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Search for pair production of vector-like top quarks in events with one lepton, jets, and missing transverse momentum in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector

The ATLAS Collaboration

The results of a search for vector-like top quarks using events with exactly one lepton, at least four jets, and large missing transverse momentum are reported. The search is optimised for pair production of vector-like top quarks in the $Z(\rightarrow\nu\nu)t+X$ decay channel. LHC pp collision data at a centre-of-mass energy of $\sqrt{s} = 13$ TeV recorded by the ATLAS detector in 2015 and 2016 are used, corresponding to an integrated luminosity of 36.1 fb^{-1} . No significant excess over the Standard Model expectation is seen and upper limits on the production cross-section of a vector-like T quark pair as a function of the T quark mass are derived. The observed (expected) 95% CL lower limits on the T mass are 870 GeV (890 GeV) for the weak-isospin singlet model, 1.05 TeV (1.06 TeV) for the weak-isospin doublet model and 1.16 TeV (1.17 TeV) for the pure Zt decay mode. Limits are also set on the mass as a function of the decay branching ratios, excluding large parts of the parameter space for masses below 1 TeV.

1 Introduction

A number of theories beyond the Standard Model (SM) of particle physics address the naturalness problem [1] and offer mechanisms through which the quadratic divergences, which arise from the radiative corrections to the Higgs boson mass, are resolved. A straightforward extension of the SM is the inclusion of a heavy fourth generation. However, fourth-generation quarks with SM-like chiral couplings are excluded as they contribute through loops to the couplings of the Higgs boson, altering the Higgs boson production cross-sections to values incompatible with observation [2, 3]. These constraints on chiral quarks can be evaded by vector-like quarks (VLQs) [4, 5], hypothetical spin-1/2 coloured particles whose left-handed and right-handed states have the same electroweak coupling. Vector-like quarks could dampen the unnaturally large quadratic corrections to the Higgs boson mass by contributing significantly to loop corrections. They appear mainly in the “Little Higgs” [6, 7] and “Composite Higgs” [8] classes of models.

In this analysis, a vector-like top quark partner (T) with a charge of $Q = +2/3|e|$ is searched for. When assuming couplings to only the third generation of quarks [9], as favoured by their large masses [10], the three possible decay modes are $T \rightarrow Zt$, $T \rightarrow Ht$, and $T \rightarrow Wb$. For T quark masses above about 0.8 TeV the branching ratios converge to $B(T \rightarrow Wb) \simeq 50\%$ and $B(T \rightarrow Zt) \simeq B(T \rightarrow Ht) \simeq 25\%$ for a weak-isospin singlet model and to $B(T \rightarrow Zt) \simeq B(T \rightarrow Ht) \simeq 50\%$ for a model with a weak-isospin doublet of vector-like quarks. The doublet prediction is valid for a $(X^{5/3}, T)$ doublet, where the superscript refers to the charge of the particle, as well as for a $(T, B^{-1/3})$ doublet, as long as the generalised CKM (Cabibbo-Kobayashi-Maskawa) matrix elements fulfil $|V_{Tb}| \ll |V_{Bt}|$ [9, 11]. In addition to these two models, the case of arbitrary branching ratios of the three possible decay modes is considered.

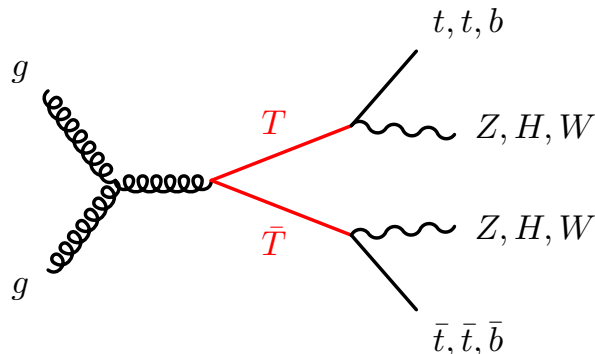


Figure 1: Representative diagram for the production and decay of a vector-like top quark pair.

Vector-like top (VLT) quarks could be produced singly or in pairs at the CERN Large Hadron Collider (LHC) [12]. This analysis targets the pair production $pp \rightarrow T\bar{T}$ channel, as shown in Figure 1. The production cross-section is predicted to be 0.044 ± 0.005 pb for a T quark mass of 1 TeV, calculated at next-to-next-to-leading order (NNLO) in quantum chromodynamics (QCD) including next-to-next-to-leading logarithmic (NNLL) soft-gluon resummation using Top++ 2.0 [13–18]. Previous searches for pair-produced vector-like T quarks by the ATLAS and CMS collaborations at centre-of-mass energies of 8 TeV [19–22] and 13 TeV [23] set lower limits on the VLT mass in the range of 550–900 GeV, at the 95% confidence level (CL), depending on the branching ratio considered.

This analysis focuses on the channel $T\bar{T} \rightarrow Zt + X$, where the Z boson decays into a neutrino pair and exactly one charged lepton is produced in either the top quark decay or from the other leg of the VLT pair de-

cay. This channel gives rise to a final state with one lepton, multiple jets and a high missing transverse momentum (E_T^{miss}) mainly due to the invisibly decaying Z boson. A single-bin signal region (SR) is defined by an event selection that maximises the sensitivity to this particular channel. Control regions (CRs) and validation regions (VRs) are defined that are enriched in the various background processes. They are orthogonal to the SR and orthogonal to each other. The statistical interpretation is based on a simultaneous fit to the CRs and the SR, in which the background normalisations and a possible signal contribution are determined, while taking into account the experimental and theoretical systematic uncertainties.

2 ATLAS detector and data sample

The ATLAS detector [24] is a multi-purpose particle detector at the LHC with nearly 4π coverage around the collision point.¹ Closest to the beam is the inner detector (ID), which provides charged-particle tracking in the range $|\eta| < 2.5$. During the LHC shutdown between Run 1 and Run 2, a new innermost layer of silicon pixels was added, which improves the track impact parameter resolution and vertex position resolution performance [25, 26]. The ID is surrounded by a superconducting solenoid providing a 2 T axial magnetic field, followed by an electromagnetic lead/liquid-argon (LAr) sampling calorimeter and a hadronic (steel/scintillator-tile) calorimeter. The endcap and forward regions are instrumented with LAr calorimeters for both the electromagnetic and hadronic energy measurements up to $|\eta| = 4.9$. The outer part of the detector consists of a muon spectrometer (MS) with high-precision tracking chambers for coverage up to $|\eta| = 2.7$, fast detectors for triggering over $|\eta| < 2.4$, and three large superconducting toroidal magnets with eight coils each. Events are selected by a two-level trigger system consisting of a hardware-based trigger for the first level and a software-based system for the second level [27].

The data used in this analysis were recorded in 2015 and 2016, corresponding to an integrated luminosity of 36.1 fb^{-1} in total, with an uncertainty of 3.2%, derived following a methodology similar to that in Ref. [28]. The data were collected using triggers that select events with high missing transverse momentum, with online thresholds of 70 GeV in 2015 and 90 GeV to 110 GeV in 2016. The triggers have an efficiency greater than 99% for an offline E_T^{miss} requirement of at least 300 GeV.

3 Signal modelling and Monte Carlo simulation

Monte Carlo (MC) simulated events are used for the description of the backgrounds and to model the VLT signals. Signal samples are generated at leading order (LO) with Proros v2.2 [9, 11], interfaced with PYTHIA 8.186 [29] for the parton shower (PS) and hadronisation. The samples are produced assuming vector-like T quark couplings according to the weak-isospin singlet model, but with equal branching ratios into each of the three decay modes (Zt , Ht , Wb). Desired branching ratios are obtained by reweighting the samples based on generator information. To test potential kinematic biases from the assumed couplings, a comparison to a sample in which the T quark is in a weak-isospin doublet was carried out. A slightly higher acceptance is observed in the doublet case. This effect is neglected in the analysis and results in slightly more conservative limits for the doublet model.

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

For the background samples, several matrix element event generators are combined with parton shower and hadronisation programs. POWHEG-Box v2 [30–33] interfaced to PYTHIA v6.428 [34] is used to simulate $t\bar{t}$ production as well as single-top production in association with a W boson, while electroweak t -channel single-top quark events are generated using the POWHEG-Box v1 generator. Events containing W bosons with associated jets (W +jets) are simulated using the SHERPA v2.2.0 event generator [35–37], while for diboson events SHERPA v2.1.1 is used. For the simulation of $t\bar{t}$ events with additional vector bosons ($t\bar{t}+V$) the MADGRAPH5_aMC@NLO v2.3.2 [38] event generator interfaced with PYTHIA 8 is used.

All MC samples are normalised using the highest-order inclusive cross-sections available at $\sqrt{s} = 13$ TeV. The parton distribution function (PDF) sets used are CT10 [39] for the POWHEG-Box and SHERPA v2.1.1 generators, NNPDF 3.0 NNLO [40] for SHERPA v2.2.0, and NNPDF 2.3 LO [41] for PROTONS and MADGRAPH5_aMC@NLO. The samples produced with PROTONS, MADGRAPH5_aMC@NLO and POWHEG-Box use EVTGEN v1.2.0 [42] for the modelling of b -hadron decays. All simulated samples are processed with the full simulation of the ATLAS detector [43] using GEANT 4 [44], and with varying numbers of simulated minimum-bias interactions generated with PYTHIA 8 overlaid on the hard-scattering event to account for the multiple pp interactions in the same or nearby bunch crossings (pile-up). The average number of interactions per bunch crossing in simulation matches the distribution in data. Additional details of the simulation set-up can be found in Refs. [45–48].

4 Event reconstruction and object selection

Events are required to have at least one vertex candidate with at least two tracks with $p_T > 500$ MeV. The primary vertex is taken to be the vertex candidate with the largest sum of squared transverse momenta of all associated tracks. Two sets of quality and kinematic requirements are imposed on physics objects in this analysis, labelled baseline and signal requirements, where the latter label describes a tighter selection than the former.

Electron candidates are reconstructed from cell clusters in the electromagnetic calorimeter which are matched to ID tracks. Baseline electrons are required to have $p_T > 7$ GeV, $|\eta| < 2.47$, and satisfy ‘VeryLoose’ likelihood identification criteria, defined following the methodology described in Ref. [49]. Signal electrons must pass all baseline requirements, have $p_T > 28$ GeV, and satisfy the ‘Tight’ likelihood identification criteria [49]. In addition, the distance of closest approach to the beam in the transverse plane (d_0) and the longitudinal distance of this point to the primary vertex along the beam direction (z_0) are required to satisfy $|z_0 \sin \theta| < 0.5$ mm and $|d_0|/\sigma_{d_0} < 5$, where σ_{d_0} is the uncertainty in d_0 . Furthermore, signal electrons must be isolated, requiring that the scalar p_T sum of all tracks in a cone of size $\Delta R < 10 \text{ GeV}/p_T^e$ around the electron momentum, with a maximum cone size of 0.2, is lower than 6% of the electron p_T .

Muon candidates are reconstructed from combined tracks that are formed from ID and MS tracks, ID tracks matched to MS track segments, standalone MS tracks, or ID tracks matched to a calorimeter energy deposit compatible with a minimum-ionising particle (referred to as calo-tagged muons) [50]. Baseline muons are required to have $p_T > 6$ GeV, $|\eta| < 2.7$, and satisfy the ‘Loose’ identification criteria [50]. Signal muons must satisfy the ‘Medium’ identification criteria, are required to have $p_T > 28$ GeV, and impact parameters $|z_0 \sin \theta| < 0.5$ mm and $|d_0|/\sigma_{d_0} < 3$. In addition, they must be isolated, requiring that the scalar p_T sum of all tracks in a cone of size $\Delta R < 10 \text{ GeV}/p_T^\mu$ around the muon momentum, with a maximum cone size of 0.3, is lower than 6% of the muon p_T .

Jet candidates are reconstructed from topological clusters [51, 52], built from energy deposits in the calorimeters calibrated to the electromagnetic scale, using the anti- k_t algorithm with radius parameter $R = 0.4$ [53]. Baseline (signal) jets are required to have $p_T > 20$ GeV ($p_T > 25$ GeV) and $|\eta| < 4.4$ ($|\eta| < 2.5$). To reject jets originating from pile-up collisions, signal jets with $p_T < 60$ GeV and $|\eta| < 2.4$ are required to satisfy jet vertex tagger criteria [54]. If a baseline jet in an event does not pass the ‘Loose’ jet quality requirements of Ref. [55], the event is vetoed in order to suppress detector noise and non-collision backgrounds [55, 56]. A b -tagging algorithm based on multivariate techniques is used to identify jets containing b -hadrons, so-called b -jets [57, 58]. The working point used provides an average tagging efficiency of 77% for b -jets in simulated $t\bar{t}$ events, as well as a rejection factor of about 130 for light-quark flavour (u, d, s) and gluon jets and about 6 for charm jets.

Jets and associated tracks are also used to identify hadronically decaying τ leptons using the ‘Loose’ identification criteria described in Ref. [59]. The τ candidates are required to have one or three associated tracks, with total electric charge opposite to that of the selected electron or muon, $p_T > 20$ GeV, and $|\eta| < 2.5$.

The missing transverse momentum is reconstructed from the negative vector sum of the transverse momenta of baseline electrons, muons, jets, and a soft-term built from high-quality tracks that are associated with the primary vertex but not with the baseline physics objects [60, 61].

Energy deposits reconstructed as two different particle candidates are resolved by removing one of the candidates according to the following procedure:

1. Electron/jet: if a baseline electron and a baseline jet are found within $\Delta R < 0.2$ the overlapping jet is removed.
2. Muon/jet: if a baseline muon overlaps with a baseline jet within $\Delta R < 0.4$ the overlapping jet is removed if the jet has fewer than three tracks with $p_T > 500$ MeV.
3. Jet/lepton:
 - If a jet that passes the previous steps overlaps with a muon in a cone of size $\Delta R = 0.04 + 10 \text{ GeV}/p_T^\mu$, up to a maximum size of 0.4, the muon is removed.
 - If a jet that passes the previous steps overlaps with an electron in a cone of size $\Delta R = 0.4$, the electron is removed.
4. Electron/ τ : if an electron that passes the previous steps overlaps with a τ candidate in a cone of size $\Delta R = 0.1$, the τ is removed.

Large-radius jets are constructed from signal jets using the anti- k_t algorithm with $R = 1.0$. Constituent small-radius jets with p_T less than 5% of the large-radius jet p_T are removed, mainly in order to reduce the impact of soft radiation.

5 Event selection and background estimation

Events are required to have exactly one signal lepton ($L = e, \mu$), at least four signal jets and $E_T^{\text{miss}} > 300$ GeV. A veto on events with a second lepton, fulfilling the baseline requirements, is used to suppress $t\bar{t}$ events with two leptons in the final state (dileptonic $t\bar{t}$). Further event selection is performed using objects fulfilling the signal requirements described in the previous section. The azimuthal angles between the

missing transverse momentum vector \vec{E}_T^{miss} and both the leading (j_1) and sub-leading (j_2) jets, ordered in p_T , must satisfy the condition $|\Delta\phi(j_i, \vec{E}_T^{\text{miss}})| > 0.4$ with $i \in \{1, 2\}$, which rejects events with E_T^{miss} arising from mismeasured jets. In addition, at least one b -tagged jet is required.

After applying these requirements, the dominant backgrounds are single-lepton plus jets ($1L$) $t\bar{t}$ events, where the lepton originates either directly from the W decay or from a subsequent τ decay, and W +jets production. This can be seen in Figure 2, which shows a comparison of data and SM expectation as a function of E_T^{miss} and m_T^W at the so-called preselection level as defined in Table 1. Here m_T^W is defined as the transverse mass² of the signal lepton and the missing transverse momentum. Requiring m_T^W to be well above the W boson mass strongly reduces $1L$ $t\bar{t}$ events and W +jets production as can be seen from the right panel of Figure 2. The remaining events at large m_T^W are mostly from $t\bar{t}$ production where both W bosons decay leptonically. The two cases of either two leptons ($2L$) and one lepton and a hadronically decaying τ ($1L1\tau$) are shown separately.

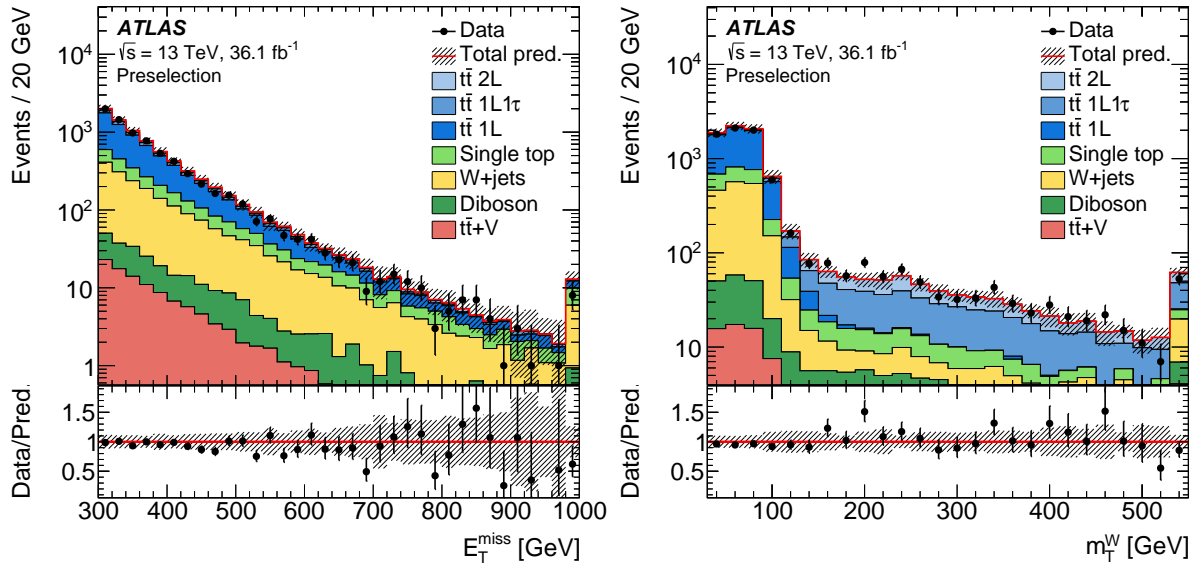


Figure 2: Comparison of data and prediction in the E_T^{miss} distribution (left) and the m_T^W distribution (right) after the preselection. The lower panels show the ratio of the data to the prediction. The error bands include statistical and systematic uncertainties. The last bin contains the overflow events.

Additional variables are used to reduce these dileptonic $t\bar{t}$ backgrounds. The m_{T2} variable [62] is a generalisation of the transverse mass applied to signatures where two or more particles are not directly detected [63, 64], defined as

$$m_{T2} \equiv \min_{\vec{q}_{Ta} + \vec{q}_{Tb} = \vec{E}_T^{\text{miss}}} \{\max(m_{Ta}, m_{Tb})\}.$$

In this formula, m_{Ta} and m_{Tb} are transverse masses calculated using two sets of one or more visible particles, denoted a and b , respectively, and all possible combinations of missing transverse momenta \vec{q}_{Ta} and \vec{q}_{Tb} , with $\vec{q}_{Ta} + \vec{q}_{Tb} = \vec{E}_T^{\text{miss}}$. This analysis uses two specific choices for the sets of visible particles a and b , and the corresponding variables are referred to as am_{T2} and m_{T2}^τ . The am_{T2} variable is used to

² The transverse mass m_T^W is defined as $m_T^W = \sqrt{2p_T^{\text{lep}} E_T^{\text{miss}} [1 - \cos(\Delta\phi)]}$, where $\Delta\phi$ is the azimuthal angle between the lepton and the missing transverse momentum direction and p_T^{lep} is the transverse momentum of the charged lepton.

suppress dileptonic $t\bar{t}$ events where one lepton goes undetected. Thus, the sets of visible particles for the am_{T2} are combinations of the identified lepton and the two jets with the highest b -tagging weights, where the lepton is combined with either jet and the combination with the lowest resulting am_{T2} is taken. For dileptonic $t\bar{t}$ events am_{T2} has a kinematic endpoint at the top quark mass but is expected to extend much higher for processes with additional sources of E_T^{miss} . The m_{T2}^τ variable targets $t\bar{t}$ events where one of the W bosons decays via a hadronically decaying τ . It is only constructed in events where a hadronically decaying τ candidate is found. The τ candidate and the signal lepton are used as the two visible particles. For these events, m_{T2}^τ is required to be greater than 80 GeV as it has a kinematic endpoint at the W boson mass for $t\bar{t}$ events. If fulfilled, the τ candidate is no longer used and instead the jet candidate, from which the τ is identified, is considered for the rest of the computations.

