.

of multiple (b -tagged) jets from the decay of the produced heavy quarks and bosons, along with the recoiling initial-state quark, which typically manifests as a forward jet. In the four-flavour scheme, and assuming that the T quark couples only to SM quarks of the third generation, this process requires an initial-state gluon to split into a $b\bar{b}$ or $t\bar{t}$ pair. Given the difference in masses between the top and bottom quarks, b -associated (or W -mediated) T -quark production is kinematically favoured over t -associated (or Z -mediated) production. However, in certain gauge representations, such as for a $(T B)$ doublet with mixing only to up-type SM singlets [14, 15], or for an $(X T)$ doublet, the coupling to W bosons vanishes, and the t -associated mode is the only allowed production channel. Therefore, both production modes are theoretically interesting, even though the parameter space in the limit of $\xi_W \rightarrow 0$ is difficult to probe due to small production cross sections. Non-resonant T -quark production (figure 1b) is subdominant compared to resonant production in the b -associated mode. By contrast, in the t -associated mode, both the resonant and non-resonant T -quark production processes have comparable cross sections, as both require the splitting of an initial-state gluon into a $t\bar{t}$ pair. The relative contribution of non-resonant production grows with resonance width, and is therefore larger at higher coupling strengths.

Physical realisations of Composite Higgs models require the presence of additional scalar [16] and vector bosons [17–19] for UV-completeness, thus opening up production and decay channels for the VLQs in addition to the ones discussed above. However, processes involving additional BSM particles are not considered in this paper, and results are interpreted in the context of a minimal extension of the Standard Model including only one VLQ multiplet [15].

The ATLAS and CMS collaborations have a broad programme of searches that has largely focused on pair production of vector-like quarks, targeting different decay modes and final states separately. A combination of all ATLAS pair production analyses using the data collected by the ATLAS detector in 2015 and 2016 delivered the most stringent limits to date on pair-produced vector-like quarks [20], with masses observed to be excluded below 1.31 TeV for T and 1.03 TeV for B for any combination of decay modes. The T (B)

singlet configuration was excluded for masses up to 1.31 (1.21) TeV, and T (B) quarks in the (T B) doublet configuration were excluded up to masses of 1.37 (1.35) TeV. Searches by both ATLAS [21–24] and CMS [25–30] targeting single vector-like quark production have set limits on the allowed vector-like quark parameter space in terms of model-dependent parameters such as coupling strengths and mixing angles. These searches have mostly focused on the b -associated single production modes for VLQs. A search by ATLAS for single VLQ production in the $T \rightarrow Wb$ channel has excluded $\sigma \times \mathcal{B}(T \rightarrow Wb)$ above ~ 100 fb for b -associated T production in the mass range of 1.0–1.9 TeV [23]. An ATLAS search [24] in the $T \rightarrow Z(\ell\ell)t$ channel has excluded $\sigma \times \mathcal{B}(T \rightarrow Zt)$ for b -associated T production above ~ 90 fb (~ 40 fb) at a mass of 1.0 TeV (2.0 TeV) in the singlet hypothesis. A CMS search for t -associated T production, also in $T \rightarrow Z(\ell\ell)t$ final states [27], has excluded $\sigma \times \mathcal{B}(T \rightarrow Zt)$ above ~ 100 fb (~ 40 fb) at a mass of 0.8 TeV (1.7 TeV) under the doublet hypothesis. Conversely, the CMS search for T production in the $T \rightarrow Z(\nu\nu)t$ channel [31] excluded $\sigma \times \mathcal{B}(T \rightarrow Zt)$ down to ~ 200 fb (~ 20 fb) at a mass of 0.6 TeV (1.8 TeV) under the singlet hypothesis, for a decay width of 30%. A recently published search by ATLAS in the all-hadronic final state [21] excludes $\sigma \times \mathcal{B}(T \rightarrow Ht)$ for b -associated T production above ~ 30 – 100 fb in the 1.0–2.3 TeV mass range for a wide range of coupling strengths.

These exclusion limits were all derived at 95% CL, assuming that the VLQs couple exclusively to SM quarks in the third generation, and production modes involving other BSM particles were not considered.

This paper presents a search for the single production of the up-type vector-like quark T , with subsequent decays into Ht with $H \rightarrow b\bar{b}$, or into Zt with $Z \rightarrow q\bar{q}$ (figure 1). Both the b - and t -associated production modes are considered in this search. The search uses 139 fb^{-1} of pp collision data at $\sqrt{s} = 13$ TeV recorded by the ATLAS Collaboration during Run 2 of the Large Hadron Collider (LHC). Data are analysed in the lepton+jets final state, characterised by an isolated electron or muon with high transverse momentum and multiple jets and b -jets. The presence of heavy hadronic boosted objects in the events is used as an important distinguishing characteristic of the signal. In the absence of a significant excess above the SM expectation, the results are used to set upper limits on the single production of T quarks for several scenarios of the mass, the universal coupling strength κ , and the relative couplings to W , Z , and Higgs bosons.

2 ATLAS detector

The ATLAS detector [32] at the LHC covers nearly the entire solid angle around the collision point.² It consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadron calorimeters, and a muon spectrometer incorporating three large superconducting air-core toroidal magnets.

²ATLAS 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. Cylindrical coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z -axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln \tan(\theta/2)$. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

The inner-detector system is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range $|\eta| < 2.5$. The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit normally being in the insertable B-layer installed before Run 2 [33, 34]. It is followed by the silicon microstrip tracker, which usually provides eight measurements per track. These silicon detectors are complemented by the transition radiation tracker (TRT), which enables radially extended track reconstruction up to $|\eta| = 2.0$. The TRT also provides electron identification information based on the fraction of hits (typically 30 in total) above a higher energy-deposit threshold corresponding to transition radiation.

The calorimeter system covers the pseudorapidity range $|\eta| < 4.9$. Within the region $|\eta| < 3.2$, electromagnetic calorimetry is provided by barrel and endcap high-granularity lead/liquid-argon (LAr) calorimeters, with an additional thin LAr presampler covering $|\eta| < 1.8$ to correct for energy loss in material upstream of the calorimeters. Hadron calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadron endcap calorimeters. The solid angle coverage is completed with forward copper/LAr and tungsten/LAr calorimeter modules optimised for electromagnetic and hadronic energy measurements respectively.

The muon spectrometer (MS) comprises separate trigger and high-precision tracking chambers measuring the deflection of muons in a magnetic field generated by the superconducting air-core toroidal magnets. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. Three layers of precision chambers, each consisting of layers of monitored drift tubes, cover the region $|\eta| < 2.7$, complemented by cathode-strip chambers in the forward region, where the background is highest. The muon trigger system covers the range $|\eta| < 2.4$ with resistive-plate chambers in the barrel, and thin-gap chambers in the endcap regions.

Interesting events are selected by the first-level trigger system implemented in custom hardware, followed by selections made by algorithms implemented in software in the high-level trigger [35]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger further reduces in order to record events to disk at about 1 kHz.

An extensive software suite [36] 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 Object reconstruction

Interaction vertices from proton-proton collisions are reconstructed from at least two tracks with transverse momentum (p_T) larger than 500 MeV that are consistent with originating from the beam collision region in the x - y plane. If more than one primary vertex candidate is found, the candidate whose associated tracks form the largest sum of squared p_T [37] is selected as the hard-scatter primary vertex.

Electron candidates [38] are reconstructed from energy clusters in the electromagnetic calorimeter associated with reconstructed tracks in the inner detector. They are required

to have $p_T > 30$ GeV and $|\eta_{\text{cluster}}| < 2.47$. Candidates in the transition region between the electromagnetic barrel and endcap calorimeters ($1.37 < |\eta_{\text{cluster}}| < 1.52$) are excluded. They are required to satisfy the “tight” likelihood-based identification criteria [38] based on calorimeter, tracking and combined variables that provide separation between electrons and jets. Muon candidates [39] are reconstructed by matching tracks in the MS to those found in the inner detector. The resulting muon candidates are re-fitted using the complete track information from both detector systems. Muon candidates are required to satisfy the “medium” identification criteria [39], and to have $p_T > 30$ GeV and $|\eta| < 2.5$. Electron (muon) candidates are matched to the primary vertex by requiring that the significance of their transverse impact parameter, d_0 , satisfies $|d_0/\sigma(d_0)| < 5(3)$, where $\sigma(d_0)$ is the measured uncertainty in d_0 , and by requiring that their longitudinal impact parameter, z_0 , satisfies $|z_0 \sin \theta| < 0.5$ mm. To further reduce the background from non-prompt leptons, photon conversions and hadrons, the lepton candidates are also required to be isolated in the tracking system and the calorimeter.

Candidate jets are reconstructed with the anti- k_t algorithm [40, 41] with a radius parameter $R = 0.4$ (referred to as “small- R jets”). The input constituents for jet reconstruction are built by combining topological clusters of energy in the calorimeter [42] with measured tracks in the inner detector using the particle-flow algorithm [43]. The reconstructed jets are then calibrated to the particle level by the application of a jet energy scale derived from simulation and *in situ* corrections based on $\sqrt{s} = 13$ TeV data [44]. Calibrated jets are required to have $p_T > 25$ GeV and $|\eta| < 4.5$. Quality criteria are imposed to reject events that contain any jets arising from non-collision sources or detector noise [45]. Jets with $|\eta| < 2.5$ are labelled “central” jets for the purposes of event selection and categorisation, while jets with $2.5 < |\eta| < 4.5$ are called “forward” jets. Requirements based on the jet-vertex tagger (JVT) [46] algorithm are imposed on central jets with $p_T < 60$ GeV and $|\eta| < 2.4$ to suppress contamination from jets that originate from pile-up interactions. Pile-up contamination for jets with $|\eta| > 2.4$ is reduced by requirements on the closely related forward JVT (fJVT) algorithm for jets with $p_T < 120$ GeV [47].

In order to identify b -hadrons in the event, variable- R [48] jets built from reconstructed tracks in the inner detector are used. Track-jets containing b -hadrons are identified (b -tagged) via the multivariate “DL1” algorithm [49], which uses information about the kinematic and topological properties of displaced tracks associated with the jet, and of secondary and tertiary decay vertices reconstructed from these tracks. For each jet, a value of the multivariate b -tagging discriminant is calculated. In this analysis, a jet is considered b -tagged if this value is above the threshold corresponding to an average 77% efficiency to tag a b -quark jet, with a light-jet³ rejection factor of ~ 112 and a charm-jet rejection factor of ~ 5 , as determined for jets with $p_T > 20$ GeV and $|\eta| < 2.5$ in simulated $t\bar{t}$ events.

Overlaps between candidate objects are removed sequentially. Firstly, electron candidates that lie within $\Delta R = 0.01$ of a muon candidate are removed to suppress contributions from muon bremsstrahlung. Overlaps between electron and jet candidates are resolved next, and finally, overlaps between remaining jet candidates and muon candidates

³Light-jet refers to a jet originating from the hadronisation of a light quark (u, d, s) or a gluon.

are removed. Clusters associated with identified electrons are not excluded during jet reconstruction. In order to avoid double-counting of electrons as jets, the closest jet whose axis is within $\Delta R = 0.2$ of an electron is discarded. If the electron is within $\Delta R = 0.4$ of the axis of any jet after this initial removal, the jet is retained and the electron is removed. The overlap removal procedure applied to the remaining jet candidates and muon candidates is designed to remove those muons that are likely to have arisen in the decay chain of hadrons and to retain the overlapping jet instead. Jets and muons may also appear in close proximity when the jet results from high- p_T muon bremsstrahlung, and in such cases the jet should be removed and the muon retained. Such jets are characterised by having very few matching inner-detector tracks. Selected muons that satisfy $\Delta R(\mu, \text{jet}) < 0.04 + 10 \text{ GeV}/p_T^\mu$ are rejected if the jet has at least three tracks originating from the primary vertex; otherwise the jet is removed and the muon is kept.

The candidate small- R jets surviving the overlap removal procedure discussed above are used as inputs for further jet reclustering [50] using the variable- R jet reconstruction algorithm with $\rho = 550 \text{ GeV}$. The parameter ρ controls the evolution of the effective size of the reclustered jet as $R = \rho/p_T$. Since the input constituents of these reclustered jets are already calibrated, no further calibration of them is required. Uncertainties in the energy and mass scales and resolutions of the constituent small- R jets are propagated to the kinematics of the reclustered (RC) jets. In order to suppress contributions from pile-up and soft radiation, the RC jets are trimmed [51] by removing all small- R (sub)jets within a RC jet that have p_T below 5% of the p_T of the reclustered jet. Due to the pile-up suppression and $p_T > 25 \text{ GeV}$ requirements imposed on the small- R jets, the average fraction of small- R jets removed by the trimming requirement is less than 1%. The resulting RC jets are required to have $|\eta| < 2.0$ and are used to identify high- p_T hadronically decaying top quark, Higgs boson or W/Z boson candidates by placing requirements on their transverse momentum, mass, and number of constituents. Hadronically decaying top-quark candidates are reconstructed as RC jets with $p_T > 400 \text{ GeV}$ and mass larger than 140 GeV. Top-quark candidates with $p_T < 700 \text{ GeV}$ are required to contain at least two constituent subjets. Higgs boson candidates are reconstructed as RC jets with $p_T > 350 \text{ GeV}$, a mass between 105 and 140 GeV, and a p_T -dependent requirement on the number of subjets (exactly two for $p_T < 600 \text{ GeV}$, and one or two for $p_T > 600 \text{ GeV}$). RC jets are tagged as arising from a W or Z boson if they have $p_T > 350 \text{ GeV}$, and a mass between 70 and 105 GeV. Furthermore, candidate W/Z (V boson) RC jets are required to have exactly two subjets if they have $p_T < 450 \text{ GeV}$, while candidates with one or two subjets are allowed at higher p_T . In the following, these are referred to as “ t -tagged”, “ H -tagged” and “ V -tagged” jets, respectively, while the term “jet” without further qualifiers is used to refer to central small- R jets.

The missing transverse momentum \vec{p}_T^{miss} (with magnitude E_T^{miss}) is defined as the negative vector sum of the \vec{p}_T of all selected and calibrated objects in the event, including a term to account for energy from soft particles in the event which are not associated with any of the selected objects. This soft term is calculated from inner-detector tracks matched to the selected primary vertex to make it more resilient to contamination from pile-up interactions [52].

To reconstruct boosted leptonic top-quark candidates in the event, the lepton and \vec{p}_T^{miss} in the event are first used to construct a leptonic W -boson candidate. The azimuthal direction and p_T of the neutrino daughter of the W boson are then chosen to be the same as the azimuthal direction and magnitude of the missing transverse momentum, and the neutrino p_z is determined by imposing a W mass constraint on the lepton-neutrino system. This amounts to solving a quadratic equation. If two solutions exist to the quadratic equation, the one with the lowest neutrino p_z is chosen. If no solution exists, the E_T^{miss} value is shifted until the equation has a unique solution. The leptonic W -boson candidate thus constructed is combined with a candidate b -jet in a two-step process. First, the b -tagged track-jet that is closest to the leptonic W -boson candidate in η - ϕ space is identified. Then, the closest small- R jet to this b -tagged jet with $\Delta R < 0.4$ is found and combined with the leptonic W -boson candidate. The b -jet is required to be within $\Delta R = 1.5$ of the leptonic W -boson candidate. Furthermore, in order to avoid double-counting, any b -jet within $\Delta R = 1.0$ of a t -tagged, H -tagged or V -tagged jet is not considered for leptonic top-quark reconstruction. The reconstructed leptonic top-quark candidate is required to have $p_T > 300$ GeV. The average reconstruction efficiency with these requirements in signal events is around 50%.

