

Search for scalar leptoquarks in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS experiment

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G Aad,
T Abajyan,



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PAPER

Search for scalar leptoquarks in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS experiment

The ATLAS Collaboration

Keywords: leptoquark, ATLAS, LHC

Abstract

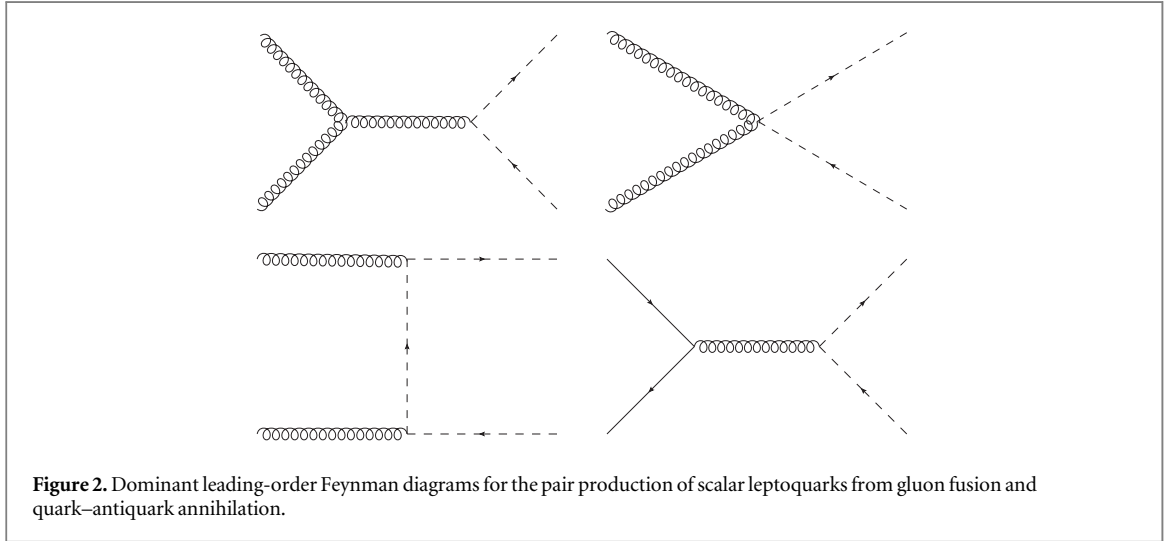
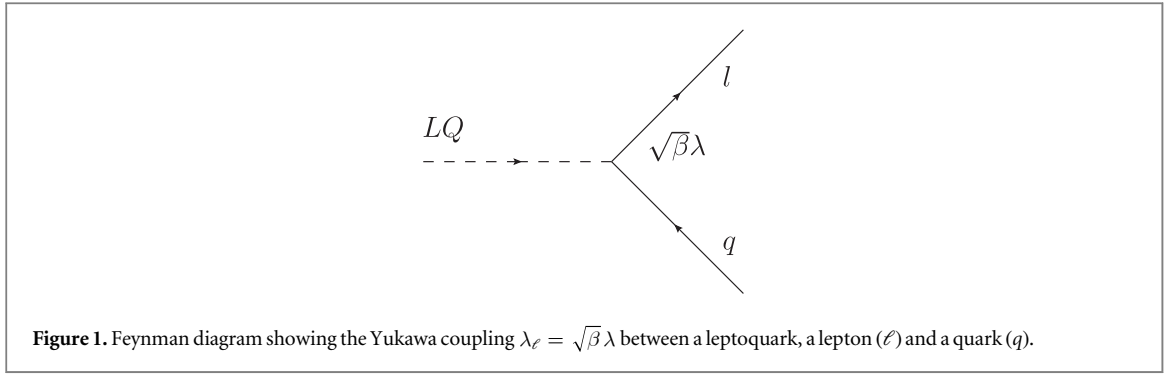
An inclusive search for a new-physics signature of lepton-jet resonances has been performed by the ATLAS experiment. Scalar leptoquarks, pair-produced in pp collisions at $\sqrt{s} = 13$ TeV at the large hadron collider, have been considered. An integrated luminosity of 3.2 fb^{-1} , corresponding to the full 2015 dataset was used. First (second) generation leptoquarks were sought in events with two electrons (muons) and two or more jets. The observed event yield in each channel is consistent with Standard Model background expectations. The observed (expected) lower limits on the leptoquark mass at 95% confidence level are 1100 and 1050 GeV (1160 and 1040 GeV) for first and second generation leptoquarks, respectively, assuming a branching ratio into a charged lepton and a quark of 100%. Upper limits on the aforementioned branching ratio are also given as a function of leptoquark mass. Compared with the results of earlier ATLAS searches, the sensitivity is increased for leptoquark masses above 860 GeV, and the observed exclusion limits confirm and extend the published results.

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1. Introduction

The large hadron collider (LHC) Run 2 has provided the possibility to study pp collisions at 13 TeV centre-of-mass energy for the first time, and has thus opened a new discovery window for physics beyond the standard model (SM). The presented analysis is an inclusive search for new physics phenomena resulting in final state signatures of lepton-jet resonances in the first 3.2 fb^{-1} of 13 TeV data collected by the ATLAS detector. Such phenomena may not have been kinematically accessible at the lower Run 1 centre-of-mass energy of 8 TeV. As a benchmark signal model, scalar leptoquarks decaying to jets and leptons were used.



Leptoquarks (LQs) feature in a number of theories [1–7] which extend the SM, such as grand unified theories and models with quark and lepton substructure. LQs possess non-zero baryon and lepton numbers and their existence would provide a connection between quarks and leptons. This could help explain the observed similarity of the quark and lepton sectors in the SM. LQs carry a colour-triplet charge and a fractional electric charge [8]. They can be scalar or vector bosons and they decay directly to lepton–quark pairs. The analysis presented in this paper focuses on the pair production of scalar leptoquarks.

A single Yukawa coupling (λ_ℓ) governs the interaction strength between a scalar LQ and a given quark (q) and lepton (ℓ) pair. A Feynman diagram showing a LQ decay is shown in figure 1. The couplings are determined by two free parameters of the model: the branching ratio into charged leptons, β , and the coupling parameter, λ . The coupling to a charged lepton and a quark is given by $\lambda_\ell = \sqrt{\beta} \lambda$, the coupling to a neutrino and a quark by $\lambda_\nu = \sqrt{1 - \beta} \lambda$. The pair-production cross section of leptoquarks in pp collisions is largely insensitive to the coupling values, since the basic processes of LQ pair-production are gluon fusion and quark–antiquark annihilation. Example LO diagrams are shown in figure 2. At a centre-of-mass energy of $\sqrt{s} = 13$ TeV, gluon fusion is the dominant process. For LQ masses (m_{LQ}) up to a few hundred GeV, it contributes up to 95% of the total cross section. Above $m_{LQ} = 1.5$ TeV, the contribution from quark–antiquark annihilation amounts to about 30% [9]. Therefore, the parameter of interest — apart from the LQ mass — is the branching ratio β .

The signal benchmark model for LQ production used in this analysis is the minimal Buchmüller–Rückl–Wyler model (mBRW) [10]. In this approach a number of constraints are imposed on the LQ properties. Lepton number and baryon number are separately conserved to prevent fast proton decay. The LQ couplings are also considered to be purely chiral. Furthermore, it is assumed that LQs belong to three generations (first, second and third) which interact only with lepton–quark pairs within the same generation. With this assumption, lepton-flavour violation is suppressed. However, in a more generic picture of leptoquarks, a LQ may couple to a quark and a lepton belonging to different generations [11]. Although the results of this search were not explicitly interpreted in this type of model, the event selections used were designed to retain sensitivity to leptoquark models in which decays into first or second generation leptons and bottom-quarks (b) are possible.

Previous searches for pair-produced LQs have been performed by the ATLAS and CMS collaborations [12–24] at $\sqrt{s} = 7$ and 8 TeV. The existence of scalar LQs with masses up to 1050 and 1000 GeV (for $\beta = 1$) for first-

and second-generation scalar LQs, respectively, is excluded at 95% confidence level (CL) by ATLAS [20] in a study performed at $\sqrt{s}=8$ TeV using 20 fb^{-1} of integrated luminosity. The CMS experiment similarly excluded first- and second-generation scalar leptoquarks up to masses of 1010 GeV and 1080 GeV (for $\beta = 1$), respectively [21].

In this paper, searches for the pair-production of leptoquarks of the first (LQ1) and second (LQ2) generations, based on events containing exactly two electrons or muons and at least two jets (denoted by $eejj$ and $\mu\mu jj$, respectively), are reported. In order to keep the search as inclusive as possible, it was not required that the charges of the two leptons in an event must be opposite. Similarly, no selections on the jet flavour were introduced so as not to exclude possible $\text{LQ} \rightarrow e b$ and $\text{LQ} \rightarrow \mu b$ decays.

2. The ATLAS detector

The ATLAS experiment [25] is a multi-purpose detector with a forward-backward symmetric cylindrical geometry and nearly 4π coverage in solid angle²²⁵. The three major sub-components of ATLAS are the tracking detector, the calorimeter and the muon spectrometer (MS). Charged-particle tracks and vertices are reconstructed by the inner detector (ID) tracking system, comprising silicon pixel (including the newly installed innermost pixel layer), and microstrip detectors covering the pseudorapidity range $|\eta| < 2.5$, and a straw tube tracker that covers $|\eta| < 2.0$. The ID is immersed in a homogeneous 2 T magnetic field provided by a solenoid. Electron, photon, jet and τ lepton energies are measured with sampling calorimeters. The ATLAS calorimeter system covers a pseudorapidity range of $|\eta| < 4.9$. Within the region $|\eta| < 3.2$, electromagnetic calorimetry is provided by barrel and endcap high-granularity lead/liquid argon (LAr) calorimeters, with an additional thin LAr presampler covering $|\eta| < 1.8$, to correct for energy loss in material upstream of the calorimeters. Hadronic calorimetry is provided by a steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadronic endcap calorimeters. The forward region ($3.1 < |\eta| < 4.9$) is instrumented by a LAr calorimeter with copper (electromagnetic) and tungsten (hadronic) absorbers. Surrounding the calorimeters is a MS with superconducting air-core toroids, providing bending powers of 3 Tm in the barrel and 6 Tm in the endcaps. The MS includes a system of precision tracking chambers providing coverage over $|\eta| < 2.7$. Three stations of precision tracking chambers are used to measure the curvature of tracks. The MS also contains detectors with triggering capabilities over $|\eta| < 2.4$ to provide fast muon identification and momentum measurements.

The ATLAS two-level trigger system is used to select events considered in this paper. The first-level trigger is hardware-based while the second, high-level trigger is implemented in software and employs algorithms similar to those used offline in the full event reconstruction.

3. Signal and background simulations

The PYTHIA 8.160 [26] Monte Carlo (MC) model, based on leading-order (LO) matrix-element calculations supplemented with parton showers, was used with the ATLASA14 [27] set of tuned parameters (tune) for the underlying event, together with the NNPDF23LO [28] parton distribution functions (PDFs), to produce simulated samples of pair-produced first- and second-generation scalar LQs. Leptoquarks of the first (second) generation decay to $e^+e^-u\bar{u}$ ($\mu^+\mu^-c\bar{c}$) final states. Samples were produced for LQ masses in the range of 500–1500 GeV. As was also done in the previous ATLAS publication [20], the value of the coupling parameter λ was set to $\sqrt{0.01 \times 4\pi\alpha}$, where α is the fine-structure constant. This value of λ determines the leptoquark natural width, which is less than 100 MeV and is smaller than the detector resolution for the reconstruction of leptoquark mass. It also leads to a LQ lifetime sufficiently small such that LQs in the mass range considered in this work would decay promptly. Next-to-leading-order (NLO) calculations [9] of the cross sections for scalar leptoquark pair-production were used to normalise the signal samples.

The dominant SM backgrounds arise from processes which can produce a final state containing two reconstructed high transverse momentum (p_T) leptons (electrons or muons) and jets. Simulated samples were made of Drell–Yan production ($q\bar{q} \rightarrow Z/\gamma^* \rightarrow \ell^+\ell^-$) and the production of $t\bar{t}$, diboson (WW, WZ, and ZZ) and single top-quarks in association with a W boson.

Drell–Yan events with associated jets were simulated using the SHERPA 2.1.1 [29] generator. Matrix elements were calculated for up to two partons at NLO and four partons at LO using the COMIX [30] and OPENLOOPS [31] matrix-element generators and merged with the SHERPA parton shower [32] using the ME+PS@NLO

²²⁵ 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 z-axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln \tan(\theta/2)$.

prescription [33]. The CT10 PDF set [34] was used in conjunction with dedicated parton-shower tuning developed by the authors of SHERPA [32].

For the generation of $t\bar{t}$ and single top quarks in the Wt channel, the POWHEG-BOX v2 generator [35–38] with the CT10 PDF set in the matrix-element calculations was used. For both processes the parton shower, fragmentation, and the underlying event were simulated using PYTHIA 6.428 [39] with the PERUGIA 2012 tune [40] and using the CTEQ6L1 PDF set [41]. The top-quark mass was set to 172.5 GeV. The EVTGEN v1.2.0 program [42] was used to simulate the bottom and charm hadron decays.

Diboson processes with four charged leptons, three charged leptons + one neutrino or two charged leptons and two neutrinos were simulated using the SHERPA 2.1.1 generator. Matrix elements contain all diagrams with four electroweak vertices. They were calculated for up to one (4ℓ , $2\ell + 2\nu$) or zero partons ($3\ell + 1\nu$) at NLO and up to three partons at LO using the COMIX and OPENLOOPS matrix element generators and merged with the SHERPA parton shower using the ME+PS@NLO prescription. Diboson processes with one of the bosons decaying hadronically and the other leptonically were simulated using the same SHERPA version.

All samples of simulated events include the effect of multiple proton–proton interactions in the same or neighbouring bunch crossings (pile-up) which were modelled by overlaying simulated minimum-bias events on each generated signal and background event. These multiple interactions were simulated with the soft QCD processes of PYTHIA 8.186 [26] using tune A2 [43] and the MSTW2008LO PDF set [44]. The number of overlaid events was chosen to match the average number of interactions per pp bunch crossing observed in the data as it evolved throughout the data-taking period (giving an average of 14 interactions per crossing for the whole data-taking period). The SM background samples were processed through the GEANT4-based detector simulation [45, 46], while a fast simulation using a parameterisation of the performance of the calorimeters [47] and GEANT4 for the other parts of the detector was used for the signal samples and some samples used for studies of systematic uncertainties. The standard ATLAS reconstruction software was used for both simulated and collision data.

Estimates of the cross sections of background processes were taken from the following theoretical predictions. Single-top production was calculated at NLO+next-to-next-to-leading-logarithm (NNLL) accuracy [48]. Estimates of Drell–Yan and $t\bar{t}$ production cross sections at NLO [29] and NLO+NNLO [49] accuracy, respectively, were used.

4. Physics object definition

The electron energy was measured using its associated cluster of electromagnetic-calorimeter cells with significant energy deposits, whereas the direction was determined by the track associated with this cluster. To identify and select electrons, requirements were placed on the shape of the cluster, on the quality of the associated track, and on the degree of matching between the track and cluster. Electron candidates must have transverse energy $E_T > 30$ GeV and $|\eta| < 2.47$. Electron candidates associated with clusters in the transition region between the barrel and endcap calorimeters ($1.37 < |\eta| < 1.52$) were not considered. All electrons must be reconstructed with a cluster-based or a combined cluster- and track-based algorithm [50]. Furthermore, the impact parameters of the electron track relative to the beam line were required to satisfy $|d_0/\sigma_{d_0}| < 5$ and $|z_0 \sin \theta| < 0.5$ mm, where d_0 , σ_{d_0} and z_0 are the transverse impact parameter, its uncertainty, and the longitudinal impact parameter, respectively. In addition, electron isolation requirements were imposed on the summed transverse momentum of tracks (transverse energy of clusters) in a cone around the electron track (cluster barycentre). The radius of the cone around the track is $\Delta R = 10 \text{ GeV}/p_T$ for $p_T > 50$ GeV and 0.2 otherwise²²⁶. For the cluster isolation, a fixed cone radius size of 0.2 is used. The efficiency of these isolation criteria is higher than 99%. The reconstruction efficiency is higher than 98% in most regions of transverse momentum and pseudorapidity. The identification efficiency varies between 75% and 92%, rising as a function of E_T [51]. All of these efficiencies refer to the efficiency for a single electron, independent of the specific event topology.

Muon tracks were reconstructed independently in the ID and the MS. These muon tracks were required to have a minimum number of associated hits in each system and to satisfy geometrical and momentum matching criteria. The two tracks were then used as input to a combined fit which takes into account the energy loss in the calorimeter and multiple-scattering effects [52]. To improve momentum resolution and ensure a reliable measurement at very high momenta, muon tracks were required to have at least three hits in each of the three precision chambers in the MS. Tracks which traverse precision chambers with poor alignment were rejected. Finally, measurements of charge over momentum, performed independently in the ID and MS, were required to agree within seven standard deviations of the sum in quadrature of the uncertainties in the corresponding ID

²²⁶ Here, $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ is a cone defined by differences in pseudorapidity and azimuthal angle. p_T is given in GeV.

and MS measurements. Muon candidates were required to have $p_T > 40$ GeV and $|\eta| < 2.5$. Those falling in the overlap region of the MS barrel and endcap ($1.01 < |\eta| < 1.10$) were rejected due to the potential p_T mismeasurement resulting from relative barrel-endcap misalignment. Muon candidates were required to fulfil $|d_0/\sigma_{d_0}| < 3$ and $|z_0 \sin \theta| < 0.5$ mm. In order to reduce the background from light- and heavy-hadron decays within jets, muons were required to fulfil isolation requirements. The track-based isolation variable used is the sum of the transverse momenta of the tracks in a cone around the muon of size $\Delta R = 10 \text{ GeV}/p_T^\mu$, excluding the muon itself and with p_T^μ in GeV. The isolation efficiency is greater than 99%. The efficiency for reconstructing and identifying muons using the criteria described above is typically greater than 80% for the transverse momentum and pseudorapidity selections used in this work [53]. As for electrons, these efficiencies refer to single objects.

