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Search for pair production of heavy vector-like quarks decaying to high- p_T W bosons and b quarks in the lepton-plus-jets final state in pp collisions at $\sqrt{s}=13$ TeV with the ATLAS detector

The ATLAS Collaboration

A search is presented for the pair production of heavy vector-like T quarks, primarily targeting the T quark decays to a W boson and a b -quark. The search is based on 36.1 fb^{-1} of pp collisions at $\sqrt{s} = 13$ TeV recorded in 2015 and 2016 with the ATLAS detector at the CERN Large Hadron Collider. Data are analysed in the lepton-plus-jets final state, including at least one b -tagged jet and a large-radius jet identified as originating from the hadronic decay of a high-momentum W boson. No significant deviation from the Standard Model expectation is observed in the reconstructed T mass distribution. The observed 95% confidence level lower limit on the T mass are 1350 GeV assuming 100% branching ratio to Wb . In the SU(2) singlet scenario, the lower mass limit is 1170 GeV. This search is also sensitive to a heavy vector-like B quark decaying to Wt and other final states. The results are thus reinterpreted to provide a 95% confidence level lower limit on the B quark mass at 1250 GeV assuming 100% branching ratio to Wt ; in the SU(2) singlet scenario, the limit is 1080 GeV. Mass limits on both T and B production are also set as a function of the decay branching ratios. The 100% branching ratio limits are found to be applicable to heavy vector-like Y and X production that decay to Wb and Wt , respectively.

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1 Introduction

The discovery of the Higgs boson by the ATLAS and CMS collaborations is a major milestone in high-energy physics [1, 2]. However, the underlying nature of electroweak symmetry breaking remains unknown. Naturalness arguments [3] require that quadratic divergences arising from radiative corrections to the Higgs boson mass are cancelled by a new mechanism to avoid fine-tuning. This paper presents a search for pair production of vector-like quarks (VLQs) decaying into third-generation quarks using the pp collision data collected at the Large Hadron Collider (LHC) in 2015 and 2016 at a centre-of-mass energy of 13 TeV.

Several new mechanisms have been proposed in theories beyond the Standard Model (BSM). In supersymmetry, the cancellation comes from assigning superpartners to the Standard Model (SM) bosons and fermions. Alternatively, Little Higgs [4, 5] and Composite Higgs [6, 7] models introduce a spontaneously broken global symmetry, with the Higgs boson emerging as a pseudo Nambu–Goldstone boson [8]. These latter models predict the existence of VLQs, defined as colour-triplet spin-1/2 fermions whose left- and right-handed chiral components have the same transformation properties under the weak-isospin $SU(2)$ gauge group [9, 10]. Depending on the model, vector-like quarks are produced in $SU(2)$ singlets, doublets or triplets of flavours T , B , X or Y , in which the first two have the same charge as the SM top and b quarks while the vector-like Y and X quarks have charge¹ $-4/3$ and $5/3$. In addition, in these models, VLQs are expected to couple preferentially to third-generation quarks [9, 11] and can have flavour-changing neutral-current decays in addition to the charged-current decays characteristic of chiral quarks. As a result, an up-type T quark can decay not only to a W boson and a b quark, but also to a Z or Higgs boson and a top quark ($T \rightarrow Wb, Zt$, and Ht). Similarly, a down-type B quark can decay to a Z or Higgs boson and a b quark, in addition to decaying to a W boson and a top quark ($B \rightarrow Wt, Zb$, and Hb). Instead, due to their charge, vector-like Y quarks decay exclusively to Wb while vector-like X quarks decay exclusively to Wt . To be consistent with the results from precision electroweak measurements a small mass-splitting between VLQs belonging to the same $SU(2)$ multiplet is required, but no requirement is placed on which member of the doublet is heavier [12]. Cascade decays such as $T \rightarrow WB \rightarrow WWt$ are thus assumed to be kinematically forbidden. Decays of VLQs into final states with first and second generation quarks, although not favoured, are not excluded [13, 14].

This search targets the $T \rightarrow Wb$ decay mode, although it is sensitive to a wide range of branching ratios to the other two decay modes as well as to vector-like B , X and Y production. Previous searches in this decay mode by the ATLAS and CMS collaborations did not observe a significant deviation from the SM predictions. Those searches excluded VLQ masses below 740 GeV for any combination of branching ratios and below 920 GeV for the assumption of $\mathcal{B}(T \rightarrow Wb) = 1$ [15, 16]. A recent search by the ATLAS collaboration at $\sqrt{s} = 13$ TeV sets a lower limit of 1160 GeV on the vector-like T quark mass for the pure Zt mode [17].

The event selection is optimised for $T\bar{T}$ production with subsequent decay to two high- p_T W bosons and two b -quarks, where one of the W bosons decays leptonically and the other decays hadronically. To suppress the SM background, boosted jet reconstruction techniques [18, 19] are used to improve the identification of high- p_T W bosons decaying hadronically while rejecting events with hadronically decaying, high- p_T top-quarks.

The $T\bar{T}$ system is reconstructed and the mass of the semi-leptonically decaying VLQ candidate is used to discriminate between SM and VLQ events. Finally, a profile likelihood fit is used to test for the presence

¹ All charges are quoted in units of e .

of a VLQ signal as a function of T and B quark masses and decay branching ratios. The results are found to be equally applicable to either singlet or doublet weak-isospin configurations as well as applicable to the decays of X and Y .

2 ATLAS detector

The ATLAS detector [20] at the LHC is a multipurpose particle detector with a forward-backward symmetric cylindrical geometry that covers nearly the entire solid angle around the collision point. It consists of an inner detector surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner detector covers the pseudorapidity range² $|\eta| < 2.5$. It consists of a silicon pixel detector, including the insertable B-layer installed after Run 1 of the LHC [21, 22], and a silicon microstrip detector surrounding the pixel detector, followed by a transition radiation straw-tube tracker. Lead/liquid-argon sampling calorimeters provide electromagnetic energy measurements with high granularity and a hadronic (steel/scintillator-tile) calorimeter covers the central pseudorapidity range ($|\eta| < 1.7$). The end-cap and forward regions are instrumented with liquid-argon calorimeters for both the electromagnetic and hadronic energy measurements up to $|\eta| = 4.9$. The outer part of the detector consists of a muon spectrometer with high-precision tracking chambers for coverage up to $|\eta| = 2.7$, fast detectors for triggering over $|\eta| < 2.4$, and three large superconducting toroid magnets with eight coils each. The ATLAS detector has a two-level trigger system to select events for offline analysis [23].

3 Data and simulation

This search utilises a data set corresponding to $36.1 \pm 1.2 \text{ fb}^{-1}$ of integrated luminosity from pp collisions at $\sqrt{s} = 13 \text{ TeV}$ collected by the ATLAS experiment, with 3.2 fb^{-1} collected in 2015 and 32.9 fb^{-1} collected in 2016 [24]. Data are only used if all ATLAS detector subsystems were operational. In all simulated events used in this search, the top quark and Higgs boson masses were set to 172.5 GeV and 125 GeV, respectively.

Simulated $T\bar{T}$ events were generated with the leading-order (LO) generator PROTONS v2.2 [25] using the NNPDF2.3 LO parton distribution function (PDF) set and a set of tuned parameters called the A14 tune [26] for the underlying-event description and passed to PYTHIA 8.186 [27] for parton showering and fragmentation. The samples were generated for an SU(2) singlet T VLQ, but with equal branching ratios of the T quark to each final state. To check the dependence of the results on the weak-isospin of the VLQ, one sample was also generated using the SU(2) doublet model including only the T contributions. The signal samples are normalised to pair-production cross-sections computed using TOP++ v2.0 [28], including next-to-next-to-leading-order (NNLO) quantum chromodynamics (QCD) corrections and soft-gluon resummation to NNLL accuracy [29–34], and using the MSTW 2008 NNLO PDF set. Their cross-sections vary from $3.38 \pm 0.25 \text{ pb}$ ($m_T = 500 \text{ GeV}$) to $3.50 \pm 0.43 \text{ fb}$ ($m_T = 1400 \text{ GeV}$). Theoretical

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

uncertainties are evaluated from variations of the factorisation and renormalisation scales, as well as from uncertainties in the PDFs and α_s . The latter two represent the largest contribution to the overall theoretical uncertainty in the signal cross-sections and are calculated using the PDF4LHC [35] prescription with the MSTW 2008 68% CL NNLO, CT10 NNLO [36, 37] and NNPDF2.3 [38] 5f FFN PDF sets. Two benchmark signal scenarios are considered, along with a full scan of the branching-ratio plane. The first benchmark corresponds to a T quark that decays 100% to Wb and the second corresponds to the SU(2) singlet T quark scenario, which predicts branching ratios of $\sim 50\%$, $\sim 25\%$, $\sim 25\%$ to Wb , Zt and Ht , respectively [12]. Samples were also generated for $B\bar{B}$ production for the reinterpretation of this search. They were produced using the same generator and normalised in the same way as $T\bar{T}$. As with $T\bar{T}$, two benchmark signal scenarios are considered, along with a full scan of the branching-ratio plane. The first benchmark assumes $\mathcal{B}(B \rightarrow Wt) = 1$ – which also corresponds to the SU(2) (B, T) doublet hypothesis – and the second corresponds to the SU(2) singlet B quark scenario, which predicts branching ratios of $\sim 50\%$, $\sim 25\%$, $\sim 25\%$ to Wt , Zb and Hb , respectively [12].

The main SM backgrounds that are studied using simulated samples are due to $t\bar{t}$, W +jets, Z +jets, diboson, single top quark, and $t\bar{t}+V$ ($V = W, Z$) production. The multi-jet background is estimated using a data-driven technique discussed in Section 5.4. The nominal $t\bar{t}$ MC sample was generated with POWHEG-Box v2 interfaced with PYTHIA 6.428 [39, 40] for the parton shower and hadronisation, using the PERUGIA2012 tune [41] and the CT10 PDF set, and setting the h_{damp} parameter to the mass of the top quark. To estimate $t\bar{t}$ modelling uncertainties, described in Section 6.3, additional samples were generated using POWHEG-Box v2 interfaced with HERWIG++ 2.7.1 [42], POWHEG-Box v2 interfaced with PYTHIA 8.186, and MG5_AMC@NLO 2.1.1 interfaced with PYTHIA 8.186 [43]. Further, samples with POWHEG-Box v2 interfaced with PYTHIA 6.428 were generated varying the factorisation and normalisation scales by 2 and 0.5, as well as the next-to-leading-order (NLO) radiation factor, h_{damp} , between m_{top} and twice m_{top} . The $t\bar{t}$ samples are normalised to the NNLO cross-section, including NNLO QCD corrections and soft-gluon resummation to NNLL accuracy, as done for the signal samples.

Single top quark production (called ‘single top’ in the following) in the Wt - and s -channels was also generated with POWHEG-Box v2 interfaced with PYTHIA 6.428, while single top production in the t -channel was generated with POWHEG-Box v1 interfaced with PYTHIA 6.428 for the parton shower and hadronisation. Single-top samples were generated using the PERUGIA2012 tune and the CT10 PDF set. The single top cross-sections for the t - and s -channels are normalised to their next-to-leading-order (NLO) predictions, while for the Wt -channel the cross-section is normalised to its NLO+NNLL prediction [44]. For W +jets, Z +jets, and diboson (WW , WZ , ZZ) samples, the SHERPA 2.2.1 generator [45] was used with the CT10 PDF set. The W +jets and Z +jets production samples are normalised to the NNLO cross-sections [46–48]. For diboson production, the generator cross-sections (already at NLO) are used for sample normalisation. The $t\bar{t}+V$ background is modelled using samples produced with MG5_AMC@NLO 2.1.1 interfaced with PYTHIA 8.186, using the A14 tune and the NNPDF2.3 LO PDF set. The $t\bar{t}+V$ samples are normalised to their respective NLO cross-sections [43].

All simulated samples were produced using the ATLAS simulation infrastructure [49], using the full GEANT4 [50] simulation of the ATLAS detector and reconstructed with the same software as used for the data. Multiple overlaid proton–proton collisions in the same or nearby bunch crossings (pile-up) were simulated at rates matching that of the data; they were modelled as low p_T multi-jet production using the PYTHIA 8.186 generator and tune A2 [51].

4 Analysis object selection

Reconstructed objects are defined by combining information from different detector subsystems. This section outlines the criteria used to identify and select the reconstructed objects used in the analysis. Events are required to have at least one vertex candidate with at least two tracks with $p_T > 500$ MeV. The primary vertex is taken to be the vertex candidate with the largest sum of squared transverse momenta of all associated tracks.

To reconstruct jets, three-dimensional energy clusters in the calorimeter, assumed to represent massless particles coming from the primary vertex, are grouped together using the anti- k_t clustering algorithm [52–54] with a radius parameter of 0.4 (1.0) for small- R (large- R) jets. Small- R jets and large- R jets are clustered independently.

Small- R jets are calibrated using an energy- and η -dependent calibration scheme, with *in situ* corrections based on data [55], and are selected if they have $p_T > 25$ GeV and $|\eta| < 2.5$. A multivariate jet vertex tagger (JVT) selectively removes small- R jets that are identified as having originated from pile-up collisions rather than the hard scatter [56]. Jets containing b -hadrons are identified via an algorithm that uses multivariate techniques to combine information from the impact parameters of displaced tracks as well as topological properties of secondary and tertiary decay vertices reconstructed within the jet. A jet is considered b -tagged if the value for the multivariate discriminant is above the threshold corresponding to an efficiency of 77% for tagging a b -quark-initiated jet. The corresponding light-jet rejection factor is ~ 130 and the charm-jet rejection factor is ~ 6 , as determined for jets with $p_T > 20$ GeV and $|\eta| < 2.5$ in simulated $t\bar{t}$ events.

Large- R jets are built using the energy clusters in the calorimeter [57, 58] and then trimmed [59] to mitigate the effects of contamination from multiple interactions and improve background rejection. The jet energy and pseudorapidity are further calibrated to account for residual detector effects using energy and pseudorapidity dependent calibration factors derived from simulation. The k_t -based trimming algorithm reclusters the jet constituents into subjects with a finer-grained resolution (the R -parameter for subjects is set to $R_{\text{sub}} = 0.2$). Subjects that contribute less than 5% to the p_T of the large- R jets are discarded. The properties (e.g. transverse momentum and invariant mass) of the jet are recalculated using only the constituents of the remaining subjects. Trimmed large- R jets are only considered if they have $p_T > 200$ GeV and $|\eta| < 2.0$. To identify large- R jets that are likely to have originated from the hadronic decay of W bosons (W_{had}) and not from the hadronic decay of top quarks or multi-jet background, jet substructure information is exploited using the ratio of the energy correlation functions $D_2^{\beta=1}$ [60, 61] and jet mass [58]. Selected large- R jets must pass both the substructure and mass requirements of the 50%-efficient W -tagging working point [18]. To reduce the contribution from the $t\bar{t}$ background, the W_{had} candidate must not overlap any b -tagged small- R jets within $\Delta R < 1.0$. If multiple large- R jets satisfy the above requirements, the one with a mass closest to the mass of the W boson is selected as the W_{had} candidate.

Electrons are reconstructed from energy deposits in the electromagnetic calorimeter matched to inner detector tracks. Electron candidates are required to satisfy likelihood-based identification criteria [62] and must have $p_T^{\text{lep}} > 30$ GeV and $|\eta| < 2.47$. Electron candidates in the transition region between the barrel and endcap electromagnetic calorimeters, $1.37 < |\eta| < 1.52$, are excluded from this analysis. A lepton isolation requirement is implemented by calculating the quantity $I_R = \sum_{\Delta R(\text{track,lep}) < R_{\text{cut}}} p_T^{\text{track}}$, where R_{cut} is the smaller of $10 \text{ GeV}/p_T^{\text{lep}}$ and 0.2; the track associated with the lepton is excluded from the calculation. The electron must satisfy $I_R < 0.06 \cdot p_T^{\text{lep}}$. Additionally, electrons are required to have a track

satisfying $\frac{|d_0|}{\sigma_{d_0}} < 5$ and $|z_0 \sin \theta| < 0.5$ mm, where d_0 is the transverse impact parameter and z_0 is the r - ϕ projection of the impact point onto the z -axis. An overlap-removal procedure prevents double-counting of energy between an electron and nearby jets by removing jets if the separation between the electron and jet is within $\Delta R < 0.2$ and removing electrons if the separation is within $0.2 < \Delta R < 0.4$. In addition, a large- R jet is removed if the separation between the electron and the large- R jet is within $\Delta R < 1.0$.

Muons are reconstructed from an inner detector track matched to muon spectrometer tracks or track segments [63]. Candidate muons are required to pass quality specifications based on information from the muon spectrometer and inner detector. Furthermore, muons are required to be isolated from detector activity using the same criterion that is applied to electrons and their associated tracks must satisfy $|z_0 \sin \theta| < 0.5$ mm and $\frac{|d_0|}{\sigma_{d_0}} < 3$. Muons are selected if they have $p_T > 30$ GeV and $|\eta| < 2.5$. An overlap-removal procedure is also applied to muons and jets. If a muon and a jet with at least three tracks are separated by $\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_T^\mu)$ the muon is removed; if the jet has fewer than three tracks, the jet is removed.

For a given reconstructed event, the magnitude of the negative vector sum of the p_T of all reconstructed leptons and small- R jets is defined as the missing transverse momentum (E_T^{miss}) [64]. An extra term is included to account for ‘soft’ energy from inner detector tracks that are not matched to any of the selected objects but are consistent with originating from the primary vertex.

The four-momentum of the neutrino can be analytically determined in each event using the missing transverse momentum vector \vec{E}_T^{miss} and assuming the lepton–neutrino system has an invariant mass equal to that of the W boson. Nearly half of the events are found to produce two complex solutions. When complex solutions are obtained, a real solution is determined by minimising a χ^2 parameter based on the difference between the mass of the lepton–neutrino system and the measured value of the W boson mass. In the case of two real solutions, the solution with the smaller absolute value of the longitudinal momentum is used.

5 Analysis strategy

This search targets the decay of pair-produced VLQs, $T\bar{T}$, where one T quark decays to Wb and the other decays to Wb , Zt or Ht . Since previous searches from ATLAS and CMS have excluded VLQs decaying to Wb at 95% confidence level (CL) for masses below 920 GeV, this search focuses on the decays of higher-mass VLQs. The final state consists of a high- p_T charged lepton and missing transverse momentum from the decay of one of the W bosons, a high-momentum large- R jet from the hadronically decaying W boson, and multiple b -tagged jets. The event preselection is described in Section 5.1 and the reconstruction of the $T\bar{T}$ system is discussed in Section 5.2. The classification of events into signal and control regions follows in Section 5.3.

The search for the $B\bar{B}$ signal uses the same selection criteria, with no further optimization.

5.1 Event preselection

Events are required to pass a single-electron or single-muon trigger. The 2015 data were collected using electron triggers with E_T thresholds of 24, 60, and 120 GeV. The 2016 data were collected using electron triggers with E_T thresholds of 26, 60, and 140 GeV. For the 2015 electron triggers, the highest- E_T trigger

had a looser quality requirement on the trigger object than the triggers with lower E_T thresholds. For the 2016 electron triggers, the trigger with the lowest E_T threshold had stringent requirements on the quality of the trigger object, as well as requirements on its isolation from other activity in the detector. The highest and second highest E_T triggers had no requirement on isolation and had progressively looser quality requirements. Muon triggers with p_T thresholds of 20 (26) GeV and requirements on isolation were used in 2015 (2016). Additionally, a high- p_T muon trigger with a threshold of 50 GeV and no isolation requirement was used in both 2015 and 2016 data.

In addition to the trigger requirement, events must have at least one primary vertex with at least two associated tracks. Exactly one lepton candidate (electron or muon), as described in Section 4, is required. Signal events are expected to have a high jet multiplicity, since they include two b -jets as well as one jet from the hadronic decay of the W boson. Therefore, at least three small- R jets are required, of which at least one must be b -tagged. At least one boosted hadronic W candidate is required and the E_T^{miss} is required to be greater than 60 GeV.

After this selection, backgrounds with large contributions include $t\bar{t}$, W +jets, and single-top events. Other SM processes, including diboson, Z +jets, $t\bar{t}V$ and multi-jet production, make a smaller but non-negligible contribution; these small backgrounds are collectively referred to as ‘Others’.

5.2 $T\bar{T}$ reconstruction

After preselection, the four-momenta of the hadronic and semi-leptonic VLQ candidates are reconstructed using the selected lepton candidates, large- R jets, small- R jets, and missing transverse momentum of the event. VLQ candidates ($T \rightarrow Wb$) are formed by pairing each W boson candidate with a b -quark candidate. If there are two or more b -tagged jets in the event, the two highest- p_T b -tagged jets are selected as the b -quark candidates. Both possible pairings of the b -quark candidates with the W_{had} and semi-leptonically decaying W boson (W_{lep}) candidates are tested and the pairing that minimises the absolute value of the mass difference between the semi-leptonically and hadronically reconstructed VLQ candidates, $|\Delta m|$, is chosen. If the event has only one b -tagged jet, that jet is used as one of the b -quark candidates and then all permutations with the remaining small- R jets are tested to find the configuration that minimises $|\Delta m|$.