4 Data sample and event preselection

As described in section 1, this search is based on a dataset of pp collisions at $\sqrt{s} = 13$ TeV with 25 ns bunch spacing collected by the ATLAS experiment during the 2015–2018 data-taking period, corresponding to an integrated luminosity of 139 fb^{-1} . Only events recorded with a single-electron trigger, a single-muon trigger, or a E_T^{miss} trigger under stable beam conditions and for which all detector subsystems were operational are considered [53].

Single-lepton triggers [54, 55] with low p_T threshold and lepton isolation requirements are combined in a logical OR with higher-threshold triggers without isolation requirements to give maximum efficiency. For muons, triggers with a p_T threshold of 20 (26) GeV in 2015 (2016–2018) and isolation requirements, are combined with triggers with a 50 GeV threshold with no isolation requirement. A trigger with a 60 GeV threshold was added for the 2017–2018 data-taking period. The lowest p_T threshold for electron triggers was 24 (26) GeV in 2015 (2016–2018), while the highest p_T threshold varied from 120 GeV to 300 GeV during the data-taking period. The E_T^{miss} trigger [56] used an E_T^{miss} threshold of 70 GeV in the HLT in 2015 and a run-period-dependent E_T^{miss} threshold varying between 90 GeV and 110 GeV in other years.

Events satisfying the trigger selection are required to have at least one primary vertex candidate, and exactly one selected electron or muon. For events that only pass a single-lepton trigger, the selected lepton is required to match the lepton reconstructed by the trigger within $\Delta R < 0.15$. Events that do not satisfy the single-lepton trigger acceptance or matching conditions are selected only if they pass the E_T^{miss} trigger requirements and the offline reconstructed E_T^{miss} is above 200 GeV. The combination of single-lepton and E_T^{miss} triggers maximises the efficiency of the trigger selection.

In addition to the above, events are required to have at least three small- R jets and at least one b -tagged variable-radius jet. All selected small- R jets are considered for the purpose of event selection and categorisation, including those used to build RC jets.

Preselection requirements
Single-lepton or E_T^{miss} trigger
=1 isolated e OR μ
≥ 3 jets
≥ 1 b -tagged jets
$E_T^{\text{miss}} > 20$ GeV
$E_T^{\text{miss}} + m_T^W > 60$ GeV
$m_{\text{eff}} > 600$ GeV

Table 1. Summary of preselection requirements.

The background from multijet production is suppressed by placing requirements on E_T^{miss} as well as on the transverse mass of the lepton and E_T^{miss} system (m_T^W):⁴ $E_T^{\text{miss}} > 20$ GeV and $E_T^{\text{miss}} + m_T^W > 60$ GeV.

In order to select events that are kinematically close to those expected from signal, an additional selection is placed on the “effective mass” (m_{eff}) observable, which is defined as the scalar sum of the p_T of all central small- R jets and leptons in the event and the E_T^{miss} . All events considered in the analysis are required to have $m_{\text{eff}} > 600$ GeV.

The above requirements are referred to as the “preselection” and are summarised in table 1.

5 Signal and background modelling

Signal and background processes were modelled using Monte Carlo (MC) simulations. In the simulation, the masses of the top quark and Higgs boson were set to 172.5 GeV and 125 GeV, respectively. All simulated samples, except those produced with the SHERPA [57] event generator, utilised the EVTGEN program [58] to model the decays of heavy-flavour hadrons. While EVTGEN 1.2.0 was used for $t\bar{t}W$ and $t\bar{t}Z$ samples, EVTGEN 1.6.0 was used for all the other samples. In samples where the parton showering and hadronisation were modelled with PYTHIA 8 [59], a set of tuned parameters called the A14 tune [60] was used for underlying-event modelling, and the NNPDF2.3LO parton distribution function (PDF) set [61] was used for the showering and hadronisation processes. The H7UE parameter tune [62] was used instead for samples that employ HERWIG 7 for hadronisation and showering, with the MMHT2014LO PDF set [63].

To model the effects of pile-up, events from minimum-bias interactions were generated using the PYTHIA 8.186 event generator and overlaid on the simulated hard-scatter events according to the luminosity profile of the recorded data. The generated events were processed through a simulation [64] of the ATLAS detector geometry and response using

⁴ $m_T^W = \sqrt{2p_T^\ell E_T^{\text{miss}}(1 - \cos \Delta\phi)}$, where p_T^ℓ is the transverse momentum (energy) of the muon (electron) and $\Delta\phi$ is the azimuthal angle separation between the lepton and the direction of the missing transverse momentum.

GEANT4 [65]. A faster simulation, where the full GEANT4 simulation of the calorimeter response is replaced by a detailed parameterisation of the shower shapes [66], was adopted for some of the samples used to estimate systematic uncertainties. In these cases, the systematic uncertainties were estimated by comparing these alternative samples with versions of the nominal samples that were also processed through the same fast detector simulation. Simulated events are processed through the same reconstruction software as the data, and corrections are applied so that the object identification efficiencies, energy scales and energy resolutions match those determined from data control samples.

5.1 Signal modelling

Single production of T quarks was simulated with samples produced at leading order in the four-flavour scheme with MADGRAPH5_AMC@NLO 2.3.3 [67], using NNPDF3.0LO [68] PDF sets. The generator was interfaced to PYTHIA 8.212 [69] for the modelling of parton showering and hadronisation. The matrix elements were calculated according to the phenomenological model given in ref. [15] and all tree-level processes are included. The VLQs are assumed to couple exclusively to SM quarks of the third generation. Separate samples are generated for $T(\rightarrow Ht)qb$, $T(\rightarrow Zt)qb$, $T(\rightarrow Ht)qt$, and $T(\rightarrow Zt)qt$ processes in the 1.0–2.3 TeV mass range at fixed values of mass and κ . Matrix-element-based event weights [70] calculated during the generation are used to reweight the events in each sample to other values of mass and κ , to fill out a grid in the mass- κ plane. Samples at specific values of the relative couplings ξ_W , ξ_Z and ξ_H are obtained by reweighting the samples for the individual production and decay modes according to their corresponding branching fractions and combining them. All signal samples are normalised to cross sections calculated at next-to-leading order (NLO) [71] in quantum chromodynamics (QCD). Since the NLO cross sections were computed in a narrow-width approximation, a correction factor is applied to them to account for finite-width effects [72] and an additional correction is applied to account for non-resonant T -quark production [73]. A change in the dynamic scale in MADGRAPH at the threshold $\Gamma_T/m_T = 0.1$ leads to a discontinuity in the computed cross section [73]. As a result, two different parameterisations of the cross section are available: $\sigma_{\text{low}}(\Gamma_T/m_T)$ for the $\Gamma_T/m_T < 0.1$ regime, and $\sigma_{\text{high}}(\Gamma_T/m_T)$ for $\Gamma_T/m_T > 0.1$. An averaging procedure is used in order to obtain a smooth cross section $\sigma(\Gamma_T/m_T)$ across the mass and coupling grid:

$$\sigma(\Gamma_T/m_T) = \begin{cases} \sigma_{\text{low}}(\Gamma_T/m_T) + \frac{1}{2}(\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1)), & \text{if } \Gamma_T/m_T < 0.1 \\ \sigma_{\text{high}}(\Gamma_T/m_T) - \frac{1}{2}(\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1)), & \text{if } \Gamma_T/m_T \geq 0.1 \end{cases}$$

An additional uncertainty of $\frac{1}{2}(\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1))$ is assigned to the cross section at every point to account for this choice.

5.2 Background modelling

After preselection, the main source of background is the production of $t\bar{t}$. The production of a top quark in association with a W boson (Wt) makes significant contributions in regimes of high transverse momentum. The remaining background contributions originate mostly from W +jets processes.

The production of $t\bar{t}$ and single-top-quark events was modelled using the POWHEG BOX v2 [74–77] generator at NLO with the NNPDF3.0NLO [68] PDF set. The h_{damp} parameter⁵ for $t\bar{t}$ samples was set to $1.5 m_{\text{top}}$ [78]. The events were interfaced to PYTHIA 8.230 [69] to model the parton shower, hadronisation, and underlying event.

Samples to model Wt production were generated using the diagram removal scheme [79], which is designed to remove interference and overlap with $t\bar{t}$ production. The related uncertainty is estimated by comparison with an alternative sample generated using the diagram subtraction scheme [78, 79] and the same generator set-up as the nominal sample. Separate samples were generated to model s -channel and t -channel single top-quark production.

The uncertainty associated with using the chosen parton shower and hadronisation model is evaluated by comparing the sample from the nominal generator set-up with a sample also produced with the POWHEG BOX v2 [74–77] generator using the NNPDF3.0NLO [68] PDF set, but with the events interfaced with HERWIG 7.04 [62, 80] to model the parton shower and hadronisation.

To assess the uncertainty in the matching of NLO matrix elements and parton showers for $t\bar{t}$ samples, the POWHEG BOX sample is compared with a sample of events generated with MADGRAPH5_AMC@NLO 2.6.0 interfaced with PYTHIA 8.230 [69]. The samples used to estimate this uncertainty for single top-quark production were generated with MADGRAPH5_AMC@NLO 2.6.2, also interfaced with PYTHIA 8.230 [69]. For both samples, the NNPDF3.0NLO set of PDFs [68] was used in the matrix-element calculations.

The $t\bar{t}$ samples were generated inclusively, but events are categorised depending on the flavour content of additional particle jets not originating from the decay of the $t\bar{t}$ system (see ref. [81] for details). Events labelled as either $t\bar{t}+\geq 1b$ or $t\bar{t}+\geq 1c$ are generically referred to in the rest of the paper as $t\bar{t}$ +HF events, where HF stands for “heavy flavour”. The remaining events are labelled as $t\bar{t}$ +light-jets events, including those with no additional jets.

The inclusive cross section for $t\bar{t}$ production was corrected to the theory prediction at next-to-next-to-leading order (NNLO) in QCD including the resummation of next-to-next-to-leading logarithmic (NNLL) soft-gluon terms calculated using TOP++ 2.0 [82–88]. For proton-proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross section corresponds to $\sigma(t\bar{t})_{\text{NNLO+NNLL}} = 832 \pm 51$ pb using a top-quark mass of $m_{\text{top}} = 172.5$ GeV. The cross-section uncertainties due to the PDF and α_s were calculated using the PDF4LHC15 prescription [89] with the MSTW2008NNLO [90, 91], CT10NNLO [92, 93] and NNPDF2.3LO [61] PDF sets in the five-flavour scheme, and were added in quadrature to the effect of the factorisation and renormalisation scale uncertainties.

The production of $W/Z(V)$ +jets was simulated with the SHERPA 2.2.1 [94] generator using NLO matrix elements for up to two partons, and leading-order (LO) matrix elements for up to four partons, calculated with the Comix [95] and OPENLOOPS 1 [96–98] libraries. They were matched with the SHERPA parton shower [99] using the MEPS@NLO prescription [100–103] and the set of tuned parameters developed by the SHERPA authors. The

⁵The h_{damp} parameter is a resummation damping factor and one of the parameters that controls the matching of POWHEG BOX matrix elements to the parton shower and thus effectively regulates the high- p_T radiation against which the $t\bar{t}$ system recoils.

NNPDF3.0NNLO set of PDFs [68] was used and the samples are normalised to a NNLO prediction [104].

Samples of diboson final states (VV) were simulated with the SHERPA 2.2.1 or 2.2.2 [94] generator depending on the process, including off-shell effects and Higgs boson contributions, where appropriate. Only processes with at least one lepton in the final state are considered in this search. Fully leptonic final states and semileptonic final states, where one boson decays leptonically and the other hadronically, were generated using matrix elements at NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional parton emissions. Samples for the loop-induced processes $gg \rightarrow VV$ were generated using LO-accurate matrix elements for up to one additional parton emission for both the cases of fully leptonic and semileptonic final states. The matrix-element calculations were matched and merged with the SHERPA parton shower based on Catani-Seymour dipole factorisation [95, 99] using the MEPS@NLO prescription [100–103]. The virtual QCD corrections were provided by the OPENLOOPS 1 library [96–98]. The NNPDF3.0NNLO set of PDFs was used [68], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

The production of $t\bar{t}W$ and $t\bar{t}Z$ events was modelled using the MADGRAPH5_AMC@NLO 2.3.3 [67] generator at NLO with the NNPDF3.0NLO [68] PDF set. The events were interfaced to PYTHIA 8.210 [69]. The production of $t\bar{t}H$ events was modelled using the POWHEG BOX v2 [74–77, 105] generator at NLO with the NNPDF3.0NLO [68] PDF set. The production of tH events was modelled using the MADGRAPH5_AMC@NLO 2.3.3 [67] generator at NLO with the NNPDF3.0NLO [68] PDF set. Events in both of these samples were interfaced with PYTHIA 8.230 [69] for showering and hadronisation. The production of four-top-quark events in the SM was simulated at LO using MADGRAPH5_AMC@NLO 2.2.2 and the NNPDF2.3LO PDF set, interfaced to PYTHIA 8.186 in combination with the A14 underlying-event tune, and normalised to the NLO theoretical cross section.

Multijet events were generated using PYTHIA 8.230 [69] with leading-order matrix elements for dijet production and interfaced to a p_T -ordered parton shower. Events from this simulation are normalised to data in a multijet-enriched region obtained by inverting the requirements on the E_T^{miss} and m_T^W observables in the preselection, and also requiring the lepton p_T to be below 100 GeV.

