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# Search for leptoquarks decaying into the $b\tau$ final state in $pp$ collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

A search for leptoquarks decaying into the  $b\tau$  final state is performed using Run 2 proton–proton collision data from the Large Hadron Collider, corresponding to an integrated luminosity of  $139 \text{ fb}^{-1}$  at  $\sqrt{s} = 13$  TeV recorded by the ATLAS detector. The benchmark models considered in this search are vector leptoquarks with electric charge of  $2/3e$  and scalar leptoquarks with an electric charge of  $4/3e$ . No significant excess above the Standard Model prediction is observed, and 95% confidence level upper limits are set on the cross-section times branching fraction of leptoquarks decaying into  $b\tau$ . For the vector leptoquark production two models are considered: the Yang–Mills and Minimal coupling models. In the Yang–Mills (Minimal coupling) scenario, vector leptoquarks with a mass below 1.58 (1.35) TeV are excluded for a gauge coupling of 1.0 and below 2.05 (1.99) TeV for a gauge coupling of 2.5. In the case of scalar leptoquarks, masses below 1.28 TeV (1.53 TeV) are excluded for a Yukawa coupling of 1.0 (2.5). Finally, an interpretation of the results with minimal model dependence is performed for each of the signal region categories, and limits on the visible cross-section for beyond the Standard Model processes are provided.

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## 1 Introduction

The existing similarities between the structure of the quark and lepton sectors in the Standard Model (SM) suggest the possibility of a new underlying symmetry in particle physics. Leptoquarks (LQs) that couple to both quarks and leptons, with non-zero baryon and lepton numbers, and fractional electric charges are predicted by several beyond the SM theories that attempt to unify the fundamental interactions, such as technicolour [1–3], composite models [4], and grand unification [5–7].

Recent results reported by BaBar [8, 9], Belle [10] and LHCb [11] show hints of deviations from lepton-flavour universality in  $B$ -meson decays into final states with  $D^*$  mesons, which could be caused by the existence of LQs. The 4.2 standard deviation disagreement with respect to the SM prediction observed in the anomalous muon magnetic moment measurement [12], though significantly reduced when updated lattice quantum chromodynamics (QCD) calculations [13] are considered, could be caused by LQ contributions to the muon magnetic moment [14].

In light of the lepton-flavour universality anomalies observed in the  $B$ -meson decays, the couplings of LQs to third-generation quarks and leptons are expected to be large [15]. At the LHC, third-generation LQs can be produced singly via quark–gluon fusion and quark–gluon scattering or in pairs via the gluon–gluon fusion process, as shown in the Feynman diagrams in Figure 1; the single LQ production motivates the search for third generation LQs via the channel  $bg \rightarrow \text{LQ}\tau \rightarrow b\tau\tau$ . The search presented in this paper is optimised for the single LQ production, while LQ pair and non-resonant production processes are also considered since they can also contribute to the  $b\tau\tau$  final state. The single LQ production contribution becomes larger than that from LQ pair production at high LQ mass and coupling values. The results are obtained from proton–proton collision data at a centre-of-mass energy of  $\sqrt{s} = 13$  TeV collected by the

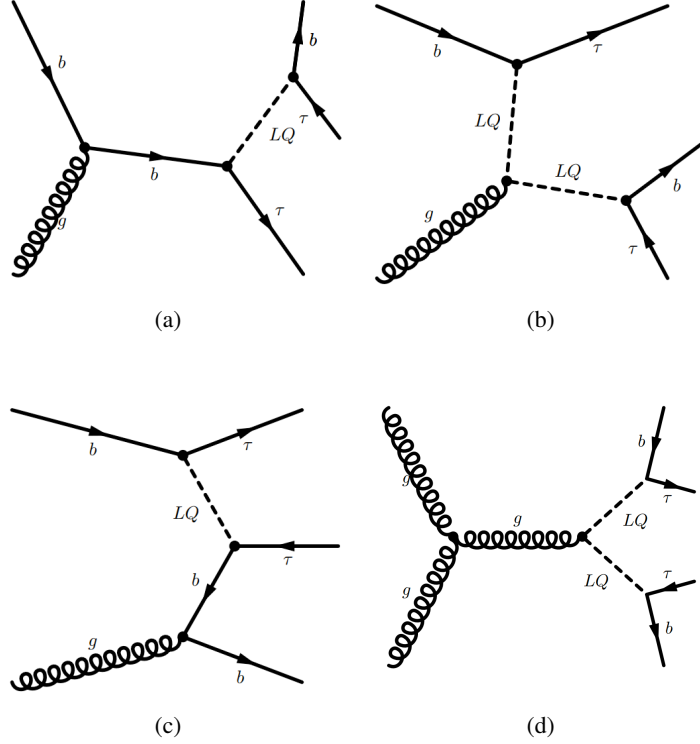


Figure 1: Illustrative Feynman diagrams of (a,b) single LQ production, (c) non-resonant LQ production, and (d) LQ pair production.

ATLAS detector [16, 17] at the LHC [18] during Run 2 between 2015 and 2018, corresponding to a total integrated luminosity of  $139 \text{ fb}^{-1}$ .

The vector LQ model chosen for this search is the  $U_1$  model [19], a  $SU(2)_L$  singlet with fermion number  $F = 3B + L = 0$ , where  $B$  and  $L$  are the baryon and lepton numbers respectively, and an electric charge of  $2/3e$ . The interaction part of  $U_1$  model Lagrangian is:

$$\mathcal{L}_{U_1} \supset -ig_s(1 - \kappa)U_{1\mu}^\dagger T^a U_{1\nu} G^{a\mu\nu} + \frac{g_U}{\sqrt{2}}[U_1^\mu (\beta_L^{ij} \bar{q}_L^i \gamma_\mu \ell_L^j + \beta_R^{ij} \bar{d}_R^i \gamma_\mu e_R^j) + \text{h.c.}],$$

where  $T^a = \lambda^a/2$  with  $\lambda^a (a = 1, \dots, 8)$  are the Gell-Mann matrices,  $g_s$  is the QCD coupling,  $q_L$  ( $\ell_L$ ) denotes the left-handed quark (lepton) doublets and  $d_R$  ( $e_R$ ) denotes the right-handed down-type quark (charge-lepton) singlets. The  $i$  and  $j$  indices represent the flavour generation. A summation over the colour indices is performed and omitted for clarity. The term  $-ig_s(1 - \kappa)U_{1\mu}^\dagger T^a U_{1\nu} G^{a\mu\nu}$  describes the interaction between  $U_1$  leptoquarks and SM gluon gauge fields  $G^{a\mu\nu}$ . In this analysis, two vector LQ scenarios are considered: the Yang–Mills ( $U_1^{\text{YM}}$ ) coupling scenario,  $\kappa = 0$ , and the Minimal ( $U_1^{\text{MIN}}$ ) coupling scenario,  $\kappa = 1$ . The  $\beta_L^{ij}$  and  $\beta_R^{ij}$  parameters describe the coupling between  $U_1$  leptoquarks and left-handed or right-handed charged leptons and quarks, respectively. In the framework of the  $U_1^{\text{YM}}$  and  $U_1^{\text{MIN}}$  scenarios, the probability to decay into the  $b$ -quark and  $\tau$ -lepton final state is predicted to be the same as to decay into the top-quark and neutrino final state. Hence, the branching fraction  $\mathcal{B}$  of the LQ decays into a  $b$ -quark and a  $\tau$ -lepton is set to 0.5. In this search, all of  $\beta_R^{ij}$  are set to zero,  $\beta_L^{33}$  is set to one and other  $\beta_L^{ij}$  are set to

zero, such that each LQ decays into a  $b$ -quark and a  $\tau$ -lepton or into a top-quark and a neutrino. Due to these choices, the gauge coupling ( $\lambda$ ) between  $U_1$  leptoquarks and third-generation charged leptons and quarks can be written as  $\lambda = g_U \beta_L^{33} / \sqrt{2}$ .

The scalar LQ model  $\tilde{S}_1$  is also considered, with  $F = 3B + L = -2$  and electric charge of  $4/3e$  [20, 21]. There are three parameters in this model: the branching fraction  $\mathcal{B}$  into charged leptons, the LQ to  $\tau b$  Yukawa coupling parameter  $\lambda$ , and the mass term of the LQ. Following Ref. [21], the Lagrangian terms for  $\tilde{S}_1$  LQs related to this analysis are:

$$\mathcal{L}_{\tilde{S}_1} \supset +\lambda^{ij} \bar{d}_R^{Ci} \tilde{S}_1 e_R^j + \text{h.c.},$$

where  $C$  in the superscript stands for the charge conjugation operation. The terms  $e_R$  and  $d_R$  are the right-handed charged leptons and down-type quarks and  $\lambda^{ij}$  represents the Yukawa couplings between  $\tilde{S}_1$ , charged leptons, and quarks, where the  $ij$  refers to the generations of the quark and charged lepton. In the framework of the  $\tilde{S}_1$  model, the only non-zero Yukawa coupling considered in this paper is the coupling to a  $b$ -quark and a  $\tau$ -lepton. Since only the coupling to the third-generation charged lepton and quark is considered,  $\lambda^{33} = \lambda$  is assumed to be different from zero, while the rest of the  $\lambda^{ij}$  are set to zero.

Most of the previous searches for LQs performed by the ATLAS [22–28] and CMS [29–32] collaborations have been conducted on different final states compared to this search. For third generation LQs, the CMS Collaboration has recently published results of searches for LQs decaying into  $\tau\nu$  and  $b\tau$  [33]. The ATLAS Collaboration performed a search for pair produced scalar LQs in  $b\tau b\tau$  final states with  $36 \text{ fb}^{-1}$  of proton–proton collision data at  $\sqrt{s} = 13 \text{ TeV}$  that excluded scalar LQs with masses below 1 TeV, assuming a LQ to  $b\tau$  branching fraction equal to one [34].

The analysis described in this paper is the first search by the ATLAS Collaboration for singly produced LQs decaying into  $b\tau$ . The search is performed over a LQ mass ( $m_{\text{LQ}}$ ) in the range of 0.4 TeV to 2.5 TeV. The  $\lambda$  range is chosen to be between 0.5 and 2.5 to cover possible regions where LQs could explain the anomalies observed in the  $B$ -meson decay and is extended to large  $\lambda$  where the single LQ production channel provides a significant contribution compared to the pair-production process.

The analysis starts from the selection of a pair of oppositely charged  $\tau$ -leptons produced in association with a jet identified as containing a  $b$ -hadron ( $b$ -jet). The main backgrounds to the search are the  $t\bar{t}$  and  $tW$  production processes. Two signatures are considered, containing either a  $\tau_{\text{lep}}\tau_{\text{had}}$  or  $\tau_{\text{had}}\tau_{\text{had}}$  pair, where  $\tau_{\text{had}}$  ( $\tau_{\text{lep}}$ ) refers to a  $\tau$ -lepton decaying into hadrons and a neutrino (two neutrinos and an electron or a muon). In each of these two analysis channels, events are classified, based on the transverse momentum ( $p_T$ ) of the  $b$ -jet, in two categories of low and high  $b$ -jet  $p_T$ . The search for LQs is only performed in the high  $b$ -jet  $p_T$  category, where the contribution from the non-resonant LQ processes is small. The non-resonant contribution can be significantly modified by the interference contribution, which depends on the signal model parameters. The effect of the interference with SM diagrams, such as those from  $Z/\gamma^*(\rightarrow \tau\tau) + b$ -jet [35, 36], is expected to be small in the high  $b$ -jet  $p_T$  category and it is neglected. Due to the lack of detailed studies of the interference effect, an additional search is performed considering both high and low  $b$ -jet  $p_T$  categories and not relying on a specific LQ model choice for its signal description (henceforth called ‘model-independent’), and covering a wider range of beyond-SM signatures. For this search, the results are expressed in terms of the visible cross-section of the beyond-SM signal.

The next sections discuss the ATLAS detector in Section 2, data and simulated samples in Section 3, followed by the object reconstruction and definitions in Section 4. Section 5 discusses the overall analysis

strategy and event selection, then Section 6 goes into more details of the background estimation methods. The systematic uncertainties are discussed in Section 7 followed by the results in Section 8, with the conclusion in Section 9.

## 2 The ATLAS Detector

The ATLAS detector [16] at the LHC covers nearly the entire solid angle around the collision point.<sup>1</sup> 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.

The inner-detector system (ID) is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range of  $|\eta| < 2.5$ . 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 [17, 37]. 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 of  $|\eta| < 4.9$ . 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 by 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 Tm across most of the detector. A set of precision chambers covers the region  $|\eta| < 2.7$  with three layers of monitored drift tubes, complemented by cathode-strip chambers in the forward region, where the background is highest. The muon trigger system covers the range of  $|\eta| < 2.4$  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 [38]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger reduces in order to record events to disk at about 1 kHz.