Table 1: Overview of the event selections for the signal region (SR) and the background control regions for $t\bar{t}$ (TCR) and W +jets (WCR) processes. For jet p_T and large-radius jet masses the numbers refer to the objects ordered in p_T .

Variable	Preselection	SR	TCR	WCR
E_T^{miss}	> 300 GeV	> 350 GeV	> 300 GeV	
m_T^W	> 30 GeV	> 170 GeV	$\in [30, 90]$ GeV	
am_{T2}	–	> 175 GeV	> 100 GeV	
m_{T2}^τ	–	> 80 GeV	> 80 GeV	
$H_{T,\text{sig}}^{\text{miss}}$	–	> 12	–	
Jet p_T	> 25 GeV	$> 120, 80, 50, 25$ GeV	$> 120, 80, 50, 25$ GeV	
$ \Delta\phi(j_i, E_T^{\text{miss}}) , i = 1, 2$	> 0.4	> 0.4	> 0.4	
# b -tagged jets	≥ 1	≥ 1	≥ 1	$= 0$
# large-radius jets	–	≥ 2	≥ 2	
Large-radius jet mass	–	$> 80, 60$ GeV	$> 80, 60$ GeV	
Large-radius jet p_T	–	> 290 GeV if $E_T^{\text{miss}} < 450$ GeV > 200 GeV if $E_T^{\text{miss}} > 450$ GeV	> 200 GeV	

The $H_{T,\text{sig}}^{\text{miss}}$ [65] variable is used to reduce the number of events with mis-reconstructed E_T^{miss} . It is defined as $H_{T,\text{sig}}^{\text{miss}} \equiv (H_T^{\text{miss}} - 100 \text{ GeV})/\sigma_{H_T^{\text{miss}}}$, where the exact value of the constant has no impact on this analysis and was optimised for the search mentioned above [66]. Here H_T^{miss} is the magnitude of the vectorial sum of the signal lepton and jets transverse momenta and $\sigma_{H_T^{\text{miss}}}$ is the approximate resolution of H_T^{miss} , computed using the per-event jet energy resolution [67].

5.1 Signal region selection

The signal region selection is optimised to target a benchmark signal with a T quark mass of 1 TeV, a branching ratio for the $T \rightarrow Zt$ decay of 80%, and equal branching ratios for the other two decay modes ($T \rightarrow Ht, T \rightarrow Wb$). This benchmark signal was chosen due to its mass being at the expected sensitivity reach of this analysis, and its high branching ratio into the required Zt decay mode, while at the same time allowing for decays into other final states. A summary of the SR selection is given in Table 1. Due to the invisible decay of the Z boson, a high- E_T^{miss} requirement of at least 350 GeV is set. As discussed above, the m_T^W and am_{T2} variables are used to reduce the $t\bar{t}$ and W +jets backgrounds. The properties of large-radius jets are used to exploit the structure of the high-mass VLT decay. At least two large-radius jets with high p_T and large mass are required. These target a hadronically decaying top quark, or the

subsequent hadronic W boson decay, as well as a second, hadronically decaying massive boson. At very high E_T^{miss} the backgrounds are sufficiently reduced to allow looser requirements on the large-radius jet p_T . For the benchmark signal, 13.4 ± 0.5 events are expected in the SR, with 95% of them containing an invisibly decaying Z boson. This number decreases to 75% for the singlet model with a T quark mass of 1 TeV, where $B(T \rightarrow Zt) \simeq 25\%$. The efficiency of the full event selection for the benchmark signal is 1%, taking all decay modes into account. For events with $Z \rightarrow \nu\bar{\nu}$ and one leptonically decaying W boson from a top quark decay, the selection efficiency is about 10%.

5.2 Background estimation

The dominant background in the SR is due to $t\bar{t}$ production, followed by about equal contributions from W +jets and single-top production. In order to derive the normalisation of the $t\bar{t}$ and W +jets processes from data, dedicated control regions are defined and referred to as TCR and WCR, respectively. The background normalisation and a possible signal contribution are determined simultaneously in a maximum-likelihood fit to the event yields in the signal region and the control regions.

The CRs are defined by modifying the requirement on m_T^W to a window around the W boson mass, ensuring orthogonality between the CRs and the SR. Requirements on E_T^{miss} , am_{T2} , $H_{T,\text{sig}}^{\text{miss}}$ and the large- R jet p_T are loosened in order to increase the statistical power of the CRs. In the W +jets control region, a veto on b -tagged jets is used to enrich the W +jets contribution and make the selection orthogonal to the $t\bar{t}$ control region. Table 1 details the CR selection in comparison to the SR requirements. The normalisation factors, obtained in a fit to the control regions, for $t\bar{t}$ and W +jets are $\mu_{t\bar{t}} = 1.05 \pm 0.17$ and $\mu_{W+\text{jets}} = 0.70 \pm 0.10$, where the error includes both the statistical and systematic uncertainties. Applying these normalisation factors, a comparison of data and simulation in the E_T^{miss} and $H_{T,\text{sig}}^{\text{miss}}$ distributions is shown in both CRs in Figure 3. The normalisation factors, in particular the one for W +jets, are tested further as described in Section 5.3 and Section 6.

The single-top background is taken from simulation. Additional backgrounds considered in the analysis are diboson production as well as $t\bar{t}$ production in association with a vector boson. These backgrounds make a small contribution to the SR and are also taken from simulation. Rare backgrounds, such as the associated production of $t\bar{t}$ with a Higgs boson, contribute less than 1% to the total expected background in the SR and are not considered further. The contribution of multi-jet events is negligible after the requirements on E_T^{miss} and $|\Delta\phi(j_i, \vec{E}_T^{\text{miss}})|$.

5.3 Background validation

The background estimates are tested in validation regions, which are not included in the maximum-likelihood fit. The background normalisation factors determined in the CRs are applied in the VRs. All VRs are defined by requiring exactly one large-radius jet, to ensure orthogonality with the event selection defining the signal and control regions. Furthermore, some SR requirements are relaxed in order to increase the statistical power. Three VRs are defined, for the $t\bar{t}$, single-top and W +jets processes. The definitions are summarised in Table 2. No indication of mismodelling is observed in any of the VRs. For example, the E_T^{miss} and m_T^W distributions are shown in Figure 4.

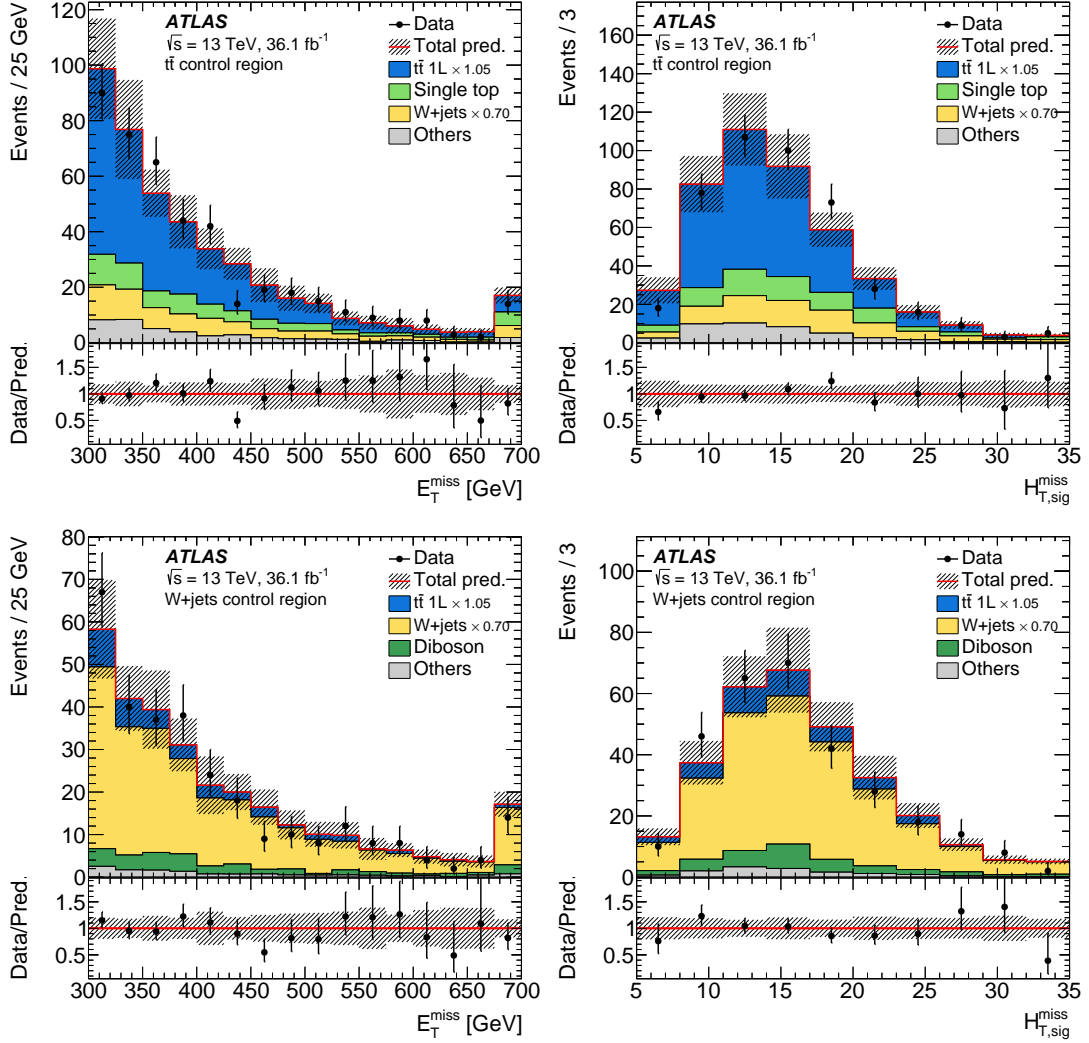


Figure 3: Comparison of data and prediction in the E_T^{miss} distribution (left) and the $H_{T,\text{sig}}^{\text{miss}}$ distribution (right) in the $t\bar{t}$ (top) and the W +jets control regions (bottom). The $t\bar{t}$ and W +jets normalisation factors are applied as indicated in the legend. The lower panels show the ratio of the data to the prediction. The error bands include statistical and systematic uncertainties. The last bin contains the overflow events. For the $H_{T,\text{sig}}^{\text{miss}}$ distributions the first bin also contains underflow events.

6 Systematic uncertainties

Systematic uncertainties from experimental sources and from the theoretical predictions affect the signal and background estimates. They are included as nuisance parameters with Gaussian constraints and are profiled in the likelihood fits that determine the background normalisation factors and the possible signal contribution. The uncertainties are not constrained further in the fits as the analysis has as many bins as free parameters. The uncertainties in the $t\bar{t}$ and W +jets backgrounds in the SR result from the relative difference of each systematic source in the SR to the respective CR due to the normalisation in the fit. In general the systematic uncertainties are smaller than the statistical uncertainties.

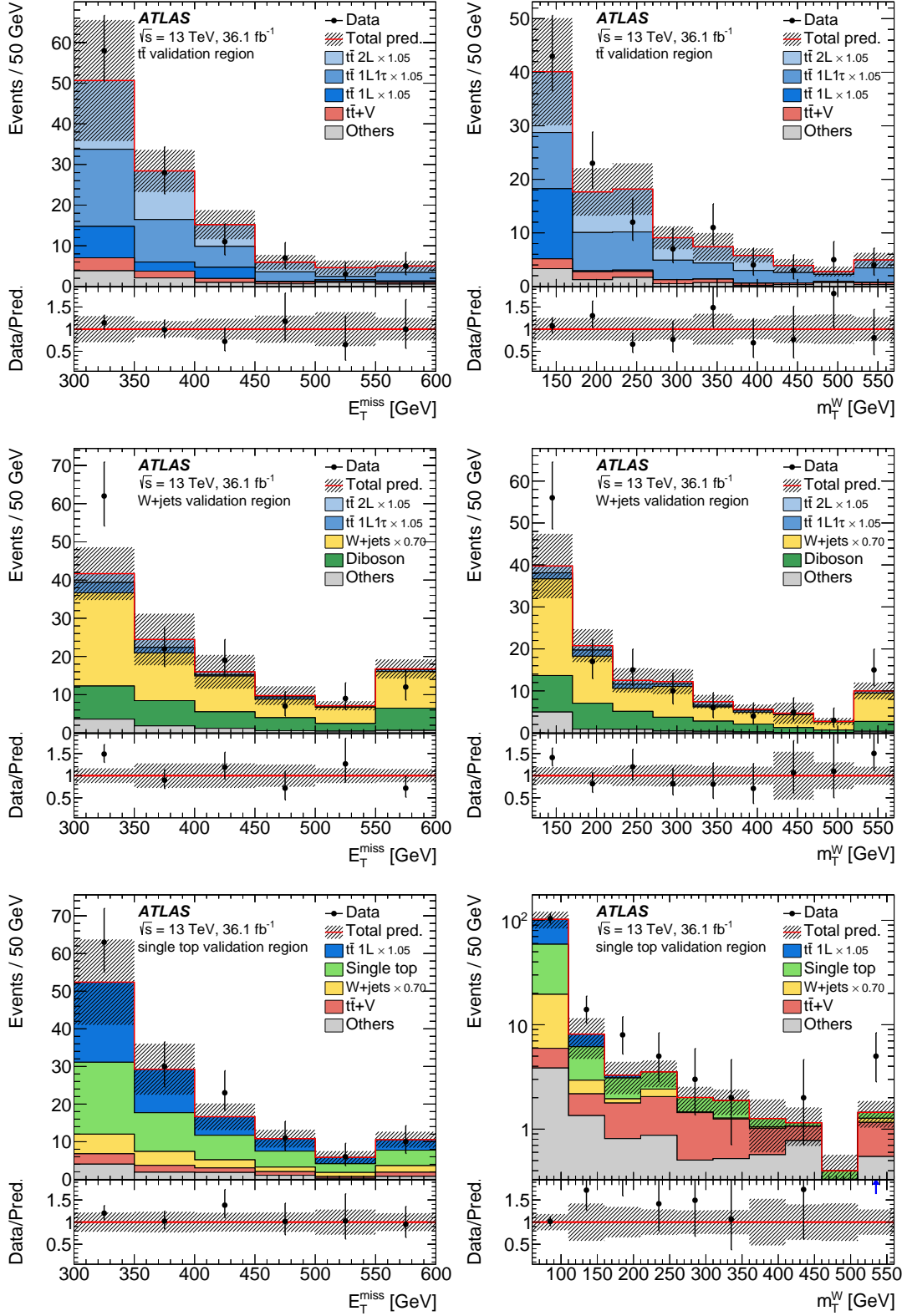


Figure 4: Comparison of data and prediction in the E_T^{miss} distribution (left) and the m_T^W distribution (right) in the $t\bar{t}$ (top), W +jets (middle) and single-top validation regions (bottom). The $t\bar{t}$ and W +jets normalisation factors are applied as indicated in the legend. The lower panels show the ratio of the data to the prediction. The error bands include statistical and systematic uncertainties. The last bin contains the overflow events.

Table 2: Overview of the event selections for the $t\bar{t}$ (TVR), W +jets (WVR) and single-top (STVR) validation regions, compared to the signal region. For jet p_T and large-radius jet masses the numbers refer to the objects ordered in p_T .

Variable	Signal Region	TVR	WVR	STVR
E_T^{miss}	> 350 GeV	> 300 GeV		
m_T^W	> 170 GeV	> 120 GeV		> 60 GeV
am_{T2}	> 175 GeV	$\in [100, 200]$ GeV	> 100 GeV	> 200 GeV
m_{T2}^c	> 80 GeV		> 80 GeV	
$H_{T,\text{sig}}^{\text{miss}}$	> 12	-		
Jet p_T	$> 120, 80, 50, 25$ GeV	$> 120, 80, 50, 25$ GeV		
$ \Delta\phi(j_i, E_T^{\text{miss}}) , i = 1, 2$	> 0.4	> 0.4		
# b -tagged jets	≥ 1	≥ 1	$= 0$	≥ 2
# large-radius jets	≥ 2	$= 1$		
Large-radius jet mass	$> 80, 60$ GeV	> 80 GeV		
Large-radius jet p_T	> 290 GeV if $E_T^{\text{miss}} < 450$ GeV	> 200 GeV		
	> 200 GeV if $E_T^{\text{miss}} > 450$ GeV			

Dominant experimental uncertainties come from imperfect knowledge of the scale and resolution of both jet energies and masses as well as the modelling of the b -tagging efficiency for b -jets, c -jets and light-flavour jets. The jet energy scale uncertainty is split into three components [68]. The relative uncertainty in the estimated background yields in the SR from these sources is 1%–5%. In addition, the uncertainty in the mass scale and the resolution of the small-radius jets is considered. It has a small effect on the background, but affects the signal because hadronically decaying Z and W bosons can be reconstructed as a single small-radius jet. Additional small experimental uncertainties are due to the scale and resolution of the E_T^{miss} soft-term, which captures all tracks not associated with calibrated objects in the event, the modelling of lepton-related quantities, the trigger efficiency, as well as the uncertainty in the integrated luminosity and the pile-up profile.

The uncertainties in the modelling of the $t\bar{t}$ background come from the choice of MC event generator, the hadronisation and fragmentation modelling, and the amount of initial- and final-state radiation. The MC generator uncertainty is estimated by comparing events produced with POWHEG-Box and with MADGRAPH5_aMC@NLO, both in conjunction with Herwig++ [69], and is the dominant uncertainty in the $t\bar{t}$ modelling, amounting to an uncertainty of 17% in the total background yield in the SR. The hadronisation and fragmentation uncertainty is about 13%, assessed by comparing events generated with POWHEG-Box and hadronised with either PYTHIA or Herwig++. POWHEG-Box–PYTHIA samples with different parton-shower radiation settings, different settings of QCD radiation at NLO accuracy, and factorisation and renormalisation scales varied by factors of 0.5 and 2 [47] yield an uncertainty of 11%.

The uncertainty in the modelling of the W +jets process is estimated by comparing the nominal simulation to a MADGRAPH5_aMC@NLO simulation. In addition, the effects of independently varying the scales for the renormalisation, factorisation, and resummation by factors of 0.5 and 2 are taken into account. Also, the scale of the matching scheme related to the merging of matrix elements and parton showers is varied between 15 GeV and 30 GeV. Since the W +jets background is normalised in a CR with a veto on b -tagged jets, additional uncertainties of about 30% in the flavour composition of the W +jets events are applied in all regions requiring at least one b -tagged jet. These uncertainties are based on the measurement reported

Table 3: Breakdown of the leading systematic uncertainties in the total background prediction in the signal region. The statistical precision is included in uncertainties derived from the comparison of MC samples. The individual uncertainties are correlated, and do not necessarily add in quadrature to the total background uncertainty.