6 Analysis strategy

The search described in this paper targets the production of a single T quark that decays to a leptonically decaying top quark and a hadronically decaying Higgs or Z boson. Both b -associated and t -associated single- T production are considered in the search. The four resulting production and decay modes are:

1. $T(\rightarrow Zt)qb$: b -associated T production with $T \rightarrow Zt$ decay
2. $T(\rightarrow Ht)qb$: b -associated T production with $T \rightarrow Ht$ decay

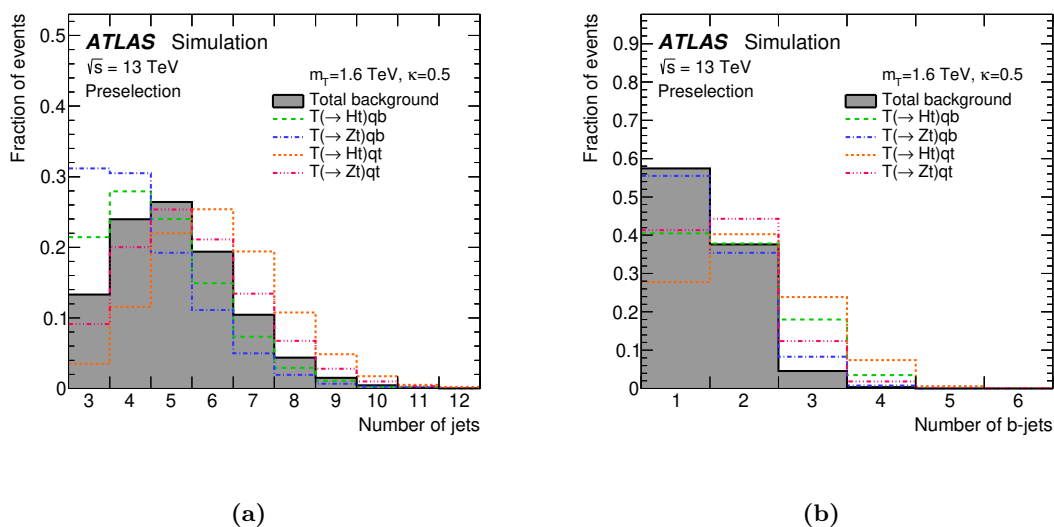


Figure 2. Comparison of the shape of the distribution of (a) the central jet multiplicity, and (b) the b -tagged jet multiplicity in the preselection region, between the total background (filled area) and the signal scenarios considered in this search for T quarks with a mass of 1.6 TeV and $\kappa = 0.5$. The last bin in each distribution contains the overflow.

3. $T(\rightarrow Zt)qt$: t -associated T production with $T \rightarrow Zt$ decay
4. $T(\rightarrow Ht)qt$: t -associated T production with $T \rightarrow Ht$ decay

To test for the presence of signal, a likelihood fit is performed on the distribution of the m_{eff} variable (defined in section 4) across a set of 24 “fit regions” constructed from events in the preselection sample. These regions are summarised in table 2. The fit regions are designed to be pure in one or more of the four targeted signal modes, or in specific background processes. The combined use of these regions in the fit allows the search to retain sensitivity to all of the processes that can occur simultaneously in a benchmark model, and the signal-depleted regions serve to improve the description of the expected background. In the following, the strategy and motivation behind the event categorisation model is described.

Different T -quark production modes can be distinguished by the number of jets in the final state, as illustrated in figure 2a. For b -associated signal production with a leptonically decaying top quark and hadronically decaying Higgs or Z boson, four central jets are expected in the final state at leading order in the four-flavour scheme. However, some of these jets can merge due to the collimation of the decay daughters from boosted Higgs or Z bosons. Furthermore, the initial b -quark from gluon splitting can sometimes be produced at high pseudorapidity and therefore not be reconstructed in the central region. Conversely, since exactly one lepton is required to be present in the final state, one of the top quarks in events with t -associated production can be expected to decay hadronically, producing extra jets. Based on these arguments, the basic category of regions targeting b -associated production modes (henceforth labelled as LJ, standing for “Low Jet multiplicity”) are

Fit regions				
Jet mult.	b -tag mult.	Region	Targeted signal / bkg	
3–5	1	LJ, 1b, $\geq 1f_j$, $0(t_h+t_l)$, 0H, $\geq 1V$	$T(\rightarrow Zt)qb$	
		LJ, 1b, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, 0H, $\geq 1V$		
	2	LJ, 2b, $\geq 1f_j$, $0(t_h+t_l)$, 0H, $\geq 1V$		
		LJ, 2b, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, 0H, $\geq 1V$		
	3	LJ, 3b, $\geq 1f_j$, $0(t_h+t_l)$, $\geq 1H$, 0V		$T(\rightarrow Ht)qb$
		LJ, 3b, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $\geq 1H$, 0V		
		LJ, 3b, $\geq 1f_j$, $\geq 1t_h$, $0t_l$, $\geq 1H$, 0V		
	≥ 4	LJ, $\geq 4b$, $\geq 1f_j$, $0(t_h+t_l)$, $\geq 1H$, 0V		
		LJ, $\geq 4b$, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $\geq 1H$, 0V		
		LJ, $\geq 4b$, $\geq 1f_j$, $\geq 1t_h$, $0t_l$, $\geq 1H$, 0V		
		LJ, $\geq 4b$, 0fj, $\geq 1t_l$, 0H, $0(V+t_h)$	$t\bar{t}+\geq 1b$, $t\bar{t}+\geq 1c$	
≥ 6	1	HJ, 1b, $\geq 1f_j$, $0t_h$, $1t_l$, 0H, $\geq 1V$	$T(\rightarrow Zt)qt$	
		HJ, 1b, $\geq 1f_j$, $1t_h$, $0t_l$, 0H, $\geq 1V$		
		HJ, 1b, $\geq 1f_j$, $\geq 2(t_h+t_l)$, 0H, $\geq 1V$		
	2	HJ, 2b, $\geq 1f_j$, $0t_h$, $1t_l$, 0H, $\geq 1V$		
		HJ, 2b, $\geq 1f_j$, $1t_h$, $0t_l$, 0H, $\geq 1V$		
		HJ, 2b, $\geq 1f_j$, $\geq 2(t_h+t_l)$, 0H, $\geq 1V$		
	3	HJ, 3b, $\geq 1f_j$, $1t_l$, $\geq 1H$, $0(V+t_h)$		$T(\rightarrow Ht)qt$
		HJ, 3b, $\geq 1f_j$, $0t_l$, $\geq 1H$, $1(V+t_h)$		
		HJ, 3b, $\geq 1f_j$, $\geq 1H$, $\geq 2(V+t_l+t_h)$		
	≥ 4	HJ, $\geq 4b$, $\geq 1f_j$, $1t_l$, $\geq 1H$, $0(V+t_h)$		
HJ, $\geq 4b$, $\geq 1f_j$, $0t_l$, $\geq 1H$, $1(V+t_h)$				
HJ, $\geq 4b$, $\geq 1f_j$, $\geq 1H$, $\geq 2(V+t_l+t_h)$				
		HJ, $\geq 4b$, 0fj, $\geq 1t_l$, 0H, $0(V+t_h)$	$t\bar{t}+\geq 1b$, $t\bar{t}+\geq 1c$	

Table 2. Definition of the 24 regions (referred to as “fit regions”) that enter the likelihood fit. Events are categorised in terms of jet (j), b -tagged jet (b), forward jet (fj), V -tagged jet (V), Higgs-tagged jet (H), hadronic top-tagged jet (t_h), and leptonic top-quark candidate (t_l) multiplicities.

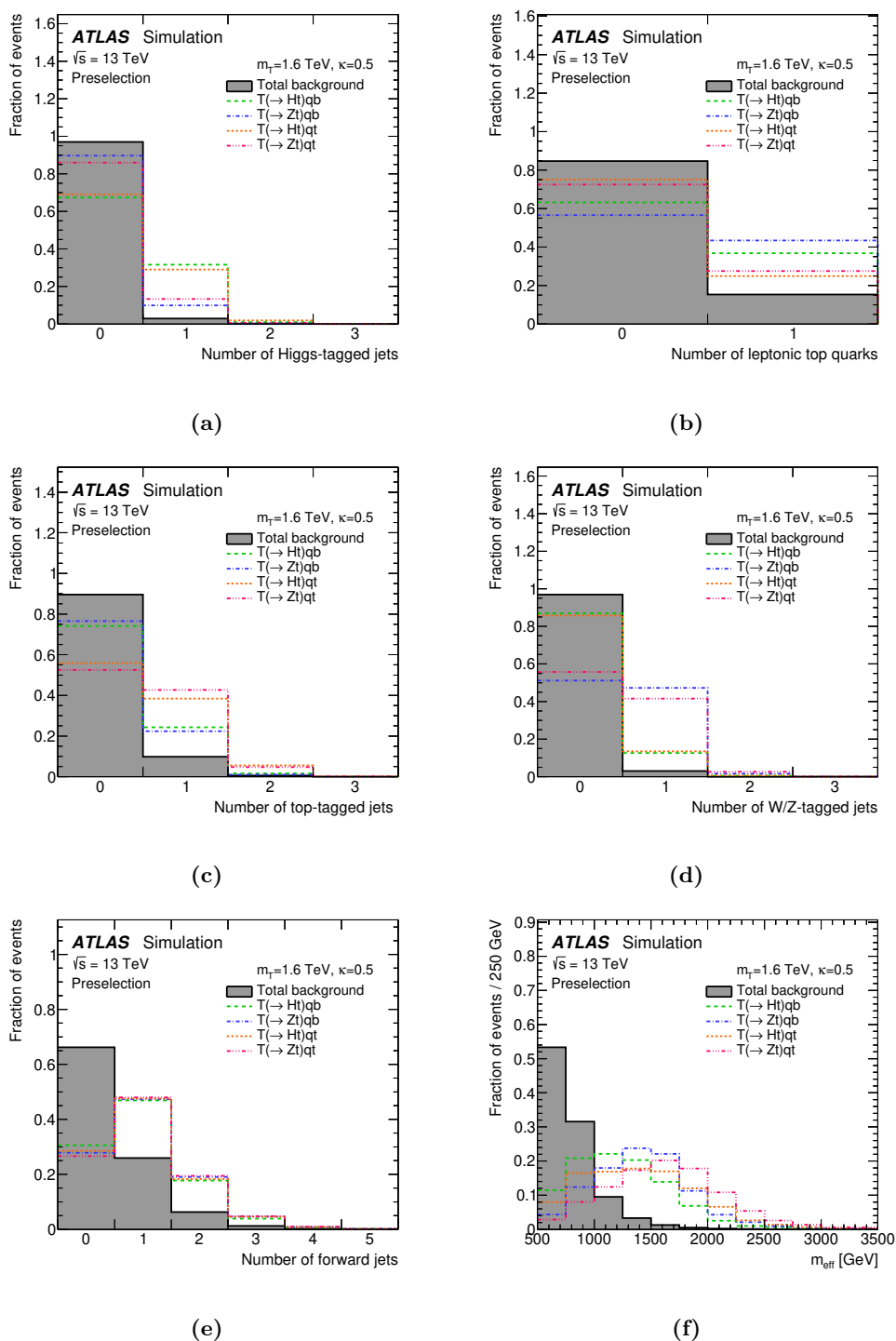


Figure 3. Comparison of the shape of the distribution of (a) Higgs-tagged jet multiplicity, (b) leptonic top-quark candidate multiplicity, (c) hadronic top-tagged jet multiplicity, (d) W/Z -tagged jet multiplicity, (e) the forward jet multiplicity, and (f) the effective mass m_{eff} , between the total background (filled area) and the signal scenarios considered in this search for a T with a mass of 1.6 TeV and $\kappa = 0.5$, in the preselection region. The last bin in each distribution contains the overflow.

required to have 3–5 jets, while regions targeting t -associated production modes (henceforth labelled as HJ, standing for “High Jet multiplicity”) are required to have ≥ 6 jets.

The different T -quark decay modes are characterised by differences in the multiplicity of b -tagged jets (figure 2b). Events with $T \rightarrow Zt$ decays typically contain fewer b -jets than events with $T \rightarrow Ht$ decays, due to the dominant Higgs boson decay to bottom-quark pairs. Accordingly, regions targeting $T \rightarrow Zt$ decays are required to have exactly 1 or 2 b -tagged jets, while events with exactly 3 or ≥ 4 b -tagged jets are used to target $T \rightarrow Ht$ decays.

Since the top quark, Z boson or Higgs boson daughters of the heavy T quark are often produced at high- p_T in boosted states, signal events are characterised by high multiplicities of tagged boosted objects. The distribution of the multiplicities of H -tagged (H) jets, leptonic top-quark (t_l) candidates, t -tagged (t_h) jets, and V -tagged (V) jets in the preselection region are shown in figures 3a–3d. The specific requirements on the multiplicities of these boosted objects that are applied in each fit region are tailored to the signal or background process targeted by that particular region. For example, regions in the $\geq 3b$ categories are designed to be sensitive to $T \rightarrow Ht$ signals, and therefore at least one H -tagged jet is required in these regions. Conversely, at least one V -tagged jet is required in all regions of the 1–2b category, since these regions target $T \rightarrow Zt$ decays. Signal events with t -associated T -quark production contain an additional top quark that can decay hadronically. Therefore, the presence of a hadronic top-tagged jet is required in some signal regions. Events can also have V -tagged jets arising from semi-boosted hadronic top quarks, in cases where the decay products of the top quark are not collimated enough to produce a t -tagged jet. Finally, an LJ region and HJ region are used in the fit to constrain the normalisation of $t\bar{t} + \geq 1b$ and $t\bar{t} + \geq 1c$ backgrounds, requiring $\geq 4b$ and no boosted hadronic objects.

As discussed in section 1, the initial quark recoiling from the gauge boson in single- T production often emerges at high pseudorapidity, resulting in the presence of jets in the forward region (figure 3e). Thus, at least one forward jet (fj) is required in the signal-enriched fit regions to increase the signal purity. On the other hand, a 0fj requirement is applied in the regions used to control the $t\bar{t} + \geq 1b$ and $t\bar{t} + \geq 1c$ background normalisations, in order to deplete the signal fraction in those regions.

Background predictions in the fit regions are validated in a set of 20 validation regions, designed to be statistically independent of the fit regions and yet kinematically similar to them (table 3). These regions are created by adopting a combination of inverted tagged boosted-object multiplicity requirements, or specifically vetoing forward jets. The maximum allowed signal contamination in the overall yield in each validation region is required to be $< 10\%$, assuming a signal cross section of 100 fb. This value was chosen as an upper bound on the allowed cross section in the considered mass range, corresponding to the observed exclusion limits from previous searches.