An extensive software suite [39] 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.

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

### 3 Data and Monte Carlo Samples

The data were collected using unprescaled single-lepton and single  $\tau_{\text{had}}$  triggers. A more detailed description of the triggers used in the analysis for each data-taking period is given in Section 5. Quality criteria are applied to events to ensure that the data were not affected by any hardware- or software-related issues [40].

Monte Carlo (MC) simulated events of single LQs decaying into  $b\tau$  were produced for masses ranging from 0.4 TeV to 2.5 TeV. The signal samples were produced at leading order (LO) in QCD in the five-flavour scheme using the `MADGRAPH5_AMC@NLO 2.8.1` [41] generator with the `NNPDF3.0NNLO` [42] parton distribution function (PDF) followed by parton showering and hadronisation with `PYTHIA 8.244` [43] using the A14 set of tuned parameters (tune) [44] and the `NNPDF2.3LO` PDF set. Single scalar and vector LQ signal samples were produced with coupling parameters  $\lambda$  from 0.5 to 2.5. The intrinsic width of the LQs increases quadratically with  $\lambda$  and linearly as a function of  $m_{\text{LQ}}$ . In the considered range of parameters, the LQ width is 16% or less of the LQ mass. The simulated signal events do not include interference effects with the SM processes. For the vector LQ signal two samples were produced for each  $\lambda$ , one with Yang–Mills coupling ( $\kappa = 0$ ) and the other with minimal coupling ( $\kappa = 1$ ). The implementation of the signal model is based on that described in Refs. [20, 21, 45].

Simulated events with pair produced scalar LQs were generated at next-to-leading order (NLO) in QCD with `MADGRAPH5_AMC@NLO 2.6.0`, using the LQ model described in Ref. [46], which adds parton showers to the fixed-order NLO QCD calculations [47, 48] interfaced to `PYTHIA 8.230` for the parton shower (PS) and hadronisation. Parton luminosities are provided by the five-flavour scheme `NNPDF3.0NLO` PDF set with a value of the strong coupling constant  $\alpha_s = 0.118$ , and the underlying event was modelled with the A14 tune. The LQ pair-production cross-sections were obtained from the calculation of direct top-squark pair production assuming that all other supersymmetric particles are heavier, since the production modes of this process are the same as the LQ pair production. The cross-sections were computed at approximate next-to-next-to-leading order (NNLO) in QCD with resummation of next-to-next-to-leading logarithmic (NNLL) soft gluon terms [49–52]. The cross-sections do not include lepton  $t$ -channel contributions, which are neglected in Ref. [46] and may lead to corrections at the percent level [53].

Simulated events with pair-produced vector LQs were generated with `MADGRAPH5_AMC@NLO 2.6.0` at LO in QCD, using the LQ model of Ref. [19] and the `NNPDF3.0NLO` PDF set with  $\alpha_s = 0.118$ . Decays of the LQs were performed with `MADSPIN`, while PS and hadronisation were simulated using `PYTHIA 8.244` with the A14 tune. Since no higher-order cross-sections are available for this model, the LO `MADGRAPH5_AMC@NLO` cross-sections were used.

Several simulation samples are used to model the expected background processes. These include  $t\bar{t}$ , single top-quark,  $Z$ +jets,  $W$ +jets, and diboson events.

The production of  $t\bar{t}$  simulated events was performed with the `POWHEG Box v2` [54–57] generator at NLO with the `NNPDF3.0NLO` PDF set [58] and the  $h_{\text{damp}}$  parameter<sup>2</sup> set to  $1.5 m_{\text{top}}$  [59], with  $m_{\text{top}} = 172.5$  GeV. The events were interfaced to `PYTHIA 8.230` [60] to model the PS, hadronisation, and underlying event, with parameters set according to the A14 tune and using the `NNPDF2.3LO` set of PDFs. The  $t\bar{t}$  sample was normalised to the cross-section prediction at NNLO in QCD including the resummation of NNLL calculated using `TOP++ 2.0` [61–67].

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<sup>2</sup> The  $h_{\text{damp}}$  parameter is a resummation damping factor and one of the parameters that controls the matching of `POWHEG` matrix elements to the PS and thus effectively regulates the high- $p_T$  radiation against which the  $t\bar{t}$  system recoils.



Single top-quark  $s$ -channel ( $t$ -channel) production was simulated using the POWHEG BOX v2 generator at NLO in QCD in the five-flavour (four-flavour) scheme with the NNPDF3.0<sub>NLO</sub> set of PDFs. The events were interfaced with PYTHIA 8.230 using the A14 tune and the NNPDF2.3<sub>LO</sub> PDF set. The samples were normalised to the theory prediction calculated at NLO in QCD with HATHOR 2.1 [68, 69]. Similarly, the associated production of top quarks with  $W$  bosons ( $tW$ ) was modelled by the POWHEG BOX v2 generator at NLO in QCD using the five-flavour scheme and the NNPDF3.0<sub>NLO</sub> set of PDFs. The diagram removal scheme [70] was used 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 [59, 70]. The events were interfaced to PYTHIA 8.230 using the A14 tune and the NNPDF2.3<sub>LO</sub> set of PDFs.

For the production of  $Z/\gamma^*$  sample, the POWHEG BOX v1 [55–57, 71] generator was used for the simulation at NLO accuracy of the hard-scattering processes of  $Z$  boson production and decay into the electron, muon, and  $\tau$ -lepton channels. It was interfaced to PYTHIA 8.186 for the modelling of the PS, hadronisation, and underlying event, with parameters set according to the AZNLO tune [72]. The CT10<sub>NLO</sub> PDF set [73] was used for the hard-scattering processes, whereas the CTEQ6L1 PDF set [74] was used for the PS. The effect of QED final-state radiation was simulated with PHOTOS++ 3.52 [75, 76].

The production of  $W$ +jets events was generated with SHERPA 2.2.1 [77]. In this set-up, NLO-accurate matrix elements for up to two partons and LO-accurate matrix elements for up to four partons were calculated with the Comix [78] and OPENLOOPS [79–81] libraries. The default SHERPA PS [82] based on Catani–Seymour dipole factorisation and the cluster hadronisation model [83] were used. They employed the dedicated set of tuned parameters developed by the SHERPA authors and the NNPDF3.0<sub>NNLO</sub> PDF set [58]. The NLO matrix elements for a given jet multiplicity were matched to the PS using a colour-exact variant of the MC@NLO algorithm [84]. Different jet multiplicities were then merged into an inclusive sample using an improved CKKW matching procedure [85, 86] that is extended to NLO accuracy using the MEPS@NLO prescription [87].

Diboson production was simulated with the SHERPA 2.2.1 or 2.2.2 generator depending on the process. 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 emission 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 fully leptonic and semileptonic final states. The matrix element calculations were matched and merged with the SHERPA PS based on Catani–Seymour dipole factorisation using the MEPS@NLO prescription. The virtual QCD corrections were provided by the OPENLOOPS library. The NNPDF3.0<sub>NNLO</sub> set of PDFs were used, along with the dedicated set of tuned PS parameters developed by the SHERPA authors. The samples were normalised to a NLO prediction.

A summary of all the features used for the simulation of the signal and background processes is shown in Table 1. In all samples except those produced with SHERPA 2.2.1 or SHERPA 2.2.2, decays of heavy-flavour hadrons were modelled with EVTGEN 1.2.0 or EVTGEN 1.6.0 program [88], depending on the process. All samples of simulated events were processed through the ATLAS detector simulation [89] based on GEANT4 [90]. The effects of multiple interactions in the same and nearby bunch crossings (pile-up) were modelled by overlaying minimum-bias events simulated using the soft QCD processes of PYTHIA 8.186 [91] with the A3 tune [92] and the NNPDF2.3<sub>LO</sub> PDF set.

Table 1: Overview of the MC generators used for the main signal and background samples. The last column specifies the order in QCD for the cross-section calculation used for the normalisation of the simulated samples.

Process	Generator		PDF set		Tune	Normalisation
	ME	PS	ME	PS		
LQ $\rightarrow b\tau$	MadGraph5_aMC@NLO	PYTHIA 8.244	NNPDF3.0NNLO	NNPDF2.3LO	A14	LO
Scalar LQLQ $\rightarrow b\tau b\tau$	MadGraph5_aMC@NLO	PYTHIA 8.230	NNPDF3.0NNLO	NNPDF2.3LO	A14	NNLO + NNLL
Vector LQLQ $\rightarrow b\tau b\tau$	MadGraph5_aMC@NLO	PYTHIA 8.244	NNPDF3.0NNLO	NNPDF2.3LO	A14	LO
$t\bar{t}$	POWHEG BOX v2	PYTHIA 8.230	NNPDF3.0NNLO	NNPDF2.3LO	A14	NNLO + NNLL
Single top	POWHEG BOX v2	PYTHIA 8.230	NNPDF3.0NNLO	NNPDF2.3LO	A14	NLO
$Z/\gamma^*$	POWHEG BOX v1	PYTHIA 8.186	CT10NLO	CTEQ6L1	AZNLO	NLO
W+jets	SHERPA 2.2.1		NNPDF3.0NNLO		SHERPA	NNLO
Diboson	SHERPA 2.2.1/SHERPA 2.2.2		NNPDF3.0NNLO		SHERPA	NLO

## 4 Object Reconstruction and Identification

Tracks measured in the ID are used to reconstruct the interaction vertices [93]. The primary vertex of the hard interaction is chosen as the proton–proton vertex candidate with the highest sum of the squared transverse momenta of the associated tracks.

Electrons are reconstructed from topological clusters of energy deposits in the electromagnetic calorimeter that are matched to a track reconstructed in the ID [94]. In the  $\tau_{\text{lep}}\tau_{\text{had}}$  ( $\tau_{\text{had}}\tau_{\text{had}}$ ) final state, the selected (rejected) electrons are required to satisfy the ‘medium’ (‘loose’) identification criteria and have  $p_{\text{T}} > 20$  GeV (15 GeV). Moreover, electrons are required to be within  $|\eta_{\text{cluster}}| = 2.47$  with the exclusion of the region between the barrel and endcap calorimeters ( $1.37 < |\eta_{\text{cluster}}| < 1.52$ ). An additional ‘loose’ isolation criterion [94] is also required, which has an efficiency of 90% for candidates with  $p_{\text{T}} > 15$  GeV, increasing to more than 98% for candidates with  $p_{\text{T}} > 30$  GeV.

Muons are reconstructed from signals in the MS matched with tracks inside the ID. In the  $\tau_{\text{lep}}\tau_{\text{had}}$  final state, the selected muons are required to satisfy the ‘medium’ identification criteria with an average efficiency of 97%, and have  $p_{\text{T}} > 25$  GeV (7 GeV) and  $|\eta| < 2.5$ . In the  $\tau_{\text{had}}\tau_{\text{had}}$  channel, muons are rejected if they satisfy the ‘loose’ identification criteria. A ‘tight’ isolation criterion [95] based on track information and having an average efficiency of 89% is also applied.

Jets are reconstructed with a particle-flow algorithm, which combines energy deposits in the calorimeter with ID tracks [96], using the anti- $k_{\text{t}}$  algorithm [97, 98] with a radius parameter  $R = 0.4$ . Only jets with  $|\eta| < 2.5$  and  $p_{\text{T}} > 25$  GeV are considered. The ‘tight’ working point of the jet vertex tagger (JVT) [99] algorithm is selected to remove jets with  $p_{\text{T}} < 60$  GeV and  $|\eta| < 2.4$  that are identified as not being associated with the primary vertex of the hard interaction. Jets containing  $b$ -hadrons are identified using the DL1r  $b$ -tagging algorithm [100, 101]. A 70% efficiency working point is used, with the efficiencies being measured in simulated  $t\bar{t}$  events. The corresponding rejection factors (defined as the reciprocal of the efficiency values) for  $b$ -tagged jets initiated by  $c$ -quarks and light partons are 9.4 and 390 respectively.

