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ATLAS Collaboration; Newman, Paul

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Searches for lepton-flavour-violating decays of the Higgs boson in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector

The ATLAS Collaboration^{*}



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ABSTRACT

This Letter presents direct searches for lepton flavour violation in Higgs boson decays, $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$, performed with the ATLAS detector at the LHC. The searches are based on a data sample of proton–proton collisions at a centre-of-mass energy $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 36.1 fb^{-1} . No significant excess is observed above the expected background from Standard Model processes. The observed (median expected) 95% confidence-level upper limits on the lepton-flavour-violating branching ratios are 0.47% ($0.34^{+0.13}_{-0.10}\%$) and 0.28% ($0.37^{+0.14}_{-0.10}\%$) for $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$, respectively.

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1. Introduction

The search for processes beyond the Standard Model (SM) is one of the main goals of the Large Hadron Collider (LHC) programme at CERN. A possible sign of such processes is lepton flavour violation (LFV) in decays of the Higgs boson [1,2]. Many beyond-SM theories predict LFV decays of the Higgs boson, such as supersymmetry [3,4], other models with more than one Higgs doublet [5,6], composite Higgs models [7], models with flavour symmetries [8] or warped extra dimensions [9–11] models and others [12,13].

In this Letter, searches for LFV decays of the Higgs boson, $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$, at the LHC with the ATLAS experiment are presented. Studies are based on proton–proton (pp) collision data recorded in 2015–2016 at a centre-of-mass energy $\sqrt{s} = 13$ TeV. The dataset corresponds to an integrated luminosity of 36.1 fb^{-1} .

Previous ATLAS searches [14,15] placed an upper limit of 1.04% (1.43%) on the $H \rightarrow e\tau$ ($H \rightarrow \mu\tau$) branching ratio (\mathcal{B}) with a 95% confidence level (CL) using Run 1 data collected at $\sqrt{s} = 8$ TeV, corresponding to an integrated luminosity of 20.3 fb^{-1} . The CMS Collaboration recently provided 95% CL upper limits on these branching ratios of 0.61% and 0.25%, respectively, using data collected at $\sqrt{s} = 13$ TeV, with an integrated luminosity of 35.9 fb^{-1} [16].

The searches presented here involve both leptonic ($\tau \rightarrow \ell' \nu \bar{\nu}^1$) and hadronic ($\tau \rightarrow \text{hadrons} + \nu$) decays of τ -leptons, denoted $\tau_{\ell'}$ and τ_{had} respectively. The dilepton final state $\ell\tau_{\ell'}$ only considers pairs of different-flavour leptons. Same-flavour lepton pairs are

rejected due to the large lepton pair-production Drell-Yan background. Two channels are considered for each of the two searches: $e\tau_{\mu}$ and $e\tau_{\text{had}}$ for the $H \rightarrow e\tau$ search, $\mu\tau_e$ and $\mu\tau_{\text{had}}$ for the $H \rightarrow \mu\tau$ search. The analysis is designed such that any potential LFV signal overlap between the $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ searches is negligible. Many methods are reused from the measurement of the Higgs boson cross-section in the $H \rightarrow \tau\tau$ final state [17].

The ATLAS detector² is described in Refs. [18–20]. It consists of an inner tracking detector covering the range $|\eta| < 2.5$, surrounded by a superconducting solenoid providing a 2 T axial magnetic field, high-granularity electromagnetic ($|\eta| < 3.2$) and hadronic calorimeters ($|\eta| < 4.9$), and a muon spectrometer (MS) which covers the range $|\eta| < 2.7$ and includes fast trigger chambers ($|\eta| < 2.4$) and superconducting toroidal magnets.

2. Simulation samples

Samples of Monte Carlo (MC) simulated events are used to optimize the event selection, and to model the signal and several of the background processes. The samples were produced with the ATLAS simulation infrastructure [21] using the full detector simulation performed by the GEANT4 [22] toolkit. The Higgs boson mass was set to $m_H = 125$ GeV [23]. The four leading Higgs boson production mechanisms are considered: the gluon–gluon fusion (ggF), vector-boson fusion (VBF) and two associated production modes

² ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point in the centre of the detector and the z-axis along the beam pipe. The azimuthal angle ϕ runs around the beam pipe, the pseudorapidity is defined in terms of the polar angle θ as $\eta \equiv -\ln \tan(\theta/2)$. Angular distance in the η - ϕ space is defined as $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

^{*} E-mail address: atlas.publications@cern.ch.

¹ Unless explicitly mentioned otherwise, leptons (denoted by ℓ or ℓ') refer to electrons or muons.

Table 1
Generators used to describe the signal and background processes, parton distribution function (PDF) sets for the hard process, and models used for parton showering, hadronization and the underlying event (UEPS). The orders of the total cross-sections used to normalize the events are also given. More details are given in Ref. [17].

| Process | Generator | PDF | UEPS | Cross-section order |
|----------------|-----------------------------------|---------------------|-------------------|--|
| ggF | Powheg-Box v2 [26–30] NNLOPS [31] | PDF4LHC15 [32] NNLO | Pythia 8.212 [25] | N ³ LO QCD + NLO EW [33–36] |
| VBF | Powheg-Box v2 MiNLO [30] | PDF4LHC15 NLO | Pythia 8.212 | ~NNLO QCD + NLO EW [37–39] |
| WH, ZH | Powheg-Box v2 MiNLO | PDF4LHC15 NLO | Pythia 8.212 | NNLO QCD + NLO EW [40–42] |
| W/Z + jets | Sherpa 2.2.1 [43] | NNPDF30NNLO [44] | Sherpa 2.2.1 [45] | NNLO [46,47] |
| $VV/V\gamma^*$ | Sherpa 2.2.1 | NNPDF30NNLO | Sherpa 2.2.1 | NNLO |
| $t\bar{t}$ | Powheg-Box v2 [26–28,48] | CT10 [49] | Pythia 6.428 [50] | NNLO+NNLL [51] |
| Single t | Powheg-Box v1 [52,53] | CT10 | Pythia 6.428 | NLO [54–56] |

(WH, ZH), while the others give negligible contributions and are ignored. The cross-sections of all Higgs boson production processes were normalized to the SM predictions [24]. The LFV Higgs boson decays as well as the $H \rightarrow \tau\tau$ and $H \rightarrow WW$ background decays were modelled with Pythia 8 [25]. Other background processes involve electroweak production of W/Z bosons via VBF, Drell–Yan production of W/Z in association with jet(s) as well as diboson, single top-quark and top-quark pair ($t\bar{t}$) production. The MC generators used for the SM $H \rightarrow \tau\tau$ cross-section measurement [17] were also employed here for all background components. The generators and parton shower models used to simulate different processes are summarized in Table 1.

3. Object reconstruction

The correct identification of $H \rightarrow \ell\tau$ events requires reconstruction of several different objects (electrons, muons, and jets, including those initiated by hadronic decays of τ -leptons) and the missing transverse momentum \vec{p}_T^{miss} , whose magnitude is called E_T^{miss} .

Electrons are reconstructed by matching tracks in the inner detector to clustered energy deposits in the electromagnetic calorimeter [57]. Loose likelihood-based identification [58], $p_T > 15$ GeV and fiducial volume requirements ($|\eta| < 2.47$, excluding the transition region between the barrel and the endcap calorimeters $1.37 < |\eta| < 1.52$) are applied. Medium identification, corresponding to an efficiency of 87% at $p_T = 20$ GeV, is imposed for the baseline electron selection.

Muons are identified by tracks reconstructed in the inner detector and matched to tracks in the MS. Loose identification [59], $p_T > 10$ GeV and $|\eta| < 2.5$ requirements are applied. Medium identification (efficiency of 96.1% for muons with $p_T > 20$ GeV) is imposed for the baseline muon selection.

Isolation criteria exploiting calorimeter and track-based information are applied to both electrons and muons. The gradient working point is used, featuring an efficiency of 90% (99%) obtained for leptons with $p_T > 25$ GeV (60 GeV) originating from the $Z \rightarrow \ell\ell$ process [58,59].

Jets are reconstructed using the anti- k_t algorithm [60] as implemented by the FastJet [61] package. The algorithm is applied to topological clusters of calorimeter cells [62] with a radius parameter $R = 0.4$. Only jets with $p_T > 20$ GeV and $|\eta| < 4.5$ are considered. Jets from other pp interactions in the same and neighbouring bunch crossings (pile-up) are suppressed using jet vertex tagger (JVT) algorithms [63,64]. Jets containing b -hadrons (b -jets) are identified by the MV2c20 algorithm [65,66] in the central region ($|\eta| < 2.4$). A working point corresponding to 85% average efficiency determined for b -jets in $t\bar{t}$ simulated events is chosen, rejection factors are 2.8 and 28 against c -jets and light-flavour jets respectively.

The reconstruction of the object formed by the visible products of the τ_{had} decay ($\tau_{\text{had-vis}}$) begins from jets reconstructed by

the anti- k_t jet algorithm with a radius parameter $R = 0.4$. Information from the inner detector tracks associated with the energy deposits in the calorimeter is incorporated in the reconstruction. Only $\tau_{\text{had-vis}}$ candidates with $p_T > 20$ GeV and $|\eta| < 2.5$ are considered.³ One or three associated tracks with an absolute total charge $|q| = 1$ are required. An identification algorithm [67,68] based on boosted decision trees (BDT) [69–71] is used to reject $\tau_{\text{had-vis}}$ candidates arising from misidentification of jets or from decays of hadrons with b - or c -quark content. Unless otherwise indicated, a tight identification (ID) working point is used for the $\tau_{\text{had-vis}}$, corresponding to an efficiency of 60% (45%) for 1-prong (3-prong) candidates. Jets corresponding to identified $\tau_{\text{had-vis}}$ candidates are removed from the jet collection. The $\tau_{\text{had-vis}}$ candidates with one track overlapping with an electron candidate with high ID score, as determined by a multivariate (MVA) approach, are rejected. Leptonic τ -decays are reconstructed as electrons or muons.

Events considered in the analysis are triggered with single-electron or single-muon triggers. The p_T thresholds depend on the isolation requirement and data-taking period [72,73]. The lowest trigger thresholds correspond to 25 – 27 GeV (electrons) and 21 – 27 GeV (muons).

4. Event selection and categorization

Events selected in the $\ell\tau_{\ell'}$ channel contain exactly one electron and one muon of opposite-sign (OS) charges. Similarly in the $\ell\tau_{\text{had}}$ channel, a lepton and a $\tau_{\text{had-vis}}$ of OS charges are required, and events with more than one baseline lepton are rejected. The selection criteria are summarized in Table 2 for the analysis categories as well as the control regions (CRs), which are described in Section 5.

In the $\ell\tau_{\ell'}$ channel, ℓ_1 and ℓ_2 denote the leading and subleading lepton in p_T , respectively. Events where the leading lepton is an electron (muon) are used in the search for $H \rightarrow e\tau_\mu$ ($H \rightarrow \mu\tau_e$). A requirement on the dilepton invariant mass, equal to the invariant mass of the lepton and the visible τ -decay products, m_{vis} , reduces backgrounds with top quarks, and the criterion applied to the track-to-cluster p_T ratio of the electron reduces the $Z \rightarrow \mu\mu$ background where a muon deposits a large amount of energy in the electromagnetic calorimeter and is misidentified as an electron in the $\mu\tau_e$ channel. The contribution from the $H \rightarrow \tau\tau$ decay is reduced by the asymmetric p_T selection of the two leptons.

In the $\ell\tau_{\text{had}}$ channel, the criterion based on the azimuthal separations of lepton- E_T^{miss} and $\tau_{\text{had-vis}}-E_T^{\text{miss}}$, $\sum_{i=\ell, \tau_{\text{had-vis}}} \cos \Delta\phi(i, E_T^{\text{miss}})$, reduces the W + jets background whereas the requirement on $|\Delta\eta(\ell, \tau_{\text{had-vis}})|$ reduces backgrounds with misidentified $\tau_{\text{had-vis}}$ candidates.

For both channels of each search, a b -veto requirement reduces the single-top-quark and $t\bar{t}$ backgrounds. Events are further cate-

³ The transition region in η is excluded, similarly to electrons.

Table 2

Baseline event selection and further categorization for the $\ell\tau_{\nu'}$ and $\ell\tau_{\text{had}}$ channels. The same criteria are also used for the control region (CR) definitions in the $\ell\tau_{\nu'}$ channel (Section 5), but one requirement of the baseline selection is inverted to achieve orthogonal event selection. There is no CR in the $\ell\tau_{\text{had}}$ channel.

| Selection | $\ell\tau_{\nu'}$ | $\ell\tau_{\text{had}}$ |
|-----------------------------|---|--|
| Baseline | exactly 1e and 1 μ , OS | exactly 1 ℓ and 1 $\tau_{\text{had-vis}}$, OS |
| | $p_T^{\ell_1} > 45$ GeV | $p_T^{\ell} > 27.3$ GeV |
| | $p_T^{\ell_2} > 15$ GeV | $p_T^{\tau_{\text{had-vis}}} > 25$ GeV, $ \eta^{\tau_{\text{had-vis}}} < 2.4$ |
| | $30 \text{ GeV} < m_{\text{vis}} < 150$ GeV | $\sum_{i=\ell, \tau_{\text{had-vis}}} \cos \Delta\phi(i, E_T^{\text{miss}}) > -0.35$ |
| | $p_T^e(\text{track})/p_T^e(\text{cluster}) < 1.2$ ($\mu\tau_e$ only) | $ \Delta\eta(\ell, \tau_{\text{had-vis}}) < 2$ |
| | b -veto (for jets with $p_T > 25$ GeV and $ \eta < 2.4$) | |
| VBF | Baseline | |
| | ≥ 2 jets, $p_T^j_1 > 40$ GeV, $p_T^j_2 > 30$ GeV | |
| | $ \Delta\eta(j_1, j_2) > 3$, $m(j_1, j_2) > 400$ GeV | $p_T^{\tau_{\text{had-vis}}} > 45$ GeV |
| Non-VBF | Baseline plus fail VBF categorization | |
| | $m_T(\ell_1, E_T^{\text{miss}}) > 50$ GeV | – |
| | $m_T(\ell_2, E_T^{\text{miss}}) < 40$ GeV | – |
| | $ \Delta\phi(\ell_2, E_T^{\text{miss}}) < 1.0$ | – |
| | $p_T^{\tau}/p_T^{\ell_1} > 0.5$ | – |
| Top-quark CR | inverted b -veto: | |
| VBF and non-VBF | ≥ 1 b -tagged jet ($p_T > 25$ GeV and $ \eta < 2.4$) | |
| $Z \rightarrow \tau\tau$ CR | inverted $p_T^{\ell_1}$ requirement: | |
| VBF and non-VBF | $35 \text{ GeV} < p_T^{\ell_1} < 45$ GeV | |

gorized into VBF (with a focus on the VBF production of the Higgs boson) and non-VBF categories. The VBF selection is based on the kinematics of the two jets with the highest p_T , where j_1 and j_2 denote the leading and subleading jet in p_T , respectively. The variables $m(j_1, j_2)$ and $\Delta\eta(j_1, j_2)$ stand for the invariant mass and η separation of these two jets. The non-VBF category contains events failing the VBF selection. In the dilepton channel, additional selection criteria are applied to further reject background events in this category. These criteria are also listed in Table 2, where m_T stands for the transverse mass⁴ of the two objects listed in parentheses, and p_T^{τ} represents the magnitude of the vector sum of $p_T^{\ell_2}$ and E_T^{miss} . The requirement on $p_T^{\tau}/p_T^{\ell_1}$ reduces the background arising from jets misidentified as leptons. The VBF and non-VBF categories in each of the $\ell\tau_{\nu'}$ and $\ell\tau_{\text{had}}$ channels give rise to four signal regions in each search.

The analysis exploits BDT algorithms to enhance the signal separation from the background in the individual searches, channels and categories. The components of the four-momenta of the analysis objects as well as derived event variables (e.g. invariant masses and angular separations) are the input variables of the BDT discriminant. Correlations between these input variables have been carefully checked, highly correlated variables have been removed and the remaining ones are ranked according to their discrimination power [74,75]. The list of variables is then optimized, removing the lowest-ranked variables with marginal contribution to the sensitivity. The final list of variables is presented in Table 3 for each channel and category. The invariant mass of the Higgs boson reconstructed under the $H \rightarrow \ell\tau$ decay hypothesis exhibits the highest signal-to-background separation power and it helps to distinguish LFV signal from $H \rightarrow \tau\tau$ and $H \rightarrow WW$ backgrounds. For the $\ell\tau_{\nu'}$ channel the invariant mass is reconstructed with the MMC algorithm [76] and is denoted by m_{MMC} ; for the $\ell\tau_{\text{had}}$ channel it is reconstructed with the collinear approximation [76] and is denoted by m_{coll} . The analysis CRs are used to validate the level of

agreement between data and simulated distributions of the BDT score and input variables, as well as their correlations.

5. Background modelling

The most significant backgrounds in the search are from events with $Z \rightarrow \tau\tau$ decays or with (single or pair-produced) top quarks, especially in the $\ell\tau_{\nu'}$ channel, as well as from events with misidentified objects, which are estimated using data-driven (d.d.) techniques. The relative contribution from misidentified objects to the total background yield is 5–25% in the $\ell\tau_{\nu'}$ channel and 25–45% in the $\ell\tau_{\text{had}}$ channel, depending on the search and the analysis category. The shapes of distributions from the $Z \rightarrow \tau\tau$ and top-quark (single-top-quark and $t\bar{t}$) processes are modelled by simulation in both the $\ell\tau_{\nu'}$ and $\ell\tau_{\text{had}}$ decay channels. In the $\ell\tau_{\nu'}$ channel, the relative contributions of $Z \rightarrow \tau\tau$ and top-quark production processes are 20–35% and 20–55%, respectively; the top-quark background dominates in the VBF category. In the $\ell\tau_{\text{had}}$ channel, the top-quark background fraction is 1–10%, while the $Z \rightarrow \tau\tau$ process contributes to 45–55% of the total background. The individual contributions are listed in Tables 4 and 5. Smaller background components are also modelled by simulation and are grouped together: $Z \rightarrow \mu\mu$, diboson production, $H \rightarrow \tau\tau$ and $H \rightarrow WW$.

Good modelling of the background is demonstrated in Fig. 1 for a selection of important BDT input variables. Details of the background estimation techniques are given below.

5.1. $\ell\tau_{\nu'}$ channel

Two sets of CRs, as defined in Table 2, are used to constrain the normalization of $Z \rightarrow \tau\tau$ and top-quark background components. These CRs inherit their definitions from the corresponding analysis category but invert one requirement to ensure orthogonality with the nominal selection. The normalization factors are determined during the statistical analysis by fitting the event yields in all signal and control regions simultaneously. For each search, separate $Z \rightarrow \tau\tau$ normalization factors are used for the VBF and non-VBF categories. In the case of the top-quark background, in

⁴ The transverse mass of two objects is defined as $m_T = \sqrt{2p_{T1}p_{T2}(1 - \cos \Delta\phi)}$, where p_{Tj} are the individual transverse momenta and $\Delta\phi$ is the angle between the two objects in the azimuthal plane.