The choice of m_{eff} as the final fitted observable is driven by the strong signal discrimination power of this observable, as can be seen in figure 3f. Due to the presence of highly energetic jets and leptons from the decay of the T quark, the average m_{eff} in signal events is much larger than in background events. The shape of the m_{eff} distribution depends on the assumed mass m_T of the T quark, as well as on the T -quark production and decay modes. In particular, an extra factor of m_T^2/s leads to an enhancement of the partonic cross sec-

Validation regions		
Jet mult.	b -tag mult.	Region
3–5	1	LJ, 1b, 0fj, 0 t_h , 0 t_l , 0H, $\geq 1V$
		LJ, 1b, 0fj, 0 t_h , $\geq 1t_l$, 0H, $\geq 1V$
		LJ, 1b, $\geq 1fj$, $\geq 1(t_h+t_l)$, 0H, 0V
		LJ, 1b, $\geq 1fj$, $\geq 1t_h$, 0 t_l , 0H, $\geq 1V$
	2	LJ, 2b, 0fj, 0 t_h , 0 t_l , 0H, $\geq 1V$
		LJ, 2b, 0fj, 0 t_h , $\geq 1t_l$, 0H, $\geq 1V$
		LJ, 2b, $\geq 1fj$, $\geq 1(t_h+t_l)$, 0H, 0V
		LJ, 2b, $\geq 1fj$, $\geq 1t_h$, 0 t_l , 0H, $\geq 1V$
	≥ 3	LJ, $\geq 3b$, 0fj, 0(t_h+t_l), $\geq 1H$, 0V
LJ, $\geq 3b$, $\geq 1fj$, 0H, $\geq 1(V+t_l+t_h)$		
≥ 6	1	HJ, 1b, 0fj, 1(t_h+t_l), 0H, $\geq 1V$
		HJ, 1b, 0fj, $\geq 2(t_h+t_l)$, 0H, $\geq 1V$
		HJ, 1b, $\geq 1fj$, 0 t_h , 0 t_l , $\geq 1H$, $\geq 1V$
		HJ, 1b, $\geq 1fj$, $\geq 2(t_h+t_l)$, $\geq 1H$, 0V
	2	HJ, 2b, 0fj, 1(t_h+t_l), 0H, $\geq 1V$
		HJ, 2b, 0fj, $\geq 2(t_h+t_l)$, 0H, $\geq 1V$
		HJ, 2b, $\geq 1fj$, 0 t_h , 0 t_l , $\geq 1H$, $\geq 1V$
		HJ, 2b, $\geq 1fj$, $\geq 2(t_h+t_l)$, $\geq 1H$, 0V
	≥ 3	HJ, $\geq 3b$, 0fj, $\geq 1H$, $\geq 1(V+t_l+t_h)$
		HJ, $\geq 3b$, $\geq 1fj$, 0H, $\geq 1(V+t_l+t_h)$

Table 3. Event categorisation into validation regions in terms of jet (j), b -tagged jet (b), forward jet (fj), V -tagged jet (V), Higgs-tagged jet (H), hadronic top-tagged jet (t_h), and leptonic top-quark candidate (t_l) multiplicities. The selection follows the same principle as the fit region categorisation defined in table 2, but maintains orthogonality by inverting either the forward jet cut or the cuts on tagged boosted objects.

tion at low centre-of-mass energies for the $T(\rightarrow Ht)qb$ and $T(\rightarrow Ht)qt$ processes [106], and consequently the m_{eff} distribution shifts to lower values.⁶ Nevertheless, the discrimination power of this observable is relatively independent of the signal model parameters, and the search is therefore sensitive across a wide range of parameter space.

7 Kinematic reweighting of background

Recent measurements of differential cross sections have demonstrated that the current simulations of $t\bar{t}$ processes overestimate the upper tail of the top-quark p_T spectrum [107, 108]. Conversely, the cross section for this process is underestimated at high jet multiplicities [107]. There are similar issues of accuracy in the modelling of W +jets processes [109] in the regime of high jet multiplicities and/or high- H_T (where H_T is defined as the scalar sum of the p_T of central jets in the event). This leads to discrepancies in the shapes of the m_{eff} and N_{jets} spectra between the data and expected background in the kinematic regimes relevant for this search. Data-driven reweighting factors are therefore used to correct the observed discrepancies in these processes. These corrections are derived using the following iterative procedure.

For a given group of background processes, a “reweighting source region” (RSR) is first identified, which is enriched in events from that process group, and depleted in signal events. Then, the reweighting factor $R_a(x)$ for any observable x , for the process group a , can be calculated as

$$R_a(x) = \frac{\text{Data}(x) - \text{MC}^{\text{non-}a}(x)}{\text{MC}^a(x)}.$$

For each group of processes, reweighting factors are first derived from the jet multiplicity distribution. After correcting the N_{jets} distribution of the process with this initial reweighting, a second set of reweighting factors is derived as a function of a reduced m_{eff} variable, which is defined as $m_{\text{eff}}^{\text{red}} = m_{\text{eff}} - (N_{\text{jets}} - 3) \times 50$ GeV. The constant value of 50 GeV approximately corresponds to the average p_T of each additional jet expected in $t\bar{t}$ events. Thus, this definition makes the shape of the reweighting functions in the $m_{\text{eff}}^{\text{red}}$ variable more consistent across N_{jets} . The residual dependence on N_{jets} is addressed by deriving the reweighting in exclusive N_{jets} bins. The $m_{\text{eff}}^{\text{red}}$ reweighting factors are parameterised by sigmoid functions to mitigate statistical fluctuations.

The subdominant $W(\ell\nu)$ +jets background process is corrected first. However, since it is difficult to isolate $W(\ell\nu)$ +jets events in the preselection sample with $\geq 1b$ selection, the correction factors for this process are extrapolated from a sample enriched in $Z(\ell\ell)$ +jets instead. This sample is obtained by selecting events containing exactly two leptons with the same flavour and opposite electric charges, and requiring the invariant mass of the lepton pair ($m_{\ell\ell}$) to be consistent with the Z boson mass (m_Z). To match the kinematic regime of the preselection more closely, events in this sample must also contain at least three small- R jets, at least one of which is b -tagged. Contamination from $t\bar{t}$ processes is suppressed by requiring $E_T^{\text{miss}} < 100$ GeV. The corrections derived from this sample are

⁶Again, m_T refers to the mass of the T quark, and s is the usual Mandelstam variable.

Reweighting source regions				
Lepton multiplicity	Jet multiplicity	b -tag multiplicity	Other requirements	Targeted background
1	≥ 3	2	—	$t\bar{t} + tW$
2	≥ 3	1	$ m_{\ell\ell} - m_Z \leq 10 \text{ GeV},$ $E_T^{\text{miss}} < 100 \text{ GeV}$	$Z+\text{jets}$

Table 4. Reweighting source regions from which the reweighting functions for $t\bar{t}$ and tW production and $W/Z+\text{jets}$ production are derived.

applied to both the $W+\text{jets}$ and $Z+\text{jets}$ events in the preselection sample, before correction factors for the $t\bar{t}$ background are derived.

Since $t\bar{t}$ events share the same final state as tW production, these two processes are grouped together for the purposes of deriving the reweighting factors. A sample enriched in $t\bar{t}$ +light-jets and tW production, selected by requiring exactly one lepton, at least three small- R jets and exactly two b -jets, is used to derive combined correction factors for both processes. The same correction factors are also applied to the $t\bar{t}+\geq 1b$ and $t\bar{t}+\geq 1c$ processes in the analysis.

The selection requirements for the RSRs are summarised in table 4.

The m_{eff} distribution in the preselection region, before and after the application of the full reweighting, is shown in figure 4. Since the preselection region is kinematically very close to the RSRs, almost perfect agreement can be seen between the data and the expected background after reweighting. As explained later in section 8, dedicated reweighting factors are derived for the alternative simulations that are used to estimate the modelling uncertainties for $t\bar{t}$, Wt and $W/Z+\text{jets}$ backgrounds. As a result, the modelling uncertainties of these background processes vanish in the RSRs, and are small in regions that are kinematically close to them. This is reflected in the small uncertainty bands seen in figure 4. The reweighted modelling uncertainties in the fit and validation regions are substantially larger, since they are kinematically further away from the RSRs.

8 Systematic uncertainties

The impact of several sources of systematic uncertainty on the normalisation of signal and background and/or the shape of the m_{eff} distributions is considered. Each systematic uncertainty is considered to be correlated across processes, channels, and bins of the signal discriminant, unless explicitly stated otherwise. Uncertainties from different sources are considered to be uncorrelated with each other.

The leading sources of uncertainty in this search arise from the modelling of the $t\bar{t}$ and single-top Wt backgrounds, the flavour-tagging efficiencies (b , c and light), and the jet mass resolution. The relative contributions of these uncertainties vary depending on the analysis region, and therefore their relative impact on the search sensitivity depends on the signal process being considered. The following sections describe each of the systematic

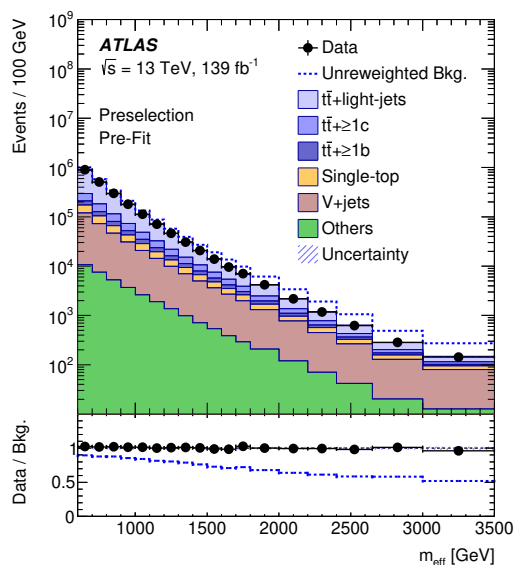


Figure 4. Comparison of the m_{eff} distribution between the data and unweighted (blue dashed line) and reweighted (stacked histograms) background predictions in the preselection region before the likelihood fit. The “others” background includes the $t\bar{t} V/H$, VH , tZ , $t\bar{t}t\bar{t}$, diboson, and multijet backgrounds. The last bin in the distribution contains the overflow. The bottom panel displays the ratios of data to the total background predictions.

uncertainties considered in this analysis. An overview of the combined impact of the different groups of systematic uncertainties is furthermore given in table 7.

8.1 Experimental uncertainties

Uncertainties associated with leptons arise from the efficiencies of the trigger selection, reconstruction, identification, and isolation criteria, as well as the lepton momentum scale and resolution. These are measured in data using $Z \rightarrow \ell^+\ell^-$, $W \rightarrow \ell\nu$ and $J/\psi \rightarrow \ell^+\ell^-$ events [39, 110]. The combined effect of all these uncertainties results in an overall normalisation uncertainty in signal and background of approximately 1%.

Uncertainties associated with jets arise from the jet energy scale (JES) and resolution (JER), the jet mass scale (JMS) and resolution (JMR), and the efficiency of the JVT requirements imposed to reject jets from pile-up. The JES and JER uncertainties are estimated by combining information from collision data, test-beam data and simulation [44, 111]. The JES (JER) uncertainties are split into 30 (8) uncorrelated components, corresponding to different physical sources. The uncertainty in the JMS is estimated by comparing each nominal sample with two corresponding alternative event samples, in which the mass of each jet is either raised or lowered by 10%, respectively. The uncertainty in the JMR is estimated by comparing each nominal sample with an alternative event sample in which the mass of each jet is smeared by a Gaussian function whose width is shifted by 20% relative to the nominal JMR. As previously mentioned, the above uncertainties associated with jets are propagated to the RC jets from which the hadronic tagged boosted objects are constructed.

The flavour-tagging efficiencies for b -, c -, and light-jets in simulation are corrected to match efficiencies measured in data control samples. Uncertainties in these efficiencies are also estimated in these auxiliary measurements, following the methods described in refs. [112–114]. A set of nine independent uncertainty sources are considered for b -jets, while five sources are considered for c -jets, and six components are considered for light-flavour jets. These components are taken to be uncorrelated among b -jets, c -jets, and light-jets. An additional extrapolation uncertainty component is considered for high- p_T jets that are outside the kinematic reach of the calibration data sample; it is taken to be correlated amongst the jet flavours. Finally, an uncertainty related to the application of the c -jet scale factors to τ -jets is considered, but has a negligible impact in this analysis.

8.2 Background modelling uncertainties

An uncertainty of $+5.5/-6.1\%$ is assigned to the inclusive $t\bar{t}$ production cross section [88], including contributions from varying the factorisation and renormalisation scales, and from uncertainties in the PDF, α_s , and the top-quark mass, all added in quadrature. Normalisation uncertainties of 50% each are assigned to the normalisation of $t\bar{t}+\geq 1b$ and $t\bar{t}+\geq 1c$ processes. These uncertainties are motivated by the observed level of agreement between data and simulation in dedicated measurements of the cross section of the $t\bar{t}+\geq 1b$ process [115]. For single-top processes, a $\pm 5\%$ uncertainty in the total cross section, estimated as a weighted average of the theoretical uncertainties in t -, Wt - and s -channel production [116–118], is included.

A number of sources of systematic uncertainty affecting the modelling of $t\bar{t}$ -jets and single-top production are considered. Uncertainties due to the choice of the NLO generator are estimated by comparing the nominal POWHEG+PYTHIA 8 samples with alternative samples generated by MADGRAPH5_AMC@NLO and showered by PYTHIA 8. The nominal samples are compared with POWHEG+HERWIG 7 samples to estimate the uncertainties in the modelling of the parton showering and hadronisation processes. The alternative samples used to evaluate modelling uncertainties are described in detail in section 5.2. The uncertainty due to initial-state radiation (ISR) is estimated by simultaneously varying the h_{damp} parameter and the renormalisation and factorisation scales, and choosing the Var3c up/down variants of the A14 tune as described in ref. [119]. The impact of final-state radiation (FSR) is evaluated by doubling or halving the renormalisation scale for emissions from the parton shower. The NNPDF3.0LO replicas are used to evaluate the PDF uncertainties for the nominal PDF. These uncertainties are all considered to be uncorrelated among $t\bar{t}$ +light-jets, $t\bar{t}+\geq 1c$, $t\bar{t}+\geq 1b$ and single-top samples, but correlated across the subcategories of the single-top background (s -channel, t -channel or tW). Furthermore, these uncertainties are treated as uncorrelated amongst LJ and HJ analysis regions and regions with 0, 1 or ≥ 2 tagged boosted objects. The impact of this correlation scheme on the search sensitivity was studied and compared with a scheme where the modelling uncertainties are correlated across all fit regions. The expected cross-section limits are around 10% higher with the current correlation scheme for low VLQ masses, whereas the impact is negligible for high mass signals.

An additional systematic uncertainty in Wt -channel production, concerning the separation between $t\bar{t}$ and Wt at NLO [79], is assessed by comparing the nominal sample, which uses the so-called “diagram removal” scheme, with an alternative sample using the “diagram subtraction” scheme.

The uncertainties in the modelling of the W/Z +jets backgrounds are estimated by varying the values of the internal renormalisation and factorisation scale parameters in SHERPA. An additional $\pm 30\%$ normalisation uncertainty for the W/Z +jets background is considered for events in analysis regions with different b -tag multiplicity (1, 2, 3, ≥ 4), uncorrelated among b -tag multiplicities. This uncertainty is based on variations of the factorisation and renormalisation scales and SHERPA matching parameters [120]. Since a dedicated reweighting of the jet multiplicity spectrum is applied to V +jets events, these uncertainties are considered to be correlated between LJ and HJ regions. Each of these uncertainties is also considered to be correlated between W +jets and Z +jets processes.

The kinematic reweighting of the main background processes (described in section 7) is also derived for each of the modelling uncertainties described above, so that each alternative background model matches the data (and the nominal background prediction) in the reweighting source regions. Thus, the role of the modelling uncertainties after this reweighting is to account for extrapolations in kinematics and background composition between the reweighting source region and the fit and validation regions.

Uncertainties in the reweighting procedure itself arise mainly from the statistical uncertainties in the reweighting source regions and the choice of the functional form for parameterisation. These uncertainties are evaluated by shifting the fitted function to $\pm 2\sigma$ from its nominal value using the uncertainties of the fitted parameters and taking their internal correlations into account. These shifts represent possible variations in both the scale and the shape of the reweighting function, although the functional form of the parameterisation is not altered.