The final discriminating variable used in the statistical analysis is m_T^{lep} , the reconstructed mass of the semi-leptonically decaying vector-like T quark candidate. This is found to provide the best expected signal sensitivity. Figure 1 shows m_T^{lep} for benchmark T and B quark signal models and $t\bar{t}$ production in the signal region (defined in Section 5.3.1) after the reconstruction algorithm is applied. The reconstructed masses for the signal and $t\bar{t}$ background are shown to peak at the generated T and top-quark masses, respectively. The tails arise from misreconstructed T candidates. As expected, the reconstruction algorithm does not reconstruct the B mass, yet the variable nonetheless provides separation power between the signal and the $t\bar{t}$ background.

5.3 Classification of event topologies

A $t\bar{t}$ control region is used to constrain the production rate of $t\bar{t}$ events as well as systematic uncertainties related to $t\bar{t}$ modelling. The signal and control regions are described in detail in Section 5.3.1 and Section 5.3.2. The scalar sum of E_T^{miss} and the transverse momenta of the lepton and all small- R jets, S_T , and the separation between the lepton and neutrino, $\Delta R(\text{lep}, \nu)$, are used to define the two regions. These regions are shown in Figure 2 after applying the event pre-selection, and described below.

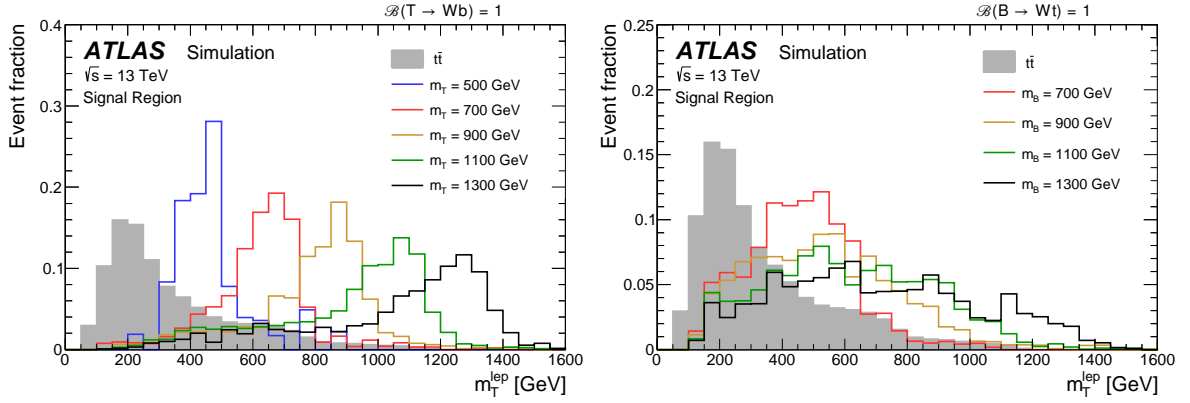


Figure 1: The reconstructed leptonic T quark mass in the signal region is shown for the $t\bar{t}$ background and a few signal mass points, for the signal models $\mathcal{B}(T \rightarrow Wb) = 1$ (left) and for the signal models $\mathcal{B}(B \rightarrow Wt) = 1$ (right). In both figures, the distributions are normalised to unity for comparison of the relative shapes at each mass point. Due to the limited Monte Carlo sample size, the $t\bar{t}$ distribution has been smoothed.

5.3.1 Signal region definition

After the event pre-selection described in Section 5.1, further requirements are applied to reduce the contribution of SM backgrounds relative to signal. Events in the signal region are selected based on their characteristic boosted topology with a high- p_T W boson and larger separation between the W boson and the b quarks. Events are required to have $\Delta R(\text{lep}, \nu) < 0.7$, arising from a boosted leptonically decaying W boson. In addition, S_T is required to be greater than 1800 GeV. This requirement is found to maximise the expected sensitivity to VLQ masses above 1 TeV. In order to reject both the $t\bar{t}$ and single-top (mostly Wt -channel) backgrounds, an additional requirement is put on the difference between the reconstructed masses of the leptonic and hadronic VLQ candidates, $|\Delta m| = |m_T^{\text{had}} - m_T^{\text{lep}}| < 300$ GeV; this selection criterion is optimised to provide the best expected sensitivity.

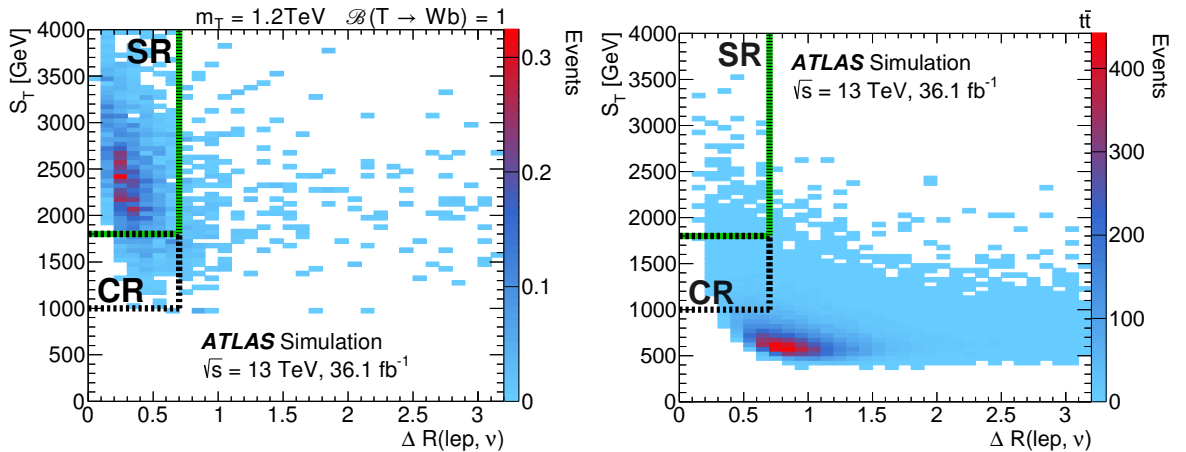


Figure 2: The signal region (SR) and control region (CR) are shown in a two-dimensional plane of S_T and $\Delta R(\text{lep}, \nu)$, overlaying the expected signal distribution for $\mathcal{B}(T \rightarrow Wb) = 1$ and a mass of 1.2 TeV (left) and overlaying the distribution of the dominant $t\bar{t}$ background (right).

The expected numbers of events in the signal region for the background processes and signal hypothesis with mass $m_T = 1$ TeV are shown in Table 1. For a signal model with $\mathcal{B}(T \rightarrow Wb) = 1$, the acceptance times efficiency of the full event selection ranges from 0.2% to 4.0% for VLQ masses from $m_T = 500$ to 1400 GeV. For the SU(2) singlet T scenario, for which $\mathcal{B}(T \rightarrow Wb)$ is approximately 50% for the mass range of interest, the signal acceptance ranges from 0.1% to 2.0%.

Table 1: Event yields for background sources and several signal models in the signal and control regions. The yields are given before the profile likelihood fit described in Section 7. The quoted uncertainties include statistical and systematic uncertainties; for the $t\bar{t}$ background no cross-section uncertainty is included. The contributions from dibosons, Z +jets, $t\bar{t}V$ and multi-jet production are included in the Others category.

Sample	Signal region	Control region
$t\bar{t}$	55 ± 26	720 ± 130
W +jets	9 ± 4	78 ± 41
Single top	15 ± 15	160 ± 110
Others	12 ± 10	82 ± 66
Total Background	91 ± 35	$1\,040 \pm 200$
Signal ($m_T = 1$ TeV, $\mathcal{B}(T \rightarrow Wb) = 1$)	45 ± 4	15 ± 2
Signal ($m_T = 1$ TeV, SU(2) singlet)	21 ± 2	8 ± 1
Signal ($m_B = 1$ TeV, $\mathcal{B}(B \rightarrow Wt) = 1$)	46 ± 4	21 ± 2
Signal ($m_B = 1$ TeV, SU(2) singlet)	18 ± 2	8 ± 1
Data	58	972

5.3.2 Control region definition

In this analysis, SM $t\bar{t}$ production is the dominant background process. To constrain the rate of $t\bar{t}$ production in the signal region, as well as to constrain some uncertainties related to $t\bar{t}$ modelling, a control region is included in the statistical analysis. This region is defined by only changing the requirement on S_T to $1000 \text{ GeV} < S_T < 1800 \text{ GeV}$. This window is chosen to be as close as possible to the signal region, while still retaining a large number of background events. Both the lower requirement on the control region and the requirement separating the signal and control regions were optimised to maximise the expected sensitivity to the signal with a mass of 1000 GeV and $\mathcal{B}(T \rightarrow Wb) = 1$.

5.4 Multi-jet background estimation

The multi-jet background originates from either the misidentification of a jet as a lepton candidate (fake lepton) or from the presence of a non-prompt lepton (e.g., from a semileptonic b - or c -hadron decay) that passes the isolation requirement. The multi-jet shape, normalisation, and related systematic uncertainties are estimated from data using the matrix method (MM) [65]. The MM exploits the difference in efficiency for prompt leptons to pass loose and tight quality requirements, obtained from W and Z boson decays, and non-prompt or fake lepton candidates, from the misidentification of photons or jets. The efficiencies, measured in dedicated control regions, are parameterised as functions of the lepton candidate p_T and η , $\Delta\phi$ between the lepton and jets, and the b -tagged jet multiplicity.

The event selection used in this analysis significantly reduces the contribution of the multi-jet background in the signal and control regions, to the point where statistical uncertainties make the MM prediction unreliable. In order to obtain a reliable prediction, the requirements on S_T and $\Delta R(\text{lep}, \nu)$ are released to 1200 GeV and 1.5, respectively. In this region the MM prediction and the small Monte Carlo derived backgrounds (diboson, Z +jets and $t\bar{t}V$) are studied and their shapes are found to be compatible. This selection is thus used to determine the ratio of the multi-jet production to the small Monte Carlo derived backgrounds. The ratio is then assumed to be the same in the signal and control regions and is used to scale those small MC derived backgrounds in order to account for the additional contribution from multi-jet backgrounds. This scaling was found to be stable under small changes to the definition of the looser selection. In the signal region, the contribution from the multi-jet background to the total background is around 6%.

6 Systematic uncertainties

The systematic uncertainties are broken down into four broad categories: luminosity and cross-section uncertainties, detector-related experimental uncertainties, uncertainties in data-driven background estimations, and modelling uncertainties in simulated background processes. Each source of uncertainty is treated as a nuisance parameter in the fit of the leptonic T mass distribution, and shape effects are taken into account where relevant. Due to the tight selection criteria applied, the analysis is limited by the statistical uncertainty; the systematic uncertainties only mildly degrade the sensitivity of the search.

6.1 Luminosity and normalisation uncertainties

The uncertainty in the combined 2015+2016 integrated luminosity is 3.2%. It is derived, following a methodology similar to that detailed in Ref. [24], from a preliminary calibration of the luminosity scale using x - y beam-separation scans performed in August 2015 and May 2016. This systematic uncertainty is applied to all backgrounds and signal that are estimated using simulated Monte Carlo events, which are normalised to the measured integrated luminosity.

Theoretical cross-section uncertainties are applied to the relevant simulated samples. The uncertainties for W/Z +jets and diboson production are 5% and 6%, respectively [47, 66]. For the largest of these backgrounds, W +jets, a total uncertainty of 50% in the normalisation is included. The pre-fit impact³ on the measured signal strength of the W +jets normalisation is less than 1%. Two additional shape uncertainties are also considered, related to the heavy-flavour content in the W +jets background. These uncertainties are derived by varying each heavy-flavour component of the W +jets background individually by a factor of 1.5, while keeping the overall normalisation fixed. For single top production, the uncertainties are taken as 6% [67, 68]. The normalisation of $t\bar{t}$ is unconstrained in the fit. For the data-driven multi-jet estimation, an uncertainty of 100% is assigned to the normalisation, corresponding to the maximum range obtained by varying the values of the cuts on S_T and $\Delta R(\text{lep}, \nu)$ when obtaining the multi-jet contribution to the ‘Others’ background.

³ The pre-fit effect on the signal strength parameter μ is calculated by fixing the corresponding uncertainty at $\theta \pm \sigma_\theta$, where θ is the initial value of the systematic uncertainty and σ_θ is its pre-fit uncertainty, and performing the fit again. The difference between the default and the modified value of μ , $\Delta\mu$, represents the effect on μ of this particular uncertainty (see section 7.1 for further details).

6.2 Detector-related uncertainties

The dominant sources of detector-related uncertainties in the signal and background yields relate to the small- R and large- R jet energy scales and resolutions. The small- R and large- R jet energy scales and their uncertainties are derived by combining information from test-beam data, LHC collision data and simulation [69]. In addition to energy scale and resolution uncertainties, there are also uncertainties in the large- R mass and substructure scales and resolutions. These are evaluated similarly to the jet energy scale and resolution uncertainties and are propagated to the W -tagging efficiencies. At $\sim 2\%$, the uncertainty in the jet energy resolution has the largest pre-fit impact on the measured signal strength, corresponding to a normalisation difference in the signal, $t\bar{t}$, and single top yields of 2%, 2%, and 14%, respectively.

Other detector-related uncertainties come from lepton trigger efficiencies, identification efficiencies, energy scales and resolutions, the $E_{\text{T}}^{\text{miss}}$ reconstruction, the b -tagging efficiency, and the JVT requirement. Uncertainties related to the efficiency for tagging c -jets have the largest pre-fit impact on the measured signal strength ($\sim 1\%$). This originates from a change in normalisation of $\sim 3\%$ on both the signal and background yields.

6.3 Generator modelling uncertainties

Modelling uncertainties are estimated for the dominant $t\bar{t}$ and single-top backgrounds. The modelling uncertainties are estimated by comparing simulated samples with different configurations, described in Section 3. The effects of extra initial and final state gluon radiation are estimated by comparing simulated samples generated with enhanced or reduced initial state radiation, changes to the h_{damp} parameter, and different radiation tunes. This uncertainty has a 12% normalisation impact on $t\bar{t}$ in the signal region, resulting in a pre-fit impact of $\sim 1\%$ on the measured signal strength. The uncertainty in the fragmentation, hadronisation and underlying-event modelling is estimated by comparing two different parton shower models, PYTHIA and HERWIG++, while keeping the same hard-scatter matrix-element generator. This causes an 18% shift in the normalisation of $t\bar{t}$ in the signal region, resulting in a pre-fit impact of $\sim 3\%$ on the measured signal strength. The uncertainty in the hard-scatter generation is estimated by comparing events generated with two different Monte Carlo generators, MG5_AMC@NLO and POWHEG, while keeping the same parton shower model. This uncertainty has a 38% normalisation impact on $t\bar{t}$ in the signal region, resulting in a pre-fit impact of only $\sim 4\%$ on the measured signal strength.

Modelling uncertainties in single top production are also included. In this analysis, Wt -channel production is the dominant contribution and the largest uncertainty comes from the method used to remove the overlap between NLO Wt production and LO $t\bar{t}$ production. The default method used is diagram removal, while the alternative method considered is diagram subtraction [70]. The full difference between the two methods is assigned as an uncertainty. This uncertainty has a 90% normalisation impact on single top in the signal region resulting in a pre-fit impact of $\sim 5\%$ on the measured signal strength.

7 Results

7.1 Statistical interpretation

The distribution of the reconstructed mass of the leptonically decaying T quark candidate, m_T^{lep} , in the signal and control regions is used to test for the presence of a signal. Hypothesis testing is performed using a modified frequentist method as implemented in RooStats [71, 72] and based on a profile likelihood which takes into account the systematic uncertainties as nuisance parameters that are fitted to the data.

The statistical analysis is based on a binned likelihood function $\mathcal{L}(\mu, \theta)$ constructed as a product of Poisson probability terms over all bins considered in the search. This function depends on the signal strength parameter μ , a multiplicative factor to the theoretical signal production cross-section, and θ , a set of nuisance parameters that encode the effect of systematic uncertainties in the signal and background expectations and are implemented in the likelihood function as Gaussian constraints. Uncertainties in each bin of the m_T^{lep} distributions due to finite size of the simulated samples are also taken into account via dedicated fit parameters and are propagated to μ . In this analysis, the normalisation of the dominant $t\bar{t}$ background is included as an unconstrained nuisance parameter; there are sufficient number of events in the control regions and low mass region of the signal region, where the signal contribution is small, to obtain a data-driven estimate of the $t\bar{t}$ normalisation. Nuisance parameters representing systematic uncertainties are only included in the likelihood if either of the following conditions are met: overall impact on the normalisation is larger than 1%, or the shape of the uncertainty varies by more than 1% between adjacent bins. This is done separately for each region and for each template (signal or background). When the bin-by-bin statistical variation of a given uncertainty is significant, a smoothing algorithm is applied.

The expected number of events in a given bin depends on μ and θ . The nuisance parameters θ adjust the expectations for signal and background according to the corresponding systematic uncertainties, and their fitted values correspond to the amounts that best fit the data. This procedure allows for a reduction of the impact of systematic uncertainties in the search sensitivity by taking advantage of the highly populated background-dominated control region (CR) included in the likelihood fit.

The test statistic q_μ is defined as the profile likelihood ratio, $q_\mu = -2\ln(\mathcal{L}(\mu, \hat{\theta}_\mu)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$, where $\hat{\mu}$ and $\hat{\theta}$ are the values of the parameters that maximise the likelihood function (with the constraint $0 \leq \hat{\mu} \leq \mu$), and $\hat{\theta}_\mu$ are the values of the nuisance parameters that maximise the likelihood function for a given value of μ . The compatibility of the observed data with the background-only hypothesis is tested by setting $\mu = 0$ in the profile likelihood ratio: $q_0 = -2\ln(\mathcal{L}(0, \hat{\theta}_0)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$. In the absence of any significant excess above the expected background, upper limits on the signal production cross-section for each of the signal scenarios considered are derived by using q_μ in the CL_s method [73, 74]. For a given signal scenario, values of the production cross-section (parameterised by μ) yielding CL_s < 0.05, where CL_s is computed using the asymptotic approximation [75], are excluded at $\geq 95\%$ CL.

7.2 Likelihood fit results

The expected and observed event yields in the signal and control regions after fitting the background-only hypothesis to data, including all uncertainties, are listed in Table 2. The total uncertainty shown in the table is the uncertainty obtained from the full fit, and is therefore not identical to the sum in quadrature of each component, due to the correlations between the fit parameters. The compatibility of the data with the

background-only hypothesis is estimated by integrating the distribution of the test statistic, approximated using the asymptotic formulae [75], above the observed value of q_0 . This value is computed for each signal scenario considered, defined by the assumed mass of the heavy quark and the three decay branching ratios. The lowest p -value is found to be $\sim 50\%$, for a T mass of 700 GeV. Thus no significant excess above the background expectation is found.

Table 2: Event yields in the signal and control regions after the background-only fit to the signal and control regions. The uncertainties include statistical and systematic uncertainties. The uncertainties in the individual background components can be larger than the uncertainty in the sum of the backgrounds, which is strongly constrained by the data.

Sample	Signal region	Control region
$t\bar{t}$	39 ± 10	700 ± 70
W +jets	8 ± 4	78 ± 38
Single top	7 ± 4	110 ± 40
Others	10 ± 7	72 ± 48
Total background	64 ± 9	970 ± 50
Data	58	972

The sensitivity of the analysis is limited by the statistical uncertainty of the data. Including all systematic uncertainties degrades the expected mass limits by only around 20 GeV and for a mass of 1 TeV, the cross-section limit increases by 4%. Individual uncertainties are generally not significantly constrained by data, except for the uncertainties associated with the $t\bar{t}$ modelling that are constrained by up to 50% of their initial size.

A comparison of the post-fit agreement between data and prediction in the signal region, Figure 3, shows a slight deficit of data in the signal region for the m_T^{lep} distribution above 700 GeV. In this context, the observed upper limits on the $T\bar{T}$ production cross-section are slightly stronger with respect to the expected sensitivity. The post-fit $t\bar{t}$ normalisation is found to be 0.93 ± 0.16 times the Monte Carlo prediction, normalised to the NNLO+NNLL cross-section.