The  $\tau_{\text{had}}$  decays are composed of a neutrino and a set of visible decay products, most frequently one or three charged pions and up to two neutral pions. The visible decay products of the  $\tau_{\text{had}}$  decay are denoted by  $\tau_{\text{had-vis}}$ . The reconstruction of the  $\tau_{\text{had-vis}}$  is seeded by jets reconstructed by the anti- $k_{\text{t}}$  algorithm [97], using calibrated topological clusters [102] as inputs, with a radius parameter of  $R = 0.4$  [103]. Reconstructed tracks are matched to  $\tau_{\text{had-vis}}$  candidates and a multivariate discriminant is used to assess whether these tracks are likely to have been produced by the charged  $\tau_{\text{had}}$  decay products, rejecting tracks originating from other interactions, nearby jets, photon conversions or misreconstructed tracks. The  $\tau_{\text{had-vis}}$  objects



are required to have one or three associated charged-particle tracks selected by this discriminant. Their charge ( $q$ ) is defined as the sum of the measured electric charges of these associated tracks and is required to be  $|q| = 1$ . The  $\tau_{\text{had-vis}}$  objects are also required to satisfy  $p_T > 20 \text{ GeV}$  and  $|\eta| < 2.5$ , excluding the region  $1.37 < |\eta| < 1.52$ . To separate the  $\tau_{\text{had-vis}}$  candidates produced by hadronic  $\tau$ -lepton decays from those due to jets initiated by quarks or gluons, a recurrent neural network (RNN) identification algorithm [104] ( $\tau_{\text{had-ID}}$ ) is constructed using information from reconstructed charged-particle tracks and calorimeter-energy clusters associated with  $\tau_{\text{had-vis}}$  candidates. This analysis uses two  $\tau_{\text{had-ID}}$  working points: ‘medium’, which has a 75% (60%) acceptance efficiency and a background rejection of 35 (240) and ‘loose’, which has a 85% (75%) acceptance efficiency and a background rejection of 21 (90) for  $\tau_{\text{had}}$  with one (three) charged-particle tracks. A ‘very loose’ working point, having a 95% acceptance efficiency, is also used for background estimation. A separate boosted decision tree discriminant (‘eBDT’) is also used to reject backgrounds arising from electrons misidentified as  $\tau_{\text{had-vis}}$ . This discriminant is built using information from the calorimeter and the ID, most notably transition radiation information from the TRT system and variables sensitive to the ratio of the energy deposited in the calorimeter to the visible momentum measured from the reconstructed tracks.

The reconstructed objects used in this analysis are not built from disjoint sets of tracks or calorimetric clusters. It is therefore possible that two different objects share most of their constituents. An overlap removal procedure is applied to resolve this ambiguity. This procedure is summarised in Table 2.

The missing transverse momentum vector,  $\vec{E}_T^{\text{miss}}$ , is reconstructed as the negative vector sum of the transverse momenta of leptons,  $\tau_{\text{had-vis}}$  and jets, and a ‘soft-term’ [105]. The soft-term is calculated as the vectorial sum of the  $\vec{p}_T$  of tracks matched to the primary vertex but not associated with a reconstructed lepton,  $\tau_{\text{had-vis}}$  or jet. The magnitude of  $\vec{E}_T^{\text{miss}}$  is referred to as the missing transverse energy,  $E_T^{\text{miss}}$ .

Table 2: Criteria applied to overlapping reconstructed objects. The criteria are listed in the order they are applied.

Object to keep	Object to remove	Criteria
Electron	Electron	If they share the same track, the electron with the highest transverse momentum is kept.
Electron	$\tau_{\text{had-vis}}$	If $\Delta R < 0.2$ , the electron is kept.
Muon	$\tau_{\text{had-vis}}$	If $\Delta R < 0.2$ , the muon is kept.
Muon	Electron	If they share a track, the electron is removed if the muon is associated with a signature in the MS, otherwise the muon is removed.
Electron	Jet	Any jet within $\Delta R = 0.2$ of an electron is removed.
Muon	Jet	Any jet within $\Delta R = 0.2$ of a muon is removed if it has fewer than three associated tracks.
Jet	Electron	Any electron within $\Delta R = 0.4$ of a jet is removed.
Jet	Muon	Any muon within $\Delta R = 0.4$ of a jet is removed.
$\tau_{\text{had-vis}}$	Jet	Any jet within $\Delta R = 0.2$ of a $\tau_{\text{had-vis}}$ is removed.

## 5 Event Selection

Events are required to contain at least one primary vertex with at least two associated tracks.

For the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel events were selected by single-lepton triggers. In 2015 single-electron triggers were active with  $p_{\text{T}}$  thresholds of 24, 60 and 120 GeV [106]. For data from 2016 onward the  $p_{\text{T}}$  thresholds are 26, 60 and 140 GeV. The single-muon triggers had  $p_{\text{T}}$  thresholds of 20 and 50 GeV for 2015, and 26 and 50 GeV from 2016 [107]. The trigger thresholds were raised to keep the trigger rates sufficiently low as the luminosity was increased. The lowest  $p_{\text{T}}$  threshold electron and muon triggers also have an isolation requirement. The lepton isolation and identification requirements loosen as the trigger  $p_{\text{T}}$  thresholds increase. Events must contain at least one  $\tau_{\text{had}}$  candidate and exactly one electron or one muon. The electron or muon must be isolated and satisfy the medium lepton identification. Events with more than one lepton satisfying the medium identification are rejected, considering electrons (muons) with a  $p_{\text{T}}$  greater than 15 (7) GeV. This helps to reject  $Z/\gamma^* \rightarrow ee/\mu\mu$  events and  $Z/\gamma^* \rightarrow \tau_{\text{lep}}\tau_{\text{lep}}$ . Furthermore, the electron and muon candidates are required to have  $p_{\text{T}} > 30$  GeV, and be matched to the trigger object that caused the event to be selected. The  $\tau_{\text{had}}$  candidate is required to have  $p_{\text{T}} > 50$  GeV, satisfy the medium  $\tau_{\text{had}}$ -ID selection and have  $|\eta| < 2.3$ . The pseudorapidity selection requirement rejects events with  $\tau_{\text{had}}$  candidates in a region with a higher background contamination and large uncertainties in the determination of the rate of electrons misidentified as  $\tau_{\text{had}}$ .

In the  $\tau_{\text{had}}\tau_{\text{had}}$  channel, events were selected by a single  $\tau_{\text{had}}$  trigger [108]. For 2015 and 2016, three single  $\tau_{\text{had}}$  triggers were available with  $p_{\text{T}}$  thresholds of 80, 125 and 160 GeV. In 2017 and 2018, due to higher instantaneous luminosity, only the  $p_{\text{T}} > 160$  GeV trigger threshold was used. The  $\tau_{\text{had}}$  identification requirements become less stringent as the trigger  $p_{\text{T}}$  thresholds rise. Events must contain at least two  $\tau_{\text{had}}$  candidates where the leading  $\tau_{\text{had}}$  candidate in  $p_{\text{T}}$  must be matched to the trigger within an angular distance of  $\Delta R = 0.2$  and have  $p_{\text{T}}$  that is at least 5 GeV above the trigger threshold. The subleading- $p_{\text{T}}$   $\tau_{\text{had}}$  candidate is required to have  $p_{\text{T}} > 65$  GeV. Identification requirements are applied to both  $\tau_{\text{had}}$  candidates; the leading- $p_{\text{T}}$   $\tau_{\text{had}}$  must satisfy the medium selection and the subleading- $p_{\text{T}}$   $\tau_{\text{had}}$  the loose selection. Events that contain any electron or muon that satisfies the loose identification requirements are rejected, which ensures orthogonality to the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel.

Events passing the previous requirements are then selected with criteria that are similar between the two channels. The two  $\tau_{\text{had}}$  or the electron/muon (denoted by  $\ell$ ) and  $\tau_{\text{had}}$  must have opposite electric charges and at least one  $b$ -tagged jet is required. The invariant mass of the visible decay products of the two  $\tau$ -leptons,  $m_{\text{vis}}(\ell, \tau_{\text{had}})$  or  $m_{\text{vis}}(\tau_{\text{had}}, \tau_{\text{had}})$ , is required to be above 100 GeV, which is effective at reducing the  $Z/\gamma^* \rightarrow \tau\tau$  background. An additional requirement  $\Delta\phi(\ell, E_{\text{T}}^{\text{miss}}) < 1.5$  is applied in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel to reduce single top and  $t\bar{t}$  events.

Events in each channel are assigned to two categories of low ( $< 200$  GeV) and high ( $> 200$  GeV) transverse momentum of the leading- $p_{\text{T}}$   $b$ -jet. The high  $b$ -jet  $p_{\text{T}}$  category is found to perform better for low-mass singly produced LQs, where the resonant contribution is dominant. Conversely, the low  $b$ -jet  $p_{\text{T}}$  category has a better acceptance for high mass signals, where the non-resonant contribution is dominant for signals with  $m_{\text{LQ}} \geq 0.9$  TeV. This split into two categories improves the analysis sensitivity by up to 30%.

The variable  $S_{\text{T}}$  is defined as the scalar  $p_{\text{T}}$  sum of the two  $\tau_{\text{had-vis}}$  (or  $\ell$  and  $\tau_{\text{had-vis}}$ ) and the leading- $p_{\text{T}}$   $b$ -jet. A minimum requirement of  $S_{\text{T}} > 300$  GeV is applied, as there is almost no improvement in sensitivity by adding events with lower  $S_{\text{T}}$  values.

The selection criteria described above define the signal regions (SR) of the analysis. The signal acceptance times efficiency of the event selection varies between 3% and 10%, depending on the LQ mass and coupling. Alternative selections define the control regions (CR), used to evaluate the contribution of the main background processes in the SR, and the validation regions (VR), used to verify the good modelling of the backgrounds. The selection requirements used for the signal, control and validation regions are summarised in Tables 3 and 4. The use of the control and validation regions in the background estimation methods is discussed more extensively in Section 6.

Table 3: Definition of signal regions (SR) and background-enriched control regions (CR) and validation regions (VR) used in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel. The symbol  $\ell$  represents the selected electron or muon candidate and  $\tau_{\text{had-vis}}$  represents the leading  $\tau_{\text{had-vis}}$  candidate.

Signal Regions	Selection	
Preselection	$\ell$ (trigger, isolated), $\tau_{\text{had-vis}}$ (medium $\tau_{\text{had-ID}}$ ), $q(\ell) \times q(\tau_{\text{had-vis}}) < 0$ , $\Delta\phi(\ell, E_{\text{T}}^{\text{miss}}) < 1.5$ , $m_{\text{vis}}(\ell, \tau_{\text{had-vis}}) > 100$ GeV, $S_{\text{T}} > 300$ GeV, at least one $b$ -jet	
High $b$ -jet $p_{\text{T}}$ SR	Leading $b$ -jet $p_{\text{T}} > 200$ GeV	
Low $b$ -jet $p_{\text{T}}$ SR	Leading $b$ -jet $p_{\text{T}} < 200$ GeV	
Control/Validation Regions	Selection	Purpose
Multijet-CR	$\ell$ (trigger, pass/fail offline isolation), $m_{\text{T}}(\ell, E_{\text{T}}^{\text{miss}}) < 30$ GeV, one $b$ -jet, $\tau_{\text{had-ID}}$ score $< 0.01$ , $E_{\text{T}}^{\text{miss}} < 50$ GeV	Measure lepton fake-factor
Top-CR	Satisfy SR except: $\Delta\phi(\ell, E_{\text{T}}^{\text{miss}}) > 2.5$ , no $S_{\text{T}}$ and lead. $b$ -jet $p_{\text{T}}$ req.	Derive top correction
SS-CR	Satisfy SR except: $q(\ell) \times q(\tau_{\text{had-vis}}) > 0$ , no $\Delta\phi(\ell, E_{\text{T}}^{\text{miss}})$ , and $S_{\text{T}}$ req.	Measure jet $\rightarrow \tau$ background scale factor
High $b$ -jet $p_{\text{T}}$ VR	Satisfy high $b$ -jet $p_{\text{T}}$ SR except: $1.5 < \Delta\phi(\ell, E_{\text{T}}^{\text{miss}}) < 2.5$ , $300$ GeV $< S_{\text{T}} < 600$ GeV	Background modelling validation
Low $b$ -jet $p_{\text{T}}$ VR	Satisfy low $b$ -jet $p_{\text{T}}$ SR except: $1.5 < \Delta\phi(\ell, E_{\text{T}}^{\text{miss}}) < 2.5$ , $300$ GeV $< S_{\text{T}} < 600$ GeV	Background modelling validation
b-tag Z-CR	Satisfy SR except: $45$ GeV $< m_{\text{vis}}(\ell, \tau_{\text{had-vis}}) < 80$ GeV, $p_{\text{T}}(\ell)/p_{\text{T}}(b\text{-jet}) > 0.8$ , $ \Delta\phi(\ell, \tau_{\text{had-vis}})  > 2.4$ , no $S_{\text{T}}$ req.	Z+ heavy-flavour jets normalisation factor

Table 4: Definition of signal regions (SR) and background-enriched control regions (CR) and validation regions (VR) used in the  $\tau_{\text{had}}\tau_{\text{had}}$  channel. The symbol  $\tau_1$  ( $\tau_2$ ) represents the leading (sub-leading)  $\tau_{\text{had-vis}}$  candidate.