Uncertainty	SR
Total background prediction	6.1
Total statistical ($\sqrt{n_{\text{exp}}}$)	± 2.5
Total background uncertainty	± 1.9 [31%]
$t\bar{t}$ MC generator	± 1.1 [17%]
$t\bar{t}$ fragmentation	± 0.8 [14%]
$t\bar{t}$ radiation	± 0.7 [11%]
MC stat. (nominal samples)	± 0.7 [11%]
$t\bar{t}$ Single-top interference	± 0.6 [11%]
Single-top radiation	± 0.4 [6.6%]
$\mu_{t\bar{t}}$	± 0.4 [6.6%]
Diboson fact. scale	± 0.4 [6.5%]
Diboson renorm. scale	± 0.4 [6.1%]
W +jets heavy flavour fraction	± 0.3 [5.3%]
Jet mass resolution	± 0.3 [5.0%]
Diboson resum. scale	± 0.3 [4.7%]
Flavour-tagging light-jet mistag rate	± 0.3 [4.5%]
Single-top fragmentation	± 0.2 [3.5%]
Flavour-tagging c -jet mistag rate	± 0.2 [3.4%]
W +jets MC generator	± 0.2 [3.1%]
$t\bar{t}$ PDF	± 0.2 [2.8%]
$\mu_{W+\text{jets}}$	± 0.2 [2.4%]
W +jets merging scale	± 0.1 [2.4%]
W +jets renorm. scale	± 0.1 [2.3%]
W +jets resum. scale	± 0.1 [2.3%]
W +jets fact. scale	± 0.1 [2.3%]
Jet energy scale (1 st component)	± 0.1 [2.0%]
$t\bar{t} + V$ cross-section	± 0.1 [1.9%]
$t\bar{t} + V$ scale	± 0.1 [1.5%]
Jet energy scale (2 nd component)	± 0.1 [1.4%]
Jet energy resolution	± 0.1 [1.3%]
Trigger efficiency	± 0.1 [1.0%]

in Ref. [70], extrapolated to higher jet multiplicities. As a further check, a region with at least one b -tagged jet is defined, which is enriched in, though not dominated by, the W +jets contribution. Good agreement between data and SM expectation is found when applying the normalisation factors obtained in the CRs. The total uncertainty in the W +jets modelling in the SR is about 40%, resulting in a 6% uncertainty in the total background estimate.

The dominant uncertainty in the single-top processes stems from the modelling of the interference between the $t\bar{t}$ and Wt processes at NLO, leading to an uncertainty of 11% in the total background yield in the SR. The uncertainty is estimated using inclusive $WWbb$ events, generated using MADGRAPH at LO, which are compared with the sum of the $t\bar{t}$ and Wt processes. To account for the different orders in α_s , the number of events in the inclusive $WWbb$ sample is scaled to the sum of the $t\bar{t}$ and Wt events after an event selection requiring only $E_T^{\text{miss}} > 200$ GeV, four jets and exactly one lepton. Uncertainties from the MC event generator, the hadronisation and fragmentation modelling, and the amount of initial- and final-state radiation are estimated in the same way as for $t\bar{t}$. Additionally, the uncertainty in the single-top cross-section is taken into account.

Since the diboson and $t\bar{t} + V$ backgrounds are not normalised in control regions, the analysis is sensitive to their respective cross-section uncertainties. Additionally, the effects of varying the renormalisation, factorisation and resummation scales are taken into account. These uncertainties have a negligible impact on the final results.

The effect of PDF uncertainties on the acceptance for the signal and the $t\bar{t}$ background is included but found to be negligible. A breakdown of the leading systematic uncertainties is summarised in Table 3.

7 Results

The number of events observed in the SR, CRs and the VRs is shown in Table 4, together with the backgrounds estimated in the simultaneous fit. The results are also summarised in the left panel of Figure 5. Good agreement of data and simulation is observed in the VRs. No significant excess above the SM background is found in the SR. The E_T^{miss} distribution in the SR for data and SM expectation is presented in the right panel of Figure 5, where the additional contribution from a T quark signal with a mass of 1.1 TeV is shown. For this particular choice of signal, an additional nine events would be expected. The largest signal contribution is expected at about half the T mass.

Upper limits on the signal cross-section as a function of the VLT mass are derived at 95% CL using profile-likelihood ratio tests following the CL_s prescription [71–73]. They are calculated for the weak-isospin singlet and doublet models, which feature mass-dependent branching ratios [4], as well as for pure $T \rightarrow Zt$ decays, using MC samples generated for 15 different VLT masses between 500 GeV and 1.4 TeV. The contribution from additional vector-like quarks, in particular from the X or B quark in the $(X^{5/3}, T)$ or (T, B) doublets, is neglected. This results in conservative limits in the case of the doublet model, where the X or B quarks are expected to always decay to a Wt final state [9], leading to about 50% more events in the SR for the case of a T quark mass of 1 TeV and a second X or B quark with the same mass. The additional contribution in the TCR is less than 10%.

The cross-section times branching ratio limits as a function of mass are shown in Figure 6 for the pure $T \rightarrow Zt$ decay, as well as for the singlet and doublet cases. Comparing the cross-section limits to the theoretical expectation, lower limits on the T quark mass can be derived. The limits are summarised in

Table 4: Number of events observed in the signal, control and validation regions, together with the estimated SM backgrounds. The normalisation factors determined in the simultaneous fit are applied. The uncertainties include all statistical and systematic sources. The individual uncertainties are correlated, and do not necessarily add in quadrature to the total background uncertainty.

Region	SR	TCR	WCR	TVR	WVR	STVR
Observed events	7	437	303	112	131	143
Fitted bkg events	6.1 ± 1.9	437 ± 21	303 ± 17	109 ± 35	127 ± 31	125 ± 27
Fitted $t\bar{t}$ events	2.5 ± 1.7	280 ± 40	38 ± 15	90 ± 40	15 ± 8	53 ± 23
Fitted W + jets events	1.1 ± 0.7	70 ± 28	224 ± 27	3.5 ± 2.0	77 ± 30	15 ± 7
Fitted singletop events	1.1 ± 0.7	63 ± 24	10 ± 5	4.2 ± 2.6	$3.3^{+3.5}_{-3.3}$	46 ± 17
Fitted $t\bar{t} + V$ events	0.91 ± 0.20	9.7 ± 1.6	1.03 ± 0.30	7.0 ± 1.4	1.9 ± 0.7	8.3 ± 1.4
Fitted diboson events	0.6 ± 0.6	11 ± 5	30 ± 12	1.3 ± 1.3	31 ± 9	1.7 ± 1.1
MC exp. bkg events	6.5	450	398	106	160	129

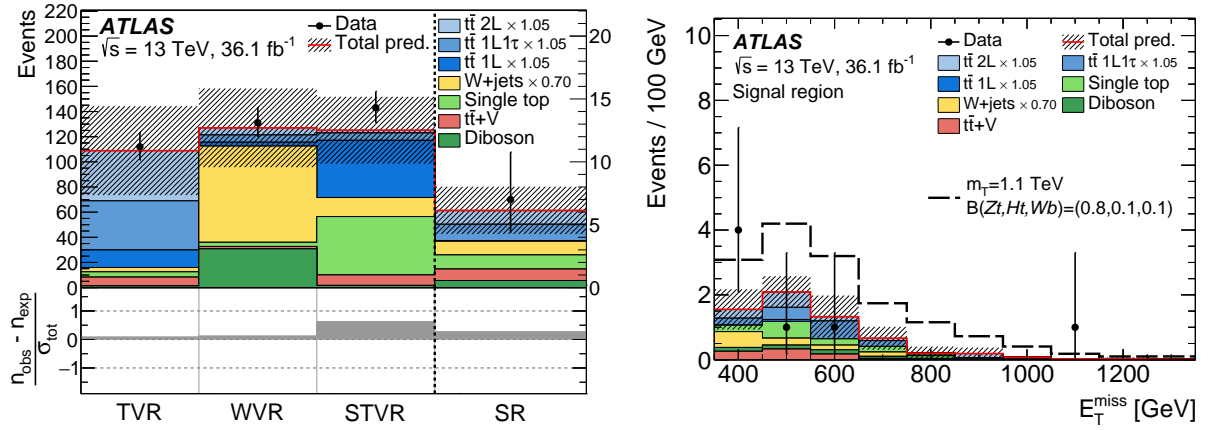


Figure 5: Left panel: Comparison of the observed data (n_{obs}) with the predicted background (n_{exp}) in the VRs and SR. The bottom panel shows the significance of the difference between data and predicted background, where the significance is based on the total uncertainty (σ_{tot}). Right panel: Comparison of data and prediction in the E_T^{miss} distribution in the SR. The error bands include statistical and systematic uncertainties. The expected shape for a signal with $m_T = 1.1$ TeV and $B(T \rightarrow Zt) = 80\%$ is added on top of the SM prediction.

Table 5. The sensitivity to the singlet model is lower due to the low $B(T \rightarrow Zt)$, which approaches 25% in the high-mass limit.

Figure 7 shows the 95% CL observed and expected lower limits on the signal mass as a function of the decay branching ratios. The highest sensitivity is found in the region of $B(T \rightarrow Zt) \approx 100\%$. The sensitivity to the mixed $ZtHt$ decay mode is larger than to the $ZtWb$ decay mode. As an example, masses of $m_T < 1$ TeV are excluded for $B(T \rightarrow Ht) < 65\%$ (70% expected) in the former decay mode and for $B(T \rightarrow Wb) < 45\%$ (50% expected) in the latter.

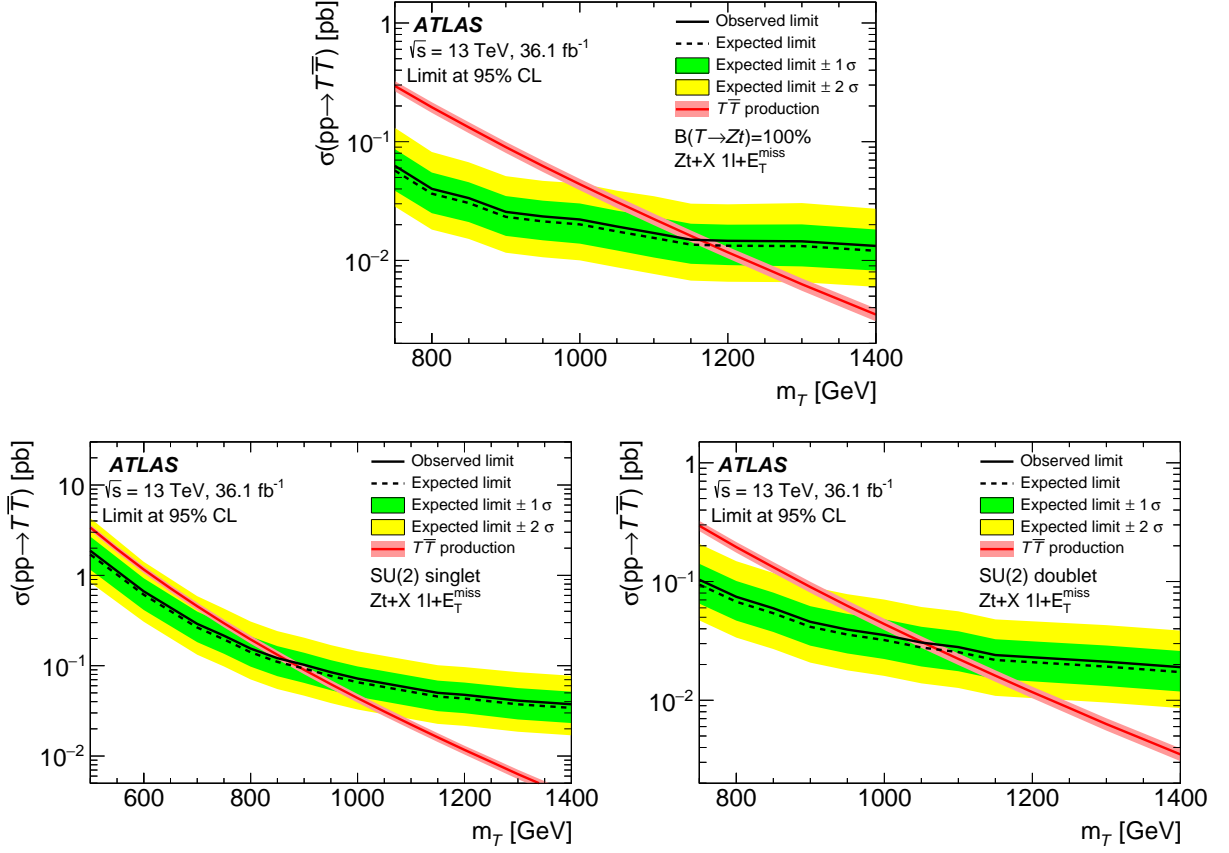


Figure 6: Observed and expected 95% CL upper limit on the cross-section times branching ratio for VLT pair production as a function of the T mass for $B(T \rightarrow Zt) = 100\%$ (top) and for branching ratios according to the singlet model (bottom left) and the doublet model (bottom right). Contributions from the X or B quark in the $(X^{5/3}, T)$ or (T, B) doublet models are neglected, leading to conservative limits. The thickness of the theory curve represents the theoretical uncertainty from PDFs, scale and the strong coupling constant α_s .

Table 5: Observed and expected 95% CL lower limits on the T quark mass for the pure $T \rightarrow Zt$, the singlet model and the doublet model. Contributions from the X or B quark in the $(X^{5/3}, T)$ or (T, B) doublet models are neglected, leading to conservative limits.

Signal	Obs. 95% CL lower mass limit	Exp. 95% CL lower mass limit
$T \rightarrow Zt$	1.16 TeV	1.17 TeV
Singlet	0.87 TeV	0.89 TeV
Doublet	1.05 TeV	1.06 TeV

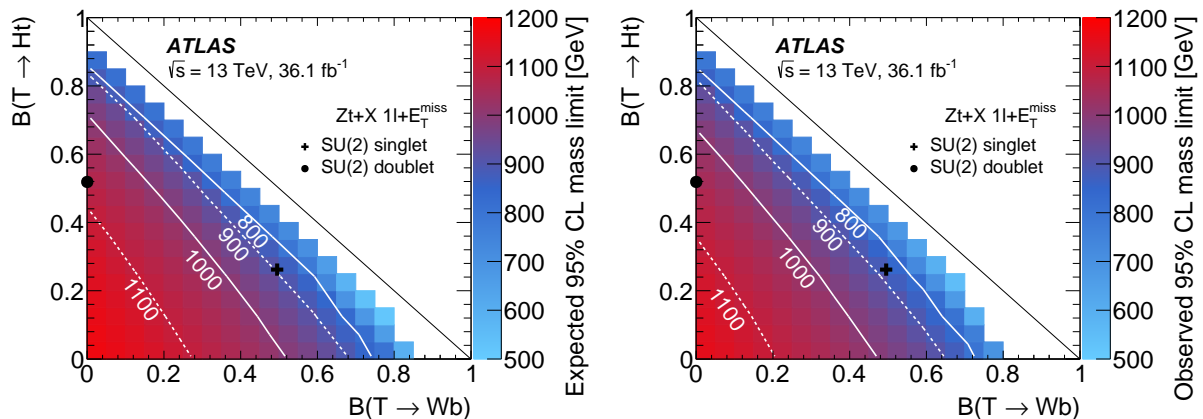


Figure 7: Expected (left) and observed (right) 95% CL lower limit on the T quark mass as a function of the decay branching ratios into Wb and Ht . The markers indicate the branching ratios in the singlet and doublet models for masses above about 0.8 TeV, where they are approximately independent of the T quark mass.

8 Conclusion

A search for the pair production of vector-like top quarks in final states with exactly one lepton, at least four jets and high missing transverse momentum is presented. The analysis follows a cut and count strategy, with a single-bin signal region and dedicated control regions for the $t\bar{t}$ and W +jets backgrounds. The search is based on 36.1 fb^{-1} of $\sqrt{s} = 13 \text{ TeV}$ LHC pp collision data recorded by ATLAS in 2015 and 2016. No significant excess above the SM background is observed in the signal region and 95% CL limits are set on the vector-like top quark mass. For the singlet and doublet models, masses below 870 GeV (890 GeV expected) and 1.05 TeV (1.06 TeV expected), respectively, are excluded. For the pure Zt decay, lower limits are set on the mass at 1.16 TeV (1.17 TeV expected). Limits are also set on the mass as a function of the decay branching ratios, excluding large parts of the parameter space for masses below 1 TeV.