7.3 Limits on VLQ pair production

Upper limits at the 95% CL on the $T\bar{T}$ production cross-section are set for two benchmark scenarios as a function of T quark mass m_T and compared to the theoretical prediction from Top++ v2.0 (Figure 4). The resulting lower limit on m_T is determined using the central value of the theoretical cross-section prediction. These results are only valid for new particles of narrow width. Assuming $\mathcal{B}(T \rightarrow Wb) = 1$, the observed (expected) lower limit is $m_T = 1350 \text{ GeV}$ (1310 GeV). For branching ratios corresponding to the SU(2) singlet T scenario, the observed (expected) 95% CL lower limit is $m_T = 1170 \text{ GeV}$ (1080 GeV). This represents a significant improvement compared to Run-1 searches [15, 16], for which the observed 95% CL limit was 920 GeV when assuming $\mathcal{B}(T \rightarrow Wb) = 1$.

To check that the results do not depend on the weak-isospin of the T quark in the simulated signal events, a sample of $T\bar{T}$ events with a mass of 1.2 TeV was generated for an SU(2) doublet T quark and compared to the nominal sample of the same mass generated with an SU(2) singlet T quark. Both the expected number of events and expected excluded cross-section are found to be consistent between those two

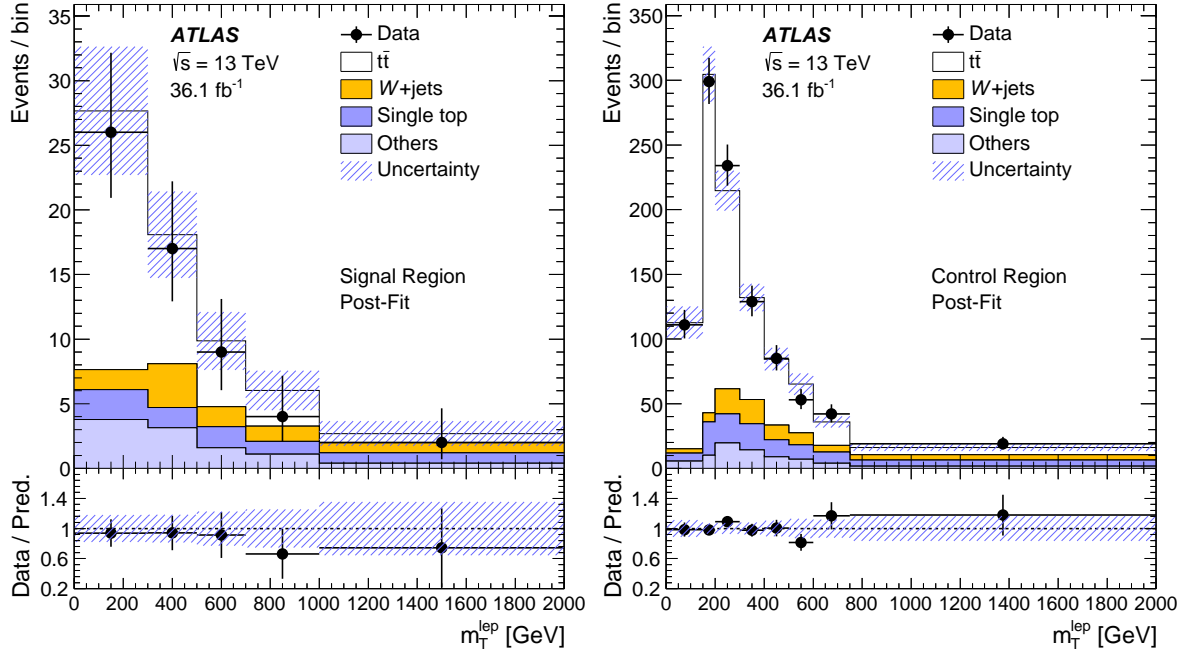


Figure 3: Fit results (background-only) for the leptonic VLQ candidate mass distributions (m_T^{lep}) in (left) the signal region and (right) the control region. The lower panel shows the ratio of data to the fitted background yields. The band represents the systematic uncertainty after the maximum-likelihood fit.

samples. Thus the limits obtained are also applicable to VLQ models with non-zero weak-isospin. As there is no explicit use of charge identification, the $\mathcal{B}(T \rightarrow Wb) = 1$ limits are found to be applicable to the pair-production of vector-like Y quarks of charge $-4/3$, which decay exclusively to Wb .

Exclusion limits on T quark pair-production are also obtained for different values of m_T and as a function of branching ratios to each of the three decays. In order to probe the complete branching-ratio plane spanned by both processes, the signal samples are weighted by the ratios of the respective branching ratios to the original branching ratios in `PROTOS`. Then, the complete analysis is repeated for each point in the \mathcal{B} plane. Figure 5 shows the corresponding expected and observed T quark mass limits in the plane $\mathcal{B}(T \rightarrow Ht)$ versus $\mathcal{B}(T \rightarrow Wb)$, obtained by linear interpolation of the calculated CL_s versus m_T .

In this search, the acceptance for VLQ $B\bar{B}$ pair production is $\sim 3\%$ for the $\mathcal{B}(B \rightarrow Wt) = 1$ scenario and $\sim 1.3\%$ for the $\text{SU}(2)$ singlet B scenario, which is similar to the $T\bar{T}$ final state. Nonetheless, the sensitivity to $B\bar{B}$ production is expected to be weaker, as the reconstructed T mass distribution is used as the final discriminant. Without any modifications to the analysis to specifically target $B\bar{B}$ production, observed (expected) lower limits at 95% CL are set at 1250 (1150) GeV when assuming $\mathcal{B}(B \rightarrow Wt) = 1$ and at 1080 (980) GeV for the $\text{SU}(2)$ singlet B scenario. This represents a significant improvement compared to Run-1 [76] and recent Run-2 searches [77] when assuming $\mathcal{B}(B \rightarrow Wt) = 1$, for which the observed 95% CL limit was 880 GeV and 1020 GeV, respectively. Being agnostic to the charge of the VLQ, the limits for $\mathcal{B}(B \rightarrow Wt) = 1$ are found to be applicable to vector-like X quarks of charge $+5/3$, which exclusively decay to Wt . Figure 6 shows the corresponding expected and observed B quark mass limits in the plane $\mathcal{B}(B \rightarrow Hb)$ versus $\mathcal{B}(B \rightarrow Wt)$, assuming $\mathcal{B}(B \rightarrow Hb) + \mathcal{B}(B \rightarrow Wt) + \mathcal{B}(B \rightarrow Zb) = 1$.

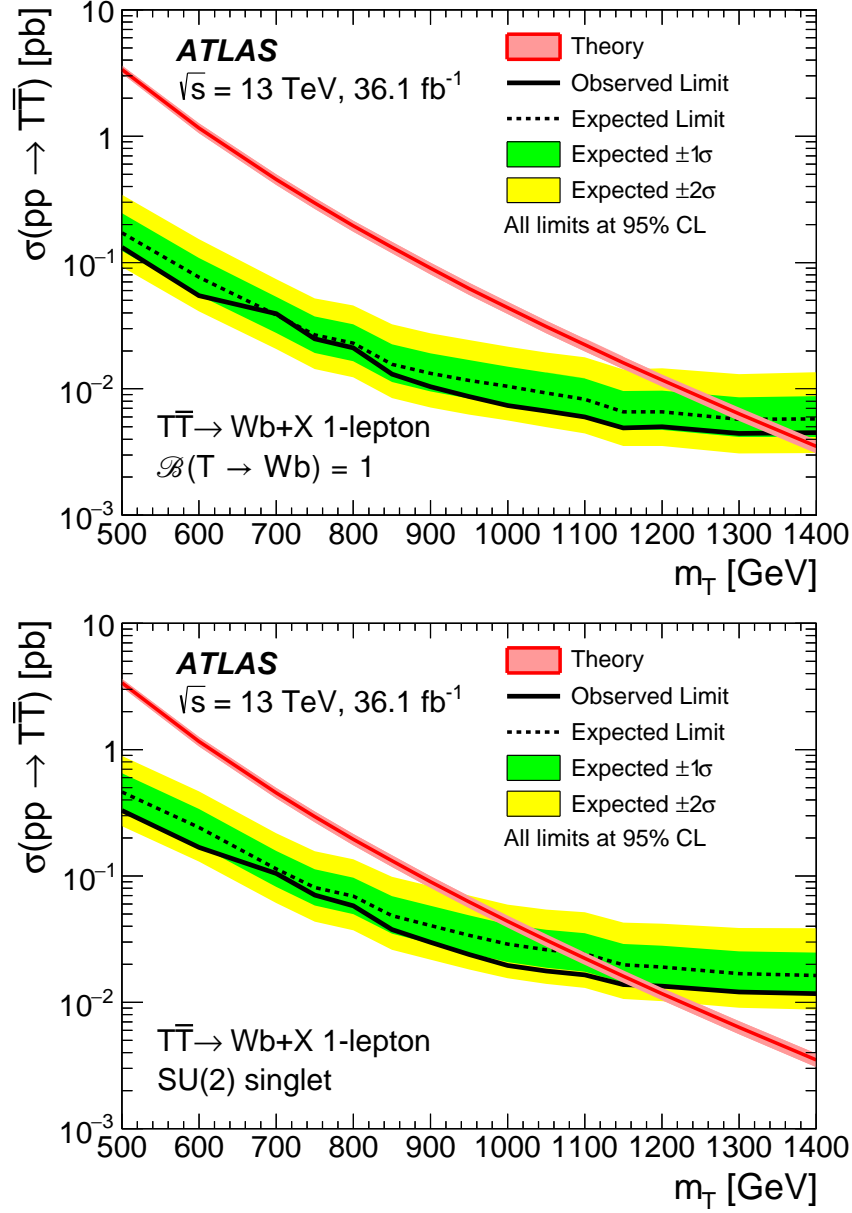


Figure 4: Expected (dashed black line) and observed (solid black line) upper limits at the 95% CL on the $T\bar{T}$ cross-section as a function of T quark mass assuming $\mathcal{B}(T \rightarrow Wb) = 1$ (top) and in the SU(2) singlet T scenario (bottom). The green and yellow bands correspond to ± 1 and ± 2 standard deviations around the expected limit. The thin red line and band show the theoretical prediction and its ± 1 standard deviation uncertainty.

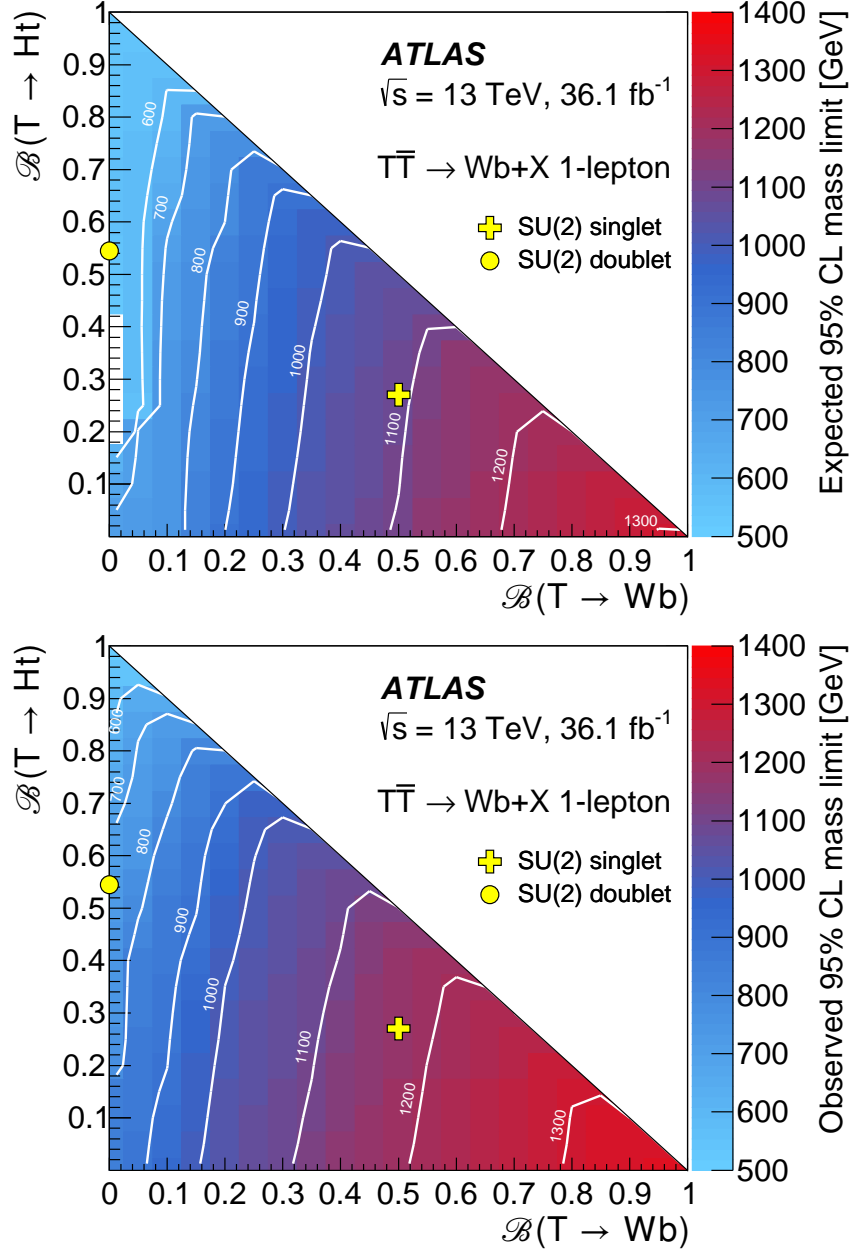


Figure 5: Expected (top) and observed (bottom) 95% CL lower limits on the mass of the T quark as a function of the decay branching ratios into $\mathcal{B}(T \rightarrow Wb)$ and $\mathcal{B}(T \rightarrow Ht)$. Contour lines are provided to guide the eye. The markers indicate the branching ratios for the SU(2) singlet and doublet scenarios with masses above $\sim 0.8 \text{ TeV}$, where they are approximately independent of the VLQ T mass. The white region is due to the limit falling below 500 GeV, the lowest simulated signal mass.

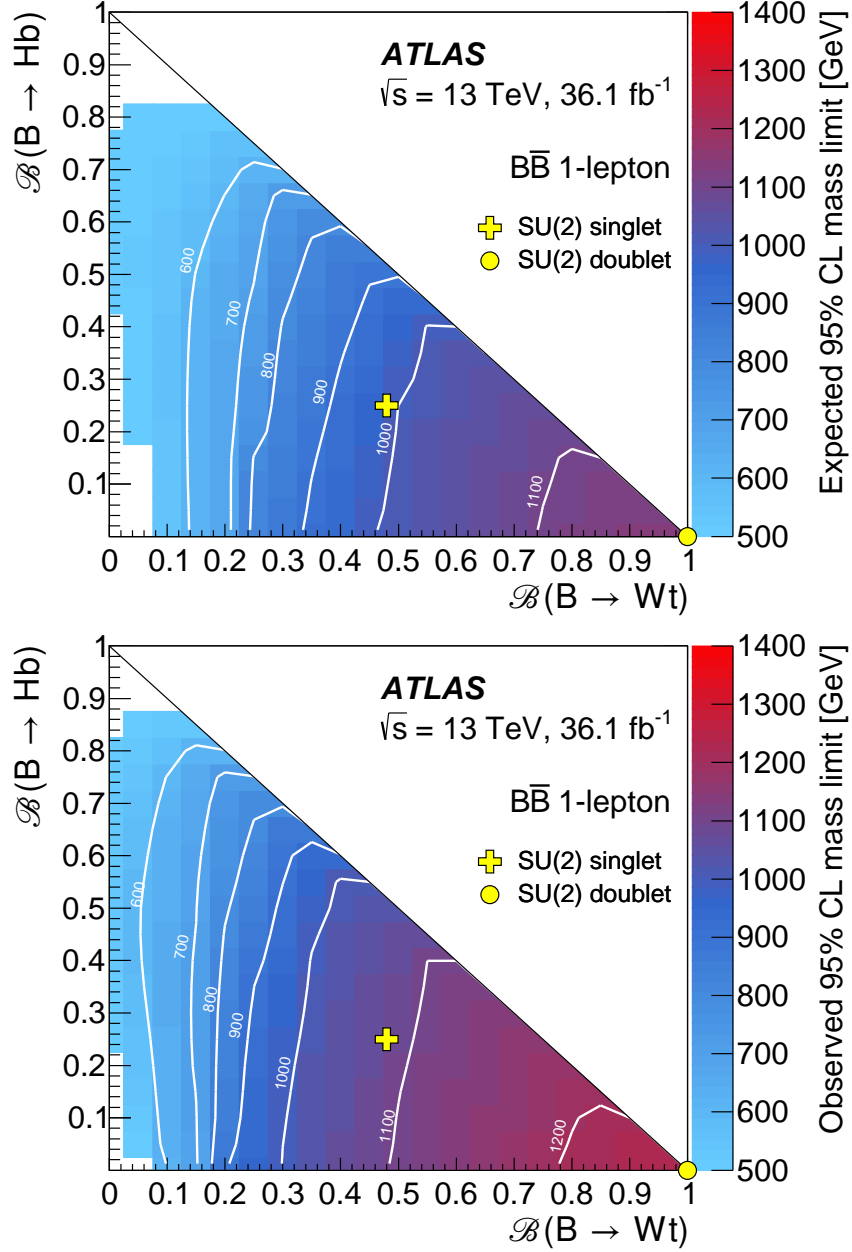


Figure 6: Expected (top) and observed (bottom) 95% CL lower limits on the mass of the B quark as a function of the decay branching ratios into $\mathcal{B}(B \rightarrow Wt)$ and $\mathcal{B}(B \rightarrow Hb)$. Contour lines are provided to guide the eye. The markers indicate the branching ratios for the SU(2) singlet and doublet scenarios with masses above $\sim 0.8 \text{ TeV}$, where they are approximately independent of the VLQ B mass. The white regions are due to the limit falling below 500 GeV, the lowest simulated signal mass.

8 Conclusions

A search for the pair production of a heavy vector-like T quark, based on pp collisions at $\sqrt{s} = 13$ TeV recorded in 2015 (3.2 fb^{-1}) and 2016 (32.9 fb^{-1}) with the ATLAS detector at the CERN Large Hadron Collider, is presented. Data are analysed in the lepton-plus-jets final state and no significant deviation from the Standard Model expectation is observed. Assuming a branching ratio $\mathcal{B}(T \rightarrow Wb) = 1$, the observed (expected) 95% CL lower limit on the vector-like quark mass is 1350 GeV (1310 GeV). For the scenario of an SU(2) singlet T quark, the observed (expected) mass limit is 1170 GeV (1080 GeV). Assuming the T quark can only decay to Wb , Zt and Ht , 95% CL lower limits are derived for various masses in the two-dimensional plane of $\mathcal{B}(T \rightarrow Wb)$ versus $\mathcal{B}(T \rightarrow Ht)$. This search is also reinterpreted to provide limits on B quark masses. These are found to be 1250 GeV (1150 GeV) assuming 100% branching ratio to Wt and 1080 GeV (980 GeV) under the SU(2) singlet B quark scenario. These limits are found to be equally applicable to VLQ Y quark and X quark production, that decay to Wb and Wt , respectively. Mass limits are also set as a function of the decay branching ratios $\mathcal{B}(T \rightarrow Hb)$ versus $\mathcal{B}(T \rightarrow Wt)$ assuming only the $B \rightarrow Wt$, $B \rightarrow Zb$ and $B \rightarrow Hb$ decay modes contribute.