Signal Regions	Selection	
Preselection	$\tau_{\text{had},1}$ (trigger, medium $\tau_{\text{had-ID}}$ ), $\tau_2$ (loose $\tau_{\text{had-ID}}$ ), $q(\tau_1) \times q(\tau_2) < 0$ , $m_{\text{vis}}(\tau_1, \tau_2) > 100$ GeV, $S_{\text{T}} > 300$ GeV, at least one $b$ -jet	
High $b$ -jet $p_{\text{T}}$ SR	Leading $b$ -jet $p_{\text{T}} > 200$ GeV	
Low $b$ -jet $p_{\text{T}}$ SR	Leading $b$ -jet $p_{\text{T}} < 200$ GeV	
Control/Validation Regions	Selection	Purpose
DJ-CR	$\tau_1$ and $\tau_2$ satisfy very loose $\tau_{\text{had-ID}}$ , $q(\tau_1) \times q(\tau_2) < 0$	Measure $\tau_{\text{had-vis}}$ fake-factor
CR-1	Satisfy SR except: $\tau_2$ fail loose $\tau_{\text{had-ID}}$	Apply $\tau_{\text{had-vis}}$ fake-factor
SS-VR	Satisfy SR except: $q(\tau_1) \times q(\tau_2) > 0$	Multijet modelling check
Z+light flavour jets VR	Satisfy SR except: 0 $b$ -jets, $\Delta\phi(\tau_1, \tau_2) > 0.25$ , $m_{\text{vis}}(\tau_1, \tau_2) < 100$ GeV, $E_{\text{T}}^{\text{miss}} > 60$ GeV	Z+light jets modelling

## 6 Background Estimation

### 6.1 $\tau_{\text{lep}}\tau_{\text{had}}$ channel

In the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel the dominant background contributions are from  $t\bar{t}$  and single top-quark events. Processes involving top quarks can produce real  $\tau$ -leptons, or jets that are misidentified as  $\tau_{\text{had}}$ , and are estimated by using simulation with data-driven corrections. The  $t\bar{t}$  and  $tW$  contributions are treated as one combined top-quark background due to their similar kinematics and final states. In the low (high)  $b$ -jet  $p_T$  SR,  $t\bar{t}$  accounts for 90% (86%) of all top-quark processes and 96% (97%) of the single top-quarks are from  $tW$ . To ensure that this background is accurately modelled, a top-quark control region (Top-CR) is defined. With respect to the SR selection, the requirements on the leading  $b$ -jet  $p_T$  and the  $S_T$  are removed, and the condition  $\Delta\phi(\ell, E_T^{\text{miss}}) < 1.5$  is replaced by  $\Delta\phi(\ell, E_T^{\text{miss}}) > 2.5$ . This results in a region with a purity of 91% in top-quark processes and negligible signal contamination. Out of all top-quark events in the Top-CR, 91% are from  $t\bar{t}$  processes and  $\sim 97\%$  of the single top-quark events are from  $tW$ , which is compatible with the composition of the SRs.

A discrepancy between the data and simulation prediction is observed in the Top-CR, with the simulation overestimating the background contribution. 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 [109, 110]. The discrepancy varies depending on  $S_T$ ; for this reason, a correction is derived as function of  $S_T$  in this region based on the ratio between data and simulation. A top-quark correction scale factor is defined in Eq. (1) and is applied to all  $t\bar{t}$  and single top-quark simulated events. The comparison between data and the background prediction in the Top-CR and the derived correction as function of  $S_T$  are shown in Figure 2, where  $t\bar{t}$  and  $tW$  events with a generated lepton reconstructed as a lepton (a ‘true’ lepton) and a jet misidentified as a  $\tau_{\text{had}}$  are included under the  $Jet \rightarrow \tau$  fake contribution. This demonstrates that the Top-CR is dominated by  $t\bar{t}$  and  $tW$  events with true leptons and  $\tau_{\text{had}}$  in the final state, thus this correction does not account for mismodelling due to jets being misidentified as  $\tau_{\text{had}}$ . The modelling of events with a true lepton and jet misidentified as a  $\tau_{\text{had}}$  in the final state is discussed later in this section.

The top-quark correction scale factor is defined as a function of  $S_T$ :

$$SF_{\text{Top}}(S_T) = \frac{(N_{\text{data}} - N_{\text{non-Top}})(S_T)}{N_{\text{Top}}(S_T)}, \quad (1)$$

where  $N_{\text{data}}$  and  $N_{\text{Top}}$  represent respectively the number of data events and of  $t\bar{t}$  plus single top-quark events predicted by simulation,  $N_{\text{Top}}$  includes events with both true and misidentified  $\tau_{\text{had}}$  in the final state and  $N_{\text{non-Top}}$  includes all the other backgrounds estimated by using simulation. The resulting correction is well fitted by a linear function, which is used to derive the correction scale factors. The correction is also derived with an alternative logarithmic function:  $SF_{\text{Top}}(S_T) = a \ln(S_T) + b$ , and the difference between the two corrections is taken as an uncertainty on the correction. Additional uncertainties related to the cross-section and acceptance of the top-quark processes, as well as the statistical and cross-section uncertainties related to the subtraction of the contribution from the other processes, are applied to account for the slight difference between the fractions of top-quark events that are due to  $t\bar{t}$  production in the Top-CR and SRs and for the extrapolation to the SR. The scale factor is applied at the per-event level to the  $t\bar{t}$  plus single top-quark events passing the selections of the signal, control or validation regions. The total uncertainty in the scale factor varies between 2% and 7% for  $S_T$  in the range of 200–800 GeV.

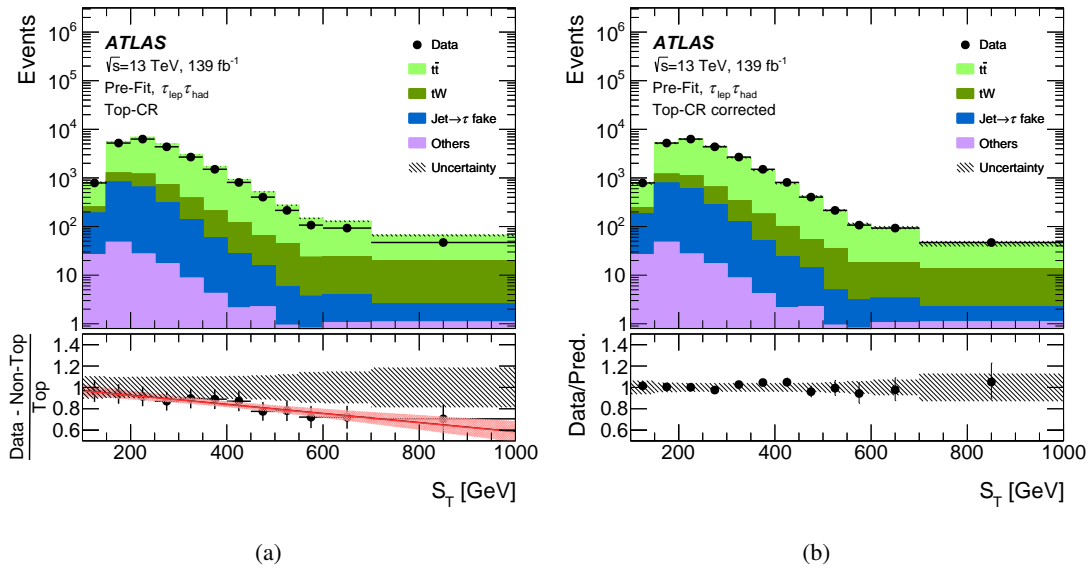


Figure 2: (a) Comparison between data and the background prediction for the  $S_T$  distribution in the Top-CR in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel. The  $t\bar{t}$  and  $tW$  contributions only include events with true leptons and  $\tau_{\text{had}}$  in the final state. The label *Jet*  $\rightarrow$   $\tau$  *fake* corresponds to events with a lepton and a quark- or gluon-initiated jet misidentified as  $\tau_{\text{had}}$ ; this contribution is estimated by using simulation. The bottom panel shows the ratio of the data to the prediction where the uncertainty shown by both the points and hatched band includes the statistical uncertainty in the data and background predictions, the theoretical uncertainty in the MC simulation predictions, and the MC subtraction uncertainty. Finally, the line and the cross dashed band show the resulting fit and the associated uncertainty. The label ‘Top’ in the bottom panel denotes the sum of  $t\bar{t}$  and  $tW$  processes, while ‘Non-Top’ refers to all other processes considered. Entries with values above the  $x$ -axis range are included in the last bin of the distribution. (b) Shows the same distribution after the top-quark correction scale factor is applied to the  $t\bar{t}$  and  $tW$  simulated events. Only the uncertainty associated to the top-quark correction and the statistical uncertainty on data and simulation are considered.

Another source of background in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel stems from multi-jet events, where jets can mimic both the  $\tau_{\text{lep}}$  and  $\tau_{\text{had}}$ . This type of background from multi-jet events is estimated via a data-driven fake-factor method by deriving a lepton fake-factor. The lepton fake-factor is measured in the multi-jet control region that is enriched in multi-jet events, but is similar kinematically to the SR. The events are still required to satisfy the single lepton trigger and to have exactly one  $b$ -jet, but the identification algorithm to reject jets misidentified as  $\tau_{\text{had}}$  is instead used to select multi-jet events by requiring an extremely low value for  $\tau_{\text{had}}$  RNN identification score (corresponding to only 1% acceptance for true  $\tau_{\text{had}}$ ). Additional selection criteria on  $m_T(\ell, E_T^{\text{miss}}) < 30$  GeV and  $E_T^{\text{miss}} < 50$  GeV are applied to increase the purity of multi-jet events relative to other backgrounds. The fake-factor is measured with a requirement on the leading  $b$ -jet  $p_T > 25$  GeV and is defined as:

$$FF_{\text{lep}}(p_T(\tau_{\text{lep}}), \eta(\tau_{\text{lep}})) = \frac{(N_{\text{data}} - N_{\text{MC}})^{\text{pass-iso}}(p_T(\tau_{\text{lep}}), \eta(\tau_{\text{lep}}))}{(N_{\text{data}} - N_{\text{MC}})^{\text{fail-iso}}(p_T(\tau_{\text{lep}}), \eta(\tau_{\text{lep}}))}.$$

The variable  $N_{\text{data}}$  is the total number of data events and  $N_{\text{MC}}$  is the number of background events predicted by simulation that contain a true  $\tau_{\text{lep}}$ . Events are split between the numerator and denominator based on whether the  $\tau_{\text{lep}}$  satisfied the lepton isolation requirement or not. The fake-factor is parameterised as

function of the  $\tau_{\text{lep}}$   $p_T$  and split into central ( $|\eta| < 1.52$ ) and forward ( $|\eta| > 1.52$ ) regions. Next, a control region is defined that has the same selection as the SR, but with the lepton isolation requirement inverted. Applying the fake-factor at the per-event level, the multi-jet estimate in each SR is then obtained by scaling the distribution in the corresponding control region where the isolation criteria are not satisfied.

