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Search for single-production of vector-like quarks decaying into Wb in the fully hadronic final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

A search for T and Y vector-like quarks produced in proton–proton collisions at a centre-of-mass energy of 13 TeV and decaying into Wb in the fully hadronic final state is presented. The search uses 139 fb^{-1} of data collected by the ATLAS detector at the LHC from 2015 to 2018. The final state is characterised by a hadronically decaying W boson with large Lorentz boost and a b-tagged jet, which are used to reconstruct the invariant mass of the vector-like quark candidate. The main background is QCD multijet production, which is estimated using a data-driven method. Upon finding no significant excess in data, mass limits at 95% confidence level are obtained as a function of the global coupling parameter, κ. The observed lower limits on the masses of Y quarks with $\kappa = 0.5$ and $\kappa = 0.7$ are 2.0 TeV and 2.4 TeV, respectively. For T quarks, the observed mass limits are 1.4 TeV for $\kappa = 0.5$ and 1.9 TeV for $\kappa = 0.7$.

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Contents

1 Introduction

The discovery of the Higgs boson [1, 2] at the Large Hadron Collider (LHC) and measurements of its width, in combination with previous experimental results, have significantly constrained the possibility of a fourth generation of chiral quarks within the Standard Model of particle physics (SM) [3]. Although the SM has been tested to high precision, certain theoretical questions still persist. One of them, the Higgs boson mass hierarchy problem, is related to the fact that the non-cancellable radiative corrections to the Higgs boson mass are proportional to the square of the 'cut-off' in the SM (the Planck scale, 10^{19} GeV), whereas the observed Higgs boson mass is 125 GeV [4, 5]. The largest contributions to these corrections originate from the loop interactions of the Higgs boson with the top quark. Various proposed beyond-the-SM (BSM) theories solve this problem by cancelling out these corrections via interactions with hypothetical particles. Vector-like quarks (VLQs) are one of those types of hypothetical spin-1/2 colour triplets. Unlike SM chiral quarks, their left- and right-handed components transform similarly under SM gauge transformations. Consequently, since VLQs do not acquire their mass via the Higgs mechanism, Higgs boson measurements do not constrain the mass of these quarks. VLQs appear in BSM models such as composite Higgs model [6] and little Higgs models [7–9]. Phenomenological renormalisable VLQ models [10] predict the existence of VLQ multiplets with fractional charges. In these models [10–13], VLQs couple primarily to the third-generation SM quarks via the SM gauge bosons. Most VLQ searches

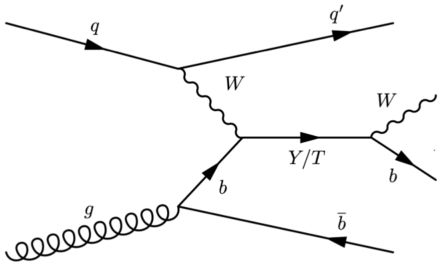


Figure 1: Leading-order Feynman diagram for the $T/Y \to Wb$ process.

in the current search programme at the LHC probe the qV decay modes, where $V = W/Z/H$ bosons and q = top (t) or bottom (b) quarks.

In this paper, a search for T and Y VLQs decaying into a Wb final state is performed using proton–proton (pp) collisions in which the probed signal is produced via Wb fusion. The T VLQ has an electric charge of $+(2/3)e$ and occurs in singlet, doublet, and triplet representations, whereas the Y VLQ with an electric charge of $-(4/3)e$ appears in doublet and triplet representations. In the final state studied here, the W boson decays hadronically. Whereas previous searches for $pp \to T/Y(\to Wb)qb + X$ have used the semileptonic final state, this is the first search using the hadronic ($W \to q\bar{q}$) decay mode. A typical lowest-order Feynman diagram for this signal process is shown in Figure 1. In the mass range relevant for this paper, the contribution from the t-channel diagram is negligible for this process [14].

The Y quark decays solely into a Wb topology with a branching fraction ($\mathcal{B}$) of 100%. The Y quark appears alongside the B VLQ, which has an electric charge of $-(1/3)e$, in the (B, Y) doublet and alongside both the B and T quarks in the (T, B, Y) triplet. The T singlet also decays via the Zt and Ht modes. The relative branching fractions are mass dependent, but for quark masses greater than 1 TeV they have a ratio of $\mathcal{B}(Wb/Zt/Ht) = 2:1:1$ [10]. The cross-section for pair-production processes is higher at lower VLQ masses; however, single-production processes start to dominate at higher masses, e.g. around 1 TeV for a coupling of 0.5. Additionally, since the production cross-section is proportional to the global coupling parameter κ, VLQ searches in the single-production mode can probe this coupling strength [12, 15]. The width (Γ) of a VLQ signal is also affected by κ.

The ATLAS and CMS collaborations have conducted extensive VLQ searches targeting both the single- and pair-production processes. The most stringent lower limits of 1.36 TeV on the mass of pair-produced T singlets arise from a $T\bar{T} \to Wb + X$ search performed using the 13 TeV pp collision data collected in 2015–2018 by the ATLAS Collaboration [16]. Similar single-production searches by ATLAS and CMS [17–27] have set limits on both the mass of the VLQs and model-dependent parameters, e.g. coupling strengths and mixing angles. The limits set on the mixing parameter $\sin\theta_\mathrm{R}$ ($\sin\theta_\mathrm{R} = 2 \cdot \sqrt{2} \cdot \kappa$) in the (B, Y)-doublet interpretation in the $T/Y \to Wb$ search by ATLAS using 2015–2016 data are comparable to limits from electroweak observables in the mass range between 0.9 TeV and 1.25 TeV [17]. In the same search, the Y quark was excluded for all masses less than 1.7 TeV for $\kappa = 0.35$. In a recent result from the ATLAS Collaboration with the 2015–2018 dataset, where a statistical combination of most $T \to Ht$ and $T \to Zt$ searches have been performed, $\kappa > 0.5$ has been excluded for m_T values up to 2.2 TeV [22]. The various limits quoted in this section are at 95% confidence level (CL).

This search for $T/Y \to Wb$ is based on the full Run 2 dataset of pp collisions at a centre-of-mass energy $\sqrt{s} = 13$ TeV collected with the ATLAS detector during 2015–2018, corresponding to an integrated luminosity of 139 fb^{-1}. The large integrated luminosity used allows probing a mass range for the T and Y VLQs from 1.0 TeV to 2.7 TeV and values of κ from 0.1 to 1. Due to the high masses probed in this analysis, the W boson from the VLQ decay is produced with large Lorentz boost. The invariant mass of the VLQ candidate is reconstructed using the hadronically decaying boosted W boson and b-tagged jet present in the final state. Compared to the previous ATLAS search for $T/Y \to Wb$ in the single-lepton channel [17], this search uses almost four times more integrated luminosity, and exploits a different decay mode, thus being complementary to it.

2 ATLAS detector

The ATLAS detector [28] at the LHC covers nearly the entire solid angle around the collision point.[1] It consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadronic 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 $|\eta| < 2.5$. The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit generally being in the insertable B-layer (IBL) installed before Run 2 [29, 30]. It is followed by the SemiConductor Tracker (SCT), 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. Hadronic calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadronic 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.

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

The luminosity is measured mainly by the LUCID–2 [31] detector that records Cherenkov light produced in the quartz windows of photomultipliers located close to the beampipe.

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 [32]. 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 complete events to disk at about 1 kHz.

A software suite [33] 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 Event reconstruction

This paper describes a search for the process $T/Y \to Wb$ where the final state is characterised by a hadronic decay of the boosted W boson. The T/Y VLQ is reconstructed using its decay products: a large-radius (large-R) jet and a small-radius (small-R) jet, both with high transverse momentum (p_{T}).

Primary interaction vertices are reconstructed from at least two tracks with $p_{\mathrm{T}} > 0.5$ GeV. For events with multiple primary vertex candidates, the one where the corresponding tracks have largest sum of squared p_{T} is chosen [34].

Large-R jets are reconstructed from three-dimensional topological clusters [35] of energy deposits in the calorimeter using the anti-k_t algorithm [36, 37] with radius parameter $R = 1.0$. These jets are calibrated to the hadronic energy scale with the local cluster weighting procedure [35]. The jets are then trimmed to reduce contributions from multiple interactions in the same and neighbouring bunch crossings (pile-up) and soft interactions by reclustering the constituents of the jet into $R = 0.2$ subjets with the k_t algorithm [38, 39] and removing constituents originating from subjets with p_{T} less than 5% of the p_{T} of the parent jet. The four-momentum of the large-R jet is recomputed from the four-momenta of the remaining constituents and corrected using Monte Carlo simulation and data [40]. The events used in this search were selected by a set of triggers requiring at least one such large-R jet [41]. This search uses large-R jets with $p_{\mathrm{T}} >$ 500 GeV and $|\eta| < 2.0$ and hence achieves maximum efficiency for these triggers.