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The ATLAS Collaboration

M. Aaboud^{137d}, G. Aad⁸⁸, B. Abbott¹¹⁵, O. Abidinov^{12,*}, B. Abeloos¹¹⁹, S.H. Abidi¹⁶¹, O.S. AbouZeid¹³⁹, N.L. Abraham¹⁵¹, H. Abramowicz¹⁵⁵, H. Abreu¹⁵⁴, R. Abreu¹¹⁸, Y. Abulaiti^{148a,148b}, B.S. Acharya^{167a,167b,a}, S. Adachi¹⁵⁷, L. Adamczyk^{41a}, J. Adelman¹¹⁰, M. Adersberger¹⁰², T. Adye¹³³, A.A. Affolder¹³⁹, Y. Afik¹⁵⁴, T. Agatonovic-Jovin¹⁴, C. Agheorghiesei^{28c}, J.A. Aguilar-Saavedra^{128a,128f}, S.P. Ahlen²⁴, F. Ahmadov^{68,b}, G. Aielli^{135a,135b}, S. Akatsuka⁷¹, H. Akerstedt^{148a,148b}, T.P.A. Åkesson⁸⁴, E. Akilli⁵², A.V. Akimov⁹⁸, G.L. Alberghi^{22a,22b}, J. Albert¹⁷², P. Albicocco⁵⁰, M.J. Alconada Verzini⁷⁴, S.C. Alderweireldt¹⁰⁸, M. Aleksa³², I.N. Aleksandrov⁶⁸, C. Alexa^{28b}, G. Alexander¹⁵⁵, T. Alexopoulos¹⁰, M. Alhroob¹¹⁵, B. Ali¹³⁰, M. Aliev^{76a,76b}, G. Alimonti^{94a}, J. Alison³³, S.P. Alkire³⁸, B.M.M. Allbrooke¹⁵¹, B.W. Allen¹¹⁸, P.P. Allport¹⁹, A. Aloisio^{106a,106b}, A. Alonso³⁹, F. Alonso⁷⁴, C. Alpigiani¹⁴⁰, A.A. Alshehri⁵⁶, M.I. Alstady⁸⁸, B. Alvarez Gonzalez³², D. Álvarez Piqueras¹⁷⁰, M.G. Alvigi^{106a,106b}, B.T. Amadio¹⁶, Y. Amaral Coutinho^{26a}, C. Amelung²⁵, D. Amidei⁹², S.P. Amor Dos Santos^{128a,128c}, S. Amoroso³², G. Amundsen²⁵, C. Anastopoulos¹⁴¹, L.S. Ancu⁵², N. Andari¹⁹, T. Andeen¹¹, C.F. Anders^{60b}, J.K. Anders⁷⁷, K.J. Anderson³³, A. Andreazza^{94a,94b}, V. Andrei^{60a}, S. Angelidakis³⁷, I. Angelozzi¹⁰⁹, A. Angerami³⁸, A.V. Anisenkov^{111,c}, N. Anjos¹³, A. Annovi^{126a,126b}, C. Antel^{60a}, M. Antonelli⁵⁰, A. Antonov^{100,*}, D.J. Antrim¹⁶⁶, F. Anulli^{134a}, M. Aoki⁶⁹, L. Aperio Bella³², G. Arabidze⁹³, Y. Arai⁶⁹, J.P. Araque^{128a}, V. Araujo Ferraz^{26a}, A.T.H. Arce⁴⁸, R.E. Ardell⁸⁰, F.A. Arduh⁷⁴, J-F. Arguin⁹⁷, S. Argyropoulos⁶⁶, M. Arik^{20a}, A.J. Armbruster³², L.J. Armitage⁷⁹, O. Arnaez¹⁶¹, H. Arnold⁵¹, M. Arratia³⁰, O. Arslan²³, A. Artamonov⁹⁹, G. Artoni¹²², S. Artz⁸⁶, S. Asai¹⁵⁷, N. Asbah⁴⁵, A. Ashkenazi¹⁵⁵, L. Asquith¹⁵¹, K. Assamagan²⁷, R. Astalos^{146a}, M. Atkinson¹⁶⁹, N.B. Atlay¹⁴³, K. Augsten¹³⁰, G. Avolio³², B. Axen¹⁶, M.K. Ayoub¹¹⁹, G. Azuelos^{97,d}, A.E. Baas^{60a}, M.J. Baca¹⁹, H. Bachacou¹³⁸, K. Bachas^{76a,76b}, M. Backes¹²², P. Bagnaia^{134a,134b}, M. Bahmani⁴², H. Bahrasemani¹⁴⁴, J.T. Baines¹³³, M. Bajic³⁹, O.K. Baker¹⁷⁹, E.M. Baldin^{111,c}, P. Balek¹⁷⁵, F. Balli¹³⁸, W.K. Balunas¹²⁴, E. Banas⁴², A. Bandyopadhyay²³, Sw. Banerjee^{176,e}, A.A.E. Bannoura¹⁷⁸, L. Barak¹⁵⁵, E.L. Barberio⁹¹, D. Barberis^{53a,53b}, M. Barbero⁸⁸, T. Barillari¹⁰³, M-S Barisits³², J.T. Barkeloo¹¹⁸, T. Barklow¹⁴⁵, N. Barlow³⁰, S.L. Barnes^{36c}, B.M. Barnett¹³³, R.M. Barnett¹⁶, Z. Barnovska-Blenessy^{36a}, A. Baroncelli^{136a}, G. Barone²⁵, A.J. Barr¹²², L. Barranco Navarro¹⁷⁰, F. Barreiro⁸⁵, J. Barreiro Guimarães da Costa^{35a}, R. Bartoldus¹⁴⁵, A.E. Barton⁷⁵, P. Bartos^{146a}, A. Basalae¹²⁵, A. Bassalat^{119,f}, R.L. Bates⁵⁶, S.J. Batista¹⁶¹, J.R. Batley³⁰, M. Battaglia¹³⁹, M. Bauce^{134a,134b}, F. Bauer¹³⁸, H.S. Bawa^{145,g}, J.B. Beacham¹¹³, M.D. Beattie⁷⁵, T. Beau⁸³, P.H. Beauchemin¹⁶⁵, P. Bechtel²³, H.P. Beck^{18,h}, H.C. Beck⁵⁷, K. Becker¹²², M. Becker⁸⁶, C. Becot¹¹², A.J. Beddall^{20e}, A. Beddall^{20b}, V.A. Bednyakov⁶⁸, M. Bedognetti¹⁰⁹, C.P. Bee¹⁵⁰, T.A. Beermann³², M. Begalli^{26a}, M. Begel²⁷, J.K. Behr⁴⁵, A.S. Bell⁸¹, G. Bella¹⁵⁵, L. Bellagamba^{22a}, A. Bellerive³¹, M. Bellomo¹⁵⁴, K. Belotskiy¹⁰⁰, O. Beltramello³², N.L. Belyaev¹⁰⁰, O. Benary^{155,*}, D. Bencheikroun^{137a}, M. Bender¹⁰², K. Bendtz^{148a,148b}, N. Benekos¹⁰, Y. Benhammou¹⁵⁵, E. Benhar Noccioli¹⁷⁹, J. Benitez⁶⁶, D.P. Benjamin⁴⁸, M. Benoit⁵², J.R. Bensinger²⁵, S. Bentvelsen¹⁰⁹, L. Beresford¹²², M. Beretta⁵⁰, D. Berge¹⁰⁹, E. Bergeas Kuutmann¹⁶⁸, N. Berger⁵, J. Beringer¹⁶, S. Berlendis⁵⁸, N.R. Bernard⁸⁹, G. Bernardi⁸³, C. Bernius¹⁴⁵, F.U. Bernlochner²³, T. Berry⁸⁰, P. Berta⁸⁶, C. Bertella^{35a}, G. Bertoli^{148a,148b}, F. Bertolucci^{126a,126b}, I.A. Bertram⁷⁵, C. Bertsche⁴⁵, D. Bertsche¹¹⁵, G.J. Besjes³⁹, O. Bessidskaia Bylund^{148a,148b}, M. Bessner⁴⁵, N. Besson¹³⁸, A. Bethani⁸⁷, S. Bethke¹⁰³, A.J. Bevan⁷⁹, J. Beyer¹⁰³, R.M. Bianchi¹²⁷, O. Biebel¹⁰², D. Biedermann¹⁷, R. Bielski⁸⁷, K. Bierwagen⁸⁶, N.V. Biesuz^{126a,126b}, M. Biglietti^{136a}, T.R.V. Billoud⁹⁷, H. Bilokon⁵⁰, M. Bindi⁵⁷, A. Bingul^{20b}, C. Bini^{134a,134b}, S. Biondi^{22a,22b}, T. Bisanz⁵⁷, C. Bittrich⁴⁷, D.M. Bjergaard⁴⁸, J.E. Black¹⁴⁵, K.M. Black²⁴, R.E. Blair⁶, T. Blazek^{146a}, I. Bloch⁴⁵, C. Blocker²⁵, A. Blue⁵⁶, W. Blum^{86,*},

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M. Curatolo⁵⁰, J. Cúth⁸⁶, S. Czekerda⁴², P. Czodrowski³², G. D'amen^{22a,22b}, S. D'Auria⁵⁶,
L. D'era⁸³, M. D'Onofrio⁷⁷, M.J. Da Cunha Sargedas De Sousa^{128a,128b}, C. Da Via⁸⁷,
W. Dabrowski^{41a}, T. Dado^{146a}, T. Dai⁹², O. Dale¹⁵, F. Dallaire⁹⁷, C. Dallapiccola⁸⁹, M. Dam³⁹,
J.R. Dandoy¹²⁴, M.F. Daneri²⁹, N.P. Dang¹⁷⁶, A.C. Daniells¹⁹, N.S. Dann⁸⁷, M. Danninger¹⁷¹,
M. Dano Hoffmann¹³⁸, V. Dao¹⁵⁰, G. Darbo^{53a}, S. Darmora⁸, J. Dassoulas³, A. Dattagupta¹¹⁸,
T. Daubney⁴⁵, W. Davey²³, C. David⁴⁵, T. Davidek¹³¹, D.R. Davis⁴⁸, P. Davison⁸¹, E. Dawe⁹¹,
I. Dawson¹⁴¹, K. De⁸, R. de Asmundis^{106a}, A. De Benedetti¹¹⁵, S. De Castro^{22a,22b}, S. De Cecco⁸³,
N. De Groot¹⁰⁸, P. de Jong¹⁰⁹, H. De la Torre⁹³, F. De Lorenzi⁶⁷, A. De Maria⁵⁷, D. De Pedis^{134a},
A. De Salvo^{134a}, U. De Sanctis^{135a,135b}, A. De Santo¹⁵¹, K. De Vasconcelos Corga⁸⁸,
J.B. De Vivie De Regie¹¹⁹, R. Debbe²⁷, C. Debenedetti¹³⁹, D.V. Dedovich⁶⁸, N. Dehghanian³,
I. Deigaard¹⁰⁹, M. Del Gaudio^{40a,40b}, J. Del Peso⁸⁵, D. Delgove¹¹⁹, F. Deliot¹³⁸, C.M. Delitzsch⁷,
A. Dell'Acqua³², L. Dell'Asta²⁴, M. Dell'Orso^{126a,126b}, M. Della Pietra^{106a,106b}, D. della Volpe⁵²,
M. Delmastro⁵, C. Delporte¹¹⁹, P.A. Delsart⁵⁸, D.A. DeMarco¹⁶¹, S. Demers¹⁷⁹, M. Demichev⁶⁸,
A. Demilly⁸³, S.P. Denisov¹³², D. Denysiuk¹³⁸, D. Derendarz⁴², J.E. Derkaoui^{137d}, F. Derue⁸³,
P. Dervan⁷⁷, K. Desch²³, C. Deterre⁴⁵, K. Dette¹⁶¹, M.R. Devesa²⁹, P.O. Deviveiros³², A. Dewhurst¹³³,
S. Dhaliwal²⁵, F.A. Di Bello⁵², A. Di Ciaccio^{135a,135b}, L. Di Ciaccio⁵, W.K. Di Clemente¹²⁴,
C. Di Donato^{106a,106b}, A. Di Girolamo³², B. Di Girolamo³², B. Di Micco^{136a,136b}, R. Di Nardo³²,
K.F. Di Petrillo⁵⁹, A. Di Simone⁵¹, R. Di Sipio¹⁶¹, D. Di Valentino³¹, C. Diaconu⁸⁸, M. Diamond¹⁶¹,
F.A. Dias³⁹, M.A. Diaz^{34a}, E.B. Diehl⁹², J. Dietrich¹⁷, S. Díez Cornell⁴⁵, A. Dimitrievska¹⁴,
J. Dingfelder²³, P. Dita^{28b}, S. Dita^{28b}, F. Dittus³², F. Djama⁸⁸, T. Djobava^{54b}, J.I. Djuvsland^{60a},
M.A.B. do Vale^{26c}, D. Dobos³², M. Dobre^{28b}, C. Doglioni⁸⁴, J. Dolejsi¹³¹, Z. Dolezal¹³¹,
M. Donadelli^{26d}, S. Donati^{126a,126b}, P. Dondero^{123a,123b}, J. Donini³⁷, J. Dopke¹³³, A. Doria^{106a},
M.T. Dova⁷⁴, A.T. Doyle⁵⁶, E. Drechsler⁵⁷, M. Dris¹⁰, Y. Du^{36b}, J. Duarte-Campderros¹⁵⁵,
A. Dubreuil⁵², E. Duchovni¹⁷⁵, G. Duckeck¹⁰², A. Ducourthial⁸³, O.A. Ducu^{97,p}, D. Duda¹⁰⁹,
A. Dudarev³², A.Ch. Dudder⁸⁶, E.M. Duffield¹⁶, L. Duflo¹¹⁹, M. Dührssen³², M. Dumancic¹⁷⁵,
A.E. Dumitriu^{28b}, A.K. Duncan⁵⁶, M. Dunford^{60a}, H. Duran Yildiz^{4a}, M. Düren⁵⁵, A. Durglishvili^{54b},
D. Duschinger⁴⁷, B. Dutta⁴⁵, M. Dyndal⁴⁵, B.S. Dziedzic⁴², C. Eckardt⁴⁵, K.M. Ecker¹⁰³, R.C. Edgar⁹²,
T. Eifert³², G. Eigen¹⁵, K. Einsweiler¹⁶, T. Ekelof¹⁶⁸, M. El Kacimi^{137c}, R. El Kosseifi⁸⁸,
V. Ellajosyula⁸⁸, M. Ellert¹⁶⁸, S. Elles⁵, F. Ellinghaus¹⁷⁸, A.A. Elliot¹⁷², N. Ellis³², J. Elmsheuser²⁷,
M. Elsing³², D. Emelianov¹³³, Y. Enari¹⁵⁷, O.C. Endner⁸⁶, J.S. Ennis¹⁷³, J. Erdmann⁴⁶, A. Ereditato¹⁸,
M. Ernst²⁷, S. Errede¹⁶⁹, M. Escalier¹¹⁹, C. Escobar¹⁷⁰, B. Esposito⁵⁰, O. Estrada Pastor¹⁷⁰,
A.I. Etienne¹³⁸, E. Etzion¹⁵⁵, H. Evans⁶⁴, A. Ezhilov¹²⁵, M. Ezzi^{137e}, F. Fabbri^{22a,22b}, L. Fabbri^{22a,22b},
V. Fabiani¹⁰⁸, G. Facini⁸¹, R.M. Fakhruddinov¹³², S. Falciano^{134a}, R.J. Falla⁸¹, J. Faltova³², Y. Fang^{35a},
M. Fanti^{94a,94b}, A. Farbin⁸, A. Farilla^{136a}, C. Farina¹²⁷, E.M. Farina^{123a,123b}, T. Farooque⁹³, S. Farrell¹⁶,
S.M. Farrington¹⁷³, P. Farthouat³², F. Fassi^{137e}, P. Fassnacht³², D. Fassouliotis⁹, M. Faucci Giannelli⁸⁰,
A. Favareto^{53a,53b}, W.J. Fawcett¹²², L. Fayard¹¹⁹, O.L. Fedin^{125,q}, W. Fedorko¹⁷¹, S. Feigl¹²¹,
L. Feligioni⁸⁸, C. Feng^{36b}, E.J. Feng³², H. Feng⁹², M.J. Fenton⁵⁶, A.B. Fenyuk¹³², L. Feremenga⁸,
P. Fernandez Martinez¹⁷⁰, S. Fernandez Perez¹³, J. Ferrando⁴⁵, A. Ferrari¹⁶⁸, P. Ferrari¹⁰⁹, R. Ferrari^{123a},
D.E. Ferreira de Lima^{60b}, A. Ferrer¹⁷⁰, D. Ferrere⁵², C. Ferretti⁹², F. Fiedler⁸⁶, A. Filipčič⁷⁸,
M. Filipuzzi⁴⁵, F. Filthaut¹⁰⁸, M. Fincke-Keeler¹⁷², K.D. Finelli¹⁵², M.C.N. Fiolhais^{128a,128c,r},
L. Fiorini¹⁷⁰, A. Fischer², C. Fischer¹³, J. Fischer¹⁷⁸, W.C. Fisher⁹³, N. Flaschel⁴⁵, I. Fleck¹⁴³,
P. Fleischmann⁹², R.R.M. Fletcher¹²⁴, T. Flick¹⁷⁸, B.M. Flierl¹⁰², L.R. Flores Castillo^{62a},
M.J. Flowerdew¹⁰³, G.T. Forcolin⁸⁷, A. Formica¹³⁸, F.A. Förster¹³, A. Forti⁸⁷, A.G. Foster¹⁹,
D. Fournier¹¹⁹, H. Fox⁷⁵, S. Fracchia¹⁴¹, P. Francavilla⁸³, M. Franchini^{22a,22b}, S. Franchino^{60a},
D. Francis³², L. Franconi¹²¹, M. Franklin⁵⁹, M. Frate¹⁶⁶, M. Fraternali^{123a,123b}, D. Freeborn⁸¹,
S.M. Fressard-Batraneanu³², B. Freund⁹⁷, D. Froidevaux³², J.A. Frost¹²², C. Fukunaga¹⁵⁸,
T. Fusayasu¹⁰⁴, J. Fuster¹⁷⁰, C. Gabaldon⁵⁸, O. Gabizon¹⁵⁴, A. Gabrielli^{22a,22b}, A. Gabrielli¹⁶,