An additional source of background are events where a lepton is produced in association with a jet that is misidentified as a  $\tau_{\text{had}}$  (*Jet*  $\rightarrow$   $\tau$  *fake*). These contribute approximately 20% to the expected background in the SR and are mostly from  $t\bar{t}$  with contributions from  $W$ +jets,  $Z$ +jets, and diboson events. To ensure that these are well modelled, a ‘same-sign’ control region (SS-CR) is defined by taking the same selection as the SR, but with a light lepton with the same electric charge as  $\tau_{\text{had}}$ . The requirements on  $\Delta\phi(\ell, E_T^{\text{miss}})$ ,  $S_T$  and the leading  $b$ -jet  $p_T$  are removed to increase the number of events in the CR. The top-quark correction scale factor derived in Eq. (1) is applied to top-quark events in this region (approximately 81% of the total). As the Top-CR used to derive that scale factor is dominated by  $t\bar{t}$  and  $tW$  events with true  $\tau$ -leptons in the final state, it does not correct for mismodelling of jets that are misidentified as a  $\tau_{\text{had}}$ . As a difference between the simulation prediction and the data is still observed, another scale factor is derived to account for any remaining differences from those backgrounds with a lepton and misidentified  $\tau_{\text{had}}$  (approximately 60% of the events in this region). The remaining events contain true  $\tau_{\text{had}}$  and are subtracted, before calculating the scale factor, by applying the top-quark correction scale factor. Then, the scale factor for events with a lepton and a jet misidentified as a  $\tau_{\text{had}}$  is defined as:

$$SF_{\text{fake-}\tau}(p_T(\tau_{\text{had-vis}}), n_{\text{track}}) = \frac{(N_{\text{data}} - N_{\text{true-}\tau})(p_T(\tau_{\text{had-vis}}), n_{\text{track}})}{N_{\text{fake-}\tau}(p_T(\tau_{\text{had-vis}}), n_{\text{track}})},$$

where  $N_{\text{true-}\tau}$  is the total number of events predicted by simulation where both the  $\tau_{\text{had}}$  and  $\tau_{\text{lep}}$  are true and  $N_{\text{fake-}\tau}$  is the number of predicted events with a jet misidentified as a  $\tau_{\text{had}}$  and a true  $\tau_{\text{lep}}$ . The scale factor is parameterised as a function of  $p_T(\tau_{\text{had-vis}})$  and the number of charged-particle tracks ( $n_{\text{track}}$ ). It is applied to any MC background event with a true lepton and a jet misidentified as a  $\tau_{\text{had}}$ . The correction is derived in the SS-CR of the  $\tau_{\mu}\tau_{\text{had}}$  channel and then applied to both  $\tau_e\tau_{\text{had}}$  and  $\tau_{\mu}\tau_{\text{had}}$ , because the  $\tau_e\tau_{\text{had}}$  SS-CR contains events with misidentified electrons, which are not well modelled by simulation. The  $SF_{\text{fake-}\tau}$  correction values are in the range of 1–1.2 (1–1.5) for  $\tau_{\text{had}}$  with one (three) charged-particle tracks.

To validate the background modelling in a region depleted in signal, high and low  $b$ -jet  $p_T$  validation regions are defined by applying the SR requirements, with the exceptions of the  $\Delta\phi(\ell, E_T^{\text{miss}}) < 1.5$  and the  $S_T > 300$  GeV criteria, that are modified into  $1.5 < \Delta\phi(\ell, E_T^{\text{miss}}) < 2.5$  and  $300 < S_T < 600$  GeV. The low (high)  $b$ -jet  $p_T$  VR consists of 82% (80%)  $t\bar{t}$  events, of 8% (10%) single top-quark events, and of 9% (9%) of events where a jet is misidentified as a  $\tau_{\text{had}}$ . Good modeling of the background is found in the validation regions; the background estimate agrees with data within the total uncertainty, as shown in Figure 3.

## 6.2 $\tau_{\text{had}}\tau_{\text{had}}$ channel

In the  $\tau_{\text{had}}\tau_{\text{had}}$  channel, the main background sources are  $Z/\gamma^* \rightarrow \tau_{\text{had}}\tau_{\text{had}}$  events, as well as top-quark processes, with  $W$  bosons decaying to  $\tau_{\text{had}}$ , or to electrons, muons or jets misidentified as  $\tau_{\text{had}}$ . Both  $Z/\gamma^* \rightarrow \tau_{\text{had}}\tau_{\text{had}}$  and top-quark backgrounds are estimated using simulation with data-driven corrections, which are discussed further below.



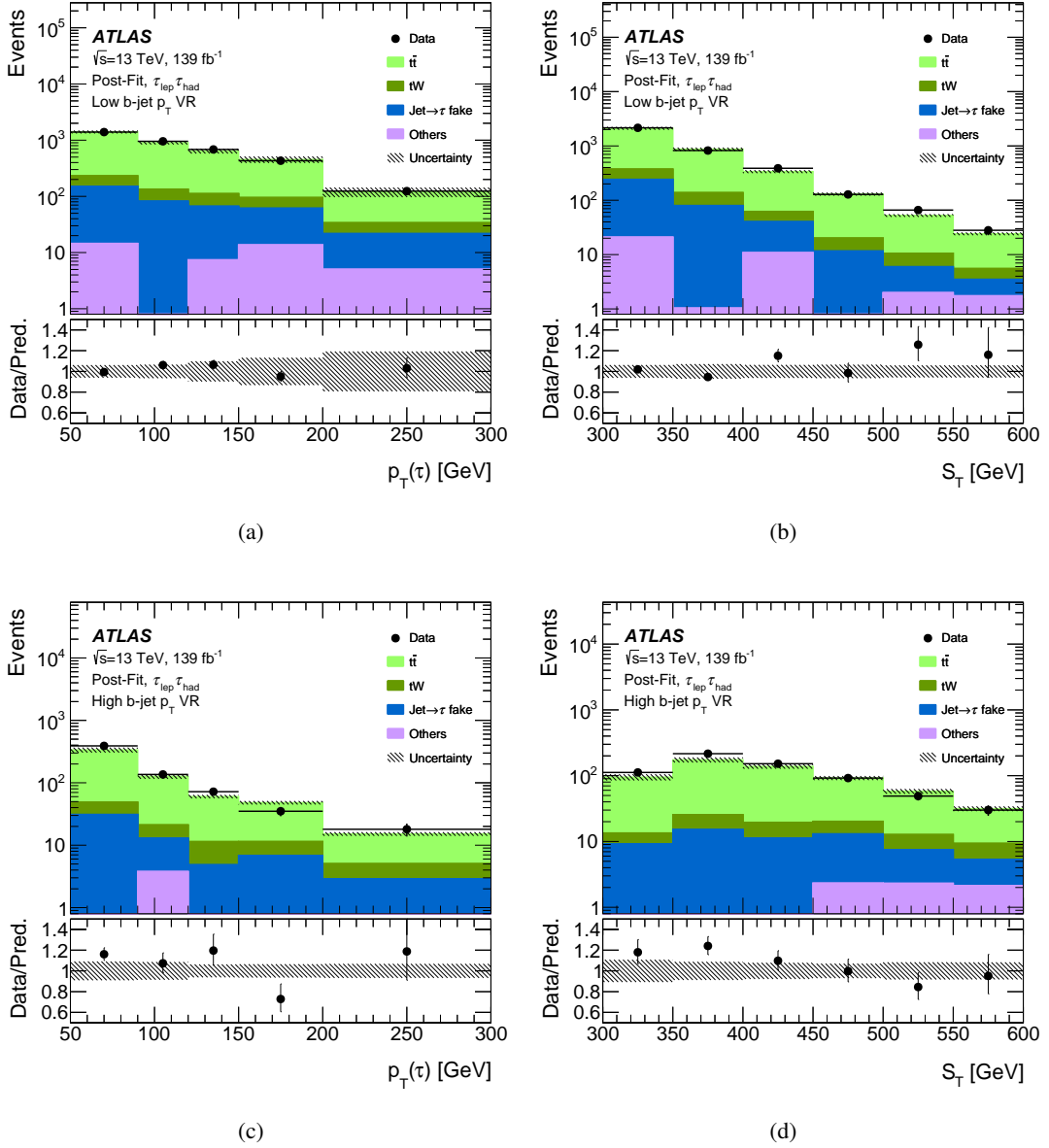


Figure 3: Comparison between data and the background prediction for the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel validation regions after applying the scale factors discussed in Section 6.1. (a) and (b) show the  $p_T(\tau)$  and  $S_T$  respectively for the low  $b$ -jet  $p_T$  category, (c) and (d) show the same for the high  $b$ -jet  $p_T$  category. The uncertainty band includes both statistical and systematic uncertainties evaluated in the fit described in Section 8. Entries with values above the  $x$ -axis range are included in the last bin of each distribution. The lower panels show the ratio of the data to the predictions.

As the mismodelling of the kinematic distributions observed in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel originates from the underlying top-quark process rather than the  $\tau_{\text{had}}$  decay, it is also expected to be present in the  $\tau_{\text{had}}\tau_{\text{had}}$  channel. However, due to small number of events in the  $\tau_{\text{had}}\tau_{\text{had}}$  channel the statistical uncertainty in the top-quark processes is comparable with the expected mismodelling. This makes it difficult to select a  $\tau_{\text{had}}\tau_{\text{had}}$ -only control region to quantify this mismodelling. Therefore, the  $S_T$ -dependent top-quark correction scale factor from Eq. (1) derived in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel is also applied to the  $\tau_{\text{had}}\tau_{\text{had}}$  channel.

The shape of the  $S_T$  distribution is checked and found to be compatible between the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels.

The  $Z/\gamma^* \rightarrow \tau_{\text{had}}\tau_{\text{had}}$  background is also modelled using simulation. Due to a known discrepancy in the simulation compared with the data for  $Z(\rightarrow \tau\tau) + \text{heavy-flavour jets}$  with at least one  $b$ - or  $c$ -jet ( $Z+\text{HF}$ ) [111], a correction factor for the normalisation of this background is derived in a  $\tau_{\text{lep}}\tau_{\text{had}}$   $b$ -tag Z-CR, defined in Table 3, which has a purity of around 60% for the  $Z+\text{HF}$  processes and is inclusive in  $p_T$  of the leading  $b$ -jet. A comparison between the data and the prediction from the simulation in the  $b$ -tag Z-CR before deriving the correction factor is shown in Figure 4.

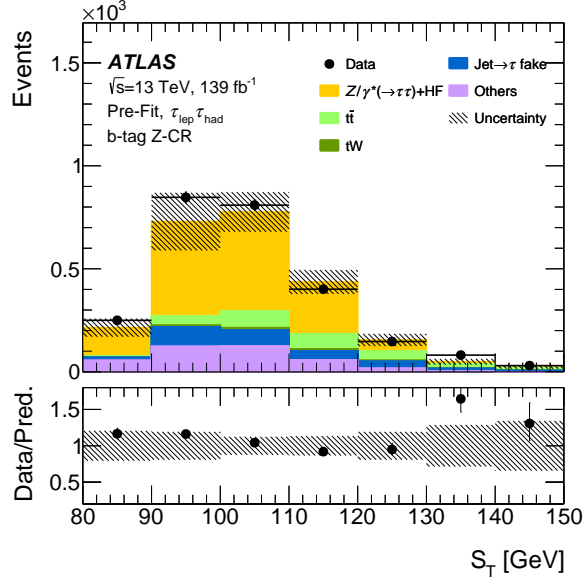


Figure 4: Comparison between data and the background prediction for the  $S_T$  distribution in the control region used for correcting the  $Z(\rightarrow \tau\tau) + \text{heavy-flavour jets}$  process. The uncertainty band includes both statistical and systematic components. Entries with values above the  $x$ -axis range are included in the last bin of the distribution. The lower panel shows the ratio of the data to the predictions.

The scale factor is derived by subtracting backgrounds estimated from simulation that are not from the  $Z+\text{HF}$  process ( $N_{\text{non-ZHF}}$ ):

$$SF_{\text{ZHF}} = \frac{N_{\text{data}} - N_{\text{non-ZHF}}}{N_{\text{ZHF}}},$$

where  $N_{\text{ZHF}}$  is the number of  $Z+\text{HF}$  events predicted by simulation.

The scale factor is applied as a normalisation to the total  $Z+\text{HF}$  contribution, with a value of  $1.13 \pm 0.23$  obtained from the control region. The uncertainty includes the statistical uncertainty, the uncertainty in the subtraction of the simulation events and the extrapolation uncertainty from the control region to the SRs. The extrapolation uncertainty is obtained by repeating the scale factor calculation in the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel using selection criteria for the control and signal regions equivalent to the ones used in the  $\tau_{\text{had}}\tau_{\text{had}}$  channel.

For  $Z(\rightarrow \tau\tau) + \text{light-flavour jets}$  ( $Z+\text{LF}$ , no  $b$ - or  $c$ -jets), the modelling is validated in a  $b$ -veto region ( $Z+\text{LF VR}$ ). This region has the same event selection as the SR, except that zero  $b$ -jets are required. In

addition, the requirements  $m_{\text{vis}} < 100$  GeV,  $E_{\text{T}}^{\text{miss}} > 60$  GeV and  $\Delta\phi(\tau, \tau) > 0.25$  are applied to ensure a high  $Z$ +LF purity. The data is found to be in agreement with the simulation within the statistical uncertainty in the data.