Small-R jets are also reconstructed with the anti-k_t algorithm, but using $R = 0.4$ and input constituents constructed by a particle-flow algorithm from calorimeter energy clusters and corresponding tracks in the ID [42]. Jets are calibrated to the particle level using corrections derived from simulation and *in situ* measurements [43]. In this analysis, both 'central' ($|\eta| < 2.5$) and 'forward' ($2.5 < |\eta| < 4.5$) small-R jets are used. For the central small-R jets with $p_{\mathrm{T}} < 60$ GeV, a jet-vertex tagging algorithm is employed to mitigate pile-up by ensuring the jets match the primary collision vertex [44]. The jet-vertex tagging is also performed for the forward jets [45]. The jet-vertex tagger's efficiency, as measured in simulated events, differs from that measured in data and thus the efficiency ratio is used as a per-event correction factor.

The large-R jet is identified as a W boson using a three-variable cut-based W-tagger [46] which is defined using jet substructure variables. The tagger is optimised for two working points (WPs), which are chosen to achieve signal efficiencies of 50% (tight) and 80% (loose), respectively [46]. Both WPs are used in this analysis. Tagging scale factors which quantify the relative tagging-efficiency differences between data and simulation are derived for both signal (W-tagged jets) and background jets (γ+jets / multijets) [47]. The signal scale factors are evaluated using $t\bar{t}$ events in the lepton-plus-jets final state.

In each event, central small-R jets which contain b-hadrons are identified using the DL1r tagging algorithm [48]. This tagger is based on a deep neural network that utilises impact-parameter information from tracks associated with the jet, as well as topological properties of their secondary and tertiary vertices. A 70% efficiency working point for identifying true b-jets in $t\bar{t}$ events is utilised in this paper. Scale factors are applied to account for remaining small tagging-efficiency discrepancies between data and simulation in this analysis [49–51].

This analysis vetoes events containing charged leptons (electrons or muons). Electron candidates are reconstructed from energy deposits in the EM calorimeter matched to charged-particle tracks in the inner detector [52]. The electrons are required to have $p_{\mathrm{T}} > 25$ GeV and $|\eta| < 2.47$, excluding the transition region between barrel and endcap calorimeters ($1.37 < |\eta| < 1.52$), and pass the 'tight' identification criteria [52]. Muon candidates are reconstructed from matching tracks in the ID and the MS [53]. The muons are required to have $p_{\mathrm{T}} > 25$ GeV and $|\eta| < 2.5$, and satisfy the 'medium' identification and 'tight' isolation criteria [53].

4 Simulated event samples

Monte Carlo (MC) simulation events are employed to model signal and background distributions. They undergo full ATLAS detector simulation using Geant4 [54] or a faster simulation with parameterised calorimeter showers [55]. In-time and out-of-time pile-up effects were simulated by overlaying minimum-bias interactions generated with Pythia 8.186 [56], adjusted to match observed pile-up conditions. EvtGen [57] modelled heavy-flavour hadron decays, except for processes generated with Sherpa [58]. Simulated events undergo the same reconstruction and analysis as data events, with small corrections to object selection efficiencies, energy scales, and resolutions are applied for better agreement with data. The main simulation settings for the MC events are discussed in this section. Signal events were generated using the faster simulation, while all SM background MC simulated events were generated with a detailed Geant4 model of the ATLAS detector.

4.1 Simulated signal events

Signal events with single T-quark production were simulated at leading-order (LO) with the MadGraph5_aMC@NLO 2.3.3 event generator [59] using the NNPDF2.3lo [60] parton distribution function (PDF) set. The samples are normalised by multiplying the LO cross-section times branching fraction for given assumed couplings by a correction factor to account for finite-width effects [61, 62], and by a K-factor to correct the LO cross-section to the next-to-leading-order (NLO) prediction computed in the narrow-width approximation [63]. The event generator was interfaced with Pythia 8.212 [64] to model parton showering, hadronisation, and the underlying event with the NNPDF2.3lo [60] PDF set and the A14 [65] set of tuned parameters (tune). The matrix-element calculations are based on the phenomenological model described in Ref. [13], which includes all tree-level processes. It is assumed that the VLQs couple exclusively to SM quarks of the third generation. Events were generated for $T(\rightarrow Wb)qb$ processes at fixed values of κ and the T-quark mass from 1.0 to 2.7 TeV. During the generation process, matrix-element-based event weights [66] were calculated. These weights are subsequently used to reweight the events in each sample to different mass (m) and κ values, effectively creating a grid in the m−κ plane. The overall acceptance times efficiency for T-quark signal events with a mass of 1.6 TeV and $\kappa = 0.5$ is 1.7%, following the kinematic cuts in the signal region described in Section 5. The Y-quark signals were not simulated separately, as the

Y-quark distributions can be obtained by multiplying the T-quark yield by a factor of two, to account for the larger branching fraction to Wb.

4.2 Simulated background events

The main background in this search comes from QCD multijet production. It is modelled using a data-driven method, with MC-based corrections to account for possible correlations inherent in the method, as detailed in Section 6. The other SM background contributions are estimated using MC simulations.

The modelling of $t\bar{t}$ events utilised the next-to-leading-order (NLO) Powheg Box v2 [67–69] generator and the NNPDF3.0nlo [70] PDF set. The events were then interfaced with Pythia 8.230, which employed the NNPDF2.3lo PDF set and the A14 tune. To regulate the effects of high-p_{T} radiation and achieve appropriate matrix element to parton shower matching, the h_{damp} parameter in Powheg Box was set to $1.5\,m_t$ [71], where $m_t = 172.5$ GeV. Corrections were applied to the top-quark kinematics to account for NLO electroweak effects and next-to-next-to leading-order (NNLO) QCD effects [72]. To ensure proper normalisation, the events were scaled to the cross-section computed at NNLO in QCD, incorporating the resummation of next-to-next-to-leading logarithmic soft gluon terms, using Top++ 2.0 [73–79].

The generation of single-top-quark events involving Wt-, t-, and s-channel processes utilised Powheg Box v2 and the NNPDF3.0nlo PDF set. Parton showering, hadronisation, and the underlying event were modelled by Pythia 8.230, using the NNPDF2.3lo PDF set and the A14 tune. To address interference between the $t\bar{t}$ and Wt final states, the 'diagram removal' (DR) scheme [80, 81] was employed. Uncertainties in modelling the interference are estimated by comparing this sample with an alternative sample generated with the 'diagram subtraction' (DS) scheme [81, 82].

The Sherpa 2.2.8 generator [83] was used to model W/Z+jets events. The matrix-element calculation incorporates up to two partons at NLO and up to four partons at LO. The merging of the matrix-element calculation with the Sherpa parton shower was achieved using the MEPS@NLO prescription [84]. The NNPDF3.0nnlo [70] PDF set was used for the matrix-element calculation. To estimate the modelling uncertainty, an alternative W+jets sample was generated using Sherpa 2.2.8, where the modelling of hadronisation is based on the Lund string model [85, 86].

5 Analysis strategy

This analysis searches for T/Y VLQs decaying into a W boson and a b-quark, where the W boson decays hadronically. Since the probed VLQs are in the TeV mass range, the W boson is boosted and thus its decay products have low angular separation and are reconstructed as a single large-R jet. The main background comes from QCD multijet production and is estimated using a data-driven method. For this estimation, four control regions, one validation region, and one signal region are defined. The reconstructed invariant mass of the VLQ (m_{VLQ}) is the discriminating variable for this analysis. For each event in the six analysis regions, m_{VLQ} is defined as the magnitude of the vector sum of the four momenta of the leading (highest-p_{T}) large-R jet and the leading small-R jet that has an angular separation of $\Delta R > 1$ from the leading large-R jet. This is motivated by the fact that a T/Y VLQ with mass greater than 1 TeV would decay into two objects with a large angular separation. The validation region is used to validate the data-driven estimate of the multijet background. Finally, the estimated multijet background, and other SM backgrounds estimated using MC simulation, are used in a binned maximum-likelihood fit in the signal region to search for a T/Y signal in the $m-\kappa$ plane.

5.1 Event preselection

Events of interest are required to have no charged leptons, as defined in Section 3, and at least one large-R jet and at least one small-R jet that do not overlap with each other. The definition of m_{VLQ} for each event ensures an angular separation of $\Delta R > 1$ for the leading small-R jet and the leading large-R jet. Signal events are expected to be characterised by the presence of high-p_{T} jets in the final state. The leading large-R jet is required to have $p_{\mathrm{T}} > 500$ GeV and the leading central small-R jet is required to have $p_{\mathrm{T}} > 350$ GeV. Events are required to contain at least one forward jet with $p_{\mathrm{T}} > 40$ GeV. This ensures considerable suppression of the multijet background. These kinematic cuts are henceforth referred to as the 'preselection'.

5.2 Event categorisation

Events passing the preselection are separated into six analysis regions: four control regions, one validation region, and one signal region. The control and validation regions are defined for the sole purpose of estimating the pre-fit multijet background using the data-driven method as described in Section 6. The control and validation regions are not used in the statistical fits.

The region categorisation is defined with two orthogonal kinematic variables, namely the b-jet multiplicity and the W-tagging WPs of the three-variable W-tagger, as shown in Figure 2. The b-jet multiplicity is calculated using b-jets defined in Section 3. Although the variables are expected to be nearly orthogonal, any departure from this ideal is accounted for in the analysis.