Since the diboson, $t\bar{t}W/Z$ and $t\bar{t}H$ processes contribute a small fraction of the events in the fit regions, their shape uncertainties have a negligible impact on the results, and only cross-section uncertainties are considered. The assigned uncertainties, due to the PDF and scale uncertainties in the NLO calculation, are $\pm 15\%$ for $t\bar{t}W/Z$ (treated as uncorrelated between LJ and HJ regions), and $+9/-12\%$ for $t\bar{t}H$. Uncertainties in the diboson background include a 5% uncertainty in the inclusive cross section calculated at NLO [121]. An additional uncorrelated 24% uncertainty in the production cross section is considered for each additional jet in the event, based on a comparison among different algorithms for merging LO matrix elements and parton showers [122]. The uncertainty estimate is based on the average jet multiplicity in each fit region, which is approximately three in the LJ regions (i.e. one additional jet from radiation) and six in the HJ regions (i.e. four additional jets from radiation). A $\pm 30\%$ normalisation uncertainty is considered for the production of additional heavy-flavour jets. Since the leading two b -tagged jets in diboson events are expected to arise from $W \rightarrow cs$ or $Z \rightarrow bb$ decays, this uncertainty is only applied to fit regions with ≥ 3 b -jets. All of these uncertainties are added in quadrature in each region, and the resulting uncertainty is treated as uncorrelated between LJ and HJ regions, as well as between low- b ($1-2b$) and high- b ($\geq 3b$) regions. The total normalisation

uncertainty for diboson processes in LJ regions is 24% and 38% in low- and high- b regions, respectively; in HJ regions it is 48% and 56% in low- and high- b regions, respectively.

9 Statistical analysis

For each benchmark scenario considered in this search, the m_{eff} distributions across all search regions are jointly analysed to test for the presence of the predicted signal. A binned likelihood function $\mathcal{L}(\mu, \theta)$ is constructed as a product of Poisson probability terms over all m_{eff} bins considered in the search.

The likelihood function depends on the signal-strength parameter μ , which multiplies the predicted production cross section for signal, and θ , a set of nuisance parameters that encode the effect of systematic uncertainties in the signal and background expectations. Therefore, the expected total number of events in a given bin depends on μ and θ .

Nuisance parameters corresponding to all systematic uncertainties are implemented in the likelihood function with Gaussian constraints. In each bin of the m_{eff} distributions, uncertainties due to the limited size of the simulated samples are also taken into account by dedicated parameters in the fit that are independent across bins. These parameters are implemented with Poisson constraints.

For a given value of μ , variations in the nuisance parameters θ allow the expectations for signal and background to change according to the corresponding systematic uncertainties. The fitted values of θ correspond to deviations from the nominal expectations that globally provide the best fit to the data. This procedure reduces the impact of systematic uncertainties on the search sensitivity and improves the background prediction by taking advantage of the highly populated background-dominated regions included in the likelihood fit.

The improvement in the background prediction is verified by performing fits under the background-only hypothesis and checking how well the data agrees with the post-fit background in validation regions that are disjoint from the regions used in the fit.

The test statistic q_μ , as implemented in a framework based on RooStats [123, 124] and HistFitter [125], is defined as the profile likelihood ratio: $q_\mu = -2 \ln(\mathcal{L}(\mu, \hat{\theta}_\mu) / \mathcal{L}(\hat{\mu}, \hat{\theta}))$. Here, $\hat{\mu}$ and $\hat{\theta}$ are the values of the parameters μ and θ that simultaneously maximise the likelihood function $\mathcal{L}(\mu, \theta)$ (subject to the constraint $0 \leq \hat{\mu} \leq \mu$), whereas $\hat{\theta}_\mu$ are the values of the nuisance parameters that maximise the likelihood function for a given value of μ . The statistic used for the discovery test, to test the compatibility of the observed data with the background-only hypothesis, is obtained by setting $\mu = 0$ in the profile likelihood ratio and leaving $\hat{\mu}$ unconstrained: $q_0 = -2 \ln(\mathcal{L}(0, \hat{\theta}_0) / \mathcal{L}(\hat{\mu}, \hat{\theta}))$. The p -value of the discovery test is given by the integral of the probability distribution of q_0 above the observed q_0 value when assuming the background-only hypothesis, and it is computed using the asymptotic approximation detailed in ref. [126]. For each signal scenario considered, the upper limit on the signal production cross section is computed using q_μ in the CL_s method [127, 128], also in the asymptotic approximation. For a given signal scenario, values of the production cross section (parameterised by μ) yielding $\text{CL}_s < 0.05$ are excluded at $\geq 95\%$ CL. The exclusion limits obtained using the asymptotic approximation are then compared with limits calculated using pseudoexperiments for 2 TeV benchmark signal points close to the

obtained constraints. The central values of the limits computed using the two methods agree within 5%, while the uncertainty bands agree within 10%–15%.

10 Results

10.1 Likelihood fits to data

A likelihood fit, as described in section 9, is performed under the background-only hypothesis. A comparison between the overall observed and expected yields in each fit region is shown, before and after the fit to data, in figure 5. As can be seen, the combined impact of the systematic uncertainties has been constrained as a result of the fit, using information from the large number of events in signal-depleted regions with different background contributions. Consequently, an improved background prediction is obtained with reduced uncertainty across regions, including those with significant fractions of expected signal events. The data and pre- and post-fit background yields in four of the most sensitive search regions are given in table 5 and table 6, respectively.

The pre- and post-fit m_{eff} distributions in these four regions are furthermore shown in figure 6 and figure 7. The post-fit agreement between the data and prediction in the fit regions is good overall. A comparison of the observed and expected yields in all validation regions, pre- and post-fit, is shown in figure 8. The pre- and post-fit m_{eff} distributions in the validation regions closest to the four selected fit regions are shown in figure 9 and figure 10. The expected background in these regions agrees with the data within uncertainties, both before and after the fit. The general post-fit improvement in the estimated background in the validation regions, which are not included in the fit, gives confidence in the background estimation procedure.

The impact of the different sources of uncertainty on the signal-strength parameter μ is reported in table 7 for a T singlet and T doublet signal near the expected sensitivity of the search. As can be seen, the results are dominated by systematic uncertainties. The largest overall impact is related to the modelling of background processes, in particular $t\bar{t}+\geq 1b$ production. The systematic uncertainty associated with jets also has a significant impact. The relative size of impacts from different sources of uncertainty differs between T singlet and T doublet signals due to their kinematic differences. Uncertainties related to $t\bar{t}+\geq 1b$ modelling and b -tagging contribute significantly more in the T doublet scenario, whereas single-top modelling has a larger impact in the T singlet scenario.

The data-driven kinematic reweighting procedure described in section 7 provides better agreement between the data and the nominal pre-fit background, and, as described in section 8, modelling uncertainties affecting the dominant background processes are also reweighted. This procedure improves the stability of the likelihood fit. However, the fit is robust against these changes to the pre-fit background model, and the post-fit values of the modelling uncertainties are not significantly impacted by the reweighting procedure.

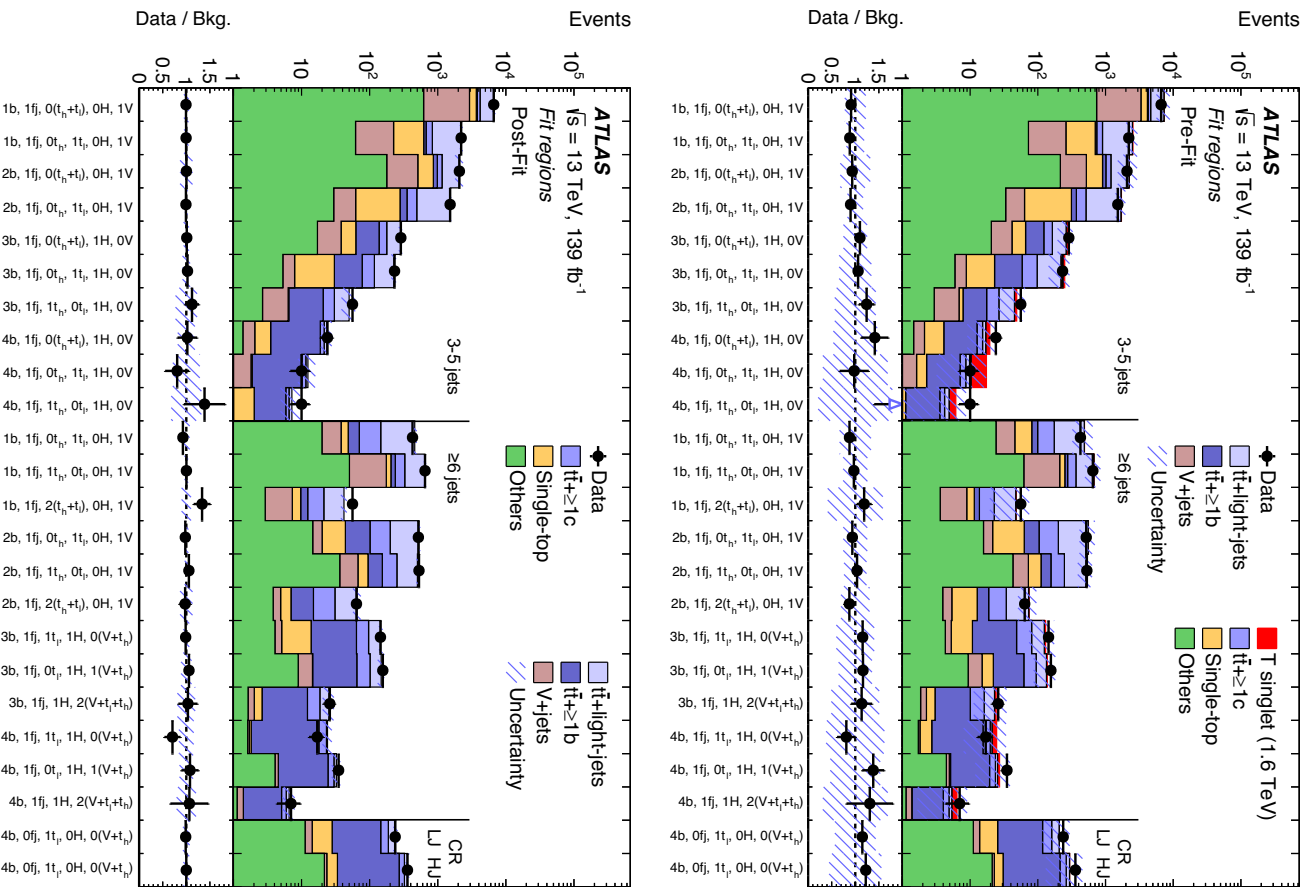


Figure 5. Comparison between the data and background prediction for the yields in each of the fit regions considered (top) pre-fit and (bottom) post-fit, performed under the background-only hypothesis. The two rightmost regions shown in the plot are the 3–5j (LJ) and $\geq 6j$ (HJ) control regions, respectively. The “others” background includes the $t\bar{t}V/H$, VH , tZ , $t\bar{t}t$, diboson, and multijet backgrounds. The expected T singlet signal (solid red) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figure. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background.

	LJ, 2b, $\geq 1f_j$, $0t_h, \geq 1t_l, 0H,$ $\geq 1V$	LJ, $\geq 4b, \geq 1f_j$, $0t_h, \geq 1t_l, \geq 1H,$ $0V$	HJ, 2b, $\geq 1f_j$, $\geq 2(t_h+t_l), 0H,$ $\geq 1V$	HJ, $\geq 4b, \geq 1f_j$, $\geq 1H,$ $\geq 2(V+t_l+t_h)$
<i>T</i> singlet ($m_T = 1.6$ TeV, $\kappa = 0.5$)	31.8 ± 4.9	7.2 ± 3.5	1.3 ± 0.4	1.0 ± 0.5
<i>T</i> doublet ($m_T = 1.6$ TeV, $\kappa = 0.5$)	21.8 ± 2.4	8.5 ± 5.6	7.3 ± 2.1	7.1 ± 4.5
$t\bar{t}$ +light-jets	1170 ± 210	1.6 ± 2	39.1 ± 9.5	0.49 ± 0.29
$t\bar{t} + \geq 1c$	143 ± 80	1.5 ± 1.3	15.3 ± 9.9	0.86 ± 0.58
$t\bar{t} + \geq 1b$	57 ± 32	4.8 ± 3.9	6.1 ± 4.3	2.6 ± 2
Single-top	250 ± 50	0.66 ± 0.87	7.3 ± 7.5	<0.001
$t\bar{t}W/Z$	13.2 ± 3.1	0.33 ± 0.19	2.5 ± 1.1	0.22 ± 0.82
$t\bar{t}H$	1.5 ± 0.2	0.51 ± 0.15	0.34 ± 0.14	0.42 ± 0.12
W +jets	25.7 ± 9.4	0.70 ± 1.3	1.2 ± 1.1	0.24 ± 0.15
Z +jets	4.4 ± 1.7	<0.001	0.25 ± 0.10	0.007 ± 0.007
Dibosons	3.8 ± 1.4	0.02 ± 0.03	0.21 ± 0.15	<0.001
Multijet	12.9 ± 7.3	0.025 ± 0.017	0.61 ± 0.46	0.16 ± 0.14
Rare backgrounds	2.0 ± 0.3	0.03 ± 0.04	0.25 ± 0.14	0.33 ± 0.06
Total background	1690 ± 280	10.2 ± 4.8	73 ± 20	5.4 ± 2.5
Data	1519	10	64	7

Table 5. Predicted and observed yields in four of the most sensitive search regions (depending on the signal scenario) considered. The background prediction is shown before the fit to data. The “rare backgrounds” category includes the VH , tZ and $t\bar{t}t\bar{t}$ backgrounds. Also shown are the signal predictions for different benchmark scenarios considered. The individual systematic uncertainties for the different background processes can be correlated, and do not necessarily add in quadrature to equal the systematic uncertainty in the total background yield. The quoted uncertainties are the sum in quadrature of statistical and systematic uncertainties in the yields.