The anti- k_t algorithm [54] with a radius parameter $R = 0.4$ was used to reconstruct jets from energy clusters in the calorimeter [55]. Jet calibration is performed using energy- and η -dependent correction factors derived from simulations together with further corrections from *in situ* measurements. The jets used in this work must satisfy $p_T > 50$ GeV and $|\eta| < 2.8$. Further selections were applied to ensure that all jets considered are well measured [56]. A description of the jet energy scale (JES) measurement and its associated systematic uncertainties can be found in [57]. Jet-flavour tagging techniques were not used in this paper and, as a consequence, good sensitivity was maintained for LQ decays into a lepton plus any quark flavour barring the top quark.

Ambiguities in the object identification during reconstruction, i.e. when a reconstructed object matched multiple object identification hypotheses (electron, muon, jet), were resolved in the following way. First, electrons were removed if they shared their track with a muon. In a second step, ambiguities between electrons and jets were removed; if the two objects had $\Delta R < 0.2$ the jet was rejected; if $0.2 < \Delta R < 0.4$ the electron was rejected. Finally, muon-jet ambiguities were resolved as follows: if the muon and jet were closer than $\Delta R = 0.4$ the jet was rejected if it has less than three tracks, otherwise the muon was rejected. For the definition of signal and control regions (see section 6) only objects remaining after this procedure were considered.

5. Dataset and event selection

Proton–proton collision data at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, collected by the ATLAS detector at the LHC during 2015, were used. After applying data quality criteria, the dataset corresponds to an integrated luminosity of 3.2 fb^{-1} .

Events considered in the search were selected by the ATLAS two-level trigger system [58]. In the $eejj$ channel, a two-electron trigger was used with an E_T threshold of 17 GeV for each electron. The $\mu\mu jj$ search used events selected by either of two single-muon triggers. The first trigger has a muon p_T threshold of 26 GeV and additional requirements on its properties. In particular, it requires the muon to be isolated, which leads to a loss in efficiency at high p_T . To retain a high trigger efficiency in the region of high p_T , the second trigger, which has a p_T threshold of 50 GeV but no additional requirements, was used. The trigger efficiencies for the $eejj$ and $\mu\mu jj$ searches exceed 90% for the object kinematics considered in this analysis.

Multiple pp interactions during bunch crossings lead to events containing a number of reconstructed vertices. The primary vertex of the event is defined as that vertex with the largest sum of squared transverse momenta of its associated tracks. Events which contain a primary vertex with at least two associated tracks satisfying $p_{T,\text{track}} > 0.4$ GeV were selected. Furthermore, MC events were given a per-event weight to correct for differences in the distribution of the average number of pp interactions per bunch crossing between data and simulation.

Only events with exactly two charged leptons and at least two jets were considered for this analysis. Scale factors were applied as event weights to correct the MC description of lepton trigger, reconstruction, identification, isolation and impact-parameter cut efficiencies. A description of the derivation of the scale factors, obtained by comparing data and MC predictions in dedicated studies, can be found in [50, 59].

6. Analysis strategy: signal, control and validation regions

The analysis presented here used signal (SR), control (CR) and validation (VR) regions to optimise signal significance and to constrain the normalisation of the main background sources. The latter are Drell–Yan events containing $Z/\gamma^* \rightarrow e^+e^-, \mu^+\mu^-$ + jets processes (hereafter termed DY+jets) and $t\bar{t}$ events in which both top quarks decay leptonically. The signal, control and validation regions were defined using the following discriminating observables:

- The dilepton invariant mass: $m_{\ell\ell}$.
- The scalar sum S_T of the transverse momentum of the two leptons and of the two leading jets.

Table 1. Definition of control, signal and validation regions. In all regions, at least two jets were required.

| Region | Channel | # <i>e</i> | # <i>μ</i> | $m_{\ell\ell}$ (GeV) | S_T (GeV) |
|---------------|-------------|------------|------------|----------------------|-------------|
| $t\bar{t}$ CR | Both | 1 | 1 | — | — |
| DY+jets CR | $eejj$ | 2 | 0 | [70, 110] | — |
| | $\mu\mu jj$ | 0 | 2 | | |
| SR | $eejj$ | 2 | 0 | >130 | >600 |
| | $\mu\mu jj$ | 0 | 2 | | |
| VR | $eejj$ | 2 | 0 | >130 | <600 |
| | $\mu\mu jj$ | 0 | 2 | | |

- The minimum invariant mass of the two lepton–jet pairs in an event, m_{LQ}^{\min} . The lepton–jet pairs were chosen such that the invariant mass difference between them was smallest. The lower mass of the two combinations was chosen as the discriminating variable following dedicated sensitivity studies.

The signal region was defined by requiring $m_{\ell\ell} > 130$ GeV and $S_T > 600$ GeV. The cut on $m_{\ell\ell}$ was chosen to reduce the DY+jets background. The cut on S_T was optimised by maximising the discovery significance [60] for LQs with masses between 500 and 1500 GeV, i.e. by performing a likelihood fit (described in more detail at the end of this section) using the m_{LQ}^{\min} distribution defined above for S_T values between 0 and 3 TeV in steps of 100 GeV. This study showed that there is little dependence of the optimised S_T value on the LQ mass when using the shape information of the mass spectrum. It was confirmed that the approach used in previous results, i.e. a cut-and-count analysis in several signal regions defined by varying cuts on the three variables mentioned above, does not give better sensitivity.

The signal selection efficiency is defined as the fraction of all simulated signal events, generated across the full phase space, that survive the trigger and the final SR selection. For leptoquarks of the first (second) generation, the overall selection efficiency rises from around 62% to 71% (38% to 43%) as the mass increases from 500 to 1500 GeV. The lower efficiency for second-generation leptoquarks is due to the muon track requirements, which demand hits in three MS stations, and which are needed to give an optimal momentum resolution at high p_T for this analysis.

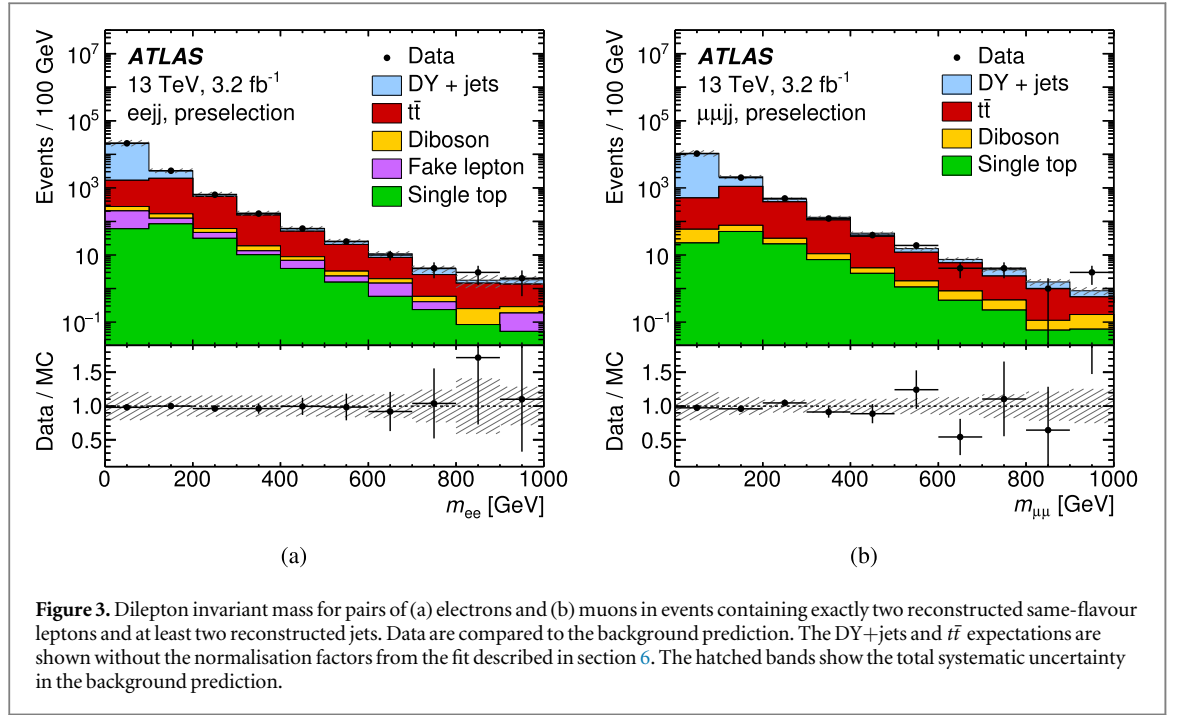
Three non-overlapping control regions with negligible signal contamination were defined. Differences in the predicted and observed event yields in these regions were used to evaluate scale factors which were used to normalise the MC predictions for the $t\bar{t}$ and DY+jets backgrounds in the SRs. The two DY+jets CRs — one for the $eejj$ and one for the $\mu\mu jj$ channel — were defined by requiring at least two jets and exactly two same-flavour leptons with a dilepton invariant mass restricted to a window around the Z boson mass: $70 < m_{\ell\ell} < 110$ GeV. The $t\bar{t}$ control region requires at least two jets, exactly one muon and exactly one electron: these events were selected with the same single-muon triggers as described in section 5. This control region is common to both channels.

Validation regions were used to verify that data and MC predictions agree in a phase space close to the signal regions, but still with a negligible signal contamination. This was achieved by applying the same selection as for the signal region, but inverting the cut on S_T , i.e. allowing only values below 600 GeV. The requirements for the various regions are collected in table 1.

For the statistical analysis, a profile-likelihood fit of signal plus background templates to the data was performed using the HistFitter package [61]. Systematic uncertainties, which are discussed in section 8, were incorporated into the likelihood as constrained nuisance parameters. The fit was performed in the CRs and the SR simultaneously and was used to extract normalisation factors, i.e. scaling corrections to the event yields predicted by theoretical cross-section calculations, described in section 3. In the CRs, only the event yield was used to extract the dominant background ($t\bar{t}$ and DY+jets) normalisation factors. In the SR, both the normalisation and the shape of m_{LQ}^{\min} distribution were used in the fit to extract the signal normalisation factor. The templates of the m_{LQ}^{\min} shape consisted of ten bins: six bins of 100 GeV width from 0 to 600 GeV and four bins of 200 GeV width that cover the range up to 1.4 TeV. The template for the signal was derived from MC predictions. For the background templates, MC predictions as well as data-driven techniques were used, as detailed in the following section.

7. Background estimation

Normalisation factors for the MC predictions of the two main SM backgrounds (DY+jets and $t\bar{t}$) were estimated with a fit to the data, as described in section 6. In total, four normalisation factors were calculated: one each for $t\bar{t}$ and DY+jets events in both the electron and muon channels.



Smaller background contributions arise from the production of a single top quark in the Wt channel, diboson events and $Z \rightarrow \tau\tau + \text{jets}$ events. These were estimated purely from simulation, i.e. their normalisation was not a free parameter in the combined fit.

Misidentified or non-prompt leptons originating from hadron decays or photon conversions can arise in multi-jet events, single top production in the s - or t -channel, $W + \text{jets}$ and $t\bar{t}$ events (with at least one top quark decaying hadronically). This fake-lepton background is negligible in the $\mu\mu jj$ channel. In the $eejj$ channel it was evaluated using the same data-driven method as in [62]. This method was used to evaluate the migration of events among four different data samples: the nominal SR and three analogous samples selected with modified electron selection criteria. The migration between different regions can be described by a matrix, the elements of which are functions of the proportions of true and fake electrons. As a simplification of [62], the fake and real rates were evaluated as a function of p_T only, since they were observed to be independent of η within the required accuracy. They were considered to be the same for all electron candidates in an event. The fake background estimation suffers from low statistical precision. Its statistical uncertainty was treated as one source of the systematic uncertainty in the total background modelling.

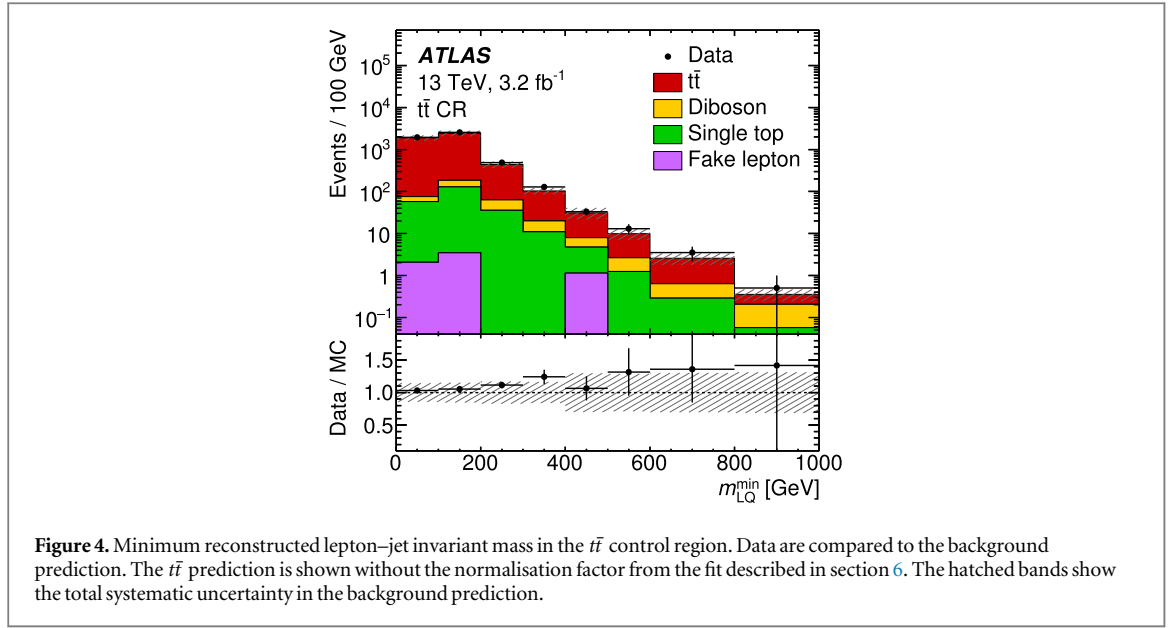
Figure 3 shows the dilepton invariant mass for pairs of electrons (a) and muons (b) in events containing exactly two reconstructed same-flavour leptons and at least two reconstructed jets, following the selections given in section 5. This selection stage is also referred to as preselection. The predictions of various background sources are compared with the data. The hatched bands show the total systematic uncertainty in the background prediction. Within the uncertainties, agreement between data and simulation is observed. Normalisation factors for the MC predictions for DY+jets and $t\bar{t}$ events are not applied in the plot.

Figure 4 shows the spectrum of the minimum reconstructed lepton-jet mass in the $t\bar{t}$ control region before the fit. Within uncertainties, the data and MC distributions are consistent.

8. Sources of systematic uncertainties

The following sources of systematic uncertainty were considered:

- The uncertainty in the integrated luminosity is 5%. It was derived following a methodology similar to that detailed in [63], from a calibration of the luminosity scale using $x\text{-}\gamma$ beam-separation scans performed in August 2015. This uncertainty affects the predicted signal event yield and those background rates for which theoretical estimates are used.
- The JES uncertainty depends on the p_T and η of the jet and on the pile-up conditions in an event. A further uncertainty in the jet energy resolution was taken into account. These sources each correspond to uncertainties in the jet energy of up to 3%. The largest resulting uncertainty in the background event yields is



about 10% in the control regions. In the signal region, the uncertainty in the event yields amounts to at most 5% for the background and less than 1% for the signal.

- The uncertainty in the lepton trigger efficiency scale factors is around 2% for the kinematic region considered here.
- Differences between the MC and data in the efficiency of the isolation requirement on the selected muons correspond to uncertainties of 1%–5% on the scale factor to correct the MC prediction. Other muon-related uncertainties arise from the momentum scale, resolution, and quality criteria and typically affect the muon event yields by around 1% in all regions for both signal and background.
- Uncertainties in the electron energy scale, identification and isolation affect the electron event yields by up to 2% in all regions for both signal and background.
- Uncertainties due to choices that have to be made in the event generation which affect final-state observables were estimated for the two major background sources: $t\bar{t}$ and $DY + \text{jets}$. These *modelling uncertainties* refer to e.g. possible differences in the generation of the hard scattering, scale dependencies, the parton shower and hadronisation and fragmentation models. Differences in the background modelling can change the event yields (total normalisation) in the CRs. Moreover, there is an uncertainty in the shape of the m_{LQ}^{\min} distribution in the signal region due to background modelling effects. This was estimated as one uncertainty per m_{LQ}^{\min} -bin in the signal region and propagated to the normalisation factor by the fit. The uncertainties were treated as uncorrelated between different bins.

The impact of modelling uncertainties in final-state predictions for $t\bar{t}$ processes was quantified by comparing various simulated samples: differences due to the parton shower as well as the hadronisation and fragmentation model were estimated by comparing the nominal sample to one that uses HERWIG++ [64], effects of additional or reduced radiation were estimated by varying the parton-shower and scale parameters within PYTHIA, and an alternative generator (AMC@NLO [65] with HERWIG++) was used to estimate differences in the hard scatter generation. The total uncertainty in the predicted $t\bar{t}$ event yield varies between 14% (in the $t\bar{t}$ CR) to about 30% (in the signal regions).

Modelling uncertainties for the $DY + \text{jets}$ background were assessed with different approaches, simulation-based, as well as data-driven in different regions of phase space. The baseline estimate used events from the $DY + \text{jets}$ control region with S_T higher than 600 GeV. In this region, the shapes of both the m_{LQ}^{\min} and S_T distributions are very similar to those in the signal region, which differs only by the cut on the dilepton invariant mass. This cut was found to not affect the shapes of the other discriminating variables. The difference between the data and the background prediction in this region was used as an estimate of the modelling uncertainty.