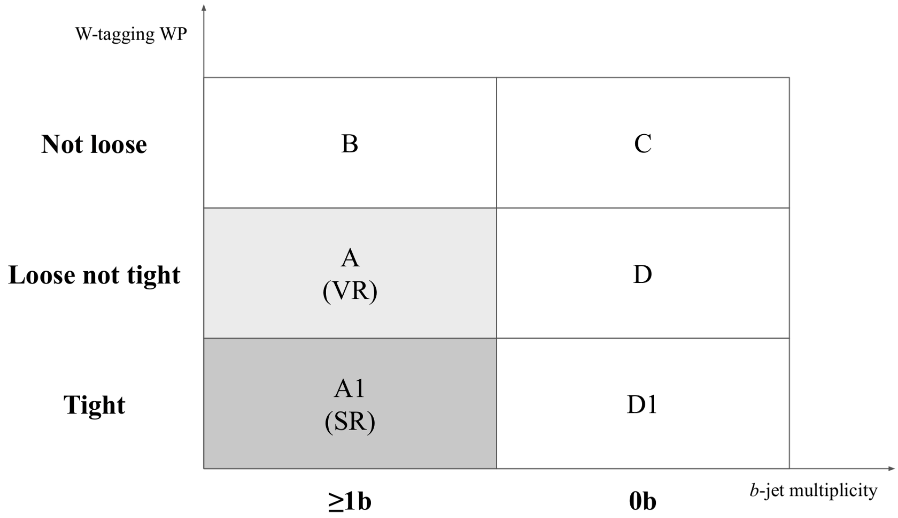


Figure 2: A representation of the signal, validation, and control regions. Region A1 is the signal region; region A is the validation region and the other four regions B, C, D, and D1 are the control regions.

Signal region Events in the signal region (SR) A1 in Figure 2 have at least one b-jet and the leading large-R jet is W-tagged using the tight WP (50% tagging efficiency). The strict requirement on the tagging efficiency improves the suppression of light-flavour multijet background events.

Validation region The validation region (VR) A is defined so as to be kinematically close to the signal region, yet orthogonal to it. Events in region A similarly contain at least one b-jet but the leading large-R jet is required to be loosely but not tightly W-tagged, i.e. these events contain a leading large-R jet that is W-tagged at the 80% WP but not at the 50% WP, thus making VR A orthogonal to SR A1.

Control regions The four control regions (CR) B, C, D, and D1 are used to constrain the shape and normalisation of the m_{VLQ} distribution of the background processes in the SR A1 and VR A. The CR B contains only events which have at least one b-jet and a leading large-R jet that is not W-tagged by the loose selection (80% WP). The three CRs C, D, and D1 contain only events that do not have any b-jets. These three regions are distinguished by their W-tagging WP requirements. The event yields in the four regions are ranked in descending order as follows: C, B, D, and D1.

For two different T-quark signals, one with mass 1.1 TeV and $\kappa = 0.25$ and the other with mass 1.5 TeV and $\kappa = 0.45$, the signal-to-background ratio is highest in the signal region and negligible in the validation and control regions. The S/B and $S/\sqrt{B}$ ratios for a 1.1 TeV signal with $\kappa = 0.25$ are 2.6% and 3.9 in the SR A1 and 0.5% and 1.8 in the VR A respectively. For a T-quark signal with mass 1.5 TeV and $\kappa = 0.45$, the S/B and $S/\sqrt{B}$ ratios are 4.8% and 5.2 in the SR A1 and 0.8% and 2.5 in the VR A respectively. In all four CRs, the S/B and $S/\sqrt{B}$ ratios for these two simulated signals are less than 0.1% and 1 respectively.

6 Data-driven estimation of the multijet background

QCD multijet production is the dominant source of background in this search. The shape and normalisation of the m_{VLQ} template for multijet events in the SR A1 and VR A in Figure 2 are estimated using a data-driven method similar to those used in Refs. [18, 87, 88]. In this method, two weakly correlated variables are used to construct the control regions. The central assumption behind the success of this method is that these control regions are pure in multijet events and have negligible non-multijet SM background contamination. Here, the multijet contribution in each bin of the m_{VLQ} distribution in SR A1 (VR A) is estimated from the multijet background in control regions B, C, and D1 (D). The projected estimate of the multijet background in a given bin i of the m_{VLQ} distribution results from the subtraction of SM MC backgrounds ($t\bar{t}$, single-top-quark, W/Z+jets) from the observed data events in each corresponding bin. Thus, the data-driven estimate for each bin i in SR A1 (VR A) can be written as

$$N_{\text{A/A1}}^{\text{multijet estimate}}[i] = R_{\text{corr}}[i] \times (N_{\text{B}}^{\text{Data}}[i] - N_{\text{B}}^{\text{SM MC backgrounds}}[i]) \times \frac{(N_{\text{D/D1}}^{\text{Data}}[i] - N_{\text{D/D1}}^{\text{SM MC backgrounds}}[i])}{(N_{\text{C}}^{\text{Data}}[i] - N_{\text{C}}^{\text{SM MC backgrounds}}[i])}\,.$$

The bin-by-bin correction factor $R_{\text{corr}}[i]$ reflects the possible correlation between the two kinematic variables, i.e. the b-jet multiplicity and W-tagging WP. The $R_{\text{corr}}[i]$ for SR A1 are calculated from the bin-by-bin ratios of simulated multijet events in the m_{VLQ} distributions for the regions specified below in Eq. (1). The overall normalisation of the m_{VLQ} distribution of the simulated multijet events in each of the four regions (A1, B, C, and D) is scaled to the estimated yield in data. This scaling is done using two single-bin likelihood fits. In the first fit, the overall normalisation of the simulated multijet events is scaled to the data yields by fixing the normalisation of other SM backgrounds for the m_{VLQ} distributions in regions A1 and B simultaneously. Similarly, the second fit fixes the normalisation of those SM backgrounds in regions C and D1 simultaneously. The normalisation scaling corrects for any mismodelling in the simulated multijet samples. The correction factor for the signal region A1 can be written as

$$R_{\text{corr}}[i] = \frac{N_{\text{A1}}^{\text{R}}[i]}{N_{\text{B}}^{\text{R}}[i]} \times \frac{N_{\text{C}}^{\text{R}}[i]}{N_{\text{D1}}^{\text{R}}[i]}\,. \tag{1}$$

Here, $N_{\text{A1/B/C/D1}}^{\text{R}}$ denotes the normalisation-scaled multijet yields in the four regions that are used to calculate R_{corr}. The corresponding $R_{\text{corr}}[i]$ for VR A is calculated by replacing N_{A1}^{R} with N_{A}^{R}, and N_{D1}^{R} with N_{D}^{R}, in Eq. (1). For this calculation of R_{corr} for VR A, the overall normalisations of the simulated multijet events are scaled to data yields by fitting regions A and B together and regions C and D together. These two single-bin fits are performed using the methodology described above for the corresponding fits for $R_{\text{corr}}[i]$ in SR A1. Thus in Eq. (1) the multijet events in each bin i of regions A1 and B are scaled by one normalisation factor, and another normalisation factor is applied bin-by-bin in regions C and D1.

The value of $R_{\text{corr}}[i]$ impacts the final multijet m_{VLQ} distribution for both SR A1 and VR A. To mitigate any statistical fluctuations in the R_{corr} distribution as a function of m_{VLQ}, a third-degree polynomial fit to the R_{corr} distribution is performed. A third-degree polynomial fit is chosen because it gives the best agreement between the data and the estimated background. The uncertainties arising from this fit are treated as systematic uncertainties. The uncertainty due to the choice of polynomial is smaller than the leading uncertainties assigned to the data-driven estimate and is neglected. The values of R_{corr} used in the final calculation of the multijet event yields for the m_{VLQ} distributions vary between 0.85 and 0.65 for SR A1 and between 0.9 and 0.7 for VR A. The final estimated yields for the multijet background in SR A1 and VR A are shown in Table 1. The uncertainties include systematic and statistical contributions as detailed in Section 7.

Table 1: Summary of observed and predicted yields in SR A1 and VR A. For the non-multijet SM backgrounds the MC predicted yields are tabulated, while for the multijet background the yields from the data-driven estimate are shown. These yields are used as inputs to the statistical fits described in Section 8. The uncertainties include systematic and statistical contributions as detailed in Section 7. The statistical and systematic uncertainties in the non-multijet SM have been propagated and assigned to the data-driven multijet estimate.

	SR A1	VR A
Single top	660 ± 570	400 ± 330
W+jets	770 ± 140	750 ± 130
$t\bar{t}$	381 ± 49	709 ± 81
Z+jets	187 ± 33	277 ± 44
Data-driven multijet estimate	$11\,220 \pm 660$	$69\,000 \pm 14\,000$
Total background	$13\,220 \pm 860$	$71\,000 \pm 14\,000$
Data	12 923	62 409

7 Systematic uncertainties

The modelling of kinematic variables such as m_{VLQ} in the signal and simulated background processes as described in Section 4 is affected by experimental uncertainties associated with the reconstruction and calibration of the underlying physics objects. These uncertainties in the simulated backgrounds are propagated to the data-driven multijet background estimate. Additionally, uncertainties are assigned to the multijet background to account for variations in the R_{corr} values and in the statistical uncertainty propagation methods. This includes the use of Gaussian uncertainty propagation and the statistical uncertainties originating from the fits used in the estimation of the multijet background. Cross-section uncertainties are included for all the simulated backgrounds.