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The ATLAS Collaboration

M. Aaboud^{137d}, G. Aad⁸⁸, B. Abbott¹¹⁵, O. Abidinov^{12,*}, B. Abeloos¹¹⁹, S.H. Abidi¹⁶¹, O.S. AbouZeid¹³⁹, N.L. Abraham¹⁵¹, H. Abramowicz¹⁵⁵, H. Abreu¹⁵⁴, R. Abreu¹¹⁸, Y. Abulaiti^{148a,148b}, B.S. Acharya^{167a,167b,a}, S. Adachi¹⁵⁷, L. Adamczyk^{41a}, J. Adelman¹¹⁰, M. Adersberger¹⁰², T. Adye¹³³, A.A. Affolder¹³⁹, T. Agatonovic-Jovin¹⁴, C. Agheorghiesei^{28c}, J.A. Aguilar-Saavedra^{128a,128f}, S.P. Ahlen²⁴, F. Ahmadov^{68,b}, G. Aielli^{135a,135b}, S. Akatsuka⁷¹, H. Akerstedt^{148a,148b}, T.P.A. Åkesson⁸⁴, E. Akilli⁵², A.V. Akimov⁹⁸, G.L. Alberghi^{22a,22b}, J. Albert¹⁷², P. Albicocco⁵⁰, M.J. Alconada Verzini⁷⁴, S.C. Alderweireldt¹⁰⁸, M. Aleksa³², I.N. Aleksandrov⁶⁸, C. Alexa^{28b}, G. Alexander¹⁵⁵, T. Alexopoulos¹⁰, M. Alhroob¹¹⁵, B. Ali¹³⁰, M. Aliev^{76a,76b}, G. Alimonti^{94a}, J. Alison³³, S.P. Alkire³⁸, B.M.M. Allbrooke¹⁵¹, B.W. Allen¹¹⁸, P.P. Allport¹⁹, A. Aloisio^{106a,106b}, A. Alonso³⁹, F. Alonso⁷⁴, C. Alpigiani¹⁴⁰, A.A. Alshehri⁵⁶, M. Alstaty⁸⁸, B. Alvarez Gonzalez³², D. Álvarez Piqueras¹⁷⁰, M.G. Alvigi^{106a,106b}, B.T. Amadio¹⁶, Y. Amaral Coutinho^{26a}, C. Amelung²⁵, D. Amidei⁹², S.P. Amor Dos Santos^{128a,128c}, A. Amorim^{128a,128b}, S. Amoroso³², G. Amundsen²⁵, C. Anastopoulos¹⁴¹, L.S. Ancu⁵², N. Andari¹⁹, T. Andeen¹¹, C.F. Anders^{60b}, J.K. Anders⁷⁷, K.J. Anderson³³, A. Andreazza^{94a,94b}, V. Andrei^{60a}, S. Angelidakis⁹, I. Angelozzi¹⁰⁹, A. Angerami³⁸, A.V. Anisenkov^{111,c}, N. Anjos¹³, A. Annovi^{126a,126b}, C. Antel^{60a}, M. Antonelli⁵⁰, A. Antonov^{100,*}, D.J. Antrim¹⁶⁶, F. Anulli^{134a}, M. Aoki⁶⁹, L. Aperio Bella³², G. Arabidze⁹³, Y. Arai⁶⁹, J.P. Araque^{128a}, V. Araujo Ferraz^{26a}, A.T.H. Arce⁴⁸, R.E. Ardell⁸⁰, F.A. Arduh⁷⁴, J-F. Arguin⁹⁷, S. Argyropoulos⁶⁶, M. Arik^{20a}, A.J. Armbruster³², L.J. Armitage⁷⁹, O. Arnaez¹⁶¹, H. Arnold⁵¹, M. Arratia³⁰, O. Arslan²³, A. Artamonov⁹⁹, G. Artoni¹²², S. Artz⁸⁶, S. Asai¹⁵⁷, N. Asbah⁴⁵, A. Ashkenazi¹⁵⁵, L. Asquith¹⁵¹, K. Assamagan²⁷, R. Astalos^{146a}, M. Atkinson¹⁶⁹, N.B. Atlay¹⁴³, K. Augsten¹³⁰, G. Avolio³², B. Axen¹⁶, M.K. Ayoub¹¹⁹, G. Azuelos^{97,d}, A.E. Baas^{60a}, M.J. Baca¹⁹, H. Bachacou¹³⁸, K. Bachas^{76a,76b}, M. Backes¹²², M. Backhaus³², P. Bagnaia^{134a,134b}, M. Bahmani⁴², H. Bahrasemani¹⁴⁴, J.T. Baines¹³³, M. Bajic³⁹, O.K. Baker¹⁷⁹, E.M. Baldin^{111,c}, P. Balek¹⁷⁵, F. Balli¹³⁸, W.K. Balunas¹²⁴, E. Banas⁴², A. Bandyopadhyay²³, Sw. Banerjee^{176,e}, A.A.E. Bannoura¹⁷⁸, L. Barak³², E.L. Barberio⁹¹, D. Barberis^{53a,53b}, M. Barbero⁸⁸, T. Barillari¹⁰³, M-S Barisits³², J.T. Barkeloo¹¹⁸, T. Barklow¹⁴⁵, N. Barlow³⁰, S.L. Barnes^{36c}, B.M. Barnett¹³³, R.M. Barnett¹⁶, Z. Barnovska-Blenessy^{36a}, A. Baroncelli^{136a}, G. Barone²⁵, A.J. Barr¹²², L. Barranco Navarro¹⁷⁰, F. Barreiro⁸⁵, J. Barreiro Guimarães da Costa^{35a}, R. Bartoldus¹⁴⁵, A.E. Barton⁷⁵, P. Bartos^{146a}, A. Basalae¹²⁵, A. Bassalat^{119,f}, R.L. Bates⁵⁶, S.J. Batista¹⁶¹, J.R. Batley³⁰, M. Battaglia¹³⁹, M. Bauce^{134a,134b}, F. Bauer¹³⁸, H.S. Bawa^{145,g}, J.B. Beacham¹¹³, M.D. Beattie⁷⁵, T. Beau⁸³, P.H. Beauchemin¹⁶⁵, P. Bechtel²³, H.P. Beck^{18,h}, H.C. Beck⁵⁷, K. Becker¹²², M. Becker⁸⁶, M. Beckingham¹⁷³, C. Becot¹¹², A.J. Beddall^{20e}, A. Beddall^{20b}, V.A. Bednyakov⁶⁸, M. Bedognetti¹⁰⁹, C.P. Bee¹⁵⁰, T.A. Beermann³², M. Begalli^{26a}, M. Begel²⁷, J.K. Behr⁴⁵, A.S. Bell⁸¹, G. Bella¹⁵⁵, L. Bellagamba^{22a}, A. Bellerive³¹, M. Bellomo¹⁵⁴, K. Belotskiy¹⁰⁰, O. Beltramello³², N.L. Belyaev¹⁰⁰, O. Benary^{155,*}, D. Benckekroun^{137a}, M. Bender¹⁰², K. Bendtz^{148a,148b}, N. Benekos¹⁰, Y. Benhammou¹⁵⁵, E. Benhar Nocchioli¹⁷⁹, J. Benitez⁶⁶, D.P. Benjamin⁴⁸, M. Benoit⁵², J.R. Bensinger²⁵, S. Bentvelsen¹⁰⁹, L. Beresford¹²², M. Beretta⁵⁰, D. Berge¹⁰⁹, E. Bergeaas Kuutmann¹⁶⁸, N. Berger⁵, J. Beringer¹⁶, S. Berlendis⁵⁸, N.R. Bernard⁸⁹, G. Bernardi⁸³, C. Bernius¹⁴⁵, F.U. Bernlochner²³, T. Berry⁸⁰, P. Berta¹³¹, C. Bertella^{35a}, G. Bertoli^{148a,148b}, F. Bertolucci^{126a,126b}, I.A. Bertram⁷⁵, C. Bertsche⁴⁵, D. Bertsche¹¹⁵, G.J. Besjes³⁹, O. Bessidskaia Bylund^{148a,148b}, M. Bessner⁴⁵, N. Besson¹³⁸, C. Betancourt⁵¹, A. Bethani⁸⁷, S. Bethke¹⁰³, A.J. Bevan⁷⁹, J. Beyer¹⁰³, R.M. Bianchi¹²⁷, O. Biebel¹⁰², D. Biedermann¹⁷, R. Bielski⁸⁷, K. Bierwagen⁸⁶, N.V. Biesuz^{126a,126b}, M. Biglietti^{136a}, T.R.V. Billoud⁹⁷, H. Bilokon⁵⁰, M. Bindi⁵⁷, A. Bingul^{20b}, C. Bini^{134a,134b}, S. Biondi^{22a,22b}, T. Bisanz⁵⁷, C. Bittrich⁴⁷, D.M. Bjergaard⁴⁸, C.W. Black¹⁵², J.E. Black¹⁴⁵, K.M. Black²⁴, R.E. Blair⁶, T. Blazek^{146a}, I. Bloch⁴⁵, C. Blocker²⁵,

A. Blue⁵⁶, W. Blum^{86,*}, U. Blumenschein⁷⁹, S. Blunier^{34a}, G.J. Bobbink¹⁰⁹, V.S. Bobrovnikov^{111,c},
 S.S. Bocchetta⁸⁴, A. Bocci⁴⁸, C. Bock¹⁰², M. Boehler⁵¹, D. Boerner¹⁷⁸, D. Bogovac¹⁰²,
 A.G. Bogdanchikov¹¹¹, C. Bohm^{148a}, V. Boisvert⁸⁰, P. Bokan^{168,i}, T. Bold^{41a}, A.S. Boldyrev¹⁰¹,
 A.E. Bolz^{60b}, M. Bomben⁸³, M. Bona⁷⁹, M. Boonekamp¹³⁸, A. Borisov¹³², G. Borissov⁷⁵, J. Bortfeldt³²,
 D. Bortoletto¹²², V. Bortolotto^{62a,62b,62c}, D. Boscherini^{22a}, M. Bosman¹³, J.D. Bossio Sola²⁹,
 J. Boudreau¹²⁷, J. Bouffard², E.V. Bouhova-Thacker⁷⁵, D. Boumediene³⁷, C. Bourdarios¹¹⁹,
 S.K. Boutle⁵⁶, A. Boveia¹¹³, J. Boyd³², I.R. Boyko⁶⁸, J. Bracinik¹⁹, A. Brandt⁸, G. Brandt⁵⁷,
 O. Brandt^{60a}, U. Bratzler¹⁵⁸, B. Brau⁸⁹, J.E. Brau¹¹⁸, W.D. Breaden Madden⁵⁶, K. Brendlinger⁴⁵,
 A.J. Brennan⁹¹, L. Brenner¹⁰⁹, R. Brenner¹⁶⁸, S. Bressler¹⁷⁵, D.L. Briglin¹⁹, T.M. Bristow⁴⁹,
 D. Britton⁵⁶, D. Britzger⁴⁵, F.M. Brochu³⁰, I. Brock²³, R. Brock⁹³, G. Brooijmans³⁸, T. Brooks⁸⁰,
 W.K. Brooks^{34b}, J. Brosamer¹⁶, E. Brost¹¹⁰, J.H. Broughton¹⁹, P.A. Bruckman de Renstrom⁴²,
 D. Bruncko^{146b}, A. Bruni^{22a}, G. Bruni^{22a}, L.S. Bruni¹⁰⁹, BH Brunt³⁰, M. Bruschi^{22a}, N. Brusino²³,
 P. Bryant³³, L. Bryngemark⁴⁵, T. Buanes¹⁵, Q. Buat¹⁴⁴, P. Buchholz¹⁴³, A.G. Buckley⁵⁶, I.A. Budagov⁶⁸,
 F. Buehrer⁵¹, M.K. Bugge¹²¹, O. Bulekov¹⁰⁰, D. Bullock⁸, T.J. Burch¹¹⁰, S. Burdin⁷⁷, C.D. Burgard⁵¹,
 A.M. Burger⁵, B. Burghgrave¹¹⁰, K. Burka⁴², S. Burke¹³³, I. Burmeister⁴⁶, J.T.P. Burr¹²², E. Busato³⁷,
 D. Büscher⁵¹, V. Büscher⁸⁶, P. Bussey⁵⁶, J.M. Butler²⁴, C.M. Buttar⁵⁶, J.M. Butterworth⁸¹, P. Butti³²,
 W. Buttinger²⁷, A. Buzatu^{35c}, A.R. Buzykaev^{111,c}, S. Cabrera Urbán¹⁷⁰, D. Caforio¹³⁰,
 V.M. Cairo^{40a,40b}, O. Cakir^{4a}, N. Calace⁵², P. Calafiura¹⁶, A. Calandri⁸⁸, G. Calderini⁸³, P. Calfayan⁶⁴,
 G. Callea^{40a,40b}, L.P. Caloba^{26a}, S. Calvente Lopez⁸⁵, D. Calvet³⁷, S. Calvet³⁷, T.P. Calvet⁸⁸,
 R. Camacho Toro³³, S. Camarda³², P. Camarri^{135a,135b}, D. Cameron¹²¹, R. Caminal Armadans¹⁶⁹,
 C. Camincher⁵⁸, S. Campana³², M. Campanelli⁸¹, A. Camplani^{94a,94b}, A. Campoverde¹⁴³,
 V. Canale^{106a,106b}, M. Cano Bret^{36c}, J. Cantero¹¹⁶, T. Cao¹⁵⁵, M.D.M. Capeans Garrido³², I. Caprini^{28b},
 M. Caprini^{28b}, M. Capua^{40a,40b}, R.M. Carbone³⁸, R. Cardarelli^{135a}, F. Cardillo⁵¹, I. Carli¹³¹, T. Carli³²,
 G. Carlino^{106a}, B.T. Carlson¹²⁷, L. Carminati^{94a,94b}, R.M.D. Carney^{148a,148b}, S. Caron¹⁰⁸, E. Carquin^{34b},
 S. Carrá^{94a,94b}, G.D. Carrillo-Montoya³², J. Carvalho^{128a,128c}, D. Casadei¹⁹, M.P. Casado^{13,j},
 M. Casolino¹³, D.W. Casper¹⁶⁶, R. Castelijin¹⁰⁹, V. Castillo Gimenez¹⁷⁰, N.F. Castro^{128a,k},
 A. Catinaccio³², J.R. Catmore¹²¹, A. Cattai³², J. Caudron²³, V. Cavaliere¹⁶⁹, E. Cavallaro¹³,
 D. Cavalli^{94a}, M. Cavalli-Sforza¹³, V. Cavasinni^{126a,126b}, E. Celebi^{20a}, F. Ceradini^{136a,136b},
 L. Cerda Alberich¹⁷⁰, A.S. Cerqueira^{26b}, A. Cerri¹⁵¹, L. Cerrito^{135a,135b}, F. Cerutti¹⁶, A. Cervelli¹⁸,
 S.A. Cetin^{20d}, A. Chafaq^{137a}, D. Chakraborty¹¹⁰, S.K. Chan⁵⁹, W.S. Chan¹⁰⁹, Y.L. Chan^{62a}, P. Chang¹⁶⁹,
 J.D. Chapman³⁰, D.G. Charlton¹⁹, C.C. Chau¹⁶¹, C.A. Chavez Barajas¹⁵¹, S. Che¹¹³,
 S. Cheatham^{167a,167c}, A. Chegwidan⁹³, S. Chekanov⁶, S.V. Chekulaev^{163a}, G.A. Chelkov^{68,l},
 M.A. Chelstowska³², C. Chen⁶⁷, H. Chen²⁷, S. Chen^{35b}, S. Chen¹⁵⁷, X. Chen^{35c,m}, Y. Chen⁷⁰,
 H.C. Cheng⁹², H.J. Cheng^{35a}, A. Cheplakov⁶⁸, E. Cheremushkina¹³², R. Cherkaoui El Moursli^{137e},
 E. Cheu⁷, K. Cheung⁶³, L. Chevalier¹³⁸, V. Chiarella⁵⁰, G. Chiarelli^{126a,126b}, G. Chiodini^{76a},
 A.S. Chisholm³², A. Chitan^{28b}, Y.H. Chiu¹⁷², M.V. Chizhov⁶⁸, K. Choi⁶⁴, A.R. Chomont³⁷,
 S. Chouridou¹⁵⁶, V. Christodoulou⁸¹, D. Chromek-Burckhart³², M.C. Chu^{62a}, J. Chudoba¹²⁹,
 A.J. Chuinard⁹⁰, J.J. Chwastowski⁴², L. Chytka¹¹⁷, A.K. Ciftci^{4a}, D. Cinca⁴⁶, V. Cindro⁷⁸, I.A. Cioara²³,
 C. Ciocca^{22a,22b}, A. Ciocio¹⁶, F. Ciotto^{106a,106b}, Z.H. Citron¹⁷⁵, M. Citterio^{94a}, M. Ciubancan^{28b},
 A. Clark⁵², B.L. Clark⁵⁹, M.R. Clark³⁸, P.J. Clark⁴⁹, R.N. Clarke¹⁶, C. Clement^{148a,148b}, Y. Coadou⁸⁸,
 M. Cobal^{167a,167c}, A. Cocco⁵², J. Cochran⁶⁷, L. Colasurdo¹⁰⁸, B. Cole³⁸, A.P. Colijn¹⁰⁹, J. Collot⁵⁸,
 T. Colombo¹⁶⁶, P. Conde Muiño^{128a,128b}, E. Coniavitis⁵¹, S.H. Connell^{147b}, I.A. Connelly⁸⁷,
 S. Constantinescu^{28b}, G. Conti³², F. Conventi^{106a,n}, M. Cooke¹⁶, A.M. Cooper-Sarkar¹²², F. Cormier¹⁷¹,
 K.J.R. Cormier¹⁶¹, M. Corradi^{134a,134b}, F. Corriveau^{90,o}, A. Cortes-Gonzalez³², G. Cortiana¹⁰³,
 G. Costa^{94a}, M.J. Costa¹⁷⁰, D. Costanzo¹⁴¹, G. Cottin³⁰, G. Cowan⁸⁰, B.E. Cox⁸⁷, K. Cranmer¹¹²,
 S.J. Crawley⁵⁶, R.A. Creager¹²⁴, G. Cree³¹, S. Crépe-Renaudin⁵⁸, F. Crescioli⁸³, W.A. Cribbs^{148a,148b},
 M. Cristinziani²³, V. Croft¹⁰⁸, G. Crosetti^{40a,40b}, A. Cueto⁸⁵, T. Cuhadar Donszelmann¹⁴¹,

A.R. Cukierman¹⁴⁵, J. Cummings¹⁷⁹, M. Curatolo⁵⁰, J. Cúth⁸⁶, P. Czodrowski³², G. D'amen^{22a,22b},
 S. D'Auria⁵⁶, L. D'eramo⁸³, M. D'Onofrio⁷⁷, M.J. Da Cunha Sargedas De Sousa^{128a,128b}, C. Da Via⁸⁷,
 W. Dabrowski^{41a}, T. Dado^{146a}, T. Dai⁹², O. Dale¹⁵, F. Dallaire⁹⁷, C. Dallapiccola⁸⁹, M. Dam³⁹,
 J.R. Dandoy¹²⁴, M.F. Daneri²⁹, N.P. Dang¹⁷⁶, A.C. Daniells¹⁹, N.S. Dann⁸⁷, M. Danninger¹⁷¹,
 M. Dano Hoffmann¹³⁸, V. Dao¹⁵⁰, G. Darbo^{53a}, S. Darmora⁸, J. Dassoulas³, A. Dattagupta¹¹⁸,
 T. Daubney⁴⁵, W. Davey²³, C. David⁴⁵, T. Davidek¹³¹, D.R. Davis⁴⁸, P. Davison⁸¹, E. Dawe⁹¹,
 I. Dawson¹⁴¹, K. De⁸, R. de Asmundis^{106a}, A. De Benedetti¹¹⁵, S. De Castro^{22a,22b}, S. De Cecco⁸³,
 N. De Groot¹⁰⁸, P. de Jong¹⁰⁹, H. De la Torre⁹³, F. De Lorenzi⁶⁷, A. De Maria⁵⁷, D. De Pedis^{134a},
 A. De Salvo^{134a}, U. De Sanctis^{135a,135b}, A. De Santo¹⁵¹, K. De Vasconcelos Corga⁸⁸,
 J.B. De Vivie De Regie¹¹⁹, W.J. Dearnaley⁷⁵, R. Debbe²⁷, C. Debenedetti¹³⁹, D.V. Dedovich⁶⁸,
 N. Dehghanian³, I. Deigaard¹⁰⁹, M. Del Gaudio^{40a,40b}, J. Del Peso⁸⁵, D. Delgove¹¹⁹, F. Deliot¹³⁸,
 C.M. Delitzsch⁵², A. Dell'Acqua³², L. Dell'Asta²⁴, M. Dell'Orso^{126a,126b}, M. Della Pietra^{106a,106b},
 D. della Volpe⁵², M. Delmastro⁵, C. Delporte¹¹⁹, P.A. Delsart⁵⁸, D.A. DeMarco¹⁶¹, S. Demers¹⁷⁹,
 M. Demichev⁶⁸, A. Demilly⁸³, S.P. Denisov¹³², D. Denysiuk¹³⁸, D. Derendarz⁴², J.E. Derkaoui^{137d},
 F. Derue⁸³, P. Dervan⁷⁷, K. Desch²³, C. Deterre⁴⁵, K. Dette⁴⁶, M.R. Devesa²⁹, P.O. Deviveiros³²,
 A. Dewhurst¹³³, S. Dhaliwal²⁵, F.A. Di Bello⁵², A. Di Ciaccio^{135a,135b}, L. Di Ciaccio⁵,
 W.K. Di Clemente¹²⁴, C. Di Donato^{106a,106b}, A. Di Girolamo³², B. Di Girolamo³², B. Di Micco^{136a,136b},
 R. Di Nardo³², K.F. Di Petrillo⁵⁹, A. Di Simone⁵¹, R. Di Sipio¹⁶¹, D. Di Valentino³¹, C. Diaconu⁸⁸,
 M. Diamond¹⁶¹, F.A. Dias³⁹, M.A. Diaz^{34a}, E.B. Diehl⁹², J. Dietrich¹⁷, S. Díez Cornell⁴⁵,
 A. Dimitrievska¹⁴, J. Dingfelder²³, P. Dita^{28b}, S. Dita^{28b}, F. Dittus³², F. Djama⁸⁸, T. Djobava^{54b},
 J.I. Djuvsland^{60a}, M.A.B. do Vale^{26c}, D. Dobos³², M. Dobre^{28b}, C. Doglioni⁸⁴, J. Dolejsi¹³¹,
 Z. Dolezal¹³¹, M. Donadelli^{26d}, S. Donati^{126a,126b}, P. Dondero^{123a,123b}, J. Donini³⁷, J. Dopke¹³³,
 A. Doria^{106a}, M.T. Dova⁷⁴, A.T. Doyle⁵⁶, E. Drechsler⁵⁷, M. Dris¹⁰, Y. Du^{36b}, J. Duarte-Campderros¹⁵⁵,
 A. Dubreuil⁵², E. Duchovni¹⁷⁵, G. Duckeck¹⁰², A. Ducourthial⁸³, O.A. Ducu^{97,p}, D. Duda¹⁰⁹,
 A. Dudarev³², A.Ch. Dudder⁸⁶, E.M. Duffield¹⁶, L. Dufлот¹¹⁹, M. Dührssen³², M. Dumancic¹⁷⁵,
 A.E. Dumitriu^{28b}, A.K. Duncan⁵⁶, M. Dunford^{60a}, H. Duran Yildiz^{4a}, M. Düren⁵⁵, A. Durglishvili^{54b},
 D. Duschinger⁴⁷, B. Dutta⁴⁵, M. Dyndal⁴⁵, B.S. Dziedzic⁴², C. Eckardt⁴⁵, K.M. Ecker¹⁰³, R.C. Edgar⁹²,
 T. Eifert³², G. Eigen¹⁵, K. Einsweiler¹⁶, T. Ekelof¹⁶⁸, M. El Kacimi^{137c}, R. El Kosseifi⁸⁸,
 V. Ellajosyula⁸⁸, M. Ellert¹⁶⁸, S. Elles⁵, F. Ellinghaus¹⁷⁸, A.A. Elliot¹⁷², N. Ellis³², J. Elmsheuser²⁷,
 M. Elsing³², D. Emelianov¹³³, Y. Enari¹⁵⁷, O.C. Endner⁸⁶, J.S. Ennis¹⁷³, J. Erdmann⁴⁶, A. Ereditato¹⁸,
 M. Ernst²⁷, S. Errede¹⁶⁹, M. Escalier¹¹⁹, C. Escobar¹⁷⁰, B. Esposito⁵⁰, O. Estrada Pastor¹⁷⁰,
 A.I. Etienne¹³⁸, E. Etzion¹⁵⁵, H. Evans⁶⁴, A. Ezhilov¹²⁵, M. Ezzi^{137e}, F. Fabbri^{22a,22b}, L. Fabbri^{22a,22b},
 V. Fabiani¹⁰⁸, G. Facini⁸¹, R.M. Fakhruddinov¹³², S. Falciano^{134a}, R.J. Falla⁸¹, J. Faltova³², Y. Fang^{35a},
 M. Fanti^{94a,94b}, A. Farbin⁸, A. Farilla^{136a}, C. Farina¹²⁷, E.M. Farina^{123a,123b}, T. Faroque⁹³, S. Farrell¹⁶,
 S.M. Farrington¹⁷³, P. Farthouat³², F. Fassi^{137e}, P. Fassnacht³², D. Fassouliotis⁹, M. Faucci Giannelli⁸⁰,
 A. Favareto^{53a,53b}, W.J. Fawcett¹²², L. Fayard¹¹⁹, O.L. Fedin^{125,q}, W. Fedorko¹⁷¹, S. Feigl¹²¹,
 L. Felgioni⁸⁸, C. Feng^{36b}, E.J. Feng³², H. Feng⁹², M.J. Fenton⁵⁶, A.B. Fenyuk¹³², L. Feremenga⁸,
 P. Fernandez Martinez¹⁷⁰, S. Fernandez Perez¹³, J. Ferrando⁴⁵, A. Ferrari¹⁶⁸, P. Ferrari¹⁰⁹, R. Ferrari^{123a},
 D.E. Ferreira de Lima^{60b}, A. Ferrer¹⁷⁰, D. Ferrere⁵², C. Ferretti⁹², F. Fiedler⁸⁶, A. Filipčič⁷⁸,
 M. Filipuzzi⁴⁵, F. Filthaut¹⁰⁸, M. Fincke-Keeler¹⁷², K.D. Finelli¹⁵², M.C.N. Fiolhais^{128a,128c,r},
 L. Fiorini¹⁷⁰, A. Fischer², C. Fischer¹³, J. Fischer¹⁷⁸, W.C. Fisher⁹³, N. Flaschel⁴⁵, I. Fleck¹⁴³,
 P. Fleischmann⁹², R.R.M. Fletcher¹²⁴, T. Flick¹⁷⁸, B.M. Flierl¹⁰², L.R. Flores Castillo^{62a},
 M.J. Flowerdew¹⁰³, G.T. Forcolin⁸⁷, A. Formica¹³⁸, F.A. Förster¹³, A. Forti⁸⁷, A.G. Foster¹⁹,
 D. Fournier¹¹⁹, H. Fox⁷⁵, S. Fracchia¹⁴¹, P. Francavilla⁸³, M. Franchini^{22a,22b}, S. Franchino^{60a},
 D. Francis³², L. Franconi¹²¹, M. Franklin⁵⁹, M. Frate¹⁶⁶, M. Fraternali^{123a,123b}, D. Freeborn⁸¹,
 S.M. Fressard-Batraneanu³², B. Freund⁹⁷, D. Froidevaux³², J.A. Frost¹²², C. Fukunaga¹⁵⁸,
 T. Fusayasu¹⁰⁴, J. Fuster¹⁷⁰, C. Gabaldon⁵⁸, O. Gabizon¹⁵⁴, A. Gabrielli^{22a,22b}, A. Gabrielli¹⁶,