	LJ, 2b, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $0H$, $\geq 1V$	LJ, $\geq 4b$, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $\geq 1H$, $0V$	HJ, 2b, $\geq 1f_j$, $\geq 2(t_h+t_l)$, $0H$, $\geq 1V$	HJ, $\geq 4b$, $\geq 1f_j$, $\geq 1H$, $\geq 2(V+t_l+t_h)$
$t\bar{t}$ +light-jets	1033 ± 72	0.6 ± 0.8	33.6 ± 4.5	0.57 ± 0.24
$t\bar{t}+\geq 1c$	144 ± 54	1.5 ± 1.0	15.6 ± 5.5	0.82 ± 0.32
$t\bar{t}+\geq 1b$	75 ± 22	8 ± 3	8.2 ± 2.3	3.8 ± 1.1
Single-top	223 ± 55	0.09 ± 0.55	2.3 ± 4.5	<0.001
$t\bar{t}W/Z$	12.1 ± 2.3	0.36 ± 0.18	2.3 ± 0.8	0.62 ± 0.76
$t\bar{t}H$	1.46 ± 0.21	0.51 ± 0.11	0.29 ± 0.08	0.40 ± 0.09
W +jets	26.6 ± 7.1	0.6 ± 1.0	0.8 ± 0.5	0.22 ± 0.13
Z +jets	4.5 ± 1.2	<0.001	0.27 ± 0.08	0.005 ± 0.006
Dibosons	3.4 ± 1.2	0.017 ± 0.029	0.17 ± 0.13	<0.001
Multijet	9.5 ± 5.7	0.018 ± 0.015	0.45 ± 0.41	0.12 ± 0.12
Rare backgrounds	2.0 ± 0.2	0.03 ± 0.03	0.22 ± 0.08	0.31 ± 0.05
Total background	1534 ± 56	12.1 ± 3.5	64 ± 8	6.8 ± 1.5
Data	1519	10	64	7

Table 6. Predicted and observed yields in four of the most sensitive search regions (depending on the signal scenario) considered. The background prediction is shown after the fit to data under the background-only hypothesis. The “rare backgrounds” category includes the VH , tZ and $t\bar{t}t$ backgrounds. The individual systematic uncertainties for the different background processes can be correlated, and do not necessarily add in quadrature to equal the systematic uncertainty in the total background yield. The quoted uncertainties are computed after taking into account correlations among nuisance parameters and among processes. The statistical uncertainty is added in quadrature to the systematic uncertainties.

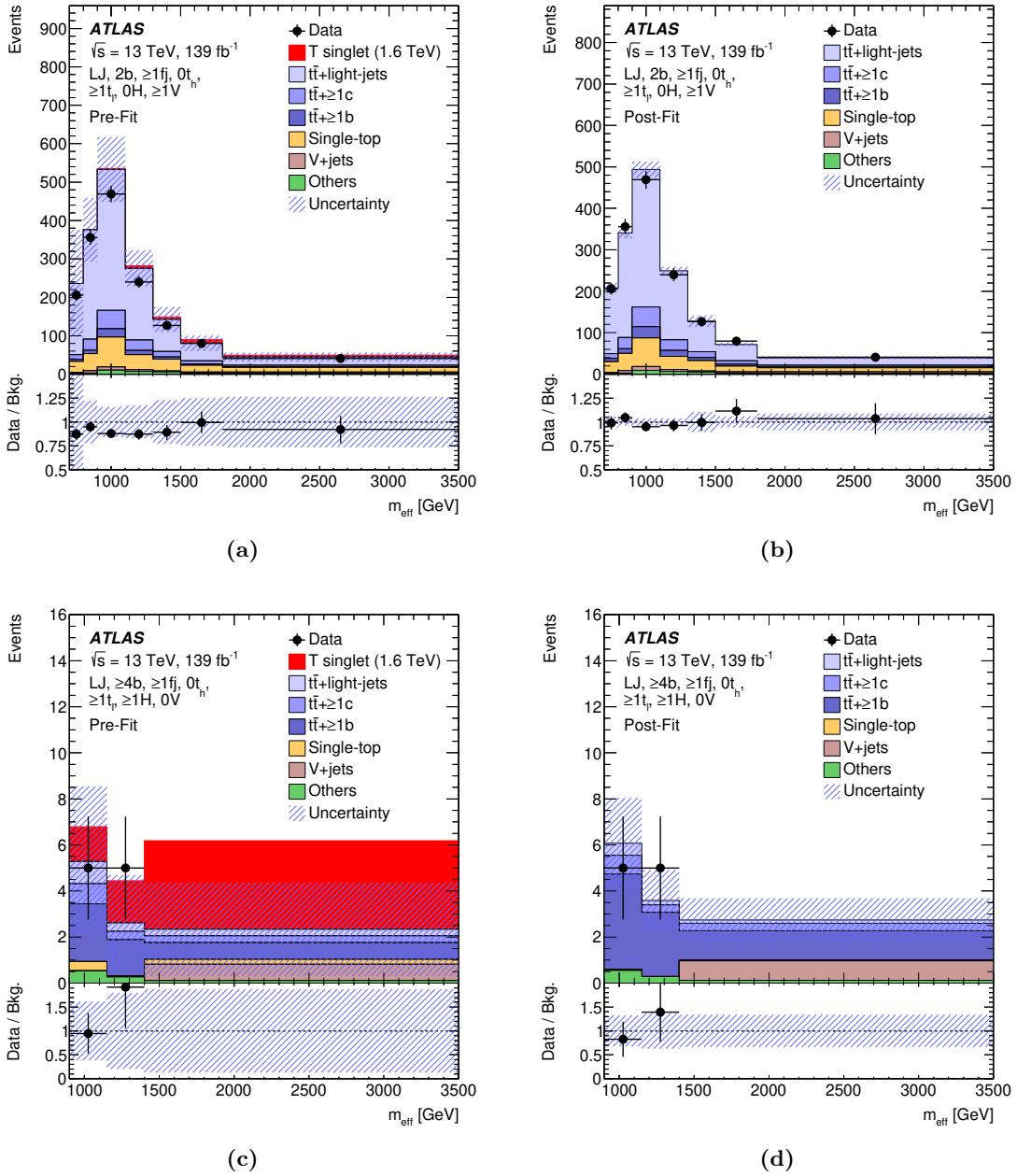


Figure 6. Comparison between the data and prediction for the m_{eff} distribution under the background-only hypothesis, in the (LJ, 2b, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, 0H, $\geq 1V$) region (a) pre-fit and (b) post-fit, and the (LJ, $\geq 4b$, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $\geq 1H$, 0V) region (c) pre-fit and (d) post-fit. The expected T singlet signal (solid red) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figures. The “others” background includes the $t\bar{t} V/H$, VH , tZ , $t\bar{t}t\bar{t}$, diboson, and multijet backgrounds. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background. The last bin in each distribution contains the overflow.

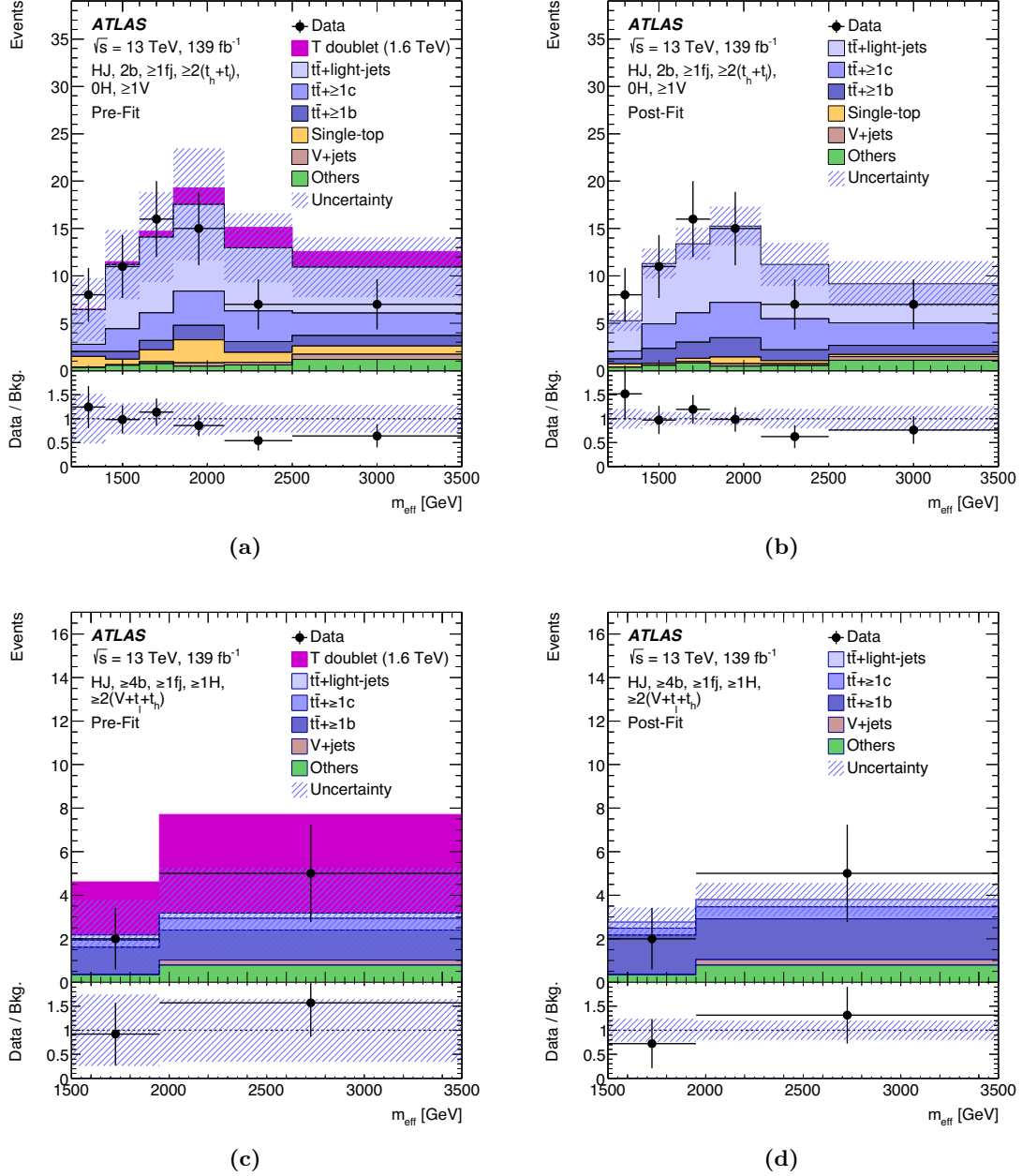


Figure 7. Comparison between the data and prediction for the m_{eff} distribution under the background-only hypothesis, in the (HJ, 2b, $\geq 1f_j$, $\geq 2(t_h+t_l)$, 0H, $\geq 1V$) region (a) pre-fit and (b) post-fit, and the (HJ, $\geq 4b$, $\geq 1f_j$, $\geq 1H$, $\geq 2(V+t_h+t_l)$) region (c) pre-fit and (d) post-fit. The expected T doublet signal (solid purple) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figures. The “others” background includes the $t\bar{t}$ V/H , VH , tZ , $t\bar{t}t\bar{t}$, diboson, and multijet backgrounds. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background. The last bin in each distribution contains the overflow.

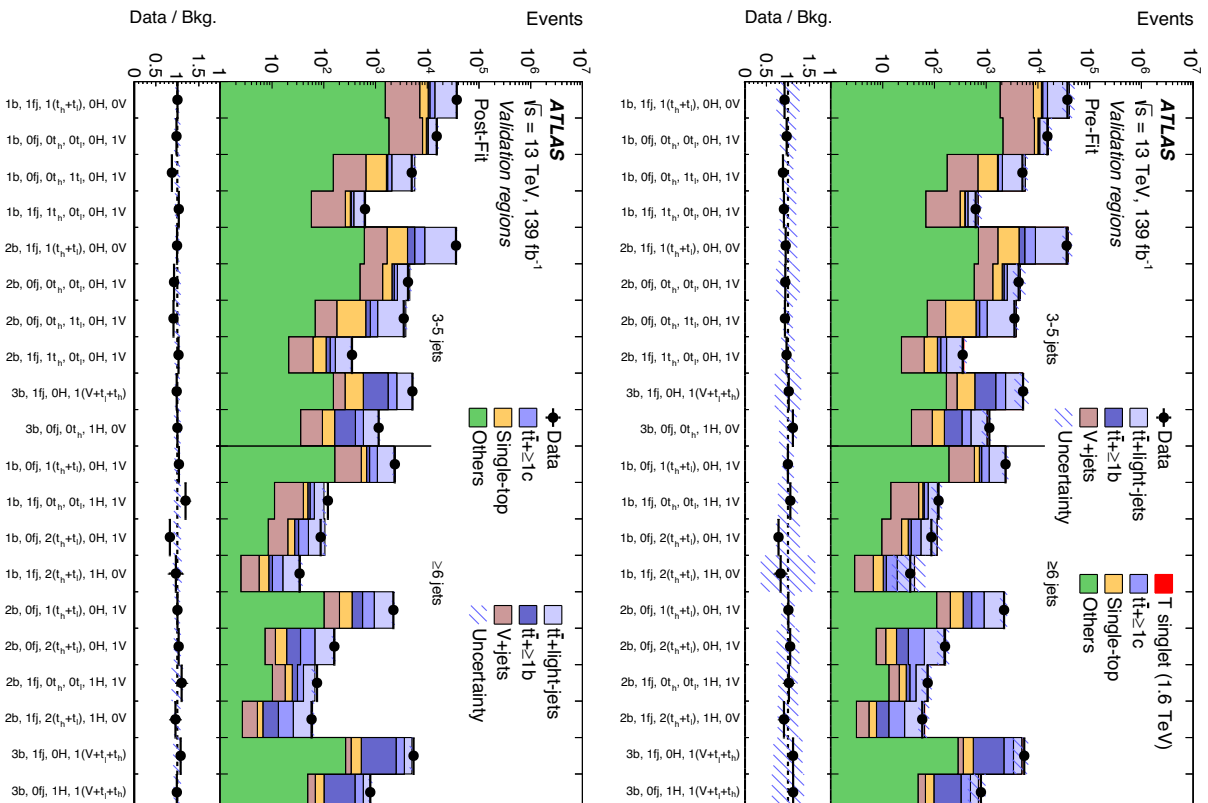


Figure 8. Comparison between the data and background prediction for the yields in each of the VRs considered (top) pre-fit and (bottom) post-fit, performed under the background-only hypothesis considering only the fit regions. The “others”² background includes the $t\bar{t}V/H$, VH , tZ , $t\bar{t}t$, diboson, and multijet backgrounds. The expected T singlet signal (solid red) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figure. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background.