Table 3

BDT input variables used in the analysis. For each channel and category, used input variables are marked with HR (indicating the five variables with the highest rank) or a bullet. Analogous variables between the two channels are listed on the same line.

| $\ell\tau_{\ell'}$ | | | $\ell\tau_{\text{had}}$ | | |
|--|-----|---------|---|-----|---------|
| Variable | VBF | non-VBF | Variable | VBF | non-VBF |
| m_{MMC} | HR | HR | m_{coll} | HR | HR |
| $p_{\text{T}}^{\ell_1}$ | • | • | p_{T}^{ℓ} | • | HR |
| $p_{\text{T}}^{\ell_2}$ | HR | HR | $p_{\text{T}}^{\tau_{\text{had-vis}}}$ | • | HR |
| $\Delta R(\ell_1, \ell_2)$ | HR | • | $\Delta R(\ell, \tau_{\text{had-vis}})$ | • | • |
| $m_{\text{T}}(\ell_1, E_{\text{T}}^{\text{miss}})$ | • | HR | $m_{\text{T}}(\ell, E_{\text{T}}^{\text{miss}})$ | HR | • |
| $m_{\text{T}}(\ell_2, E_{\text{T}}^{\text{miss}})$ | HR | • | $m_{\text{T}}(\tau_{\text{had-vis}}, E_{\text{T}}^{\text{miss}})$ | HR | HR |
| $\Delta\phi(\ell_1, E_{\text{T}}^{\text{miss}})$ | • | • | $\Delta\phi(\ell, E_{\text{T}}^{\text{miss}})$ | HR | • |
| $\Delta\phi(\ell_2, E_{\text{T}}^{\text{miss}})$ | • | HR | $\Delta\phi(\tau_{\text{had-vis}}, E_{\text{T}}^{\text{miss}})$ | • | • |
| $m(j_1, j_2)$ | • | • | $m(j_1, j_2)$ | • | • |
| $\Delta\eta(j_1, j_2)$ | HR | • | $\Delta\eta(j_1, j_2)$ | • | • |
| $p_{\text{T}}^{\tau}/p_{\text{T}}^{\ell_1}$ | • | HR | $\sum \cos \Delta\phi(i, E_{\text{T}}^{\text{miss}})$ | • | • |
| | | | $\sum_{i=\ell, \tau_{\text{had-vis}}} \cos \Delta\phi(i, E_{\text{T}}^{\text{miss}})$ | • | • |
| | | | $E_{\text{T}}^{\text{miss}}$ | HR | • |
| | | | m_{vis} | • | HR |
| | | | $\Delta\eta(\ell, \tau_{\text{had-vis}})$ | • | • |
| | | | η^{ℓ} | • | • |
| | | | $\eta^{\tau_{\text{had-vis}}}$ | • | • |
| | | | ϕ^{ℓ} | • | • |
| | | | $\phi^{\tau_{\text{had-vis}}}$ | • | • |
| | | | $\phi(E_{\text{T}}^{\text{miss}})$ | • | • |

Table 4

Event yields and predictions as determined by the background-only fit in different signal regions of the $H \rightarrow e\tau$ analysis. Uncertainties include both the statistical and systematic contributions. "Other" contains diboson, $Z \rightarrow \ell\ell$, $H \rightarrow \tau\tau$ and $H \rightarrow WW$ background processes. For the $e\tau_{\text{had}}$ channel the " $Z \rightarrow ee$ (d.d.)" component corresponds to electrons misidentified as $\tau_{\text{had-vis}}$. This contribution is summed with "Other" since there are few events in the VBF category. The uncertainty of the total background includes all correlations between channels. The normalizations of top-quark ($\ell\tau_{\ell'}$ channel only) and $Z \rightarrow \tau\tau$ background components are determined by the fit, while the expected signal event yields are given for $\mathcal{B}(H \rightarrow e\tau) = 1\%$.

| | $e\tau_{\mu}$ non-VBF | $e\tau_{\mu}$ VBF | $e\tau_{\text{had}}$ non-VBF | $e\tau_{\text{had}}$ VBF |
|---------------------------|-----------------------|-------------------|------------------------------|--------------------------|
| Signal | 379 ± 31 | 19.8 ± 2.7 | 1180 ± 110 | 25 ± 4 |
| $Z \rightarrow \tau\tau$ | 2470 ± 230 | 221 ± 34 | $73\,800 \pm 1900$ | 290 ± 40 |
| Top-quark | 1640 ± 140 | 490 ± 40 | 1580 ± 190 | 56 ± 12 |
| Mis-identified | 1330 ± 250 | 73 ± 33 | $74\,400 \pm 1600$ | 140 ± 50 |
| $Z \rightarrow ee$ (d.d.) | • | • | $15\,900 \pm 1800$ | • |
| Other | 1700 ± 80 | 220 ± 15 | 2960 ± 200 | 82 ± 13 |
| Total background | 7130 ± 100 | 1003 ± 33 | $168\,700 \pm 1000$ | 570 ± 40 |
| Data | 7128 | 992 | 168883 | 572 |

Table 5

Event yields and predictions as determined by the background-only fit in different signal regions of the $H \rightarrow \mu\tau$ analysis. Uncertainties include both the statistical and systematic contributions. "Other" contains diboson, $Z \rightarrow \ell\ell$, $H \rightarrow \tau\tau$ and $H \rightarrow WW$ background processes. The uncertainty of the total background includes all correlations between channels. The normalizations of top-quark ($\ell\tau_{\ell'}$ channel only) and $Z \rightarrow \tau\tau$ background components are determined by the fit, while the expected signal event yields are given for $\mathcal{B}(H \rightarrow \mu\tau) = 1\%$.

| | $\mu\tau_e$ non-VBF | $\mu\tau_e$ VBF | $\mu\tau_{\text{had}}$ non-VBF | $\mu\tau_{\text{had}}$ VBF |
|--------------------------|---------------------|-----------------|--------------------------------|----------------------------|
| Signal | 287 ± 23 | 14.6 ± 1.9 | 1200 ± 120 | 25 ± 5 |
| $Z \rightarrow \tau\tau$ | 1860 ± 130 | 144 ± 26 | $96\,100 \pm 2000$ | 274 ± 33 |
| Top quark | 1260 ± 130 | 390 ± 34 | 1620 ± 210 | 51 ± 10 |
| Misidentified | 1340 ± 210 | 41 ± 21 | $63\,900 \pm 1600$ | 149 ± 33 |
| Other | 1180 ± 140 | 168 ± 18 | $23\,000 \pm 1000$ | 104 ± 15 |
| Total background | 5640 ± 100 | 743 ± 29 | $184\,500 \pm 1200$ | 580 ± 30 |
| Data | 5664 | 723 | 184508 | 583 |

which leading jets are produced at a lower order of the perturbative expansion of the scattering process, a combined normalization factor across the two categories is used in the $\ell\tau_{\ell'}$ channel.

Top-quark CRs are almost exclusively composed of top-quark backgrounds: the purity is 95% across both searches and categories, with $t\bar{t}$ process accounting for more than 90% of the top-quark backgrounds. The $Z \rightarrow \tau\tau$ CRs achieved a purity of $\sim 80\%$ in the non-VBF categories, while a lower purity of $\sim 60\%$ is observed in

the VBF categories. The contributions of all other background components are normalized to their SM predictions when the likelihood fit (Section 7) is applied.

The shape and normalization of diboson and $Z \rightarrow \mu\mu$ background distributions are validated with data in dedicated regions where their contributions are enhanced. The latter process only contributes sizeably in the $\mu\tau_e$ channel, where it represents up to 10% of the total background.

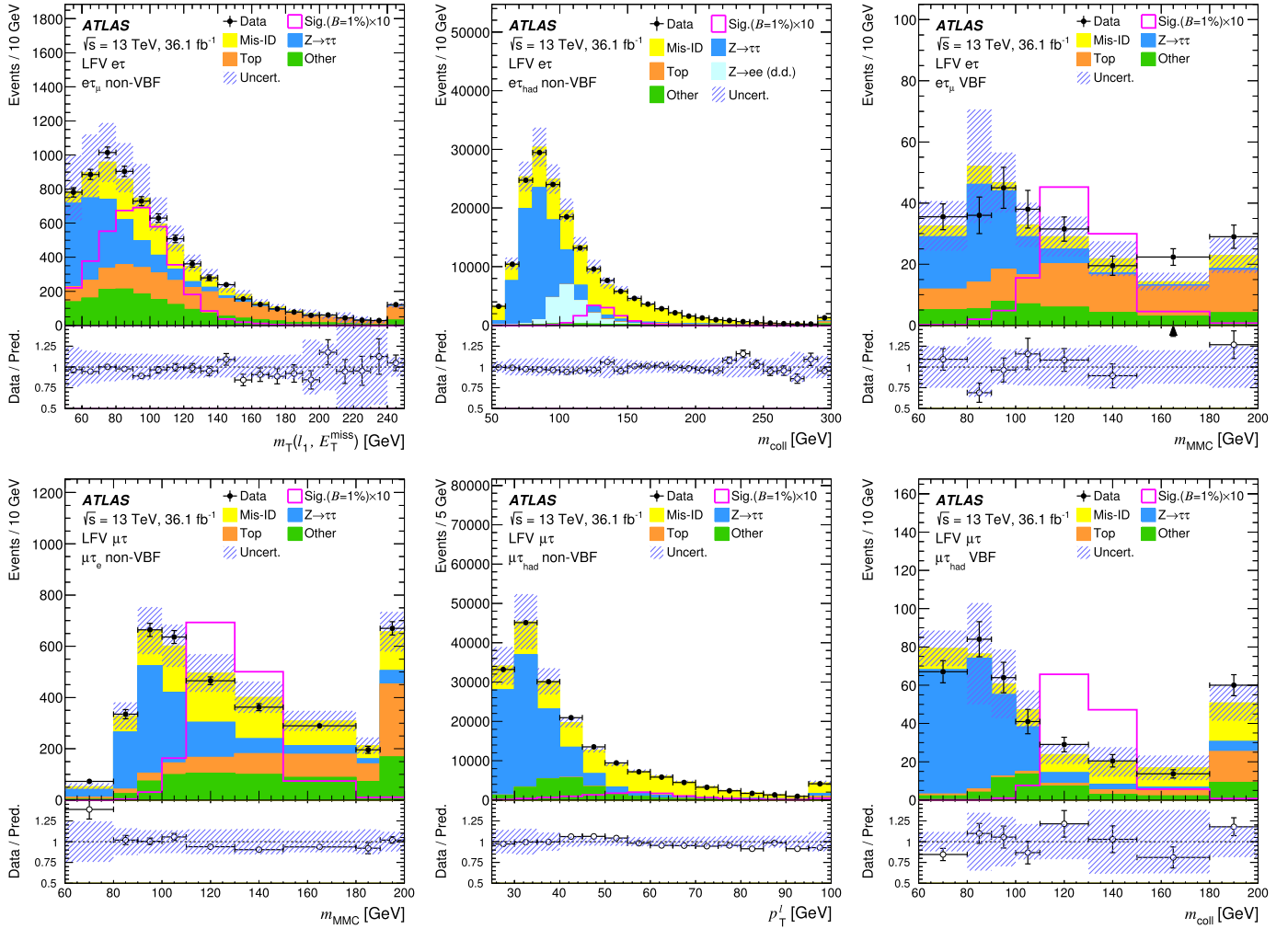


Fig. 1. Distributions of representative kinematic quantities for different searches, channels and categories, before the fit as described in Section 7 is applied. Top row: transverse mass $m_T(\ell_1, E_T^{\text{miss}})$ ($e\tau_\mu$ non-VBF), collinear mass m_{coll} ($e\tau_{\text{had}}$ non-VBF) and m_{MMC} ($e\tau_\mu$ VBF). Bottom row: m_{MMC} ($\mu\tau_e$ non-VBF), muon p_T ($\mu\tau_{\text{had}}$ non-VBF) and m_{coll} ($\mu\tau_{\text{had}}$ VBF). Entries with values that would exceed the x-axis range are included in the last bin of each distribution. The size of the combined statistical, experimental and theoretical uncertainties in the background is indicated by the hatched bands. The $H \rightarrow e\tau$ ($H \rightarrow \mu\tau$) signal overlaid in top (bottom) plots assumes $\mathcal{B}(H \rightarrow \ell\tau) = 1\%$ and is enhanced by a factor 10. In the data/background prediction ratio plots, points outside the displayed y-axis range are shown by arrows.

Another source of background comes from W + jets, top-quark and multi-jet events, where jets are misidentified as leptons. This background is estimated directly from OS data events where an inverted isolation requirement is imposed on the subleading lepton [17]. Normalization factors are applied to correct for the inverted isolation requirement. The normalization factors are derived in a dedicated region where the leptons are required to have same-sign (SS) charges. Additional corrections are made by reweighting the MC distributions of $\Delta\phi(\ell_1, E_T^{\text{miss}})$ and $\Delta\phi(\ell_2, E_T^{\text{miss}})$ to data in the SS region, which improves the modelling of azimuthal angles between leptons and the E_T^{miss} direction as well as the modelling of $m_T(\ell_2, E_T^{\text{miss}})$. A similar improvement is observed in the nominal OS region. In most of the cases, the misidentified jet mimics the lepton of lower p_T , ℓ_2 , while the fraction of events where both leptons are misidentified varies between 2% to 8% across categories. The systematic uncertainties of the estimation of the misidentified lepton background include contributions from closure tests in SS and OS regions enriched with misidentified leptons, from the corrections made to the $\Delta\phi$ distributions, and from the composition of the misidentified lepton background.

5.2. $\ell\tau_{\text{had}}$ channel

The main background contributions come from the $Z \rightarrow \tau\tau$ process and events where either a jet or an electron is misidentified as $\tau_{\text{had-vis}}$. The shape of the $Z \rightarrow \tau\tau$ background distribution is modelled by simulation, and the corresponding normalization factors are determined from the simultaneous fit of the event yields in all signal and control regions. The $Z \rightarrow \tau\tau$ normalization factors are fully correlated with those of the $\ell\tau_\nu$ channel, in each VBF and non-VBF category. Top-quark production represents less than 1% of the total background in the $\ell\tau_{\text{had}}$ channel and is determined by simulation, including its normalization, which is kept fixed in the fit.

The main contributions to jets misidentified as $\tau_{\text{had-vis}}$ come from multi-jet events and W -boson production in association with jets, and a fake-factor method is used to estimate the contribution of each component separately. A fake factor is defined as the ratio of the number of events where the highest- p_T jet is identified as a tight $\tau_{\text{had-vis}}$ candidate to the number of events where the highest- p_T jet fails to satisfy this τ -ID criterion but satisfies a looser criterion. The procedure, including systematic uncertainties, is described in Ref. [17]. Since a different τ -ID working point

is considered in this analysis, fake factors are re-derived as a function of p_T and track multiplicity of the $\tau_{\text{had-vis}}$ candidate.

Electrons misidentified as $\tau_{\text{had-vis}}$, denoted by “ $Z \rightarrow ee$ (d.d.)” in the following figures and tables, represent another background component in the $e\tau_{\text{had}}$ channel, with a contribution about five times smaller than that of jets misidentified as $\tau_{\text{had-vis}}$. While the rate of electrons misidentified as 3-prong $\tau_{\text{had-vis}}$ makes a negligible contribution and is modelled by simulation, the rate of electrons misidentified as 1-prong $\tau_{\text{had-vis}}$ is determined with a fake-factor method. This time, the fake factor is defined as the ratio of the number of events with tight τ -ID to the number of events with anti-identified $\tau_{\text{had-vis}}$ (such a candidate satisfies all criteria but the requirement on the high electron ID score is inverted). These fake factors are derived in a dedicated $Z \rightarrow ee$ enriched region defined by $|m_{\text{vis}} - m_Z| < 5$ GeV, $m_T(\ell, E_T^{\text{miss}}) < 40$ GeV, and $m_T(\tau_{\text{had-vis}}, E_T^{\text{miss}}) < 60$ GeV, where the $\tau_{\text{had-vis}}$ candidate satisfies the medium τ -ID (corresponding to an efficiency of 55% and 40% for 1-prong and 3-prong candidates, respectively) but not the tight τ -ID criterion to avoid overlap with the $\ell\tau_{\text{had}}$ signal region. These fake factors are applied to signal-like events with the anti-identified $\tau_{\text{had-vis}}$ to determine the background contribution in the categories of the analysis. The systematic uncertainties include the statistical uncertainty of the fake factors and account for looser τ -ID in the $Z \rightarrow ee$ enriched region as well as for the subtraction of the not misidentified components in this region.

6. Systematic uncertainties

The systematic uncertainties affect the normalization of signal and background, and/or the shape of their corresponding final discriminant distributions. Each source of systematic uncertainty is considered to be uncorrelated with the other sources. The effect of each systematic uncertainty is fully considered in each category, including control regions. Correlations of each systematic uncertainty are maintained across processes, channels, categories and regions. The size of the systematic uncertainties and their impact on the fitted branching ratio are discussed in Section 7. The main sources of systematic uncertainties are related to the estimation of the backgrounds originating from mis-identified leptons/jets and to the jet energy scale uncertainties.

Experimental uncertainties include those originating from the reconstruction, identification, tagging and triggering efficiencies of all physics objects as well as their momentum scale and resolution. These include effects from leptons [57–59], $\tau_{\text{had-vis}}$ [68], jets [63, 64, 77] and E_T^{miss} [78]. Uncertainties affecting the kinematics of the physics objects are propagated to the BDT input variables. The corresponding shape and normalization variations of the BDT discriminant are considered in the statistical analysis. Uncertainties of the luminosity measurement [79], pile-up modelling and uncertainties specific to mis-identified background estimation techniques mentioned in Section 5 are included.

The procedures to estimate the uncertainty of the Higgs boson production cross-sections follow the recommendations of the LHC Higgs Cross-Section Working Group [80]. Theoretical uncertainties affecting the ggF signal originate from nine sources [24]. Two sources account for yield uncertainties, which are evaluated by an overall variation of all relevant scales and are correlated across all bins of the BDT discriminant distribution [81]. Another two sources account for migration uncertainties of zero to one jet and one to at least two jets in the event [81–83], two for Higgs boson p_T shape uncertainties, one for the treatment of the top-quark mass in the loop corrections, and two for the acceptance uncertainties of ggF production in the VBF phase space from selecting exactly two and at least three jets, respectively [84, 85]. For VBF and WH, ZH production cross-sections, the uncertainties due to

missing higher-order QCD corrections are estimated by varying the factorization and renormalization scales up and down by factors of two around the nominal scale. For all signal samples, PDF uncertainties are estimated using 30 eigenvector variations and two α_s variations using the default PDF set PDF4LHC15 [32]. Uncertainties related to the simulation of the underlying event, hadronization and parton shower are estimated by comparing the acceptances when using Pythia 8.212 [25] or Herwig 7.0.3 [86, 87].

The sources of modelling uncertainties considered for the $Z \rightarrow \tau\tau$ process are the same as in Ref. [17] and their effect on the event migrations between categories and on the shape of the BDT discriminant are considered, since the overall normalizations are determined from data in the statistical analysis. These systematic uncertainties include variations of PDF sets, factorization and renormalization scales, CKKW matching [88], resummation scale and parton shower modelling. The other background processes are either normalized using data (processes with top-quarks and mis-identified leptons and $\tau_{\text{had-vis}}$ candidates) or their cross-section uncertainties have negligible impact and therefore are not included. The shape uncertainties of these backgrounds originate from experimental uncertainties only.

7. Statistical analysis

The searches for $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ are treated independently. For each search, the analysis exploits the four signal regions and the two control regions specified in Table 2. The BDT score distributions of all signal regions are analysed to test the presence of a signal, simultaneously with the event yields in control regions, which are included to constrain the normalizations of the major backgrounds estimated from simulation. The statistical analysis uses 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 parameter μ , defined as the branching ratio $\mathcal{B}(H \rightarrow \ell\tau)$, and a set of nuisance parameters θ that encode the effect of systematic uncertainties in the signal and background expectations. All nuisance parameters are implemented in the likelihood function as Gaussian or log-normal constraints. The normalization factors of the single-top-quark and $t\bar{t}$ backgrounds in the $\ell\tau_{\ell'}$ channel and of the $Z \rightarrow \tau\tau$ background component are unconstrained parameters of the fit. Estimates of the parameters of interest are calculated with the profile-likelihood-ratio test statistic \tilde{q}_μ [89], and the upper limits on the branching ratios are derived by using \tilde{q}_μ and the CL_S method [90].

The discriminant distributions after the fit in each channel are shown in Figs. 2 and 3. Good agreement between data and the background expectation is observed. The event yields after the background-only fit are summarized in Tables 4 and 5. In the non-VBF category, the yields in the $\ell\tau_{\text{had}}$ channel are larger than in the $\ell\tau_{\ell'}$ channel due to the looser selection criteria defined for the former channel (Section 4). Table 6 shows a summary of the uncertainties of $\mathcal{B}(H \rightarrow \ell\tau)$. The uncertainties associated with misidentified leptons and $\tau_{\text{had-vis}}$ candidates and those related to the jet energy scale and resolution exhibit the highest impact on the best-fit branching ratios in both searches. The combined impact from all systematic uncertainties and the data statistics ranges from 0.17% to 0.19%.

8. Results

The best-fit branching ratios and upper limits are computed while assuming $\mathcal{B}(H \rightarrow \mu\tau) = 0$ for the $H \rightarrow e\tau$ search and $\mathcal{B}(H \rightarrow e\tau) = 0$ for the $H \rightarrow \mu\tau$ search. The best-fit values of the LFV Higgs boson branching ratios are equal to $(0.15_{-0.17}^{+0.18})\%$ and $(-0.22 \pm 0.19)\%$ for the $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ search, respectively.