The result was cross-checked using simulated samples in which the renormalisation, factorisation and resummation scales, as well as the scale for matrix element and parton shower matching, were independently varied up and down by a factor of two. Within the statistical uncertainties resulting from the limited number

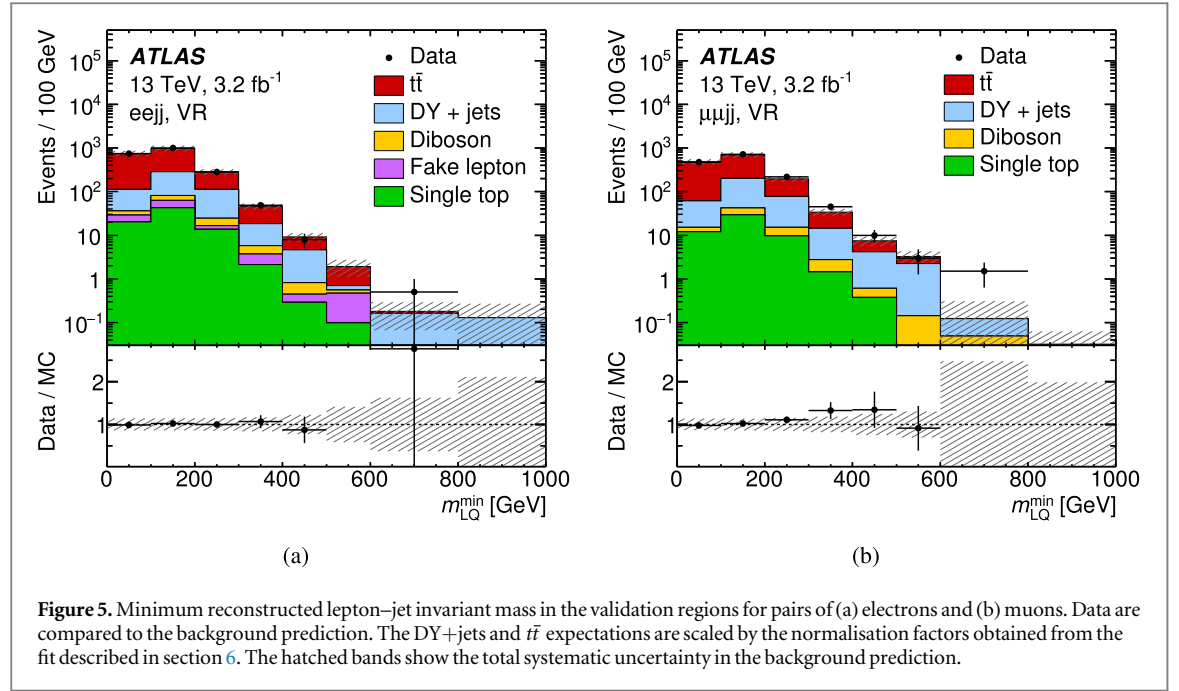


Figure 5. Minimum reconstructed lepton-jet invariant mass in the validation regions for pairs of (a) electrons and (b) muons. Data are compared to the background prediction. The DY+jets and $t\bar{t}$ expectations are scaled by the normalisation factors obtained from the fit described in section 6. The hatched bands show the total systematic uncertainty in the background prediction.

Table 2. Normalisation factors for the main backgrounds obtained from the combined fit in each of the channels.

| Channel | DY+jets | $t\bar{t}$ |
|-------------|---------------|---------------------|
| $eejj$ | 0.9 ± 0.1 | 1.0 ± 0.1 |
| $\mu\mu jj$ | 0.9 ± 0.1 | $1.0^{+0.2}_{-0.1}$ |

of events in these samples, the estimate from the data-driven approach was confirmed. The result is a 10% uncertainty in the DY+jets event yield in the control regions and 20% in each m_{LQ}^{\min} bin in the signal region.

- PDF uncertainties on the $t\bar{t}$ and DY+jets normalisation as well as the m_{LQ}^{\min} shape amount to less than 4% and do not affect the final result given the large modelling uncertainties described above.
- The effects of higher-order contributions on the signal cross section were estimated by varying the QCD renormalisation and factorisation scales, set to a common value, up and down by a factor of two, as done in [9]. One half of the difference between the predicted cross section for the increased and reduced scale choice is used as the cross section uncertainty for a given mass. This uncertainty lies in the range 12%–17% for the mass points considered in this paper.
- The impact of theoretical uncertainties related to the parton-shower algorithm and multiple-interactions tune were evaluated by varying the corresponding parameters, as specified in [66]. This leads to an uncertainty in signal acceptance of up to 2%.
- The uncertainty in the signal cross section due to the choice of PDF set was calculated as the envelope of the predictions of 40 different CTEQ6.6 NLO error sets [9]. The uncertainty ranges from 11% at $m_{LQ} = 500$ GeV to 34% at $m_{LQ} = 1500$ GeV. The predicted signal acceptance was studied using NNPDF23LO [28], CT14 [67] and MMHT14 [68] PDF sets. The acceptance is very insensitive to the choice of parton distribution function; the systematic uncertainty from this source is less than 1%.

9. Results

The results are consistent with SM expectations. The normalisation factors obtained in the fit described in section 6 are summarised in table 2. Similar results are obtained in the two channels and the normalisation factors are found to be compatible with unity within the uncertainties. The reliability of extrapolating the background predictions from the control regions to the signal region was checked in the VRs defined in section 6. The distribution of m_{LQ}^{\min} in the two validation regions is compared to the background prediction after the fit in figure 5. Within the uncertainties, the predictions are compatible with the observed data.

Table 3. Observed and predicted event yields in the signal and control regions in the $eejj$ channel. The background prediction with its total uncertainty after the fit is shown. The fit is performed using only the control regions as input. The lower part of the table shows the separate contributions from the different background processes and their total uncertainty after the fit. In addition, the expected signal event yields for $\beta = 1$ and LQ masses of 500, 1000, and 1500 GeV are given.

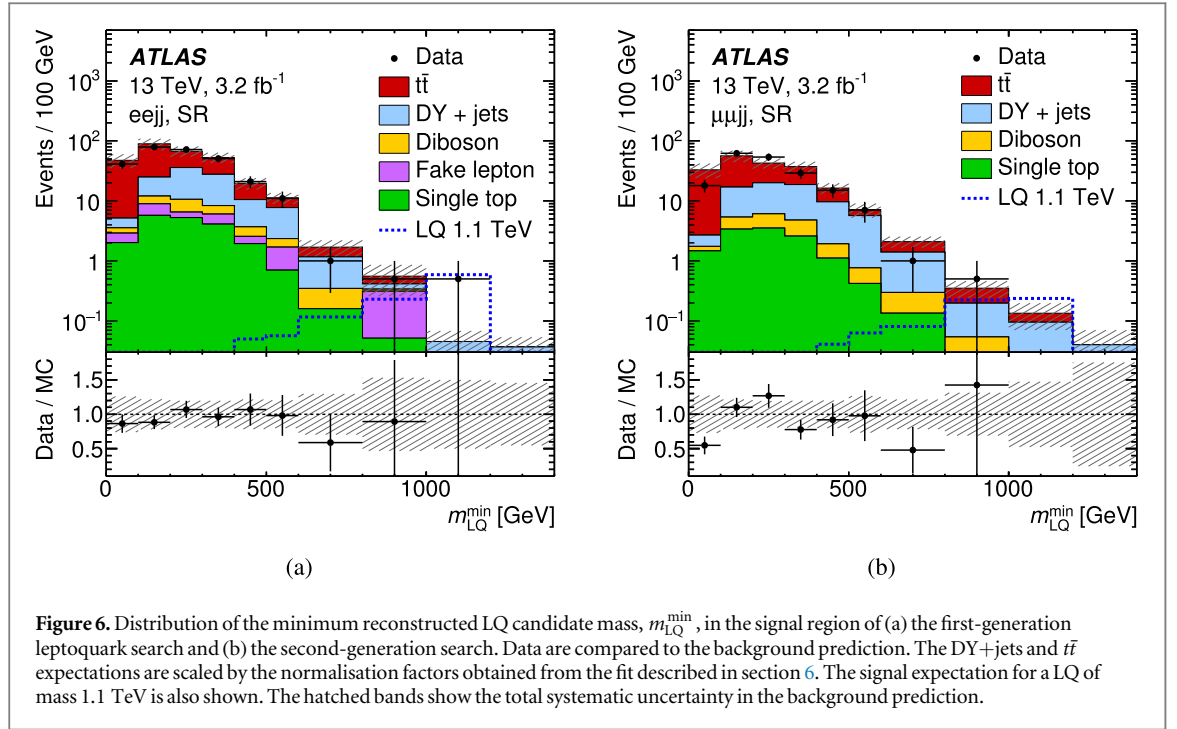
| | SR | CR DY+jets | CR $t\bar{t}$ |
|--|----------------|-----------------|---------------|
| Observed events | 279 | 20328 | 5194 |
| Total background events | 300 ± 30 | 20300 ± 200 | 5200 ± 50 |
| Fitted DY+jets events | 74 ± 7 | 19100 ± 200 | <0.01 |
| Fitted $t\bar{t}$ events | 190 ± 30 | 1060 ± 10 | 4840 ± 40 |
| MC predicted diboson events | 12.5 ± 0.6 | 63 ± 3 | 115 ± 6 |
| MC predicted single-top events | 20 ± 1 | 42 ± 2 | 230 ± 10 |
| Estimated fake-lepton events | 9 ± 4 | 120 ± 10 | 6 ± 3 |
| MC exp. signal events ($m_{LQ} = 500$ GeV) | 1000 ± 100 | 26 ± 4 | <0.01 |
| MC exp. signal events ($m_{LQ} = 1000$ GeV) | 13 ± 2 | 0.03 ± 0.00 | <0.01 |
| MC exp. signal events ($m_{LQ} = 1500$ GeV) | 0.6 ± 0.1 | <0.01 | <0.01 |

Table 4. Observed and predicted event yields in the signal and control regions in the $\mu\mu jj$ channel. The background prediction with its total uncertainty after the fit is shown. The fit is performed using only the control regions as input. The lower part of the table shows the separate contributions from the different background processes and their total uncertainty after the fit. Where no number is given, the contribution is found to be negligible. In addition, the expected signal event yields for $\beta = 1$ and LQ masses of 500, 1000, and 1500 GeV are given.

| | SR | CR DY+jets | CR $t\bar{t}$ |
|--|-----------------|-----------------|---------------|
| Observed events | 188 | 10233 | 5194 |
| Fitted background events | 200 ± 30 | 10200 ± 100 | 5200 ± 70 |
| Fitted DY+jets events | 56 ± 8 | 9800 ± 100 | 9 ± 1 |
| Fitted $t\bar{t}$ events | 120 ± 30 | 400 ± 20 | 4840 ± 80 |
| MC predicted diboson events | 8.6 ± 0.6 | 32 ± 3 | 115 ± 10 |
| MC predicted single-top events | 12.8 ± 0.9 | 18 ± 2 | 230 ± 20 |
| Estimated fake-lepton events | — | — | — |
| MC exp. signal events ($m_{LQ} = 500$ GeV) | 610 ± 40 | 25 ± 2 | 3 ± 3 |
| MC exp. signal events ($m_{LQ} = 1000$ GeV) | 8.0 ± 0.8 | 0.08 ± 0.01 | 0.1 ± 0.1 |
| MC exp. signal events ($m_{LQ} = 1500$ GeV) | 0.33 ± 0.06 | <0.01 | <0.01 |

The observed and expected event yields in the signal regions for the $eejj$ and the $\mu\mu jj$ channels, after the fits, are shown in tables 3 and 4, respectively. The values in these tables are intended to illustrate the sensitivity independent of a specific signal hypothesis and thus, in this case, the fit was performed using only the control regions as input. The resulting fit parameters (DY+jets and $t\bar{t}$ normalisation factors and values of the nuisance parameters) were transferred to the signal region, using appropriate transfer factors based on the MC models. The different contributions to the background do not necessarily exactly sum to the total quoted number of background events owing to the rounding scheme used. The dominant experimental systematic uncertainties in the background prediction arise from uncertainties on corrections to the simulated electron and muon trigger efficiencies and the JES; the latter source gives an uncertainty of 2%–4% in the signal region. The luminosity uncertainty of 5% contributes for simulated backgrounds not constrained by the fit (diboson and single-top production). The theoretical uncertainties after the fit range from 3% to 12% for the DY+jets background and from 3% to 16% for the $t\bar{t}$ background. The global fit takes correlations of the nuisance parameters into account, which results in the uncertainty in the total background being smaller than the quadratic sum of the uncertainties in the separate components. The contribution of $Z \rightarrow \tau\tau + \text{jets}$ to the background is negligible and not shown in the tables.

Figure 6 shows the SR distribution of m_{LQ}^{\min} compared to background predictions based on the combined fit in the CRs and the SR. The signal prediction for a LQ of mass 1.1 TeV is also shown. The wider signal shape in the muon channel compared to the electron channel is due the worsening of the muon momentum resolution with increasing momentum. Again, no significant deviation from the SM predictions was observed. Limits on the LQ



signal strength were derived using pseudo-experiments and following a modified frequentist CL_s method [69]. Apart from the luminosity uncertainty (5%), dominant uncertainties in the signal event yields arise from lepton scale factors and are of the order of 2%–5% at low masses and up to 10% at high masses.

In figure 7, limits on the cross section times branching ratio are shown on the left, for leptoquarks of the first (second) generation in the top (bottom) plot. The expected limit is depicted by the dashed line; the uncertainty bands result from considering all sources of systematic as well as statistical uncertainties. The observed limit is given by the solid line. The NLO pair-production cross section for $\beta = 1$ is shown as a line with a shaded band representing the uncertainties. The shaded band around it illustrates the uncertainties in the theoretical prediction due to PDF and scale uncertainties. The intersection of this line with the cross-section limits yields the lower limit on the leptoquark mass for a value of $\beta = 1$. These observed (expected) limits are found to be 1100 (1160 GeV) and 1050 GeV (1040 GeV) for first- and second-generation LQs, respectively. The observed limit for each channel is stronger than the previous bound [20] by 50 GeV. The expected limits are improved by 110 GeV for the first-generation search and by 40 GeV in the second generation search. The theoretical cross section was scaled by β^2 and then used to obtain the limits on the branching ratio as a function of the LQ mass shown on the right of figure 7. Below LQ masses of 650 GeV, the limits on β are weaker than those obtained at 8 TeV centre-of-mass energy, which are shown as the dashed-dotted line, owing to the much lower integrated luminosity collected in 2015 and the effects of background at lower LQ masses. At high masses (above 900 GeV), however, the gain in the production cross section at 13 TeV compensates for the smaller luminosity and stronger bounds than at 8 TeV are obtained. In the intermediate mass region, the results are comparable. Mass limits for various values of β are summarised in table 5.

10. Summary and conclusions

Searches for first- and second-generation scalar leptoquarks, pair-produced in pp collisions at 13 TeV centre-of-mass energy, have been performed with the ATLAS detector at the LHC. An integrated luminosity of 3.2 fb^{-1} of data was used. No significant excess above the SM background expectation was observed in either channel. The results were interpreted in the framework of the mBRW model. Mass-dependent limits were derived on the pair-production cross section times the square of the branching ratio (β^2) and on β . For $\beta = 1$, the observed (expected) LQ mass limits at 95% CL are 1100 and 1050 GeV (1160 and 1040 GeV) for first- and second-generation leptoquarks, respectively. The observed bounds are more stringent than the previous ATLAS limits by 50 GeV in each channel. This analysis is the first result at 13 TeV using the Run 2 data collected by the ATLAS experiment in a program of high precision inclusive searches for resonant signatures involving a lepton and a jet.