7.1 Experimental and theoretical uncertainties

The uncertainty in the integrated luminosity of the 2015–2018 ATLAS dataset is estimated to be 1.7% [89]. The uncertainty is derived from the baseline luminosity measurements made by the LUCID-2 detector [31]. For small-R and large-R jets, the uncertainties associated with the energy scale and resolution are evaluated using a combination of simulated events and *in situ* methods applied to the collected data [40]. In addition, a mass scale uncertainty is evaluated for the large-R jets with a forward-folding technique that uses fits to the W-boson and top-quark mass peaks [90] in simulation and data. A jet mass resolution uncertainty of 20% is applied to large-R jets by smearing the energy of the jets. This uncertainty estimate has negligible impact on the final result.

Uncertainties are assigned to correction factors for differences in b-tagging and W-tagging efficiencies between simulated events and data events. Flavour-dependent tagging uncertainties are evaluated using differences in tagging response for b-jets, c-jets, and light-flavour jets between simulation and data [49–51]. Since the high-p_{T} region is probed in this search, an additional extrapolation uncertainty is used to account for tagging inefficiencies in the range $p_{\mathrm{T}} > 400$ GeV [49]. Uncertainties in the correction factors for W-tagging arise from uncertainties related to the jet energy scale, as well as modelling uncertainties and statistical uncertainties [46]. The correction factors are extrapolated into the high-p_{T} region ($p_{\mathrm{T}} > 600$ GeV) and hence the corresponding uncertainties are also propagated.

7.2 Modelling uncertainties for simulated backgrounds

Modelling uncertainties are assigned to single-top-quark and W+jets events as they are the irreducible backgrounds secondary to the multijet background. Uncertainties related to initial-state radiation (ISR), final-state radiation (FSR), and the parton shower were assessed for the single-top samples. Due to significant interference between the Wt and $t\bar{t}$ processes, two different schemas were employed to generate the Wt MC event samples. The nominal sample uses the diagram removal method, while the variation sample uses the diagram subtraction method. The difference between these two samples is used as the uncertainty. The ISR/FSR uncertainty is determined similarly to the uncertainty estimation for $t\bar{t}$ events. For the W+jets events, an alternative sample where the modelling of hadronisation is based on the Lund string model, is used. Theoretical cross-section uncertainties in the normalisation of the simulated SM backgrounds are included. For the single-top-quark backgrounds an uncertainty of $\pm 2.5\%$ is included, for $t\bar{t}$ an uncertainty of $+2.4\%/-3.5\%$ is assigned, while for W/Z+jets a $\pm 6\%$ uncertainty is applied.

7.3 Modelling uncertainties for data-driven background estimates

The uncertainties in the data-driven method used to estimate the multijet background can be categorised according to their source. First, experimental and theoretical uncertainties from the simulated SM backgrounds are propagated through the method, and variations in these backgrounds are used to estimate the uncertainties for the multijet estimate. The variations of the simulated SM backgrounds are used in calculating the corresponding multijet event estimates for the m_{VLQ} distributions. Differences between the resulting m_{VLQ} distributions of the multijet background are used as corresponding uncertainties. Statistical uncertainties arising from Gaussian propagation from the method's arithmetic operations are assigned as separate uncertainties. The shape of the R_{corr} distributions is a function of the Pythia 8 and Sherpa dijet MC distributions used in the respective calculations. Since the final data-driven estimate depends on these distributions, uncertainties in the modelling of R_{corr} are evaluated by comparing the estimates of R_{corr} obtained by using dijet Monte Carlo samples from different generators, namely Pythia 8 and Sherpa. The difference between the Pythia 8 estimate and the Sherpa estimate is used as an uncertainty. This uncertainty is larger in the VR than in the SR, resulting in a larger fractional uncertainty in the VR in Table 1. A third-degree polynomial is fitted to model R_{corr} for the multijet estimate, based on the method described in Section 6. The statistical uncertainty arising from the polynomial fitting is also considered as a separate uncertainty. An additional non-closure uncertainty is introduced to account for shape discrepancies between the data and fitted backgrounds in the validation region. The m_{VLQ} distribution is fitted to data in the validation region under the background-only hypothesis. The post-fit distribution from the fit is shown in Figure 3. The shape of the non-closure between the data and the fitted backgrounds seen in the validation region in Figure 3 is propagated as a shape uncertainty for the multijet events in SR A1. This uncertainty is introduced to account for a similar discrepancy that may arise in the fits to data in the SR. The systematic uncertainty in the inclusive simulated SM background yield determined from the VLQ candidate invariant mass distribution after the fit to the background-only hypothesis for the non-closure uncertainty is 5.2%, and the uncertainty in the modelling of R_{corr} found by using Sherpa as the alternative MC generator is 2.2%. After injecting a nominal signal, it was checked that the distortion of the background shape is well below the shape uncertainties considered, so the expected bias is minimal.

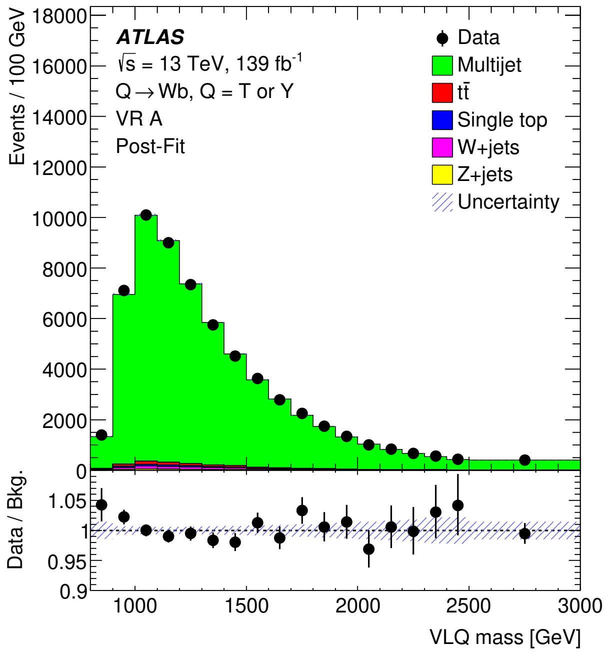


Figure 3: The post-fit distribution for m_{VLQ} in VR A after the fit to data under the background-only hypothesis. All the uncertainties are included in this fit as nuisance parameters. The lower panel depicts the ratio of data to the fitted background yields.

8 Statistical analysis and results

A binned maximum-likelihood fit is performed on the m_{VLQ} distribution in the SR A1 using the RooStats [91] framework to test the background-only hypothesis across the m–κ plane for the VLQ signals described in Section 4. The background prediction used for all these fits is the aggregation of the data-driven multijet background and the simulated SM backgrounds. The systematic uncertainties described in Section 7 are incorporated into the likelihood as nuisance parameters θ_i via multiplicative Gaussian constraints, $G(\theta_i)$ [92]. The normalisation of the multijet background, $\mu^{\mathrm{multijets}}$, is included as an unconstrained parameter of the fit.

In the fit to data under the background-only hypothesis, $\mu^{\mathrm{multijets}}$ is measured to be 0.94 ± 0.06. The post-fit distribution of m_{VLQ} in the SR A1 after the background-only fit to data is shown in Figure 4. The expected signal from a Y VLQ with mass 1.6 TeV and $\kappa = 0.5$, normalised to the total post-fit background yield, is overlaid. The post-fit yields for the backgrounds and data are listed in Table 2. The data agree with the background-only hypothesis and no significant excess of events above the SM predictions is observed. A fit to data under the signal-plus-background hypothesis found a significance of 1.1σ for a T-singlet signal with mass 1.6 TeV and $\kappa = 0.5$. In the absence of any significant excess, 95% CL limits on the VLQ production cross-section are calculated separately for each signal hypothesis in the m–κ plane using the $\mathrm{CL_s}$ method [93]. The mass limits for $Y \to W(\to q\bar{q})b$ with $\kappa = 0.5$ and $\kappa = 0.7$ are shown in Figure 5. The limits depend on κ because the total width of the m_{VLQ} distribution varies with κ. For $\kappa = 0.5$, both the expected and observed mass limits for Y quarks are 2.0 TeV, whereas for $\kappa = 0.7$ the expected and observed limits are 2.3 TeV and 2.4 TeV respectively. Figure 5 also shows the T quark's theoretical cross-section times branching fraction ($\mathcal{B}(T \to Wb) = 0.5$) as a function of its mass. The limits for the T singlet are