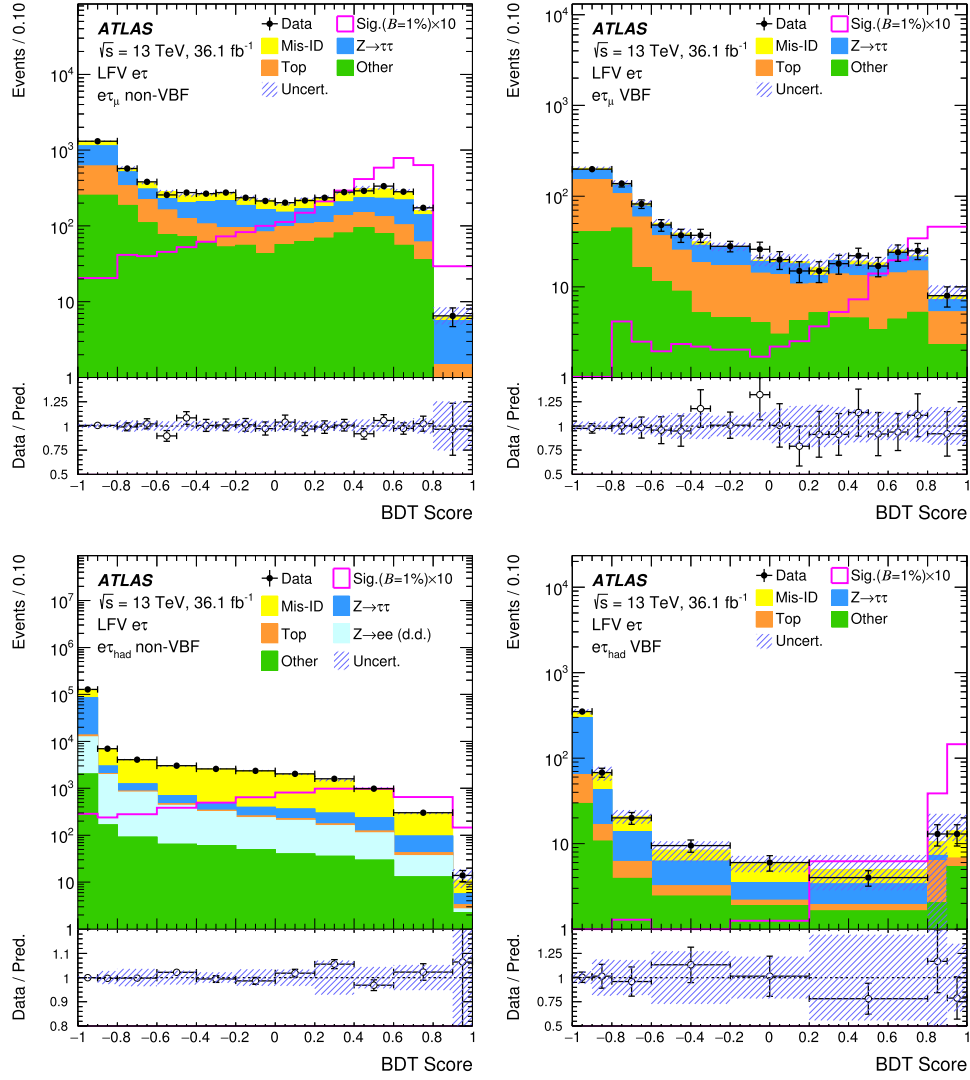


Fig. 2. Distributions of the BDT score after the background+signal fit in each signal region of the $e\tau$ search, with the LFV signal overlaid, normalized with $\mathcal{B}(H \rightarrow e\tau) = 1\%$ and enhanced by a factor 10 for visibility. The top and bottom plots display $e\tau_\mu$ and $e\tau_{\text{had}}$ BDT scores respectively, the left (right) column corresponds to the non-VBF (VBF) category. The size of the combined statistical, experimental and theoretical uncertainties of the background is indicated by the hatched bands. The binning is shown as in the statistical analysis.

Table 6

Summary of the systematic uncertainties and their impact on the best-fit value of \mathcal{B} in the $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ searches. The measured values are obtained by the fit to data, while the expected values are determined by the fit to a background-only sample.

| Source of uncertainty | Impact on $\mathcal{B}(H \rightarrow e\tau)$ [%] | | Impact on $\mathcal{B}(H \rightarrow \mu\tau)$ [%] | |
|---|--|---------------|--|---------------|
| | Measured | Expected | Measured | Expected |
| Electron | +0.05 / -0.05 | +0.06 / -0.06 | +0.03 / -0.03 | +0.02 / -0.02 |
| Muon | +0.04 / -0.04 | +0.04 / -0.04 | +0.10 / -0.10 | +0.08 / -0.10 |
| $\tau_{\text{had-vis}}$ | +0.02 / -0.02 | +0.02 / -0.02 | +0.04 / -0.04 | +0.04 / -0.05 |
| Jet | +0.09 / -0.08 | +0.09 / -0.09 | +0.11 / -0.12 | +0.11 / -0.12 |
| $E_{\text{T}}^{\text{miss}}$ | +0.02 / -0.02 | +0.02 / -0.03 | +0.05 / -0.08 | +0.03 / -0.05 |
| b -tag | +0.02 / -0.03 | +0.03 / -0.03 | +0.01 / -0.01 | +0.01 / -0.01 |
| Mis-ID backg. ($\ell\tau_{\ell'}$) | +0.08 / -0.07 | +0.09 / -0.08 | +0.07 / -0.07 | +0.07 / -0.07 |
| Mis-ID backg. ($\ell\tau_{\text{had}}$) | +0.12 / -0.11 | +0.11 / -0.12 | +0.11 / -0.11 | +0.10 / -0.10 |
| Pile-up modelling | +0.02 / -0.01 | +0.01 / -0.01 | +0.05 / -0.03 | +0.08 / -0.06 |
| Luminosity | < 0.01 | < 0.01 | < 0.01 | < 0.01 |
| Background norm. | +0.05 / -0.04 | +0.05 / -0.03 | +0.04 / -0.02 | +0.05 / -0.03 |
| Theor. uncert. (backg.) | +0.04 / -0.03 | +0.04 / -0.03 | +0.08 / -0.07 | +0.09 / -0.09 |
| Theor. uncert. (signal) | +0.01 / -0.01 | +0.01 / -0.01 | +0.04 / -0.02 | +0.02 / -0.02 |
| MC statistics | +0.04 / -0.04 | +0.03 / -0.03 | +0.04 / -0.04 | +0.05 / -0.04 |
| Full systematic | +0.17 / -0.16 | +0.17 / -0.17 | +0.18 / -0.18 | +0.19 / -0.20 |
| Data statistics | +0.07 / -0.07 | +0.07 / -0.07 | +0.07 / -0.07 | +0.08 / -0.08 |
| Total | +0.18 / -0.17 | +0.18 / -0.18 | +0.19 / -0.19 | +0.20 / -0.21 |

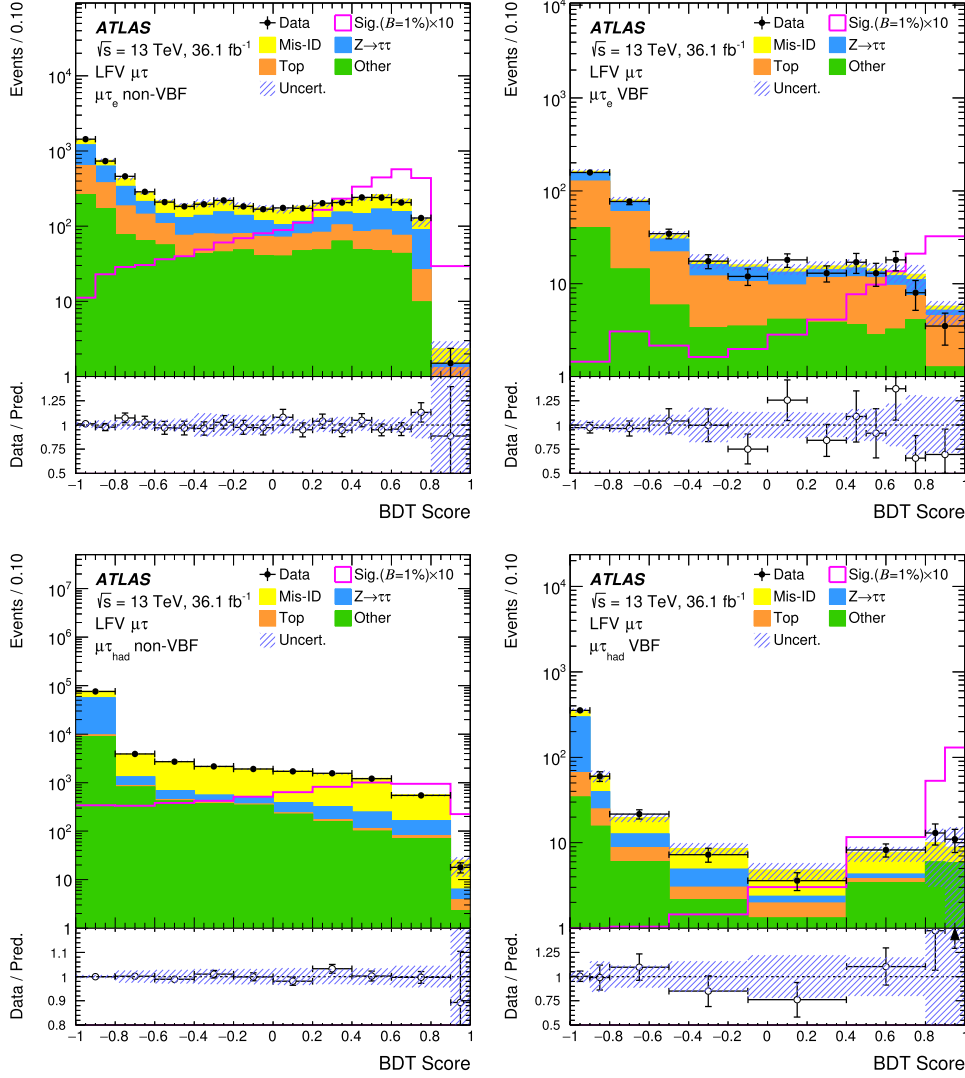


Fig. 3. Distributions of the BDT score after the background+signal fit in each signal region of the $\mu\tau$ search, with the LFV signal overlaid, normalized with $B(H \rightarrow \mu\tau) = 1\%$ and enhanced by a factor 10 for visibility. The top and bottom plots display $\mu\tau_e$ and $\mu\tau_{\text{had}}$ BDT scores respectively, the left (right) column corresponds to the non-VBF (VBF) category. The size of the combined statistical, experimental and theoretical uncertainties of the background is indicated by the hatched bands. The binning is shown as in the statistical analysis. In the data/background prediction ratio plots, points outside the displayed y-axis range are shown by arrows.

In the absence of a significant excess, upper limits on the LFV branching ratios are set for a Higgs boson with $m_H = 125$ GeV. The observed (median expected) 95% CL upper limits are 0.47% ($0.34^{+0.13}_{-0.10}\%$) and 0.28% ($0.37^{+0.14}_{-0.10}\%$) for the $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ searches, respectively. These limits are significantly lower than the corresponding Run 1 limits of Refs. [14,15]. The breakdown of contributions from different signal regions is shown in Fig. 4.

The branching ratio of the LFV Higgs boson decay is related to the non-diagonal Yukawa coupling matrix elements [91] by the formula

$$|Y_{\ell\tau}|^2 + |Y_{\tau\ell}|^2 = \frac{8\pi}{m_H} \frac{B(H \rightarrow \ell\tau)}{1 - B(H \rightarrow \ell\tau)} \Gamma_H(\text{SM}),$$

where $\Gamma_H(\text{SM}) = 4.07$ MeV [92] stands for the Higgs boson width as predicted by the Standard Model. Thus, the observed limits on the branching ratio correspond to the following limits on the coupling matrix elements: $\sqrt{|Y_{\tau\ell}|^2 + |Y_{\ell\tau}|^2} < 0.0020$, and $\sqrt{|Y_{\tau\mu}|^2 + |Y_{\mu\tau}|^2} < 0.0015$. Fig. 5 shows the limits on the individual coupling matrix elements $Y_{\tau\ell}$ and $Y_{\ell\tau}$ together with the limits from the ATLAS Run 1 analysis and from $\tau \rightarrow \ell\gamma$ searches [91,93].

9. Conclusions

Direct searches for the decays $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ are performed with proton–proton collisions recorded by the ATLAS detector at the LHC corresponding to an integrated luminosity of 36.1 fb^{-1} at a centre-of-mass energy of $\sqrt{s} = 13$ TeV. No significant excess is observed above the expected background from Standard Model processes. The observed (expected) upper limits at 95% confidence level on the branching ratios of $H \rightarrow e\tau$ and $H \rightarrow \mu\tau$ are 0.47% ($0.34^{+0.13}_{-0.10}\%$) and 0.28% ($0.37^{+0.14}_{-0.10}\%$), respectively. These limits are more stringent by a factor of 2 (5) than the corresponding limits for the $H \rightarrow e\tau$ ($H \rightarrow \mu\tau$) decay determined by ATLAS at $\sqrt{s} = 8$ TeV.

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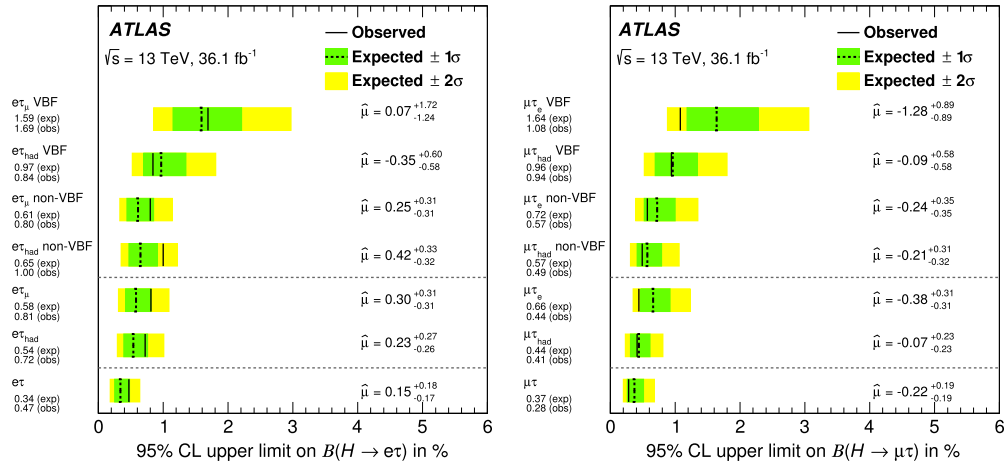


Fig. 4. Upper limits at 95% CL on the LFV branching ratios of the Higgs boson, $H \rightarrow e\tau$ (left) and $H \rightarrow \mu\tau$ (right), indicated by solid and dashed lines. Best-fit values of the branching ratios ($\hat{\mu}$) are also given, in %. The limits are computed while assuming that either $\mathcal{B}(H \rightarrow \mu\tau) = 0$ (left) or $\mathcal{B}(H \rightarrow e\tau) = 0$ (right). First, the results of the fits are shown, when only the data of an individual channel or of an individual category are used; in these cases the signal and control regions from all other channels/categories are removed from the fit. These results are finally compared with the full fit displayed in the last row.

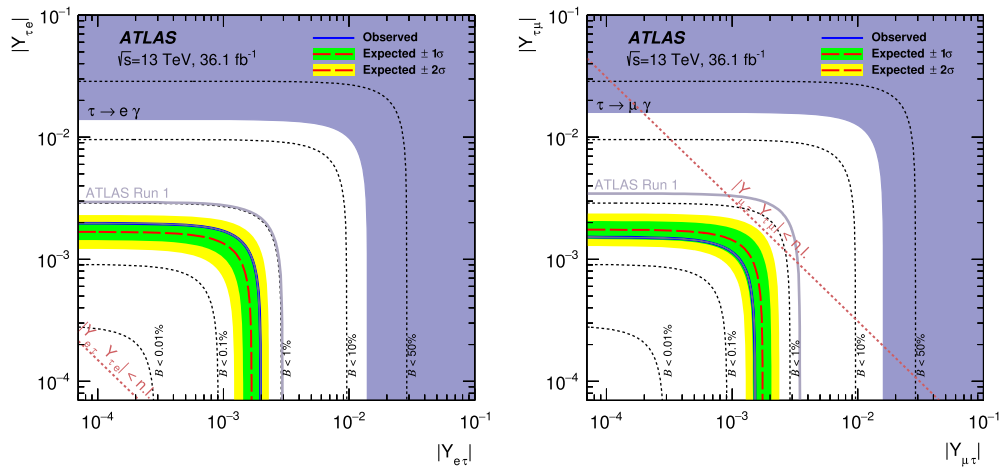


Fig. 5. Upper limits on the absolute value of the couplings $Y_{\tau e}$ and $Y_{e\tau}$ together with the limits from the ATLAS Run 1 analysis (light grey line) and the most stringent indirect limits from $\tau \rightarrow e\gamma$ searches (dark purple region). Also indicated are limits corresponding to different branching ratios (0.01%, 0.1%, 1%, 10% and 50%) and the naturalness limit (denoted n.l.) $|Y_{\tau e} Y_{e\tau}| \lesssim \frac{m_e m_\tau}{v^2}$ [91] where v is the vacuum expectation value of the Higgs field.

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 B.M. Barnett ¹⁴⁴, R.M. Barnett ¹⁸, Z. Barnovska-Blenessy ^{60a}, A. Baroncelli ^{60a}, G. Barone ²⁹, A.J. Barr ¹³⁵,
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 S. Campana ³⁶, M. Campanelli ⁹⁴, A. Camplani ⁴⁰, A. Campoverde ¹⁵¹, V. Canale ^{69a,69b}, A. Canesse ¹⁰³,
 M. Cano Bret ^{60c}, J. Cantero ¹²⁹, T. Cao ¹⁶¹, Y. Cao ¹⁷³, M.D.M. Capeans Garrido ³⁶, M. Capua ^{41b,41a},
 R. Cardarelli ^{73a}, F.C. Cardillo ¹⁴⁹, G. Carducci ^{41b,41a}, I. Carli ¹⁴³, T. Carli ³⁶, G. Carlino ^{69a}, B.T. Carlson ¹³⁹,
 L. Carminati ^{68a,68b}, R.M.D. Carney ^{45a,45b}, S. Caron ¹¹⁹, E. Carquin ^{147b}, S. Carrá ⁴⁶, J.W.S. Carter ¹⁶⁷,
 M.P. Casado ^{14,d}, A.F. Casha ¹⁶⁷, D.W. Casper ¹⁷¹, R. Castelijin ¹²⁰, F.L. Castillo ¹⁷⁴, V. Castillo Gimenez ¹⁷⁴,
 N.F. Castro ^{140a,140e}, A. Catinaccio ³⁶, J.R. Catmore ¹³⁴, A. Cattai ³⁶, J. Caudron ²⁴, V. Cavaliere ²⁹,
 E. Cavallaro ¹⁴, M. Cavalli-Sforza ¹⁴, V. Cavasinni ^{71a,71b}, E. Celebi ^{12b}, F. Ceradini ^{74a,74b},
 L. Cerda Alberich ¹⁷⁴, K. Cerny ¹³⁰, A.S. Cerqueira ^{80a}, A. Cerri ¹⁵⁶, L. Cerrito ^{73a,73b}, F. Cerutti ¹⁸,
 A. Cervelli ^{23b,23a}, S.A. Cetin ^{12b}, Z. Chadi ^{35a}, D. Chakraborty ¹²¹, S.K. Chan ⁵⁹, W.S. Chan ¹²⁰, W.Y. Chan ⁹⁰,
 J.D. Chapman ³², B. Chargeishvili ^{159b}, D.G. Charlton ²¹, T.P. Charman ⁹², C.C. Chau ³⁴, S. Che ¹²⁶,
 A. Chegwidden ¹⁰⁶, S. Chekanov ⁶, S.V. Chekulaev ^{168a}, G.A. Chelkov ^{79,au}, M.A. Chelstowska ³⁶, B. Chen ⁷⁸,
 C. Chen ^{60a}, C.H. Chen ⁷⁸, H. Chen ²⁹, J. Chen ^{60a}, J. Chen ³⁹, S. Chen ¹³⁷, S.J. Chen ^{15c}, X. Chen ^{15b,at},
 Y. Chen ⁸², Y-H. Chen ⁴⁶, H.C. Cheng ^{63a}, H.J. Cheng ^{15a,15d}, A. Cheplakov ⁷⁹, E. Cheremushkina ¹²³,
 R. Cherkaoui El Moursli ^{35e}, E. Cheu ⁷, K. Cheung ⁶⁴, T.J.A. Chevalérias ¹⁴⁵, L. Chevalier ¹⁴⁵, V. Chiarella ⁵¹,