Finally the background originating from multi-jet events, where jets are misidentified as  $\tau_{\text{had}}$ , is estimated by using a data-driven fake-factor method. A control region dominated by multi-jet events, the DJ-CR, is defined by taking events that satisfy one of the single-jet triggers (with thresholds between 15 and 420 GeV). The leading  $\tau_{\text{had-vis}}$  candidate is required to not satisfy the medium  $\tau_{\text{had}}$  identification and the subleading  $\tau_{\text{had-vis}}$  candidate is used as a probe. As for the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel, the fake-factor is measured inclusively in the leading  $b$ -jet  $p_{\text{T}}$ . The leading and subleading  $\tau_{\text{had-vis}}$  candidates are required to have opposite electric charges and have a  $p_{\text{T}} > 65$  GeV. At least one additional  $b$ -tagged jet is required, but no selection is made on the leading  $b$ -jet  $p_{\text{T}}$ . Then, the fake-factor is defined as:

$$f_{\tau_{\text{had-ID}}}(p_{\text{T}}, N_{\text{track}}) \equiv \frac{(N_{\text{data}} - N_{\text{MC}})^{\text{pass } \tau_{\text{had-ID}}}(p_{\text{T}}, N_{\text{track}})}{(N_{\text{data}} - N_{\text{MC}})^{\text{fail } \tau_{\text{had-ID}}}(p_{\text{T}}, N_{\text{track}})} \Big|_{\text{dijet}},$$

where  $N_{\text{MC}}$  includes all simulated background events. The pass or fail  $\tau_{\text{had-ID}}$  superscript refers to whether the subleading  $\tau_{\text{had-vis}}$  candidate satisfies the loose  $\tau_{\text{had-ID}}$  or not, while still satisfying the very loose requirement. For each of the SRs, the multi-jet estimate is then obtained from the CR-1 control region, composed of events in which the subleading  $\tau_{\text{had-vis}}$  candidate fails the loose  $\tau_{\text{had-ID}}$ , using the fake-factor:

$$N_{\text{multi-jet}}(p_{\text{T}}, N_{\text{track}}) = f_{\tau_{\text{had-ID}}}(p_{\text{T}}, N_{\text{track}}) \times (N_{\text{data}} - N_{\text{MC}})^{\text{fail } \tau_{\text{had-ID}}}(p_{\text{T}}, N_{\text{track}}).$$

The fake-factor is parameterised as a function of the  $p_{\text{T}}$  and number of charged-particle tracks of the subleading  $\tau_{\text{had-vis}}$  candidate. For this method to be accurate, it is important that the fail- $\tau_{\text{had-ID}}$  and multi-jet control regions have a similar composition of quark- and gluon-initiated jets. This is obtained by inspecting the shape of subleading  $\tau_{\text{had}}$  identification scores in the two regions, which depends on the quark–gluon fraction. A lower threshold than the very loose requirement is applied on this score, which ensures that the shapes of the distributions are compatible.

After the selection, the multi-jet contribution to the SR is expected to be small. This is verified with the same-sign validation regions (SS-VR). The SS-VR has the same selection as the SR, but the electric charges of the  $\tau_{\text{had}}$  candidates are required to be the same. For key distributions in the low  $b$ -jet  $p_{\text{T}}$  category, the data is found to agree with the background prediction, with approximately half of the events being from  $t\bar{t}$  and half from multi-jet background. The total predicted background in the high  $b$ -jet  $p_{\text{T}}$  SS-VR is 2.8 events (mostly from  $t\bar{t}$ ) and 4 data events are observed. The contribution of multi-jet events in the high  $b$ -jet  $p_{\text{T}}$  SS-VR of the  $\tau_{\text{had}}\tau_{\text{had}}$  channel is thus negligible.

## 7 Systematic Uncertainties

Systematic uncertainties arise from the reconstruction of the various physics objects and from theoretical or modelling uncertainties affecting the predictions for both the backgrounds and signals. These uncertainties manifest themselves in both the overall yield and shape of the final observable, and can be divided into two main groups: the experimental uncertainties and the modelling uncertainties.

The experimental uncertainties include the uncertainties related to the trigger, reconstruction, calibration and identification of electrons [94], muons [95], taus [103] and jets [99, 100, 112]; for electron and muons, additional uncertainties in the lepton isolation are considered. Uncertainties related to background with misidentified  $\tau$ -leptons are described in Section 6. Another source of experimental uncertainties is given by the luminosity measurement, whose primary measurement is obtained using the LUCID-2 detector [113]. An uncertainty value of 1.7% [114] is assigned for the combined 2015–2018 integrated luminosity.

Among the experimental uncertainties, the ones with the highest impact on the analysis sensitivity are the  $\tau_{\text{had-vis}}$  related uncertainties, with an impact on the results in the range of 30–40% depending on the LQ coupling and mass values considered. The uncertainties in the  $\tau_{\text{had-vis}}$  identification efficiency are in the range of 2% to 6%, while the eBDT efficiency uncertainties are of the order of 1% to 2%. These uncertainties are parameterised as a function of the  $\tau_{\text{had-vis}}$   $p_T$  and the number of associated tracks for the  $\tau_{\text{had-vis}}$  identification efficiency, and as a function of the  $\tau_{\text{had}}$  decay mode for the eBDT efficiency. In both cases, the uncertainties are derived in dedicated tag and probe measurements [103]. The  $\tau_{\text{had-vis}}$  reconstruction efficiency uncertainty is derived from comparisons between simulations using different detector geometries or GEANT4 physics lists; this uncertainty is parameterised as a function of true  $\tau_{\text{had-vis}}$   $p_T$  and is between 1% and 1.5%. For the  $\tau_{\text{had-vis}}$  energy scale, the total uncertainty is in the range of 1% to 4%, arising from a combination of measurements: a direct measurement with  $Z \rightarrow \tau\tau \rightarrow \mu\tau_{\text{had-vis}} + 3\nu$  events, measurements of the calorimeter response to single particles, and comparisons between simulations using different detector geometries or GEANT4 physics lists. This uncertainty is also parameterised as a function of the  $\tau_{\text{had-vis}}$   $p_T$  and the number of associated tracks.

The uncertainties in the background modelling include uncertainties in the top-quark,  $Z$ +jets and diboson backgrounds, as well as multijet events in which quark- or gluon-initiated jets are misidentified as a  $\tau_{\text{had}}$ . Among the background modelling uncertainties, the ones related to the top-quark background have the largest impact on the analysis sensitivity, with an impact on the results in the range of 40–50% depending on the LQ coupling and mass values. This uncertainty is extracted by comparing nominal and alternative  $t\bar{t}$  and single top-quark MC samples in the phase space of the SR and Top-CR. For each sample, a dedicated data-driven  $S_T$ -dependent correction is applied before the comparison. The difference between the nominal and alternative samples in the  $S_T$  distribution is taken as the uncertainty in the top-quark processes. The alternative samples have variations of the initial/final-state radiation, matrix element and PS compared to the nominal sample. To derive the initial/final-state radiation uncertainty, the generator parameters used to produce the nominal samples are varied. The matrix element to PS NLO matching uncertainty is derived by comparing the MADGRAPH5\_AMC@NLO and POWHEG predictions while keeping the same generator for the PS component. For the PS, the uncertainty is derived by a comparison with an alternative sample generated by using HERWIG for the PS while keeping the same generator for the hard-scattering simulation component. The uncertainties in the background modelling originating from the PDF and  $\alpha_S$  uncertainties are found to be less than 1% and are neglected. Finally, an uncertainty in the  $tW$  interference for the single top-quark background is estimated by comparing the nominal sample, where the diagram removal scheme is applied, to an alternative sample that uses the diagram subtraction scheme [115].

The uncertainties in the signal modelling include those from the signal cross-section and acceptance due to renormalisation scale ( $\mu_R$ ) and factorisation scale ( $\mu_F$ ) variations, PDF and  $\alpha_S$ . The  $\mu_R$  and  $\mu_F$  uncertainties are estimated through an envelope of the variations obtained from scaling  $\mu_R$  and  $\mu_F$  by a factor between 0.5 and 2, while keeping their ratio between 0.5 and 2. The uncertainties due to the NNPDF3.0<sub>NLO</sub> PDF set and  $\alpha_S$  are evaluated following the PDF4LHC recommendation [116].

Table 5: Post-fit background yields in the high  $b$ -jet  $p_T$  signal region of  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels. ‘Jet $\rightarrow\tau$  fake’ indicates the events with a true lepton and a quark- or gluon-initialized jet misidentified as a  $\tau_{\text{had}}$ . The ‘Two jet $\rightarrow\tau$  fake’ indicates the events where two jets are misidentified as  $\tau_{\text{had}}$ . ‘Others’ in  $\tau_{\text{lep}}\tau_{\text{had}}$  includes  $Z(\rightarrow\tau\tau)$ +LF jets, diboson,  $W$ +jets and  $Z(\rightarrow ee, \mu\mu)$ +jets while ‘Others’ in  $\tau_{\text{had}}\tau_{\text{had}}$  includes  $Z(\rightarrow\tau\tau)$ +LF jets, diboson and  $W$ +jets. The results are extracted from a fit assuming the background-only hypothesis.

Process	$\tau_{\text{lep}}\tau_{\text{had}}$	$\tau_{\text{had}}\tau_{\text{had}}$
$t\bar{t}$	764 $\pm$ 82	9.9 $\pm$ 2.6
Single top	65 $\pm$ 35	3.9 $\pm$ 1.0
Jet $\rightarrow\tau$ fake	215 $\pm$ 79	3.9 $\pm$ 1.0
Two jet $\rightarrow\tau$ fake	–	1.34 $\pm$ 0.27
$Z(\rightarrow\tau\tau)$ +HF jets	5.5 $\pm$ 0.4	4.6 $\pm$ 1.1
Others	9.7 $\pm$ 1.0	1.75 $\pm$ 0.30
Total	1059 $\pm$ 51	25.4 $\pm$ 4.9
Data	1053	29

## 8 Results

The distribution of the  $S_T$  variable for the events of the signal regions, defined in Tables 3 and 4 for the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels, is used as final discriminant between the leptoquark signal and the background. The statistical analysis of the data is performed using the profile likelihood ratio method [117], to test whether a model can be rejected given the observed data. As the model under test is a signal plus background hypothesis, the chosen parameter of interest is the signal strength,  $\mu$ , defined as the ratio of the observed to the predicted value of the signal cross-section times branching fraction. The likelihood function  $\mathcal{L}(\mu, \theta)$  is then constructed as a product of Poisson probability terms for each bin of the distributions. It depends on  $\mu$  and on the nuisance parameters  $\theta$ , which encode systematic uncertainties that can affect the signal and background distributions and are constrained using Gaussian probability density functions. The asymptotic approximation is used when constructing the test statistic  $\tilde{q}_\mu$  [118] from the likelihood ratio, defined as  $\tilde{q}_\mu = -2 \ln(\mathcal{L}(\mu, \hat{\theta})/\mathcal{L}(\hat{\mu}, \hat{\theta}))$  where  $\hat{\mu}$  and  $\hat{\theta}$  are the parameters that define the global maximum-likelihood function and  $\hat{\theta}$  are the nuisance parameters that give the maximum likelihood for a given value of  $\mu$ . To ensure a reliable estimation of the backgrounds in the fit model, the binning in  $S_T$  is optimised so that sufficient background events (greater than 10) are present in each bin of the pre-fit distribution. No significant excess above the background expectations is observed and corresponding limits on production cross-sections of the LQ signals are set.

For the LQ results interpretation, only the high  $b$ -jet  $p_T$  signal regions from the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels are considered and fit simultaneously. For the high  $b$ -jet  $p_T$  signal regions, the contribution from the non-resonant LQ production process is small. Therefore the interference between the LQ non-resonant processes and the SM processes is not expected to be substantial in these SRs, and it is neglected. By setting  $\mu = 0$  in the profile likelihood ratio, the test statistic can be used to check for compatibility with the background-only hypothesis. The data are first fit under the background-only hypothesis and the resulting post-fit distributions are found to be in good agreement with the data, as shown in Figure 5. Table 5 shows the yields for the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels, respectively.