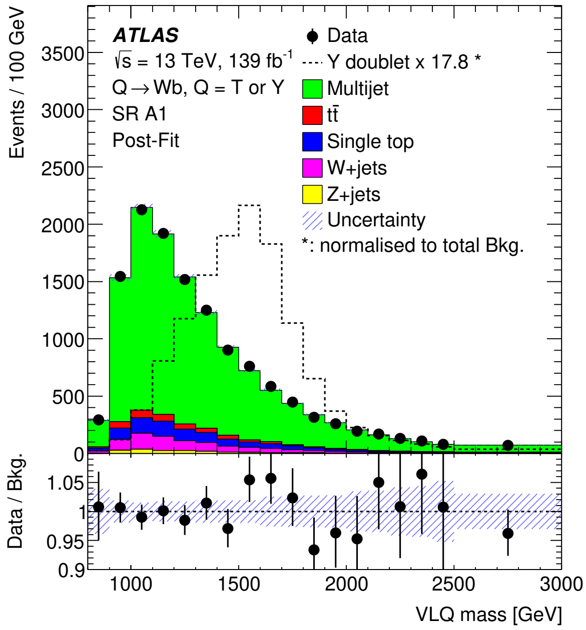


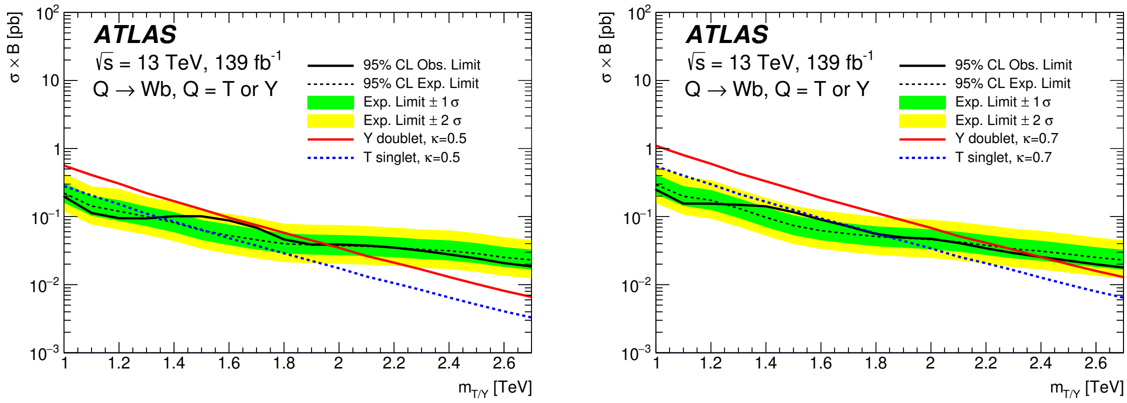
Figure 4: The post-fit distribution of m_{VLQ} in the SR A1 after the fit to data under the background-only hypothesis. All the uncertainties are included in this fit as nuisance parameters. The lower panel depicts the ratio of data to the fitted background yields. The hatched area in the lower panel represents the total uncertainty in the background, including the uncertainty in $\mu^{\mathrm{multijets}}$. The overlaid dotted-line histogram in the upper panel shows the signal from a simulated Y VLQ with mass 1.6 TeV and $\kappa = 0.5$, normalised to the total post-fit background yield.

Table 2: Post-fit background yields after the fit to data for the background-only hypothesis in the SR. The quoted uncertainties in the yields include contributions from statistical and systematic sources, and are computed taking into account correlations among nuisance parameters resulting from the fit to data.

	SR A1
Single top	870 ± 570
W+jets	780 ± 140
Z+jets	190 ± 32
$t\bar{t}$	388 ± 48
Multijet	10 690 ± 530
Total background	12 920 ± 180
Data	12 923

weaker than those for Y quarks in the (B, Y)-doublet representation. The observed mass limits for T-singlet quarks as shown in Figure 5 are 1.4 TeV for $\kappa = 0.5$ and 1.9 TeV for $\kappa = 0.7$. The limits in this search are affected more by systematic uncertainties than by statistical ones. The two uncertainties with the highest impact on the exclusion limits affect the modelling of the data-driven multijet estimate, the first being the non-closure uncertainty and the second being the uncertainty in the modelling of R_{corr} found by using Sherpa as the alternative MC generator.

The results are also interpreted in a more generalised representation of the parameter space in Figure 6,



(a) (b)

Figure 5: Expected (dotted) and observed (solid) cross-section limits times branching fraction for a Y VLQ in the (B, Y) doublet as a function of $m_{T/Y}$. Limits are computed for signals with couplings (a) $\kappa = 0.5$ and (b) $\kappa = 0.7$. The branching fraction $\mathcal{B}(Y \rightarrow Wb)$ is set to 1. The surrounding bands correspond to ± 1 and ± 2 standard deviations around the expected limit. The T-singlet quark's theoretical cross-section (corrected to NLO with the inclusion of finite-width effects) times branching fraction ($\mathcal{B}(T \rightarrow Wb) = 0.5$) as a function of the T/Y mass is also shown (dashed blue line). The mass limit for a T singlet can then be obtained by computing the intersection of those cross-section limits and the T-singlet theory cross-section curve. The limits depend on κ because the natural width of the T/Y VLQ depends on κ.

showing the largest excluded mass at a given κ. Thus, for a coupling of $\kappa = 0.3$, Y-quark masses below 1.5 TeV are excluded. For width-to-mass ratios less than 50% in the m_Y–κ plane, the Γ_Y/m_Y isolines are displayed along with the two-dimensional limits.

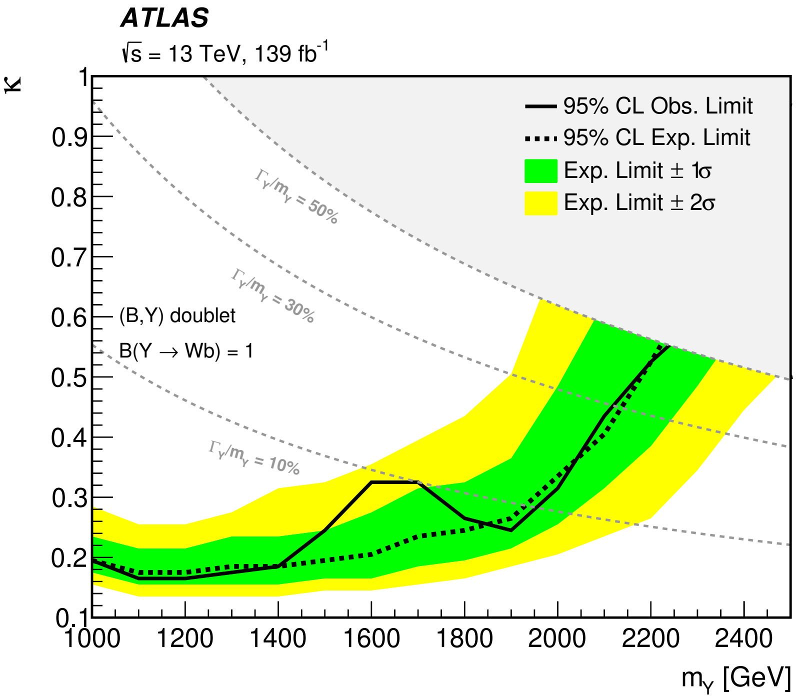


Figure 6: Observed (solid) and expected (dotted) 95% CL exclusion limits on the coupling constant κ as a function of the Y VLQ mass in the (B, Y)-doublet scenario. All κ values above the black contour lines are excluded at each mass point. The bands correspond to ± 1 and ± 2 standard deviations around the expected limit. Limits are only presented in the regime $\Gamma_Y/m_Y \leq 50\%$, where the theory calculations are known to be valid. The grey dotted isolines depict the highest (m, κ) values allowed for Y-doublet signals with various widths up to $\Gamma_Y/m_Y = 50\%$.

9 Conclusion

A search for T and Y vector-like quarks decaying into a Wb final state using proton–proton (pp) collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, is presented in this paper. The search uses 139 fb^{-1} of data recorded from 2015 to 2018 by the ATLAS experiment at the LHC. Whereas previous ATLAS searches using this topology focused on the leptonic decay mode of the W boson, this is the first search where the hadronic decay mode of the W boson is probed. This analysis searches for VLQs with masses in the TeV range. Consequently, the W boson has a large Lorentz boost, and is reconstructed using advanced tagging algorithms that use substructure information from large-R jets. The main background comes from QCD multijet production. The shape and expected yield of this background are estimated using a data-driven method. Upon finding no significant excess of events in data, mass limits as a function of the global coupling parameter κ are determined. The observed lower limits on the masses of Y quarks with $\kappa = 0.5$ and $\kappa = 0.7$ are 2.0 TeV and 2.4 TeV, respectively. For T quarks, the observed mass limits are 1.4 TeV for $\kappa = 0.5$ and 1.9 TeV for $\kappa = 0.7$. All coupling values $\kappa > 0.6$ for Y-quark masses up to 2.2 TeV in the (B, Y) doublet are excluded for narrow-width signals $(\Gamma_Y/m_Y < 50\%)$. The mass limits on the Y quark in the (B, Y)-doublet representation improve on those of the previous ATLAS search, obtained using leptonic decays of the W boson, by 0.6 TeV for $\kappa = 0.5$. Compared to the previous ATLAS search, this paper extends the search region for Y quarks from 2.0 TeV to 2.7 TeV. For the T-singlet case, with $T \to Wb$ decays, the search region is extended from 1.2 TeV to 2.7 TeV. Depending on the choice of κ, the reported mass limits are the most stringent to date for this channel.