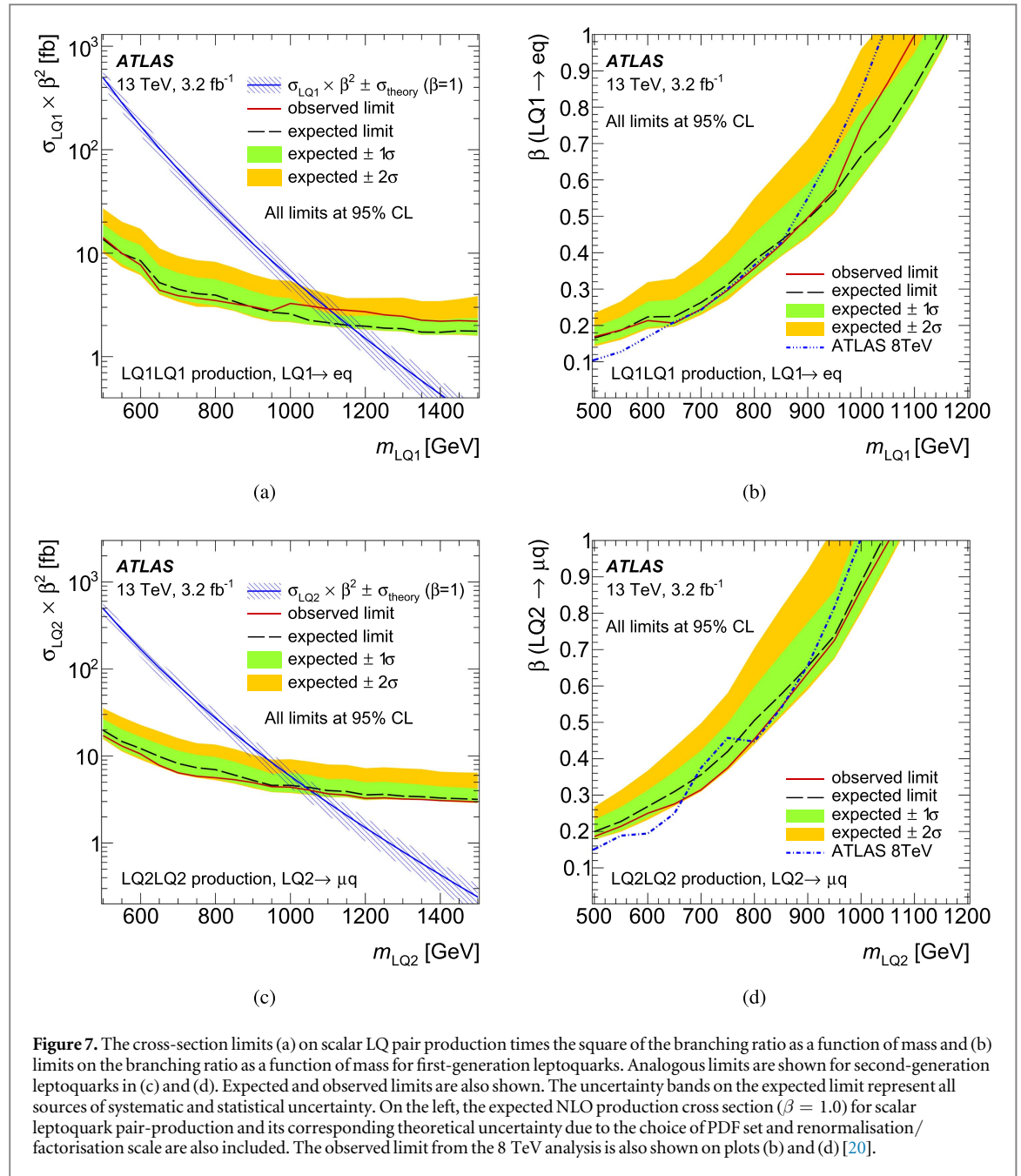


Figure 7. The cross-section limits (a) on scalar LQ pair production times the square of the branching ratio as a function of mass and (b) limits on the branching ratio as a function of mass for first-generation leptoquarks. Analogous limits are shown for second-generation leptoquarks in (c) and (d). Expected and observed limits are also shown. The uncertainty bands on the expected limit represent all sources of systematic and statistical uncertainty. On the left, the expected NLO production cross section ($\beta = 1.0$) for scalar leptoquark pair-production and its corresponding theoretical uncertainty due to the choice of PDF set and renormalisation/factorisation scale are also included. The observed limit from the 8 TeV analysis is also shown on plots (b) and (d) [20].

Table 5. Expected and observed 95% CL lower limits on first- and second-generation leptoquark masses for different assumptions of β .

| β | 95% CL limit on | | | |
|---------|-----------------|----------|-----------------|----------|
| | m_{LQ1} (GeV) | | m_{LQ2} (GeV) | |
| | Expected | Observed | Expected | Observed |
| 1.00 | 1160 | 1100 | 1040 | 1050 |
| 0.75 | 1050 | 1000 | 950 | 960 |
| 0.50 | 900 | 900 | 800 | 830 |
| 0.25 | 680 | 700 | 580 | 600 |

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The ATLAS Collaboration

M Aaboud^{136d}, G Aad⁸⁷, B Abbott¹¹⁴, J Abdallah⁶⁵, O Abidinov¹², B Abeloos¹¹⁸, R Aben¹⁰⁸, O S AbouZeid¹³⁸, N L Abraham¹⁵⁰, H Abramowicz¹⁵⁴, H Abreu¹⁵³, R Abreu¹¹⁷, Y Abulaiti^{147a,147b}, B S Acharya^{164a,164b,179}, L Adamczyk^{40a}, D L Adams²⁷, J Adelman¹⁰⁹, S Adomeit¹⁰¹, T Adye¹³², A A Affolder⁷⁶, T Agatonovic-Jovin¹⁴, J Agricola³⁶, J A Aguilar-Saavedra^{127a,127f}, S P Ahlen²⁴, F Ahmadov^{67,180}, G Aielli^{134a,134b}, H Akerstedt^{147a,147b}, T P A Åkesson⁸³, A V Akimov⁹⁷, G L Alberghi^{22a,22b}, J Albert¹⁶⁹, S Albrand⁵⁷, M J Alconada Verzini⁷³, M Aleksa³², I N Aleksandrov⁶⁷, C Alexa^{28b}, G Alexander¹⁵⁴, T Alexopoulos¹⁰, M Alhroob¹¹⁴, M Aliev^{75a,75b}, G Alimonti^{93a}, J Alison³³, S P Alkire³⁷, B M M Allbrooke¹⁵⁰, B W Allen¹¹⁷, P P Allport¹⁹, A Aloisio^{105a,105b},

A Alonso³⁸, F Alonso⁷³, C Alpigiani¹³⁹, M Alstady⁸⁷, B Alvarez Gonzalez³², D Álvarez Piqueras¹⁶⁷, M G Alviggi^{105a,105b}, B T Amadio¹⁶, K Amako⁶⁸, Y Amaral Coutinho^{26a}, C Amelung²⁵, D Amidei⁹¹, S P Amor Dos Santos^{127a,127c}, A Amorim^{127a,127b}, S Amoroso³², G Amundsen²⁵, C Anastopoulos¹⁴⁰, L S Ancu⁵¹, N Andari¹⁰⁹, T Andeen¹¹, C F Anders^{60b}, G Anders³², J K Anders⁷⁶, K J Anderson³³, A Andreazza^{93a,93b}, V Andrei^{60a}, S Angelidakis⁹, I Angelozzi¹⁰⁸, P Anger⁴⁶, A Angerami³⁷, F Anghinolfi³², A V Anisenkov^{110,181}, N Anjos¹³, A Annovi^{125a,125b}, M Antonelli⁴⁹, A Antonov⁹⁹, F Anulli^{133a}, M Aoki⁶⁸, L Aperio Bella¹⁹, G Arabidze⁹², Y Arai⁶⁸, J P Araque^{127a}, A T H Arce⁴⁷, F A Arduh⁷³, J-F Arguin⁹⁶, S Argyropoulos⁶⁵, M Arik^{20a}, A J Armbruster¹⁴⁴, L J Armitage⁷⁸, O Arnaez³², H Arnold⁵⁰, M Arratia³⁰, O Arslan²³, A Artamonov⁹⁸, G Artoni¹²¹, S Artz⁸⁵, S Asai¹⁵⁶, N Asbah⁴⁴, A Ashkenazi¹⁵⁴, B Åsman^{147a,147b}, L Asquith¹⁵⁰, K Assamagan²⁷, R Astalos^{145a}, M Atkinson¹⁶⁶, N B Atlay¹⁴², K Augsten¹²⁹, G Avolio³², B Axen¹⁶, M K Ayoub¹¹⁸, G Azuelos^{96,182}, M A Baak³², A E Baas^{60a}, M J Baca¹⁹, H Bachacou¹³⁷, K Bachas^{75a,75b}, M Backes³², M Backhaus³², P Bagiacchi^{133a,133b}, P Bagnaia^{133a,133b}, Y Bai^{35a}, J T Baines¹³², O K Baker¹⁷⁶, E M Baldin^{110,181}, P Balek¹³⁰, T Balestri¹⁴⁹, F Balli¹³⁷, W K Balunas¹²³, E Banas⁴¹, Sw Banerjee^{173,183}, A A E Bannoura¹⁷⁵, L Barak³², E L Barberio⁹⁰, D Barberis^{52a,52b}, M Barbero⁸⁷, T Barillari¹⁰², T Barklow¹⁴⁴, N Barlow³⁰, S L Barnes⁸⁶, B M Barnett¹³², R M Barnett¹⁶, Z Barnovska⁵, A Baroncelli^{135a}, G Barone²⁵, A J Barr¹²¹, L Barranco Navarro¹⁶⁷, F Barreiro⁸⁴, J Barreiro Guimarães da Costa^{35a}, R Bartoldus¹⁴⁴, A E Barton⁷⁴, P Bartos^{145a}, A Basalae¹²⁴, A Bassalat¹¹⁸, R L Bates⁵⁵, S J Batista¹⁵⁹, J R Batley³⁰, M Battaglia¹³⁸, M Baue^{133a,133b}, F Bauer¹³⁷, H S Bawa^{144,184}, J B Beacham¹¹², M D Beattie⁷⁴, T Beau⁸², P H Beauchemin¹⁶², P Bechtel²³, H P Beck^{18,185}, K Becker¹²¹, M Becker⁸⁵, M Beckingham¹⁷⁰, C Becot¹¹¹, A J Beddal^{20c}, A Beddall^{20b}, V A Bednyakov⁶⁷, M Bedognetti¹⁰⁸, C P Bee¹⁴⁹, L J Beemster¹⁰⁸, T A Beermann³², M Begel²⁷, J K Behr⁴⁴, C Belanger-Champagne⁸⁹, A S Bell⁸⁰, G Bella¹⁵⁴, L Bellagamba^{22a}, A Bellerive³¹, M Bellomo⁸⁸, K Belotskiy⁹⁹, O Beltramello³², N L Belyaev⁹⁹, O Benary¹⁵⁴, D Benchechroun^{136a}, M Bender¹⁰¹, K Bendtz^{147a,147b}, N Benekos¹⁰, Y Benhammou¹⁵⁴, E Benhar Noccioli¹⁷⁶, J Benitez⁶⁵, D P Benjamin⁴⁷, J R Bensinger²⁵, S Bentvelsen¹⁰⁸, L Beresford¹²¹, M Beretta⁴⁹, D Berge¹⁰⁸, E Bergeas Kuutmann¹⁶⁵, N Berger⁵, J Beringer¹⁶, S Berlendis⁵⁷, N R Bernard⁸⁸, C Bernius¹¹¹, F U Bernlochner²³, T Berry⁷⁹, P Berta¹³⁰, C Bertella⁸⁵, G Bertoli^{147a,147b}, F Bertolucci^{125a,125b}, I A Bertram⁷⁴, C Bertsche⁴⁴, D Bertsche¹¹⁴, G J Besjes³⁸, O Bessidskaia Bylund^{147a,147b}, M Bessner⁴⁴, N Besson¹³⁷, C Betancourt⁵⁰, S Bethke¹⁰², A J Bevan⁷⁸, W Bhimji¹⁶, R M Bianchi¹²⁶, L Bianchini²⁵, M Bianco³², O Biebel¹⁰¹, D Biedermann¹⁷, R Bielski⁸⁶, N V Biesuz^{125a,125b}, M Biglietti^{135a}, J Bilbao De Mendizabal⁵¹, H Bilokon⁴⁹, M Bindi⁵⁶, S Binet¹¹⁸, A Bingul^{20b}, C Bini^{133a,133b}, S Biondi^{22a,22b}, D M Bjergaard⁴⁷, C W Black¹⁵¹, J E Black¹⁴⁴, K M Black²⁴, D Blackburn¹³⁹, R E Blair⁶, J-B Blanchard¹³⁷, J E Blanco⁷⁹, T Blazek^{145a}, I Bloch⁴⁴, C Blocker²⁵, W Blum^{85,224}, U Blumenschein⁵⁶, S Blunier^{34a}, G J Bobbink¹⁰⁸, V S Bobrovnikov^{110,181}, S S Bocchetta⁸³, A Bocci⁴⁷, C Bock¹⁰¹, M Boehler⁵⁰, D Boerner¹⁷⁵, J A Bogaerts³², D Bogavac¹⁴, A G Bogdanchikov¹¹⁰, C Bohm^{147a}, V Boisvert⁷⁹, P Bokan¹⁴, T Bold^{40a}, A S Boldyrev^{164a,164c}, M Bomben⁸², M Bona⁷⁸, M Boonekamp¹³⁷, A Borisov¹³¹, G Borissow⁷⁴, J Bortfeldt¹⁰¹, D Bortoletto¹²¹, V Bortolotto^{62a,62b,62c}, K Bos¹⁰⁸, D Boscherini^{22a}, M Bosman¹³, J D Bossio Sola²⁹, J Boudreau¹²⁶, J Bouffard², E V Bouhova-Thacker⁷⁴, D Boumediene³⁶, C Bourdarios¹¹⁸, S K Boutle⁵⁵, A Boveia³², J Boyd³², I R Boyko⁶⁷, J Bracinik¹⁹, A Brandt⁸, G Brandt⁵⁶, O Brandt^{60a}, U Bratzler¹⁵⁷, B Brau⁸⁸, J E Brau¹¹⁷, H M Braun^{175,224}, W D Breaden Madden⁵⁵, K Brendlinger¹²³, A J Brennan⁹⁰, L Brenner¹⁰⁸, R Brenner¹⁶⁵, S Bressler¹⁷², T M Bristow⁴⁸, D Britton⁵⁵, D Britzger⁴⁴, F M Brochu³⁰, I Brock²³, R Brock⁹², G Brooijmans³⁷, T Brooks⁷⁹, W K Brooks^{34b}, J Brosamer¹⁶, E Brost¹¹⁷, J H Broughton¹⁹, P A Bruckman de Renstrom⁴¹, D Bruncko^{145b}, R Bruneliere⁵⁰, A Bruni^{22a}, G Bruni^{22a}, L S Bruni¹⁰⁸, B H Brunt³⁰, M Bruschi^{22a}, N Bruscinò²³, P Bryant³³, L Bryngemark⁸³, T Buanes¹⁵, Q Buat¹⁴³, P Buchholz¹⁴², A G Buckley⁵⁵, I A Budagov⁶⁷, F Buehrer⁵⁰, M K Bugge¹²⁰, O Bulekov⁹⁹, D Bullock⁸, H Burckhart³², S Burdin⁷⁶, C D Burgard⁵⁰, B Burghgrave¹⁰⁹, K Burka⁴¹, S Burke¹³², I Burmeister⁴⁵, E Busato³⁶, D Büscher⁵⁰, V Büscher⁸⁵, P Bussey⁵⁵, J M Butler²⁴, C M Buttar⁵⁵, J M Butterworth⁸⁰, P Butti¹⁰⁸, W Buttinger²⁷, A Buzatu⁵⁵, A R Buzykaev^{110,181}, S Cabrera Urbán¹⁶⁷, D Caforio¹²⁹, V M Cairo^{39a,39b}, O Cakir^{4a}, N Calace⁵¹, P Calafiura¹⁶, A Calandri⁸⁷, G Calderini⁸², P Calfayan¹⁰¹, L P Caloba^{26a}, D Calvet³⁶, S Calvet³⁶, T P Calvet⁸⁷, R Camacho Toro³³, S Camarda³², P Camarri^{134a,134b}, D Cameron¹²⁰, R Caminal Armadans¹⁶⁶, C Camincher⁵⁷, S Campana³², M Campanelli⁸⁰, A Camplani^{93a,93b}, A Campoverde¹⁴², V Canale^{105a,105b}, A Canepa^{160a}, M Cano Bret^{35e,35f}, J Cantero¹¹⁵, R Cantrill^{127a}, T Cao⁴², M D M Capeans Garrido³², I Caprini^{28b}, M Caprini^{28b}, M Capua^{39a,39b}, R Caputo⁸⁵, R M Carbone³⁷, R Cardarelli^{134a}, F Cardillo⁵⁰, I Carli¹³⁰, T Carli³², G Carlino^{105a}, L Carminati^{93a,93b}, S Caron¹⁰⁷, E Carquin^{34b}, G D Carrillo-Montoya³², J R Carter³⁰, J Carvalho^{127a,127c}, D Casadei¹⁹, M P Casado^{13,186}, M Casolino¹³, D W Casper¹⁶³, E Castaneda-Miranda^{146a}, R Castelijns¹⁰⁸, A Castelli¹⁰⁸, V Castillo Gimenez¹⁶⁷, N F Castro^{127a,187}, A Catinaccio³², J R Catmore¹²⁰, A Cattai³², J Caudron⁸⁵, V Cavaliere¹⁶⁶, E Cavallaro¹³, D Cavalli^{93a}, M Cavalli-Sforza¹³, V Cavasinni^{125a,125b}, F Ceradini^{135a,135b}, L Cerda Alberich¹⁶⁷, B C Cerio⁴⁷, A S Cerqueira^{26b}, A Cerri¹⁵⁰, L Cerrito⁷⁸, F Cerutti¹⁶, M Cerv³², A Cervelli¹⁸, S A Cetin^{20d}, A Chafaq^{136a}, D Chakraborty¹⁰⁹, S K Chan⁵⁹, Y L Chan^{62a}, P Chang¹⁶⁶, J D Chapman³⁰, D G Charlton¹⁹, A Chatterjee⁵¹, C C Chau¹⁵⁹, C A Chavez Barajas¹⁵⁰, S Che¹¹², S Cheatham⁷⁴, A Chegwidien⁹², S Chekanov⁶, S V Chekulaev^{160a}, G A Chelkov^{67,188}, M A Chelstowska⁹¹, C Chen⁶⁶, H Chen²⁷, K Chen¹⁴⁹, S Chen^{35c}, S Chen¹⁵⁶, X Chen^{35g}, Y Chen⁶⁹, H C Cheng⁹¹, H J Cheng^{35a}, Y Cheng³³, A Cheplakov⁶⁷, E Cheremushkina¹³¹, R Cherkaoui El Moursli^{27,224}, V Chernyatin^{27,224}, E Cheu⁷, L Chevalier¹³⁷, V Chiarella⁴⁹, G Chiarelli^{125a,125b}, G Chiodini^{75a}, A S Chisholm¹⁹, A Chitan^{28b}, M V Chizhov⁶⁷, K Choi⁶³, A R Chomont³⁶,