As good agreement is found between the data and the background expectation, upper limits are set on the

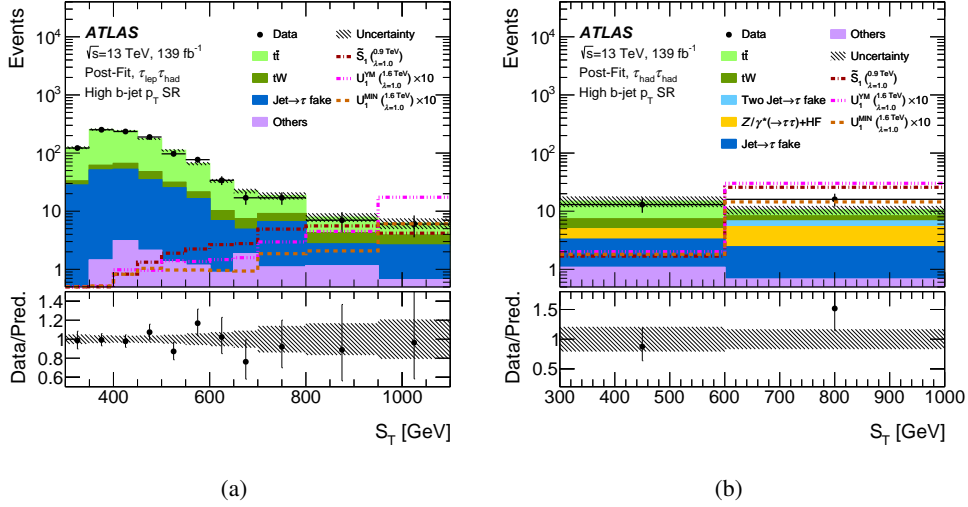


Figure 5: Post-fit distributions of the discriminating variable  $S_T$  in the high  $b$ -jet  $p_T$  signal region for the (a)  $\tau_{\text{lep}}\tau_{\text{had}}$  and (b)  $\tau_{\text{had}}\tau_{\text{had}}$  channels. The two channels are fit simultaneously considering the background-only hypothesis. The lower panels show the ratio of the data to the predictions, where the uncertainty band includes both statistical and systematic post-fit errors. Entries with values above the  $x$ -axis range are included in the last bin of each distributions. For illustrative purposes, the dotted lines show the expectation from three singly produced scalar and vector LQ signals.

cross-section assuming that the branching fraction  $\mathcal{B}(\text{LQ} \rightarrow b\tau)$  is 100% in the case of the  $\tilde{S}_1$  model and 50% for the  $U_1^{\text{YM}}$  and  $U_1^{\text{MIN}}$  scenarios. This is performed using the frequentist  $\text{CL}_s$  method [117]. A production cross-section for a given signal scenario is excluded at the 95% confidence level (CL) when  $\text{CL}_s < 0.05$ .

The results are interpreted considering all LQ production modes in the  $U_1$  model. Several values of the coupling  $\lambda$  are considered, each one with a value of the coupling parameter  $\kappa$  of 0 or 1. The exclusion limits for the single plus non-resonant plus pair vector LQ production are shown in Figure 6. The behaviour of the upper limits as a function of  $m_{\text{LQ}}$  reflects the signal acceptance times efficiency of the analysis. Figure 7 shows the vector LQ limits in the  $\lambda - m_{\text{LQ}}$  plane for each of the  $\kappa$  coupling values considered.

The same procedure is used to interpret the results for single and pair production of scalar LQs from the  $\tilde{S}_1$  model. The single  $\tilde{S}_1$  production and the combined single plus non-resonant plus pair  $\tilde{S}_1$  production are considered. The 95%  $\text{CL}_s$  limits on the  $\tilde{S}_1$  production cross-section are derived as a function of LQ mass for various assumptions on the coupling  $\lambda$  value. The single plus non-resonant plus pair  $\tilde{S}_1$  production result is shown in Figure 8. The exclusion limits in the  $\lambda - m_{\text{LQ}}$  plane are shown in Figure 9.

The observed and expected limits on the LQ mass for the various signal production modes considered are reported in Table 6. This analysis is the first ATLAS result for the search of singly produced LQs in the  $b\tau\tau$  final state. Vector LQs in the  $U_1$  Yang-Mills (Minimal coupling) model are excluded below masses of 1.56 (1.29) TeV for all  $\lambda$  values;  $\tilde{S}_1$  masses below 1.26 TeV are excluded for all  $\lambda$  values. The observed limits obtained are less stringent than the expected limits, which is mostly driven by the higher data yields relative to the predicted yields in the highest  $S_T$  bin in the  $\tau_{\text{had}}\tau_{\text{had}}$  channel. Overall the  $\tau_{\text{had}}\tau_{\text{had}}$  channel is more sensitive than the  $\tau_{\text{lep}}\tau_{\text{had}}$  channel due to the smaller background and the larger signal to background



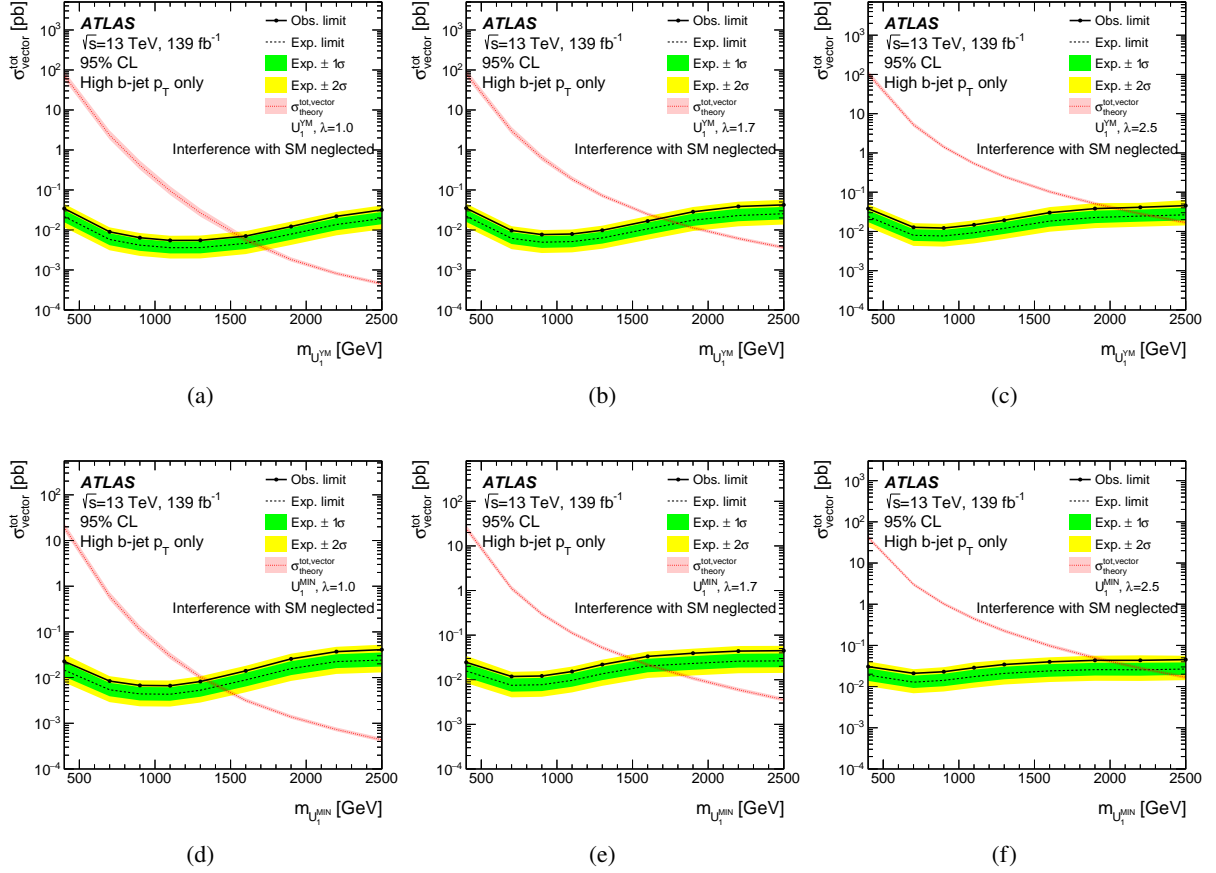


Figure 6: Observed (solid line) and expected (dashed line) 95% CL upper limits on the cross-section of single non-resonant plus pair vector LQ production from the combination of the high  $b$ -jet  $p_T$  signal region for the  $\tau_{1ep}\tau_{had}$  and  $\tau_{had}\tau_{had}$  channels. The dotted curve indicates the total theoretical predictions for singly, non-resonant and pair-produced vector LQ at LO. The top row shows the  $U_1^{YM}$  model ( $\kappa = 0$ ) with (a)  $\lambda = 1.0$ , (b)  $\lambda = 1.7$  and (c)  $\lambda = 2.5$ . The bottom row shows the  $U_1^{MIN}$  model ( $\kappa = 1$ ) with (d)  $\lambda = 1.0$ , (e)  $\lambda = 1.7$  and (f)  $\lambda = 2.5$ .

Table 6: Observed (expected) 95% lower limits on the LQ mass in high  $b$ -jet  $p_T$  signal region for the singly plus non-resonant and singly plus non-resonant plus pair produced LQs. All limits are reported in TeV.

Model	$\lambda = 1.0$	$\lambda = 1.7$	$\lambda = 2.5$
Single+non-resonant $U_1^{YM}$ production	1.31 (1.43)	1.59 (1.73)	2.03 (2.27)
Single+non-resonant $U_1^{MIN}$ production	1.15 (1.24)	1.45 (1.58)	1.98 (2.26)
Single+non-resonant+pair $U_1^{YM}$ production	1.58 (1.64)	1.70 (1.81)	2.05 (2.28)
Single+non-resonant+pair $U_1^{MIN}$ production	1.35 (1.44)	1.52 (1.63)	1.99 (2.26)
Single+non-resonant $\tilde{S}_1$ production	1.04 (1.11)	1.26 (1.38)	1.49 (1.62)
Single+non-resonant+pair $\tilde{S}_1$ production	1.28 (1.37)	1.38 (1.49)	1.53 (1.67)

ratio in the last  $S_T$  bin. This difference arises from the larger  $t\bar{t}$  background for the  $b\tau_{1ep}\tau_{had}$  final state in the most sensitive part of the  $S_T$  spectrum.

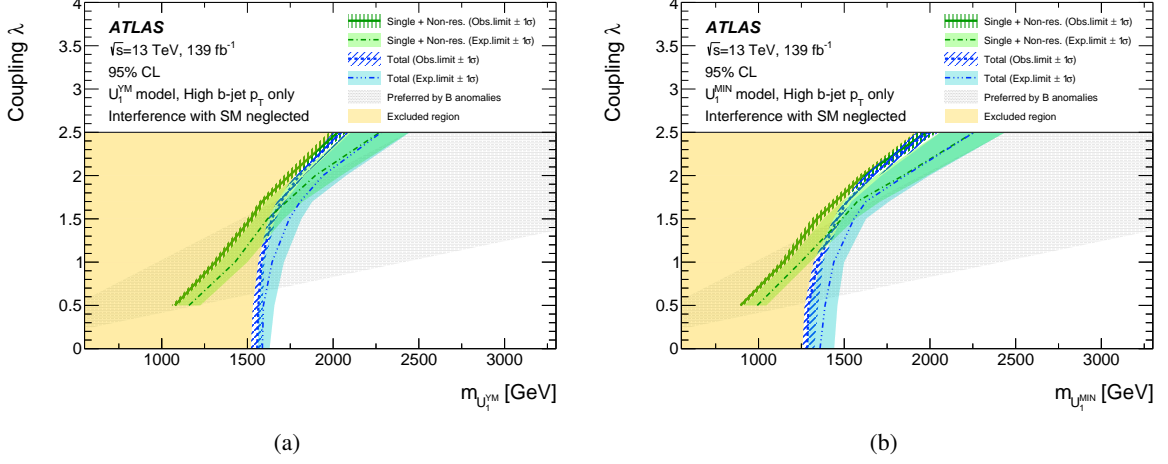


Figure 7: The two-dimensional 95% CL exclusion limits in the  $\lambda - m_{LQ}$  plane for singly plus non-resonant produced vector LQ (green lines) and for the sum, referred as *Total*, of single plus non-resonant plus pair vector LQ production (blue lines), with (a) showing the case with  $\kappa = 0$  and (b) the case with  $\kappa = 1$ . Regions to the left of the lines are excluded. The dotted area shows the preferred region where the chosen LQ model can explain observed  $B$  anomalies [119].