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Usai [8], R. Ushioda [157], M. Usman [110], F. Ustuner [53], Z. Uysal [83], V. Vacek [135], B. Vachon [106], T. Vafeiadis [37], A. Vaitkus [98], C. Valderanis [111], E. Valdes Santurio [48a,48b], M. Valente [159a], S. Valentinetti [24b,24a], A. Valero [166], E. Valiente Moreno [166], A. Vallier [91], J.A. Valls Ferrer [166], D.R. Van Arneman [117], T.R. Van Daalen [141], A. Van Der Graaf [50], P. Van Gemmeren [6], M. Van Rijnbach [37], S. Van Stroud [98], I. Van Vulpen [117], P. Vana [136], M. Vanadia [77a,77b], W. Vandelli [37], E.R. Vandewall [124], D. Vannicola [154], L. Vannoli [54], R. Vari [76a], E.W. Varnes [7], C. Varni [18b], T. Varol [151], D. Varouchas [67], L. Varriale [166], K.E. Varvell [150], M.E. Vasile [28b], L. Vaslin[85], G.A. Vasquez [168], A. Vasyukov [39], L.M. Vaughan [124], R. Vavricka[102], T. Vazquez Schroeder [37], J. Veatch [32], V. Vecchio [103], M.J. Veen [105], I. Veliscek [30], L.M. Veloce [158], F. Veloso [133a,133c], S. Veneziano [76a], A. Ventura [71a,71b], S. Ventura Gonzalez [138], A. Verbytskyi [112], M. Verducci [75a,75b], C. Vergis [96], M. Verissimo De Araujo [84b], W. Verkerke [117], J.C. Vermeulen [117], C. Vernieri [146], M. Vessella [105], M.C. Vetterli [145,ad], A. Vgenopoulos [102], N. Viaux Maira [140f], T. Vickey [142], O.E. Vickey Boeriu [142], G.H.A. Viehhauser [129], L. Vigani [64b], M. Vigl [112], M. Villa [24b,24a], M. Villaplana Perez [166], E.M. Villhauer[53], E. Vilucchi [54], M.G. Vincter [35], A. Visibile[117], C. Vittori [37], I. Vivarelli [24b,24a], E. Voevodina [112], F. Vogel [111], J.C. Voigt [51], P. Vokac [135], Yu. Volkotrub [87b], J. Von Ahnen [49], E. Von Toerne [25], B. Vormwald [37], V. Vorobel [136], K. Vorobev [38], M. Vos [166], K. Voss [144], M. Vozak [117], L. Vozdecky [123], N. Vranjes [16], M. Vranjes Milosavljevic [16], M. Vreeswijk [117], N.K. Vu [63d,63c], R. Vuillermet [37], O. Vujinovic [102], I. Vukotic [40], I.K. Vyas [35], S. Wada [160], C. Wagner[105], J.M. Wagner [18a], W. Wagner [174], S. Wahdan [174], H. Wahlberg [92], J. Walder [137], R. Walker [111], W. Walkowiak [144], A. Wall [131], E.J. Wallin [100], T. Wamorkar [6], A.Z. Wang [139], C. Wang [102], C. Wang [11], H. Wang [18a], J. Wang [65c], P. Wang [98], R. Wang [62], R. Wang [6], S.M. Wang [151], S. Wang [63b], S. Wang [14], T. Wang [63a], W.T. Wang [81], W. Wang [14], X. Wang [114a], X. Wang [165], X. Wang [63c], Y. Wang [63d], Y. Wang [114a], Y. Wang [63a], Z. Wang [108], Z. Wang [63d,52,63c], Z. Wang [108], A. Warburton [106], R.J. Ward [21], N. Warrack [60], S. Waterhouse [97], A.T. Watson [21], H. Watson [53], M.F. Watson [21], E. Watton [60,137], G. Watts [141], B.M. Waugh [98], J.M. Webb [55], C. Weber [30], H.A. Weber [19], M.S. Weber [20], S.M. Weber [64a], C. Wei [63a], Y. Wei [55], A.R. Weidberg [129], E.J. Weik [120], J. Weingarten [50], C. Weiser [55], C.J. Wells [49], T. Wenaus [30], B. Wendland [50], T. Wengler [37], N.S. Wenke[112], N. Wermes [25], M. Wessels [64a], A.M. Wharton [93], A.S. White [62], A. White [8], M.J. White [1], D. Whiteson [162], L. Wickremasinghe [127], W. Wiedenmann [173], M. Wielers [137], C. Wiglesworth [43], D.J. Wilbern[123], H.G. Wilkens [37], J.J.H. Wilkinson [33], D.M. Williams [42], H.H. Williams[131], S. Williams [33], S. Willocq [105], B.J. Wilson [103], P.J. Windischhofer [40], F.I. Winkel [31], F. Winklmeier [126], B.T. Winter [55], J.K. Winter [103], M. Wittgen[146], M. Wobisch [99], T. Wojtkowski[61], Z. Wolffs [117], J. Wollrath[162], M.W. Wolter [88], H. Wolters [133a,133c], M.C. Wong[139], E.L. Woodward [42], S.D. Worm [49], B.K. Wosiek [88], K.W. Woźniak [88], S. Wozniewski [56], K. Wraight [60], C. Wu [21], M. Wu [114b], M. Wu [116], S.L. Wu [173], X. Wu [57], Y. Wu [63a], Z. Wu [4], J. Wuerzinger [112,ab], T.R. Wyatt [103], B.M. Wynne [53], S. Xella [43], L. Xia [114a], M. Xia [15], M. Xie [63a], S. Xin [14,114c], A. Xiong [126], J. Xiong [18a], D. Xu [14], H. Xu [63a], L. Xu [63a], R. Xu [131], T. Xu [108], Y. Xu [15], Z. Xu [53], Z. Xu[114a], B. Yabsley [150], S. Yacoob [34a], Y. Yamaguchi [85], E. Yamashita [156], H. Yamauchi [160], T. Yamazaki [18a], Y. Yamazaki [86], S. Yan [60], Z. Yan [105], H.J. Yang [63c,63d], H.T. Yang [63a], S. Yang [63a], T. Yang [65c], X. Yang [37], X. Yang [14], Y. Yang [45], Y. Yang[63a], Z. Yang [63a], W-M. Yao [18a], H. Ye [114a], H. Ye [56], J. Ye [14], S. Ye [30], X. Ye [63a], Y. Yeh [98], I. Yeletskikh [39], B. Yeo [18b], M.R. Yexley [98], T.P. Yildirim [129], P. Yin [42], K. Yorita [171], S. Younas [28b], C.J.S. Young [37], C. Young [146], C. Yu [14,114c], Y. Yu [63a], J. Yuan [14,114c], M. Yuan [108], R. Yuan [63d,63c], L. Yue [98], M. Zaazoua [63a], B. Zabinski [88], E. Zaid[53], Z.K. Zak [88], T. Zakareishvili [166], S. Zambito [57], J.A. Zamora Saa [140d,140b], J. Zang [156], D. Zanzi [55], O. Zaplatilek [135], C. Zeitnitz [174], H. Zeng [14], J.C. Zeng [165], D.T. Zenger Jr [27], O. Zenin [38], T. Ženiš [29a], S. Zenz [96], S. Zerradi [36a], D. Zerwas [67], M. Zhai [14,114c], D.F. Zhang [142], J. Zhang [63b], J. Zhang [6], K. Zhang [14,114c], L. Zhang [63a], L. Zhang [114a], P. Zhang [14,114c], R. Zhang [173], S. Zhang [108], S. Zhang [91], T. Zhang [156], X. Zhang [63c], X. Zhang [63b], Y. Zhang [63c], Y. Zhang [98], Y. Zhang [114a], Z. Zhang [18a], Z. Zhang [63b], Z. Zhang [67], H. Zhao [141], T. Zhao [63b], Y. Zhao [139], Z. Zhao [63a], Z. Zhao [63a], A. Zhemchugov [39], J. Zheng [114a], K. Zheng [165], X. Zheng [63a], Z. Zheng [146], D. Zhong [165], B. Zhou [108], H. Zhou [7], N. Zhou [63c], Y. Zhou [15], Y. Zhou [114a], Y. Zhou[7], C.G. Zhu [63b], J. Zhu [108], X. Zhu[63d], Y. Zhu [63c], Y. Zhu [63a], X. Zhuang [14], K. Zhukov [69], N.I. Zimine [39], J. Zinsser [64b], M. Ziolkowski [144], L. Živković [16], A. Zoccoli [24b,24a], K. Zoch [62], T.G. Zorbas [142], O. Zormpa [47], W. Zou [42], L. Zwalinski [37].