G.P. Gach^{41a}, S. Gadatsch³², S. Gadomski⁸⁰, G. Gagliardi^{53a,53b}, L.G. Gagnon⁹⁷, C. Galea¹⁰⁸, B. Galhardo^{128a,128c}, E.J. Gallas¹²², B.J. Gallop¹³³, P. Gallus¹³⁰, G. Galster³⁹, K.K. Gan¹¹³, S. Ganguly³⁷, Y. Gao⁷⁷, Y.S. Gao^{145.g}, F.M. Garay Walls⁴⁹, C. García¹⁷⁰, J.E. García Navarro¹⁷⁰, J.A. García Pascual^{35a}, M. Garcia-Sciveres¹⁶, R.W. Gardner³³, N. Garelli¹⁴⁵, V. Garonne¹²¹, A. Gascon Bravo⁴⁵, K. Gasnikova⁴⁵, C. Gatti⁵⁰, A. Gaudiello^{53a,53b}, G. Gaudio^{123a}, I.L. Gavrilenko⁹⁸, C. Gay¹⁷¹, G. Gaycken²³, E.N. Gazis¹⁰, C.N.P. Gee¹³³, J. Geisen⁵⁷, M. Geisen⁸⁶, M.P. Geisler^{60a}, K. Gellerstedt^{148a,148b}, C. Gemme^{53a}, M.H. Genest⁵⁸, C. Geng⁹², S. Gentile^{134a,134b}, C. Gentsos¹⁵⁶, S. George⁸⁰, D. Gerbaudo¹³, A. Gershon¹⁵⁵, G. Geßner⁴⁶, S. Ghasemi¹⁴³, M. Ghneimat²³, B. Giacobbe^{22a}, S. Giagu^{134a,134b}, N. Giangiacomi^{22a,22b}, P. Giannetti^{126a,126b}, S.M. Gibson⁸⁰, M. Gignac¹⁷¹, M. Gilchriese¹⁶, D. Gillberg³¹, G. Gilles¹⁷⁸, D.M. Gingrich^{3.d}, N. Giokaris^{9,*}, M.P. Giordani^{167a,167c}, F.M. Giorgi^{22a}, P.F. Giraud¹³⁸, P. Giromini⁵⁹, D. Giugni^{94a}, F. Giuli¹²², C. Giuliani¹⁰³, M. Giulini^{60b}, B.K. Gjelsten¹²¹, S. Gkaitatzis¹⁵⁶, I. Gkialas^{9,s}, E.L. Gkoukousis¹³⁹, P. Gkoutoumis¹⁰, L.K. Gladilin¹⁰¹, C. Glasman⁸⁵, J. Glatzer¹³, P.C.F. Glaysheer⁴⁵, A. Glazov⁴⁵, M. Goblirsch-Kolb²⁵, J. Godlewski⁴², S. Goldfarb⁹¹, T. Golling⁵², D. Golubkov¹³², A. Gomes^{128a,128b,128d}, R. Gonçalo^{128a}, R. Goncalves Gama^{26a}, J. Goncalves Pinto Firmino Da Costa¹³⁸, G. Gonella⁵¹, L. Gonella¹⁹, A. Gongadze⁶⁸, S. González de la Hoz¹⁷⁰, S. Gonzalez-Sevilla⁵², L. Goossens³², P.A. Gorbounov⁹⁹, H.A. Gordon²⁷, I. Gorelov¹⁰⁷, B. Gorini³², E. Gorini^{76a,76b}, A. Gorišek⁷⁸, A.T. Goshaw⁴⁸, C. Gössling⁴⁶, M.I. Gostkin⁶⁸, C.A. Gottardo²³, C.R. Goudet¹¹⁹, D. Goujdami^{137c}, A.G. Goussiou¹⁴⁰, N. Govender^{147b,t}, E. Gozani¹⁵⁴, L. Graber⁵⁷, I. Grabowska-Bold^{41a}, P.O.J. Gradin¹⁶⁸, J. Gramling¹⁶⁶, E. Gramstad¹²¹, S. Grancagnolo¹⁷, V. Gratchev¹²⁵, P.M. Gravila^{28f}, C. Gray⁵⁶, H.M. Gray¹⁶, Z.D. Greenwood^{82,u}, C. Grefe²³, K. Gregersen⁸¹, I.M. Gregor⁴⁵, P. Grenier¹⁴⁵, K. Grevtsov⁵, J. Griffiths⁸, A.A. Grillo¹³⁹, K. Grimm⁷⁵, S. Grinstein^{13,v}, Ph. Gris³⁷, J.-F. Grivaz¹¹⁹, S. Groh⁸⁶, E. Gross¹⁷⁵, J. Grosse-Knetter⁵⁷, G.C. Grossi⁸², Z.J. Grout⁸¹, A. Grummer¹⁰⁷, L. Guan⁹², W. Guan¹⁷⁶, J. Guenther⁶⁵, F. Guescini^{163a}, D. Guest¹⁶⁶, O. Gueta¹⁵⁵, B. Gui¹¹³, E. Guido^{53a,53b}, T. Guillemin⁵, S. Guindon², U. Gul⁵⁶, C. Gumpert³², J. Guo^{36c}, W. Guo⁹², Y. Guo^{36a}, R. Gupta⁴³, S. Gupta¹²², G. Gustavino^{134a,134b}, P. Gutierrez¹¹⁵, N.G. Gutierrez Ortiz⁸¹, C. Gutschow⁸¹, C. Guyot¹³⁸, M.P. Guzik^{41a}, C. Gwenlan¹²², C.B. Gwilliam⁷⁷, A. Haas¹¹², C. Haber¹⁶, H.K. Hadavand⁸, N. Haddad^{137e}, A. Hadeef⁸⁸, S. Hageböck²³, M. Hagihara¹⁶⁴, H. Hakobyan^{180,*}, M. Haleem⁴⁵, J. Haley¹¹⁶, G. Halladjian⁹³, G.D. Hallewell⁸⁸, K. Hamacher¹⁷⁸, P. Hamal¹¹⁷, K. Hamano¹⁷², A. Hamilton^{147a}, G.N. Hamity¹⁴¹, P.G. Hamnett⁴⁵, L. Han^{36a}, S. Han^{35a}, K. Hanagaki^{69,w}, K. Hanawa¹⁵⁷, M. Hance¹³⁹, B. Haney¹²⁴, P. Hanke^{60a}, J.B. Hansen³⁹, J.D. Hansen³⁹, M.C. Hansen²³, P.H. Hansen³⁹, K. Hara¹⁶⁴, A.S. Hard¹⁷⁶, T. Harenberg¹⁷⁸, F. Hariri¹¹⁹, S. Harkusha⁹⁵, R.D. Harrington⁴⁹, P.F. Harrison¹⁷³, N.M. Hartmann¹⁰², M. Hasegawa⁷⁰, Y. Hasegawa¹⁴², A. Hasib⁴⁹, S. Hassani¹³⁸, S. Haug¹⁸, R. Hauser⁹³, L. Hauswald⁴⁷, L.B. Havener³⁸, M. Havranek¹³⁰, C.M. Hawkes¹⁹, R.J. Hawkings³², D. Hayakawa¹⁵⁹, D. Hayden⁹³, C.P. Hays¹²², J.M. Hays⁷⁹, H.S. Hayward⁷⁷, S.J. Haywood¹³³, S.J. Head¹⁹, T. Heck⁸⁶, V. Hedberg⁸⁴, L. Heelan⁸, S. Heer²³, K.K. Heidegger⁵¹, S. Heim⁴⁵, T. Heim¹⁶, B. Heinemann^{45,x}, J.J. Heinrich¹⁰², L. Heinrich¹¹², C. Heinz⁵⁵, J. Hejbal¹²⁹, L. Helary³², A. Held¹⁷¹, S. Hellman^{148a,148b}, C. Helsen³², R.C.W. Henderson⁷⁵, Y. Heng¹⁷⁶, S. Henkelmann¹⁷¹, A.M. Henriques Correia³², S. Henrot-Versille¹¹⁹, G.H. Herbert¹⁷, H. Herde²⁵, V. Herget¹⁷⁷, Y. Hernández Jiménez^{147c}, H. Herr⁸⁶, G. Herten⁵¹, R. Hertenberger¹⁰², L. Hervas³², T.C. Herwig¹²⁴, G.G. Hesketh⁸¹, N.P. Hesse^{163a}, J.W. Hetherly⁴³, S. Higashino⁶⁹, E. Higón-Rodríguez¹⁷⁰, K. Hildebrand³³, E. Hill¹⁷², J.C. Hill³⁰, K.H. Hiller⁴⁵, S.J. Hillier¹⁹, M. Hils⁴⁷, I. Hinchliffe¹⁶, M. Hirose⁵¹, D. Hirschbuehl¹⁷⁸, B. Hiti⁷⁸, O. Hladik¹²⁹, X. Hoad⁴⁹, J. Hobbs¹⁵⁰, N. Hod^{163a}, M.C. Hodgkinson¹⁴¹, P. Hodgson¹⁴¹, A. Hoecker³², M.R. Hoferkamp¹⁰⁷, F. Hoenig¹⁰², D. Hohn²³, T.R. Holmes³³, M. Homann⁴⁶, S. Honda¹⁶⁴, T. Honda⁶⁹, T.M. Hong¹²⁷, B.H. Hooberman¹⁶⁹, W.H. Hopkins¹¹⁸, Y. Horii¹⁰⁵, A.J. Horton¹⁴⁴, J.-Y. Hostachy⁵⁸, S. Hou¹⁵³, A. Hoummada^{137a}, J. Howarth⁸⁷, J. Hoya⁷⁴, M. Hrabovsky¹¹⁷, J. Hrdinka³², I. Hristova¹⁷, J. Hrivnac¹¹⁹, T. Hryn'ova⁵,

A. Hrynevich⁹⁶, P.J. Hsu⁶³, S.-C. Hsu¹⁴⁰, Q. Hu^{36a}, S. Hu^{36c}, Y. Huang^{35a}, Z. Hubacek¹³⁰, F. Hubaut⁸⁸,
 F. Huegging²³, T.B. Huffman¹²², E.W. Hughes³⁸, G. Hughes⁷⁵, M. Huhtinen³², P. Huo¹⁵⁰,
 N. Huseynov^{68,b}, J. Huston⁹³, J. Huth⁵⁹, G. Iacobucci⁵², G. Iakovidis²⁷, I. Ibragimov¹⁴³,
 L. Iconomidou-Fayard¹¹⁹, Z. Idrissi^{137e}, P. Iengo³², O. Igonkina^{109,y}, T. Iizawa¹⁷⁴, Y. Ikegami⁶⁹,
 M. Ikeno⁶⁹, Y. Ilchenko^{11,z}, D. Iliadis¹⁵⁶, N. Ilic¹⁴⁵, G. Introzzi^{123a,123b}, P. Ioannou^{9,*}, M. Iodice^{136a},
 K. Iordanidou³⁸, V. Ippolito⁵⁹, M.F. Isacson¹⁶⁸, N. Ishijima¹²⁰, M. Ishino¹⁵⁷, M. Ishitsuka¹⁵⁹,
 C. Issever¹²², S. Istin^{20a}, F. Ito¹⁶⁴, J.M. Iturbe Ponce^{62a}, R. Iuppa^{162a,162b}, H. Iwasaki⁶⁹, J.M. Izen⁴⁴,
 V. Izzo^{106a}, S. Jabbar³, P. Jackson¹, R.M. Jacobs²³, V. Jain², K.B. Jakobi⁸⁶, K. Jakobs⁵¹, S. Jakobsen⁶⁵,
 T. Jakoubek¹²⁹, D.O. Jamin¹¹⁶, D.K. Jana⁸², R. Jansky⁵², J. Janssen²³, M. Janus⁵⁷, P.A. Janus^{41a},
 G. Jarlskog⁸⁴, N. Javadov^{68,b}, T. Javůrek⁵¹, M. Javurkova⁵¹, F. Jeanneau¹³⁸, L. Jeanty¹⁶, J. Jejelava^{54a,aa},
 A. Jelinskas¹⁷³, P. Jenni^{51,ab}, C. Jeske¹⁷³, S. Jézéquel⁵, H. Ji¹⁷⁶, J. Jia¹⁵⁰, H. Jiang⁶⁷, Y. Jiang^{36a},
 Z. Jiang¹⁴⁵, S. Jiggins⁸¹, J. Jimenez Pena¹⁷⁰, S. Jin^{35a}, A. Jinaru^{28b}, O. Jinnouchi¹⁵⁹, H. Jivan^{147c},
 P. Johansson¹⁴¹, K.A. Johns⁷, C.A. Johnson⁶⁴, W.J. Johnson¹⁴⁰, K. Jon-And^{148a,148b}, R.W.L. Jones⁷⁵,
 S.D. Jones¹⁵¹, S. Jones⁷, T.J. Jones⁷⁷, J. Jongmanns^{60a}, P.M. Jorge^{128a,128b}, J. Jovicevic^{163a}, X. Ju¹⁷⁶,
 A. Juste Rozas^{13,v}, M.K. Köhler¹⁷⁵, A. Kaczmarzka⁴², M. Kado¹¹⁹, H. Kagan¹¹³, M. Kagan¹⁴⁵,
 S.J. Kahn⁸⁸, T. Kaji¹⁷⁴, E. Kajomovitz⁴⁸, C.W. Kalderon⁸⁴, A. Kaluza⁸⁶, S. Kama⁴³,
 A. Kamenshchikov¹³², N. Kanaya¹⁵⁷, L. Kanjir⁷⁸, V.A. Kantserov¹⁰⁰, J. Kanzaki⁶⁹, B. Kaplan¹¹²,
 L.S. Kaplan¹⁷⁶, D. Kar^{147c}, K. Karakostas¹⁰, N. Karastathis¹⁰, M.J. Kareem⁵⁷, E. Karentzos¹⁰,
 S.N. Karpov⁶⁸, Z.M. Karpova⁶⁸, K. Karthik¹¹², V. Kartvelishvili⁷⁵, A.N. Karyukhin¹³², K. Kasahara¹⁶⁴,
 L. Kashif¹⁷⁶, R.D. Kass¹¹³, A. Kastanas¹⁴⁹, Y. Kataoka¹⁵⁷, C. Kato¹⁵⁷, A. Katre⁵², J. Katzy⁴⁵,
 K. Kawade⁷⁰, K. Kawagoe⁷³, T. Kawamoto¹⁵⁷, G. Kawamura⁵⁷, E.F. Kay⁷⁷, V.F. Kazanin^{111,c},
 R. Keeler¹⁷², R. Kehoe⁴³, J.S. Keller³¹, J.J. Kempster⁸⁰, J. Kendrick¹⁹, H. Keoshkerian¹⁶¹, O. Kepka¹²⁹,
 B.P. Kerševan⁷⁸, S. Kersten¹⁷⁸, R.A. Keyes⁹⁰, M. Khader¹⁶⁹, F. Khalil-zada¹², A. Khanov¹¹⁶,
 A.G. Kharlamov^{111,c}, T. Kharlamova^{111,c}, A. Khodinov¹⁶⁰, T.J. Khoo⁵², V. Khovanskiy^{99,*},
 E. Khramov⁶⁸, J. Khubua^{54b,ac}, S. Kido⁷⁰, C.R. Kilby⁸⁰, H.Y. Kim⁸, S.H. Kim¹⁶⁴, Y.K. Kim³³,
 N. Kimura¹⁵⁶, O.M. Kind¹⁷, B.T. King⁷⁷, D. Kirchmeier⁴⁷, J. Kirk¹³³, A.E. Kiryunin¹⁰³,
 T. Kishimoto¹⁵⁷, D. Kisielewska^{41a}, V. Kitali⁴⁵, K. Kiuchi¹⁶⁴, O. Kivernyk⁵, E. Kladiva^{146b},
 T. Klapdor-Kleingrothaus⁵¹, M.H. Klein³⁸, M. Klein⁷⁷, U. Klein⁷⁷, K. Kleinknecht⁸⁶, P. Klimek¹¹⁰,
 A. Klimentov²⁷, R. Klingenberg⁴⁶, T. Klingl²³, T. Klioutchnikova³², E.-E. Kluge^{60a}, P. Kluit¹⁰⁹,
 S. Kluth¹⁰³, E. Kneringer⁶⁵, E.B.F.G. Knoops⁸⁸, A. Knue¹⁰³, A. Kobayashi¹⁵⁷, D. Kobayashi¹⁵⁹,
 T. Kobayashi¹⁵⁷, M. Kobel⁴⁷, M. Kocian¹⁴⁵, P. Kodys¹³¹, T. Koffas³¹, E. Koffeman¹⁰⁹, N.M. Köhler¹⁰³,
 T. Koi¹⁴⁵, M. Kolb^{60b}, I. Koletsou⁵, A.A. Komar^{98,*}, Y. Komori¹⁵⁷, T. Kondo⁶⁹, N. Kondrashova^{36c},
 K. Köneke⁵¹, A.C. König¹⁰⁸, T. Kono^{69,ad}, R. Konoplich^{112,ae}, N. Konstantinidis⁸¹, R. Kopeliansky⁶⁴,
 S. Koperny^{41a}, A.K. Kopp⁵¹, K. Korcyl⁴², K. Kordas¹⁵⁶, A. Korn⁸¹, A.A. Korol^{111,c}, I. Korolkov¹³,
 E.V. Korolkova¹⁴¹, O. Kortner¹⁰³, S. Kortner¹⁰³, T. Kosek¹³¹, V.V. Kostyukhin²³, A. Kotwal⁴⁸,
 A. Koulouris¹⁰, A. Kourkoumeli-Charalampidi^{123a,123b}, C. Kourkoumelis⁹, E. Kourlitis¹⁴¹,
 V. Kouskoura²⁷, A.B. Kowalewska⁴², R. Kowalewski¹⁷², T.Z. Kowalski^{41a}, C. Kozakai¹⁵⁷,
 W. Kozanecki¹³⁸, A.S. Kozhin¹³², V.A. Kramarenko¹⁰¹, G. Kramberger⁷⁸, D. Krasnopevtsev¹⁰⁰,
 M.W. Krasny⁸³, A. Krasznahorkay³², D. Krauss¹⁰³, J.A. Kremer^{41a}, J. Kretschmar⁷⁷, K. Kreutzfeldt⁵⁵,
 P. Krieger¹⁶¹, K. Krizka³³, K. Kroeninger⁴⁶, H. Kroha¹⁰³, J. Kroll¹²⁹, J. Kroll¹²⁴, J. Kroseberg²³,
 J. Krstic¹⁴, U. Kruchonak⁶⁸, H. Krüger²³, N. Krumnack⁶⁷, M.C. Kruse⁴⁸, T. Kubota⁹¹, H. Kucuk⁸¹,
 S. Kудay^{4b}, J.T. Kuechler¹⁷⁸, S. Kuehn³², A. Kugel^{60a}, F. Kuger¹⁷⁷, T. Kuhl⁴⁵, V. Kukhtin⁶⁸, R. Kukla⁸⁸,
 Y. Kulchitsky⁹⁵, S. Kuleshov^{34b}, Y.P. Kulinich¹⁶⁹, M. Kuna^{134a,134b}, T. Kunigo⁷¹, A. Kupco¹²⁹,
 T. Kupfer⁴⁶, O. Kuprash¹⁵⁵, H. Kurashige⁷⁰, L.L. Kurchaninov^{163a}, Y.A. Kurochkin⁹⁵, M.G. Kurth^{35a},
 V. Kus¹²⁹, E.S. Kuwertz¹⁷², M. Kuze¹⁵⁹, J. Kvita¹¹⁷, T. Kwan¹⁷², D. Kyriazopoulos¹⁴¹, A. La Rosa¹⁰³,
 J.L. La Rosa Navarro^{26d}, L. La Rotonda^{40a,40b}, F. La Ruffa^{40a,40b}, C. Lacasta¹⁷⁰, F. Lacava^{134a,134b},
 J. Lacey⁴⁵, H. Lacker¹⁷, D. Lacour⁸³, E. Ladygin⁶⁸, R. Lafaye⁵, B. Laforge⁸³, T. Lagouri¹⁷⁹, S. Lai⁵⁷,