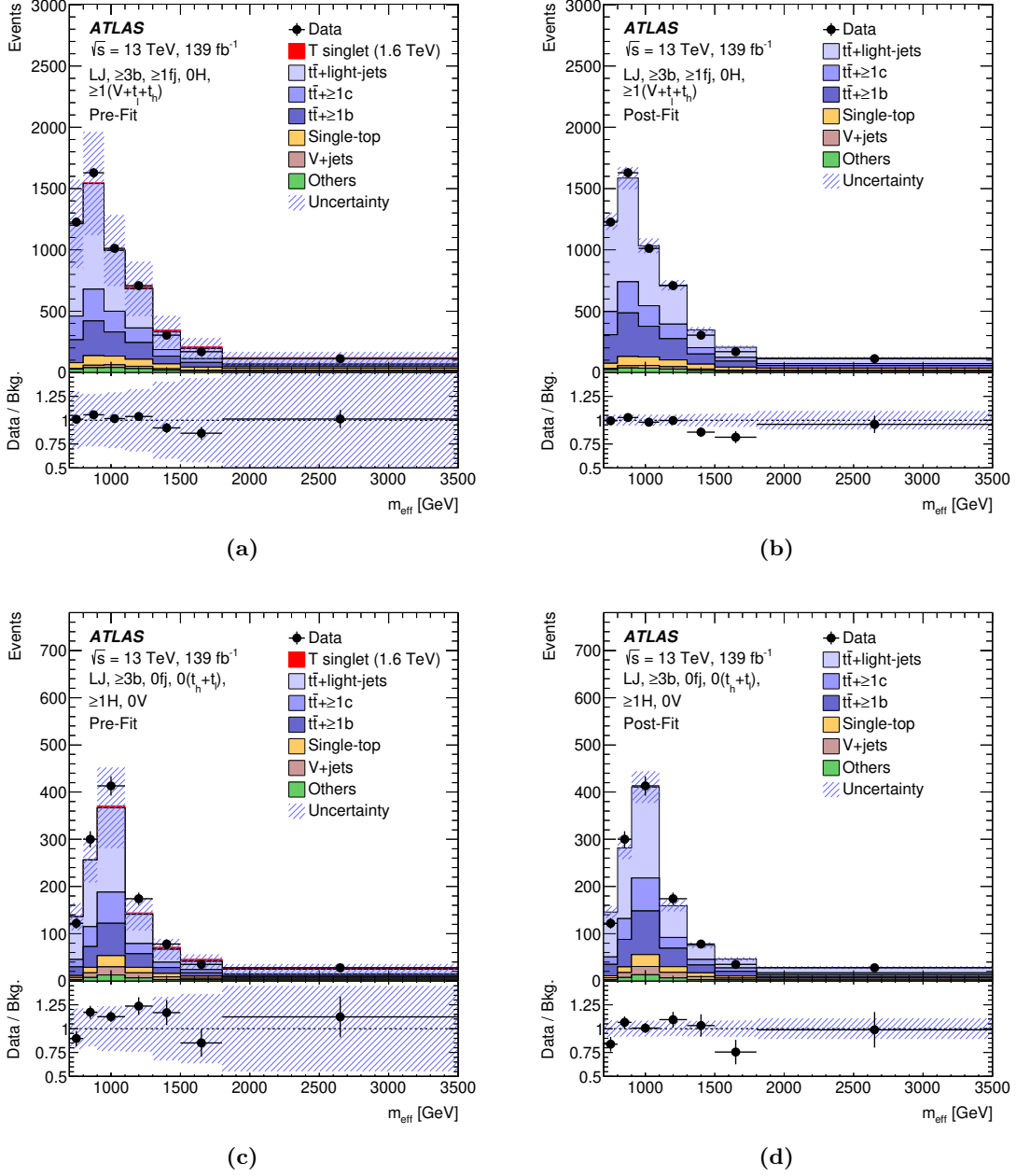


Figure 9. Comparison between the data and prediction for the m_{eff} distribution under the background-only hypothesis, in the (LJ, $\geq 3b$, $\geq 1f_j$, 0H, $\geq 1(V+t_l+t_h)$) validation region (a) pre-fit and (b) post-fit, and the (LJ, $\geq 3b$, 0fj, 0(t_h+t_l), $\geq 1H$, 0V) validation region (c) pre-fit and (d) post-fit. The expected T singlet signal (solid red) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figures. The “others” background includes the $t\bar{t} V/H$, VH , tZ , $t\bar{t}t\bar{t}$, diboson, and multijet backgrounds. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background. The last bin in each distribution contains the overflow.

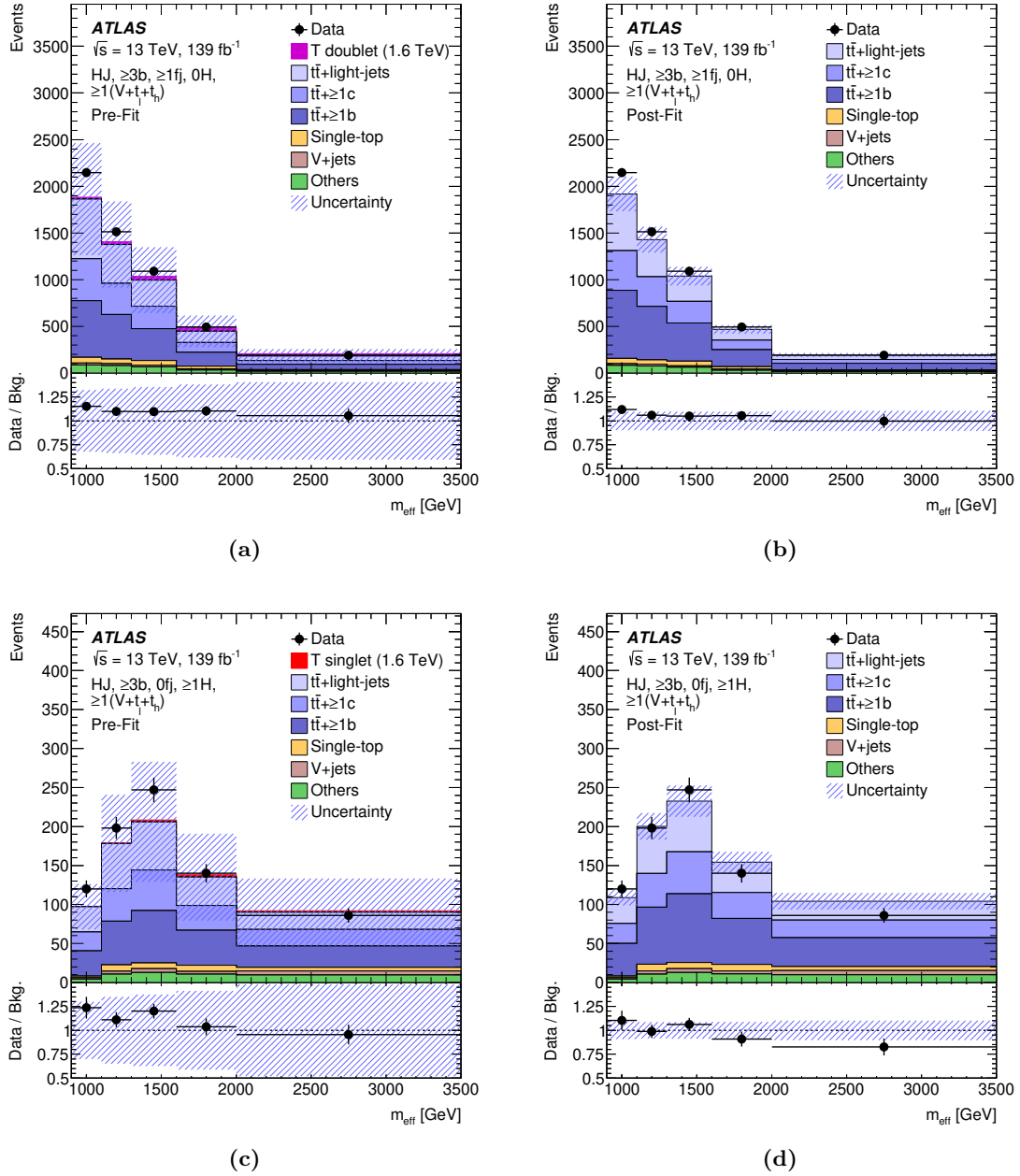


Figure 10. Comparison between the data and prediction for the m_{eff} distribution under the background-only hypothesis, in the (HJ, $\geq 3b$, $\geq 1f_j$, 0H, $\geq 1(V+t_l+t_h)$) validation region (a) pre-fit and (b) post-fit, and the (HJ, $\geq 3b$, 0fj, $\geq 1H$, $\geq 1(V+t_l+t_h)$) validation region (c) pre-fit and (d) post-fit. The expected T doublet signal (solid purple) for $m_T = 1.6$ TeV and $\kappa = 0.5$ is included in the pre-fit figures. The “others” background includes the $t\bar{t} V/H$, VH , tZ , $t\bar{t}t\bar{t}$, diboson, and multijet backgrounds. The bottom panels display the ratios of data to the total background prediction. The hashed area represents the total uncertainty in the background. The last bin in each distribution contains the overflow.

Uncertainty source	<i>T</i> singlet	<i>T</i> doublet
	$m_T = 1.5 \text{ TeV}, \kappa = 0.4$	$m_T = 1.5 \text{ TeV}, \kappa = 0.7$
	$\Delta\mu$	$\Delta\mu$
Process modelling uncertainties		
$t\bar{t}$ +light-jets	± 0.05	± 0.11
$t\bar{t} + \geq 1c$	± 0.03	± 0.08
$t\bar{t} + \geq 1b$	± 0.09	± 0.27
Single-top	± 0.12	± 0.07
W/Z +jets	± 0.03	± 0.09
Object uncertainties		
Jets	± 0.07	± 0.13
b -tagging	± 0.03	± 0.11
Other sources	± 0.02	± 0.04
Background reweighting	± 0.04	± 0.11
Total systematic uncertainty	± 0.23	± 0.33
Total statistical uncertainty	± 0.09	± 0.17

Table 7. Breakdown of the contributions to the uncertainties in μ , shown for the singlet T signal with $\kappa = 0.4$ and the doublet T signal with $\kappa = 0.7$, both with $m_T = 1.5 \text{ TeV}$. The contributions from the different sources of uncertainty are evaluated after the fit. The $\Delta\mu$ values are obtained by repeating the fit after having fixed a certain set of nuisance parameters corresponding to a group of systematic uncertainties, and then evaluating $(\Delta\mu)^2$ by subtracting the resulting squared uncertainty of μ from its squared uncertainty found in the full fit.

10.2 Limits on single vector-like quark production

No significant excess above the SM prediction is found in any of the considered regions in the background-only fit. Unconditional fits with a floating signal-strength parameter μ were also consistent with the background-only hypothesis. Upper limits at 95% CL on the single- T production cross section are derived in both the singlet (T) and doublet ($T B$) scenarios.

The observed cross-section limits at each point in the parameter space are compared with the NLO theoretical prediction to set exclusion limits on model parameters. Since the theory cross-section calculations with finite-width effects and non-resonant contributions are only reliable for relative T -quark widths (Γ_T/m_T) up to $\sim 50\%$ [106], results are presented only in this restricted regime.

The obtained limits corresponding to the singlet and doublet scenarios are shown in figure 11 and figure 12, respectively, for a set of three values of the common coupling parameter κ , chosen to approximately span the sensitivity range of the search in each scenario. The corresponding limits are also derived in the mass versus coupling plane, where exclusion contours indicate the interpolated intersection between the planes of excluded and theoretically predicted cross sections, shown in figure 13 for both the singlet and doublet scenarios. Additionally, upper limits on the production cross section of both the singlet and doublet scenarios are derived as a function of mass and coupling, as shown in figures 14 and 15. As expected, the exclusion limits on the T -quark mass are generally stronger in the singlet scenario than in the doublet scenario. All T -quark masses below 2.1 TeV (expected 1.9 TeV) are excluded for singlet T quarks at couplings $\kappa \geq 0.6$. At a mass of 1.6 TeV, κ values above 0.3 (expected 0.41) are all excluded. By comparison, the previous ATLAS search in the all-hadronic $T \rightarrow Ht$ channel has excluded κ values above ~ 0.5 (expected ~ 0.65) at a mass of 1.6 TeV [21]. In the doublet scenario, the limits on the considered mass range extend down to coupling values of $\kappa = 0.55$, corresponding to a T -quark mass limit of 1.0 TeV. Masses up to 1.68 TeV are excluded at $\kappa = 0.75$, at a relative T -quark width threshold of 50%.

The expected limits on the cross section get progressively stronger at larger masses in both scenarios, as the decay products of the T quark become more boosted, and the fraction of signal in the highest m_{eff} bins increases. The limits deteriorate at larger values of κ , since this regime corresponds to large resonance width and a larger fraction of the signal resides in the low mass regime away from the peak of the resonance. As can be seen, the observed limits exceed the expected limits in both benchmark scenarios in a few cases. These deviations are larger for the singlet scenario, reaching almost 2σ at high masses. These findings can be ascribed to downward statistical fluctuations in a few of the most signal-sensitive bins, most notably in the last bin of the (LJ, $\geq 4b$, $\geq 1f_j$, $0t_h$, $\geq 1t_l$, $\geq 1H$, $0V$) region, which has no data events, and the last few bins of the (HJ, $\geq 4b$, $\geq 1f_j$, $0t_h$, $1t_l$, $\geq 1H$, $0V$) region. The origin of these discrepancies was investigated, and no evidence of any systematic bias was found. Notably, the pre- and post-fit m_{eff} distributions in the corresponding validation regions, shown in figure 9 and figure 10, respectively, exhibit good agreement between the data and expectations. Several other fit regions with kinematic features and background compositions similar to those in the two regions mentioned above show good agreement between data and predictions. The observed discrepancies were therefore deemed to be consistent with statistical fluctuations.

Finally, the results are interpreted in a more generalised representation of the parameter space, displaying the largest excluded mass as a function of Γ_T/m_T and the relative coupling parameter ξ_W (figure 16). As discussed in section 1, the T -quark width is determined by the T -quark mass m_T and the universal coupling constant κ and is independent of the multiplet representation. The relative coupling parameter ξ_W controls the branching fraction $\mathcal{B}(T \rightarrow Wb)$. For ease of representation, the limits are shown for the assumption $\xi_Z = \xi_H$, which is valid for all VLQ multiplet scenarios in the phenomenological model discussed in section 1. Since the relative coupling constants $\xi_{W,Z,H}$ must sum to unity, the assumption of equal ξ_Z and ξ_H fully determines the values of these parameters for any given value of ξ_W .

In all of the benchmarks considered in this search, only the contributions from T -quark production were taken into account. In particular, limits presented in the doublet ($T B$) scenario neglect contributions from B -quark production. The most relevant signature of B -quark production for this analysis would occur in the $B \rightarrow Wt$ decay channel, when the top quark decays leptonically and the W boson decays hadronically. This process has a signature almost identical to the $T \rightarrow Zt$ decay signatures considered in the search, and would therefore make very similar contributions to the fit regions. By the same argument, contributions from B -quark production in the RSRs and the background control regions are expected to be negligible. Thus, the limits presented for the doublet scenario in this paper can be considered to be conservative.