[1]Department of Physics, University of Adelaide, Adelaide; Australia.
[2]Department of Physics, University of Alberta, Edmonton AB; Canada.
[3(a)]Department of Physics, Ankara University, Ankara;[(b)]Division of Physics, TOBB University of Economics and Technology, Ankara; Türkiye.
[4]LAPP, Université Savoie Mont Blanc, CNRS/IN2P3, Annecy; France.
[5]APC, Université Paris Cité, CNRS/IN2P3, Paris; France.
[6]High Energy Physics Division, Argonne National Laboratory, Argonne IL; United States of America.
[7]Department of Physics, University of Arizona, Tucson AZ; United States of America.
[8]Department of Physics, University of Texas at Arlington, Arlington TX; United States of America.
[9]Physics Department, National and Kapodistrian University of Athens, Athens; Greece.
[10]Physics Department, National Technical University of Athens, Zografou; Greece.
[11]Department of Physics, University of Texas at Austin, Austin TX; United States of America.
[12]Institute of Physics, Azerbaijan Academy of Sciences, Baku; Azerbaijan.
[13]Institut de Física d'Altes Energies (IFAE), Barcelona Institute of Science and Technology, Barcelona; Spain.

[14]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; China.
[15]Physics Department, Tsinghua University, Beijing; China.
[16]Institute of Physics, University of Belgrade, Belgrade; Serbia.
[17]Department for Physics and Technology, University of Bergen, Bergen; Norway.
[18](a)Physics Division, Lawrence Berkeley National Laboratory, Berkeley CA;(b)University of California, Berkeley CA; United States of America.
[19]Institut für Physik, Humboldt Universität zu Berlin, Berlin; Germany.
[20]Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern; Switzerland.
[21]School of Physics and Astronomy, University of Birmingham, Birmingham; United Kingdom.
[22](a)Department of Physics, Bogazici University, Istanbul;(b)Department of Physics Engineering, Gaziantep University, Gaziantep;(c)Department of Physics, Istanbul University, Istanbul; Türkiye.
[23](a)Facultad de Ciencias y Centro de Investigaciónes, Universidad Antonio Nariño, Bogotá;(b)Departamento de Física, Universidad Nacional de Colombia, Bogotá; Colombia.
[24](a)Dipartimento di Fisica e Astronomia A. Righi, Università di Bologna, Bologna;(b)INFN Sezione di Bologna; Italy.
[25]Physikalisches Institut, Universität Bonn, Bonn; Germany.
[26]Department of Physics, Boston University, Boston MA; United States of America.
[27]Department of Physics, Brandeis University, Waltham MA; United States of America.
[28](a)Transilvania University of Brasov, Brasov;(b)Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest;(c)Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi;(d)National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj-Napoca;(e)National University of Science and Technology Politechnica, Bucharest;(f)West University in Timisoara, Timisoara;(g)Faculty of Physics, University of Bucharest, Bucharest; Romania.
[29](a)Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava;(b)Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice; Slovak Republic.
[30]Physics Department, Brookhaven National Laboratory, Upton NY; United States of America.
[31]Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física, y CONICET, Instituto de Física de Buenos Aires (IFIBA), Buenos Aires; Argentina.
[32]California State University, CA; United States of America.
[33]Cavendish Laboratory, University of Cambridge, Cambridge; United Kingdom.
[34](a)Department of Physics, University of Cape Town, Cape Town;(b)iThemba Labs, Western Cape;(c)Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg;(d)National Institute of Physics, University of the Philippines Diliman (Philippines);(e)University of South Africa, Department of Physics, Pretoria;(f)University of Zululand, KwaDlangezwa;(g)School of Physics, University of the Witwatersrand, Johannesburg; South Africa.
[35]Department of Physics, Carleton University, Ottawa ON; Canada.
[36](a)Faculté des Sciences Ain Chock, Université Hassan II de Casablanca;(b)Faculté des Sciences, Université Ibn-Tofail, Kénitra;(c)Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech;(d)LPMR, Faculté des Sciences, Université Mohamed Premier, Oujda;(e)Faculté des sciences, Université Mohammed V, Rabat;(f)Institute of Applied Physics, Mohammed VI Polytechnic University, Ben Guerir; Morocco.
[37]CERN, Geneva; Switzerland.
[38]Affiliated with an institute covered by a cooperation agreement with CERN.
[39]Affiliated with an international laboratory covered by a cooperation agreement with CERN.
[40]Enrico Fermi Institute, University of Chicago, Chicago IL; United States of America.

[41]LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand; France.
[42]Nevis Laboratory, Columbia University, Irvington NY; United States of America.
[43]Niels Bohr Institute, University of Copenhagen, Copenhagen; Denmark.
[44][(a)]Dipartimento di Fisica, Università della Calabria, Rende;[(b)]INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati; Italy.
[45]Physics Department, Southern Methodist University, Dallas TX; United States of America.
[46]Physics Department, University of Texas at Dallas, Richardson TX; United States of America.
[47]National Centre for Scientific Research "Demokritos", Agia Paraskevi; Greece.
[48][(a)]Department of Physics, Stockholm University;[(b)]Oskar Klein Centre, Stockholm; Sweden.
[49]Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen; Germany.
[50]Fakultät Physik , Technische Universität Dortmund, Dortmund; Germany.
[51]Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden; Germany.
[52]Department of Physics, Duke University, Durham NC; United States of America.
[53]SUPA - School of Physics and Astronomy, University of Edinburgh, Edinburgh; United Kingdom.
[54]INFN e Laboratori Nazionali di Frascati, Frascati; Italy.
[55]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg; Germany.
[56]II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen; Germany.
[57]Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève; Switzerland.
[58][(a)]Dipartimento di Fisica, Università di Genova, Genova;[(b)]INFN Sezione di Genova; Italy.
[59]II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen; Germany.
[60]SUPA - School of Physics and Astronomy, University of Glasgow, Glasgow; United Kingdom.
[61]LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble; France.
[62]Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge MA; United States of America.
[63][(a)]Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Hefei;[(b)]Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE), Shandong University, Qingdao;[(c)]School of Physics and Astronomy, Shanghai Jiao Tong University, Key Laboratory for Particle Astrophysics and Cosmology (MOE), SKLPPC, Shanghai;[(d)]Tsung-Dao Lee Institute, Shanghai;[(e)]School of Physics and Microelectronics, Zhengzhou University; China.
[64][(a)]Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg;[(b)]Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg; Germany.
[65][(a)]Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong;[(b)]Department of Physics, University of Hong Kong, Hong Kong;[(c)]Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong; China.
[66]Department of Physics, National Tsing Hua University, Hsinchu; Taiwan.
[67]IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay; France.
[68]Centro Nacional de Microelectrónica (IMB-CNM-CSIC), Barcelona; Spain.
[69]Department of Physics, Indiana University, Bloomington IN; United States of America.
[70][(a)]INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine;[(b)]ICTP, Trieste;[(c)]Dipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine; Italy.
[71][(a)]INFN Sezione di Lecce;[(b)]Dipartimento di Matematica e Fisica, Università del Salento, Lecce; Italy.
[72][(a)]INFN Sezione di Milano;[(b)]Dipartimento di Fisica, Università di Milano, Milano; Italy.
[73][(a)]INFN Sezione di Napoli;[(b)]Dipartimento di Fisica, Università di Napoli, Napoli; Italy.
[74][(a)]INFN Sezione di Pavia;[(b)]Dipartimento di Fisica, Università di Pavia, Pavia; Italy.
[75][(a)]INFN Sezione di Pisa;[(b)]Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa; Italy.
[76][(a)]INFN Sezione di Roma;[(b)]Dipartimento di Fisica, Sapienza Università di Roma, Roma; Italy.

[77(a)]INFN Sezione di Roma Tor Vergata;[(b)]Dipartimento di Fisica, Università di Roma Tor Vergata, Roma; Italy.
[78(a)]INFN Sezione di Roma Tre;[(b)]Dipartimento di Matematica e Fisica, Università Roma Tre, Roma; Italy.
[79(a)]INFN-TIFPA;[(b)]Università degli Studi di Trento, Trento; Italy.
[80]Universität Innsbruck, Department of Astro and Particle Physics, Innsbruck; Austria.
[81]University of Iowa, Iowa City IA; United States of America.
[82]Department of Physics and Astronomy, Iowa State University, Ames IA; United States of America.
[83]Istinye University, Sariyer, Istanbul; Türkiye.
[84(a)]Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora;[(b)]Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro;[(c)]Instituto de Física, Universidade de São Paulo, São Paulo;[(d)]Rio de Janeiro State University, Rio de Janeiro;[(e)]Federal University of Bahia, Bahia; Brazil.
[85]KEK, High Energy Accelerator Research Organization, Tsukuba; Japan.
[86]Graduate School of Science, Kobe University, Kobe; Japan.
[87(a)]AGH University of Krakow, Faculty of Physics and Applied Computer Science, Krakow;[(b)]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow; Poland.
[88]Institute of Nuclear Physics Polish Academy of Sciences, Krakow; Poland.
[89]Faculty of Science, Kyoto University, Kyoto; Japan.
[90]Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka ; Japan.
[91]L2IT, Université de Toulouse, CNRS/IN2P3, UPS, Toulouse; France.
[92]Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata; Argentina.
[93]Physics Department, Lancaster University, Lancaster; United Kingdom.
[94]Oliver Lodge Laboratory, University of Liverpool, Liverpool; United Kingdom.
[95]Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana; Slovenia.
[96]School of Physics and Astronomy, Queen Mary University of London, London; United Kingdom.
[97]Department of Physics, Royal Holloway University of London, Egham; United Kingdom.
[98]Department of Physics and Astronomy, University College London, London; United Kingdom.
[99]Louisiana Tech University, Ruston LA; United States of America.
[100]Fysiska institutionen, Lunds universitet, Lund; Sweden.
[101]Departamento de Física Teorica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid; Spain.
[102]Institut für Physik, Universität Mainz, Mainz; Germany.
[103]School of Physics and Astronomy, University of Manchester, Manchester; United Kingdom.
[104]CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille; France.
[105]Department of Physics, University of Massachusetts, Amherst MA; United States of America.
[106]Department of Physics, McGill University, Montreal QC; Canada.
[107]School of Physics, University of Melbourne, Victoria; Australia.
[108]Department of Physics, University of Michigan, Ann Arbor MI; United States of America.
[109]Department of Physics and Astronomy, Michigan State University, East Lansing MI; United States of America.
[110]Group of Particle Physics, University of Montreal, Montreal QC; Canada.
[111]Fakultät für Physik, Ludwig-Maximilians-Universität München, München; Germany.
[112]Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München; Germany.
[113]Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya; Japan.
[114(a)]Department of Physics, Nanjing University, Nanjing;[(b)]School of Science, Shenzhen Campus of Sun