S. Lammers⁶⁴, W. Lampl⁷, E. Lançon²⁷, U. Landgraf⁵¹, M.P.J. Landon⁷⁹, M.C. Lanfermann⁵²,
 V.S. Lang^{60a}, J.C. Lange¹³, R.J. Langenberg³², A.J. Lankford¹⁶⁶, F. Lanni²⁷, K. Lantsch²³,
 A. Lanza^{123a}, A. Lapertosa^{53a,53b}, S. Laplace⁸³, J.F. Laporte¹³⁸, T. Lari^{94a}, F. Lasagni Manghi^{22a,22b},
 M. Lassnig³², P. Laurelli⁵⁰, W. Lavrijsen¹⁶, A.T. Law¹³⁹, P. Laycock⁷⁷, T. Lazovich⁵⁹,
 M. Lazzaroni^{94a,94b}, B. Le⁹¹, O. Le Dortz⁸³, E. Le Guirrec⁸⁸, E.P. Le Quilleuc¹³⁸, M. LeBlanc¹⁷²,
 T. LeCompte⁶, F. Ledroit-Guillon⁵⁸, C.A. Lee²⁷, G.R. Lee^{133,af}, S.C. Lee¹⁵³, L. Lee⁵⁹, B. Lefebvre⁹⁰,
 G. Lefebvre⁸³, M. Lefebvre¹⁷², F. Legger¹⁰², C. Leggett¹⁶, G. Lehmann Miotto³², X. Lei⁷,
 W.A. Leight⁴⁵, M.A.L. Leite^{26d}, R. Leitner¹³¹, D. Lellouch¹⁷⁵, B. Lemmer⁵⁷, K.J.C. Leney⁸¹, T. Lenz²³,
 B. Lenzi³², R. Leone⁷, S. Leone^{126a,126b}, C. Leonidopoulos⁴⁹, G. Lerner¹⁵¹, C. Leroy⁹⁷,
 A.A.J. Lesage¹³⁸, C.G. Lester³⁰, M. Levchenko¹²⁵, J. Levêque⁵, D. Levin⁹², L.J. Levinson¹⁷⁵,
 M. Levy¹⁹, D. Lewis⁷⁹, B. Li^{36a,ag}, Changqiao Li^{36a}, H. Li¹⁵⁰, L. Li^{36c}, Q. Li^{35a}, S. Li⁴⁸, X. Li^{36c},
 Y. Li¹⁴³, Z. Liang^{35a}, B. Liberti^{135a}, A. Liblong¹⁶¹, K. Lie^{62c}, J. Liebal²³, W. Liebig¹⁵, A. Limosani¹⁵²,
 S.C. Lin¹⁸², T.H. Lin⁸⁶, B.E. Lindquist¹⁵⁰, A.E. Lioni⁵², E. Lipeles¹²⁴, A. Lipniacka¹⁵, M. Lisovyi^{60b},
 T.M. Liss^{169,ah}, A. Lister¹⁷¹, A.M. Litke¹³⁹, B. Liu^{153,ai}, H. Liu⁹², H. Liu²⁷, J.K.K. Liu¹²², J. Liu^{36b},
 J.B. Liu^{36a}, K. Liu⁸⁸, L. Liu¹⁶⁹, M. Liu^{36a}, Y.L. Liu^{36a}, Y. Liu^{36a}, M. Livan^{123a,123b}, A. Lleres⁵⁸,
 J. Llorente Merino^{35a}, S.L. Lloyd⁷⁹, C.Y. Lo^{62b}, F. Lo Sterzo¹⁵³, E.M. Lobodzinska⁴⁵, P. Loch⁷,
 F.K. Loebinger⁸⁷, A. Loesle⁵¹, K.M. Loew²⁵, A. Loginov^{179,*}, T. Lohse¹⁷, K. Lohwasser¹⁴¹,
 M. Lokajicek¹²⁹, B.A. Long²⁴, J.D. Long¹⁶⁹, R.E. Long⁷⁵, L. Longo^{76a,76b}, K.A. Looper¹¹³,
 J.A. Lopez^{34b}, D. Lopez Mateos⁵⁹, I. Lopez Paz¹³, A. Lopez Solis⁸³, J. Lorenz¹⁰²,
 N. Lorenzo Martinez⁵, M. Losada²¹, P.J. Lösel¹⁰², X. Lou^{35a}, A. Lounis¹¹⁹, J. Love⁶, P.A. Love⁷⁵,
 H. Lu^{62a}, N. Lu⁹², Y.J. Lu⁶³, H.J. Lubatti¹⁴⁰, C. Luci^{134a,134b}, A. Lucotte⁵⁸, C. Luedtke⁵¹, F. Luehring⁶⁴,
 W. Lukas⁶⁵, L. Luminari^{134a}, O. Lundberg^{148a,148b}, B. Lund-Jensen¹⁴⁹, M.S. Lutz⁸⁹, P.M. Luzi⁸³,
 D. Lynn²⁷, R. Lysak¹²⁹, E. Lytken⁸⁴, F. Lyu^{35a}, V. Lyubushkin⁶⁸, H. Ma²⁷, L.L. Ma^{36b}, Y. Ma^{36b},
 G. Maccarrone⁵⁰, A. Macchiolo¹⁰³, C.M. Macdonald¹⁴¹, B. Maček⁷⁸, J. Machado Miguens^{124,128b},
 D. Madaffari¹⁷⁰, R. Madar³⁷, W.F. Mader⁴⁷, A. Madsen⁴⁵, J. Maeda⁷⁰, S. Maeland¹⁵, T. Maeno²⁷,
 A.S. Maevskiy¹⁰¹, V. Magerl⁵¹, J. Mahlstedt¹⁰⁹, C. Maiani¹¹⁹, C. Maidantchik^{26a}, A.A. Maier¹⁰³,
 T. Maier¹⁰², A. Maio^{128a,128b,128d}, O. Majersky^{146a}, S. Majewski¹¹⁸, Y. Makida⁶⁹, N. Makovec¹¹⁹,
 B. Malaescu⁸³, Pa. Malecki⁴², V.P. Maleev¹²⁵, F. Malek⁵⁸, U. Mallik⁶⁶, D. Malon⁶, C. Malone³⁰,
 S. Maltezos¹⁰, S. Malyukov³², J. Mamuzic¹⁷⁰, G. Mancini⁵⁰, I. Mandić⁷⁸, J. Maneira^{128a,128b},
 L. Manhaes de Andrade Filho^{26b}, J. Manjarres Ramos⁴⁷, K.H. Mankinen⁸⁴, A. Mann¹⁰², A. Manousos³²,
 B. Mansoulie¹³⁸, J.D. Mansour^{35a}, R. Mantifel⁹⁰, M. Mantoani⁵⁷, S. Manzoni^{94a,94b}, L. Mapelli³²,
 G. Marceca²⁹, L. March⁵², L. Marchese¹²², G. Marchiori⁸³, M. Marcisovsky¹²⁹, M. Marjanovic³⁷,
 D.E. Marley⁹², F. Marroquim^{26a}, S.P. Marsden⁸⁷, Z. Marshall¹⁶, M.U.F. Martensson¹⁶⁸,
 S. Marti-Garcia¹⁷⁰, C.B. Martin¹¹³, T.A. Martin¹⁷³, V.J. Martin⁴⁹, B. Martin dit Latour¹⁵,
 M. Martinez^{13,v}, V.I. Martinez Outschoorn¹⁶⁹, S. Martin-Haugh¹³³, V.S. Martoiu^{28b}, A.C. Martyniuk⁸¹,
 A. Marzin³², L. Masetti⁸⁶, T. Mashimo¹⁵⁷, R. Mashinistov⁹⁸, J. Masik⁸⁷, A.L. Maslennikov^{111,c},
 L. Massa^{135a,135b}, P. Mastrandrea⁵, A. Mastroberardino^{40a,40b}, T. Masubuchi¹⁵⁷, P. Mättig¹⁷⁸,
 J. Maurer^{28b}, S.J. Maxfield⁷⁷, D.A. Maximov^{111,c}, R. Mazini¹⁵³, I. Maznas¹⁵⁶, S.M. Mazza^{94a,94b},
 N.C. Mc Fadden¹⁰⁷, G. Mc Goldrick¹⁶¹, S.P. Mc Kee⁹², A. McCarn⁹², R.L. McCarthy¹⁵⁰,
 T.G. McCarthy¹⁰³, L.I. McClymont⁸¹, E.F. McDonald⁹¹, J.A. Mcfayden⁸¹, G. Mchedlidze⁵⁷,
 S.J. McMahan¹³³, P.C. McNamara⁹¹, R.A. McPherson^{172,o}, S. Meehan¹⁴⁰, T.J. Megy⁵¹, S. Mehlhase¹⁰²,
 A. Mehta⁷⁷, T. Meideck⁵⁸, K. Meier^{60a}, B. Meirose⁴⁴, D. Melini^{170,aj}, B.R. Mellado Garcia^{147c},
 J.D. Mellenthin⁵⁷, M. Melo^{146a}, F. Meloni¹⁸, A. Melzer²³, S.B. Menary⁸⁷, L. Meng⁷⁷, X.T. Meng⁹²,
 A. Mengarelli^{22a,22b}, S. Menke¹⁰³, E. Meoni^{40a,40b}, S. Mergelmeyer¹⁷, P. Mermod⁵², L. Merola^{106a,106b},
 C. Meroni^{94a}, F.S. Merritt³³, A. Messina^{134a,134b}, J. Metcalfe⁶, A.S. Mete¹⁶⁶, C. Meyer¹²⁴, J-P. Meyer¹³⁸,
 J. Meyer¹⁰⁹, H. Meyer Zu Theenhausen^{60a}, F. Miano¹⁵¹, R.P. Middleton¹³³, S. Miglioranzi^{53a,53b},
 L. Mijović⁴⁹, G. Mikenberg¹⁷⁵, M. Mikestikova¹²⁹, M. Mikuž⁷⁸, M. Milesi⁹¹, A. Milic¹⁶¹,

D.W. Miller³³, C. Mills⁴⁹, A. Milov¹⁷⁵, D.A. Milstead^{148a,148b}, A.A. Minaenko¹³², Y. Minami¹⁵⁷,
 I.A. Minashvili⁶⁸, A.I. Mincer¹¹², B. Mindur^{41a}, M. Mineev⁶⁸, Y. Minegishi¹⁵⁷, Y. Ming¹⁷⁶, L.M. Mir¹³,
 K.P. Mistry¹²⁴, T. Mitani¹⁷⁴, J. Mitrevski¹⁰², V.A. Mitsou¹⁷⁰, A. Miucci¹⁸, P.S. Miyagawa¹⁴¹,
 A. Mizukami⁶⁹, J.U. Mjörnmark⁸⁴, T. Mkrtchyan¹⁸⁰, M. Mlynarikova¹³¹, T. Moa^{148a,148b},
 K. Mochizuki⁹⁷, P. Mogg⁵¹, S. Mohapatra³⁸, S. Molander^{148a,148b}, R. Moles-Valls²³, R. Monden⁷¹,
 M.C. Mondragon⁹³, K. Mönig⁴⁵, J. Monk³⁹, E. Monnier⁸⁸, A. Montalbano¹⁵⁰, J. Montejo Berlingen³²,
 F. Monticelli⁷⁴, S. Monzani^{94a,94b}, R.W. Moore³, N. Morange¹¹⁹, D. Moreno²¹, M. Moreno Llácer³²,
 P. Morettini^{53a}, S. Morgenstern³², D. Mori¹⁴⁴, T. Mori¹⁵⁷, M. Morii⁵⁹, M. Morinaga¹⁵⁷, V. Morisbak¹²¹,
 A.K. Morley³², G. Mornacchi³², J.D. Morris⁷⁹, L. Morvaj¹⁵⁰, P. Moschovakos¹⁰, M. Mosidze^{54b},
 H.J. Moss¹⁴¹, J. Moss^{145.ak}, K. Motohashi¹⁵⁹, R. Mount¹⁴⁵, E. Mountricha²⁷, E.J.W. Moyses⁸⁹,
 S. Muanza⁸⁸, F. Mueller¹⁰³, J. Mueller¹²⁷, R.S.P. Mueller¹⁰², D. Muenstermann⁷⁵, P. Mullen⁵⁶,
 G.A. Mullier¹⁸, F.J. Munoz Sanchez⁸⁷, W.J. Murray^{173,133}, H. Musheghyan³², M. Muškinja⁷⁸,
 A.G. Myagkov^{132.al}, M. Myska¹³⁰, B.P. Nachman¹⁶, O. Nackenhorst⁵², K. Nagai¹²², R. Nagai^{69.ad},
 K. Nagano⁶⁹, Y. Nagasaka⁶¹, K. Nagata¹⁶⁴, M. Nagel⁵¹, E. Nagy⁸⁸, A.M. Nairz³², Y. Nakahama¹⁰⁵,
 K. Nakamura⁶⁹, T. Nakamura¹⁵⁷, I. Nakano¹¹⁴, R.F. Naranjo Garcia⁴⁵, R. Narayan¹¹,
 D.I. Narrias Villar^{60a}, I. Naryshkin¹²⁵, T. Naumann⁴⁵, G. Navarro²¹, R. Nayyar⁷, H.A. Neal⁹²,
 P.Yu. Nechaeva⁹⁸, T.J. Neep¹³⁸, A. Negri^{123a,123b}, M. Negrini^{22a}, S. Nektarijevic¹⁰⁸, C. Nellist¹¹⁹,
 A. Nelson¹⁶⁶, M.E. Nelson¹²², S. Nemecek¹²⁹, P. Nemethy¹¹², M. Nessi^{32.am}, M.S. Neubauer¹⁶⁹,
 M. Neumann¹⁷⁸, P.R. Newman¹⁹, T.Y. Ng^{62c}, T. Nguyen Manh⁹⁷, R.B. Nickerson¹²², R. Nicolaidou¹³⁸,
 J. Nielsen¹³⁹, V. Nikolaenko^{132.al}, I. Nikolic-Audit⁸³, K. Nikolopoulos¹⁹, J.K. Nilsen¹²¹, P. Nilsson²⁷,
 Y. Ninomiya¹⁵⁷, A. Nisati^{134a}, N. Nishu^{35c}, R. Nisius¹⁰³, I. Nitsche⁴⁶, T. Nitta¹⁷⁴, T. Nobe¹⁵⁷,
 Y. Noguchi⁷¹, M. Nomachi¹²⁰, I. Nomidis³¹, M.A. Nomura²⁷, T. Nooney⁷⁹, M. Nordberg³²,
 N. Norjoharuddeen¹²², O. Novgorodova⁴⁷, S. Nowak¹⁰³, M. Nozaki⁶⁹, L. Nozka¹¹⁷, K. Ntekas¹⁶⁶,
 E. Nurse⁸¹, F. Nuti⁹¹, K. O'connor²⁵, D.C. O'Neil¹⁴⁴, A.A. O'Rourke⁴⁵, V. O'Shea⁵⁶, F.G. Oakham^{31.d},
 H. Oberlack¹⁰³, T. Obermann²³, J. Ocariz⁸³, A. Ochi⁷⁰, I. Ochoa³⁸, J.P. Ochoa-Ricoux^{34a}, S. Oda⁷³,
 S. Odaka⁶⁹, A. Oh⁸⁷, S.H. Oh⁴⁸, C.C. Ohm¹⁶, H. Ohman¹⁶⁸, H. Oide^{53a,53b}, H. Okawa¹⁶⁴,
 Y. Okumura¹⁵⁷, T. Okuyama⁶⁹, A. Olariu^{28b}, L.F. Oleiro Seabra^{128a}, S.A. Olivares Pino⁴⁹,
 D. Oliveira Damazio²⁷, A. Olszewski⁴², J. Olszowska⁴², A. Onofre^{128a,128e}, K. Onogi¹⁰⁵,
 P.U.E. Onyisi^{11.z}, H. Oppen¹²¹, M.J. Oreglia³³, Y. Oren¹⁵⁵, D. Orestano^{136a,136b}, N. Orlando^{62b},
 R.S. Orr¹⁶¹, B. Osculati^{53a,53b,*}, R. Ospanov^{36a}, G. Otero y Garzon²⁹, H. Otono⁷³, M. Ouchrif^{137d},
 F. Ould-Saada¹²¹, A. Ouraou¹³⁸, K.P. Oussoren¹⁰⁹, Q. Ouyang^{35a}, M. Owen⁵⁶, R.E. Owen¹⁹,
 V.E. Ozcan^{20a}, N. Ozturk⁸, K. Pachal¹⁴⁴, A. Pacheco Pages¹³, L. Pacheco Rodriguez¹³⁸,
 C. Padilla Aranda¹³, S. Pagan Griso¹⁶, M. Paganini¹⁷⁹, F. Paige²⁷, G. Palacino⁶⁴, S. Palazzo^{40a,40b},
 S. Palestini³², M. Palka^{41b}, D. Pallin³⁷, E.St. Panagiotopoulou¹⁰, I. Panagoulas¹⁰, C.E. Pandini⁸³,
 J.G. Panduro Vazquez⁸⁰, P. Pani³², S. Panitkin²⁷, D. Pantea^{28b}, L. Paolozzi⁵², Th.D. Papadopoulou¹⁰,
 K. Papageorgiou^{9.s}, A. Paramonov⁶, D. Paredes Hernandez¹⁷⁹, A.J. Parker⁷⁵, M.A. Parker³⁰,
 K.A. Parker⁴⁵, F. Parodi^{53a,53b}, J.A. Parsons³⁸, U. Parzefall⁵¹, V.R. Pascuzzi¹⁶¹, J.M. Pasner¹³⁹,
 E. Pasqualucci^{134a}, S. Passaggio^{53a}, Fr. Pastore⁸⁰, S. Pataraiia⁸⁶, J.R. Pater⁸⁷, T. Pauly³², B. Pearson¹⁰³,
 S. Pedraza Lopez¹⁷⁰, R. Pedro^{128a,128b}, S.V. Peleganchuk^{111.c}, O. Penc¹²⁹, C. Peng^{35a}, H. Peng^{36a},
 J. Penwell⁶⁴, B.S. Peralva^{26b}, M.M. Perego¹³⁸, D.V. Perepelitsa²⁷, F. Peri¹⁷, L. Perini^{94a,94b},
 H. Pernegger³², S. Perrella^{106a,106b}, R. Peschke⁴⁵, V.D. Peshekhonov^{68,*}, K. Peters⁴⁵, R.F.Y. Peters⁸⁷,
 B.A. Petersen³², T.C. Petersen³⁹, E. Petit⁵⁸, A. Petridis¹, C. Petridou¹⁵⁶, P. Petroff¹¹⁹, E. Petrolo^{134a},
 M. Petrov¹²², F. Petrucci^{136a,136b}, N.E. Pettersson⁸⁹, A. Peyaud¹³⁸, R. Pezoa^{34b}, F.H. Phillips⁹³,
 P.W. Phillips¹³³, G. Piacquadio¹⁵⁰, E. Pianori¹⁷³, A. Picazio⁸⁹, E. Piccaro⁷⁹, M.A. Pickering¹²²,
 R. Piegai²⁹, J.E. Pilcher³³, A.D. Pilkington⁸⁷, A.W.J. Pin⁸⁷, M. Pinamonti^{135a,135b}, J.L. Pinfold³,
 H. Pirumov⁴⁵, M. Pitt¹⁷⁵, L. Plazak^{146a}, M.-A. Pleier²⁷, V. Pleskot⁸⁶, E. Plotnikova⁶⁸, D. Pluth⁶⁷,
 P. Podberezko¹¹¹, R. Poettgen^{148a,148b}, R. Poggi^{123a,123b}, L. Poggioli¹¹⁹, D. Pohl²³, G. Polesello^{123a},