G. Chiarelli ^{71a}, G. Chiodini ^{67a}, A.S. Chisholm ^{36,21}, A. Chitan ^{27b}, I. Chiu ¹⁶³, Y.H. Chiu ¹⁷⁶, M.V. Chizhov ⁷⁹, K. Choi ⁶⁵, A.R. Chomont ^{72a,72b}, S. Chouridou ¹⁶², Y.S. Chow ¹²⁰, M.C. Chu ^{63a}, X. Chu ^{15a}, J. Chudoba ¹⁴¹, A.J. Chuinard ¹⁰³, J.J. Chwastowski ⁸⁴, L. Chytka ¹³⁰, K.M. Ciesla ⁸⁴, D. Cinca ⁴⁷, V. Cindro ⁹¹, I.A. Cioară ^{27b}, A. Ciocio ¹⁸, F. Ciroto ^{69a,69b}, Z.H. Citron ¹⁸⁰, M. Citterio ^{68a}, D.A. Ciubotaru ^{27b}, B.M. Ciungu ¹⁶⁷, A. Clark ⁵⁴, M.R. Clark ³⁹, P.J. Clark ⁵⁰, C. Clement ^{45a,45b}, Y. Coadou ¹⁰¹, M. Cobal ^{66a,66c}, A. Coccaro ^{55b}, J. Cochran ⁷⁸, H. Cohen ¹⁶¹, A.E.C. Coimbra ³⁶, L. Colasurdo ¹¹⁹, B. Cole ³⁹, A.P. Colijn ¹²⁰, J. Collot ⁵⁸, P. Conde Muiño ^{140a,e}, E. Coniavitis ⁵², S.H. Connell ^{33b}, I.A. Connelly ⁵⁷, S. Constantinescu ^{27b}, F. Conventi ^{69a,aw}, A.M. Cooper-Sarkar ¹³⁵, F. Cormier ¹⁷⁵, K.J.R. Cormier ¹⁶⁷, L.D. Corpe ⁹⁴, M. Corradi ^{72a,72b}, E.E. Corrigan ⁹⁶, F. Corriveau ^{103,ab}, A. Cortes-Gonzalez ³⁶, M.J. Costa ¹⁷⁴, F. Costanza ⁵, D. Costanzo ¹⁴⁹, G. Cowan ⁹³, J.W. Cowley ³², J. Crane ¹⁰⁰, K. Cranmer ¹²⁴, S.J. Crawley ⁵⁷, R.A. Creager ¹³⁷, S. Crépe-Renaudin ⁵⁸, F. Crescioli ¹³⁶, M. Cristinziani ²⁴, V. Croft ¹²⁰, G. Crosetti ^{41b,41a}, A. Cueto ⁵, T. Cuhadar Donszelmann ¹⁴⁹, A.R. Cukierman ¹⁵³, S. Czokierda ⁸⁴, P. Czodrowski ³⁶, M.J. Da Cunha Sargedas De Sousa ^{60b}, J.V. Da Fonseca Pinto ^{80b}, C. Da Via ¹⁰⁰, W. Dabrowski ^{83a}, T. Dado ^{28a}, S. Dahbi ^{35e}, T. Dai ¹⁰⁵, C. Dallapiccola ¹⁰², M. Dam ⁴⁰, G. D'amen ^{23b,23a}, V. D'Amico ^{74a,74b}, J. Damp ⁹⁹, J.R. Dandoy ¹³⁷, M.F. Daneri ³⁰, N.P. Dang ¹⁸¹, N.D. Dann ¹⁰⁰, M. Danninger ¹⁷⁵, V. Dao ³⁶, G. Darbo ^{55b}, O. Dartsis ⁵, A. Dattagupta ¹³¹, T. Daubney ⁴⁶, S. D'Auria ^{68a,68b}, W. Davey ²⁴, C. David ⁴⁶, T. Davidek ¹⁴³, D.R. Davis ⁴⁹, I. Dawson ¹⁴⁹, K. De ⁸, R. De Asmundis ^{69a}, M. De Beurs ¹²⁰, S. De Castro ^{23b,23a}, S. De Cecco ^{72a,72b}, N. De Groot ¹¹⁹, P. de Jong ¹²⁰, H. De la Torre ¹⁰⁶, A. De Maria ^{15c}, D. De Pedis ^{72a}, A. De Salvo ^{72a}, U. De Sanctis ^{73a,73b}, M. De Santis ^{73a,73b}, A. De Santo ¹⁵⁶, K. De Vasconcelos Corga ¹⁰¹, J.B. De Vivie De Regie ¹³², C. Debenedetti ¹⁴⁶, D.V. Dedovich ⁷⁹, A.M. Deiana ⁴², M. Del Gaudio ^{41b,41a}, J. Del Peso ⁹⁸, Y. Delabat Diaz ⁴⁶, D. Delgove ¹³², F. Deliot ^{145,p}, C.M. Delitzsch ⁷, M. Della Pietra ^{69a,69b}, D. Della Volpe ⁵⁴, A. Dell'Acqua ³⁶, L. Dell'Asta ^{73a,73b}, M. Delmastro ⁵, C. Delporte ¹³², P.A. Delsart ⁵⁸, D.A. DeMarco ¹⁶⁷, S. Demers ¹⁸³, M. Demichev ⁷⁹, G. Demontigny ¹⁰⁹, S.P. Denisov ¹²³, D. Denysiuk ¹²⁰, L. D'Eramo ¹³⁶, D. Derendarz ⁸⁴, J.E. Derkaoui ^{35d}, F. Derue ¹³⁶, P. Dervan ⁹⁰, K. Desch ²⁴, C. Deterre ⁴⁶, K. Dette ¹⁶⁷, C. Deutsch ²⁴, M.R. Devesa ³⁰, P.O. Deviveiros ³⁶, A. Dewhurst ¹⁴⁴, F.A. Di Bello ⁵⁴, A. Di Ciaccio ^{73a,73b}, L. Di Ciaccio ⁵, W.K. Di Clemente ¹³⁷, C. Di Donato ^{69a,69b}, A. Di Girolamo ³⁶, G. Di Gregorio ^{71a,71b}, B. Di Micco ^{74a,74b}, R. Di Nardo ¹⁰², K.F. Di Petrillo ⁵⁹, R. Di Sipio ¹⁶⁷, D. Di Valentino ³⁴, C. Diaconu ¹⁰¹, F.A. Dias ⁴⁰, T. Dias Do Vale ^{140a}, M.A. Diaz ^{147a}, J. Dickinson ¹⁸, E.B. Diehl ¹⁰⁵, J. Dietrich ¹⁹, S. Díez Cornell ⁴⁶, A. Dimitrievska ¹⁸, W. Ding ^{15b}, J. Dingfelder ²⁴, F. Dittus ³⁶, F. Djama ¹⁰¹, T. Djobava ^{159b}, J.I. Djuvsland ¹⁷, M.A.B. Do Vale ^{80c}, M. Dobre ^{27b}, D. Dodsworth ²⁶, C. Doglioni ⁹⁶, J. Dolejsi ¹⁴³, Z. Dolezal ¹⁴³, M. Donadelli ^{80d}, B. Dong ^{60c}, J. Donini ³⁸, A. D'onofrio ⁹², M. D'Onofrio ⁹⁰, J. Dopke ¹⁴⁴, A. Doria ^{69a}, M.T. Dova ⁸⁸, A.T. Doyle ⁵⁷, E. Drechsler ¹⁵², E. Dreyer ¹⁵², T. Dreyer ⁵³, A.S. Drobac ¹⁷⁰, Y. Duan ^{60b}, F. Dubinin ¹¹⁰, M. Dubovsky ^{28a}, A. Dubreuil ⁵⁴, E. Duchovni ¹⁸⁰, G. Duckeck ¹¹⁴, A. Ducourthial ¹³⁶, O.A. Ducu ¹⁰⁹, D. Duda ¹¹⁵, A. Dudarev ³⁶, A.C. Dudder ⁹⁹, E.M. Duffield ¹⁸, L. Duflost ¹³², M. Dührssen ³⁶, C. Dülsen ¹⁸², M. Dumancic ¹⁸⁰, A.E. Dumitriu ^{27b}, A.K. Duncan ⁵⁷, M. Dunford ^{61a}, A. Duperrin ¹⁰¹, H. Duran Yildiz ^{4a}, M. Düren ⁵⁶, A. Durglishvili ^{159b}, D. Duschinger ⁴⁸, B. Dutta ⁴⁶, D. Duvnjak ¹, G.I. Dyckes ¹³⁷, M. Dyndal ³⁶, S. Dysch ¹⁰⁰, B.S. Dziedzic ⁸⁴, K.M. Ecker ¹¹⁵, R.C. Edgar ¹⁰⁵, M.G. Eggleston ⁴⁹, T. Eifert ³⁶, G. Eigen ¹⁷, K. Einsweiler ¹⁸, T. Ekelof ¹⁷², H. El Jarrari ^{35e}, M. El Kacimi ^{35c}, R. El Kosseifi ¹⁰¹, V. Ellajosyula ¹⁷², M. Ellert ¹⁷², F. Ellinghaus ¹⁸², A.A. Elliot ⁹², N. Ellis ³⁶, J. Elmsheuser ²⁹, M. Elsing ³⁶, D. Emelianov ¹⁴⁴, A. Emerman ³⁹, Y. Enari ¹⁶³, M.B. Epland ⁴⁹, J. Erdmann ⁴⁷, A. Ereditato ²⁰, M. Errenst ³⁶, M. Escalier ¹³², C. Escobar ¹⁷⁴, O. Estrada Pastor ¹⁷⁴, E. Etzion ¹⁶¹, H. Evans ⁶⁵, A. Ezhilov ¹³⁸, F. Fabbri ⁵⁷, L. Fabbri ^{23b,23a}, V. Fabiani ¹¹⁹, G. Facini ⁹⁴, R.M. Faisca Rodrigues Pereira ^{140a}, R.M. Fakhruddinov ¹²³, S. Falciano ^{72a}, P.J. Falke ⁵, S. Falke ⁵, J. Faltova ¹⁴³, Y. Fang ^{15a}, Y. Fang ^{15a}, G. Fanourakis ⁴⁴, M. Fantì ^{68a,68b}, M. Faraj ^{66a,66c}, A. Farbin ⁸, A. Farilla ^{74a}, E.M. Farina ^{70a,70b}, T. Farooque ¹⁰⁶, S. Farrell ¹⁸, S.M. Farrington ⁵⁰, P. Farthouat ³⁶, F. Fassi ^{35e}, P. Fassnacht ³⁶, D. Fassouliotis ⁹, M. Faucci Giannelli ⁵⁰, W.J. Fawcett ³², L. Fayard ¹³², O.L. Fedin ^{138,n}, W. Fedorko ¹⁷⁵, M. Feickert ⁴², L. Felgioni ¹⁰¹, A. Fell ¹⁴⁹, C. Feng ^{60b}, E.J. Feng ³⁶, M. Feng ⁴⁹, M.J. Fenton ⁵⁷, A.B. Fenyuk ¹²³, J. Ferrando ⁴⁶, A. Ferrante ¹⁷³, A. Ferrari ¹⁷², P. Ferrari ¹²⁰, R. Ferrari ^{70a}, D.E. Ferreira de Lima ^{61b}, A. Ferrer ¹⁷⁴, D. Ferrere ⁵⁴, C. Ferretti ¹⁰⁵, F. Fiedler ⁹⁹, A. Filipčič ⁹¹, F. Filthaut ¹¹⁹, K.D. Finelli ²⁵, M.C.N. Fiolhais ^{140a}, L. Fiorini ¹⁷⁴, F. Fischer ¹¹⁴, W.C. Fisher ¹⁰⁶, I. Fleck ¹⁵¹, P. Fleischmann ¹⁰⁵, R.R.M. Fletcher ¹³⁷, T. Flick ¹⁸², B.M. Flierl ¹¹⁴, L.F. Flores ¹³⁷, L.R. Flores Castillo ^{63a}, F.M. Follega ^{75a,75b},

N. Fomin ¹⁷, J.H. Foo ¹⁶⁷, G.T. Forcolin ^{75a,75b}, A. Formica ¹⁴⁵, F.A. Förster ¹⁴, A.C. Forti ¹⁰⁰, A.G. Foster ²¹,
 M.G. Foti ¹³⁵, D. Fournier ¹³², H. Fox ⁸⁹, P. Francavilla ^{71a,71b}, S. Francescato ^{72a,72b}, M. Franchini ^{23b,23a},
 S. Franchino ^{61a}, D. Francis ³⁶, L. Franconi ²⁰, M. Franklin ⁵⁹, A.N. Fray ⁹², P.M. Freeman ²¹, B. Freund ¹⁰⁹,
 W.S. Freund ^{80b}, E.M. Freundlich ⁴⁷, D.C. Frizzell ¹²⁸, D. Froidevaux ³⁶, J.A. Frost ¹³⁵, C. Fukunaga ¹⁶⁴,
 E. Fullana Torregrosa ¹⁷⁴, E. Fumagalli ^{55b,55a}, T. Fusayasu ¹¹⁶, J. Fuster ¹⁷⁴, A. Gabrielli ^{23b,23a},
 A. Gabrielli ¹⁸, G.P. Gach ^{83a}, S. Gadatsch ⁵⁴, P. Gadow ¹¹⁵, G. Gagliardi ^{55b,55a}, L.G. Gagnon ¹⁰⁹, C. Galea ^{27b},
 B. Galhardo ^{140a}, G.E. Gallardo ¹³⁵, E.J. Gallas ¹³⁵, B.J. Gallop ¹⁴⁴, G. Galster ⁴⁰, R. Gamboa Goni ⁹²,
 K.K. Gan ¹²⁶, S. Ganguly ¹⁸⁰, J. Gao ^{60a}, Y. Gao ⁵⁰, Y.S. Gao ^{31,k}, C. García ¹⁷⁴, J.E. García Navarro ¹⁷⁴,
 J.A. García Pascual ^{15a}, C. Garcia-Argos ⁵², M. Garcia-Sciveres ¹⁸, R.W. Gardner ³⁷, N. Garelli ¹⁵³,
 S. Gargiulo ⁵², V. Garonne ¹³⁴, A. Gaudiello ^{55b,55a}, G. Gaudio ^{70a}, I.L. Gavrilenko ¹¹⁰, A. Gavrilyuk ¹¹¹,
 C. Gay ¹⁷⁵, G. Gaycken ⁴⁶, E.N. Gazis ¹⁰, A.A. Geanta ^{27b}, C.N.P. Gee ¹⁴⁴, J. Geisen ⁵³, M. Geisen ⁹⁹,
 M.P. Geisler ^{61a}, C. Gemme ^{55b}, M.H. Genest ⁵⁸, C. Geng ¹⁰⁵, S. Gentile ^{72a,72b}, S. George ⁹³, T. Gerialis ⁴⁴,
 L.O. Gerlach ⁵³, P. Gessinger-Befurt ⁹⁹, G. Gessner ⁴⁷, S. Ghasemi ¹⁵¹, M. Ghasemi Bostanabad ¹⁷⁶,
 M. Ghneimat ²⁴, A. Ghosh ¹³², A. Ghosh ⁷⁷, B. Giacobbe ^{23b}, S. Giagu ^{72a,72b}, N. Giangiacomi ^{23b,23a},
 P. Giannetti ^{71a}, A. Giannini ^{69a,69b}, G. Giannini ¹⁴, S.M. Gibson ⁹³, M. Gignac ¹⁴⁶, D. Gillberg ³⁴,
 G. Gilles ¹⁸², D.M. Gingrich ^{3,av}, M.P. Giordani ^{66a,66c}, F.M. Giorgi ^{23b}, P.F. Giraud ¹⁴⁵, G. Giugliarelli ^{66a,66c},
 D. Giugni ^{68a}, F. Giuli ^{73a,73b}, S. Gkaitatzis ¹⁶², I. Gkialas ^{9,g}, E.L. Gkoukousis ¹⁴, P. Gkoutoumis ¹⁰,
 L.K. Gladilin ¹¹³, C. Glasman ⁹⁸, J. Glatzer ¹⁴, P.C.F. Glaysher ⁴⁶, A. Glazov ⁴⁶, G.R. Gledhill ¹³¹,
 M. Goblirsch-Kolb ²⁶, S. Goldfarb ¹⁰⁴, T. Golling ⁵⁴, D. Golubkov ¹²³, A. Gomes ^{140a,140b},
 R. Goncalves Gama ⁵³, R. Gonçalves ^{140a,140b}, G. Gonella ⁵², L. Gonella ²¹, A. Gongadze ⁷⁹, F. Gonnella ²¹,
 J.L. Gonski ⁵⁹, S. González de la Hoz ¹⁷⁴, S. Gonzalez-Sevilla ⁵⁴, G.R. Gonzalvo Rodriguez ¹⁷⁴,
 L. Goossens ³⁶, P.A. Gorbounov ¹¹¹, H.A. Gordon ²⁹, B. Gorini ³⁶, E. Gorini ^{67a,67b}, A. Gorišek ⁹¹,
 A.T. Goshaw ⁴⁹, C. Gössling ⁴⁷, M.I. Gostkin ⁷⁹, C.A. Gottardo ¹¹⁹, M. Gouighri ^{35b}, D. Goujdami ^{35c},
 A.G. Goussiou ¹⁴⁸, N. Govender ^{33b}, C. Goy ⁵, E. Gozani ¹⁶⁰, I. Grabowska-Bold ^{83a}, E.C. Graham ⁹⁰,
 J. Gramling ¹⁷¹, E. Gramstad ¹³⁴, S. Grancagnolo ¹⁹, M. Grandi ¹⁵⁶, V. Gratchev ¹³⁸, P.M. Gravila ^{27f},
 F.G. Gravili ^{67a,67b}, C. Gray ⁵⁷, H.M. Gray ¹⁸, C. Grefe ²⁴, K. Gregersen ⁹⁶, I.M. Gregor ⁴⁶, P. Grenier ¹⁵³,
 K. Grevtsov ⁴⁶, C. Grieco ¹⁴, N.A. Grieser ¹²⁸, J. Griffiths ⁸, A.A. Grillo ¹⁴⁶, K. Grimm ^{31,j}, S. Grinstein ^{14,w},
 J.-F. Grivaz ¹³², S. Groh ⁹⁹, E. Gross ¹⁸⁰, J. Grosse-Knetter ⁵³, Z.J. Grout ⁹⁴, C. Grud ¹⁰⁵, A. Grummer ¹¹⁸,
 L. Guan ¹⁰⁵, W. Guan ¹⁸¹, J. Guenther ³⁶, A. Guerguichon ¹³², J.G.R. Guerrero Rojas ¹⁷⁴, F. Guescini ¹¹⁵,
 D. Guest ¹⁷¹, R. Gugel ⁵², T. Guillemin ⁵, S. Guindon ³⁶, U. Gul ⁵⁷, J. Guo ^{60c}, W. Guo ¹⁰⁵, Y. Guo ^{60a,r},
 Z. Guo ¹⁰¹, R. Gupta ⁴⁶, S. Gurbuz ^{12c}, G. Gustavino ¹²⁸, P. Gutierrez ¹²⁸, C. Gutsche ⁹⁴, C. Guyot ¹⁴⁵,
 C. Gwenlan ¹³⁵, C.B. Gwilliam ⁹⁰, A. Haas ¹²⁴, C. Haber ¹⁸, H.K. Hadavand ⁸, N. Haddad ^{35e}, A. Hadeef ^{60a},
 S. Hageböck ³⁶, M. Haleem ¹⁷⁷, J. Haley ¹²⁹, G. Halladjian ¹⁰⁶, G.D. Hallewell ¹⁰¹, K. Hamacher ¹⁸²,
 P. Hamal ¹³⁰, K. Hamano ¹⁷⁶, H. Hamdaoui ^{35e}, G.N. Hamity ¹⁴⁹, K. Han ^{60a,ai}, L. Han ^{60a}, S. Han ^{15a,15d},
 Y.F. Han ¹⁶⁷, K. Hanagaki ^{81,u}, M. Hance ¹⁴⁶, D.M. Handl ¹¹⁴, B. Haney ¹³⁷, R. Hankache ¹³⁶, P. Hanke ^{61a},
 E. Hansen ⁹⁶, J.B. Hansen ⁴⁰, J.D. Hansen ⁴⁰, M.C. Hansen ²⁴, P.H. Hansen ⁴⁰, E.C. Hanson ¹⁰⁰, K. Hara ¹⁶⁹,
 A.S. Hard ¹⁸¹, T. Harenberg ¹⁸², S. Harkusha ¹⁰⁷, P.F. Harrison ¹⁷⁸, N.M. Hartmann ¹¹⁴, Y. Hasegawa ¹⁵⁰,
 A. Hasib ⁵⁰, S. Hassani ¹⁴⁵, S. Haug ²⁰, R. Hauser ¹⁰⁶, L.B. Havener ³⁹, M. Havranek ¹⁴², C.M. Hawkes ²¹,
 R.J. Hawkins ³⁶, D. Hayden ¹⁰⁶, C. Hayes ¹⁵⁵, R.L. Hayes ¹⁷⁵, C.P. Hays ¹³⁵, J.M. Hays ⁹², H.S. Hayward ⁹⁰,
 S.J. Haywood ¹⁴⁴, F. He ^{60a}, M.P. Heath ⁵⁰, V. Hedberg ⁹⁶, L. Heelan ⁸, S. Heer ²⁴, K.K. Heidegger ⁵²,
 W.D. Heidorn ⁷⁸, J. Heilman ³⁴, S. Heim ⁴⁶, T. Heim ¹⁸, B. Heinemann ^{46,aq}, J.J. Heinrich ¹³¹, L. Heinrich ³⁶,
 C. Heinz ⁵⁶, J. Hejbal ¹⁴¹, L. Helary ^{61b}, A. Held ¹⁷⁵, S. Hellesund ¹³⁴, C.M. Helling ¹⁴⁶, S. Hellman ^{45a,45b},
 C. Hensens ³⁶, R.C.W. Henderson ⁸⁹, Y. Heng ¹⁸¹, S. Henkelmann ¹⁷⁵, A.M. Henriques Correia ³⁶,
 G.H. Herbert ¹⁹, H. Herde ²⁶, V. Herget ¹⁷⁷, Y. Hernández Jiménez ^{33c}, H. Herr ⁹⁹, M.G. Herrmann ¹¹⁴,
 T. Herrmann ⁴⁸, G. Herten ⁵², R. Hertenberger ¹¹⁴, L. Hervas ³⁶, T.C. Herwig ¹³⁷, G.G. Hesketh ⁹⁴,
 N.P. Hessey ^{168a}, A. Higashida ¹⁶³, S. Higashino ⁸¹, E. Higón-Rodríguez ¹⁷⁴, K. Hildebrand ³⁷, E. Hill ¹⁷⁶,
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 M. Hirose ¹³³, S. Hirose ⁵², D. Hirschbuehl ¹⁸², B. Hiti ⁹¹, O. Hladik ¹⁴¹, D.R. Hlaluku ^{33c}, X. Hoad ⁵⁰,
 J. Hobbs ¹⁵⁵, N. Hod ¹⁸⁰, M.C. Hodgkinson ¹⁴⁹, A. Hoecker ³⁶, F. Hoenig ¹¹⁴, D. Hohn ⁵², D. Hohov ¹³²,
 T.R. Holmes ³⁷, M. Holzbock ¹¹⁴, L.B.A.H. Hommels ³², S. Honda ¹⁶⁹, T.M. Hong ¹³⁹, A. Hönle ¹¹⁵,
 B.H. Hooberman ¹⁷³, W.H. Hopkins ⁶, Y. Horii ¹¹⁷, P. Horn ⁴⁸, L.A. Horyn ³⁷, S. Hou ¹⁵⁸, A. Hoummada ^{35a},
 J. Howarth ¹⁰⁰, J. Hoya ⁸⁸, M. Hrabovsky ¹³⁰, J. Hrdinka ⁷⁶, I. Hristova ¹⁹, J. Hrivnac ¹³², A. Hrynevich ¹⁰⁸,