G.P. Gach^{41a}, S. Gadatsch³², S. Gadomski⁸⁰, G. Gagliardi^{53a,53b}, L.G. Gagnon⁹⁷, C. Galea¹⁰⁸, B. Galhardo^{128a,128c}, E.J. Gallas¹²², B.J. Gallop¹³³, P. Gallus¹³⁰, G. Galster³⁹, K.K. Gan¹¹³, S. Ganguly³⁷, Y. Gao⁷⁷, Y.S. Gao^{145,g}, F.M. Garay Walls^{34a}, C. García¹⁷⁰, J.E. García Navarro¹⁷⁰, J.A. García Pascual^{35a}, M. Garcia-Sciveres¹⁶, R.W. Gardner³³, N. Garelli¹⁴⁵, V. Garonne¹²¹, A. Gascon Bravo⁴⁵, K. Gasnikova⁴⁵, C. Gatti⁵⁰, A. Gaudiello^{53a,53b}, G. Gaudio^{123a}, I.L. Gavrilenko⁹⁸, C. Gay¹⁷¹, G. Gaycken²³, E.N. Gazis¹⁰, C.N.P. Gee¹³³, J. Geisen⁵⁷, M. Geisen⁸⁶, M.P. Geisler^{60a}, K. Gellerstedt^{148a,148b}, C. Gemme^{53a}, M.H. Genest⁵⁸, C. Geng⁹², S. Gentile^{134a,134b}, C. Gentsos¹⁵⁶, S. George⁸⁰, D. Gerbaudo¹³, A. Gershon¹⁵⁵, G. Geßner⁴⁶, S. Ghasemi¹⁴³, M. Ghneimat²³, B. Giacobbe^{22a}, S. Giagu^{134a,134b}, N. Giangiacomi^{22a,22b}, P. Giannetti^{126a,126b}, S.M. Gibson⁸⁰, M. Gignac¹⁷¹, M. Gilchriese¹⁶, D. Gillberg³¹, G. Gilles¹⁷⁸, D.M. Gingrich^{3,d}, M.P. Giordani^{167a,167c}, F.M. Giorgi^{22a}, P.F. Giraud¹³⁸, P. Giromini⁵⁹, G. Giugliarelli^{167a,167c}, D. Giugni^{94a}, F. Giuli¹²², C. Giuliani¹⁰³, M. Giulini^{60b}, B.K. Gjølsten¹²¹, S. Gkaitatzis¹⁵⁶, I. Gkialas^{9,s}, E.L. Gkoukousis¹³, P. Gkoutoumis¹⁰, L.K. Gladilin¹⁰¹, C. Glasman⁸⁵, J. Glatzer¹³, P.C.F. Glaysheer⁴⁵, A. Glazov⁴⁵, M. Goblirsch-Kolb²⁵, J. Godlewski⁴², S. Goldfarb⁹¹, T. Golling⁵², D. Golubkov¹³², A. Gomes^{128a,128b,128d}, R. Gonçalo^{128a}, R. Goncalves Gama^{26a}, J. Goncalves Pinto Firmino Da Costa¹³⁸, G. Gonella⁵¹, L. Gonella¹⁹, A. Gongadze⁶⁸, S. González de la Hoz¹⁷⁰, S. Gonzalez-Sevilla⁵², L. Goossens³², P.A. Gorbounov⁹⁹, H.A. Gordon²⁷, I. Gorelov¹⁰⁷, B. Gorini³², E. Gorini^{76a,76b}, A. Gorišek⁷⁸, A.T. Goshaw⁴⁸, C. Gössling⁴⁶, M.I. Gostkin⁶⁸, C.A. Gottardo²³, C.R. Goudet¹¹⁹, D. Goujdami^{137c}, A.G. Goussiou¹⁴⁰, N. Govender^{147b,t}, E. Gozani¹⁵⁴, L. Graber⁵⁷, I. Grabowska-Bold^{41a}, P.O.J. Gradin¹⁶⁸, J. Gramling¹⁶⁶, E. Gramstad¹²¹, S. Grancagnolo¹⁷, V. Gratchev¹²⁵, P.M. Gravila^{28f}, C. Gray⁵⁶, H.M. Gray¹⁶, Z.D. Greenwood^{82,u}, C. Grefe²³, K. Gregersen⁸¹, I.M. Gregor⁴⁵, P. Grenier¹⁴⁵, K. Grevtsov⁵, J. Griffiths⁸, A.A. Grillo¹³⁹, K. Grimm⁷⁵, S. Grinstein^{13,v}, Ph. Gris³⁷, J.-F. Grivaz¹¹⁹, S. Groh⁸⁶, E. Gross¹⁷⁵, J. Grosse-Knetter⁵⁷, G.C. Grossi⁸², Z.J. Grout⁸¹, A. Grummer¹⁰⁷, L. Guan⁹², W. Guan¹⁷⁶, J. Guenther⁶⁵, F. Guescini^{163a}, D. Guest¹⁶⁶, O. Gueta¹⁵⁵, B. Gui¹¹³, E. Guido^{53a,53b}, T. Guillemin⁵, S. Guindon², U. Gul⁵⁶, C. Gumpert³², J. Guo^{36c}, W. Guo⁹², Y. Guo^{36a}, R. Gupta⁴³, S. Gupta¹²², G. Gustavino¹¹⁵, B.J. Gutelman¹⁵⁴, P. Gutierrez¹¹⁵, N.G. Gutierrez Ortiz⁸¹, C. Gutsche⁸¹, C. Guyot¹³⁸, M.P. Guzik^{41a}, C. Gwenlan¹²², C.B. Gwilliam⁷⁷, A. Haas¹¹², C. Haber¹⁶, H.K. Hadavand⁸, N. Haddad^{137e}, A. Hadeef⁸⁸, S. Hageböck²³, M. Hagihara¹⁶⁴, H. Hakobyan^{180,*}, M. Haleem⁴⁵, J. Haley¹¹⁶, G. Halladjian⁹³, G.D. Hallewell⁸⁸, K. Hamacher¹⁷⁸, P. Hamal¹¹⁷, K. Hamano¹⁷², A. Hamilton^{147a}, G.N. Hamity¹⁴¹, P.G. Hamnett⁴⁵, L. Han^{36a}, S. Han^{35a}, K. Hanagaki^{69,w}, K. Hanawa¹⁵⁷, M. Hance¹³⁹, B. Haney¹²⁴, P. Hanke^{60a}, J.B. Hansen³⁹, J.D. Hansen³⁹, M.C. Hansen²³, P.H. Hansen³⁹, K. Hara¹⁶⁴, A.S. Hard¹⁷⁶, T. Harenberg¹⁷⁸, F. Hariri¹¹⁹, S. Harkusha⁹⁵, R.D. Harrington⁴⁹, P.F. Harrison¹⁷³, N.M. Hartmann¹⁰², Y. Hasegawa¹⁴², A. Hasib⁴⁹, S. Hassani¹³⁸, S. Haug¹⁸, R. Hauser⁹³, L. Hauswald⁴⁷, L.B. Havener³⁸, M. Havranek¹³⁰, C.M. Hawkes¹⁹, R.J. Hawkings³², D. Hayakawa¹⁵⁹, D. Hayden⁹³, C.P. Hays¹²², J.M. Hays⁷⁹, H.S. Hayward⁷⁷, S.J. Haywood¹³³, S.J. Head¹⁹, T. Heck⁸⁶, V. Hedberg⁸⁴, L. Heelan⁸, S. Heer²³, K.K. Heidegger⁵¹, S. Heim⁴⁵, T. Heim¹⁶, B. Heinemann^{45,x}, J.J. Heinrich¹⁰², L. Heinrich¹¹², C. Heinz⁵⁵, J. Hejbal¹²⁹, L. Helary³², A. Held¹⁷¹, S. Hellman^{148a,148b}, C. Helsens³², R.C.W. Henderson⁷⁵, Y. Heng¹⁷⁶, S. Henkelmann¹⁷¹, A.M. Henriques Correia³², S. Henrot-Versille¹¹⁹, G.H. Herbert¹⁷, H. Herde²⁵, V. Herget¹⁷⁷, Y. Hernández Jiménez^{147c}, H. Herr⁸⁶, G. Herten⁵¹, R. Hertenberger¹⁰², L. Hervas³², T.C. Herwig¹²⁴, G.G. Hesketh⁸¹, N.P. Hessey^{163a}, J.W. Hetherly⁴³, S. Higashino⁶⁹, E. Higón-Rodríguez¹⁷⁰, K. Hildebrand³³, E. Hill¹⁷², J.C. Hill³⁰, K.H. Hiller⁴⁵, S.J. Hillier¹⁹, M. Hils⁴⁷, I. Hinchliffe¹⁶, M. Hirose⁵¹, D. Hirschbuehl¹⁷⁸, B. Hiti⁷⁸, O. Hladik¹²⁹, X. Hoad⁴⁹, J. Hobbs¹⁵⁰, N. Hod^{163a}, M.C. Hodgkinson¹⁴¹, P. Hodgson¹⁴¹, A. Hoecker³², M.R. Hoferkamp¹⁰⁷, F. Hoenig¹⁰², D. Hohn²³, T.R. Holmes³³, M. Homann⁴⁶, S. Honda¹⁶⁴, T. Honda⁶⁹, T.M. Hong¹²⁷, B.H. Hooberman¹⁶⁹, W.H. Hopkins¹¹⁸, Y. Horii¹⁰⁵, A.J. Horton¹⁴⁴, J.-Y. Hostachy⁵⁸, S. Hou¹⁵³, A. Hoummada^{137a}, J. Howarth⁸⁷, J. Hoya⁷⁴, M. Hrabovsky¹¹⁷, J. Hrdinka³², I. Hristova¹⁷, J. Hrivnac¹¹⁹, T. Hryn'ova⁵,

A. Hrynevich⁹⁶, P.J. Hsu⁶³, S.-C. Hsu¹⁴⁰, Q. Hu^{36a}, S. Hu^{36c}, Y. Huang^{35a}, Z. Hubacek¹³⁰, F. Hubaut⁸⁸, F. Huegging²³, T.B. Huffman¹²², E.W. Hughes³⁸, G. Hughes⁷⁵, M. Huhtinen³², P. Huo¹⁵⁰, N. Huseynov^{68,b}, J. Huston⁹³, J. Huth⁵⁹, G. Iacobucci⁵², G. Iakovidis²⁷, I. Ibragimov¹⁴³, L. Iconomidou-Fayard¹¹⁹, Z. Idrissi^{137e}, P. Iengo³², O. Igonkina^{109,y}, T. Iizawa¹⁷⁴, Y. Ikegami⁶⁹, M. Ikeno⁶⁹, Y. Ilchenko^{11,z}, D. Iliadis¹⁵⁶, N. Ilic¹⁴⁵, G. Introzzi^{123a,123b}, P. Ioannou^{9,*}, M. Iodice^{136a}, K. Iordanidou³⁸, V. Ippolito⁵⁹, M.F. Isacson¹⁶⁸, N. Ishijima¹²⁰, M. Ishino¹⁵⁷, M. Ishitsuka¹⁵⁹, C. Issever¹²², S. Istin^{20a}, F. Ito¹⁶⁴, J.M. Iturbe Ponce^{62a}, R. Iuppa^{162a,162b}, H. Iwasaki⁶⁹, J.M. Izen⁴⁴, V. Izzo^{106a}, S. Jabbar³, P. Jackson¹, R.M. Jacobs²³, V. Jain², K.B. Jakobi⁸⁶, K. Jakobs⁵¹, S. Jakobsen⁶⁵, T. Jakoubek¹²⁹, D.O. Jamin¹¹⁶, D.K. Jana⁸², R. Jansky⁵², J. Janssen²³, M. Janus⁵⁷, P.A. Janus^{41a}, G. Jarlskog⁸⁴, N. Javadov^{68,b}, T. Javůrek⁵¹, M. Javurkova⁵¹, F. Jeanneau¹³⁸, L. Jeanty¹⁶, J. Jejelava^{54a,aa}, A. Jelinskas¹⁷³, P. Jenni^{51,ab}, C. Jeske¹⁷³, S. Jézéquel⁵, H. Ji¹⁷⁶, J. Jia¹⁵⁰, H. Jiang⁶⁷, Y. Jiang^{36a}, Z. Jiang¹⁴⁵, S. Jiggins⁸¹, J. Jimenez Pena¹⁷⁰, S. Jin^{35a}, A. Jinaru^{28b}, O. Jinnouchi¹⁵⁹, H. Jivan^{147c}, P. Johansson¹⁴¹, K.A. Johns⁷, C.A. Johnson⁶⁴, W.J. Johnson¹⁴⁰, K. Jon-And^{148a,148b}, R.W.L. Jones⁷⁵, S.D. Jones¹⁵¹, S. Jones⁷, T.J. Jones⁷⁷, J. Jongmanns^{60a}, P.M. Jorge^{128a,128b}, J. Jovicevic^{163a}, X. Ju¹⁷⁶, A. Juste Rozas^{13,v}, M.K. Köhler¹⁷⁵, A. Kaczmarska⁴², M. Kado¹¹⁹, H. Kagan¹¹³, M. Kagan¹⁴⁵, S.J. Kahn⁸⁸, T. Kaji¹⁷⁴, E. Kajomovitz⁴⁸, C.W. Kalderon⁸⁴, A. Kaluza⁸⁶, S. Kama⁴³, A. Kamenshchikov¹³², N. Kanaya¹⁵⁷, L. Kanjir⁷⁸, V.A. Kantserov¹⁰⁰, J. Kanzaki⁶⁹, B. Kaplan¹¹², L.S. Kaplan¹⁷⁶, D. Kar^{147c}, K. Karakostas¹⁰, N. Karastathis¹⁰, M.J. Kareem⁵⁷, E. Karentzos¹⁰, S.N. Karpov⁶⁸, Z.M. Karpova⁶⁸, K. Karthik¹¹², V. Kartvelishvili⁷⁵, A.N. Karyukhin¹³², K. Kasahara¹⁶⁴, L. Kashif¹⁷⁶, R.D. Kass¹¹³, A. Kastanas¹⁴⁹, Y. Kataoka¹⁵⁷, C. Kato¹⁵⁷, A. Katre⁵², J. Katzy⁴⁵, K. Kawade⁷⁰, K. Kawagoe⁷³, T. Kawamoto¹⁵⁷, G. Kawamura⁵⁷, E.F. Kay⁷⁷, V.F. Kazanin^{111,c}, R. Keeler¹⁷², R. Kehoe⁴³, J.S. Keller³¹, E. Kellermann⁸⁴, J.J. Kempster⁸⁰, J. Kendrick¹⁹, H. Keoshkerian¹⁶¹, O. Kepka¹²⁹, B.P. Kerševan⁷⁸, S. Kersten¹⁷⁸, R.A. Keyes⁹⁰, M. Khader¹⁶⁹, F. Khalil-zada¹², A. Khanov¹¹⁶, A.G. Kharlamov^{111,c}, T. Kharlamova^{111,c}, A. Khodinov¹⁶⁰, T.J. Khoo⁵², V. Khovanskiy^{99,*}, E. Khramov⁶⁸, J. Khubua^{54b,ac}, S. Kido⁷⁰, C.R. Kilby⁸⁰, H.Y. Kim⁸, S.H. Kim¹⁶⁴, Y.K. Kim³³, N. Kimura¹⁵⁶, O.M. Kind¹⁷, B.T. King⁷⁷, D. Kirchmeier⁴⁷, J. Kirk¹³³, A.E. Kiryunin¹⁰³, T. Kishimoto¹⁵⁷, D. Kisielewska^{41a}, V. Kitali⁴⁵, O. Kivernyk⁵, E. Kladiva^{146b}, T. Klapdor-Kleingrothaus⁵¹, M.H. Klein³⁸, M. Klein⁷⁷, U. Klein⁷⁷, K. Kleinknecht⁸⁶, P. Klimek¹¹⁰, A. Klimentov²⁷, R. Klingenberg⁴⁶, T. Klingl²³, T. Klioutchnikova³², E.-E. Kluge^{60a}, P. Kluit¹⁰⁹, S. Kluth¹⁰³, E. Kneringer⁶⁵, E.B.F.G. Knoops⁸⁸, A. Knue¹⁰³, A. Kobayashi¹⁵⁷, D. Kobayashi¹⁵⁹, T. Kobayashi¹⁵⁷, M. Kobel⁴⁷, M. Kocian¹⁴⁵, P. Kodys¹³¹, T. Koffas³¹, E. Koffeman¹⁰⁹, N.M. Köhler¹⁰³, T. Koi¹⁴⁵, M. Kolb^{60b}, I. Koletsou⁵, A.A. Komar^{98,*}, T. Kondo⁶⁹, N. Kondrashova^{36c}, K. Köneke⁵¹, A.C. König¹⁰⁸, T. Kono^{69,ad}, R. Konoplich^{112,ae}, N. Konstantinidis⁸¹, R. Kopeliansky⁶⁴, S. Koperny^{41a}, A.K. Kopp⁵¹, K. Korcyl⁴², K. Kordas¹⁵⁶, A. Korn⁸¹, A.A. Korol^{111,c}, I. Korolkov¹³, E.V. Korolkova¹⁴¹, O. Kortner¹⁰³, S. Kortner¹⁰³, T. Kosek¹³¹, V.V. Kostyukhin²³, A. Kotwal⁴⁸, A. Koulouris¹⁰, A. Kourkumeli-Charalampidi^{123a,123b}, C. Kourkumelis⁹, E. Kourlitis¹⁴¹, V. Kouskoura²⁷, A.B. Kowalewska⁴², R. Kowalewski¹⁷², T.Z. Kowalski^{41a}, C. Kozakai¹⁵⁷, W. Kozanecki¹³⁸, A.S. Kozhin¹³², V.A. Kramarenko¹⁰¹, G. Kramberger⁷⁸, D. Krasnopevtsev¹⁰⁰, M.W. Krasny⁸³, A. Krasznahorkay³², D. Krauss¹⁰³, J.A. Kremer^{41a}, J. Kretzschmar⁷⁷, K. Kreutzfeldt⁵⁵, P. Krieger¹⁶¹, K. Krizka³³, K. Kroeninger⁴⁶, H. Kroha¹⁰³, J. Kroll¹²⁹, J. Kroll¹²⁴, J. Kroseberg²³, J. Krstic¹⁴, U. Kruchonak⁶⁸, H. Krüger²³, N. Krumnack⁶⁷, M.C. Kruse⁴⁸, T. Kubota⁹¹, H. Kucuk⁸¹, S. Kudah^{4b}, J.T. Kuechler¹⁷⁸, S. Kuehn³², A. Kugel^{60a}, F. Kuger¹⁷⁷, T. Kuhl⁴⁵, V. Kukhtin⁶⁸, R. Kukla⁸⁸, Y. Kulchitsky⁹⁵, S. Kuleshov^{34b}, Y.P. Kulinich¹⁶⁹, M. Kuna^{134a,134b}, T. Kunigo⁷¹, A. Kupco¹²⁹, T. Kupfer⁴⁶, O. Kuprash¹⁵⁵, H. Kurashige⁷⁰, L.L. Kurchaninov^{163a}, Y.A. Kurochkin⁹⁵, M.G. Kurth^{35a}, V. Kus¹²⁹, E.S. Kuwertz¹⁷², M. Kuze¹⁵⁹, J. Kvita¹¹⁷, T. Kwan¹⁷², D. Kyriazopoulos¹⁴¹, A. La Rosa¹⁰³, J.L. La Rosa Navarro^{26d}, L. La Rotonda^{40a,40b}, F. La Ruffa^{40a,40b}, C. Lacasta¹⁷⁰, F. Lacava^{134a,134b}, J. Lacey⁴⁵, H. Lacker¹⁷, D. Lacour⁸³, E. Ladygin⁶⁸, R. Lafaye⁵, B. Laforge⁸³, T. Lagouri¹⁷⁹, S. Lai⁵⁷,

S. Lammers⁶⁴, W. Lampl⁷, E. Lançon²⁷, U. Landgraf⁵¹, M.P.J. Landon⁷⁹, M.C. Lanfermann⁵²,
 V.S. Lang^{60a}, J.C. Lange¹³, R.J. Langenberg³², A.J. Lankford¹⁶⁶, F. Lanni²⁷, K. Lantzsch²³,
 A. Lanza^{123a}, A. Lapertosa^{53a,53b}, S. Laplace⁸³, J.F. Laporte¹³⁸, T. Lari^{94a}, F. Lasagni Manghi^{22a,22b},
 M. Lassnig³², T.S. Lau^{62a}, P. Laurelli⁵⁰, W. Lavrijsen¹⁶, A.T. Law¹³⁹, P. Laycock⁷⁷, T. Lazovich⁵⁹,
 M. Lazzaroni^{94a,94b}, B. Le⁹¹, O. Le Dortz⁸³, E. Le Guirrec⁸⁸, E.P. Le Quilleuc¹³⁸, M. LeBlanc¹⁷²,
 T. LeCompte⁶, F. Ledroit-Guillon⁵⁸, C.A. Lee²⁷, G.R. Lee^{133,af}, S.C. Lee¹⁵³, L. Lee⁵⁹, B. Lefebvre⁹⁰,
 G. Lefebvre⁸³, M. Lefebvre¹⁷², F. Legger¹⁰², C. Leggett¹⁶, G. Lehmann Miotto³², X. Lei⁷,
 W.A. Leight⁴⁵, M.A.L. Leite^{26d}, R. Leitner¹³¹, D. Lellouch¹⁷⁵, B. Lemmer⁵⁷, K.J.C. Leney⁸¹, T. Lenz²³,
 B. Lenzi³², R. Leone⁷, S. Leone^{126a,126b}, C. Leonidopoulos⁴⁹, G. Lerner¹⁵¹, C. Leroy⁹⁷,
 A.A.J. Lesage¹³⁸, C.G. Lester³⁰, M. Levchenko¹²⁵, J. Levêque⁵, D. Levin⁹², L.J. Levinson¹⁷⁵,
 M. Levy¹⁹, D. Lewis⁷⁹, B. Li^{36a,ag}, Changqiao Li^{36a}, H. Li¹⁵⁰, L. Li^{36c}, Q. Li^{35a}, Q. Li^{36a}, S. Li⁴⁸,
 X. Li^{36c}, Y. Li¹⁴³, Z. Liang^{35a}, B. Liberti^{135a}, A. Liblong¹⁶¹, K. Lie^{62c}, J. Liebal²³, W. Liebig¹⁵,
 A. Limosani¹⁵², S.C. Lin¹⁸², T.H. Lin⁸⁶, B.E. Lindquist¹⁵⁰, A.E. Lioni⁵², E. Lipeles¹²⁴, A. Lipniacka¹⁵,
 M. Lisovy^{60b}, T.M. Liss^{169,ah}, A. Lister¹⁷¹, A.M. Litke¹³⁹, B. Liu⁶⁷, H. Liu⁹², H. Liu²⁷, J.K.K. Liu¹²²,
 J. Liu^{36b}, J.B. Liu^{36a}, K. Liu⁸⁸, L. Liu¹⁶⁹, M. Liu^{36a}, Y.L. Liu^{36a}, Y. Liu^{36a}, M. Livan^{123a,123b},
 A. Lleres⁵⁸, J. Llorente Merino^{35a}, S.L. Lloyd⁷⁹, C.Y. Lo^{62b}, F. Lo Sterzo¹⁵³, E.M. Lobodzinska⁴⁵,
 P. Loch⁷, F.K. Loebinger⁸⁷, A. Loesle⁵¹, K.M. Loew²⁵, A. Loginov^{179,*}, T. Lohse¹⁷, K. Lohwasser¹⁴¹,
 M. Lokajicek¹²⁹, B.A. Long²⁴, J.D. Long¹⁶⁹, R.E. Long⁷⁵, L. Longo^{76a,76b}, K.A. Looper¹¹³,
 J.A. Lopez^{34b}, D. Lopez Mateos⁵⁹, I. Lopez Paz¹³, A. Lopez Solis⁸³, J. Lorenz¹⁰²,
 N. Lorenzo Martinez⁵, M. Losada²¹, P.J. Lösel¹⁰², X. Lou^{35a}, A. Lounis¹¹⁹, J. Love⁶, P.A. Love⁷⁵,
 H. Lu^{62a}, N. Lu⁹², Y.J. Lu⁶³, H.J. Lubatti¹⁴⁰, C. Luci^{134a,134b}, A. Lucotte⁵⁸, C. Luedtke⁵¹, F. Luehring⁶⁴,
 W. Lukas⁶⁵, L. Luminari^{134a}, O. Lundberg^{148a,148b}, B. Lund-Jensen¹⁴⁹, M.S. Lutz⁸⁹, P.M. Luzi⁸³,
 D. Lynn²⁷, R. Lysak¹²⁹, E. Lytken⁸⁴, F. Lyu^{35a}, V. Lyubushkin⁶⁸, H. Ma²⁷, L.L. Ma^{36b}, Y. Ma^{36b},
 G. Maccarrone⁵⁰, A. Macchiolo¹⁰³, C.M. Macdonald¹⁴¹, B. Maček⁷⁸, J. Machado Miguens^{124,128b},
 D. Madaffari¹⁷⁰, R. Madar³⁷, W.F. Mader⁴⁷, A. Madsen⁴⁵, J. Maeda⁷⁰, S. Maeland¹⁵, T. Maeno²⁷,
 A.S. Maevskiy¹⁰¹, V. Magerl⁵¹, J. Mahlstedt¹⁰⁹, C. Maiani¹¹⁹, C. Maidantchik^{26a}, A.A. Maier¹⁰³,
 T. Maier¹⁰², A. Maio^{128a,128b,128d}, O. Majersky^{146a}, S. Majewski¹¹⁸, Y. Makida⁶⁹, N. Makovec¹¹⁹,
 B. Malaescu⁸³, Pa. Malecki⁴², V.P. Maleev¹²⁵, F. Malek⁵⁸, U. Mallik⁶⁶, D. Malon⁶, C. Malone³⁰,
 S. Maltezos¹⁰, S. Malyukov³², J. Mamuzic¹⁷⁰, G. Mancini⁵⁰, I. Mandić⁷⁸, J. Maneira^{128a,128b},
 L. Manhaes de Andrade Filho^{26b}, J. Manjarres Ramos⁴⁷, K.H. Mankinen⁸⁴, A. Mann¹⁰², A. Manousos³²,
 B. Mansoulie¹³⁸, J.D. Mansour^{35a}, R. Mantifel⁹⁰, M. Mantoani⁵⁷, S. Manzoni^{94a,94b}, L. Mapelli³²,
 G. Marceca²⁹, L. March⁵², L. Marchese¹²², G. Marchiori⁸³, M. Marcisovsky¹²⁹, M. Marjanovic³⁷,
 D.E. Marley⁹², F. Marroquim^{26a}, S.P. Marsden⁸⁷, Z. Marshall¹⁶, M.U.F. Martensson¹⁶⁸,
 S. Marti-Garcia¹⁷⁰, C.B. Martin¹¹³, T.A. Martin¹⁷³, V.J. Martin⁴⁹, B. Martin dit Latour¹⁵,
 M. Martinez^{13,v}, V.I. Martinez Outschoorn¹⁶⁹, S. Martin-Haugh¹³³, V.S. Martoiu^{28b}, A.C. Martyniuk⁸¹,
 A. Marzin³², L. Masetti⁸⁶, T. Mashimo¹⁵⁷, R. Mashinistov⁹⁸, J. Masik⁸⁷, A.L. Maslennikov^{111,c},
 L. Massa^{135a,135b}, P. Mastrandrea⁵, A. Mastroberardino^{40a,40b}, T. Masubuchi¹⁵⁷, P. Mättig¹⁷⁸,
 J. Maurer^{28b}, S.J. Maxfield⁷⁷, D.A. Maximov^{111,c}, R. Mazini¹⁵³, I. Maznas¹⁵⁶, S.M. Mazza^{94a,94b},
 N.C. Mc Fadden¹⁰⁷, G. Mc Goldrick¹⁶¹, S.P. Mc Kee⁹², A. McCarn⁹², R.L. McCarthy¹⁵⁰,
 T.G. McCarthy¹⁰³, L.I. McClymont⁸¹, E.F. McDonald⁹¹, J.A. Mcfayden³², G. Mchedlidze⁵⁷,
 S.J. McMahon¹³³, P.C. McNamara⁹¹, R.A. McPherson^{172,o}, S. Meehan¹⁴⁰, T.J. Megy⁵¹, S. Mehlhase¹⁰²,
 A. Mehta⁷⁷, T. Meideck⁵⁸, K. Meier^{60a}, B. Meirose⁴⁴, D. Melini^{170,ai}, B.R. Mellado Garcia^{147c},
 J.D. Mellenthin⁵⁷, M. Melo^{146a}, F. Meloni¹⁸, A. Melzer²³, S.B. Menary⁸⁷, L. Meng⁷⁷, X.T. Meng⁹²,
 A. Mengarelli^{22a,22b}, S. Menke¹⁰³, E. Meoni^{40a,40b}, S. Mergelmeyer¹⁷, C. Merlassino¹⁸, P. Mermod⁵²,
 L. Merola^{106a,106b}, C. Meroni^{94a}, F.S. Merritt³³, A. Messina^{134a,134b}, J. Metcalfe⁶, A.S. Mete¹⁶⁶,
 C. Meyer¹²⁴, J-P. Meyer¹³⁸, J. Meyer¹⁰⁹, H. Meyer Zu Theenhausen^{60a}, F. Miano¹⁵¹, R.P. Middleton¹³³,
 S. Miglioranzi^{53a,53b}, L. Mijović⁴⁹, G. Mikenberg¹⁷⁵, M. Mikestikova¹²⁹, M. Mikuž⁷⁸, M. Milesi⁹¹,