S Chouridou⁹, B K B Chow¹⁰¹, V Christodoulou⁸⁰, D Chromek-Burckhart³², J Chudoba¹²⁸, A J Chuinard⁸⁹, J J Chwastowski⁴¹, L Chytka¹¹⁶, G Ciapetti^{133a,133b}, A K Ciftci^{4a}, D Cinca⁵⁵, V Cindro⁷⁷, I A Cioara²³, A Ciochio¹⁶, F Ciotto^{105a,105b}, Z H Citron¹⁷², M Citterio^{93a}, M Ciubancan^{28b}, A Clark⁵¹, B L Clark⁵⁹, M R Clark³⁷, P J Clark⁴⁸, R N Clarke¹⁶, C Clement^{147a,147b}, Y Coadou⁸⁷, M Cobal^{164a,164c}, A Coccaro⁵¹, J Cochran⁶⁶, L Coffey²⁵, L Colasurdo¹⁰⁷, B Cole³⁷, A P Colijn¹⁰⁸, J Collot⁵⁷, T Colombo³², G Compostella¹⁰², P Conde Muino^{127a,127b}, E Coniavitis⁵⁰, S H Connell^{146b}, I A Connelly⁷⁹, V Consorti⁵⁰, S Constantinescu^{28b}, G Conti³², F Conventi^{105a,189}, M Cooke¹⁶, B D Cooper⁸⁰, A M Cooper-Sarkar¹²¹, K J R Cormier¹⁵⁹, T Cornelissen¹⁷⁵, M Corradi^{133a,133b}, F Corriveau^{89,190}, A Corso-Radu¹⁶³, A Cortes-Gonzalez¹³, G Cortiana¹⁰², G Costa^{93a}, M J Costa¹⁶⁷, D Costanzo¹⁴⁰, G Cottin³⁰, G Cowan⁷⁹, B E Cox⁸⁶, K Cranmer¹¹¹, S J Crawley⁵⁵, G Cree³¹, S Crépé-Renaudin⁵⁷, F Crescioli⁸², W A Cribbs^{147a,147b}, M Crispin Ortuzar¹²¹, M Cristinziani²³, V Croft¹⁰⁷, G Crosetti^{39a,39b}, T Cuhadar Donszelmann¹⁴⁰, J Cummings¹⁷⁶, M Curatolo⁴⁹, J Cúth⁸⁵, C Cuthbert¹⁵¹, H Czirr¹⁴², P Czodrowski³, G D'amen^{22a,22b}, S D'Auria⁵⁵, M D'Onofrio⁷⁶, M J Da Cunha Sargedas De Sousa^{127a,127b}, C Da Via⁸⁶, W Dabrowski^{40a}, T Dado^{145a}, T Dai⁹¹, O Dale¹⁵, F Dallaire⁹⁶, C Dallapiccola⁸⁸, M Dam³⁸, J R Dandoy³³, N P Dang⁵⁰, A C Daniells¹⁹, N S Dann⁸⁶, M Danninger¹⁶⁸, M Dano Hoffmann¹³⁷, V Dao⁵⁰, G Darbo^{52a}, S Darmora⁸, J Dassoulas³, A Dattagupta⁶³, W Davey²³, C David¹⁶⁹, T Davidek¹³⁰, M Davies¹⁵⁴, P Davison⁸⁰, E Dawe⁹⁰, I Dawson¹⁴⁰, R K Daya-Ishmukhametova⁸⁸, K De⁸, R de Asmundis^{105a}, A De Benedetti¹¹⁴, S De Castro^{22a,22b}, S De Cecco⁸², N De Groot¹⁰⁷, P de Jong¹⁰⁸, H De la Torre⁸⁴, F De Lorenzi⁶⁶, A De Maria⁵⁶, D De Pedis^{133a}, A De Salvo^{133a}, U De Sanctis¹⁵⁰, A De Santo¹⁵⁰, J B De Vivie De Regie¹¹⁸, W J Dearnaley⁷⁴, R Debbé²⁷, C Debenedetti¹³⁸, D V Dedovich⁶⁷, N Dehghanian³, I Deigaard¹⁰⁸, M Del Gaudio^{39a,39b}, J Del Peso⁸⁴, T Del Prete^{125a,125b}, D Delgove¹¹⁸, F Deliot¹³⁷, C M Delitzsch⁵¹, M Deliyergiyev⁷⁷, A Dell'Acqua³², L Dell'Asta²⁴, M Dell'Orso^{125a,125b}, M Della Pietra^{105a,189}, D della Volpe⁵¹, M Delmastro⁵, P A Delsart⁵⁷, C Deluca¹⁰⁸, D A DeMarco¹⁵⁹, S Demers¹⁷⁶, M Demichev⁶⁷, A Demilly⁸², S P Denisov¹³¹, D Denysiuk¹³⁷, D Derendarz⁴¹, J E Derkaoui^{136d}, F Derue⁸², P Dervan⁷⁶, K Desch²³, C Deterre⁴⁴, K Dette⁴⁵, P O Deviveiros³², A Dewhurst¹³², S Dhaliwal²⁵, A Di Ciaccio^{134a,134b}, L Di Ciaccio⁵, W K Di Clemente¹²³, C Di Donato^{133a,133b}, A Di Girolamo³², B Di Girolamo³², B Di Micco^{135a,135b}, R Di Nardo³², A Di Simone⁵⁰, R Di Sipio¹⁵⁹, D Di Valentino³¹, C Diaconu⁸⁷, M Diamond¹⁵⁹, F A Dias⁴⁸, M A Diaz^{34a}, E B Diehl⁹¹, J Dietrich¹⁷, S Diglio⁸⁷, A Dimitrievska¹⁴, J Dingfelder²³, P Dita^{28b}, S Dita^{28b}, F Dittus³², F Djama⁸⁷, T Djobava^{53b}, J I Djuvsland^{60a}, M A B do Vale^{26c}, D Dobos³², M Dobre^{28b}, C Doglioni⁸³, T Dohmae¹⁵⁶, J Dolejsi¹³⁰, Z Dolezal¹³⁰, B A Dolgoshein^{99,224}, M Donadelli^{26d}, S Donati^{125a,125b}, P Dondero^{122a,122b}, J Donini³⁶, J Dopke¹³², A Doria^{105a}, M T Dova⁷³, A T Doyle⁵⁵, E Drechsler⁵⁶, M Dris¹⁰, Y Du^{35d}, J Duarte-Campderros¹⁵⁴, E Duchovni¹⁷², G Duckeck¹⁰¹, O A Ducu^{96,191}, D Duda¹⁰⁸, A Dudarev³², E M Duffield¹⁶, L Duflot¹¹⁸, L Duguid⁷⁹, M Dührssen³², M Dumancic¹⁷², M Dunford^{60a}, H Duran Yildiz^{4a}, M Düren⁵⁴, A Durglishvili^{53b}, D Duschinger⁴⁶, B Dutta⁴⁴, M Dyndal⁴⁴, C Eckardt⁴⁴, K M Ecker¹⁰², R C Edgar⁹¹, N C Edwards⁴⁸, T Eifert³², G Eigen¹⁵, K Einsweiler¹⁶, V Ellajosyula⁸⁷, M Ellert¹⁶⁵, S Elles⁵, F Ellinghaus¹⁷⁵, A A Elliot¹⁶⁹, N Ellis³², J Elmsheuser²⁷, M Elsing³², D Emelianov¹³², Y Enari¹⁵⁶, O C Endner⁸⁵, M Endo¹¹⁹, J S Ennis¹⁷⁰, J Erdmann⁴⁵, A Ereditato¹⁸, G Ernis¹⁷⁵, J Ernst², M Ernst²⁷, S Errede¹⁶⁶, E Ertel⁸⁵, M Escalier¹¹⁸, H Esch⁴⁵, C Escobar¹²⁶, B Esposito⁴⁹, A I Etienne¹³⁷, E Etzion¹⁵⁴, H Evans⁶³, A Ezhilov¹²⁴, F Fabbri^{22a,22b}, L Fabbri^{22a,22b}, G Facini³³, R M Fakhrutdinov¹³¹, S Falciano^{133a}, R J Falla⁸⁰, J Faltova¹³⁰, Y Fang^{35a}, M Fantì^{93a,93b}, A Farbin⁸, A Farilla^{135a}, C Farina¹²⁶, T Farooque¹³, S Farrell¹⁶, S M Farrington¹⁷⁰, P Farthouat³², F Fassi^{136c}, P Fassnacht³², D Fassouliotis⁹, M Fauci Giannelli⁷⁹, A Favareto^{52a,52b}, W J Fawcett¹²¹, L Fayard¹¹⁸, O L Fedin^{124,192}, W Fedorko¹⁶⁸, S Feigl¹²⁰, L Feligioni⁸⁷, C Feng^{35d}, E J Feng³², H Feng⁹¹, A B Fenyyuk¹³¹, L Feremenga⁸, P Fernandez Martinez¹⁶⁷, S Fernandez Perez¹³, J Ferrando⁵⁵, A Ferrari¹⁶⁵, P Ferrari¹⁰⁸, R Ferrari^{122a}, D E Ferreira de Lima^{60b}, A Ferrer¹⁶⁷, D Ferrere⁵¹, C Ferretti⁹¹, A Ferretto Parodi^{52a,52b}, F Fiedler⁸⁵, A Filipčič⁷⁷, M Filipuzzi⁴⁴, F Filthaut¹⁰⁷, M Fincke-Keeler¹⁶⁹, K D Finelli¹⁵¹, M C N Fiolhais^{127a,127c}, L Fiorini¹⁶⁷, A Firan⁴², A Fischer², C Fischer¹³, J Fischer¹⁷⁵, W C Fisher⁹², N Flaschel⁴⁴, I Fleck¹⁴², P Fleischmann⁹¹, G T Fletcher¹⁴⁰, R R M Fletcher¹²³, T Flick¹⁷⁵, A Floderus⁸³, L R Flores Castillo^{62a}, M J Flowerdew¹⁰², G T Forcolin⁸⁶, A Formica¹³⁷, A Forti⁸⁶, A G Foster¹⁹, D Fournier¹¹⁸, H Fox⁷⁴, S Fracchia¹³, P Francavilla⁸², M Franchini^{22a,22b}, D Francis³², L Franconi¹²⁰, M Franklin⁵⁹, M Frate¹⁶³, M Fraternali^{122a,122b}, D Freeborn⁸⁰, S M Fressard-Batraneanu³², F Friedrich⁴⁶, D Froidevaux³², J A Frost¹²¹, C Fukunaga¹⁵⁷, E Fullana Torregrosa⁸⁵, T Fusayasu¹⁰³, J Fuster¹⁶⁷, C Gabaldon⁵⁷, O Gabizon¹⁷⁵, A Gabrielli^{22a,22b}, A Gabrielli¹⁶, G P Gach^{40a}, S Gadatsch³², S Gadomski⁵¹, G Gagliardi^{52a,52b}, L G Gagnon⁹⁶, P Gagnon⁶³, C Galea¹⁰⁷, B Galhardo^{127a,127c}, E J Gallas¹²¹, B J Gallop¹³², P Gallus¹²⁹, G Galster³⁸, K K Gan¹¹², J Gao^{35b,87}, Y Gao⁴⁸, Y S Gao^{144,184}, F M Garay Walls⁴⁸, C García¹⁶⁷, J E García Navarro¹⁶⁷, M Garcia-Sciveres¹⁶, R W Gardner³³, N Garelli¹⁴⁴, V Garonne¹²⁰, A Gascon Bravo⁴⁴, C Gatti⁴⁹, A Gaudiello^{52a,52b}, G Gaudio^{122a}, B Gaur¹⁴², L Gauthier⁹⁶, I L Gavrilenko⁹⁷, C Gay¹⁶⁸, G Gaycken²³, E N Gazis¹⁰, Z Gecse¹⁶⁸, C N P Gee¹³², Ch Geich-Gimbel²³, M Geisen⁸⁵, M P Geisler^{60a}, C Gemme^{52a}, M H Genest⁵⁷, C Geng^{35b,193}, S Gentile^{133a,133b}, S George⁷⁹, D Gerbaudo¹³, A Gershon¹⁵⁴, S Ghasemi¹⁴², H Ghazlane^{136b}, M Ghneimat²³, B Giacobbe^{22a}, S Giagu^{133a,133b}, P Giannetti^{125a,125b}, B Gibbard²⁷, S M Gibson⁷⁹, M Gignac¹⁶⁸, M Gilchriese¹⁶, T P S Gillam³⁰, D Gillberg³¹, G Gilles¹⁷⁵, D M Gingrich^{3,182}, N Giokaris⁹, M P Giordani^{164a,164c}, F M Giorgi^{22a}, F M Giorgi¹⁷, P F Giraud¹³⁷, P Giromini⁵⁹, D Giugni^{93a}, F Giulì¹²¹, C Giuliani¹⁰², M Giulini^{60b}, B K Gjølsten¹²⁰,