T. Hryn'ova⁵, P.J. Hsu⁶⁴, S.-C. Hsu¹⁴⁸, Q. Hu²⁹, S. Hu^{60c}, D.P. Huang⁹⁴, Y. Huang^{15a}, Z. Hubacek¹⁴², F. Hubaut¹⁰¹, M. Huebner²⁴, F. Huegging²⁴, T.B. Huffman¹³⁵, M. Huhtinen³⁶, R.F.H. Hunter³⁴, P. Huo¹⁵⁵, A.M. Hupe³⁴, N. Huseynov^{79,ad}, J. Huston¹⁰⁶, J. Huth⁵⁹, R. Hyneman¹⁰⁵, S. Hyrych^{28a}, G. Iacobucci⁵⁴, G. Iakovidis²⁹, I. Ibragimov¹⁵¹, L. Iconomidou-Fayard¹³², Z. Idrissi^{35e}, P.I. Iengo³⁶, R. Ignazzi⁴⁰, O. Igonkina^{120,y,*}, R. Iguchi¹⁶³, T. Iizawa⁵⁴, Y. Ikegami⁸¹, M. Ikeno⁸¹, D. Iliadis¹⁶², N. Ilic¹¹⁹, F. Iltzsche⁴⁸, G. Introzzi^{70a,70b}, M. Iodice^{74a}, K. Iordanidou^{168a}, V. Ippolito^{72a,72b}, M.F. Isacson¹⁷², M. Ishino¹⁶³, W. Islam¹²⁹, C. Issever¹³⁵, S. Istin¹⁶⁰, F. Ito¹⁶⁹, J.M. Iturbe Ponce^{63a}, R. Iuppa^{75a,75b}, A. Ivina¹⁸⁰, H. Iwasaki⁸¹, J.M. Izen⁴³, V. Izzo^{69a}, P. Jacka¹⁴¹, P. Jackson¹, R.M. Jacobs²⁴, B.P. Jaeger¹⁵², V. Jain², G. Jäkel¹⁸², K.B. Jakobi⁹⁹, K. Jakobs⁵², S. Jakobsen⁷⁶, T. Jakoubek¹⁴¹, J. Jamieson⁵⁷, K.W. Janas^{83a}, R. Jansky⁵⁴, J. Janssen²⁴, M. Janus⁵³, P.A. Janus^{83a}, G. Jarlskog⁹⁶, N. Javadov^{79,ad}, T. Javůrek³⁶, M. Javurkova⁵², F. Jeanneau¹⁴⁵, L. Jeanty¹³¹, J. Jejelava^{159a,ae}, A. Jelinskas¹⁷⁸, P. Jenni^{52,a}, J. Jeong⁴⁶, N. Jeong⁴⁶, S. Jézéquel⁵, H. Ji¹⁸¹, J. Jia¹⁵⁵, H. Jiang⁷⁸, Y. Jiang^{60a}, Z. Jiang^{153,o}, S. Jiggins⁵², F.A. Jimenez Morales³⁸, J. Jimenez Pena¹¹⁵, S. Jin^{15c}, A. Jinaru^{27b}, O. Jinnouchi¹⁶⁵, H. Jivan^{33c}, P. Johansson¹⁴⁹, K.A. Johns⁷, C.A. Johnson⁶⁵, K. Jon-And^{45a,45b}, R.W.L. Jones⁸⁹, S.D. Jones¹⁵⁶, S. Jones⁷, T.J. Jones⁹⁰, J. Jongmanns^{61a}, P.M. Jorge^{140a}, J. Jovicevic³⁶, X. Ju¹⁸, J.J. Jungeburth¹¹⁵, A. Juste Rozas^{14,w}, A. Kaczmarska⁸⁴, M. Kado^{72a,72b}, H. Kagan¹²⁶, M. Kagan¹⁵³, C. Kahra⁹⁹, T. Kaji¹⁷⁹, E. Kajomovitz¹⁶⁰, C.W. Kalderon⁹⁶, A. Kaluza⁹⁹, A. Kamenshchikov¹²³, L. Kanjir⁹¹, Y. Kano¹⁶³, V.A. Kantserov¹¹², J. Kanzaki⁸¹, L.S. Kaplan¹⁸¹, D. Kar^{33c}, K. Karava¹³⁵, M.J. Kareem^{168b}, S.N. Karpov⁷⁹, Z.M. Karpova⁷⁹, V. Kartvelishvili⁸⁹, A.N. Karyukhin¹²³, L. Kashif¹⁸¹, R.D. Kass¹²⁶, A. Kastanas^{45a,45b}, C. Kato^{60d,60c}, J. Katzy⁴⁶, K. Kawade¹⁵⁰, K. Kawagoe⁸⁷, T. Kawaguchi¹¹⁷, T. Kawamoto¹⁶³, G. Kawamura⁵³, E.F. Kay¹⁷⁶, V.F. Kazanin^{122b,122a}, R. Keeler¹⁷⁶, R. Kehoe⁴², J.S. Keller³⁴, E. Kellermann⁹⁶, D. Kelsey¹⁵⁶, J.J. Kempster²¹, J. Kendrick²¹, O. Kepka¹⁴¹, S. Kersten¹⁸², B.P. Kerševan⁹¹, S. Ketabchi Haghighat¹⁶⁷, M. Khader¹⁷³, F. Khalil-Zada¹³, M. Khandoga¹⁴⁵, A. Khanov¹²⁹, A.G. Kharlamov^{122b,122a}, T. Kharlamova^{122b,122a}, E.E. Khoda¹⁷⁵, A. Khodinov¹⁶⁶, T.J. Khoo⁵⁴, E. Khramov⁷⁹, J. Khubua^{159b}, S. Kido⁸², M. Kiehn⁵⁴, C.R. Kilby⁹³, Y.K. Kim³⁷, N. Kimura^{66a,66c}, O.M. Kind¹⁹, B.T. King^{90,*}, D. Kirchmeier⁴⁸, J. Kirk¹⁴⁴, A.E. Kiryunin¹¹⁵, T. Kishimoto¹⁶³, D.P. Kisliuk¹⁶⁷, V. Kitali⁴⁶, O. Kivernyk⁵, T. Klapdor-Kleingrothaus⁵², M. Klassen^{61a}, M.H. Klein¹⁰⁵, M. Klein⁹⁰, U. Klein⁹⁰, K. Kleinknecht⁹⁹, P. Klimek¹²¹, A. Klimentov²⁹, T. Klingl²⁴, T. Klioutchnikova³⁶, F.F. Klitzner¹¹⁴, P. Kluit¹²⁰, S. Kluth¹¹⁵, E. Kneringer⁷⁶, E.B.F.G. Knoop¹⁰¹, A. Knue⁵², D. Kobayashi⁸⁷, T. Kobayashi¹⁶³, M. Kobel⁴⁸, M. Kocian¹⁵³, P. Kodys¹⁴³, P.T. Koenig²⁴, T. Koffas³⁴, N.M. Köhler³⁶, T. Koi¹⁵³, M. Kolb^{61b}, I. Koletsou⁵, T. Komarek¹³⁰, T. Kondo⁸¹, N. Kondrashova^{60c}, K. Köneke⁵², A.C. König¹¹⁹, T. Kono¹²⁵, R. Konoplich^{124,al}, V. Konstantinides⁹⁴, N. Konstantinidis⁹⁴, B. Konya⁹⁶, R. Kopeliansky⁶⁵, S. Koperny^{83a}, K. Korcyl⁸⁴, K. Kordas¹⁶², G. Koren¹⁶¹, A. Korn⁹⁴, I. Korolkov¹⁴, E.V. Korolkova¹⁴⁹, N. Korotkova¹¹³, O. Kortner¹¹⁵, S. Kortner¹¹⁵, T. Kosek¹⁴³, V.V. Kostyukhin²⁴, A. Kotwal⁴⁹, A. Koulouris¹⁰, A. Kourkoumeli-Charalampidi^{70a,70b}, C. Kourkoumelis⁹, E. Kourlitis¹⁴⁹, V. Kouskoura²⁹, A.B. Kowalewska⁸⁴, R. Kowalewski¹⁷⁶, C. Kozakai¹⁶³, W. Kozanecki¹⁴⁵, A.S. Kozhin¹²³, V.A. Kramarenko¹¹³, G. Kramberger⁹¹, D. Krasnopevtsev^{60a}, M.W. Krasny¹³⁶, A. Krasznahorkay³⁶, D. Krauss¹¹⁵, J.A. Kremer^{83a}, J. Kretschmar⁹⁰, P. Krieger¹⁶⁷, F. Krieter¹¹⁴, A. Krishnan^{61b}, K. Krizka¹⁸, K. Kroeninger⁴⁷, H. Kroha¹¹⁵, J. Kroll¹⁴¹, J. Kroll¹³⁷, J. Krstic¹⁶, U. Kruchonak⁷⁹, H. Krüger²⁴, N. Krumnack⁷⁸, M.C. Kruse⁴⁹, J.A. Krzysiak⁸⁴, T. Kubota¹⁰⁴, O. Kuchinskaia¹⁶⁶, S. Kuday^{4b}, J.T. Kuechler⁴⁶, S. Kuehn³⁶, A. Kugel^{61a}, T. Kuhl⁴⁶, V. Kukhtin⁷⁹, R. Kukla¹⁰¹, Y. Kulchitsky^{107,ah}, S. Kuleshov^{147b}, Y.P. Kulinich¹⁷³, M. Kuna⁵⁸, T. Kunigo⁸⁵, A. Kupco¹⁴¹, T. Kupfer⁴⁷, O. Kuprash⁵², H. Kurashige⁸², L.L. Kurchaninov^{168a}, Y.A. Kurochkin¹⁰⁷, A. Kurova¹¹², M.G. Kurth^{15a,15d}, E.S. Kuwertz³⁶, M. Kuze¹⁶⁵, A.K. Kvam¹⁴⁸, J. Kvita¹³⁰, T. Kwan¹⁰³, A. La Rosa¹¹⁵, L. La Rotonda^{41b,41a}, F. La Ruffa^{41b,41a}, C. Lacasta¹⁷⁴, F. Lacava^{72a,72b}, D.P.J. Lack¹⁰⁰, H. Lacker¹⁹, D. Lacour¹³⁶, E. Ladygin⁷⁹, R. Lafaye⁵, B. Laforge¹³⁶, T. Lagouri^{33c}, S. Lai⁵³, S. Lammers⁶⁵, W. Lampl⁷, C. Lampoudis¹⁶², E. Lançon²⁹, U. Landgraf⁵², M.P.J. Landon⁹², M.C. Lanfermann⁵⁴, V.S. Lang⁴⁶, J.C. Lange⁵³, R.J. Langenberg³⁶, A.J. Lankford¹⁷¹, F. Lanni²⁹, K. Lantsch²⁴, A. Lanza^{70a}, A. Lapertosa^{55b,55a}, S. Laplace¹³⁶, J.F. Laporte¹⁴⁵, T. Lari^{68a}, F. Lasagni Manghi^{23b,23a}, M. Lassnig³⁶, T.S. Lau^{63a}, A. Laudrain¹³², A. Laurier³⁴, M. Lavorgna^{69a,69b}, M. Lazzaroni^{68a,68b}, B. Le¹⁰⁴, O. Le Dortz¹³⁶, E. Le Guirriec¹⁰¹, M. LeBlanc⁷, T. LeCompte⁶, F. Ledroit-Guillon⁵⁸, C.A. Lee²⁹, G.R. Lee¹⁷, L. Lee⁵⁹, S.C. Lee¹⁵⁸, S.J. Lee³⁴, B. Lefebvre^{168a}, M. Lefebvre¹⁷⁶, F. Legger¹¹⁴, C. Leggett¹⁸, K. Lehmann¹⁵², N. Lehmann¹⁸²,

G. Lehmann Miotto³⁶, W.A. Leight⁴⁶, A. Leisos^{162,v}, M.A.L. Leite^{80d}, C.E. Leitgeb¹¹⁴, R. Leitner¹⁴³, D. Lellouch^{180,*}, K.J.C. Leney⁴², T. Lenz²⁴, B. Lenzi³⁶, R. Leone⁷, S. Leone^{71a}, C. Leonidopoulos⁵⁰, A. Leopold¹³⁶, G. Lerner¹⁵⁶, C. Leroy¹⁰⁹, R. Les¹⁶⁷, C.G. Lester³², M. Levchenko¹³⁸, J. Levêque⁵, D. Levin¹⁰⁵, L.J. Levinson¹⁸⁰, D.J. Lewis²¹, B. Li^{15b}, B. Li¹⁰⁵, C.-Q. Li^{60a}, F. Li^{60c}, H. Li^{60a}, H. Li^{60b}, J. Li^{60c}, K. Li¹⁵³, L. Li^{60c}, M. Li^{15a}, Q. Li^{15a,15d}, Q.Y. Li^{60a}, S. Li^{60d,60c}, X. Li⁴⁶, Y. Li⁴⁶, Z. Li^{60b}, Z. Liang^{15a}, B. Liberti^{73a}, A. Liblong¹⁶⁷, K. Lie^{63c}, S. Liem¹²⁰, C.Y. Lin³², K. Lin¹⁰⁶, T.H. Lin⁹⁹, R.A. Linck⁶⁵, J.H. Lindon²¹, A.L. Lioni⁵⁴, E. Lipeles¹³⁷, A. Lipniacka¹⁷, M. Lisovyi^{61b}, T.M. Liss^{173,as}, A. Lister¹⁷⁵, A.M. Litke¹⁴⁶, J.D. Little⁸, B. Liu⁷⁸, B.L. Liu⁶, H.B. Liu²⁹, H. Liu¹⁰⁵, J.B. Liu^{60a}, J.K.K. Liu¹³⁵, K. Liu¹³⁶, M. Liu^{60a}, P. Liu¹⁸, Y. Liu^{15a,15d}, Y.L. Liu¹⁰⁵, Y.W. Liu^{60a}, M. Livan^{70a,70b}, A. Lleres⁵⁸, J. Llorente Merino^{15a}, S.L. Lloyd⁹², C.Y. Lo^{63b}, F. Lo Sterzo⁴², E.M. Lobodzinska⁴⁶, P. Loch⁷, S. Loffredo^{73a,73b}, T. Lohse¹⁹, K. Lohwasser¹⁴⁹, M. Lokajicek¹⁴¹, J.D. Long¹⁷³, R.E. Long⁸⁹, L. Longo³⁶, K.A.Looper¹²⁶, J.A. Lopez^{147b}, I. Lopez Paz¹⁰⁰, A. Lopez Solis¹⁴⁹, J. Lorenz¹¹⁴, N. Lorenzo Martinez⁵, M. Losada²², P.J. Lösel¹¹⁴, A. Lösle⁵², X. Lou⁴⁶, X. Lou^{15a}, A. Lounis¹³², J. Love⁶, P.A. Love⁸⁹, J.J. Lozano Bahilo¹⁷⁴, M. Lu^{60a}, Y.J. Lu⁶⁴, H.J. Lubatti¹⁴⁸, C. Luci^{72a,72b}, A. Lucotte⁵⁸, C. Luedtke⁵², F. Luehring⁶⁵, I. Luise¹³⁶, L. Luminari^{72a}, B. Lund-Jensen¹⁵⁴, M.S. Lutz¹⁰², D. Lynn²⁹, R. Lysak¹⁴¹, E. Lytken⁹⁶, F. Lyu^{15a}, V. Lyubushkin⁷⁹, T. Lyubushkina⁷⁹, H. Ma²⁹, L.L. Ma^{60b}, Y. Ma^{60b}, G. Maccarrone⁵¹, A. Macchiolo¹¹⁵, C.M. Macdonald¹⁴⁹, J. Machado Miguens¹³⁷, D. Madaffari¹⁷⁴, R. Madar³⁸, W.F. Mader⁴⁸, N. Madysa⁴⁸, J. Maeda⁸², S. Maeland¹⁷, T. Maeno²⁹, M. Maerker⁴⁸, A.S. Maevskiy¹¹³, V. Magerl⁵², N. Magini⁷⁸, D.J. Mahon³⁹, C. Maidantchik^{80b}, T. Maier¹¹⁴, A. Maio^{140a,140b,140d}, O. Majersky^{28a}, S. Majewski¹³¹, Y. Makida⁸¹, N. Makovec¹³², B. Malaescu¹³⁶, Pa. Malecki⁸⁴, V.P. Maleev¹³⁸, F. Malek⁵⁸, U. Mallik⁷⁷, D. Malon⁶, C. Malone³², S. Maltezos¹⁰, S. Malyukov³⁶, J. Mamuzic¹⁷⁴, G. Mancini⁵¹, I. Mandić⁹¹, L. Manhaes de Andrade Filho^{80a}, I.M. Maniatis¹⁶², J. Manjarres Ramos⁴⁸, K.H. Mankinen⁹⁶, A. Mann¹¹⁴, A. Manousos⁷⁶, B. Mansoulie¹⁴⁵, I. Manthos¹⁶², S. Manzoni¹²⁰, A. Marantis¹⁶², G. Marceca³⁰, L. Marchese¹³⁵, G. Marchiori¹³⁶, M. Marcisovsky¹⁴¹, C. Marcon⁹⁶, C.A. Marin Tobon³⁶, M. Marjanovic³⁸, F. Marroquim^{80b}, Z. Marshall¹⁸, M.U.F. Martensson¹⁷², S. Marti-Garcia¹⁷⁴, C.B. Martin¹²⁶, T.A. Martin¹⁷⁸, V.J. Martin⁵⁰, B. Martin dit Latour¹⁷, L. Martinelli^{74a,74b}, M. Martinez^{14,w}, V.I. Martinez Outschoorn¹⁰², S. Martin-Haugh¹⁴⁴, V.S. Martouli^{27b}, A.C. Martyniuk⁹⁴, A. Marzin³⁶, S.R. Maschek¹¹⁵, L. Masetti⁹⁹, T. Mashimo¹⁶³, R. Mashinistov¹¹⁰, J. Masik¹⁰⁰, A.L. Maslennikov^{122b,122a}, L. Massa^{73a,73b}, P. Massarotti^{69a,69b}, P. Mastrandrea^{71a,71b}, A. Mastroberardino^{41b,41a}, T. Masubuchi¹⁶³, D. Matakias¹⁰, A. Matic¹¹⁴, P. Mättig²⁴, J. Maurer^{27b}, B. Maček⁹¹, S.J. Maxfield⁹⁰, D.A. Maximov^{122b,122a}, R. Mazini¹⁵⁸, I. Maznas¹⁶², S.M. Mazza¹⁴⁶, S.P. Mc Kee¹⁰⁵, T.G. McCarthy¹¹⁵, W.P. McCormack¹⁸, E.F. McDonald¹⁰⁴, J.A. Mcfayden³⁶, M.A. McKay⁴², K.D. McLean¹⁷⁶, S.J. McMahon¹⁴⁴, P.C. McNamara¹⁰⁴, C.J. McNicol¹⁷⁸, R.A. McPherson^{176,ab}, J.E. Mdhlluli^{33c}, Z.A. Meadows¹⁰², S. Meehan³⁶, T. Megy⁵², S. Mehlhase¹¹⁴, A. Mehta⁹⁰, T. Meideck⁵⁸, B. Meirose⁴³, D. Melini¹⁷⁴, B.R. Mellado Garcia^{33c}, J.D. Mellenthin⁵³, M. Melo^{28a}, F. Meloni⁴⁶, A. Melzer²⁴, S.B. Menary¹⁰⁰, E.D. Mendes Gouveia^{140a,140e}, L. Meng³⁶, X.T. Meng¹⁰⁵, S. Menke¹¹⁵, E. Meoni^{41b,41a}, S. Mergelmeyer¹⁹, S.A.M. Merkt¹³⁹, C. Merlassino²⁰, P. Mermoud⁵⁴, L. Merola^{69a,69b}, C. Meroni^{68a}, O. Meshkov^{113,110}, J.K.R. Meshreki¹⁵¹, A. Messina^{72a,72b}, J. Metcalfe⁶, A.S. Mete¹⁷¹, C. Meyer⁶⁵, J. Meyer¹⁶⁰, J.-P. Meyer¹⁴⁵, H. Meyer Zu Theenhausen^{61a}, F. Miano¹⁵⁶, M. Michetti¹⁹, R.P. Middleton¹⁴⁴, L. Mijović⁵⁰, G. Mikenberg¹⁸⁰, M. Mikesikova¹⁴¹, M. Mikuz⁹¹, H. Mildner¹⁴⁹, M. Milesi¹⁰⁴, A. Milic¹⁶⁷, D.A. Millar⁹², D.W. Miller³⁷, A. Milov¹⁸⁰, D.A. Milstead^{45a,45b}, R.A. Mina^{153,o}, A.A. Minaenko¹²³, M. Miñano Moya¹⁷⁴, I.A. Minashvili^{159b}, A.I. Mincer¹²⁴, B. Mindur^{83a}, M. Mineev⁷⁹, Y. Minegishi¹⁶³, Y. Ming¹⁸¹, L.M. Mir¹⁴, A. Mirto^{67a,67b}, K.P. Mistry¹³⁷, T. Mitani¹⁷⁹, J. Mitrevski¹¹⁴, V.A. Mitsou¹⁷⁴, M. Mittal^{60c}, O. Miu¹⁶⁷, A. Miucci²⁰, P.S. Miyagawa¹⁴⁹, A. Mizukami⁸¹, J.U. Mjörnmark⁹⁶, T. Mkrtchyan¹⁸⁴, M. Mlynarikova¹⁴³, T. Moa^{45a,45b}, K. Mochizuki¹⁰⁹, P. Mogg⁵², S. Mohapatra³⁹, R. Moles-Valls²⁴, M.C. Mondragon¹⁰⁶, K. Mönig⁴⁶, J. Monk⁴⁰, E. Monnier¹⁰¹, A. Montalbano¹⁵², J. Montejo Berlingen³⁶, M. Montella⁹⁴, F. Monticelli⁸⁸, S. Monzani^{68a}, N. Morange¹³², D. Moreno²², M. Moreno Llácer³⁶, C. Moreno Martinez¹⁴, P. Morettini^{55b}, M. Morgenstern¹²⁰, S. Morgenstern⁴⁸, D. Mori¹⁵², M. Morii⁵⁹, M. Morinaga¹⁷⁹, V. Morisbak¹³⁴, A.K. Morley³⁶, G. Mornacchi³⁶, A.P. Morris⁹⁴, L. Morvaj¹⁵⁵, P. Moschovakos³⁶, B. Moser¹²⁰, M. Mosidze^{159b}, T. Moskalets¹⁴⁵, H.J. Moss¹⁴⁹, J. Moss^{31,l}, E.J.W. Moyse¹⁰², S. Muanza¹⁰¹, J. Mueller¹³⁹, R.S.P. Mueller¹¹⁴, D. Muenstermann⁸⁹, G.A. Mullier⁹⁶, J.L. Munoz Martinez¹⁴,