A. Milic¹⁶¹, D.A. Millar⁷⁹, D.W. Miller³³, C. Mills⁴⁹, A. Milov¹⁷⁵, D.A. Milstead^{148a,148b},
 A.A. Minaenko¹³², Y. Minami¹⁵⁷, I.A. Minashvili⁶⁸, A.I. Mincer¹¹², B. Mindur^{41a}, M. Mineev⁶⁸,
 Y. Minegishi¹⁵⁷, Y. Ming¹⁷⁶, L.M. Mir¹³, K.P. Mistry¹²⁴, T. Mitani¹⁷⁴, J. Mitrevski¹⁰², V.A. Mitsou¹⁷⁰,
 A. Miucci¹⁸, P.S. Miyagawa¹⁴¹, A. Mizukami⁶⁹, J.U. Mjörnmark⁸⁴, T. Mkrtchyan¹⁸⁰,
 M. Mlynarikova¹³¹, T. Moa^{148a,148b}, K. Mochizuki⁹⁷, P. Mogg⁵¹, S. Mohapatra³⁸, S. Molander^{148a,148b},
 R. Moles-Valls²³, M.C. Mondragon⁹³, K. Mönig⁴⁵, J. Monk³⁹, E. Monnier⁸⁸, A. Montalbano¹⁵⁰,
 J. Montejó Berlingen³², F. Monticelli⁷⁴, S. Monzani^{94a,94b}, R.W. Moore³, N. Morange¹¹⁹, D. Moreno²¹,
 M. Moreno Llácer³², P. Moretini^{53a}, S. Morgenstern³², D. Mori¹⁴⁴, T. Mori¹⁵⁷, M. Morii⁵⁹,
 M. Morinaga¹⁷⁴, V. Morisbak¹²¹, A.K. Morley³², G. Mornacchi³², J.D. Morris⁷⁹, L. Morvaj¹⁵⁰,
 P. Moschovakos¹⁰, M. Mosidze^{54b}, H.J. Moss¹⁴¹, J. Moss^{145,aj}, K. Motohashi¹⁵⁹, R. Mount¹⁴⁵,
 E. Mountricha²⁷, E.J.W. Moyse⁸⁹, S. Muanza⁸⁸, F. Mueller¹⁰³, J. Mueller¹²⁷, R.S.P. Mueller¹⁰²,
 D. Muenstermann⁷⁵, P. Mullen⁵⁶, G.A. Mullier¹⁸, F.J. Munoz Sanchez⁸⁷, W.J. Murray^{173,133},
 H. Musheghyan³², M. Muškinja⁷⁸, A.G. Myagkov^{132,ak}, M. Myska¹³⁰, B.P. Nachman¹⁶,
 O. Nackenhorst⁵², K. Nagai¹²², R. Nagai^{69,ad}, K. Nagano⁶⁹, Y. Nagasaka⁶¹, K. Nagata¹⁶⁴, M. Nagel⁵¹,
 E. Nagy⁸⁸, A.M. Nairz³², Y. Nakahama¹⁰⁵, K. Nakamura⁶⁹, T. Nakamura¹⁵⁷, I. Nakano¹¹⁴,
 R.F. Naranjo Garcia⁴⁵, R. Narayan¹¹, D.I. Narrias Villar^{60a}, I. Naryshkin¹²⁵, T. Naumann⁴⁵,
 G. Navarro²¹, R. Nayyar⁷, H.A. Neal⁹², P.Yu. Nechaeva⁹⁸, T.J. Neep¹³⁸, A. Negri^{123a,123b}, M. Negrini^{22a},
 S. Nektarijevic¹⁰⁸, C. Nellist¹¹⁹, A. Nelson¹⁶⁶, M.E. Nelson¹²², S. Nemecek¹²⁹, P. Nemethy¹¹²,
 M. Nessi^{32,al}, M.S. Neubauer¹⁶⁹, M. Neumann¹⁷⁸, P.R. Newman¹⁹, T.Y. Ng^{62c}, T. Nguyen Manh⁹⁷,
 R.B. Nickerson¹²², R. Nicolaidou¹³⁸, J. Nielsen¹³⁹, V. Nikolaenko^{132,ak}, I. Nikolic-Audit⁸³,
 K. Nikolopoulos¹⁹, J.K. Nilsen¹²¹, P. Nilsson²⁷, Y. Ninomiya¹⁵⁷, A. Nisati^{134a}, N. Nishu^{35c}, R. Nisius¹⁰³,
 I. Nitsche⁴⁶, T. Nitta¹⁷⁴, T. Nobe¹⁵⁷, Y. Noguchi⁷¹, M. Nomachi¹²⁰, I. Nomidis³¹, M.A. Nomura²⁷,
 T. Nooney⁷⁹, M. Nordberg³², N. Norjoharuddeen¹²², O. Novgorodova⁴⁷, S. Nowak¹⁰³, M. Nozaki⁶⁹,
 L. Nozka¹¹⁷, K. Ntekas¹⁶⁶, E. Nurse⁸¹, F. Nuti⁹¹, K. O'connor²⁵, D.C. O'Neil¹⁴⁴, A.A. O'Rourke⁴⁵,
 V. O'Shea⁵⁶, F.G. Oakham^{31,d}, H. Oberlack¹⁰³, T. Obermann²³, J. Ocariz⁸³, A. Ochi⁷⁰, I. Ochoa³⁸,
 J.P. Ochoa-Ricoux^{34a}, S. Oda⁷³, S. Odaka⁶⁹, A. Oh⁸⁷, S.H. Oh⁴⁸, C.C. Ohm¹⁶, H. Ohman¹⁶⁸,
 H. Oide^{53a,53b}, H. Okawa¹⁶⁴, Y. Okumura¹⁵⁷, T. Okuyama⁶⁹, A. Olariu^{28b}, L.F. Oleiro Seabra^{128a},
 S.A. Olivares Pino^{34a}, D. Oliveira Damazio²⁷, A. Olszewski⁴², J. Olszowska⁴², A. Onofre^{128a,128e},
 K. Onogi¹⁰⁵, P.U.E. Onyisi^{11,z}, H. Oppen¹²¹, M.J. Oreglia³³, Y. Oren¹⁵⁵, D. Orestano^{136a,136b},
 N. Orlando^{62b}, R.S. Orr¹⁶¹, B. Osculati^{53a,53b,*}, R. Ospanov^{36a}, G. Otero y Garzon²⁹, H. Otono⁷³,
 M. Ouchrif^{137d}, F. Ould-Saada¹²¹, A. Ouraou¹³⁸, K.P. Oussoren¹⁰⁹, Q. Ouyang^{35a}, M. Owen⁵⁶,
 R.E. Owen¹⁹, V.E. Ozcan^{20a}, N. Ozturk⁸, K. Pachal¹⁴⁴, A. Pacheco Pages¹³, L. Pacheco Rodriguez¹³⁸,
 C. Padilla Aranda¹³, S. Pagan Griso¹⁶, M. Paganini¹⁷⁹, F. Paige²⁷, G. Palacino⁶⁴, S. Palazzo^{40a,40b},
 S. Palestini³², M. Palka^{41b}, D. Pallin³⁷, E.St. Panagiotopoulou¹⁰, I. Panagoulas¹⁰, C.E. Pandini^{126a,126b},
 J.G. Panduro Vazquez⁸⁰, P. Pani³², S. Panitkin²⁷, D. Pantea^{28b}, L. Paolozzi⁵², Th.D. Papadopoulou¹⁰,
 K. Papageorgiou^{9,s}, A. Paramonov⁶, D. Paredes Hernandez¹⁷⁹, A.J. Parker⁷⁵, M.A. Parker³⁰,
 K.A. Parker⁴⁵, F. Parodi^{53a,53b}, J.A. Parsons³⁸, U. Parzefall⁵¹, V.R. Pascuzzi¹⁶¹, J.M. Pasner¹³⁹,
 E. Pasqualucci^{134a}, S. Passaggio^{53a}, Fr. Pastore⁸⁰, S. Patariaia⁸⁶, J.R. Pater⁸⁷, T. Pauly³², B. Pearson¹⁰³,
 S. Pedraza Lopez¹⁷⁰, R. Pedro^{128a,128b}, S.V. Peleganchuk^{111,c}, O. Penc¹²⁹, C. Peng^{35a}, H. Peng^{36a},
 J. Penwell⁶⁴, B.S. Peralva^{26b}, M.M. Perego¹³⁸, D.V. Perepelitsa²⁷, F. Peri¹⁷, L. Perini^{94a,94b},
 H. Pernegger³², S. Perrella^{106a,106b}, R. Peschke⁴⁵, V.D. Peshekhonov^{68,*}, K. Peters⁴⁵, R.F.Y. Peters⁸⁷,
 B.A. Petersen³², T.C. Petersen³⁹, E. Petit⁵⁸, A. Petridis¹, C. Petridou¹⁵⁶, P. Petroff¹¹⁹, E. Petrollo^{134a},
 M. Petrov¹²², F. Petrucci^{136a,136b}, N.E. Pettersson⁸⁹, A. Peyaud¹³⁸, R. Pezoa^{34b}, F.H. Phillips⁹³,
 P.W. Phillips¹³³, G. Piacquadio¹⁵⁰, E. Pianori¹⁷³, A. Picazio⁸⁹, E. Piccaro⁷⁹, M.A. Pickering¹²²,
 R. Piegai²⁹, J.E. Pilcher³³, A.D. Pilkington⁸⁷, A.W.J. Pin⁸⁷, M. Pinamonti^{135a,135b}, J.L. Pinfold³,
 H. Pirumov⁴⁵, M. Pitt¹⁷⁵, L. Plazak^{146a}, M.-A. Pleier²⁷, V. Pleskot⁸⁶, E. Plotnikova⁶⁸, D. Pluth⁶⁷,
 P. Podberezko¹¹¹, R. Poettgen⁸⁴, R. Poggi^{123a,123b}, L. Poggioli¹¹⁹, I. Pogrebnyak⁹³, D. Pohl²³,

G. Polesello^{123a}, A. Poley⁴⁵, A. Policicchio^{40a,40b}, R. Polifka³², A. Polini^{22a}, C.S. Pollard⁵⁶, V. Polychronakos²⁷, K. Pommès³², D. Ponomarenko¹⁰⁰, L. Pontecorvo^{134a}, G.A. Popeneciu^{28d}, S. Pospisil¹³⁰, K. Potamianos¹⁶, I.N. Potrap⁶⁸, C.J. Potter³⁰, T. Poulsen⁸⁴, J. Poveda³², M.E. Pozo Astigarraga³², P. Pralavorio⁸⁸, A. Pranko¹⁶, S. Prell⁶⁷, D. Price⁸⁷, M. Primavera^{76a}, S. Prince⁹⁰, N. Proklova¹⁰⁰, K. Prokofiev^{62c}, F. Prokoshin^{34b}, S. Protopopescu²⁷, J. Proudfoot⁶, M. Przybycien^{41a}, A. Puri¹⁶⁹, P. Puzo¹¹⁹, J. Qian⁹², G. Qin⁵⁶, Y. Qin⁸⁷, A. Quadt⁵⁷, M. Queitsch-Maitland⁴⁵, D. Quilty⁵⁶, S. Raddum¹²¹, V. Radeka²⁷, V. Radescu¹²², S.K. Radhakrishnan¹⁵⁰, P. Radloff¹¹⁸, P. Rados⁹¹, F. Ragusa^{94a,94b}, G. Rahal¹⁸¹, J.A. Raine⁸⁷, S. Rajagopalan²⁷, C. Rangel-Smith¹⁶⁸, T. Rashid¹¹⁹, S. Raspopov⁵, M.G. Ratti^{94a,94b}, D.M. Rauch⁴⁵, F. Rauscher¹⁰², S. Rave⁸⁶, I. Ravinovich¹⁷⁵, J.H. Rawling⁸⁷, M. Raymond³², A.L. Read¹²¹, N.P. Readioff⁵⁸, M. Reale^{76a,76b}, D.M. Rebuzzi^{123a,123b}, A. Redelbach¹⁷⁷, G. Redlinger²⁷, R. Reece¹³⁹, R.G. Reed^{147c}, K. Reeves⁴⁴, L. Rehnisch¹⁷, J. Reichert¹²⁴, A. Reiss⁸⁶, C. Rembser³², H. Ren^{35a}, M. Rescigno^{134a}, S. Resconi^{94a}, E.D. Resseguie¹²⁴, S. Rettie¹⁷¹, E. Reynolds¹⁹, O.L. Rezanova^{111,c}, P. Reznicek¹³¹, R. Rezvani⁹⁷, R. Richter¹⁰³, S. Richter⁸¹, E. Richter-Was^{41b}, O. Ricken²³, M. Rideli⁸³, P. Rieck¹⁰³, C.J. Riegel¹⁷⁸, J. Rieger⁵⁷, O. Rifki¹¹⁵, M. Rijssenbeek¹⁵⁰, A. Rimoldi^{123a,123b}, M. Rimoldi¹⁸, L. Rinaldi^{22a}, G. Ripellino¹⁴⁹, B. Ristic³², E. Ritsch³², I. Riu¹³, F. Rizatdinova¹¹⁶, E. Rizvi⁷⁹, C. Rizzi¹³, R.T. Roberts⁸⁷, S.H. Robertson^{90,o}, A. Robichaud-Veronneau⁹⁰, D. Robinson³⁰, J.E.M. Robinson⁴⁵, A. Robson⁵⁶, E. Rocco⁸⁶, C. Roda^{126a,126b}, Y. Rodina^{88,am}, S. Rodriguez Bosca¹⁷⁰, A. Rodriguez Perez¹³, D. Rodriguez Rodriguez¹⁷⁰, S. Roe³², C.S. Rogan⁵⁹, O. Röhne¹²¹, J. Roloff⁵⁹, A. Romaniouk¹⁰⁰, M. Romano^{22a,22b}, S.M. Romano Saez³⁷, E. Romero Adam¹⁷⁰, N. Rompotis⁷⁷, M. Ronzani⁵¹, L. Roos⁸³, S. Rosati^{134a}, K. Rosbach⁵¹, P. Rose¹³⁹, N.-A. Rosien⁵⁷, E. Rossi^{106a,106b}, L.P. Rossi^{53a}, J.H.N. Rosten³⁰, R. Rosten¹⁴⁰, M. Rotaru^{28b}, J. Rothberg¹⁴⁰, D. Rousseau¹¹⁹, A. Rozanov⁸⁸, Y. Rozen¹⁵⁴, X. Ruan^{147c}, F. Rubbo¹⁴⁵, F. Rühr⁵¹, A. Ruiz-Martinez³¹, Z. Rurikova⁵¹, N.A. Rusakovich⁶⁸, H.L. Russell⁹⁰, J.P. Rutherford⁷, N. Ruthmann³², Y.F. Ryabov¹²⁵, M. Rybar¹⁶⁹, G. Rybkin¹¹⁹, S. Ryu⁶, A. Ryzhov¹³², G.F. Rzehorz⁵⁷, A.F. Saavedra¹⁵², G. Sabato¹⁰⁹, S. Sacerdoti²⁹, H.F.-W. Sadrozinski¹³⁹, R. Sadykov⁶⁸, F. Safai Tehrani^{134a}, P. Saha¹¹⁰, M. Sahinsoy^{60a}, M. Saimpert⁴⁵, M. Saito¹⁵⁷, T. Saito¹⁵⁷, H. Sakamoto¹⁵⁷, Y. Sakurai¹⁷⁴, G. Salamanna^{136a,136b}, J.E. Salazar Loyola^{34b}, D. Salek¹⁰⁹, P.H. Sales De Bruin¹⁶⁸, D. Salihagic¹⁰³, A. Salnikov¹⁴⁵, J. Salt¹⁷⁰, D. Salvatore^{40a,40b}, F. Salvatore¹⁵¹, A. Salvucci^{62a,62b,62c}, A. Salzburger³², D. Sammel⁵¹, D. Sampsonidis¹⁵⁶, D. Sampsonidou¹⁵⁶, J. Sánchez¹⁷⁰, V. Sanchez Martinez¹⁷⁰, A. Sanchez Pineda^{167a,167c}, H. Sandaker¹²¹, R.L. Sandbach⁷⁹, C.O. Sander⁴⁵, M. Sandhoff¹⁷⁸, C. Sandoval²¹, D.P.C. Sankey¹³³, M. Sannino^{53a,53b}, Y. Sano¹⁰⁵, A. Sansoni⁵⁰, C. Santoni³⁷, H. Santos^{128a}, I. Santoyo Castillo¹⁵¹, A. Saponov⁶⁸, J.G. Saraiva^{128a,128d}, B. Sarrazin²³, O. Sasaki⁶⁹, K. Sato¹⁶⁴, E. Sauvan⁵, G. Savage⁸⁰, P. Savard^{161,d}, N. Savić¹⁰³, C. Sawyer¹³³, L. Sawyer^{82,u}, J. Saxon³³, C. Sbarra^{22a}, A. Sbrizzi^{22a,22b}, T. Scanlon⁸¹, D.A. Scannicchio¹⁶⁶, J. Schaarschmidt¹⁴⁰, P. Schacht¹⁰³, B.M. Schachtner¹⁰², D. Schaefer³², L. Schaefer¹²⁴, R. Schaefer⁴⁵, J. Schaeffer⁸⁶, S. Schaepe²³, S. Schaetzel^{60b}, U. Schäfer⁸⁶, A.C. Schaffer¹¹⁹, D. Schaile¹⁰², R.D. Schamberger¹⁵⁰, V.A. Schegelsky¹²⁵, D. Scheirich¹³¹, M. Schernau¹⁶⁶, C. Schiavi^{53a,53b}, S. Schier¹³⁹, L.K. Schildgen²³, C. Schillo⁵¹, M. Schioppa^{40a,40b}, S. Schlenker³², K.R. Schmidt-Sommerfeld¹⁰³, K. Schmieden³², C. Schmitt⁸⁶, S. Schmitt⁴⁵, S. Schmitz⁸⁶, U. Schnoor⁵¹, L. Schoeffel¹³⁸, A. Schoening^{60b}, B.D. Schoenrock⁹³, E. Schopf²³, M. Schott⁸⁶, J.F.P. Schouwenberg¹⁰⁸, J. Schovancova³², S. Schramm⁵², N. Schuh⁸⁶, A. Schulte⁸⁶, M.J. Schultens²³, H.-C. Schultz-Coulon^{60a}, H. Schulz¹⁷, M. Schumacher⁵¹, B.A. Schumm¹³⁹, Ph. Schune¹³⁸, A. Schwartzman¹⁴⁵, T.A. Schwarz⁹², H. Schweiger⁸⁷, Ph. Schwemling¹³⁸, R. Schwienhorst⁹³, J. Schwindling¹³⁸, A. Sciandra²³, G. Sciolla²⁵, M. Scornajenghi^{40a,40b}, F. Scuri^{126a,126b}, F. Scutti⁹¹, J. Searcy⁹², P. Seema²³, S.C. Seidel¹⁰⁷, A. Seiden¹³⁹, J.M. Seixas^{26a}, G. Sekhniaidze^{106a}, K. Sekhon⁹², S.J. Sekula⁴³, N. Semprini-Cesari^{22a,22b}, S. Senkin³⁷, C. Serfon¹²¹, L. Serin¹¹⁹, L. Serkin^{167a,167b}, M. Sessa^{136a,136b}, R. Seuster¹⁷², H. Severini¹¹⁵, T. Sfiligoj⁷⁸, F. Sforza¹⁶⁵,