S Gkaitatzis¹⁵⁵, I Gkialas¹⁵⁵, E L Gkoukousis¹¹⁸, L K Gladilin¹⁰⁰, C Glasman⁸⁴, J Glatzer³², P C F Glaysheer⁴⁸, A Glazov⁴⁴, M Goblirsch-Kolb¹⁰², J Godlewski⁴¹, S Goldfarb⁹¹, T Golling⁵¹, D Golubkov¹³¹, A Gomes^{127a,127b,127d}, R Gonçalves^{127a}, J Goncalves Pinto Firmino Da Costa¹³⁷, G Gonella⁵⁰, L Gonella¹⁹, A Gongadze⁶⁷, S González de la Hoz¹⁶⁷, G Gonzalez Parra¹³, S Gonzalez-Sevilla⁵¹, L Goossens³², P A Gorbounov⁹⁸, H A Gordon²⁷, I Gorelov¹⁰⁶, B Gorini³², E Gorini^{75a,75b}, A Gorišek⁷⁷, E Gornicki⁴¹, A T Goshaw⁴⁷, C Gössling⁴⁵, M I Gostkin⁶⁷, C R Goudet¹¹⁸, D Goujdami^{136c}, A G Goussiou¹³⁹, N Govender^{146b,194}, E Gozani¹⁵³, L Graber⁵⁶, I Grabowska-Bold^{40a}, P O J Gradin⁵⁷, P Grafström^{22a,22b}, J Gramling⁵¹, E Gramstad¹²⁰, S Grancagnolo¹⁷, V Gratchev¹²⁴, P M Gravila^{28e}, H M Gray³², E Graziani^{135a}, Z D Greenwood^{81,195}, C Greife²³, K Gregersen⁸⁰, I M Gregor⁴⁴, P Grenier¹⁴⁴, K Grevtsov⁵, J Griffiths⁸, A A Grillo¹³⁸, K Grimm⁷⁴, S Grinstein^{13,196}, Ph Gris³⁶, J-F Grivaz¹¹⁸, S Groh⁸⁵, J P Grohs⁴⁶, E Gross¹⁷², J Grosse-Knetter⁵⁶, G C Grossi⁸¹, Z J Grout¹⁵⁰, L Guan⁹¹, W Guan¹⁷³, J Guenther¹²⁹, F Guescini⁵¹, D Guest¹⁶³, O Gueta¹⁵⁴, E Guido^{52a,52b}, T Guillemin⁵, S Guindon², U Gul⁵⁵, C Gumpert³², J Guo^{35e,35f}, Y Guo^{35b,193}, S Gupta¹²¹, G Gustavino^{133a,133b}, P Gutierrez¹¹⁴, N G Gutierrez Ortiz⁸⁰, C Gutschow⁴⁶, C Guyot¹³⁷, C Gwenlan¹²¹, C B Gwilliam⁷⁶, A Haas¹¹¹, C Haber¹⁶, H K Hadavand⁸, N Haddad^{136e}, A Hadeef⁸⁷, P Haefner²³, S Hageböck²³, Z Hajduk⁴¹, H Hakobyan^{177,224}, M Haleem⁴⁴, J Haley¹¹⁵, G Halladjian⁹², G D Hallowell⁸⁷, K Hamacher¹⁷⁵, P Hamal¹¹⁶, K Hamano¹⁶⁹, A Hamilton^{146a}, G N Hamity¹⁴⁰, P G Hamnett⁴⁴, L Han^{35b}, K Hanagaki^{168,197}, K Hanawa¹⁵⁶, M Hance¹³⁸, B Haney¹²³, P Hanke^{60a}, R Hanna¹³⁷, J B Hansen³⁸, J D Hansen³⁸, M C Hansen²³, P H Hansen³⁸, K Hara¹⁶¹, A S Hard¹⁷³, T Harenberg¹⁷⁵, F Hariri¹¹⁸, S Harkusha⁹⁴, R D Harrington⁴⁸, P F Harrison¹⁷⁰, F Hartjes¹⁰⁸, N M Hartmann¹⁰¹, M Hasegawa⁶⁹, Y Hasegawa¹⁴¹, A Hasib¹¹⁴, S Hassani¹³⁷, S Haug¹⁸, R Hauser⁹², L Hauswald⁴⁶, M Havranek¹²⁸, C M Hawkes¹⁹, R J Hawkings³², D Hayden⁹², C P Hays¹²¹, J M Hays⁷⁸, H S Hayward⁷⁶, S J Haywood¹³², S J Head¹⁹, T Heck⁸⁵, V Hedberg⁸³, L Heelan⁸, S Heim¹²³, T Heim¹⁶, B Heinemann¹⁶, J J Heinrich¹⁰¹, L Heinrich¹¹¹, C Heinz⁵⁴, J Hejbal¹²⁸, L Helary²⁴, S Hellman^{147a,147b}, C Helsen³², J Henderson¹²¹, R C W Henderson⁷⁴, Y Heng¹⁷³, S Henkelmann¹⁶⁸, A M Henriques Correia³², S Henrot-Versille¹¹⁸, G H Herbert¹⁷, Y Hernández Jiménez¹⁶⁷, G Herten⁵⁰, R Hertenberger¹⁰¹, L Hervas³², G G Hesketh⁸⁰, N P Hessey¹⁰⁸, J W Hetherly⁴², R Hickling⁷⁸, E Higón-Rodríguez¹⁶⁷, E Hill¹⁶⁹, J C Hill³⁰, K H Hiller⁴⁴, S J Hillier¹⁹, I Hinchliffe¹⁶, E Hines¹²³, R R Hinman¹⁶, M Hirose¹⁵⁸, D Hirschbuehl¹⁷⁵, J Hobbs¹⁴⁹, N Hod^{160a}, M C Hodgkinson¹⁴⁰, P Hodgson¹⁴⁰, A Hoecker³², M R Hoefkamp¹⁰⁶, F Hoenig¹⁰¹, D Hohn²³, T R Holmes¹⁶, M Homann⁴⁵, T M Hong¹²⁶, B H Hooberman¹⁶⁶, W H Hopkins¹¹⁷, Y Horii¹⁰⁴, A J Horton¹⁴³, J-Y Hostachy⁵⁷, S Hou¹⁵², A Hoummada^{136a}, J Howarth⁴⁴, M Hrabovsky¹¹⁶, I Hristova¹⁷, J Hrivnac¹¹⁸, T Hryn'ova⁵, A Hrynevich⁹⁵, C Hsu^{146c}, P J Hsu^{152,198}, S-C Hsu¹³⁹, D Hu³⁷, Q Hu^{35b}, Y Huang⁴⁴, Z Hubacek¹²⁹, F Hubaut⁸⁷, F Huegging²³, T B Huffman¹²¹, E W Hughes³⁷, G Hughes⁷⁴, M Huhtinen³², T A Hülsing⁸⁵, P Huo¹⁴⁹, N Huseynov^{67,180}, J Huston⁹², J Huth⁵⁹, G Iacobucci⁵¹, G Iakovidis²⁷, I Ibragimov¹⁴², L Iconomidou-Fayard¹¹⁸, E Ideal¹⁷⁶, Z Idriissi^{136e}, P Iengo³², O Igonkina^{108,199}, T Iizawa¹⁷¹, Y Ikegami⁶⁸, M Ikeno⁶⁸, Y Ilchenko^{11,200}, D Iliadis¹⁵⁵, N Ilic¹⁴⁴, T Ince¹⁰², G Introzzi^{122a,122b}, P Ioannou^{9,224}, M Iodice^{135a}, K Iordanidou³⁷, V Ippolito⁵⁹, M Ishino⁷⁰, M Ishitsuka¹⁵⁸, R Ishmukhametov¹¹², C Issever¹²¹, S Istin^{20a}, F Ito¹⁶¹, J M Iturbe Ponce⁸⁶, R Iuppa^{134a,134b}, W Iwanski⁴¹, H Iwasaki⁶⁸, J M Izen⁴³, V Izzo^{105a}, S Jabbar³, B Jackson¹²³, M Jackson⁷⁶, P Jackson¹, V Jain², K B Jakobi⁸⁵, K Jakobs⁵⁰, S Jakobsen³², T Jakoubek¹²⁸, D O Jamin¹¹⁵, D K Jana⁸¹, E Jansen⁸⁰, R Jansky⁶⁴, J Janssen²³, M Janus⁵⁶, G Jarlskog⁸³, N Javadov^{67,180}, T Javůrek⁵⁰, F Jeanneau¹³⁷, L Jeanty¹⁶, J Jejelava^{53a,201}, G-Y Jeng¹⁵¹, D Jennens⁹⁰, P Jenni^{50,202}, J Jentzsch⁴⁵, C Jeske¹⁷⁰, S Jézéquel⁵, H Ji¹⁷³, J Jia¹⁴⁹, H Jiang⁶⁶, Y Jiang^{35b}, S Jiggins⁸⁰, J Jimenez Pena¹⁶⁷, S Jin^{35a}, A Jinaru^{28b}, O Jinnouchi¹⁵⁸, P Johansson¹⁴⁰, K A Johns⁷, W J Johnson¹³⁹, K Jon-And^{147a,147b}, G Jones¹⁷⁰, R W L Jones⁷⁴, S Jones⁷, T J Jones⁷, J Jongmanns^{60a}, P M Jorge^{127a,127b}, J Jovicevic^{160a}, X Ju¹⁷³, A Juste Rozas^{13,196}, M K Köhler¹⁷², A Kaczmarska⁴¹, M Kado¹¹⁸, H Kagan¹¹², M Kagan¹⁴⁴, S J Kahn⁸⁷, E Kajomovitz⁴⁷, C W Kalderon¹²¹, A Kaluza⁸⁵, S Kama⁴², A Kamenshchikov¹³¹, N Kanaya¹⁵⁶, S Kaneti³⁰, L Kanjir⁷⁷, V A Kantserov⁹⁹, J Kanzaki⁶⁸, B Kaplan¹¹¹, L S Kaplan¹⁷³, A Kapliy³³, D Kar^{146c}, K Karakostas¹⁰, A Karamaoun³, N Karastathis¹⁰, M J Kareem⁵⁶, E Karentzos¹⁰, M Karneviskiy⁸⁵, S N Karpov⁶⁷, Z M Karpova⁶⁷, K Karthik¹¹¹, V Kartvelishvili⁷⁴, A N Karyukhin¹³¹, K Kasahara¹⁶¹, L Kashif¹⁷³, R D Kass¹¹², A Kastanas¹⁵, Y Kataoka¹⁵⁶, C Kato¹⁵⁶, A Katre⁵¹, J Katzy⁴⁴, K Kawagoe⁷², T Kawamoto¹⁵⁶, G Kawamura⁵⁶, S Kazama¹⁵⁶, V F Kazanin^{110,181}, R Keeler¹⁶⁹, R Kehoe⁴², J S Keller⁷⁹, J J Kempster⁷⁹, K Kentaro¹⁰⁴, H Keoshkerian¹⁵⁹, O Kepka¹²⁸, B P Kerševan⁷⁷, S Kersten¹⁷⁵, R A Keyes⁸⁹, F Khalil-zada¹², A Khanov¹¹⁵, A G Kharlamov^{110,181}, T J Khoo⁵¹, V Khovanskiy⁹⁸, E Khramov⁶⁷, J Khubua^{53b,203}, S Kido⁶⁹, H Y Kim⁸, S H Kim¹⁶¹, Y K Kim³³, N Kimura¹⁵⁵, O M Kind¹⁷, B T King⁷⁶, M King¹⁶⁷, S B King¹⁶⁸, J Kirk¹³², A E Kiryunin¹⁰², T Kishimoto⁶⁹, D Kisielevska^{40a}, F Kiss⁵⁰, K Kiuchi¹⁶¹, O Kivernyk¹³⁷, E Kladiiva^{145b}, M H Klein³⁷, M Klein⁷⁶, U Klein⁷⁶, K Kleinknecht⁸⁵, P Klimek^{147a,147b}, A Klimentov²⁷, R Klingenberg⁴⁵, J A Klinger¹⁴⁰, T Klioutchnikova³², E-E Kluge^{60a}, P Kluit¹⁰⁸, S Kluth¹⁰², J Knapik⁴¹, E Kneringer⁶⁴, E B F G Knoops⁸⁷, A Knue⁵⁵, A Kobayashi¹⁵⁶, D Kobayashi¹⁵⁸, T Kobayashi¹⁵⁶, M Kobel⁴⁶, M Kocian¹⁴⁴, P Kodys¹³⁰, T Koffas³¹, E Koffeman¹⁰⁸, T Koi¹⁴⁴, H Kolanoski¹⁷, M Kolb^{60b}, I Koletsou⁵, A A Komar^{97,224}, Y Komori¹⁵⁶, T Kondo⁶⁸, N Kondrashova⁴⁴, K Köneke⁸⁵, A C König¹⁰⁷, T Kono^{68,204}, R Konoplich^{111,205}, N Konstantinidis⁸⁰, R Kopeliansky⁶³, S Koperny^{40a}, L Köpke⁸⁵, A K Kopp⁵⁰, K Korcyl⁴¹, K Kordas¹⁵⁵, A Korn⁸⁰, A A Korol^{110,181}, I Korolkov¹³, E V Korolkova¹⁴⁰, O Kortner¹⁰², S Kortner¹⁰², T Kosek¹³⁰, V V Kostyukhin²³, A Kotwal⁴⁷, A Kourkouveli-Charalampidi¹⁵⁵, C Kourkouvelis⁹, V Kouskoura²⁷, A B Kowalewska⁴¹, R Kowalewski¹⁶⁹, T Z Kowalski^{40a}, C Kozakai¹⁵⁶

W Kozanecki¹³⁷, A S Kozhin¹³¹, V A Kramarenko¹⁰⁰, G Kramberger⁷⁷, D Krasnopevtsev⁹⁹, M W Krasny⁸², A Krasznahorkay³², J K Kraus²³, A Kravchenko²⁷, M Kretz^{60c}, J Kretzschmar⁷⁶, K Kreutzfeldt⁵⁴, P Krieger¹⁵⁹, K Krizka³³, K Kroeninger⁴⁵, H Kroha¹⁰², J Kroll¹²³, J Kroseberg²³, J Krstic¹⁴, U Kruchonak⁶⁷, H Krüger²³, N Krumnack⁶⁶, A Kruse¹⁷³, M C Kruse⁴⁷, M Kruskal²⁴, T Kubota⁹⁰, H Kucuk⁸⁰, S Kuday^{4b}, J T Kuechler¹⁷⁵, S Kuehn⁵⁰, A Kugel^{60c}, F Kuger¹⁷⁴, A Kuhl¹³⁸, T Kuhl⁴⁴, V Kukhtin⁶⁷, R Kukla¹³⁷, Y Kulchitsky⁹⁴, S Kuleshov^{34b}, M Kuna^{133a,133b}, T Kunigo⁷⁰, A Kupco¹²⁸, H Kurashige⁶⁹, Y A Kurochkin⁹⁴, V Kus¹²⁸, E S Kuwertz¹⁶⁹, M Kuze¹⁵⁸, J Kvita¹¹⁶, T Kwan¹⁶⁹, D Kyriazopoulos¹⁴⁰, A La Rosa¹⁰², J L La Rosa Navarro^{26d}, L La Rotonda^{39a,39b}, C Lacasta¹⁶⁷, F Lacava^{133a,133b}, J Lacey³¹, H Lacker¹⁷, D Lacour⁸², V R Lacuesta¹⁶⁷, E Ladygin⁶⁷, R Lafaye⁵, B Laforge⁸², T Lagouri¹⁷⁶, S Lai⁵⁶, S Lammers⁶³, W Lampl⁷, E Lançon¹³⁷, U Landgraf⁵⁰, M P J Landon⁷⁸, V S Lang^{60a}, J C Lange¹³, A J Lankford¹⁶³, F Lanni²⁷, K Lantzsch²³, A Lanza^{122a}, S Laplace⁸², C Lapoire³², J F Laporte¹³⁷, T Lari^{93a}, F Lasagni Manghi^{22a,22b}, M Lassnig³², P Laurelli⁴⁹, W Lavrijsen¹⁶, A T Law¹³⁸, P Laycock⁷⁶, T Lazovich⁵⁹, M Lazzaroni^{93a,93b}, B Le⁹⁰, O Le Dortz⁸², E Le Guirriec⁸⁷, E P Le Quilleuc¹³⁷, M LeBlanc¹⁶⁹, T LeCompte⁶, F Ledroit-Guillon⁵⁷, C A Lee²⁷, S C Lee¹⁵², L Lee¹, G Lefebvre⁸², M Lefebvre¹⁶⁹, F Legger¹⁰¹, C Leggett¹⁶, A Lehan⁷⁶, G Lehmann Miotto³², X Lei⁷, W A Leight³¹, A Leisos^{155,206}, A G Leister¹⁷⁶, M A L Leite^{26d}, R Leitner¹³⁰, D Lellouch¹⁷², B Lemmer⁵⁶, K J C Leney⁸⁰, T Lenz²³, B Lenzi³², R Leone⁷, S Leone^{125a,125b}, C Leonidopoulos⁴⁸, S Leontsinis¹⁰, G Lerner¹⁵⁰, C Leroy⁹⁶, A A J Lesage¹³⁷, C G Lester³⁰, M Levchenko¹²⁴, J Levêque⁵, D Levin⁹¹, L J Levinson¹⁷², M Levy¹⁹, D Lewis⁷⁸, A M Leyko²³, M Leyton⁴³, B Li^{35b,193}, H Li¹⁴⁹, H L Li³³, L Li⁴⁷, L Li^{35c,35f}, Q Li^{35a}, S Li⁴⁷, X Li⁸⁶, Y Li¹⁴², Z Liang^{35a}, B Liberti^{134a}, A Liblong¹⁵⁹, P Lichard³², K Lie¹⁶⁶, J Liebal²³, W Liebig¹⁵, A Limosani¹⁵¹, S C Lin^{152,207}, T H Lin⁸⁵, B E Lindquist¹⁴⁹, A E Lioni⁵¹, E Lipeles¹²³, A Lipniacka¹⁵, M Lisovyi^{60b}, T M Liss¹⁶⁶, A Lister¹⁶⁸, A M Litke¹³⁸, B Liu^{152,208}, D Liu¹⁵², H Liu⁹¹, H Liu²⁷, J Liu⁸⁷, J B Liu^{35b}, K Liu⁸⁷, L Liu¹⁶⁶, M Liu⁴⁷, M Liu^{35b}, Y L Liu^{35b}, Y Liu^{35b}, M Livan^{122a,122b}, A Lleres⁵⁷, J Llorente Merino^{35a}, S L Lloyd⁷⁸, F Lo Sterzo¹⁵², E Lobodzinska⁴⁴, P Loch⁷, W S Lockman¹³⁸, F K Loebinger⁸⁶, A E Loevschall-Jensen³⁸, K M Loew²⁵, A Loginov¹⁷⁶, T Lohse¹⁷, K Lohwasser⁴⁴, M Lokajicek¹²⁸, B A Long²⁴, J D Long¹⁶⁶, R E Long⁷⁴, L Longo^{75a,75b}, K A Looper¹¹², L Lopes^{127a}, D Lopez Mateos⁵⁹, B Lopez Paredes¹⁴⁰, I Lopez Paz¹³, A Lopez Solis⁸², J Lorenz¹⁰¹, N Lorenzo Martinez⁶³, M Losada²¹, P J Lösel¹⁰¹, X Lou^{35a}, A Lounis¹¹⁸, J Love⁶, P A Love⁷⁴, H Lu^{62a}, N Lu⁹¹, H J Lubatti¹³⁹, C Luci^{133a,133b}, A Lucotte⁵⁷, C Luedtke⁵⁰, F Luehring⁶³, W Lukas⁶⁴, L Luminari^{133a}, O Lundberg^{147a,147b}, B Lund-Jensen¹⁴⁸, P M Luzi⁸², D Lynn²⁷, R Lysak¹²⁸, E Lytken⁸³, V Lyubushkin⁶⁷, H Ma²⁷, L L Ma^{35d}, Y Ma^{35d}, G Maccarrone⁴⁹, A Macchiolo¹⁰², C M Macdonald¹⁴⁰, B Maček⁷⁷, J Machado Miguens^{123,127b}, D Madaffari⁸⁷, R Madar³⁶, H J Maddocks¹⁶⁵, W F Mader⁴⁶, A Madsen⁴⁴, J Maeda⁶⁹, S Maeland¹⁵, T Maeno²⁷, A Maevskiy¹⁰⁰, E Magradze⁵⁶, J Mahlstedt¹⁰⁸, C Maiani¹¹⁸, C Maidantchik^{26a}, A A Maier¹⁰², T Maier¹⁰¹, A Maio^{127a,127b,127d}, S Majewski¹¹⁷, Y Makida⁶⁸, N Makovec¹¹⁸, B Malaescu⁸², Pa Malecki⁴¹, V P Maleev¹²⁴, F Malek⁵⁷, U Mallik⁶⁵, D Malon⁶, C Malone¹⁴⁴, S Maltezos¹⁰, S Malyukov³², J Mamuzic¹⁶⁷, G Mancini⁴⁹, B Mandelli³², L Mandelli^{93a}, I Mandić⁷⁷, J Maneira^{127a,127b}, L Manhaes de Andrade Filho^{26b}, J Manjarres Ramos^{160b}, A Mann¹⁰¹, A Manousos³², B Mansoulie¹³⁷, J D Mansour^{35a}, R Mantifel⁸⁹, M Mantoani⁵⁶, S Manzoni^{93a,93b}, L Mapelli³², G Marceca²⁹, L March⁵¹, G Marchiori⁸², M Marcisovsky¹²⁸, M Marjanovic¹⁴, D E Marley⁹¹, F Marroquim^{26a}, S P Marsden⁸⁶, Z Marshall¹⁶, S Marti-Garcia¹⁶⁷, B Martin⁹², T A Martin¹⁷⁰, V J Martin⁴⁸, B Martin dit Latour¹⁵, M Martinez^{13,196}, S Martin-Haugh¹³², V S Martoiu^{28b}, A C Martyniuk⁸⁰, M Marx¹³⁹, A Marzin³², L Masetti⁸⁵, T Mashimo¹⁵⁶, R Mashinistov⁹⁷, J Masik⁸⁶, A L Maslennikov^{110,181}, I Massa^{22a,22b}, L Massa^{22a,22b}, P Mastrandrea⁵, A Mastroberardino^{39a,39b}, T Masubuchi¹⁵⁶, P Mättig¹⁷⁵, J Mattmann⁸⁵, J Maurer^{28b}, S J Maxfield⁷⁶, D A Maximov^{110,181}, R Mazini¹⁵², S M Mazza^{93a,93b}, N C Mc Fadden¹⁰⁶, G Mc Goldrick¹⁵⁹, S P Mc Kee⁹¹, A McCarn⁹¹, R L McCarthy¹⁴⁹, T G McCarthy¹⁰², L I McClymont⁸⁰, E F McDonald⁹⁰, K W McFarlane^{58,224}, J A Mcfayden⁸⁰, G Mchedlidze⁵⁶, S J McMahon¹³², R A McPherson^{169,190}, M Medinnis⁴⁴, S Meehan¹³⁹, S Mehlhase¹⁰¹, A Mehta⁷⁶, K Meier^{60a}, C Meineck¹⁰¹, B Meirose⁴³, D Melini¹⁶⁷, B R Mellado Garcia^{146c}, M Melo^{145a}, F Meloni¹⁸, A Mengarelli^{22a,22b}, S Menke¹⁰², E Meoni¹⁶², S Mergelmeyer¹⁷, P Mermod⁵¹, L Merola^{105a,105b}, C Meroni^{93a}, F S Merritt³³, A Messina^{133a,133b}, J Metcalfe⁶, A S Mete¹⁶³, C Meyer⁸⁵, C Meyer¹²³, J-P Meyer¹³⁷, J Meyer¹⁰⁸, H Meyer Zu Theenhausen^{60a}, F Miano¹⁵⁰, R P Middleton¹³², S Miglioni^{52a,52b}, L Mijovic²³, G Mikenberg¹⁷², M Mikestikova¹²⁸, M Mikuz⁷⁷, M Milesi⁹⁰, A Milic⁶⁴, D W Miller³³, C Mills⁴⁸, A Milov¹⁷², D A Milstead^{147a,147b}, A A Minaenko¹³¹, Y Minami¹⁵⁶, I A Minashvili⁶⁷, A I Mincer¹¹¹, B Mindur^{40a}, M Mineev⁶⁷, Y Ming¹⁷³, L M Mir¹³, K P Mistry¹²³, T Mitani¹⁷¹, J Mitrevski¹⁰¹, V A Mitsou¹⁶⁷, A Miucci⁵¹, P S Miyagawa¹⁴⁰, J U Mjörnmark⁸³, T Moa^{147a,147b}, K Mochizuki⁹⁶, S Mohapatra³⁷, S Molander^{147a,147b}, R Moles-Valls²³, R Monden⁹², M C Mondragon⁹², K Mönig⁴⁴, J Monk³⁸, E Monnier⁸⁷, A Montalbano¹⁴⁹, J Montejó Berlingen³², F Monticelli⁷³, S Monzani^{93a,93b}, R W Moore³, N Morange¹¹⁸, D Moreno²¹, M Moreno Llacer⁵⁶, P Morettini^{52a}, D Mori¹⁴³, T Mori¹⁵⁶, M Morii⁵⁹, M Morinaga¹⁵⁶, V Morisbak¹²⁰, S Moritz⁸⁵, A K Morley¹⁵¹, G Mornacchi³², J D Morris⁷⁸, S S Mortensen³⁸, L Morvaj¹⁴⁹, M Mosidze^{53b}, J Moss¹⁴⁴, K Motohashi¹⁵⁸, R Mount¹⁴⁴, E Mountricha²⁷, S V Mouraviev^{97,224}, E J W Moyse⁸⁸, S Muanza⁸⁷, R D Mudd¹⁹, F Mueller¹⁰², J Mueller¹²⁶, R S P Mueller¹⁰¹, T Mueller³⁰, D Muenstermann⁷⁴, P Mullen⁵⁵, G A Mullier¹⁸, F J Munoz Sanchez⁸⁶, J A Murillo Quijada¹⁹, W J Murray^{170,132}, H Musheghyan⁵⁶, M Muškinja⁷⁷, A G Myagkov^{131,209}, M Myska¹²⁹, B P Nachman¹⁴⁴, O Nackenhorst⁵¹, K Nagai¹²¹, R Nagai^{68,204}, K Nagano⁶⁸, Y Nagasaka⁶¹, K Nagata¹⁶¹, M Nagel⁵⁰, E Nagy⁸⁷, A M Nairz³², Y Nakahama³², K Nakamura⁶⁸, T Nakamura¹⁵⁶, I Nakano¹¹³, H Namasivayam⁴³,