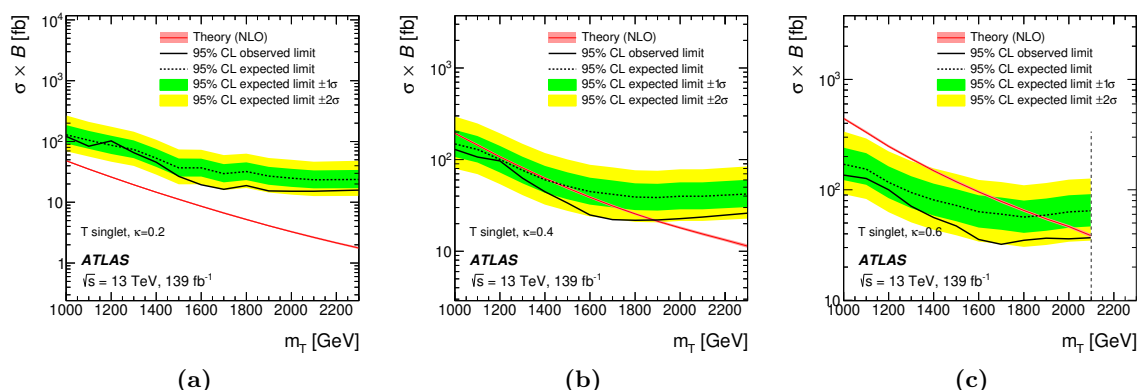


Figure 11. Observed (solid black line) and expected (dashed black line) 95% CL upper limits on the single- T production cross section as a function of the T -quark mass in the singlet scenario with the common coupling parameter (a) $\kappa = 0.2$, (b) $\kappa = 0.4$, and (c) $\kappa = 0.6$. The surrounding shaded bands correspond to ± 1 and ± 2 standard deviations around the expected limit. The red line shows the NLO theoretical cross-section prediction, with the surrounding shaded band representing the corresponding uncertainty. Limits are only presented in the regime $\Gamma_T/m_T \leq 50\%$, where the theory calculations are known to be valid, as indicated by the vertical grey dashed line.

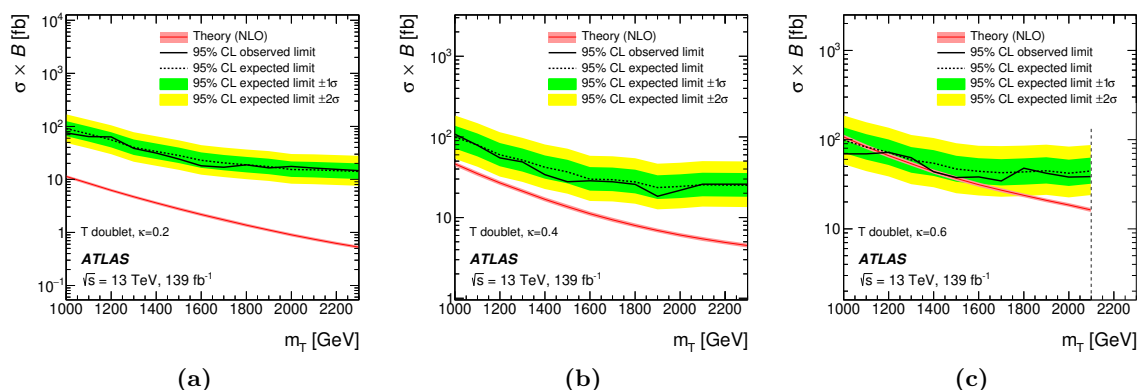


Figure 12. Observed (solid black line) and expected (dashed black line) 95% CL upper limits on the single- T production cross section as a function of the T -quark mass in the doublet scenario with the common coupling parameter (a) $\kappa = 0.2$, (b) $\kappa = 0.4$, and (c) $\kappa = 0.6$. The surrounding shaded bands correspond to ± 1 and ± 2 standard deviations around the expected limit. The red line shows the NLO theoretical cross-section prediction, with the surrounding shaded band representing the corresponding uncertainty. Limits are only presented in the regime $\Gamma_T/m_T \leq 50\%$, where the theory calculations are known to be valid, as indicated by the vertical grey dashed line.

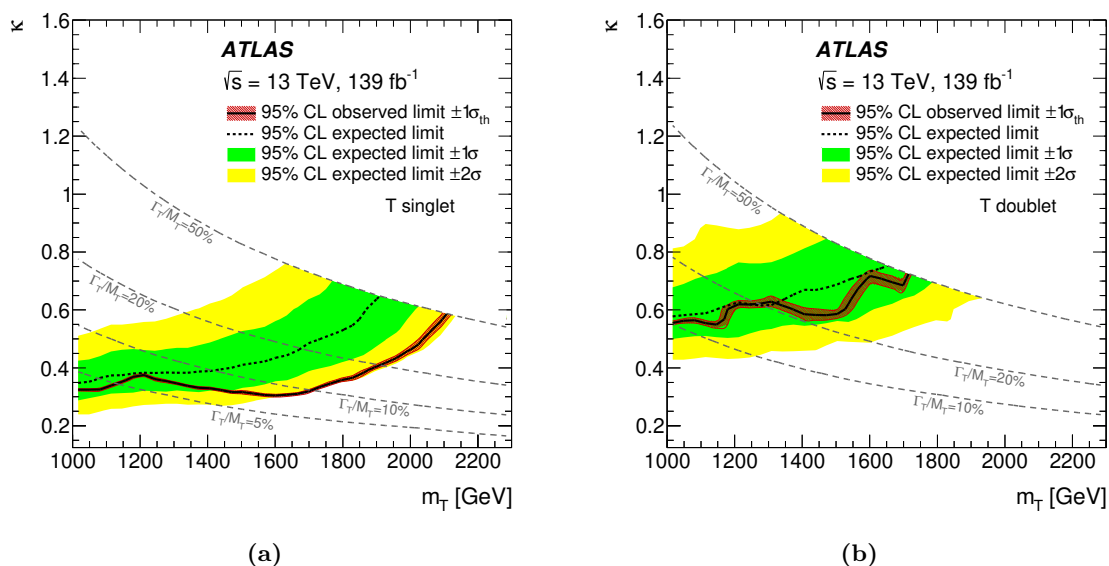


Figure 13. Observed (solid black line) and expected (dashed black line) 95% CL exclusion limits on the universal coupling constant κ as a function of the T -quark mass in the (a) SU(2) singlet and (b) SU(2) doublet scenarios. All values of κ above the black contour lines are excluded at each mass point. The shaded bands correspond to ± 1 and ± 2 standard deviations around the expected limit. The red hashed area around the observed limit corresponds to the theoretical uncertainty of the NLO cross-section prediction. The grey dashed lines represent configurations of (m_T, κ) resulting in equal values of the relative resonance width Γ_T/m_T . Limits are only presented in the regime $\Gamma_T/m_T \leq 50\%$, where the theory calculations are known to be valid.

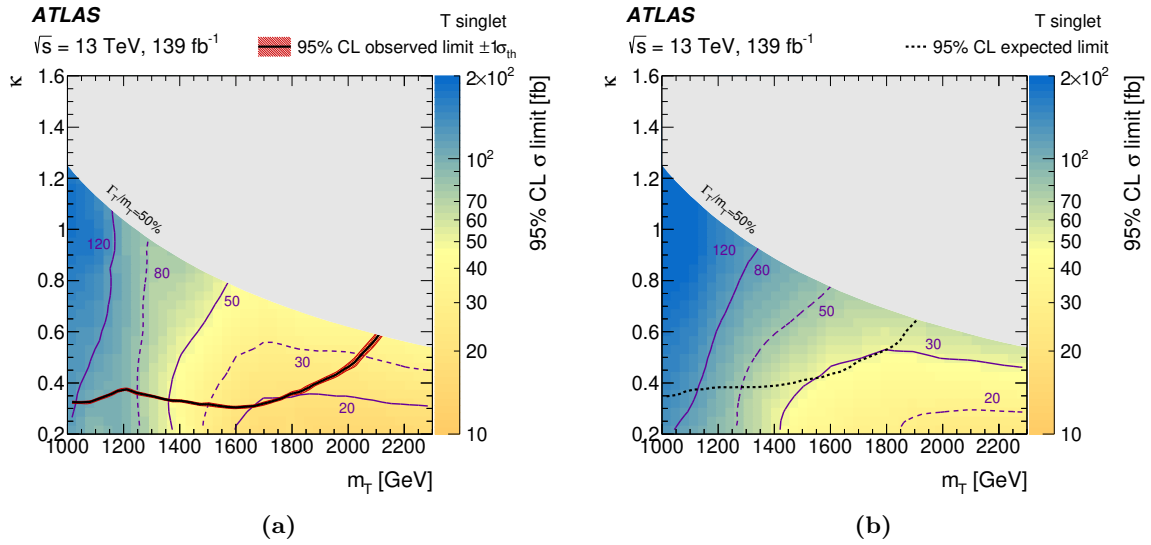


Figure 14. (a) Observed and (b) expected 95% CL exclusion limits on the cross section times branching ratio of single T -quark production as a function of the universal coupling constant κ and the T -quark mass in the $SU(2)$ singlet scenario. The red hashed area around the observed limit corresponds to the theoretical uncertainty of the NLO cross-section prediction. All values of κ above the black contour line are excluded at each mass point. The purple contour lines denote exclusion limits of equal cross section times branching ratio in units of fb. Limits are only presented in the regime $\Gamma_T/m_T \leq 50\%$, where the theory calculations are known to be valid.

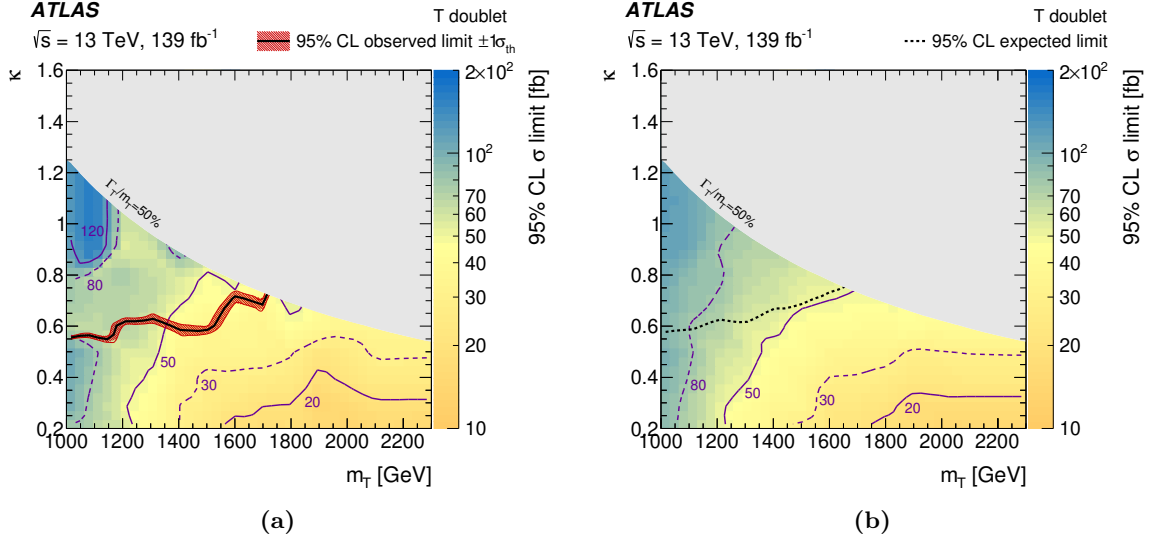


Figure 15. (a) Observed and (b) expected 95% CL exclusion limits on the cross section times branching ratio of single T -quark production as a function of the universal coupling constant κ and the T -quark mass in the SU(2) doublet scenario. The red hashed area around the observed limit corresponds to the theoretical uncertainty of the NLO cross-section prediction. All values of κ above the black contour line are excluded at each mass point. The purple contour lines denote exclusion limits of equal cross section times branching ratio in units of fb. Limits are only presented in the regime $\Gamma_T/m_T \leq 50\%$, where the theory calculations are known to be valid.

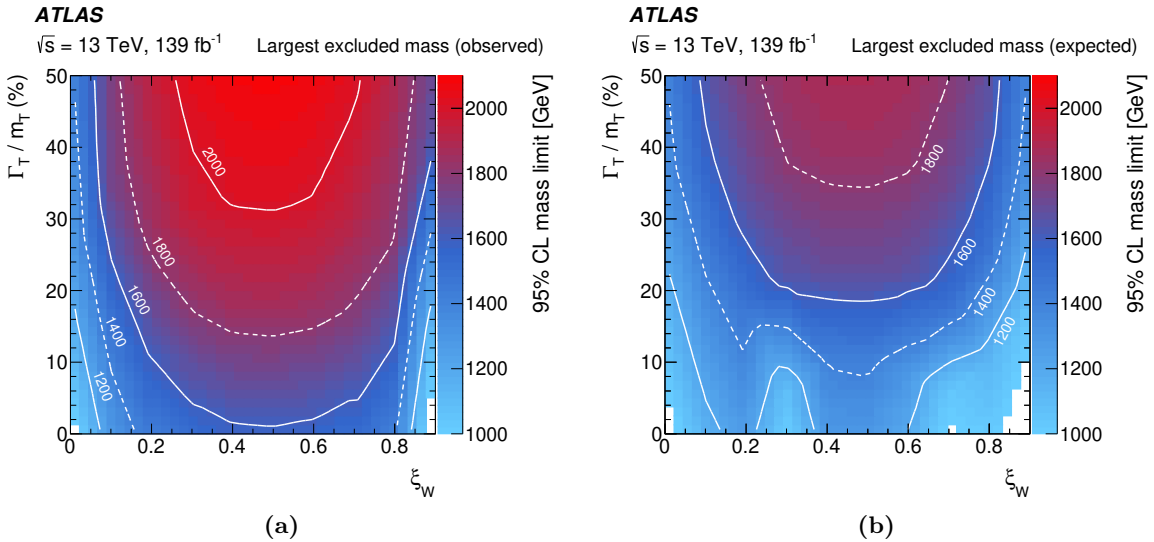


Figure 16. (a) Observed and (b) expected upper limits at 95% CL on the T -quark mass as a function of the relative resonance width (Γ_T/m_T) and the relative coupling parameter ξ_W , for the assumption $\mathcal{B}(T \rightarrow Ht) = \mathcal{B}(T \rightarrow Zt)$. The white contour lines denote exclusion limits of equal mass in units of GeV. The white regions represent points in parameter space that are not excluded for any mass in the considered range.

11 Conclusion

A search for the single production of up-type vector-like quarks (T), with subsequent decays $T \rightarrow Ht$ with $H \rightarrow b\bar{b}$ or $T \rightarrow Zt$ with $Z \rightarrow q\bar{q}$, is presented. The search uses pp collision data at $\sqrt{s} = 13$ TeV, collected by the ATLAS detector at the LHC during the 2015–2018 Run 2 data-taking period. The recorded dataset corresponds to an integrated luminosity of 139 fb^{-1} . Events are analysed in the lepton+jets final state, characterised by the presence of a single lepton and multiple jets and b -jets in the event. The search exploits the presence of boosted, hadronically decaying Higgs and vector bosons, and hadronically or leptonically decaying top quarks in signal events.

No significant excess above Standard Model expectations is observed, and 95% CL upper limits are set on the production cross section of single T quarks. The results are interpreted in benchmark scenarios to set limits on the mass and universal coupling strength (κ) of the vector-like quark. For singlet T quarks, all masses below 2.1 TeV are excluded at couplings $\kappa \geq 0.6$, while the limits extend down to $\kappa = 0.3$ for a T -quark mass of 1.6 TeV. For T quarks in the doublet scenario, where the production cross section is much lower, coupling values as low as $\kappa = 0.55$ are excluded at a T -quark mass of 1.0 TeV. The limits extend up to 1.68 TeV and $\kappa = 0.75$, at a threshold of 50% relative T -quark width.

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