A. Sfyrila⁵², E. Shabalina⁵⁷, N.W. Shaikh^{148a,148b}, L.Y. Shan^{35a}, R. Shang¹⁶⁹, J.T. Shank²⁴, M. Shapiro¹⁶,
 P.B. Shatalov⁹⁹, K. Shaw^{167a,167b}, S.M. Shaw⁸⁷, A. Shcherbakova^{148a,148b}, C.Y. Shehu¹⁵¹, Y. Shen¹¹⁵,
 N. Sherafati³¹, P. Sherwood⁸¹, L. Shi^{153,an}, S. Shimizu⁷⁰, C.O. Shimmin¹⁷⁹, M. Shimojima¹⁰⁴,
 I.P.J. Shipsey¹²², S. Shirabe⁷³, M. Shiyakova^{68,ao}, J. Shlomi¹⁷⁵, A. Shmeleva⁹⁸, D. Shoaleh Saadi⁹⁷,
 M.J. Shochet³³, S. Shojaii^{94a}, D.R. Shope¹¹⁵, S. Shrestha¹¹³, E. Shulga¹⁰⁰, M.A. Shupe⁷, P. Sicho¹²⁹,
 A.M. Sickles¹⁶⁹, P.E. Sidebo¹⁴⁹, E. Sideras Haddad^{147c}, O. Sidiropoulou¹⁷⁷, A. Sidoti^{22a,22b}, F. Siegert⁴⁷,
 Dj. Sijacki¹⁴, J. Silva^{128a,128d}, S.B. Silverstein^{148a}, V. Simak¹³⁰, Lj. Simic¹⁴, S. Simion¹¹⁹, E. Simioni⁸⁶,
 B. Simmons⁸¹, M. Simon⁸⁶, P. Sinervo¹⁶¹, N.B. Sinev¹¹⁸, M. Sioli^{22a,22b}, G. Siragusa¹⁷⁷, I. Siral⁹²,
 S.Yu. Sivoklov¹⁰¹, J. Sjölin^{148a,148b}, M.B. Skinner⁷⁵, P. Skubic¹¹⁵, M. Slater¹⁹, T. Slavicek¹³⁰,
 M. Slawinska⁴², K. Sliwa¹⁶⁵, R. Slovak¹³¹, V. Smakhtin¹⁷⁵, B.H. Smart⁵, J. Smiesko^{146a}, N. Smirnov¹⁰⁰,
 S.Yu. Smirnov¹⁰⁰, Y. Smirnov¹⁰⁰, L.N. Smirnova^{101,ap}, O. Smirnova⁸⁴, J.W. Smith⁵⁷, M.N.K. Smith³⁸,
 R.W. Smith³⁸, M. Smizanska⁷⁵, K. Smolek¹³⁰, A.A. Snesarev⁹⁸, I.M. Snyder¹¹⁸, S. Snyder²⁷,
 R. Sobie^{172,o}, F. Socher⁴⁷, A. Soffer¹⁵⁵, A. Søggaard⁴⁹, D.A. Soh¹⁵³, G. Sokhrannyi⁷⁸,
 C.A. Solans Sanchez³², M. Solar¹³⁰, E.Yu. Soldatov¹⁰⁰, U. Soldevila¹⁷⁰, A.A. Solodkov¹³²,
 A. Soloshenko⁶⁸, O.V. Solovyanov¹³², V. Solovyev¹²⁵, P. Sommer⁵¹, H. Son¹⁶⁵, A. Sopczak¹³⁰,
 D. Sosa^{60b}, C.L. Sotiropoulou^{126a,126b}, R. Soualah^{167a,167c}, A.M. Soukharev^{111,c}, D. South⁴⁵,
 B.C. Sowden⁸⁰, S. Spagnolo^{76a,76b}, M. Spalla^{126a,126b}, M. Spangenberg¹⁷³, F. Spanò⁸⁰, D. Sperlich¹⁷,
 F. Spettel¹⁰³, T.M. Spieker^{60a}, R. Spighi^{22a}, G. Spigo³², L.A. Spiller⁹¹, M. Spousta¹³¹, R.D. St. Denis^{56,*},
 A. Stabile^{94a}, R. Stamen^{60a}, S. Stamm¹⁷, E. Stanecka⁴², R.W. Stanek⁶, C. Stanescu^{136a},
 M.M. Stanitzki⁴⁵, B.S. Stapf¹⁰⁹, S. Stapnes¹²¹, E.A. Starchenko¹³², G.H. Stark³³, J. Stark⁵⁸, S.H. Stark³⁹,
 P. Staroba¹²⁹, P. Starovoitov^{60a}, S. Stärz³², R. Staszewski⁴², P. Steinberg²⁷, B. Stelzer¹⁴⁴, H.J. Stelzer³²,
 O. Stelzer-Chilton^{163a}, H. Stenzel⁵⁵, G.A. Stewart⁵⁶, M.C. Stockton¹¹⁸, M. Stoebe⁹⁰, G. Stoicea^{28b},
 P. Stolte⁵⁷, S. Stonjek¹⁰³, A.R. Stradling⁸, A. Straessner⁴⁷, M.E. Stramaglia¹⁸, J. Strandberg¹⁴⁹,
 S. Strandberg^{148a,148b}, M. Strauss¹¹⁵, P. Strizenec^{146b}, R. Ströhmer¹⁷⁷, D.M. Strom¹¹⁸, R. Stroynowski⁴³,
 A. Strubig⁴⁹, S.A. Stucci²⁷, B. Stugu¹⁵, N.A. Styles⁴⁵, D. Su¹⁴⁵, J. Su¹²⁷, S. Suchek^{60a}, Y. Sugaya¹²⁰,
 M. Suk¹³⁰, V.V. Sulin⁹⁸, DMS Sultan^{162a,162b}, S. Sultansoy^{4c}, T. Sumida⁷¹, S. Sun⁵⁹, X. Sun³,
 K. Suruliz¹⁵¹, C.J.E. Suster¹⁵², M.R. Sutton¹⁵¹, S. Suzuki⁶⁹, M. Svatos¹²⁹, M. Swiatkowski³³,
 S.P. Swift², I. Sykora^{146a}, T. Sykora¹³¹, D. Ta⁵¹, K. Tackmann⁴⁵, J. Taenzer¹⁵⁵, A. Taffard¹⁶⁶,
 R. Tafirout^{163a}, E. Tahirovic⁷⁹, N. Taiblum¹⁵⁵, H. Takai²⁷, R. Takashima⁷², E.H. Takasugi¹⁰³,
 T. Takeshita¹⁴², Y. Takubo⁶⁹, M. Talby⁸⁸, A.A. Talyshv^{111,c}, J. Tanaka¹⁵⁷, M. Tanaka¹⁵⁹, R. Tanaka¹¹⁹,
 S. Tanaka⁶⁹, R. Tanioka⁷⁰, B.B. Tannenwald¹¹³, S. Tapia Araya^{34b}, S. Tapprogge⁸⁶, S. Tarem¹⁵⁴,
 G.F. Tartarelli^{94a}, P. Tas¹³¹, M. Tasevsky¹²⁹, T. Tashiro⁷¹, E. Tassi^{40a,40b}, A. Tavares Delgado^{128a,128b},
 Y. Tayalati^{137e}, A.C. Taylor¹⁰⁷, A.J. Taylor⁴⁹, G.N. Taylor⁹¹, P.T.E. Taylor⁹¹, W. Taylor^{163b},
 P. Teixeira-Dias⁸⁰, D. Temple¹⁴⁴, H. Ten Kate³², P.K. Teng¹⁵³, J.J. Teoh¹²⁰, F. Tepel¹⁷⁸, S. Terada⁶⁹,
 K. Terashi¹⁵⁷, J. Terron⁸⁵, S. Terzo¹³, M. Testa⁵⁰, R.J. Teuscher^{161,o}, T. Theveniaux-Pelzer⁸⁸,
 F. Thiele³⁹, J.P. Thomas¹⁹, J. Thomas-Wilsker⁸⁰, P.D. Thompson¹⁹, A.S. Thompson⁵⁶, L.A. Thomsen¹⁷⁹,
 E. Thomson¹²⁴, M.J. Tibbetts¹⁶, R.E. Ticse Torres⁸⁸, V.O. Tikhomirov^{98,aq}, Yu.A. Tikhonov^{111,c},
 S. Timoshenko¹⁰⁰, P. Tipton¹⁷⁹, S. Tisserant⁸⁸, K. Todome¹⁵⁹, S. Todorova-Nova⁵, S. Todt⁴⁷, J. Tojo⁷³,
 S. Tokár^{146a}, K. Tokushuku⁶⁹, E. Tolley⁵⁹, L. Tomlinson⁸⁷, M. Tomoto¹⁰⁵, L. Tompkins^{145,ar},
 K. Toms¹⁰⁷, B. Tong⁵⁹, P. Tornambe⁵¹, E. Torrence¹¹⁸, H. Torres⁴⁷, E. Torró Pastor¹⁴⁰, J. Toth^{88,as},
 F. Touchard⁸⁸, D.R. Tovey¹⁴¹, C.J. Treado¹¹², T. Trefzger¹⁷⁷, F. Tresoldi¹⁵¹, A. Tricoli²⁷,
 I.M. Trigger^{163a}, S. Trincas-Duvoid⁸³, M.F. Tripiana¹³, W. Trischuk¹⁶¹, B. Trocmé⁵⁸, A. Trofymov⁴⁵,
 C. Troncon^{94a}, M. Trottier-McDonald¹⁶, M. Trovatelli¹⁷², L. Truong^{147b}, M. Trzebinski⁴², A. Trzupek⁴²,
 K.W. Tsang^{62a}, J.C.-L. Tseng¹²², P.V. Tsiareshka⁹⁵, G. Tsipolitis¹⁰, N. Tsirintanis⁹, S. Tsiskaridze¹³,
 V. Tsiskaridze⁵¹, E.G. Tskhadadze^{54a}, K.M. Tsui^{62a}, I.I. Tsukerman⁹⁹, V. Tsulaia¹⁶, S. Tsuno⁶⁹,
 D. Tsybychev¹⁵⁰, Y. Tu^{62b}, A. Tudorache^{28b}, V. Tudorache^{28b}, T.T. Tulbure^{28a}, A.N. Tuna⁵⁹,
 S.A. Tupputi^{22a,22b}, S. Turchikhin⁶⁸, D. Turgeman¹⁷⁵, I. Turk Cakir^{4b,at}, R. Turra^{94a}, P.M. Tuts³⁸,

G. Uccchielli^{22a,22b}, I. Ueda⁶⁹, M. Ughetto^{148a,148b}, F. Ukegawa¹⁶⁴, G. Unal³², A. Undrus²⁷, G. Unel¹⁶⁶, F.C. Ungaro⁹¹, Y. Unno⁶⁹, C. Unverdorben¹⁰², J. Urban^{146b}, P. Urquijo⁹¹, P. Urrejola⁸⁶, G. Usai⁸, J. Usui⁶⁹, L. Vacavant⁸⁸, V. Vacek¹³⁰, B. Vachon⁹⁰, K.O.H. Vadla¹²¹, A. Vaidya⁸¹, C. Valderanis¹⁰², E. Valdes Santurio^{148a,148b}, M. Valente⁵², S. Valentinetti^{22a,22b}, A. Valero¹⁷⁰, L. Valéry¹³, S. Valkar¹³¹, A. Vallier⁵, J.A. Valls Ferrer¹⁷⁰, W. Van Den Wollenberg¹⁰⁹, H. van der Graaf¹⁰⁹, P. van Gemmeren⁶, J. Van Nieuwkoop¹⁴⁴, I. van Vulpen¹⁰⁹, M.C. van Woerden¹⁰⁹, M. Vanadia^{135a,135b}, W. Vandelli³², A. Vaniachine¹⁶⁰, P. Vankov¹⁰⁹, G. Vardanyan¹⁸⁰, R. Vari^{134a}, E.W. Varnes⁷, C. Varni^{53a,53b}, T. Varol⁴³, D. Varouchas¹¹⁹, A. Vartapetian⁸, K.E. Varvell¹⁵², J.G. Vasquez¹⁷⁹, G.A. Vasquez^{34b}, F. Vazeille³⁷, T. Vazquez Schroeder⁹⁰, J. Veatch⁵⁷, V. Veeraraghavan⁷, L.M. Veloce¹⁶¹, F. Veloso^{128a,128c}, S. Veneziano^{134a}, A. Ventura^{76a,76b}, M. Venturi¹⁷², N. Venturi³², A. Venturini²⁵, V. Vercesi^{123a}, M. Verducci^{136a,136b}, W. Verkerke¹⁰⁹, A.T. Vermeulen¹⁰⁹, J.C. Vermeulen¹⁰⁹, M.C. Vetterli^{144,d}, N. Viaux Maira^{34b}, O. Viazlo⁸⁴, I. Vichou^{169,*}, T. Vickey¹⁴¹, O.E. Vickey Boeriu¹⁴¹, G.H.A. Viehhauser¹²², S. Viel¹⁶, L. Vigani¹²², M. Villa^{22a,22b}, M. Villaplana Perez^{94a,94b}, E. Vilucchi⁵⁰, M.G. Vinciter³¹, V.B. Vinogradov⁶⁸, A. Vishwakarma⁴⁵, C. Vittori^{22a,22b}, I. Vivarelli¹⁵¹, S. Vlachos¹⁰, M. Vogel¹⁷⁸, P. Vokac¹³⁰, G. Volpi^{126a,126b}, H. von der Schmitt¹⁰³, E. von Toerne²³, V. Vorobel¹³¹, K. Vorobev¹⁰⁰, M. Vos¹⁷⁰, R. Voss³², J.H. Vosseveld⁷⁷, N. Vranjes¹⁴, M. Vranjes Milosavljevic¹⁴, V. Vrba¹³⁰, M. Vreeswijk¹⁰⁹, R. Vuillermet³², I. Vukotic³³, P. Wagner²³, W. Wagner¹⁷⁸, J. Wagner-Kuhr¹⁰², H. Wahlberg⁷⁴, S. Wahrmund⁴⁷, J. Walder⁷⁵, R. Walker¹⁰², W. Walkowiak¹⁴³, V. Wallangen^{148a,148b}, C. Wang^{35b}, C. Wang^{36b,au}, F. Wang¹⁷⁶, H. Wang¹⁶, H. Wang³, J. Wang⁴⁵, J. Wang¹⁵², Q. Wang¹¹⁵, R. Wang⁶, S.M. Wang¹⁵³, T. Wang³⁸, W. Wang^{153,av}, W. Wang^{36a}, Z. Wang^{36c}, C. Wanotayaroj¹¹⁸, A. Warburton⁹⁰, C.P. Ward³⁰, D.R. Wardrope⁸¹, A. Washbrook⁴⁹, P.M. Watkins¹⁹, A.T. Watson¹⁹, M.F. Watson¹⁹, G. Watts¹⁴⁰, S. Watts⁸⁷, B.M. Waugh⁸¹, A.F. Webb¹¹, S. Webb⁸⁶, M.S. Weber¹⁸, S.W. Weber¹⁷⁷, S.A. Weber³¹, J.S. Webster⁶, A.R. Weidberg¹²², B. Weinert⁶⁴, J. Weingarten⁵⁷, M. Weirich⁸⁶, C. Weiser⁵¹, H. Weits¹⁰⁹, P.S. Wells³², T. Wenaus²⁷, T. Wengler³², S. Wenig³², N. Wermes²³, M.D. Werner⁶⁷, P. Werner³², M. Wessels^{60a}, T.D. Weston¹⁸, K. Whalen¹¹⁸, N.L. Whallon¹⁴⁰, A.M. Wharton⁷⁵, A.S. White⁹², A. White⁸, M.J. White¹, R. White^{34b}, D. Whiteson¹⁶⁶, B.W. Whitmore⁷⁵, F.J. Wickens¹³³, W. Wiedenmann¹⁷⁶, M. Wielders¹³³, C. Wigglesworth³⁹, L.A.M. Wiik-Fuchs⁵¹, A. Wildauer¹⁰³, F. Wilk⁸⁷, H.G. Wilkens³², H.H. Williams¹²⁴, S. Williams¹⁰⁹, C. Willis⁹³, S. Willocq⁸⁹, J.A. Wilson¹⁹, I. Wingerter-Seez⁵, E. Winkels¹⁵¹, F. Winklmeier¹¹⁸, O.J. Winston¹⁵¹, B.T. Winter²³, M. Wittgen¹⁴⁵, M. Wobisch^{82,u}, T.M.H. Wolf¹⁰⁹, R. Wolff⁸⁸, M.W. Wolter⁴², H. Wolters^{128a,128c}, V.W.S. Wong¹⁷¹, S.D. Worm¹⁹, B.K. Wosiek⁴², J. Wotschack³², K.W. Wozniak⁴², M. Wu³³, S.L. Wu¹⁷⁶, X. Wu⁵², Y. Wu⁹², T.R. Wyatt⁸⁷, B.M. Wynne⁴⁹, S. Xella³⁹, Z. Xi⁹², L. Xia^{35c}, D. Xu^{35a}, L. Xu²⁷, T. Xu¹³⁸, B. Yabsley¹⁵², S. Yacoob^{147a}, D. Yamaguchi¹⁵⁹, Y. Yamaguchi¹⁵⁹, A. Yamamoto⁶⁹, S. Yamamoto¹⁵⁷, T. Yamanaka¹⁵⁷, F. Yamane⁷⁰, M. Yamatani¹⁵⁷, Y. Yamazaki⁷⁰, Z. Yan²⁴, H. Yang^{36c}, H. Yang¹⁶, Y. Yang¹⁵³, Z. Yang¹⁵, W-M. Yao¹⁶, Y.C. Yap⁸³, Y. Yasu⁶⁹, E. Yatsenko⁵, K.H. Yau Wong²³, J. Ye⁴³, S. Ye²⁷, I. Yeletsikh⁶⁸, E. Yigitbasi²⁴, E. Yildirim⁸⁶, K. Yorita¹⁷⁴, K. Yoshihara¹²⁴, C. Young¹⁴⁵, C.J.S. Young³², J. Yu⁸, J. Yu⁶⁷, S.P.Y. Yuen²³, I. Yusuff^{30,aw}, B. Zabinski⁴², G. Zacharis¹⁰, R. Zaidan¹³, A.M. Zaitsev^{132,ak}, N. Zakharchuk⁴⁵, J. Zalieckas¹⁵, A. Zaman¹⁵⁰, S. Zambito⁵⁹, D. Zanzi⁹¹, C. Zeitnitz¹⁷⁸, G. Zemaityte¹²², A. Zemla^{41a}, J.C. Zeng¹⁶⁹, Q. Zeng¹⁴⁵, O. Zenin¹³², T. Ženiš^{146a}, D. Zerwas¹¹⁹, D. Zhang⁹², F. Zhang¹⁷⁶, G. Zhang^{36a,ax}, H. Zhang^{35b}, J. Zhang⁶, L. Zhang⁵¹, L. Zhang^{36a}, M. Zhang¹⁶⁹, P. Zhang^{35b}, R. Zhang²³, R. Zhang^{36a,au}, X. Zhang^{36b}, Y. Zhang^{35a}, Z. Zhang¹¹⁹, X. Zhao⁴³, Y. Zhao^{36b,ay}, Z. Zhao^{36a}, A. Zhemchugov⁶⁸, B. Zhou⁹², C. Zhou¹⁷⁶, L. Zhou⁴³, M. Zhou^{35a}, M. Zhou¹⁵⁰, N. Zhou^{35c}, C.G. Zhu^{36b}, H. Zhu^{35a}, J. Zhu⁹², Y. Zhu^{36a}, X. Zhuang^{35a}, K. Zhukov⁹⁸, A. Zibell¹⁷⁷, D. Zieminska⁶⁴, N.I. Zimine⁶⁸, C. Zimmermann⁸⁶, S. Zimmermann⁵¹, Z. Zinonos¹⁰³, M. Zinser⁸⁶, M. Ziolkowski¹⁴³, L. Živković¹⁴, G. Zobernig¹⁷⁶, A. Zoccoli^{22a,22b}, R. Zou³³, M. zur Nedden¹⁷, L. Zwalinski³².