F.J. Munoz Sanchez¹⁰⁰, P. Murin^{28b}, W.J. Murray^{178,144}, A. Murrone^{68a,68b}, M. Muškinja¹⁸, C. Mwewa^{33a}, A.G. Myagkov^{123.am}, J. Myers¹³¹, M. Myska¹⁴², B.P. Nachman¹⁸, O. Nackenhorst⁴⁷, A. Nag Nag⁴⁸, K. Nagai¹³⁵, K. Nagano⁸¹, Y. Nagasaka⁶², M. Nagel⁵², E. Nagy¹⁰¹, A.M. Nairz³⁶, Y. Nakahama¹¹⁷, K. Nakamura⁸¹, T. Nakamura¹⁶³, I. Nakano¹²⁷, H. Nanjo¹³³, F. Napolitano^{61a}, R.F. Naranjo Garcia⁴⁶, R. Narayan⁴², I. Naryshkin¹³⁸, T. Naumann⁴⁶, G. Navarro²², H.A. Neal^{105,*}, P.Y. Nechaeva¹¹⁰, F. Nechansky⁴⁶, T.J. Neep²¹, A. Negri^{70a,70b}, M. Negrini^{23b}, C. Nellist⁵³, M.E. Nelson¹³⁵, S. Nemecek¹⁴¹, P. Nemethy¹²⁴, M. Nessi^{36.c}, M.S. Neubauer¹⁷³, M. Neumann¹⁸², P.R. Newman²¹, Y.S. Ng¹⁹, Y.W.Y. Ng¹⁷¹, B. Ngair^{35e}, H.D.N. Nguyen¹⁰¹, T. Nguyen Manh¹⁰⁹, E. Nibigira³⁸, R.B. Nickerson¹³⁵, R. Nicolaidou¹⁴⁵, D.S. Nielsen⁴⁰, J. Nielsen¹⁴⁶, N. Nikiforou¹¹, V. Nikolaenko^{123.am}, I. Nikolic-Audit¹³⁶, K. Nikolopoulos²¹, P. Nilsson²⁹, H.R. Nindhito⁵⁴, Y. Ninomiya⁸¹, A. Nisati^{72a}, N. Nishu^{60c}, R. Nisius¹¹⁵, I. Nitsche⁴⁷, T. Nitta¹⁷⁹, T. Nobe¹⁶³, Y. Noguchi⁸⁵, I. Nomidis¹³⁶, M.A. Nomura²⁹, M. Nordberg³⁶, N. Norjoharuddeen¹³⁵, T. Novak⁹¹, O. Novgorodova⁴⁸, R. Novotny¹⁴², L. Nozka¹³⁰, K. Ntekas¹⁷¹, E. Nurse⁹⁴, F.G. Oakham^{34.av}, H. Oberlack¹¹⁵, J. Ocariz¹³⁶, A. Ochi⁸², I. Ochoa³⁹, J.P. Ochoa-Ricoux^{147a}, K. O'Connor²⁶, S. Oda⁸⁷, S. Odaka⁸¹, S. Oerdek⁵³, A. Ogrodnik^{83a}, A. Oh¹⁰⁰, S.H. Oh⁴⁹, C.C. Ohm¹⁵⁴, H. Oide¹⁶⁵, M.L. Ojeda¹⁶⁷, H. Okawa¹⁶⁹, Y. Okazaki⁸⁵, Y. Okumura¹⁶³, T. Okuyama⁸¹, A. Olariu^{27b}, L.F. Oleiro Seabra^{140a}, S.A. Olivares Pino^{147a}, D. Oliveira Damazio²⁹, J.L. Oliver¹, M.J.R. Olsson¹⁷¹, A. Olszewski⁸⁴, J. Olszowska⁸⁴, D.C. O'Neil¹⁵², A.P. O'Neill¹³⁵, A. Onofre^{140a,140e}, P.U.E. Onyisi¹¹, H. Oppen¹³⁴, M.J. Oreglia³⁷, G.E. Orellana⁸⁸, Y. Oren¹⁶¹, D. Orestano^{74a,74b}, N. Orlando¹⁴, R.S. Orr¹⁶⁷, V. O'Shea⁵⁷, R. Ospanov^{60a}, G. Otero y Garzon³⁰, H. Otono⁸⁷, P.S. Ott^{61a}, M. Ouchrif^{35d}, J. Ouellette²⁹, F. Ould-Saada¹³⁴, A. Ouraou¹⁴⁵, Q. Ouyang^{15a}, M. Owen⁵⁷, R.E. Owen²¹, V.E. Ozcan^{12c}, N. Ozturk⁸, J. Pacalt¹³⁰, H.A. Pacey³², K. Pachal⁴⁹, A. Pacheco Pages¹⁴, C. Padilla Aranda¹⁴, S. Pagan Griso¹⁸, M. Paganini¹⁸³, G. Palacino⁶⁵, S. Palazzo⁵⁰, S. Palestini³⁶, M. Palka^{83b}, D. Pallin³⁸, I. Panagoulas¹⁰, C.E. Pandini³⁶, J.G. Panduro Vazquez⁹³, P. Pani⁴⁶, G. Panizzo^{66a,66c}, L. Paolozzi⁵⁴, C. Papadatos¹⁰⁹, K. Papageorgiou^{9.g}, S. Parajuli⁴³, A. Paramonov⁶, D. Paredes Hernandez^{63b}, S.R. Paredes Saenz¹³⁵, B. Parida¹⁶⁶, T.H. Park¹⁶⁷, A.J. Parker⁸⁹, M.A. Parker³², F. Parodi^{55b,55a}, E.W.P. Parrish¹²¹, J.A. Parsons³⁹, U. Parzefall⁵², L. Pascual Dominguez¹³⁶, V.R. Pascuzzi¹⁶⁷, J.M.P. Pasner¹⁴⁶, E. Pasqualucci^{72a}, S. Passaggio^{55b}, F. Pastore⁹³, P. Pasuwan^{45a,45b}, S. Pataria⁹⁹, J.R. Pater¹⁰⁰, A. Pathak^{181.i}, T. Pauly³⁶, B. Pearson¹¹⁵, M. Pedersen¹³⁴, L. Pedraza Diaz¹¹⁹, R. Pedro^{140a}, T. Peiffer⁵³, S.V. Peleganchuk^{122b,122a}, O. Penc¹⁴¹, H. Peng^{60a}, B.S. Peralva^{80a}, M.M. Perego¹³², A.P. Pereira Peixoto^{140a}, D.V. Perepelitsa²⁹, F. Peri¹⁹, L. Perini^{68a,68b}, H. Pernegger³⁶, S. Perrella^{69a,69b}, K. Peters⁴⁶, R.F.Y. Peters¹⁰⁰, B.A. Petersen³⁶, T.C. Petersen⁴⁰, E. Petit¹⁰¹, A. Petridis¹, C. Petridou¹⁶², P. Petroff¹³², M. Petrov¹³⁵, F. Petrucci^{74a,74b}, M. Pettee¹⁸³, N.E. Pettersson¹⁰², K. Petukhova¹⁴³, A. Peyaud¹⁴⁵, R. Pezoa^{147b}, L. Pezzotti^{70a,70b}, T. Pham¹⁰⁴, F.H. Phillips¹⁰⁶, P.W. Phillips¹⁴⁴, M.W. Phipps¹⁷³, G. Piacquadio¹⁵⁵, E. Pianori¹⁸, A. Picazio¹⁰², R.H. Pickles¹⁰⁰, R. Piegai³⁰, D. Pietreanu^{27b}, J.E. Pilcher³⁷, A.D. Pilkington¹⁰⁰, M. Pinamonti^{73a,73b}, J.L. Pinfold³, M. Pitt¹⁶¹, L. Pizzimento^{73a,73b}, M.-A. Pleier²⁹, V. Pleskot¹⁴³, E. Plotnikova⁷⁹, P. Podberezko^{122b,122a}, R. Poettgen⁹⁶, R. Poggi⁵⁴, L. Poggioli¹³², I. Pogrebnyak¹⁰⁶, D. Pohl²⁴, I. Pokharel⁵³, G. Polesello^{70a}, A. Poley¹⁸, A. Policicchio^{72a,72b}, R. Polifka¹⁴³, A. Polini^{23b}, C.S. Pollard⁴⁶, V. Polychronakos²⁹, D. Ponomarenko¹¹², L. Pontecorvo³⁶, S. Popa^{27a}, G.A. Popeneciu^{27d}, L. Portales⁵, D.M. Portillo Quintero⁵⁸, S. Pospisil¹⁴², K. Potamianos⁴⁶, I.N. Potrap⁷⁹, C.J. Potter³², H. Potti¹¹, T. Poulsen⁹⁶, J. Poveda³⁶, T.D. Powell¹⁴⁹, G. Pownall⁴⁶, M.E. Pozo Astigarraga³⁶, P. Pralavorio¹⁰¹, S. Prell⁷⁸, D. Price¹⁰⁰, M. Primavera^{67a}, S. Prince¹⁰³, M.L. Proffitt¹⁴⁸, N. Proklova¹¹², K. Prokofiev^{63c}, F. Prokoshin⁷⁹, S. Protopopescu²⁹, J. Proudfoot⁶, M. Przybycien^{83a}, D. Pudzha¹³⁸, A. Puri¹⁷³, P. Puzo¹³², J. Qian¹⁰⁵, Y. Qin¹⁰⁰, A. Quadt⁵³, M. Queitsch-Maitland⁴⁶, A. Qureshi¹, M. Racko^{28a}, P. Rados¹⁰⁴, F. Ragusa^{68a,68b}, G. Rahal⁹⁷, J.A. Raine⁵⁴, S. Rajagopalan²⁹, A. Ramirez Morales⁹², K. Ran^{15a,15d}, T. Rashid¹³², S. Raspopov⁵, D.M. Rauch⁴⁶, F. Rauscher¹¹⁴, S. Rave⁹⁹, B. Ravina¹⁴⁹, I. Ravinovich¹⁸⁰, J.H. Rawling¹⁰⁰, M. Raymond³⁶, A.L. Read¹³⁴, N.P. Readioff⁵⁸, M. Reale^{67a,67b}, D.M. Rebuszi^{70a,70b}, A. Redelbach¹⁷⁷, G. Redlinger²⁹, K. Reeves⁴³, L. Rehnisch¹⁹, J. Reichert¹³⁷, D. Reikher¹⁶¹, A. Reiss⁹⁹, A. Rej¹⁵¹, C. Rembser³⁶, M. Renda^{27b}, M. Rescigno^{72a}, S. Resconi^{68a}, E.D. Resseguie¹³⁷, S. Rettie¹⁷⁵, E. Reynolds²¹, O.L. Rezanova^{122b,122a}, P. Reznicek¹⁴³, E. Ricci^{75a,75b}, R. Richter¹¹⁵, S. Richter⁴⁶, E. Richter-Was^{83b}, O. Ricken²⁴, M. Ridel¹³⁶, P. Rieck¹¹⁵, C.J. Riegel¹⁸², O. Rifki⁴⁶, M. Rijssenbeek¹⁵⁵, A. Rimoldi^{70a,70b}, M. Rimoldi⁴⁶, L. Rinaldi^{23b},