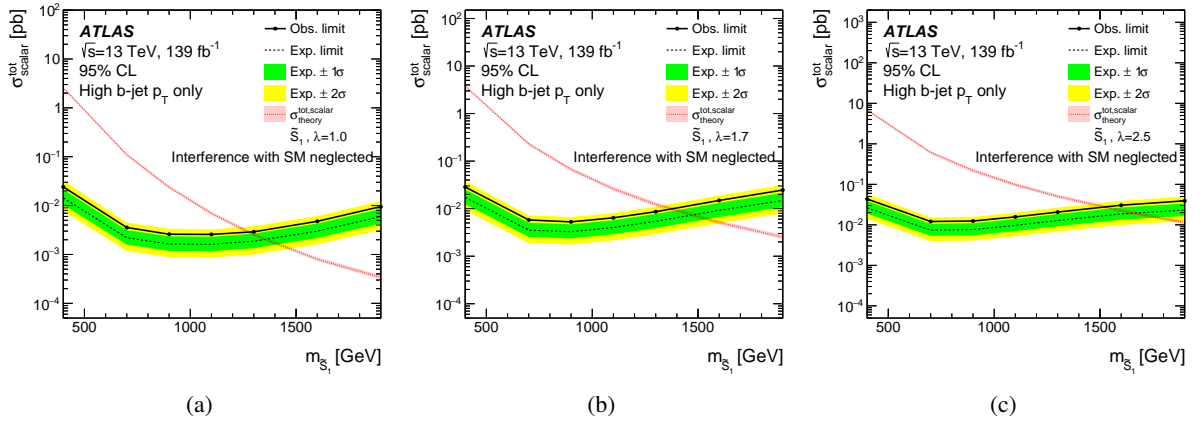


Figure 8: Observed (solid line) and expected (dashed line) 95% CL upper limits for (a)  $\lambda = 1.0$ , (b)  $\lambda = 1.7$  and (c)  $\lambda = 2.5$  on the cross-section of single plus non-resonant plus pair  $\tilde{S}_1$  production hypotheses from the combination of the high  $b$ -jet  $p_T$  signal region for the  $\tau_{ep}\tau_{had}$  and  $\tau_{had}\tau_{had}$  channels. The dotted curve indicates the total theoretical predictions for singly, non-resonant and pair-produced scalar LQ. The prediction for singly plus non-resonant produced  $\tilde{S}_1$  (pair-produced  $\tilde{S}_1$ ) is calculated at LO (NNLO+NNLL).

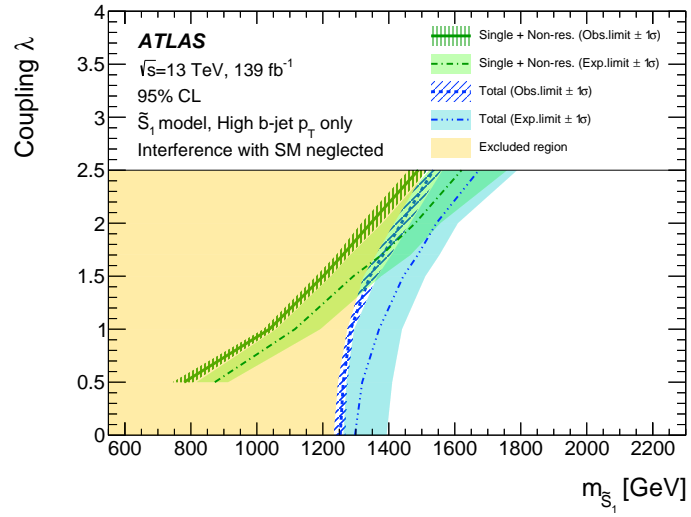
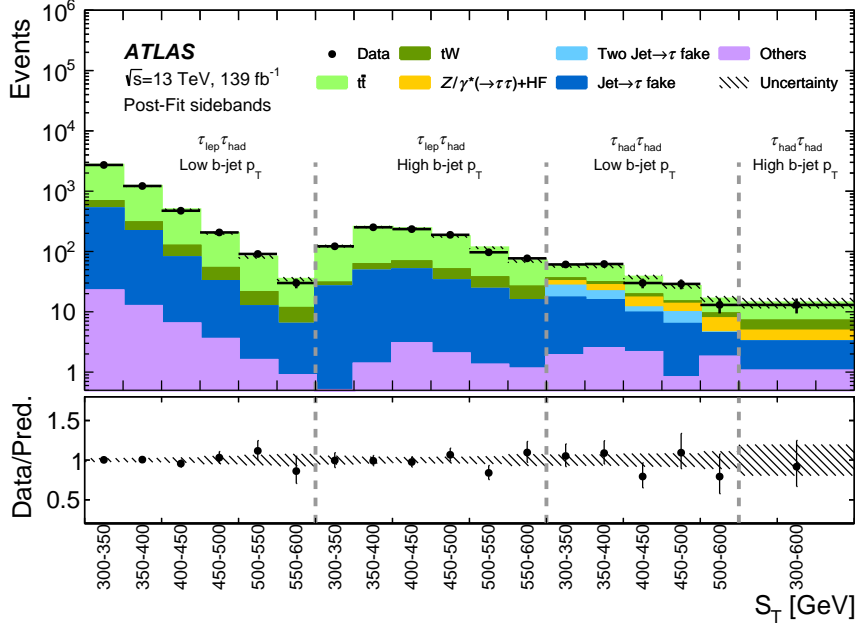


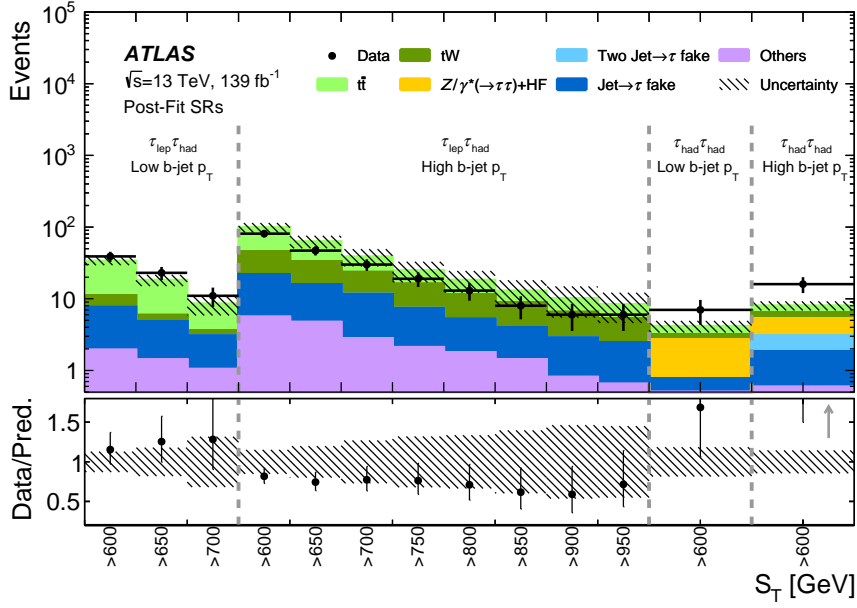
Figure 9: The two-dimensional 95% CL exclusion limits in the  $\lambda - m_{LQ}$  plane for singly plus non-resonant produced  $\tilde{S}_1$  (green lines) and for the sum, referred as *Total*, of single plus non-resonant plus pair vector LQ production (blue lines). Regions to the left of the lines are excluded.

An additional model-independent search considering both the high and low  $b$ -jet  $p_T$  signal regions in the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels is performed. For each of these regions, the events with  $S_T < 600$  GeV form a sideband region, while a signal region is defined by counting the number of events with a  $S_T$  value above a variable threshold. Four sideband regions, one for each channel and for each  $b$ -jet  $p_T$  signal region, are fit simultaneously considering the background-only hypothesis. The fit results are then used to predict the background contribution in the signal region. Figure 10 shows the post-fit distributions of the  $S_T$  variable in the sideband region and the background composition in each channel as a function of the  $S_T$  lower bound threshold used to define the signal regions.

Since no significant excess is observed in any of the signal regions, a signal-plus-background fit is performed considering a generic signal in the signal region. As for the LQs search, the parameter of interest of the statistical analysis is the signal strength  $\mu$ , and the results are translated into upper limits on the number of signal events and, dividing them by the integrated luminosity, they can be expressed in terms of upper limits on the visible cross-section,  $\sigma_{\text{vis}}$ . Figure 11 shows the limit values of the visible cross-section as a function of  $S_T$  lower bound threshold in each signal category. The visible cross-section limits can be reinterpreted as limits on specific physics models as long as the selection efficiency and acceptance of the model (including any uncertainties in these values) for a specific signal region definition used in this analysis is known. By dividing the visible cross-section limits given here by this efficiency and acceptance, upper limits on the cross-section can be derived.



(a)



(b)

Figure 10: (a) Post-fit distributions of the discriminating variable  $S_T$  in the sideband regions for the high and low  $b$ -jet  $p_T$  signal regions for the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels. The distributions are fit simultaneously considering the background-only hypothesis. (b) Observed and predicted yields as function of the  $S_T$  threshold used to define the signal regions for the high and low  $b$ -jet  $p_T$  signal regions for the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels. The results have been extracted by projecting the results from the fit to the sideband regions assuming the background-only hypothesis in the context of the model-independent search. The lower panel shows the ratio of the data to the predictions.

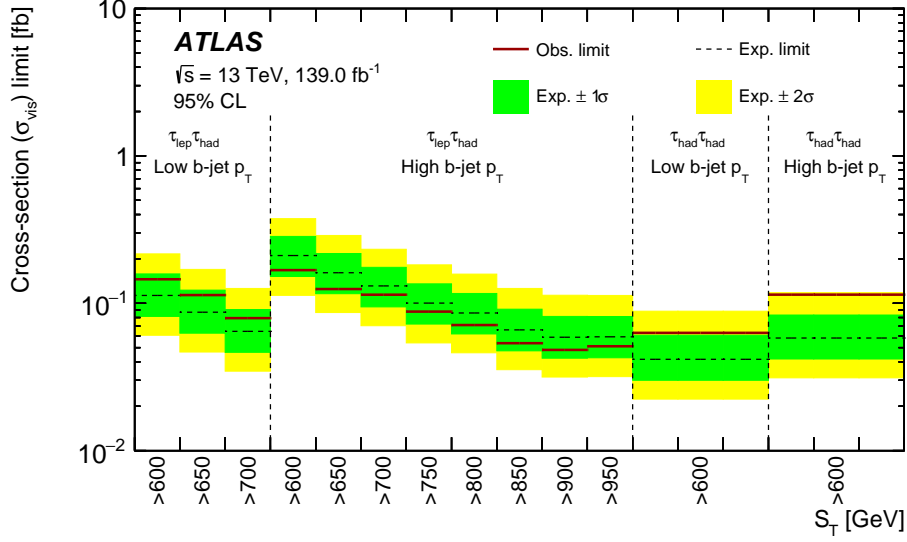


Figure 11: Observed (solid line) and expected (dashed line) 95% upper limits on the visible cross-section,  $\sigma_{\text{vis}}$ , obtained from the model-independent search by a signal-plus-background fit in the high and low  $b$ -jet  $p_T$  signal regions for the  $\tau_{\text{lep}}\tau_{\text{had}}$  and  $\tau_{\text{had}}\tau_{\text{had}}$  channels.

## 9 Conclusion

A search for scalar and vector leptoquarks is performed in the  $b\tau\tau$  final state using  $pp$  collision data at  $\sqrt{s} = 13$  TeV recorded by the ATLAS detector at the LHC from 2015 to 2018 corresponding to an integrated luminosity of  $139 \text{ fb}^{-1}$ . Final states including one leptonic and one hadronic  $\tau$ -lepton decay or two hadronic  $\tau$ -leptons decays are considered. In each of these two final states, events are classified, based on the  $p_T$  of the  $b$ -jet, in two signal regions of low and high  $b$ -jet  $p_T$ . The benchmark model is  $U_1$  for vector leptoquarks in the Yang–Mills or Minimal coupling scenarios with  $\lambda$  between 0.5 and 2.5. For scalar leptoquarks the benchmark model is  $\tilde{S}_1$ , with values of the  $\lambda$  parameter ranging between 0.5 and 2.5.

Upper limits at 95% CL on the cross-section for leptoquarks produced via either single plus non-resonant production, or considering all production modes (including pair production), and decaying into  $b\tau$  are set. The results have been extracted considering only the high  $b$ -jet signal region and the combination of both final states. For the Yang–Mills coupling, the observed (expected) lower limits on the leptoquark mass are 1.58 (1.64) TeV for  $\lambda = 1.0$ , 1.70 (1.81) TeV for  $\lambda = 1.7$ , and 2.05 (2.28) TeV for  $\lambda = 2.5$ , considering all leptoquark production modes. In the Minimal coupling case, considering all leptoquark production modes, the lower limits are 1.35 (1.44) TeV for  $\lambda = 1.0$ , 1.52 (1.63) TeV for  $\lambda = 1.7$  and 1.99 (2.26) TeV for  $\lambda = 2.5$ . The observed (expected) lower limits, considering all leptoquark production modes in the  $\tilde{S}_1$  model, are 1.28 (1.37) TeV for  $\lambda = 1.0$ , 1.38 (1.49) TeV for  $\lambda = 1.7$  and 1.53 (1.67) TeV for  $\lambda = 2.5$ .

An interpretation of the results in a model-independent scenario is also performed for each of the signal region categories. The 95% confidence level limits on the visible cross-section vary between 0.17 fb and  $4.8 \cdot 10^{-2}$  fb as function of the event variable  $S_T$  ranging from  $S_T > 600$  GeV to  $S_T > 950$  GeV.



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