A. Poley⁴⁵, A. Policicchio^{40a,40b}, R. Polifka³², A. Polini^{22a}, C.S. Pollard⁵⁶, V. Polychronakos²⁷,
 K. Pommès³², D. Ponomarenko¹⁰⁰, L. Pontecorvo^{134a}, G.A. Popeneciu^{28d}, A. Poppleton³²,
 S. Pospisil¹³⁰, K. Potamianos¹⁶, I.N. Potrap⁶⁸, C.J. Potter³⁰, G. Poulard³², T. Poulsen⁸⁴, J. Poveda³²,
 M.E. Pozo Astigarraga³², P. Pralavorio⁸⁸, A. Pranko¹⁶, S. Prell⁶⁷, D. Price⁸⁷, M. Primavera^{76a},
 S. Prince⁹⁰, N. Proklova¹⁰⁰, K. Prokofiev^{62c}, F. Prokoshin^{34b}, S. Protopopescu²⁷, J. Proudfoot⁶,
 M. Przybycien^{41a}, A. Puri¹⁶⁹, P. Puzo¹¹⁹, J. Qian⁹², G. Qin⁵⁶, Y. Qin⁸⁷, A. Quadt⁵⁷,
 M. Queitsch-Maitland⁴⁵, D. Quilty⁵⁶, S. Raddum¹²¹, V. Radeka²⁷, V. Radescu¹²²,
 S.K. Radhakrishnan¹⁵⁰, P. Radloff¹¹⁸, P. Rados⁹¹, F. Ragusa^{94a,94b}, G. Rahal¹⁸¹, J.A. Raine⁸⁷,
 S. Rajagopalan²⁷, C. Rangel-Smith¹⁶⁸, T. Rashid¹¹⁹, S. Raspopov⁵, M.G. Ratti^{94a,94b}, D.M. Rauch⁴⁵,
 F. Rauscher¹⁰², S. Rave⁸⁶, I. Ravinovich¹⁷⁵, J.H. Rawling⁸⁷, M. Raymond³², A.L. Read¹²¹,
 N.P. Radoiff⁵⁸, M. Reale^{76a,76b}, D.M. Rebuffi^{123a,123b}, A. Redelbach¹⁷⁷, G. Redlinger²⁷, R. Reece¹³⁹,
 R.G. Reed^{147c}, K. Reeves⁴⁴, L. Rehnisch¹⁷, J. Reichert¹²⁴, A. Reiss⁸⁶, C. Rembser³², H. Ren^{35a},
 M. Rescigno^{134a}, S. Resconi^{94a}, E.D. Resseguie¹²⁴, S. Rettie¹⁷¹, E. Reynolds¹⁹, O.L. Rezanova^{111,c},
 P. Reznicek¹³¹, R. Rezvani⁹⁷, R. Richter¹⁰³, S. Richter⁸¹, E. Richter-Was^{41b}, O. Ricken²³, M. Ridel⁸³,
 P. Rieck¹⁰³, C.J. Riegel¹⁷⁸, J. Rieger⁵⁷, O. Rifki¹¹⁵, M. Rijssenbeek¹⁵⁰, A. Rimoldi^{123a,123b},
 M. Rimoldi¹⁸, L. Rinaldi^{22a}, G. Ripellino¹⁴⁹, B. Ristic³², E. Ritsch³², I. Riu¹³, F. Rizatdinova¹¹⁶,
 E. Rizvi⁷⁹, C. Rizzi¹³, R.T. Roberts⁸⁷, S.H. Robertson^{90,o}, A. Robichaud-Veronneau⁹⁰, D. Robinson³⁰,
 J.E.M. Robinson⁴⁵, A. Robson⁵⁶, E. Rocco⁸⁶, C. Roda^{126a,126b}, Y. Rodina^{88,an}, S. Rodriguez Bosca¹⁷⁰,
 A. Rodriguez Perez¹³, D. Rodriguez Rodriguez¹⁷⁰, S. Roe³², C.S. Rogan⁵⁹, O. Röhne¹²¹, J. Roloff⁵⁹,
 A. Romaniouk¹⁰⁰, M. Romano^{22a,22b}, S.M. Romano Saez³⁷, E. Romero Adam¹⁷⁰, N. Rompotis⁷⁷,
 M. Ronzani⁵¹, L. Roos⁸³, S. Rosati^{134a}, K. Rosbach⁵¹, P. Rose¹³⁹, N.-A. Rosien⁵⁷, E. Rossi^{106a,106b},
 L.P. Rossi^{53a}, J.H.N. Rosten³⁰, R. Rosten¹⁴⁰, M. Rotaru^{28b}, J. Rothberg¹⁴⁰, D. Rousseau¹¹⁹,
 A. Rozanov⁸⁸, Y. Rozen¹⁵⁴, X. Ruan^{147c}, F. Rubbo¹⁴⁵, F. Rühr⁵¹, A. Ruiz-Martinez³¹, Z. Rurikova⁵¹,
 N.A. Rusakovich⁶⁸, H.L. Russell⁹⁰, J.P. Rutherford⁷, N. Ruthmann³², Y.F. Ryabov¹²⁵, M. Rybar¹⁶⁹,
 G. Rybkin¹¹⁹, S. Ryu⁶, A. Ryzhov¹³², G.F. Rzehorz⁵⁷, A.F. Saavedra¹⁵², G. Sabato¹⁰⁹, S. Sacerdoti²⁹,
 H.F-W. Sadrozinski¹³⁹, R. Sadykov⁶⁸, F. Safai Tehrani^{134a}, P. Saha¹¹⁰, M. Sahinsoy^{60a}, M. Saimpert⁴⁵,
 M. Saito¹⁵⁷, T. Saito¹⁵⁷, H. Sakamoto¹⁵⁷, Y. Sakurai¹⁷⁴, G. Salamanna^{136a,136b}, J.E. Salazar Loyola^{34b},
 D. Salek¹⁰⁹, P.H. Sales De Bruin¹⁶⁸, D. Salihagic¹⁰³, A. Salnikov¹⁴⁵, J. Salt¹⁷⁰, D. Salvatore^{40a,40b},
 F. Salvatore¹⁵¹, A. Salvucci^{62a,62b,62c}, A. Salzburger³², D. Sammel⁵¹, D. Sampsonidis¹⁵⁶,
 D. Sampsonidou¹⁵⁶, J. Sánchez¹⁷⁰, V. Sanchez Martinez¹⁷⁰, A. Sanchez Pineda^{167a,167c}, H. Sandaker¹²¹,
 R.L. Sandbach⁷⁹, C.O. Sander⁴⁵, M. Sandhoff¹⁷⁸, C. Sandoval²¹, D.P.C. Sankey¹³³, M. Sannino^{53a,53b},
 Y. Sano¹⁰⁵, A. Sansoni⁵⁰, C. Santoni³⁷, H. Santos^{128a}, I. Santoyo Castillo¹⁵¹, A. Saponov⁶⁸,
 J.G. Saraiva^{128a,128d}, B. Sarrazin²³, O. Sasaki⁶⁹, K. Sato¹⁶⁴, E. Sauvan⁵, G. Savage⁸⁰, P. Savard^{161,d},
 N. Savic¹⁰³, C. Sawyer¹³³, L. Sawyer^{82,u}, J. Saxon³³, C. Sbarra^{22a}, A. Sbrizzi^{22a,22b}, T. Scanlon⁸¹,
 D.A. Scannicchio¹⁶⁶, M. Scarcella¹⁵², J. Schaarschmidt¹⁴⁰, P. Schacht¹⁰³, B.M. Schachtner¹⁰²,
 D. Schaefer³², L. Schaefer¹²⁴, R. Schaefer⁴⁵, J. Schaeffer⁸⁶, S. Schaepe²³, S. Schaezel^{160b}, U. Schäfer⁸⁶,
 A.C. Schaffer¹¹⁹, D. Schaile¹⁰², R.D. Chamberger¹⁵⁰, V.A. Schegelsky¹²⁵, D. Scheirich¹³¹,
 M. Schernau¹⁶⁶, C. Schiavi^{53a,53b}, S. Schier¹³⁹, L.K. Schildgen²³, C. Schillo⁵¹, M. Schioppa^{40a,40b},
 S. Schlenker³², K.R. Schmidt-Sommerfeld¹⁰³, K. Schmieden³², C. Schmitt⁸⁶, S. Schmitt⁴⁵,
 S. Schmitz⁸⁶, U. Schnoor⁵¹, L. Schoeffel¹³⁸, A. Schoening^{60b}, B.D. Schoenrock⁹³, E. Schopf²³,
 M. Schott⁸⁶, J.F.P. Schouwenberg¹⁰⁸, J. Schovancova³², S. Schramm⁵², N. Schuh⁸⁶, A. Schulte⁸⁶,
 M.J. Schultens²³, H.-C. Schultz-Coulon^{60a}, H. Schulz¹⁷, M. Schumacher⁵¹, B.A. Schumm¹³⁹,
 Ph. Schune¹³⁸, A. Schwartzman¹⁴⁵, T.A. Schwarz⁹², H. Schweiger⁸⁷, Ph. Schwemling¹³⁸,
 R. Schwienhorst⁹³, J. Schwindling¹³⁸, A. Sciandra²³, G. Sciolla²⁵, M. Scornajenghi^{40a,40b},
 F. Scuri^{126a,126b}, F. Scutti⁹¹, J. Searcy⁹², P. Seema²³, S.C. Seidel¹⁰⁷, A. Seiden¹³⁹, J.M. Seixas^{26a},
 G. Sekhniadze^{106a}, K. Sekhon⁹², S.J. Sekula⁴³, N. Semprini-Cesari^{22a,22b}, S. Senkin³⁷, C. Serfon¹²¹,
 L. Serin¹¹⁹, L. Serkin^{167a,167b}, M. Sessa^{136a,136b}, R. Seuster¹⁷², H. Severini¹¹⁵, T. Sfiligoj⁷⁸, F. Sforza³²,

A. Sfyrla⁵², E. Shabalina⁵⁷, N.W. Shaikh^{148a,148b}, L.Y. Shan^{35a}, R. Shang¹⁶⁹, J.T. Shank²⁴, M. Shapiro¹⁶,
 P.B. Shatalov⁹⁹, K. Shaw^{167a,167b}, S.M. Shaw⁸⁷, A. Shcherbakova^{148a,148b}, C.Y. Shehu¹⁵¹, Y. Shen¹¹⁵,
 N. Sherafati³¹, P. Sherwood⁸¹, L. Shi^{153,ao}, S. Shimizu⁷⁰, C.O. Shimmin¹⁷⁹, M. Shimojima¹⁰⁴,
 I.P.J. Shipsey¹²², S. Shirabe⁷³, M. Shiyakova^{68,ap}, J. Shlomi¹⁷⁵, A. Shmeleva⁹⁸, D. Shoaleh Saadi⁹⁷,
 M.J. Shochet³³, S. Shojaii^{94a}, D.R. Shope¹¹⁵, S. Shrestha¹¹³, E. Shulga¹⁰⁰, M.A. Shupe⁷, P. Sicho¹²⁹,
 A.M. Sickles¹⁶⁹, P.E. Sidebo¹⁴⁹, E. Sideras Haddad^{147c}, O. Sidiropoulou¹⁷⁷, A. Sidoti^{22a,22b}, F. Siegert⁴⁷,
 Dj. Sijacki¹⁴, J. Silva^{128a,128d}, S.B. Silverstein^{148a}, V. Simak¹³⁰, Lj. Simic¹⁴, S. Simion¹¹⁹, E. Simioni⁸⁶,
 B. Simmons⁸¹, M. Simon⁸⁶, P. Sinervo¹⁶¹, N.B. Sinev¹¹⁸, M. Sioli^{22a,22b}, G. Siragusa¹⁷⁷, I. Siral⁹²,
 S.Yu. Sivoklov¹⁰¹, J. Sjölin^{148a,148b}, M.B. Skinner⁷⁵, P. Skubic¹¹⁵, M. Slater¹⁹, T. Slavicek¹³⁰,
 M. Slawinska⁴², K. Sliwa¹⁶⁵, R. Slovak¹³¹, V. Smakhtin¹⁷⁵, B.H. Smart⁵, J. Smiesko^{146a}, N. Smirnov¹⁰⁰,
 S.Yu. Smirnov¹⁰⁰, Y. Smirnov¹⁰⁰, L.N. Smirnova^{101,aa}, O. Smirnova⁸⁴, J.W. Smith⁵⁷, M.N.K. Smith³⁸,
 R.W. Smith³⁸, M. Smizanska⁷⁵, K. Smolek¹³⁰, A.A. Snesarev⁹⁸, I.M. Snyder¹¹⁸, S. Snyder²⁷,
 R. Sobie^{172,o}, F. Socher⁴⁷, A. Soffer¹⁵⁵, A. Søggaard⁴⁹, D.A. Soh¹⁵³, G. Sokhrannyi⁷⁸,
 C.A. Solans Sanchez³², M. Solar¹³⁰, E.Yu. Soldatov¹⁰⁰, U. Soldevila¹⁷⁰, A.A. Solodkov¹³²,
 A. Soloshenko⁶⁸, O.V. Solovyanov¹³², V. Solovyev¹²⁵, P. Sommer⁵¹, H. Son¹⁶⁵, A. Sopczak¹³⁰,
 D. Sosa^{60b}, C.L. Sotiropoulou^{126a,126b}, R. Soualah^{167a,167c}, A.M. Soukharev^{111,c}, D. South⁴⁵,
 B.C. Sowden⁸⁰, S. Spagnolo^{76a,76b}, M. Spalla^{126a,126b}, M. Spangenberg¹⁷³, F. Spanò⁸⁰, D. Sperlich¹⁷,
 F. Spettel¹⁰³, T.M. Spieker^{60a}, R. Spighi^{22a}, G. Spigo³², L.A. Spiller⁹¹, M. Spousta¹³¹, R.D. St. Denis^{56,*},
 A. Stabile^{94a}, R. Stamen^{60a}, S. Stamm¹⁷, E. Stanecka⁴², R.W. Stanek⁶, C. Stanescu^{136a},
 M.M. Stanitzki⁴⁵, B.S. Stapf¹⁰⁹, S. Stapnes¹²¹, E.A. Starchenko¹³², G.H. Stark³³, J. Stark⁵⁸, S.H. Stark³⁹,
 P. Staroba¹²⁹, P. Starovoitov^{60a}, S. Stärz³², R. Staszewski⁴², P. Steinberg²⁷, B. Stelzer¹⁴⁴, H.J. Stelzer³²,
 O. Stelzer-Chilton^{163a}, H. Stenzel⁵⁵, G.A. Stewart⁵⁶, M.C. Stockton¹¹⁸, M. Stoebe⁹⁰, G. Stoica^{28b},
 P. Stolte⁵⁷, S. Stonjek¹⁰³, A.R. Stradling⁸, A. Straessner⁴⁷, M.E. Stramaglia¹⁸, J. Strandberg¹⁴⁹,
 S. Strandberg^{148a,148b}, M. Strauss¹¹⁵, P. Strizenec^{146b}, R. Ströhmer¹⁷⁷, D.M. Strom¹¹⁸, R. Stroynowski⁴³,
 A. Strubig⁴⁹, S.A. Stucci²⁷, B. Stugu¹⁵, N.A. Styles⁴⁵, D. Su¹⁴⁵, J. Su¹²⁷, S. Suchek^{60a}, Y. Sugaya¹²⁰,
 M. Suk¹³⁰, V.V. Sulin⁹⁸, DMS Sultan^{162a,162b}, S. Sultansoy^{4c}, T. Sumida⁷¹, S. Sun⁵⁹, X. Sun³,
 K. Suruliz¹⁵¹, C.J.E. Suster¹⁵², M.R. Sutton¹⁵¹, S. Suzuki⁶⁹, M. Svatos¹²⁹, M. Swiatlowski³³,
 S.P. Swift², I. Sykora^{146a}, T. Sykora¹³¹, D. Ta⁵¹, K. Tackmann⁴⁵, J. Taenzer¹⁵⁵, A. Taffard¹⁶⁶,
 R. Tafirout^{163a}, N. Taiblum¹⁵⁵, H. Takai²⁷, R. Takashima⁷², E.H. Takasugi¹⁰³, T. Takeshita¹⁴²,
 Y. Takubo⁶⁹, M. Talby⁸⁸, A.A. Talyshev^{111,c}, J. Tanaka¹⁵⁷, M. Tanaka¹⁵⁹, R. Tanaka¹¹⁹, S. Tanaka⁶⁹,
 R. Tanioka⁷⁰, B.B. Tannenwald¹¹³, S. Tapia Araya^{34b}, S. Tapprogge⁸⁶, S. Tarem¹⁵⁴, G.F. Tartarelli^{94a},
 P. Tas¹³¹, M. Tasevsky¹²⁹, T. Tashiro⁷¹, E. Tassi^{40a,40b}, A. Tavares Delgado^{128a,128b}, Y. Tayalati^{137e},
 A.C. Taylor¹⁰⁷, G.N. Taylor⁹¹, P.T.E. Taylor⁹¹, W. Taylor^{163b}, P. Teixeira-Dias⁸⁰, D. Temple¹⁴⁴,
 H. Ten Kate³², P.K. Teng¹⁵³, J.J. Teoh¹²⁰, F. Tepel¹⁷⁸, S. Terada⁶⁹, K. Terashi¹⁵⁷, J. Terron⁸⁵, S. Terzo¹³,
 M. Testa⁵⁰, R.J. Teuscher^{161,o}, T. Theveneaux-Pelzer⁸⁸, F. Thiele³⁹, J.P. Thomas¹⁹, J. Thomas-Wilsker⁸⁰,
 P.D. Thompson¹⁹, A.S. Thompson⁵⁶, L.A. Thomsen¹⁷⁹, E. Thomson¹²⁴, M.J. Tibbetts¹⁶,
 R.E. Ticse Torres⁸⁸, V.O. Tikhomirov^{98,ar}, Yu.A. Tikhonov^{111,c}, S. Timoshenko¹⁰⁰, P. Tipton¹⁷⁹,
 S. Tisserant⁸⁸, K. Todome¹⁵⁹, S. Todorova-Nova⁵, S. Todt⁴⁷, J. Tojo⁷³, S. Tokár^{146a}, K. Tokushuku⁶⁹,
 E. Tolley⁵⁹, L. Tomlinson⁸⁷, M. Tomoto¹⁰⁵, L. Tompkins^{145,as}, K. Toms¹⁰⁷, B. Tong⁵⁹, P. Tornambe⁵¹,
 E. Torrence¹¹⁸, H. Torres¹⁴⁴, E. Torró Pastor¹⁴⁰, J. Toth^{88,at}, F. Touchard⁸⁸, D.R. Tovey¹⁴¹,
 C.J. Treado¹¹², T. Trefzger¹⁷⁷, F. Tresoldi¹⁵¹, A. Tricoli²⁷, I.M. Trigger^{163a}, S. Trincav-Duvoid⁸³,
 M.F. Tripiana¹³, W. Trischuk¹⁶¹, B. Trocmé⁵⁸, A. Trofymov⁴⁵, C. Troncon^{94a}, M. Trotter-McDonald¹⁶,
 M. Trovatelli¹⁷², L. Truong^{147b}, M. Trzebinski⁴², A. Trzupek⁴², K.W. Tsang^{62a}, J.C.-L. Tseng¹²²,
 P.V. Tsiarehka⁹⁵, G. Tsiapolitis¹⁰, N. Tsirintanis⁹, S. Tsiskaridze¹³, V. Tsiskaridze⁵¹,
 E.G. Tskhadadze^{54a}, K.M. Tsui^{62a}, I.I. Tsukerman⁹⁹, V. Tsulaia¹⁶, S. Tsuno⁶⁹, D. Tsybychev¹⁵⁰,
 Y. Tu^{62b}, A. Tudorache^{28b}, V. Tudorache^{28b}, T.T. Tulbure^{28a}, A.N. Tuna⁵⁹, S.A. Tuppuri^{22a,22b},
 S. Turchikhin⁶⁸, D. Turgeman¹⁷⁵, I. Turk Cakir^{4b,au}, R. Turra^{94a}, P.M. Tuts³⁸, G. Ucchielli^{22a,22b},