G. Ripellino ¹⁵⁴, I. Riu ¹⁴, J.C. Rivera Vergara ¹⁷⁶, F. Rizatdinova ¹²⁹, E. Rizvi ⁹², C. Rizzi ³⁶, R.T. Roberts ¹⁰⁰, S.H. Robertson ^{103,ab}, M. Robin ⁴⁶, D. Robinson ³², J.E.M. Robinson ⁴⁶, C.M. Robles Gajardo ^{147b}, A. Robson ⁵⁷, E. Rocco ⁹⁹, C. Roda ^{71a,71b}, S. Rodriguez Bosca ¹⁷⁴, A. Rodriguez Perez ¹⁴, D. Rodriguez Rodriguez ¹⁷⁴, A.M. Rodríguez Vera ^{168b}, S. Roe ³⁶, O. Røhne ¹³⁴, R. Röhrig ¹¹⁵, C.P.A. Roland ⁶⁵, J. Roloff ⁵⁹, A. Romaniouk ¹¹², M. Romano ^{23b,23a}, N. Rompotis ⁹⁰, M. Ronzani ¹²⁴, L. Roos ¹³⁶, S. Rosati ^{72a}, K. Rosbach ⁵², G. Rosin ¹⁰², B.J. Rosser ¹³⁷, E. Rossi ⁴⁶, E. Rossi ^{74a,74b}, E. Rossi ^{69a,69b}, L.P. Rossi ^{55b}, L. Rossini ^{68a,68b}, R. Rosten ¹⁴, M. Rotaru ^{27b}, J. Rothberg ¹⁴⁸, D. Rousseau ¹³², G. Rovelli ^{70a,70b}, A. Roy ¹¹, D. Roy ^{33c}, A. Rozanov ¹⁰¹, Y. Rozen ¹⁶⁰, X. Ruan ^{33c}, F. Rubbo ¹⁵³, F. Rühr ⁵², A. Ruiz-Martinez ¹⁷⁴, A. Rummler ³⁶, Z. Rurikova ⁵², N.A. Rusakovich ⁷⁹, H.L. Russell ¹⁰³, L. Rustige ^{38,47}, J.P. Rutherford ⁷, E.M. Rüttinger ¹⁴⁹, Y.F. Ryabov ¹³⁸, M. Rybar ³⁹, G. Rybkin ¹³², E.B. Rye ¹³⁴, A. Ryzhov ¹²³, G.F. Rzehorz ⁵³, P. Sabatini ⁵³, G. Sabato ¹²⁰, S. Sacerdoti ¹³², H.F-W. Sadrozinski ¹⁴⁶, R. Sadykov ⁷⁹, F. Safai Tehrani ^{72a}, B. Safarzadeh Samani ¹⁵⁶, P. Saha ¹²¹, S. Saha ¹⁰³, M. Sahinsoy ^{61a}, A. Sahu ¹⁸², M. Saimpert ⁴⁶, M. Saito ¹⁶³, T. Saito ¹⁶³, H. Sakamoto ¹⁶³, A. Sakharov ^{124,al}, D. Salamani ⁵⁴, G. Salamanna ^{74a,74b}, J.E. Salazar Loyola ^{147b}, P.H. Sales De Bruin ¹⁷², A. Salnikov ¹⁵³, J. Salt ¹⁷⁴, D. Salvatore ^{41b,41a}, F. Salvatore ¹⁵⁶, A. Salvucci ^{63a,63b,63c}, A. Salzburger ³⁶, J. Samarati ³⁶, D. Sammel ⁵², D. Sampsonidis ¹⁶², D. Sampsonidou ¹⁶², J. Sánchez ¹⁷⁴, A. Sanchez Pineda ^{66a,66c}, H. Sandaker ¹³⁴, C.O. Sander ⁴⁶, I.G. Sanderswood ⁸⁹, M. Sandhoff ¹⁸², C. Sandoval ²², D.P.C. Sankey ¹⁴⁴, M. Sannino ^{55b,55a}, Y. Sano ¹¹⁷, A. Sansoni ⁵¹, C. Santoni ³⁸, H. Santos ^{140a,140b}, S.N. Santpur ¹⁸, A. Santra ¹⁷⁴, A. Saprosov ⁷⁹, J.G. Saraiva ^{140a,140d}, O. Sasaki ⁸¹, K. Sato ¹⁶⁹, F. Sauerburger ⁵², E. Sauvan ⁵, P. Savard ^{167,av}, N. Savic ¹¹⁵, R. Sawada ¹⁶³, C. Sawyer ¹⁴⁴, L. Sawyer ^{95,aj}, C. Sbarra ^{23b}, A. Sbrizzi ^{23a}, T. Scanlon ⁹⁴, J. Schaarschmidt ¹⁴⁸, P. Schacht ¹¹⁵, B.M. Schachtner ¹¹⁴, D. Schaefer ³⁷, L. Schaefer ¹³⁷, J. Schaeffer ⁹⁹, S. Schaepe ³⁶, U. Schäfer ⁹⁹, A.C. Schaffer ¹³², D. Schaile ¹¹⁴, R.D. Schamberger ¹⁵⁵, N. Scharmberg ¹⁰⁰, V.A. Schegelsky ¹³⁸, D. Scheirich ¹⁴³, F. Schenck ¹⁹, M. Schernau ¹⁷¹, C. Schiavi ^{55b,55a}, S. Schier ¹⁴⁶, L.K. Schildgen ²⁴, Z.M. Schillaci ²⁶, E.J. Schioppa ³⁶, M. Schioppa ^{41b,41a}, K.E. Schleicher ⁵², S. Schlenker ³⁶, K.R. Schmidt-Sommerfeld ¹¹⁵, K. Schmieden ³⁶, C. Schmitt ⁹⁹, S. Schmitt ⁴⁶, S. Schmitz ⁹⁹, J.C. Schmoekel ⁴⁶, U. Schnoor ⁵², L. Schoeffel ¹⁴⁵, A. Schoening ^{61b}, P.G. Scholer ⁵², E. Schopf ¹³⁵, M. Schott ⁹⁹, J.F.P. Schouwenberg ¹¹⁹, J. Schovancova ³⁶, S. Schramm ⁵⁴, F. Schroeder ¹⁸², A. Schulte ⁹⁹, H-C. Schultz-Coulon ^{61a}, M. Schumacher ⁵², B.A. Schumm ¹⁴⁶, Ph. Schune ¹⁴⁵, A. Schwartzman ¹⁵³, T.A. Schwarz ¹⁰⁵, Ph. Schwemling ¹⁴⁵, R. Schwiendhorst ¹⁰⁶, A. Sciandra ¹⁴⁶, G. Sciolla ²⁶, M. Scodeggio ⁴⁶, M. Scornajenghi ^{41b,41a}, F. Scuri ^{71a}, F. Scutti ¹⁰⁴, L.M. Scyboz ¹¹⁵, C.D. Sebastiani ^{72a,72b}, P. Seema ¹⁹, S.C. Seidel ¹¹⁸, A. Seiden ¹⁴⁶, B.D. Seidlitz ²⁹, T. Seiss ³⁷, J.M. Seixas ^{80b}, G. Sekhniaidze ^{69a}, K. Sekhon ¹⁰⁵, S.J. Sekula ⁴², N. Semprini-Cesari ^{23b,23a}, S. Sen ⁴⁹, S. Senkin ³⁸, C. Serfon ⁷⁶, L. Serin ¹³², L. Serkin ^{66a,66b}, M. Sessa ^{60a}, H. Severini ¹²⁸, F. Sforza ^{55b,55a}, A. Sfyrta ⁵⁴, E. Shabalina ⁵³, J.D. Shahinian ¹⁴⁶, N.W. Shaikh ^{45a,45b}, D. Shaked Renous ¹⁸⁰, L.Y. Shan ^{15a}, R. Shang ¹⁷³, J.T. Shank ²⁵, M. Shapiro ¹⁸, A. Sharma ¹³⁵, A.S. Sharma ¹, P.B. Shatalov ¹¹¹, K. Shaw ¹⁵⁶, S.M. Shaw ¹⁰⁰, A. Shcherbakova ¹³⁸, M. Shehade ¹⁸⁰, Y. Shen ¹²⁸, N. Sherafati ³⁴, A.D. Sherman ²⁵, P. Sherwood ⁹⁴, L. Shi ^{158,ar}, S. Shimizu ⁸¹, C.O. Shimmin ¹⁸³, Y. Shimogama ¹⁷⁹, M. Shimojima ¹¹⁶, I.P.J. Shipsey ¹³⁵, S. Shirabe ⁸⁷, M. Shiyakova ^{79,z}, J. Shlomi ¹⁸⁰, A. Shmeleva ¹¹⁰, M.J. Shochet ³⁷, S. Shojaii ¹⁰⁴, D.R. Shope ¹²⁸, S. Shrestha ¹²⁶, E.M. Shrif ^{33c}, E. Shulga ¹⁸⁰, P. Sicho ¹⁴¹, A.M. Sickles ¹⁷³, P.E. Sidebo ¹⁵⁴, E. Sideras Haddad ^{33c}, O. Sidiropoulou ³⁶, A. Sidoti ^{23b,23a}, F. Siegert ⁴⁸, Dj. Sijacki ¹⁶, M. Silva Jr. ¹⁸¹, M.V. Silva Oliveira ^{80a}, S.B. Silverstein ^{45a}, S. Simion ¹³², E. Simioni ⁹⁹, R. Simoniello ⁹⁹, S. Simsek ^{12b}, P. Sinervo ¹⁶⁷, V. Sinetckii ^{113,110}, N.B. Sinev ¹³¹, M. Sioli ^{23b,23a}, I. Siral ¹⁰⁵, S.Yu. Sivoklov ¹¹³, J. Sjölin ^{45a,45b}, E. Skorda ⁹⁶, P. Skubic ¹²⁸, M. Slawinska ⁸⁴, K. Sliwa ¹⁷⁰, R. Slovak ¹⁴³, V. Smakhtin ¹⁸⁰, B.H. Smart ¹⁴⁴, J. Smiesko ^{28a}, N. Smirnov ¹¹², S.Yu. Smirnov ¹¹², Y. Smirnov ¹¹², L.N. Smirnova ^{113,s}, O. Smirnova ⁹⁶, J.W. Smith ⁵³, M. Smizanska ⁸⁹, K. Smolek ¹⁴², A. Smykiewicz ⁸⁴, A.A. Snesarev ¹¹⁰, H.L. Snoek ¹²⁰, I.M. Snyder ¹³¹, S. Snyder ²⁹, R. Sobie ^{176,ab}, A. Soffer ¹⁶¹, A. Søgaard ⁵⁰, F. Sohns ⁵³, C.A. Solans Sanchez ³⁶, E.Yu. Soldatov ¹¹², U. Soldevila ¹⁷⁴, A.A. Solodkov ¹²³, A. Soloshenko ⁷⁹, O.V. Solovyanov ¹²³, V. Solovyev ¹³⁸, P. Sommer ¹⁴⁹, H. Son ¹⁷⁰, W. Song ¹⁴⁴, W.Y. Song ^{168b}, A. Sopczak ¹⁴², F. Sopkova ^{28b}, C.L. Sotiropoulou ^{71a,71b}, S. Sottocornola ^{70a,70b}, R. Soualah ^{66a,66c,f}, A.M. Soukharev ^{122b,122a}, D. South ⁴⁶, S. Spagnolo ^{67a,67b}, M. Spalla ¹¹⁵, M. Spangenberg ¹⁷⁸, F. Spanò ⁹³, D. Sperlich ⁵², T.M. Spieker ^{61a}, R. Spighi ^{23b}, G. Spigo ³⁶, M. Spina ¹⁵⁶, D.P. Spiteri ⁵⁷, M. Spousta ¹⁴³, A. Stabile ^{68a,68b}, B.L. Stamas ¹²¹, R. Stamen ^{61a}, M. Stamenkovic ¹²⁰, E. Stanecka ⁸⁴, B. Stanislaus ¹³⁵, M.M. Stanitzki ⁴⁶, M. Stankaityte ¹³⁵, B. Stapf ¹²⁰, E.A. Starchenko ¹²³,

G.H. Stark¹⁴⁶, J. Stark⁵⁸, S.H. Stark⁴⁰, P. Staroba¹⁴¹, P. Starovoitov^{61a}, S. Stärz¹⁰³, R. Staszewski⁸⁴, G. Stavropoulos⁴⁴, M. Stegler⁴⁶, P. Steinberg²⁹, A.L. Steinhebel¹³¹, B. Stelzer¹⁵², H.J. Stelzer¹³⁹, O. Stelzer-Chilton^{168a}, H. Stenzel⁵⁶, T.J. Stevenson¹⁵⁶, G.A. Stewart³⁶, M.C. Stockton³⁶, G. Stoicea^{27b}, M. Stolarski^{140a}, S. Stonjek¹¹⁵, A. Straessner⁴⁸, J. Strandberg¹⁵⁴, S. Strandberg^{45a,45b}, M. Strauss¹²⁸, P. Strizenec^{28b}, R. Ströhmer¹⁷⁷, D.M. Strom¹³¹, R. Stroynowski⁴², A. Strubig⁵⁰, S.A. Stucci²⁹, B. Stugu¹⁷, J. Stupak¹²⁸, N.A. Styles⁴⁶, D. Su¹⁵³, S. Suchek^{61a}, V.V. Sulin¹¹⁰, M.J. Sullivan⁹⁰, D.M.S. Sultan⁵⁴, S. Sultansoy^{4c}, T. Sumida⁸⁵, S. Sun¹⁰⁵, X. Sun³, K. Suruliz¹⁵⁶, C.J.E. Suster¹⁵⁷, M.R. Sutton¹⁵⁶, S. Suzuki⁸¹, M. Svatos¹⁴¹, M. Swiatlowski³⁷, S.P. Swift², T. Swirski¹⁷⁷, A. Sydorenko⁹⁹, I. Sykora^{28a}, M. Sykora¹⁴³, T. Sykora¹⁴³, D. Ta⁹⁹, K. Tackmann^{46,x}, J. Taenzer¹⁶¹, A. Taffard¹⁷¹, R. Tafirout^{168a}, H. Takai²⁹, R. Takashima⁸⁶, K. Takeda⁸², T. Takeshita¹⁵⁰, E.P. Takeva⁵⁰, Y. Takubo⁸¹, M. Talby¹⁰¹, A.A. Talyshev^{122b,122a}, N.M. Tamir¹⁶¹, J. Tanaka¹⁶³, M. Tanaka¹⁶⁵, R. Tanaka¹³², S. Tapia Araya¹⁷³, S. Tapprogge⁹⁹, A. Tarek Abouelfadl Mohamed¹³⁶, S. Tarem¹⁶⁰, G. Tarna^{27b,b}, G.F. Tartarelli^{68a}, P. Tas¹⁴³, M. Tasevsky¹⁴¹, T. Tashiro⁸⁵, E. Tassi^{41b,41a}, A. Tavares Delgado^{140a,140b}, Y. Tayalati^{35e}, A.J. Taylor⁵⁰, G.N. Taylor¹⁰⁴, W. Taylor^{168b}, A.S. Tee⁸⁹, R. Teixeira De Lima¹⁵³, P. Teixeira-Dias⁹³, H. Ten Kate³⁶, J.J. Teoh¹²⁰, S. Terada⁸¹, K. Terashi¹⁶³, J. Terron⁹⁸, S. Terzo¹⁴, M. Testa⁵¹, R.J. Teuscher^{167,ab}, S.J. Thais¹⁸³, T. Theveneaux-Pelzer⁴⁶, F. Thiele⁴⁰, D.W. Thomas⁹³, J.O. Thomas⁴², J.P. Thomas²¹, A.S. Thompson⁵⁷, P.D. Thompson²¹, L.A. Thomsen¹⁸³, E. Thomson¹³⁷, E.J. Thorpe⁹², Y. Tian³⁹, R.E. Ticse Torres⁵³, V.O. Tikhomirov^{110,an}, Yu.A. Tikhonov^{122b,122a}, S. Timoshenko¹¹², P. Tipton¹⁸³, S. Tisserant¹⁰¹, K. Todome^{23b,23a}, S. Todorova-Nova⁵, S. Todt⁴⁸, J. Tojo⁸⁷, S. Tokár^{28a}, K. Tokushuku⁸¹, E. Tolley¹²⁶, K.G. Tomiwa^{33c}, M. Tomoto¹¹⁷, L. Tompkins^{153,o}, K. Toms¹¹⁸, B. Tong⁵⁹, P. Tornambe¹⁰², E. Torrence¹³¹, H. Torres⁴⁸, E. Torrón Pastor¹⁴⁸, C. Toscirì¹³⁵, J. Toth^{101,aa}, D.R. Tovey¹⁴⁹, A. Traeet¹⁷, C.J. Treado¹²⁴, T. Trefzger¹⁷⁷, F. Tresoldi¹⁵⁶, A. Tricoli²⁹, I.M. Trigger^{168a}, S. Trincaz-Duvoid¹³⁶, W. Trischuk¹⁶⁷, B. Trocmé⁵⁸, A. Trofymov¹³², C. Troncon^{68a}, M. Trovatelli¹⁷⁶, F. Trovato¹⁵⁶, L. Truong^{33b}, M. Trzebinski⁸⁴, A. Trzupek⁸⁴, F. Tsai⁴⁶, J.C-L. Tseng¹³⁵, P.V. Tsiarehka^{107,ah}, A. Tsirigotis¹⁶², N. Tsirintanis⁹, V. Tsiskaridze¹⁵⁵, E.G. Tskhadadze^{159a}, M. Tsopoulou¹⁶², I.I. Tsukerman¹¹¹, V. Tsulaia¹⁸, S. Tsuno⁸¹, D. Tsybychev¹⁵⁵, Y. Tu^{63b}, A. Tudorache^{27b}, V. Tudorache^{27b}, T.T. Tulbure^{27a}, A.N. Tuna⁵⁹, S. Turchikhin⁷⁹, D. Turgeman¹⁸⁰, I. Turk Cakir^{4b,t}, R.J. Turner²¹, R.T. Turra^{68a}, P.M. Tuts³⁹, S. Tzamarias¹⁶², E. Tzovara⁹⁹, G. Uccielli⁴⁷, K. Uchida¹⁶³, I. Ueda⁸¹, M. Ughetto^{45a,45b}, F. Ukegawa¹⁶⁹, G. Unal³⁶, A. Undrus²⁹, G. Unel¹⁷¹, F.C. Ungaro¹⁰⁴, Y. Unno⁸¹, K. Uno¹⁶³, J. Urban^{28b}, P. Urquijo¹⁰⁴, G. Usai⁸, Z. Uysal^{12d}, L. Vacavant¹⁰¹, V. Vacek¹⁴², B. Vachon¹⁰³, K.O.H. Vadla¹³⁴, A. Vaidya⁹⁴, C. Valderanis¹¹⁴, E. Valdes Santurio^{45a,45b}, M. Valente⁵⁴, S. Valentineti^{23b,23a}, A. Valero¹⁷⁴, L. Valéry⁴⁶, R.A. Vallance²¹, A. Vallier³⁶, J.A. Valls Ferrer¹⁷⁴, T.R. Van Daalen¹⁴, P. Van Gemmeren⁶, I. Van Vulpen¹²⁰, M. Vanadia^{73a,73b}, W. Vandelli³⁶, A. Vaniachine¹⁶⁶, D. Vannicola^{72a,72b}, R. Vari^{72a}, E.W. Varnes⁷, C. Varni^{55b,55a}, T. Varol⁴², D. Varouchas¹³², K.E. Varvell¹⁵⁷, M.E. Vasile^{27b}, G.A. Vasquez¹⁷⁶, J.G. Vasquez¹⁸³, F. Vazeille³⁸, D. Vazquez Furelos¹⁴, T. Vazquez Schroeder³⁶, J. Veatch⁵³, V. Vecchio^{74a,74b}, M.J. Veen¹²⁰, L.M. Veloce¹⁶⁷, F. Veloso^{140a,140c}, S. Veneziano^{72a}, A. Ventura^{67a,67b}, N. Venturi³⁶, A. Verbytskyi¹¹⁵, V. Vercesi^{70a}, M. Verducci^{71a,71b}, C.M. Vergel Infante⁷⁸, C. Vergis²⁴, W. Verkerke¹²⁰, A.T. Vermeulen¹²⁰, J.C. Vermeulen¹²⁰, M.C. Vetterli^{152,av}, N. Viaux Maira^{147b}, M. Vicente Barreto Pinto⁵⁴, T. Vickey¹⁴⁹, O.E. Vickey Boeriu¹⁴⁹, G.H.A. Viehhauser¹³⁵, L. Vigani^{61b}, M. Villa^{23b,23a}, M. Villaplana Perez^{68a,68b}, E. Vilucchi⁵¹, M.G. Vincker³⁴, V.B. Vinogradov⁷⁹, G.S. Virdee²¹, A. Vishwakarma⁴⁶, C. Vittori^{23b,23a}, I. Vivarelli¹⁵⁶, M. Vogel¹⁸², P. Vokac¹⁴², S.E. von Buddenbrock^{33c}, E. Von Toerne²⁴, V. Vorobel¹⁴³, K. Vorobev¹¹², M. Vos¹⁷⁴, J.H. Vosseveld⁹⁰, M. Vozak¹⁰⁰, N. Vranjes¹⁶, M. Vranjes Milosavljevic¹⁶, V. Vrba¹⁴², M. Vreeswijk¹²⁰, T. Šfiligoj⁹¹, R. Vuillermet³⁶, I. Vukotic³⁷, T. Ženiš^{28a}, L. Živković¹⁶, P. Wagner²⁴, W. Wagner¹⁸², J. Wagner-Kuhr¹¹⁴, S. Wahdan¹⁸², H. Wahlberg⁸⁸, V.M. Walbrecht¹¹⁵, J. Walder⁸⁹, R. Walker¹¹⁴, S.D. Walker⁹³, W. Walkowiak¹⁵¹, V. Wallangen^{45a,45b}, A.M. Wang⁵⁹, C. Wang^{60c}, C. Wang^{60b}, F. Wang¹⁸¹, H. Wang¹⁸, H. Wang³, J. Wang¹⁵⁷, J. Wang^{61b}, P. Wang⁴², Q. Wang¹²⁸, R.-J. Wang⁹⁹, R. Wang^{60a}, R. Wang⁶, S.M. Wang¹⁵⁸, W.T. Wang^{60a}, W. Wang^{15c,ac}, W.X. Wang^{60a,ac}, Y. Wang^{60a,ak}, Z. Wang^{60c}, C. Wanotayaroj⁴⁶, A. Warburton¹⁰³, C.P. Ward³², D.R. Wardrope⁹⁴, N. Warrack⁵⁷, A. Washbrook⁵⁰, A.T. Watson²¹, M.F. Watson²¹, G. Watts¹⁴⁸, B.M. Waugh⁹⁴, A.F. Webb¹¹, S. Webb⁹⁹, C. Weber¹⁸³, M.S. Weber²⁰, S.A. Weber³⁴, S.M. Weber^{61a}, A.R. Weidberg¹³⁵, J. Weingarten⁴⁷, M. Weirich⁹⁹, C. Weiser⁵², P.S. Wells³⁶, T. Wenaus²⁹, T. Wengler³⁶