R F Naranjo Garcia⁴⁴, R Narayan¹¹, D I Narrias Villar^{60a}, I Naryshkin¹²⁴, T Naumann⁴⁴, G Navarro²¹, R Nayyar⁷, H A Neal⁹¹, P Yu Nechaeva⁹⁷, T J Neep⁸⁶, P D Nef⁴⁴, A Negri^{122a,122b}, M Negrini^{22a}, S Nektarijevic¹⁰⁷, C Nellist¹¹⁸, A Nelson¹⁶³, S Nemecek¹²⁸, P Nemethy¹¹¹, A A Nepomuceno^{26a}, M Nessi^{32,210}, M S Neubauer¹⁶⁶, M Neumann¹⁷⁵, R M Neves¹¹¹, P Nevski²⁷, P R Newman¹⁹, D H Nguyen⁶, T Nguyen Manh⁹⁶, R B Nickerson¹²¹, R Nicolaidou¹³⁷, J Nielsen¹³⁸, A Nikiforov¹⁷, V Nikolaenko^{131,209}, I Nikolic-Audit⁸², K Nikolopoulos¹⁹, J K Nilsen¹²⁰, P Nilsson²⁷, Y Ninomiya¹⁵⁶, A Nisati^{133a}, R Nisius¹⁰², T Nobe¹⁵⁶, L Nodulman⁶, M Nomachi¹¹⁹, I Nomidis³¹, T Nooney⁷⁸, S Norberg¹¹⁴, M Nordberg³², N Norjoharuddeen¹²¹, O Novgorodova⁴⁶, S Nowak¹⁰², M Nozaki⁶⁸, L Nozka¹¹⁶, K Ntekas¹⁰, E Nurse⁸⁰, F Nuti⁹⁰, F O'grady⁷, D C O'Neil¹⁴³, A A O'Rourke⁴⁴, V O'Shea⁵⁵, F G Oakham^{31,182}, H Oberlack¹⁰², T Obermann²³, J Ocariz⁸², A Ochi⁶⁹, I Ochoa³⁷, J P Ochoa-Ricoux^{34a}, S Oda⁷², S Odaka⁶⁸, H Ogren⁶³, A Oh⁸⁶, S H Oh⁴⁷, C C Ohm¹⁶, H Ohman¹⁶⁵, H Oide³², H Okawa¹⁶¹, Y Okumura³³, T Okuyama⁶⁸, A Olariu^{28b}, L F Oleiro Seabra^{127a}, S A Olivares Pino⁴⁸, D Oliveira Damazio²⁷, A Olszewski⁴¹, J Olszowska⁴¹, A Onofre^{127a,127c}, K Onogi¹⁰⁴, P U E Onyisi^{11,200}, M J Oreglia³³, Y Oren¹⁵⁴, D Orestano^{135a,135b}, N Orlando^{62b}, R S Orr¹⁵⁹, B Osculati^{52a,52b}, R Ospanov⁸⁶, G Otero y Garzon²⁹, H Otono⁷², M Ouchrif^{136d}, F Ould-Saada¹²⁰, A Ouraou¹³⁷, K P Oussoren¹⁰⁸, Q Ouyang^{35a}, M Owen⁵⁵, R E Owen¹⁹, V E Ozcan^{20a}, N Ozturk⁸, K Pachal¹⁴³, A Pacheco Pages¹³, C Padilla Aranda¹³, M Pagáčová⁵⁰, S Pagan Griso¹⁶, F Paige²⁷, P Pais⁸⁸, K Pajchel¹²⁰, G Palacino^{160b}, S Palestini³², M Palka^{40b}, D Pallin³⁶, A Palma^{127a,127b}, E St Panagiotopoulou¹⁰, C E Pandini⁸², J G Panduro Vazquez⁷⁹, P Pani^{147a,147b}, S Panitkin²⁷, D Pantea^{28b}, L Paolozzi⁵¹, Th D Papadopoulos¹⁰, K Papageorgiou¹⁵⁵, A Paramonov⁶, D Paredes Hernandez¹⁷⁶, A J Parker⁷⁴, M A Parker³⁰, K A Parker¹⁴⁰, F Parodi^{52a,52b}, J A Parsons³⁷, U Parzefall⁵⁰, V R Pascuzzi¹⁵⁹, E Pasqualucci^{133a}, S Passaggio^{52a}, Fr Pastore⁷⁹, G Pásztor^{31,211}, S Pataria¹⁷⁵, J R Pater⁸⁶, T Pauly³², J Pearce¹⁶⁹, B Pearson¹¹⁴, L E Pedersen³⁸, M Pedersen¹²⁰, S Pedraza Lopez¹⁶⁷, R Pedro^{127a,127b}, S V Peleganchuk^{110,181}, D Pelikan¹⁶⁵, O Penc¹²⁸, C Peng^{35a}, H Peng^{35b}, J Penwell⁶³, B S Peralva^{26b}, M M Perego¹³⁷, D V Perepelitsa²⁷, E Perez Codina^{160a}, L Perini^{93a,93b}, H Pernegger³², S Perrella^{105a,105b}, R Peschke⁴⁴, V D Peshekhonov⁶⁷, K Peters⁴⁴, R F Y Peters⁸⁶, B A Petersen³², T C Petersen³⁸, E Petit⁵⁷, A Petridis¹, C Petridou¹⁵⁵, P Petroff¹¹⁸, E Petrolo^{133a}, M Petrov¹²¹, F Petrucci^{135a,135b}, N E Pettersson⁸⁸, A Peyaud¹³⁷, R Pezoa^{34b}, P W Phillips¹³², G Piacquadio¹⁴⁴, E Pianori¹⁷⁰, A Picazio⁸⁸, E Piccaro⁷⁸, M Piccinini^{22a,22b}, M A Pickering¹²¹, R Piegai²⁹, J E Pilcher³³, A D Pilkington⁸⁶, A W J Pin⁸⁶, M Pinamonti^{164a,164c,212}, J L Pinfold³, A Pingel³⁸, S Pires⁸², H Pirumov⁴⁴, M Pitt¹⁷², L Plazak^{145a}, M-A Pleier²⁷, V Pleskot⁸⁵, E Plotnikova⁶⁷, P Plucinski⁹², D Pluth⁶⁶, R Poettgen^{147a,147b}, L Poggioli¹¹⁸, D Pohl²³, G Polesello^{122a}, A Poley⁴⁴, A Policicchio^{39a,39b}, R Polifka¹⁵⁹, A Polini^{22a}, C S Pollard⁵⁵, V Polychronakos²⁷, K Pommès³², L Pontecorvo^{133a}, B G Pope⁹², G A Popeneciu^{28c}, D S Popovic¹⁴, A Poppleton³², S Pospisil¹²⁹, K Potamianos¹⁶, I N Potrap⁶⁷, C J Potter³⁰, C T Potter¹¹⁷, G Poulard³², J Poveda³², V Pozdnyakov⁶⁷, M E Pozo Astigarraga³², P Pralavorio⁸⁷, A Pranko¹⁶, S Prell⁶⁶, D Price⁸⁶, L E Price⁶, M Primavera^{75a}, S Prince⁸⁹, M Proissl⁴⁸, K Prokofiev^{62c}, F Prokoshin^{34b}, S Protopopescu²⁷, J Proudfoot⁶, M Przybicien^{40a}, D Puddu^{135a,135b}, M Purohit^{27,213}, P Puzo¹¹⁸, J Qian⁹¹, G Qin⁵⁵, Y Qin⁸⁶, A Quadt⁵⁶, W B Quayle^{164a,164b}, M Queitsch-Maitland⁸⁶, D Quilty⁵⁵, S Raddum¹²⁰, V Radeka²⁷, V Radescu^{60b}, S K Radhakrishnan¹⁴⁹, P Radloff¹¹⁷, P Rados⁹⁰, F Ragusa^{93a,93b}, G Rahal¹⁷⁸, J A Raine⁸⁶, S Rajagopalan²⁷, M Rammensee³², C Rangel-Smith¹⁶⁵, M G Ratti^{93a,93b}, F Rauscher¹⁰¹, S Rave⁸⁵, T Ravenscroft⁵⁵, I Ravinovich¹⁷², M Raymond³², A L Read¹²⁰, N P Readioff⁷⁶, M Reale^{75a,75b}, D M Rebuffi^{122a,122b}, A Redelbach¹⁷⁴, G Redlinger²⁷, R Reece¹³⁸, K Reeves⁴³, L Rehnisch¹⁷, J Reichert¹²³, H Reisin²⁹, C Rembser³², H Ren^{35a}, M Rescigno^{133a}, S Resconi^{93a}, O L Rezanova^{110,181}, P Reznicek¹³⁰, R Rezvani⁹⁶, R Richter¹⁰², S Richter⁸⁰, E Richter-Was^{40b}, O Ricken²³, M Ridet⁸², P Rieck¹⁷, C J Riegel¹⁷⁵, J Rieger⁵⁶, O Rifki¹¹⁴, M Rijssenbeek¹⁴⁹, A Rimoldi^{122a,122b}, M Rimoldi¹⁸, L Rinaldi^{22a}, B Ristic⁵¹, E Ritsch³², I Riu¹³, F Rizatdinova¹¹⁵, E Rizvi⁷⁸, C Rizzi¹³, S H Robertson^{89,190}, A Robichaud-Veronneau⁸⁹, D Robinson³⁰, J E M Robinson⁴⁴, A Robson⁵⁵, C Roda^{125a,125b}, Y Rodina⁸⁷, A Rodriguez Perez¹³, D Rodriguez Rodriguez¹⁶⁷, S Roe³², C S Rogan⁵⁹, O Röhne¹²⁰, A Romaniouk⁹⁹, M Romano^{22a,22b}, S M Romano Saez³⁶, E Romero Adam¹⁶⁷, N Rompotis¹³⁹, M Ronzani⁵⁰, L Roos⁸², E Ros¹⁶⁷, S Rosati^{133a}, K Rosbach⁵⁰, P Rose¹³⁸, O Rosenthal¹⁴², N-A Rosien⁵⁶, V Rossetti^{147a,147b}, E Rossi^{105a,105b}, L P Rossi^{52a}, J H N Rosten³⁰, R Rosten¹³⁹, M Rotaru^{28b}, I Roth¹⁷², J Rothberg¹³⁹, D Rousseau¹¹⁸, C R Royon¹³⁷, A Rozanov⁸⁷, Y Rozen¹⁵³, X Ruan^{146c}, F Rubbo¹⁴⁴, M S Rudolph¹⁵⁹, F Rühr⁵⁰, A Ruiz-Martinez³¹, Z Rurikova⁵⁰, N A Rusakovich⁶⁷, A Ruschke¹⁰¹, H L Russell¹³⁹, J P Rutherford⁷, N Ruthmann³², Y F Ryabov¹²⁴, M Rybar¹⁶⁶, G Rybkin¹¹⁸, S Ryu⁶, A Ryzhov¹³¹, G F Rzehorz⁵⁶, A F Saavedra¹⁵¹, G Sabato¹⁰⁸, S Sacerdoti²⁹, H F-W Sadrozinski¹³⁸, R Sadykov⁶⁷, F Safai Tehrani^{133a}, P Saha¹⁰⁹, M Sahinsoy^{60a}, M Saimpert¹³⁷, T Saito¹⁵⁶, H Sakamoto¹⁵⁶, Y Sakurai¹⁷¹, G Salamanna^{135a,135b}, A Salamon^{134a,134b}, J E Salazar Loyola^{34b}, D Salek¹⁰⁸, P H Sales De Bruin¹³⁹, D Salihagic¹⁰², A Salnikov¹⁴⁴, J Salt², D Salvatore^{39a,39b}, F Salvatore¹⁵⁰, A Salvucci^{62a}, A Salzburger³², D Sammel⁵⁰, D Sampsonidis¹⁵⁵, A Sanchez^{105a,105b}, J Sánchez¹⁶⁷, V Sanchez Martinez¹⁶⁷, H Sandaker¹²⁰, R L Sandbach⁴⁹, H G Sander⁸⁵, M Sandhoff¹⁷⁵, C Sandoval²¹, R Sandstroem¹⁰², D P C Sankey¹³², M Sannino^{52a,52b}, A Sansoni⁴⁹, C Santoni³⁶, R Santonico^{134a,134b}, H Santos^{127a}, I Santoyo Castillo¹⁵⁰, K Sapp¹²⁶, A Saprnov⁶⁷, J G Saraiva^{127a,127d}, B Sarrazin²³, O Sasaki⁶⁸, Y Sasaki¹⁵⁶, K Sato¹⁶¹, G Sauvage^{5,224}, E Sauvan⁵, G Savage⁷⁹, P Savard^{159,182}, C Sawyer¹³², L Sawyer^{81,195}, J Saxon³³, C Sbarra^{22a}, A Sbrizzi^{22a,22b}, T Scanlon⁸⁰, D A Scannicchio¹⁶³, M Scarcella¹⁵¹, V Scarfone^{39a,39b}, J Schaarschmidt¹⁷², P Schacht¹⁰², B M Schachtner¹⁰¹, D Schaefer³², R Schaefer⁴⁴, J Schaeffer⁸⁵, S Schaepe²³, S Schaetzel^{60b}, U Schäfer⁸⁵, A C Schaffer¹¹⁸, D Schaile¹⁰¹,