I. Ueda⁶⁹, M. Ughetto^{148a,148b}, F. Ukegawa¹⁶⁴, G. Unal³², A. Undrus²⁷, G. Unel¹⁶⁶, F.C. Ungaro⁹¹,
 Y. Unno⁶⁹, C. Unverdorben¹⁰², J. Urban^{146b}, P. Urquijo⁹¹, P. Urrejola⁸⁶, G. Usai⁸, J. Usui⁶⁹,
 L. Vacavant⁸⁸, V. Vacek¹³⁰, B. Vachon⁹⁰, K.O.H. Vadla¹²¹, A. Vaidya⁸¹, C. Valderanis¹⁰²,
 E. Valdes Santurio^{148a,148b}, S. Valentinetti^{22a,22b}, A. Valero¹⁷⁰, L. Valéry¹³, S. Valkar¹³¹, A. Vallier⁵,
 J.A. Valls Ferrer¹⁷⁰, W. Van Den Wollenberg¹⁰⁹, H. van der Graaf¹⁰⁹, P. van Gemmeren⁶,
 J. Van Nieuwkoop¹⁴⁴, I. van Vulpen¹⁰⁹, M.C. van Woerden¹⁰⁹, M. Vanadia^{135a,135b}, W. Vandelli³²,
 A. Vaniachine¹⁶⁰, P. Vankov¹⁰⁹, G. Vardanyan¹⁸⁰, R. Vari^{134a}, E.W. Varnes⁷, C. Varni^{53a,53b}, T. Varol⁴³,
 D. Varouchas¹¹⁹, A. Vartapetian⁸, K.E. Varvell¹⁵², J.G. Vasquez¹⁷⁹, G.A. Vasquez^{34b}, F. Vazeille³⁷,
 T. Vazquez Schroeder⁹⁰, J. Veatch⁵⁷, V. Veeraraghavan⁷, L.M. Veloce¹⁶¹, F. Veloso^{128a,128c},
 S. Veneziano^{134a}, A. Ventura^{76a,76b}, M. Venturi¹⁷², N. Venturi³², A. Venturini²⁵, V. Vercesi^{123a},
 M. Verducci^{136a,136b}, W. Verkerke¹⁰⁹, A.T. Vermeulen¹⁰⁹, J.C. Vermeulen¹⁰⁹, M.C. Vetterli^{144,d},
 N. Viaux Maira^{34b}, O. Viazlo⁸⁴, I. Vichou^{169,*}, T. Vickey¹⁴¹, O.E. Vickey Boeriu¹⁴¹,
 G.H.A. Viehhauser¹²², S. Viel¹⁶, L. Vigani¹²², M. Villa^{22a,22b}, M. Villaplana Perez^{94a,94b}, E. Vilucchi⁵⁰,
 M.G. Vincter³¹, V.B. Vinogradov⁶⁸, A. Vishwakarma⁴⁵, C. Vittori^{22a,22b}, I. Vivarelli¹⁵¹, S. Vlachos¹⁰,
 M. Vogel¹⁷⁸, P. Vokac¹³⁰, G. Volpi^{126a,126b}, H. von der Schmitt¹⁰³, E. von Toerne²³, V. Vorobel¹³¹,
 K. Vorobev¹⁰⁰, M. Vos¹⁷⁰, R. Voss³², J.H. Vosseveld⁷⁷, N. Vranjes¹⁴, M. Vranjes Milosavljevic¹⁴,
 V. Vrba¹³⁰, M. Vreeswijk¹⁰⁹, R. Vuillermet³², I. Vukotic³³, P. Wagner²³, W. Wagner¹⁷⁸,
 J. Wagner-Kuhr¹⁰², H. Wahlberg⁷⁴, S. Wahrmund⁴⁷, J. Wakabayashi¹⁰⁵, J. Walder⁷⁵, R. Walker¹⁰²,
 W. Walkowiak¹⁴³, V. Wallangen^{148a,148b}, C. Wang^{35b}, C. Wang^{36b,aw}, F. Wang¹⁷⁶, H. Wang¹⁶, H. Wang³,
 J. Wang⁴⁵, J. Wang¹⁵², Q. Wang¹¹⁵, R. Wang⁶, S.M. Wang¹⁵³, T. Wang³⁸, W. Wang^{153,aw}, W. Wang^{36a},
 Z. Wang^{36c}, C. Wanotayaroj¹¹⁸, A. Warburton⁹⁰, C.P. Ward³⁰, D.R. Wardrope⁸¹, A. Washbrook⁴⁹,
 P.M. Watkins¹⁹, A.T. Watson¹⁹, M.F. Watson¹⁹, G. Watts¹⁴⁰, S. Watts⁸⁷, B.M. Waugh⁸¹, A.F. Webb¹¹,
 S. Webb⁸⁶, M.S. Weber¹⁸, S.W. Weber¹⁷⁷, S.A. Weber³¹, J.S. Webster⁶, A.R. Weidberg¹²², B. Weinert⁶⁴,
 J. Weingarten⁵⁷, M. Weirich⁸⁶, C. Weiser⁵¹, H. Weits¹⁰⁹, P.S. Wells³², T. Wenaus²⁷, T. Wengler³²,
 S. Wenig³², N. Wermes²³, M.D. Werner⁶⁷, P. Werner³², M. Wessels^{60a}, K. Whalen¹¹⁸, N.L. Whallon¹⁴⁰,
 A.M. Wharton⁷⁵, A.S. White⁹², A. White⁸, M.J. White¹, R. White^{34b}, D. Whiteson¹⁶⁶,
 B.W. Whitmore⁷⁵, F.J. Wickens¹³³, W. Wiedenmann¹⁷⁶, M. Wielers¹³³, C. Wiglesworth³⁹,
 L.A.M. Wiik-Fuchs⁵¹, A. Wildauer¹⁰³, F. Wilk⁸⁷, H.G. Wilkens³², H.H. Williams¹²⁴, S. Williams¹⁰⁹,
 C. Willis⁹³, S. Willocq⁸⁹, J.A. Wilson¹⁹, I. Wingerter-Seez⁵, E. Winkels¹⁵¹, F. Winklmeier¹¹⁸,
 O.J. Winston¹⁵¹, B.T. Winter²³, M. Wittgen¹⁴⁵, M. Wobisch^{82,u}, T.M.H. Wolf¹⁰⁹, R. Wolff⁸⁸,
 M.W. Wolter⁴², H. Wolters^{128a,128c}, V.W.S. Wong¹⁷¹, S.D. Worm¹⁹, B.K. Wosiek⁴², J. Wotschack³²,
 K.W. Wozniak⁴², M. Wu³³, S.L. Wu¹⁷⁶, X. Wu⁵², Y. Wu⁹², T.R. Wyatt⁸⁷, B.M. Wynne⁴⁹, S. Xella³⁹,
 Z. Xi⁹², L. Xia^{35c}, D. Xu^{35a}, L. Xu²⁷, T. Xu¹³⁸, B. Yabsley¹⁵², S. Yacoob^{147a}, D. Yamaguchi¹⁵⁹,
 Y. Yamaguchi¹²⁰, A. Yamamoto⁶⁹, S. Yamamoto¹⁵⁷, T. Yamanaka¹⁵⁷, M. Yamatani¹⁵⁷, K. Yamauchi¹⁰⁵,
 Y. Yamazaki⁷⁰, Z. Yan²⁴, H. Yang^{36c}, H. Yang¹⁶, Y. Yang¹⁵³, Z. Yang¹⁵, W-M. Yao¹⁶, Y.C. Yap⁸³,
 Y. Yasu⁶⁹, E. Yatsenko⁵, K.H. Yau Wong²³, J. Ye⁴³, S. Ye²⁷, I. Yeletsikh⁶⁸, E. Yigitbasi²⁴,
 E. Yildirim⁸⁶, K. Yorita¹⁷⁴, K. Yoshihara¹²⁴, C. Young¹⁴⁵, C.J.S. Young³², J. Yu⁸, J. Yu⁶⁷, S.P.Y. Yuen²³,
 I. Yusuff^{30,ax}, B. Zabinski⁴², G. Zacharis¹⁰, R. Zaidan¹³, A.M. Zaitsev^{132,al}, N. Zakharchuk⁴⁵,
 J. Zalieckas¹⁵, A. Zaman¹⁵⁰, S. Zambito⁵⁹, D. Zanzi⁹¹, C. Zeitnitz¹⁷⁸, G. Zemaityte¹²², A. Zemla^{41a},
 J.C. Zeng¹⁶⁹, Q. Zeng¹⁴⁵, O. Zenin¹³², T. Ženiš^{146a}, D. Zerwas¹¹⁹, D. Zhang⁹², F. Zhang¹⁷⁶,
 G. Zhang^{36a,ay}, H. Zhang^{35b}, J. Zhang⁶, L. Zhang⁵¹, L. Zhang^{36a}, M. Zhang¹⁶⁹, P. Zhang^{35b}, R. Zhang²³,
 R. Zhang^{36a,av}, X. Zhang^{36b}, Y. Zhang^{35a}, Z. Zhang¹¹⁹, X. Zhao⁴³, Y. Zhao^{36b,az}, Z. Zhao^{36a},
 A. Zhemchugov⁶⁸, B. Zhou⁹², C. Zhou¹⁷⁶, L. Zhou⁴³, M. Zhou^{35a}, M. Zhou¹⁵⁰, N. Zhou^{35c},
 C.G. Zhu^{36b}, H. Zhu^{35a}, J. Zhu⁹², Y. Zhu^{36a}, X. Zhuang^{35a}, K. Zhukov⁹⁸, A. Zibell¹⁷⁷, D. Zieminska⁶⁴,
 N.I. Zimine⁶⁸, C. Zimmermann⁸⁶, S. Zimmermann⁵¹, Z. Zinonos¹⁰³, M. Zinser⁸⁶, M. Ziolkowski¹⁴³,
 L. Živković¹⁴, G. Zobernig¹⁷⁶, A. Zoccoli^{22a,22b}, R. Zou³³, M. zur Nedden¹⁷, L. Zwalinski³².

- ¹ Department of Physics, University of Adelaide, Adelaide, Australia
- ² Physics Department, SUNY Albany, Albany NY, United States of America
- ³ Department of Physics, University of Alberta, Edmonton AB, Canada
- ⁴ ^(a) Department of Physics, Ankara University, Ankara; ^(b) Istanbul Aydin University, Istanbul; ^(c) Division of Physics, TOBB University of Economics and Technology, Ankara, Turkey
- ⁵ LAPP, CNRS/IN2P3 and Université Savoie Mont Blanc, Annecy-le-Vieux, France
- ⁶ High Energy Physics Division, Argonne National Laboratory, Argonne IL, United States of America
- ⁷ Department of Physics, University of Arizona, Tucson AZ, United States of America
- ⁸ Department of Physics, The University of Texas at Arlington, Arlington TX, United States of America
- ⁹ Physics Department, National and Kapodistrian University of Athens, Athens, Greece
- ¹⁰ Physics Department, National Technical University of Athens, Zografou, Greece
- ¹¹ Department of Physics, The University of Texas at Austin, Austin TX, United States of America
- ¹² Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan
- ¹³ Institut de Física d'Altes Energies (IFAE), The Barcelona Institute of Science and Technology, Barcelona, Spain
- ¹⁴ Institute of Physics, University of Belgrade, Belgrade, Serbia
- ¹⁵ Department for Physics and Technology, University of Bergen, Bergen, Norway
- ¹⁶ Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley CA, United States of America
- ¹⁷ Department of Physics, Humboldt University, Berlin, Germany
- ¹⁸ Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland
- ¹⁹ School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom
- ²⁰ ^(a) Department of Physics, Bogazici University, Istanbul; ^(b) Department of Physics Engineering, Gaziantep University, Gaziantep; ^(d) Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul; ^(e) Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey
- ²¹ Centro de Investigaciones, Universidad Antonio Narino, Bogota, Colombia
- ²² ^(a) INFN Sezione di Bologna; ^(b) Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy
- ²³ Physikalisches Institut, University of Bonn, Bonn, Germany
- ²⁴ Department of Physics, Boston University, Boston MA, United States of America
- ²⁵ Department of Physics, Brandeis University, Waltham MA, United States of America
- ²⁶ ^(a) Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro; ^(b) Electrical Circuits Department, Federal University of Juiz de Fora (UFJF), Juiz de Fora; ^(c) Federal University of Sao Joao del Rei (UFSJ), Sao Joao del Rei; ^(d) Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil
- ²⁷ Physics Department, Brookhaven National Laboratory, Upton NY, United States of America
- ²⁸ ^(a) Transilvania University of Brasov, Brasov; ^(b) Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest; ^(c) Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi; ^(d) National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj Napoca; ^(e) University Politehnica Bucharest, Bucharest; ^(f) West University in Timisoara, Timisoara, Romania
- ²⁹ Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina
- ³⁰ Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
- ³¹ Department of Physics, Carleton University, Ottawa ON, Canada
- ³² CERN, Geneva, Switzerland
- ³³ Enrico Fermi Institute, University of Chicago, Chicago IL, United States of America

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

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

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

- Rabat; ^(c) Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech; ^(d) Faculté des Sciences, Université Mohamed Premier and LTPM, Oujda; ^(e) Faculté des sciences, Université Mohammed V, Rabat, Morocco
- ¹³⁸ DSM/IRFU (Institut de Recherches sur les Lois Fondamentales de l'Univers), CEA Saclay (Commissariat à l'Energie Atomique et aux Energies Alternatives), Gif-sur-Yvette, France
- ¹³⁹ Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA, United States of America
- ¹⁴⁰ Department of Physics, University of Washington, Seattle WA, United States of America
- ¹⁴¹ Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom
- ¹⁴² Department of Physics, Shinshu University, Nagano, Japan
- ¹⁴³ Department Physik, Universität Siegen, Siegen, Germany
- ¹⁴⁴ Department of Physics, Simon Fraser University, Burnaby BC, Canada
- ¹⁴⁵ SLAC National Accelerator Laboratory, Stanford CA, United States of America
- ¹⁴⁶ ^(a) Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava; ^(b) Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic
- ¹⁴⁷ ^(a) Department of Physics, University of Cape Town, Cape Town; ^(b) Department of Physics, University of Johannesburg, Johannesburg; ^(c) School of Physics, University of the Witwatersrand, Johannesburg, South Africa
- ¹⁴⁸ ^(a) Department of Physics, Stockholm University; ^(b) The Oskar Klein Centre, Stockholm, Sweden
- ¹⁴⁹ Physics Department, Royal Institute of Technology, Stockholm, Sweden
- ¹⁵⁰ Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook NY, United States of America
- ¹⁵¹ Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom
- ¹⁵² School of Physics, University of Sydney, Sydney, Australia
- ¹⁵³ Institute of Physics, Academia Sinica, Taipei, Taiwan
- ¹⁵⁴ Department of Physics, Technion: Israel Institute of Technology, Haifa, Israel
- ¹⁵⁵ Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel
- ¹⁵⁶ Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
- ¹⁵⁷ International Center for Elementary Particle Physics and Department of Physics, The University of Tokyo, Tokyo, Japan
- ¹⁵⁸ Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan
- ¹⁵⁹ Department of Physics, Tokyo Institute of Technology, Tokyo, Japan
- ¹⁶⁰ Tomsk State University, Tomsk, Russia
- ¹⁶¹ Department of Physics, University of Toronto, Toronto ON, Canada
- ¹⁶² ^(a) INFN-TIFPA; ^(b) University of Trento, Trento, Italy
- ¹⁶³ ^(a) TRIUMF, Vancouver BC; ^(b) Department of Physics and Astronomy, York University, Toronto ON, Canada
- ¹⁶⁴ Faculty of Pure and Applied Sciences, and Center for Integrated Research in Fundamental Science and Engineering, University of Tsukuba, Tsukuba, Japan
- ¹⁶⁵ Department of Physics and Astronomy, Tufts University, Medford MA, United States of America
- ¹⁶⁶ Department of Physics and Astronomy, University of California Irvine, Irvine CA, United States of America
- ¹⁶⁷ ^(a) INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; ^(b) ICTP, Trieste; ^(c) Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy
- ¹⁶⁸ Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden

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

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