S. Wenig³⁶, N. Wermes²⁴, M.D. Werner⁷⁸, M. Wessels^{61a}, T.D. Weston²⁰, K. Whalen¹³¹, N.L. Whallon¹⁴⁸, A.M. Wharton⁸⁹, A.S. White¹⁰⁵, A. White⁸, M.J. White¹, D. Whiteson¹⁷¹, B.W. Whitmore⁸⁹, W. Wiedenmann¹⁸¹, M. Wielers¹⁴⁴, N. Wieseotte⁹⁹, C. Wiglesworth⁴⁰, L.A.M. Wiik-Fuchs⁵², F. Wilk¹⁰⁰, H.G. Wilkens³⁶, L.J. Wilkins⁹³, H.H. Williams¹³⁷, S. Williams³², C. Willis¹⁰⁶, S. Willocq¹⁰², J.A. Wilson²¹, I. Wingerter-Seez⁵, E. Winkels¹⁵⁶, F. Winklmeier¹³¹, O.J. Winston¹⁵⁶, B.T. Winter⁵², M. Wittgen¹⁵³, M. Wobisch⁹⁵, A. Wolf⁹⁹, T.M.H. Wolf¹²⁰, R. Wolff¹⁰¹, R.W. Wölker¹³⁵, J. Wollrath⁵², M.W. Wolter⁸⁴, H. Wolters^{140a,140c}, V.W.S. Wong¹⁷⁵, N.L. Woods¹⁴⁶, S.D. Worm²¹, B.K. Wosiek⁸⁴, K.W. Woźniak⁸⁴, K. Wraight⁵⁷, S.L. Wu¹⁸¹, X. Wu⁵⁴, Y. Wu^{60a}, T.R. Wyatt¹⁰⁰, B.M. Wynne⁵⁰, S. Xella⁴⁰, Z. Xi¹⁰⁵, L. Xia¹⁷⁸, X. Xiao¹⁰⁵, D. Xu^{15a}, H. Xu^{60a,b}, L. Xu²⁹, T. Xu¹⁴⁵, W. Xu¹⁰⁵, Z. Xu^{60b}, Z. Xu¹⁵³, B. Yabsley¹⁵⁷, S. Yacoob^{33a}, K. Yajima¹³³, D.P. Yallup⁹⁴, D. Yamaguchi¹⁶⁵, Y. Yamaguchi¹⁶⁵, A. Yamamoto⁸¹, M. Yamatani¹⁶³, T. Yamazaki¹⁶³, Y. Yamazaki⁸², Z. Yan²⁵, H.J. Yang^{60c,60d}, H.T. Yang¹⁸, S. Yang⁷⁷, X. Yang^{60b,58}, Y. Yang¹⁶³, W-M. Yao¹⁸, Y.C. Yap⁴⁶, Y. Yasu⁸¹, E. Yatsenko^{60c,60d}, J. Ye⁴², S. Ye²⁹, I. Yeletsikh⁷⁹, M.R. Yexley⁸⁹, E. Yigitbasi²⁵, K. Yorita¹⁷⁹, K. Yoshihara¹³⁷, C.J.S. Young³⁶, C. Young¹⁵³, J. Yu⁷⁸, R. Yuan^{60b,h}, X. Yue^{61a}, S.P.Y. Yuen²⁴, B. Zabinski⁸⁴, G. Zacharis¹⁰, E. Zaffaroni⁵⁴, J. Zahreddine¹³⁶, A.M. Zaitsev^{123.am}, T. Zakareishvili^{159b}, N. Zakharchuk³⁴, S. Zambito⁵⁹, D. Zanzi³⁶, D.R. Zaripovas⁵⁷, S.V. Zeißner⁴⁷, C. Zeitnitz¹⁸², G. Zemaityte¹³⁵, J.C. Zeng¹⁷³, O. Zenin¹²³, D. Zerwas¹³², M. Zgubič¹³⁵, D.F. Zhang^{15b}, F. Zhang¹⁸¹, G. Zhang^{15b}, H. Zhang^{15c}, J. Zhang⁶, L. Zhang^{15c}, L. Zhang^{60a}, M. Zhang¹⁷³, R. Zhang²⁴, X. Zhang^{60b}, Y. Zhang^{15a,15d}, Z. Zhang^{63a}, Z. Zhang¹³², P. Zhao⁴⁹, Y. Zhao^{60b}, Z. Zhao^{60a}, A. Zhemchugov⁷⁹, Z. Zheng¹⁰⁵, D. Zhong¹⁷³, B. Zhou¹⁰⁵, C. Zhou¹⁸¹, M.S. Zhou^{15a,15d}, M. Zhou¹⁵⁵, N. Zhou^{60c}, Y. Zhou⁷, C.G. Zhu^{60b}, H.L. Zhu^{60a}, H. Zhu^{15a}, J. Zhu¹⁰⁵, Y. Zhu^{60a}, X. Zhuang^{15a}, K. Zhukov¹¹⁰, V. Zhulanov^{122b,122a}, D. Zieminska⁶⁵, N.I. Zimine⁷⁹, S. Zimmermann⁵², Z. Zinonos¹¹⁵, M. Ziolkowski¹⁵¹, G. Zobernig¹⁸¹, A. Zoccoli^{23b,23a}, K. Zoch⁵³, T.G. Zorbas¹⁴⁹, R. Zou³⁷, L. Zwalinski³⁶

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, Université Grenoble Alpes, Université Savoie Mont Blanc, CNRS/IN2P3, Annecy, France

⁶ High Energy Physics Division, Argonne National Laboratory, Argonne, IL, United States of America

⁷ Department of Physics, University of Arizona, Tucson, AZ, United States of America

⁸ Department of Physics, University of Texas at Arlington, Arlington, TX, United States of America

⁹ Physics Department, National and Kapodistrian University of Athens, Athens, Greece

¹⁰ Physics Department, National Technical University of Athens, Zografou, Greece

¹¹ Department of Physics, University of Texas at Austin, Austin, TX, United States of America

¹² (a) Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul; (b) Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul; (c) Department of Physics, Bogazici University, Istanbul; (d) Department of Physics Engineering, Gaziantep University, Gaziantep, Turkey

¹³ Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan

¹⁴ Institut de Física d'Altes Energies (IFAE), Barcelona Institute of Science and Technology, Barcelona, Spain

¹⁵ (a) Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; (b) Physics Department, Tsinghua University, Beijing; (c) Department of Physics, Nanjing University, Nanjing;

(d) University of Chinese Academy of Science (UCAS), Beijing, China

¹⁶ Institute of Physics, University of Belgrade, Belgrade, Serbia

¹⁷ Department for Physics and Technology, University of Bergen, Bergen, Norway

¹⁸ Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley, CA, United States of America

¹⁹ Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany

²⁰ Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland

²¹ School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom

²² Facultad de Ciencias y Centro de Investigaciones, Universidad Antonio Nariño, Bogota, Colombia

²³ (a) INFN Bologna and Università di Bologna, Dipartimento di Fisica; (b) INFN Sezione di Bologna, Italy

²⁴ Physikalisches Institut, Universität Bonn, Bonn, Germany

²⁵ Department of Physics, Boston University, Boston, MA, United States of America

²⁶ Department of Physics, Brandeis University, Waltham, MA, United States of America

²⁷ (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

²⁸ (a) Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava; (b) Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of

Sciences, Kosice, Slovak Republic

²⁹ Physics Department, Brookhaven National Laboratory, Upton, NY, United States of America

³⁰ Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina

³¹ California State University, CA, United States of America

³² Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

³³ (a) Department of Physics, University of Cape Town, Cape Town; (b) Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg; (c) School of Physics,

University of the Witwatersrand, Johannesburg, South Africa

³⁴ Department of Physics, Carleton University, Ottawa, ON, Canada

³⁵ (a) Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies – Université Hassan II, Casablanca; (b) Faculté des Sciences, Université Ibn-Tofail, Kénitra;

(c) Faculté des Sciences Semailia, Université Cadi Ayyad, LPHEA, Marrakech; (d) Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda; (e) Faculté des sciences, Université

Mohammed V, Rabat, Morocco

- ³⁶ CERN, Geneva, Switzerland
- ³⁷ Enrico Fermi Institute, University of Chicago, Chicago, IL, United States of America
- ³⁸ LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand, France
- ³⁹ Nevis Laboratory, Columbia University, Irvington, NY, United States of America
- ⁴⁰ Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
- ⁴¹ ^(a) Dipartimento di Fisica, Università della Calabria, Rende; ^(b) INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Italy
- ⁴² Physics Department, Southern Methodist University, Dallas, TX, United States of America
- ⁴³ Physics Department, University of Texas at Dallas, Richardson, TX, United States of America
- ⁴⁴ National Centre for Scientific Research "Demokritos", Agia Paraskevi, Greece
- ⁴⁵ ^(a) Department of Physics, Stockholm University; ^(b) Oskar Klein Centre, Stockholm, Sweden
- ⁴⁶ Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen, Germany
- ⁴⁷ Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
- ⁴⁸ Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
- ⁴⁹ Department of Physics, Duke University, Durham, NC, United States of America
- ⁵⁰ SUPA – School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom
- ⁵¹ INFN e Laboratori Nazionali di Frascati, Frascati, Italy
- ⁵² Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany
- ⁵³ II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany
- ⁵⁴ Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland
- ⁵⁵ ^(a) Dipartimento di Fisica, Università di Genova, Genova; ^(b) INFN Sezione di Genova, Italy
- ⁵⁶ II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
- ⁵⁷ SUPA – School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom
- ⁵⁸ LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble, France
- ⁵⁹ Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, MA, United States of America
- ⁶⁰ ^(a) Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Hefei; ^(b) Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE), Shandong University, Qingdao; ^(c) School of Physics and Astronomy, Shanghai Jiao Tong University, KLPPAC-MoE, SKLPPC, Shanghai; ^(d) Tsung-Dao Lee Institute, Shanghai, China
- ⁶¹ ^(a) Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg; ^(b) Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
- ⁶² Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
- ⁶³ ^(a) Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; ^(b) Department of Physics, University of Hong Kong, Hong Kong; ^(c) Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China
- ⁶⁴ Department of Physics, National Tsing Hua University, Hsinchu, Taiwan
- ⁶⁵ Department of Physics, Indiana University, Bloomington, IN, United States of America
- ⁶⁶ ^(a) INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; ^(b) ICTP, Trieste; ^(c) Dipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine, Italy
- ⁶⁷ ^(a) INFN Sezione di Lecce; ^(b) Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy
- ⁶⁸ ^(a) INFN Sezione di Milano; ^(b) Dipartimento di Fisica, Università di Milano, Milano, Italy
- ⁶⁹ ^(a) INFN Sezione di Napoli; ^(b) Dipartimento di Fisica, Università di Napoli, Napoli, Italy
- ⁷⁰ ^(a) INFN Sezione di Pavia; ^(b) Dipartimento di Fisica, Università di Pavia, Pavia, Italy
- ⁷¹ ^(a) INFN Sezione di Pisa; ^(b) Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy
- ⁷² ^(a) INFN Sezione di Roma; ^(b) Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy
- ⁷³ ^(a) INFN Sezione di Roma Tor Vergata; ^(b) Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy
- ⁷⁴ ^(a) INFN Sezione di Roma Tre; ^(b) Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy
- ⁷⁵ ^(a) INFN-TIFPA; ^(b) Università degli Studi di Trento, Trento, Italy
- ⁷⁶ Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria
- ⁷⁷ University of Iowa, Iowa City, IA, United States of America
- ⁷⁸ Department of Physics and Astronomy, Iowa State University, Ames, IA, United States of America
- ⁷⁹ Joint Institute for Nuclear Research, Dubna, Russia
- ⁸⁰ ^(a) Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora; ^(b) Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro;
- ^(c) Universidade Federal de São João del Rei (UFSJ), São João del Rei; ^(d) Instituto de Física, Universidade de São Paulo, São Paulo, Brazil
- ⁸¹ KEK, High Energy Accelerator Research Organization, Tsukuba, Japan
- ⁸² Graduate School of Science, Kobe University, Kobe, Japan
- ⁸³ ^(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
- ⁸⁴ Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
- ⁸⁵ Faculty of Science, Kyoto University, Kyoto, Japan
- ⁸⁶ Kyoto University of Education, Kyoto, Japan
- ⁸⁷ Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan
- ⁸⁸ Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
- ⁸⁹ Physics Department, Lancaster University, Lancaster, United Kingdom
- ⁹⁰ Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom
- ⁹¹ Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia
- ⁹² School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom
- ⁹³ Department of Physics, Royal Holloway University of London, Egham, United Kingdom
- ⁹⁴ Department of Physics and Astronomy, University College London, London, United Kingdom
- ⁹⁵ Louisiana Tech University, Ruston, LA, United States of America
- ⁹⁶ Fysiska institutionen, Lunds universitet, Lund, Sweden
- ⁹⁷ Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France
- ⁹⁸ Departamento de Física Teórica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid, Spain
- ⁹⁹ Institut für Physik, Universität Mainz, Mainz, Germany
- ¹⁰⁰ School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom
- ¹⁰¹ CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France
- ¹⁰² Department of Physics, University of Massachusetts, Amherst, MA, United States of America
- ¹⁰³ Department of Physics, McGill University, Montreal, QC, Canada
- ¹⁰⁴ School of Physics, University of Melbourne, Victoria, Australia
- ¹⁰⁵ Department of Physics, University of Michigan, Ann Arbor, MI, United States of America
- ¹⁰⁶ Department of Physics and Astronomy, Michigan State University, East Lansing, MI, United States of America
- ¹⁰⁷ B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus
- ¹⁰⁸ Research Institute for Nuclear Problems of Byelorussian State University, Minsk, Belarus
- ¹⁰⁹ Group of Particle Physics, University of Montreal, Montreal, QC, Canada

- 110 P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia
 111 Institute for Theoretical and Experimental Physics of the National Research Centre Kurchatov Institute, Moscow, Russia
 112 National Research Nuclear University MEPhI, Moscow, Russia
 113 D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia
 114 Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany
 115 Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany
 116 Nagasaki Institute of Applied Science, Nagasaki, Japan
 117 Graduate School of Science and Kobayashi–Maskawa Institute, Nagoya University, Nagoya, Japan
 118 Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM, United States of America
 119 Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands
 120 Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands
 121 Department of Physics, Northern Illinois University, DeKalb, IL, United States of America
 122 ^(a) Budker Institute of Nuclear Physics and NSU, SB RAS, Novosibirsk; ^(b) Novosibirsk State University Novosibirsk, Russia
 123 Institute for High Energy Physics of the National Research Centre Kurchatov Institute, Protvino, Russia
 124 Department of Physics, New York University, New York, NY, United States of America
 125 Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo, Japan
 126 Ohio State University, Columbus, OH, United States of America
 127 Faculty of Science, Okayama University, Okayama, Japan
 128 Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK, United States of America
 129 Department of Physics, Oklahoma State University, Stillwater, OK, United States of America
 130 Palacký University, RCPTM, Joint Laboratory of Optics, Olomouc, Czech Republic
 131 Center for High Energy Physics, University of Oregon, Eugene, OR, United States of America
 132 LAL, Université Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France
 133 Graduate School of Science, Osaka University, Osaka, Japan
 134 Department of Physics, University of Oslo, Oslo, Norway
 135 Department of Physics, Oxford University, Oxford, United Kingdom
 136 LPNHE, Sorbonne Université, Paris Diderot Sorbonne Paris Cité, CNRS/IN2P3, Paris, France
 137 Department of Physics, University of Pennsylvania, Philadelphia, PA, United States of America
 138 Konstantinov Nuclear Physics Institute of National Research Centre “Kurchatov Institute”, PNPI, St. Petersburg, Russia
 139 Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA, United States of America
 140 ^(a) Laboratório de Instrumentação e Física Experimental de Partículas – LIP; ^(b) Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa; ^(c) Departamento de Física, Universidade de Coimbra, Coimbra; ^(d) Centro de Física Nuclear da Universidade de Lisboa, Lisboa; ^(e) Departamento de Física, Universidade do Minho, Braga; ^(f) Universidad de Granada, Granada (Spain); ^(g) Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal
 141 Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic
 142 Czech Technical University in Prague, Prague, Czech Republic
 143 Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic
 144 Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom
 145 IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France
 146 Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, CA, United States of America
 147 ^(a) Departamento de Física, Pontificia Universidad Católica de Chile, Santiago; ^(b) Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
 148 Department of Physics, University of Washington, Seattle, WA, United States of America
 149 Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom
 150 Department of Physics, Shinshu University, Nagano, Japan
 151 Department Physik, Universität Siegen, Siegen, Germany
 152 Department of Physics, Simon Fraser University, Burnaby, BC, Canada
 153 SLAC National Accelerator Laboratory, Stanford, CA, United States of America
 154 Physics Department, Royal Institute of Technology, Stockholm, Sweden
 155 Departments of Physics and Astronomy, Stony Brook University, Stony Brook, NY, United States of America
 156 Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom
 157 School of Physics, University of Sydney, Sydney, Australia
 158 Institute of Physics, Academia Sinica, Taipei, Taiwan
 159 ^(a) E. Andronikashvili Institute of Physics, Iv. Javakishvili Tbilisi State University, Tbilisi; ^(b) High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
 160 Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel
 161 Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel
 162 Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
 163 International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo, Japan
 164 Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan
 165 Department of Physics, Tokyo Institute of Technology, Tokyo, Japan
 166 Tomsk State University, Tomsk, Russia
 167 Department of Physics, University of Toronto, Toronto, ON, Canada
 168 ^(a) TRIUMF, Vancouver, BC; ^(b) Department of Physics and Astronomy, York University, Toronto, ON, Canada
 169 Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan
 170 Department of Physics and Astronomy, Tufts University, Medford, MA, United States of America
 171 Department of Physics and Astronomy, University of California Irvine, Irvine, CA, United States of America
 172 Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden
 173 Department of Physics, University of Illinois, Urbana, IL, United States of America
 174 Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia – CSIC, Valencia, Spain
 175 Department of Physics, University of British Columbia, Vancouver, BC, Canada
 176 Department of Physics and Astronomy, University of Victoria, Victoria, BC, Canada
 177 Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg, Germany
 178 Department of Physics, University of Warwick, Coventry, United Kingdom
 179 Waseda University, Tokyo, Japan
 180 Department of Particle Physics, Weizmann Institute of Science, Rehovot, Israel
 181 Department of Physics, University of Wisconsin, Madison, WI, United States of America
 182 Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany
 183 Department of Physics, Yale University, New Haven, CT, United States of America
 184 Yerevan Physics Institute, Yerevan, Armenia

- ^a Also at CERN, Geneva; Switzerland.
- ^b Also at CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille; France.
- ^c Also at Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève; Switzerland.
- ^d Also at Departament de Física de la Universitat Autònoma de Barcelona, Barcelona; Spain.
- ^e Also at Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, Lisboa; Portugal.
- ^f Also at Department of Applied Physics and Astronomy, University of Sharjah, Sharjah; United Arab Emirates.
- ^g Also at Department of Financial and Management Engineering, University of the Aegean, Chios; Greece.
- ^h Also at Department of Physics and Astronomy, Michigan State University, East Lansing MI; United States of America.
- ⁱ Also at Department of Physics and Astronomy, University of Louisville, Louisville, KY; United States of America.
- ^j Also at Department of Physics, California State University, East Bay; United States of America.
- ^k Also at Department of Physics, California State University, Fresno; United States of America.
- ^l Also at Department of Physics, California State University, Sacramento; United States of America.
- ^m Also at Department of Physics, King's College London, London; United Kingdom.
- ⁿ Also at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg; Russia.
- ^o Also at Department of Physics, Stanford University, Stanford CA; United States of America.
- ^p Also at Department of Physics, University of Adelaide, Adelaide; Australia.
- ^q Also at Department of Physics, University of Fribourg, Fribourg; Switzerland.
- ^r Also at Department of Physics, University of Michigan, Ann Arbor MI; United States of America.
- ^s Also at Faculty of Physics, M.V. Lomonosov Moscow State University, Moscow; Russia.
- ^t Also at Giresun University, Faculty of Engineering, Giresun; Turkey.
- ^u Also at Graduate School of Science, Osaka University, Osaka; Japan.
- ^v Also at Hellenic Open University, Patras; Greece.
- ^w Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona; Spain.
- ^x Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg; Germany.
- ^y Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen; Netherlands.
- ^z Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia; Bulgaria.
- ^{aa} Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest; Hungary.
- ^{ab} Also at Institute of Particle Physics (IPP); Canada.
- ^{ac} Also at Institute of Physics, Academia Sinica, Taipei; Taiwan.
- ^{ad} Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku; Azerbaijan.
- ^{ae} Also at Institute of Theoretical Physics, Iliia State University, Tbilisi; Georgia.
- ^{af} Also at Instituto de Física Teórica, IFT-UAM/CSIC, Madrid; Spain.
- ^{ag} Also at Istanbul University, Dept. of Physics, Istanbul; Turkey.
- ^{ah} Also at Joint Institute for Nuclear Research, Dubna; Russia.
- ^{ai} Also at LAL, Université Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay; France.
- ^{aj} Also at Louisiana Tech University, Ruston LA; United States of America.
- ^{ak} Also at LPNHE, Sorbonne Université, Paris Diderot Sorbonne Paris Cité, CNRS/IN2P3, Paris; France.
- ^{al} Also at Manhattan College, New York NY; United States of America.
- ^{am} Also at Moscow Institute of Physics and Technology State University, Dolgoprudny; Russia.
- ^{an} Also at National Research Nuclear University MEPhI, Moscow; Russia.
- ^{ao} Also at Physics Department, An-Najah National University, Nablus; Palestine.
- ^{ap} Also at Physics Dept, University of South Africa, Pretoria; South Africa.
- ^{aq} Also at Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg; Germany.
- ^{ar} Also at School of Physics, Sun Yat-sen University, Guangzhou; China.
- ^{as} Also at The City College of New York, New York NY; United States of America.
- ^{at} Also at The Collaborative Innovation Center of Quantum Matter (CICQM), Beijing; China.
- ^{au} Also at Tomsk State University, Tomsk, and Moscow Institute of Physics and Technology State University, Dolgoprudny; Russia.
- ^{av} Also at TRIUMF, Vancouver BC; Canada.
- ^{aw} Also at Università di Napoli Parthenope, Napoli; Italy.
- * Deceased.