Yat-sen University;[c]University of Chinese Academy of Science (UCAS), Beijing; China.
[115]Department of Physics and Astronomy, University of New Mexico, Albuquerque NM; United States of America.
[116]Institute for Mathematics, Astrophysics and Particle Physics, Radboud University/Nikhef, Nijmegen; Netherlands.
[117]Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam; Netherlands.
[118]Department of Physics, Northern Illinois University, DeKalb IL; United States of America.
[119][a]New York University Abu Dhabi, Abu Dhabi;[b]United Arab Emirates University, Al Ain; United Arab Emirates.
[120]Department of Physics, New York University, New York NY; United States of America.
[121]Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo; Japan.
[122]Ohio State University, Columbus OH; United States of America.
[123]Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman OK; United States of America.
[124]Department of Physics, Oklahoma State University, Stillwater OK; United States of America.
[125]Palacký University, Joint Laboratory of Optics, Olomouc; Czech Republic.
[126]Institute for Fundamental Science, University of Oregon, Eugene, OR; United States of America.
[127]Graduate School of Science, Osaka University, Osaka; Japan.
[128]Department of Physics, University of Oslo, Oslo; Norway.
[129]Department of Physics, Oxford University, Oxford; United Kingdom.
[130]LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris; France.
[131]Department of Physics, University of Pennsylvania, Philadelphia PA; United States of America.
[132]Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh PA; United States of America.
[133][a]Laboratório de Instrumentação e Física Experimental de Partículas - LIP, Lisboa;[b]Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa;[c]Departamento de Física, Universidade de Coimbra, Coimbra;[d]Centro de Física Nuclear da Universidade de Lisboa, Lisboa;[e]Departamento de Física, Universidade do Minho, Braga;[f]Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada (Spain);[g]Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, Lisboa; Portugal.
[134]Institute of Physics of the Czech Academy of Sciences, Prague; Czech Republic.
[135]Czech Technical University in Prague, Prague; Czech Republic.
[136]Charles University, Faculty of Mathematics and Physics, Prague; Czech Republic.
[137]Particle Physics Department, Rutherford Appleton Laboratory, Didcot; United Kingdom.
[138]IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette; France.
[139]Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA; United States of America.
[140][a]Departamento de Física, Pontificia Universidad Católica de Chile, Santiago;[b]Millennium Institute for Subatomic physics at high energy frontier (SAPHIR), Santiago;[c]Instituto de Investigación Multidisciplinario en Ciencia y Tecnología, y Departamento de Física, Universidad de La Serena;[d]Universidad Andres Bello, Department of Physics, Santiago;[e]Instituto de Alta Investigación, Universidad de Tarapacá, Arica;[f]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso; Chile.
[141]Department of Physics, University of Washington, Seattle WA; United States of America.
[142]Department of Physics and Astronomy, University of Sheffield, Sheffield; United Kingdom.
[143]Department of Physics, Shinshu University, Nagano; Japan.

[144]Department Physik, Universität Siegen, Siegen; Germany.
[145]Department of Physics, Simon Fraser University, Burnaby BC; Canada.
[146]SLAC National Accelerator Laboratory, Stanford CA; United States of America.
[147]Department of Physics, Royal Institute of Technology, Stockholm; Sweden.
[148]Departments of Physics and Astronomy, Stony Brook University, Stony Brook NY; United States of America.
[149]Department of Physics and Astronomy, University of Sussex, Brighton; United Kingdom.
[150]School of Physics, University of Sydney, Sydney; Australia.
[151]Institute of Physics, Academia Sinica, Taipei; Taiwan.
[152(a)]E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi;[(b)]High Energy Physics Institute, Tbilisi State University, Tbilisi;[(c)]University of Georgia, Tbilisi; Georgia.
[153]Department of Physics, Technion, Israel Institute of Technology, Haifa; Israel.
[154]Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv; Israel.
[155]Department of Physics, Aristotle University of Thessaloniki, Thessaloniki; Greece.
[156]International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo; Japan.
[157]Department of Physics, Tokyo Institute of Technology, Tokyo; Japan.
[158]Department of Physics, University of Toronto, Toronto ON; Canada.
[159(a)]TRIUMF, Vancouver BC;[(b)]Department of Physics and Astronomy, York University, Toronto ON; Canada.
[160]Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba; Japan.
[161]Department of Physics and Astronomy, Tufts University, Medford MA; United States of America.
[162]Department of Physics and Astronomy, University of California Irvine, Irvine CA; United States of America.
[163]University of Sharjah, Sharjah; United Arab Emirates.
[164]Department of Physics and Astronomy, University of Uppsala, Uppsala; Sweden.
[165]Department of Physics, University of Illinois, Urbana IL; United States of America.
[166]Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia - CSIC, Valencia; Spain.
[167]Department of Physics, University of British Columbia, Vancouver BC; Canada.
[168]Department of Physics and Astronomy, University of Victoria, Victoria BC; Canada.
[169]Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg; Germany.
[170]Department of Physics, University of Warwick, Coventry; United Kingdom.
[171]Waseda University, Tokyo; Japan.
[172]Department of Particle Physics and Astrophysics, Weizmann Institute of Science, Rehovot; Israel.
[173]Department of Physics, University of Wisconsin, Madison WI; United States of America.
[174]Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal; Germany.
[175]Department of Physics, Yale University, New Haven CT; United States of America.
[a] Also Affiliated with an institute covered by a cooperation agreement with CERN.
[b] Also at An-Najah National University, Nablus; Palestine.
[c] Also at Borough of Manhattan Community College, City University of New York, New York NY; United States of America.
[d] Also at Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki; Greece.
[e] Also at CERN, Geneva; Switzerland.
[f] Also at CMD-AC UNEC Research Center, Azerbaijan State University of Economics (UNEC); Azerbaijan.

[g] Also at Départment de Physique Nucléaire et Corpusculaire, Université de Genève, Genève; Switzerland.
[h] Also at Departament de Fisica de la Universitat Autonoma de Barcelona, Barcelona; Spain.
[i] Also at Department of Financial and Management Engineering, University of the Aegean, Chios; Greece.
[j] Also at Department of Physics, California State University, Sacramento; United States of America.
[k] Also at Department of Physics, King's College London, London; United Kingdom.
[l] Also at Department of Physics, Stanford University, Stanford CA; United States of America.
[m] Also at Department of Physics, Stellenbosch University; South Africa.
[n] Also at Department of Physics, University of Fribourg, Fribourg; Switzerland.
[o] Also at Department of Physics, University of Thessaly; Greece.
[p] Also at Department of Physics, Westmont College, Santa Barbara; United States of America.
[q] Also at Faculty of Physics, Sofia University, 'St. Kliment Ohridski', Sofia; Bulgaria.
[r] Also at Hellenic Open University, Patras; Greece.
[s] Also at Imam Mohammad Ibn Saud Islamic University; Saudi Arabia.
[t] Also at Institucio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona; Spain.
[u] Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg; Germany.
[v] Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia; Bulgaria.
[w] Also at Institute of Applied Physics, Mohammed VI Polytechnic University, Ben Guerir; Morocco.
[x] Also at Institute of Particle Physics (IPP); Canada.
[y] Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku; Azerbaijan.
[z] Also at Institute of Theoretical Physics, Ilia State University, Tbilisi; Georgia.
[aa] Also at National Institute of Physics, University of the Philippines Diliman (Philippines); Philippines.
[ab] Also at Technical University of Munich, Munich; Germany.
[ac] Also at The Collaborative Innovation Center of Quantum Matter (CICQM), Beijing; China.
[ad] Also at TRIUMF, Vancouver BC; Canada.
[ae] Also at Università di Napoli Parthenope, Napoli; Italy.
[af] Also at University of Colorado Boulder, Department of Physics, Colorado; United States of America.
[ag] Also at Washington College, Chestertown, MD; United States of America.
[ah] Also at Yeditepe University, Physics Department, Istanbul; Türkiye.
[*] Deceased