- ¹ Department of Physics, University of Adelaide, Adelaide, Australia
- ² Physics Department, SUNY Albany, Albany NY, United States of America
- ³ Department of Physics, University of Alberta, Edmonton AB, Canada
- ⁴ ^(a) Department of Physics, Ankara University, Ankara; ^(b) Istanbul Aydin University, Istanbul; ^(c) Division of Physics, TOBB University of Economics and Technology, Ankara, Turkey
- ⁵ LAPP, CNRS/IN2P3 and Université Savoie Mont Blanc, Annecy-le-Vieux, 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, The 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, The 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), The Barcelona Institute of Science and Technology, Barcelona, Spain
- ¹⁴ Institute of Physics, University of Belgrade, Belgrade, Serbia
- ¹⁵ Department for Physics and Technology, University of Bergen, Bergen, Norway
- ¹⁶ Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley CA, United States of America
- ¹⁷ Department of Physics, Humboldt University, Berlin, Germany
- ¹⁸ Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland
- ¹⁹ School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom
- ²⁰ ^(a) Department of Physics, Bogazici University, Istanbul; ^(b) Department of Physics Engineering, Gaziantep University, Gaziantep; ^(d) Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul; ^(e) Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey
- ²¹ Centro de Investigaciones, Universidad Antonio Narino, Bogota, Colombia
- ²² ^(a) INFN Sezione di Bologna; ^(b) Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy
- ²³ Physikalisches Institut, University of Bonn, Bonn, Germany
- ²⁴ Department of Physics, Boston University, Boston MA, United States of America
- ²⁵ Department of Physics, Brandeis University, Waltham MA, United States of America
- ²⁶ ^(a) Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro; ^(b) Electrical Circuits Department, Federal University of Juiz de Fora (UFJF), Juiz de Fora; ^(c) Federal University of Sao Joao del Rei (UFSJ), Sao Joao del Rei; ^(d) Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil
- ²⁷ Physics Department, Brookhaven National Laboratory, Upton NY, 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) University Politehnica Bucharest, Bucharest; ^(f) West University in Timisoara, Timisoara, Romania
- ²⁹ Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina
- ³⁰ Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
- ³¹ Department of Physics, Carleton University, Ottawa ON, Canada
- ³² CERN, Geneva, Switzerland
- ³³ Enrico Fermi Institute, University of Chicago, Chicago IL, United States of America

- ³⁴ (a) Departamento de Física, Pontificia Universidad Católica de Chile, Santiago; (b) Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
- ³⁵ (a) Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; (b) Department of Physics, Nanjing University, Jiangsu; (c) Physics Department, Tsinghua University, Beijing 100084, China
- ³⁶ (a) Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Anhui; (b) School of Physics, Shandong University, Shandong; (c) Department of Physics and Astronomy, Key Laboratory for Particle Physics, Astrophysics and Cosmology, Ministry of Education; Shanghai Key Laboratory for Particle Physics and Cosmology, Shanghai Jiao Tong University, Shanghai(also at PKU-CHEP), China
- ³⁷ Université Clermont Auvergne, CNRS/IN2P3, LPC, Clermont-Ferrand, France
- ³⁸ Nevis Laboratory, Columbia University, Irvington NY, United States of America
- ³⁹ Niels Bohr Institute, University of Copenhagen, Kobenhavn, Denmark
- ⁴⁰ (a) INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati; (b) Dipartimento di Fisica, Università della Calabria, Rende, Italy
- ⁴¹ (a) AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow; (b) Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
- ⁴² Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
- ⁴³ Physics Department, Southern Methodist University, Dallas TX, United States of America
- ⁴⁴ Physics Department, University of Texas at Dallas, Richardson TX, United States of America
- ⁴⁵ DESY, Hamburg and Zeuthen, Germany
- ⁴⁶ Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
- ⁴⁷ Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
- ⁴⁸ Department of Physics, Duke University, Durham NC, United States of America
- ⁴⁹ SUPA - School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom
- ⁵⁰ INFN e Laboratori Nazionali di Frascati, Frascati, Italy
- ⁵¹ Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
- ⁵² Departement de Physique Nucleaire et Corpusculaire, Université de Genève, Geneva, Switzerland
- ⁵³ (a) INFN Sezione di Genova; (b) Dipartimento di Fisica, Università di Genova, Genova, Italy
- ⁵⁴ (a) E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi; (b) High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
- ⁵⁵ II Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
- ⁵⁶ SUPA - School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom
- ⁵⁷ II Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
- ⁵⁸ Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France
- ⁵⁹ Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge MA, United States of America
- ⁶⁰ (a) Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg; (b) Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
- ⁶¹ Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
- ⁶² (a) Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong; (b) Department of Physics, The University of Hong Kong, Hong Kong; (c) Department of Physics and Institute for Advanced Study, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China
- ⁶³ Department of Physics, National Tsing Hua University, Taiwan, Taiwan
- ⁶⁴ Department of Physics, Indiana University, Bloomington IN, United States of America

- ⁶⁵ Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria
- ⁶⁶ University of Iowa, Iowa City IA, United States of America
- ⁶⁷ Department of Physics and Astronomy, Iowa State University, Ames IA, United States of America
- ⁶⁸ Joint Institute for Nuclear Research, JINR Dubna, Dubna, Russia
- ⁶⁹ KEK, High Energy Accelerator Research Organization, Tsukuba, Japan
- ⁷⁰ Graduate School of Science, Kobe University, Kobe, Japan
- ⁷¹ Faculty of Science, Kyoto University, Kyoto, Japan
- ⁷² Kyoto University of Education, Kyoto, Japan
- ⁷³ Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan
- ⁷⁴ Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
- ⁷⁵ Physics Department, Lancaster University, Lancaster, United Kingdom
- ⁷⁶ ^(a) INFN Sezione di Lecce; ^(b) Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy
- ⁷⁷ Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom
- ⁷⁸ Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia
- ⁷⁹ School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom
- ⁸⁰ Department of Physics, Royal Holloway University of London, Surrey, United Kingdom
- ⁸¹ Department of Physics and Astronomy, University College London, London, United Kingdom
- ⁸² Louisiana Tech University, Ruston LA, United States of America
- ⁸³ Laboratoire de Physique Nucléaire et de Hautes Energies, UPMC and Université Paris-Diderot and CNRS/IN2P3, Paris, France
- ⁸⁴ Fysiska institutionen, Lunds universitet, Lund, Sweden
- ⁸⁵ Departamento de Física Teórica C-15, Universidad Autónoma de Madrid, Madrid, Spain
- ⁸⁶ Institut für Physik, Universität Mainz, Mainz, Germany
- ⁸⁷ School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom
- ⁸⁸ CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
- ⁸⁹ Department of Physics, University of Massachusetts, Amherst MA, United States of America
- ⁹⁰ Department of Physics, McGill University, Montreal QC, Canada
- ⁹¹ School of Physics, University of Melbourne, Victoria, Australia
- ⁹² Department of Physics, The University of Michigan, Ann Arbor MI, United States of America
- ⁹³ Department of Physics and Astronomy, Michigan State University, East Lansing MI, United States of America
- ⁹⁴ ^(a) INFN Sezione di Milano; ^(b) Dipartimento di Fisica, Università di Milano, Milano, Italy
- ⁹⁵ B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Republic of Belarus
- ⁹⁶ Research Institute for Nuclear Problems of Byelorussian State University, Minsk, Republic of Belarus
- ⁹⁷ Group of Particle Physics, University of Montreal, Montreal QC, Canada
- ⁹⁸ P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia
- ⁹⁹ Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia
- ¹⁰⁰ National Research Nuclear University MEPhI, Moscow, Russia
- ¹⁰¹ D.V. Skobel'syn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia
- ¹⁰² Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany
- ¹⁰³ Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany
- ¹⁰⁴ Nagasaki Institute of Applied Science, Nagasaki, Japan

- ¹⁰⁵ Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan
- ¹⁰⁶ ^(a) INFN Sezione di Napoli; ^(b) Dipartimento di Fisica, Università di Napoli, Napoli, Italy
- ¹⁰⁷ Department of Physics and Astronomy, University of New Mexico, Albuquerque NM, United States of America
- ¹⁰⁸ Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands
- ¹⁰⁹ Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands
- ¹¹⁰ Department of Physics, Northern Illinois University, DeKalb IL, United States of America
- ¹¹¹ Budker Institute of Nuclear Physics, SB RAS, Novosibirsk, Russia
- ¹¹² Department of Physics, New York University, New York NY, United States of America
- ¹¹³ Ohio State University, Columbus OH, United States of America
- ¹¹⁴ Faculty of Science, Okayama University, Okayama, Japan
- ¹¹⁵ Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman OK, United States of America
- ¹¹⁶ Department of Physics, Oklahoma State University, Stillwater OK, United States of America
- ¹¹⁷ Palacký University, RCPTM, Olomouc, Czech Republic
- ¹¹⁸ Center for High Energy Physics, University of Oregon, Eugene OR, United States of America
- ¹¹⁹ LAL, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France
- ¹²⁰ Graduate School of Science, Osaka University, Osaka, Japan
- ¹²¹ Department of Physics, University of Oslo, Oslo, Norway
- ¹²² Department of Physics, Oxford University, Oxford, United Kingdom
- ¹²³ ^(a) INFN Sezione di Pavia; ^(b) Dipartimento di Fisica, Università di Pavia, Pavia, Italy
- ¹²⁴ Department of Physics, University of Pennsylvania, Philadelphia PA, United States of America
- ¹²⁵ National Research Centre "Kurchatov Institute" B.P.Konstantinov Petersburg Nuclear Physics Institute, St. Petersburg, Russia
- ¹²⁶ ^(a) INFN Sezione di Pisa; ^(b) Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy
- ¹²⁷ Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh PA, United States of America
- ¹²⁸ ^(a) Laboratório de Instrumentação e Física Experimental de Partículas - LIP, Lisboa; ^(b) Faculdade de Ciências, Universidade de Lisboa, Lisboa; ^(c) Department of Physics, University of 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 and CAFPE, Universidad de Granada, Granada; ^(g) Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal
- ¹²⁹ Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic
- ¹³⁰ Czech Technical University in Prague, Praha, Czech Republic
- ¹³¹ Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic
- ¹³² State Research Center Institute for High Energy Physics (Protvino), NRC KI, Russia
- ¹³³ Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom
- ¹³⁴ ^(a) INFN Sezione di Roma; ^(b) Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy
- ¹³⁵ ^(a) INFN Sezione di Roma Tor Vergata; ^(b) Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy
- ¹³⁶ ^(a) INFN Sezione di Roma Tre; ^(b) Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy
- ¹³⁷ ^(a) Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies - Université Hassan II, Casablanca; ^(b) Centre National de l'Energie des Sciences Techniques Nucleaires,

Rabat; ^(c) Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech; ^(d) Faculté des Sciences, Université Mohamed Premier and LTPM, Oujda; ^(e) Faculté des sciences, Université Mohammed V, Rabat, Morocco

¹³⁸ DSM/IRFU (Institut de Recherches sur les Lois Fondamentales de l'Univers), CEA Saclay (Commissariat à l'Energie Atomique et aux Energies Alternatives), Gif-sur-Yvette, France

¹³⁹ Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA, United States of America

¹⁴⁰ Department of Physics, University of Washington, Seattle WA, United States of America

¹⁴¹ Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

¹⁴² Department of Physics, Shinshu University, Nagano, Japan

¹⁴³ Department Physik, Universität Siegen, Siegen, Germany

¹⁴⁴ Department of Physics, Simon Fraser University, Burnaby BC, Canada

¹⁴⁵ SLAC National Accelerator Laboratory, Stanford CA, United States of America

¹⁴⁶ ^(a) Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava; ^(b) Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic

¹⁴⁷ ^(a) Department of Physics, University of Cape Town, Cape Town; ^(b) Department of Physics, University of Johannesburg, Johannesburg; ^(c) School of Physics, University of the Witwatersrand, Johannesburg, South Africa

¹⁴⁸ ^(a) Department of Physics, Stockholm University; ^(b) The Oskar Klein Centre, Stockholm, Sweden

¹⁴⁹ Physics Department, Royal Institute of Technology, Stockholm, Sweden

¹⁵⁰ Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook NY, United States of America

¹⁵¹ Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom

¹⁵² School of Physics, University of Sydney, Sydney, Australia

¹⁵³ Institute of Physics, Academia Sinica, Taipei, Taiwan

¹⁵⁴ Department of Physics, Technion: Israel Institute of Technology, Haifa, Israel

¹⁵⁵ Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel

¹⁵⁶ Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

¹⁵⁷ International Center for Elementary Particle Physics and Department of Physics, The University of Tokyo, Tokyo, Japan

¹⁵⁸ Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan

¹⁵⁹ Department of Physics, Tokyo Institute of Technology, Tokyo, Japan

¹⁶⁰ Tomsk State University, Tomsk, Russia

¹⁶¹ Department of Physics, University of Toronto, Toronto ON, Canada

¹⁶² ^(a) INFN-TIFPA; ^(b) University of Trento, Trento, Italy

¹⁶³ ^(a) TRIUMF, Vancouver BC; ^(b) Department of Physics and Astronomy, York University, Toronto ON, Canada

¹⁶⁴ Faculty of Pure and Applied Sciences, and Center for Integrated Research in Fundamental Science and Engineering, University of Tsukuba, Tsukuba, Japan

¹⁶⁵ Department of Physics and Astronomy, Tufts University, Medford MA, United States of America

¹⁶⁶ Department of Physics and Astronomy, University of California Irvine, Irvine CA, United States of America

¹⁶⁷ ^(a) INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; ^(b) ICTP, Trieste; ^(c) Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy

¹⁶⁸ Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden

- ¹⁶⁹ Department of Physics, University of Illinois, Urbana IL, United States of America
- ¹⁷⁰ Instituto de Fisica Corpuscular (IFIC), Centro Mixto Universidad de Valencia - CSIC, Spain
- ¹⁷¹ Department of Physics, University of British Columbia, Vancouver BC, Canada
- ¹⁷² Department of Physics and Astronomy, University of Victoria, Victoria BC, Canada
- ¹⁷³ Department of Physics, University of Warwick, Coventry, United Kingdom
- ¹⁷⁴ Waseda University, Tokyo, Japan
- ¹⁷⁵ Department of Particle Physics, The Weizmann Institute of Science, Rehovot, Israel
- ¹⁷⁶ Department of Physics, University of Wisconsin, Madison WI, United States of America
- ¹⁷⁷ Fakultät für Physik und Astronomie, Julius-Maximilians-Universität, Würzburg, Germany
- ¹⁷⁸ Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany
- ¹⁷⁹ Department of Physics, Yale University, New Haven CT, United States of America
- ¹⁸⁰ Yerevan Physics Institute, Yerevan, Armenia
- ¹⁸¹ Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France
- ¹⁸² Academia Sinica Grid Computing, Institute of Physics, Academia Sinica, Taipei, Taiwan
- ^a Also at Department of Physics, King's College London, London, United Kingdom
- ^b Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan
- ^c Also at Novosibirsk State University, Novosibirsk, Russia
- ^d Also at TRIUMF, Vancouver BC, Canada
- ^e Also at Department of Physics & Astronomy, University of Louisville, Louisville, KY, United States of America
- ^f Also at Physics Department, An-Najah National University, Nablus, Palestine
- ^g Also at Department of Physics, California State University, Fresno CA, United States of America
- ^h Also at Department of Physics, University of Fribourg, Fribourg, Switzerland
- ⁱ Also at II Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
- ^j Also at Departament de Fisica de la Universitat Autònoma de Barcelona, Barcelona, Spain
- ^k Also at Departamento de Fisica e Astronomia, Faculdade de Ciencias, Universidade do Porto, Portugal
- ^l Also at Tomsk State University, Tomsk, Russia
- ^m Also at The Collaborative Innovation Center of Quantum Matter (CICQM), Beijing, China
- ⁿ Also at Università di Napoli Parthenope, Napoli, Italy
- ^o Also at Institute of Particle Physics (IPP), Canada
- ^p Also at Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania
- ^q Also at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg, Russia
- ^r Also at Borough of Manhattan Community College, City University of New York, New York City, United States of America
- ^s Also at Department of Financial and Management Engineering, University of the Aegean, Chios, Greece
- ^t Also at Centre for High Performance Computing, CSIR Campus, Rosebank, Cape Town, South Africa
- ^u Also at Louisiana Tech University, Ruston LA, United States of America
- ^v Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain
- ^w Also at Graduate School of Science, Osaka University, Osaka, Japan
- ^x Also at Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
- ^y Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands
- ^z Also at Department of Physics, The University of Texas at Austin, Austin TX, United States of America
- ^{aa} Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia

- ab* Also at CERN, Geneva, Switzerland
- ac* Also at Georgian Technical University (GTU), Tbilisi, Georgia
- ad* Also at Ochadai Academic Production, Ochanomizu University, Tokyo, Japan
- ae* Also at Manhattan College, New York NY, United States of America
- af* Also at Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile
- ag* Also at Department of Physics, The University of Michigan, Ann Arbor MI, United States of America
- ah* Also at The City College of New York, New York NY, United States of America
- ai* Also at Departamento de Física Teórica y del Cosmos and CAFPE, Universidad de Granada, Granada, Portugal
- aj* Also at Department of Physics, California State University, Sacramento CA, United States of America
- ak* Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia
- al* Also at Département de Physique Nucleaire et Corpusculaire, Université de Genève, Geneva, Switzerland
- am* Also at Institut de Física d'Altes Energies (IFAE), The Barcelona Institute of Science and Technology, Barcelona, Spain
- an* Also at School of Physics, Sun Yat-sen University, Guangzhou, China
- ao* Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria
- ap* Also at Faculty of Physics, M.V.Lomonosov Moscow State University, Moscow, Russia
- aq* Also at National Research Nuclear University MEPhI, Moscow, Russia
- ar* Also at Department of Physics, Stanford University, Stanford CA, United States of America
- as* Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary
- at* Also at Giresun University, Faculty of Engineering, Turkey
- au* Also at CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
- av* Also at Department of Physics, Nanjing University, Jiangsu, China
- aw* Also at University of Malaya, Department of Physics, Kuala Lumpur, Malaysia
- ax* Also at Institute of Physics, Academia Sinica, Taipei, Taiwan
- ay* Also at LAL, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France
- * Deceased