R D Schamberger¹⁴⁹, V Scharf^{50a}, V A Schegelsky¹²⁴, D Scheirich¹³⁰, M Schernau¹⁶³, C Schiavi^{52a,52b}, S Schier¹³⁸, C Schillo⁵⁰, M Schioppa^{39a,39b}, S Schlenker³², K R Schmidt-Sommerfeld¹⁰², K Schmieden³², C Schmitt⁸⁵, S Schmitt⁴⁴, S Schmitz⁸⁵, B Schneider^{160a}, U Schnoor⁵⁰, L Schoeffel¹³⁷, A Schoening^{60b}, B D Schoenrock⁹², E Schopf²³, M Schott⁸⁵, J Schovancova⁸, S Schramm⁵¹, M Schreyer¹⁷⁴, N Schuh⁸⁵, M J Schultens²³, H-C Schultz-Coulon^{60a}, H Schulz¹⁷, M Schumacher⁵⁰, B A Schumm¹³⁸, Ph Schune¹³⁷, A Schwartzman¹⁴⁴, T A Schwarz⁹¹, Ph Schwegler¹⁰², H Schweiger⁸⁶, Ph Schwemling¹³⁷, R Schwienhorst⁹², J Schwindling¹³⁷, T Schwindt²³, G Sciolla²⁵, F Scuri^{125a,125b}, F Scutti⁹⁰, J Searcy⁹¹, P Seema²³, S C Seidel¹⁰⁶, A Seiden¹³⁸, F Seifert¹²⁹, J M Seixas^{26a}, G Sekhniadze^{105a}, K Sekhon⁹¹, S J Sekula⁴², D M Seliverstov^{124,224}, N Semprini-Cesari^{22a,22b}, C Serfon¹²⁰, L Serin¹¹⁸, L Serkin^{164a,164b}, M Sessa^{135a,135b}, R Seuster¹⁶⁹, H Severini¹¹⁴, T Sfiligoi⁷⁷, F Sforza³², A Sfyrila⁵¹, E Shabalina⁵⁶, N W Shaikh^{147a,147b}, L Y Shan^{35a}, R Shang¹⁶⁶, J T Shank²⁴, M Shapiro¹⁶, P B Shatalov⁹⁸, K Shaw^{164a,164b}, S M Shaw⁸⁶, A Shcherbakova^{147a,147b}, C Y Shehu¹⁵⁰, P Sherwood⁸⁰, L Shi^{152,224}, S Shimizu⁶⁹, C O Shimmin¹⁶³, M Shimojima¹⁰³, M Shiyakova^{67,215}, A Shmeleva⁹⁷, D Shoaleh Saadi⁹⁶, M J Shochet³³, S Shojai^{93a,93b}, S Shrestha¹¹², E Shulga⁹⁹, M A Shupe⁷, P Sicho¹²⁸, A M Sickles¹⁶⁶, P E Sidebo¹⁴⁸, O Sidiropoulou¹⁷⁴, D Sidorov¹¹⁵, A Sidoti^{22a,22b}, F Siegert⁴⁶, Dj Sijacki¹⁴, J Silva^{127a,127d}, S B Silverstein^{147a}, V Simak¹²⁹, O Simard⁵, Lj Simic¹⁴, S Simion¹¹⁸, E Simioni⁸⁵, B Simmons⁸⁰, D Simon³⁶, M Simon⁸⁵, P Sinervo¹⁵⁹, N B Sinev¹¹⁷, M Sioli^{22a,22b}, G Siragusa¹⁷⁴, S Yu Sivoklokov¹⁰⁰, J Sjölin^{147a,147b}, T B Sjursten¹⁵, M B Skinner⁷⁴, H P Skottowe⁵⁹, P Skubic¹¹⁴, M Slater¹⁹, T Slavicek¹²⁹, M Slawinska¹⁰⁸, K Sliwa¹⁶², R Slovak¹³⁰, V Smakhtin¹⁷², B H Smart⁵, L Smestad¹⁵, J Smiesko^{145a}, S Yu Smirnov⁹⁹, Y Smirnov⁹⁹, L N Smirnova^{100,216}, O Smirnova⁸³, M N K Smith³⁷, R W Smith³⁷, M Smizanska⁷⁴, K Smolek¹²⁹, A A Snesarev⁹⁷, S Snyder²⁷, R Sobie^{169,190}, F Socher⁴⁶, A Soffer¹⁵⁴, D A Soh¹⁵², G Sokhrannyi⁷⁷, C A Solans Sanchez³², M Solar¹²⁹, E Yu Soldatov⁹⁹, U Soldevila¹⁶⁷, A A Solodkov¹³¹, A Soloshenko⁶⁷, O V Solovyanov¹³¹, V Solovyev¹²⁴, P Sommer⁵⁰, H Son¹⁶², H Y Song^{35b,217}, A Sood¹⁶, A Sopczak¹²⁹, V Sopko¹²⁹, V Sorin¹³, D Sosa^{60b}, C L Sotiropoulou^{125a,125b}, R Soualah^{164a,164c}, A M Soukharev^{110,181}, D South⁴⁴, B C Sowden⁷⁹, S Spagnolo^{75a,75b}, M Spalla^{125a,125b}, M Spangenberg¹⁷⁰, F Spanò⁷⁹, D Sperlich¹⁷, F Spettel¹⁰², R Spighi^{22a}, G Spigo³², L A Spiller⁹⁰, M Spousta¹³⁰, R D St Denis^{55,224}, A Stabile^{93a}, R Stamen^{60a}, S Stamm¹⁷, E Stanecka⁴¹, R W Stanek⁶, C Stanescu^{135a}, M Stanescu-Bellu⁴⁴, M M Stanitzki⁴⁴, S Stapnes¹²⁰, E A Starchenko¹³¹, G H Stark³³, J Stark⁵⁷, P Staroba¹²⁸, P Starovoitov^{60a}, S Stärz³², R Staszewski⁴¹, P Steinberg²⁷, B Stelzer¹⁴³, H J Stelzer³², O Stelzer-Chilton^{160a}, H Stenzel⁵⁴, G A Stewart⁵⁵, J A Stillings²³, M C Stockton⁸⁹, M Stoebe⁸⁹, G Stoicea^{28b}, P Stolte⁵⁶, S Stonjek¹⁰², A R Stradling⁸, A Straessner⁴⁶, M E Stramaglia¹⁸, J Strandberg¹⁴⁸, S Strandberg^{147a,147b}, A Strandlie¹²⁰, M Strauss¹¹⁴, P Strizenc^{145b}, R Ströhmer¹⁷⁴, D M Strom¹¹⁷, R Stroynowski⁴², A Strubig¹⁰⁷, S A Stucci¹⁸, B Stugu¹⁵, N A Styles⁴⁴, D Su¹⁴⁴, J Su¹²⁶, R Subramaniam⁸¹, S Suchek^{60a}, Y Sugaya¹¹⁹, M Suk¹²⁹, V V Sulin⁹⁷, S Sultansoy^{4c}, T Sumida⁷⁰, S Sun⁵⁹, X Sun^{35a}, J E Sundermann⁵⁰, K Suruliz¹⁵⁰, G Susinno^{39a,39b}, M R Sutton¹⁵⁰, S Suzuki⁶⁸, M Svatos¹²⁸, M Swiatlowski³³, I Sykora^{145a}, T Sykora¹³⁰, D Ta⁵⁰, C Taccini^{135a,135b}, K Tackmann⁴⁴, J Taenzer¹⁵⁹, A Taffard¹⁶³, R Tafiout^{160a}, N Taiblum¹⁵⁴, H Takai²⁷, R Takashima⁷¹, T Takeshita¹⁴¹, Y Takubo⁶⁸, M Talby⁸⁷, A A Talyshev^{110,181}, K G Tan⁹⁰, J Tanaka¹⁵⁶, R Tanaka¹¹⁸, S Tanaka⁶⁸, B B Tannenwald¹¹², S Tapia Araya^{34b}, S Tapprogge⁸⁵, S Tarem¹⁵³, G F Tartarelli^{93a}, P Tas¹³⁰, M Tasevsky¹²⁸, T Tashiro⁷⁰, E Tassi^{39a,39b}, A Tavares Delgado^{127a,127b}, Y Tayalati^{136d}, A C Taylor¹⁰⁶, G N Taylor⁹⁰, P T E Taylor⁹⁰, W Taylor^{160b}, F A Teischinger³², P Teixeira-Dias⁷⁹, K K Temming⁵⁰, D Temple¹⁴³, H Ten Kate³², P K Teng¹⁵², J J Teoh¹¹⁹, F Tepel¹⁷⁵, S Terada⁶⁸, K Terashi¹⁵⁶, J Terron⁸⁴, S Terzo¹⁰², M Testa⁴⁹, R J Teuscher^{159,190}, T Theveneaux-Pelzer⁸⁷, J P Thomas¹⁹, J Thomas-Wilsker⁷⁹, E N Thompson³⁷, P D Thompson¹⁹, A S Thompson⁵⁵, L A Thomsen¹⁷⁶, E Thomson¹²³, M Thomson³⁰, M J Tibbetts¹⁶, R E Ticse Torres⁸⁷, V O Tikhomirov^{97,218}, Yu A Tikhonov^{110,181}, S Timoshenko⁹⁹, P Tipton¹⁷⁶, S Tisserant⁸⁷, K Todome¹⁵⁸, T Todorov^{5,224}, S Todorova-Nova¹³⁰, J Tojo⁷², S Tokár^{145a}, K Tokushuku⁶⁸, E Tolley⁵⁹, L Tomlinson⁸⁶, M Tomoto¹⁰⁴, L Tompkins^{144,219}, K Toms¹⁰⁶, B Tong⁵⁹, E Torrence¹¹⁷, H Torres¹⁴³, E Torró Pastor¹³⁹, J Toth^{87,220}, F Touchard⁸⁷, D R Tovey¹⁴⁰, T Trefzger¹⁷⁴, A Tricoli²⁷, I M Trigger^{160a}, S Trincas-Duvoid⁸², M F Tripania¹³, W Trischuk¹⁵⁹, B Trocme⁵⁷, A Trofymov⁴⁴, C Troncon^{93a}, M Trottier-McDonald¹⁶, M Trovatelli¹⁶⁹, L Truong^{164a,164c}, M Trzebinski⁴¹, A Trzupek⁴¹, J C-L Tseng¹²¹, P V Tsiareshka⁹⁴, G Tsiopolitis¹⁰, N Tsirintanis⁹, S Tsiskaridze¹³, V Tsiskaridze⁵⁰, E G Tskhadadze^{53a}, K M Tsui^{62a}, I I Tsukerman⁹⁸, V Tsulaia¹⁶, S Tsuno⁶⁸, D Tsybychev¹⁴⁹, A Tudorache^{28b}, V Tudorache^{28b}, A N Tuna⁵⁹, S A Tupputi^{22a,22b}, S Turchikhin^{100,216}, D Turecek¹²⁹, D Turgeman¹⁷², R Turra^{93a,93b}, A J Turvey⁴², P M Tuts³⁷, M Tyndel¹³², G Uccielli^{22a,22b}, I Ueda¹⁵⁶, R Ueno³¹, M Ughetto^{147a,147b}, F Ukegawa¹⁶¹, G Unal³², A Undrus²⁷, G Unel¹⁶³, F C Ungaro⁹⁰, Y Unno⁶⁸, C Unverdorben¹⁰¹, J Urban^{145b}, P Urquijo⁹⁰, P Urrejola⁸⁵, G Usai⁸, A Usanova⁶⁴, L Vacavant⁸⁷, V Vacek¹²⁹, B Vachon⁸⁹, C Valderanis¹⁰¹, E Valdes Santurio^{147a,147b}, N Valencic¹⁰⁸, S Valentinetti^{22a,22b}, A Valero¹⁶⁷, L Valery¹³, S Valkar¹³⁰, S Vallecorsa⁵¹, J A Valls Ferrer¹⁶⁷, W Van Den Wollenberg¹⁰⁸, P C Van Der Deijl¹⁰⁸, R van der Geer¹⁰⁸, H van der Graaf¹⁰⁸, N van Eldik¹⁵³, P van Gemmeren⁶, J Van Nieuwkoop¹⁴³, I van Vulpen¹⁰⁸, M C van Woerden³², M Vanadia^{133a,133b}, W Vandelli³², R Vanguri¹²³, A Vaniachine¹³¹, P Vankov¹⁰⁸, G Vardanyan¹⁷⁷, R Vari^{133a}, E W Varnes⁷, T Varol⁴², D Varouchas⁸², A Vartapetian⁸, K E Varvell¹⁵¹, J G Vasquez¹⁷⁶, F Vazeille³⁶, T Vazquez Schroeder⁸⁹, J Veatch⁵⁶, L M Veloce¹⁵⁹, F Veloso^{127a,127c}, S Veneziano^{133a}, A Ventura^{75a,75b}, M Venturi¹⁶⁹, N Venturi¹⁵⁹, A Venturini²⁵, V Vercesi^{122a}, M Verducci^{133a,133b}, W Verkerke¹⁰⁸, J C Vermeulen¹⁰⁸, A Vest^{46,221}, M C Vetterli^{143,182}, O Viazlo⁸³, I Vichou¹⁶⁶, T Vickey¹⁴⁰, O E Vickey Boeriu¹⁴⁰, G H A Viehhauser¹²¹, S Viel¹⁶,

L Vigani¹²¹, R Vigne⁶⁴, M Villa^{22a,22b}, M Villaplana Perez^{93a,93b}, E Vilucchi⁴⁹, M G Vinciter³¹, V B Vinogradov⁶⁷, C Vittori^{22a,22b}, I Vivarelli¹⁵⁰, S Vlachos¹⁰, M Vlasak¹²⁹, M Vogel¹⁷⁵, P Vokac¹²⁹, G Volpi^{125a,125b}, M Volpi⁹⁰, H von der Schmitt¹⁰², E von Toerne²³, V Vorobel¹³⁰, K Vorobev⁹⁹, M Vos¹⁶⁷, R Voss³², J H Vossebeld⁷⁶, N Vranjes¹⁴, M Vranjes Milosavljevic¹⁴, V Vrba¹²⁸, M Vreeswijk¹⁰⁸, R Vuillermet³², I Vukotic³³, Z Vykydal¹²⁹, P Wagner²³, W Wagner¹⁷⁵, H Wahlberg⁷³, S Wahrmund⁴⁶, J Wakabayashi¹⁰⁴, J Walder⁷⁴, R Walker¹⁰¹, W Walkowiak¹⁴², V Wallangen^{147a,147b}, C Wang^{35c}, C Wang^{35d,87}, F Wang¹⁷³, H Wang¹⁶, H Wang⁴², J Wang⁴⁴, J Wang¹⁵¹, K Wang⁸⁹, R Wang⁶, S M Wang¹⁵², T Wang²³, T Wang³⁷, W Wang^{35b}, X Wang¹⁷⁶, C Wanotayaroj¹¹⁷, A Warburton⁸⁹, C P Ward³⁰, D R Wardrope⁸⁰, A Washbrook⁴⁸, P M Watkins¹⁹, A T Watson¹⁹, M F Watson¹⁹, G Watts¹³⁹, S Watts⁸⁶, B M Waugh⁸⁰, S Webb⁸⁵, M S Weber¹⁸, S W Weber¹⁷⁴, J S Webster⁶, A R Weidberg¹²¹, B Weinert⁶³, J Weingarten⁵⁶, C Weiser⁵⁰, H Weits¹⁰⁸, P S Wells³², T Wenaus²⁷, T Wengler³², S Wenig³², N Vermes²³, M Werner⁵⁰, M D Werner⁶⁶, P Werner³², M Wessels^{60a}, J Wetter¹⁶², K Whalen¹¹⁷, N L Whallon¹³⁹, A M Wharton⁷⁴, A White⁸, M J White¹, R White^{34b}, D Whiteson¹⁶³, F J Wickens¹³², W Wiedenmann¹⁷³, M Wielers¹³², P Wienemann²³, C Wigglesworth³⁸, L A M Wiik-Fuchs²³, A Wildauer¹⁰², F Wilk⁸⁶, H G Wilkens³², H H Williams¹²³, S Williams¹⁰⁸, C Willis⁹², S Willocq⁸⁸, J A Wilson¹⁹, I Wingerter-Seez⁵, F Winklmeier¹¹⁷, O J Winston¹⁵⁰, B T Winter²³, M Wittgen¹⁴⁴, J Wittkowski¹⁰¹, S J Wollstadt⁸⁵, M W Wolter⁴¹, H Wolters^{127a,127c}, B K Wosiek⁴¹, J Wotschack³², M J Woudstra⁸⁶, K W Wozniak⁴¹, M Wu⁵⁷, M Wu³³, S L Wu¹⁷³, X Wu⁵¹, Y Wu⁹¹, T R Wyatt⁸⁶, B M Wynne⁴⁸, S Xella³⁸, D Xu^{35a}, L Xu²⁷, B Yabsley¹⁵¹, S Yacoob^{146a}, R Yakabe⁶⁹, D Yamaguchi¹⁵⁸, Y Yamaguchi¹¹⁹, A Yamamoto⁶⁸, S Yamamoto¹⁵⁶, T Yamanaka¹⁵⁶, K Yamauchi¹⁰⁴, Y Yamazaki⁶⁹, Z Yan²⁴, H Yang^{35e,35f}, H Yang¹⁷³, Y Yang¹⁵², Z Yang¹⁵, W-M Yao¹⁶, Y C Yap⁸², Y Yasu⁶⁸, E Yatsenko⁵, K H Yau Wong²³, J Ye⁴², S Ye²⁷, I Yeletsikh⁶⁷, A L Yen⁵⁹, E Yildirim⁸⁵, K Yorita¹⁷¹, R Yoshida⁶, K Yoshihara¹²³, C Young¹⁴⁴, C J S Young³², S Youssef²⁴, D R Yu¹⁶, J Yu⁸, J M Yu⁹¹, J Yu⁶⁶, L Yuan⁶⁹, S P Y Yuen²³, I Yusuff^{30,222}, B Zabinski⁴¹, R Zaidan^{35d}, A M Zaitsev^{131,209}, N Zakharuk⁴⁴, J Zalieckas¹⁵, A Zaman¹⁴⁹, S Zambito⁵⁹, L Zanello^{133a,133b}, D Zanzi⁹⁰, C Zeitnitz¹⁷⁵, M Zeman¹²⁹, A Zemla^{40a}, J C Zeng¹⁶⁶, Q Zeng¹⁴⁴, K Zengel²⁵, O Zenin¹³¹, T Ženiš^{145a}, D Zerwas¹¹⁸, D Zhang⁹¹, F Zhang¹⁷³, G Zhang^{35b,217}, H Zhang^{35c}, J Zhang⁶, L Zhang³⁰, R Zhang²³, R Zhang^{35b,223}, X Zhang^{35d}, Z Zhang¹¹⁸, X Zhao⁴², Y Zhao^{35d}, Z Zhao^{35b}, A Zhemchugov⁶⁷, J Zhong¹²¹, B Zhou⁹¹, C Zhou⁴⁷, L Zhou³⁷, L Zhou⁴², M Zhou¹⁴⁹, N Zhou^{35g}, C G Zhu^{35d}, H Zhu^{35a}, J Zhu⁹¹, Y Zhu^{35b}, X Zhuang^{35a}, K Zhukov⁹⁷, A Zibell¹⁷⁴, D Zieminska⁶³, N I Zimine⁶⁷, C Zimmermann⁸⁵, S Zimmermann⁵⁰, Z Zinonos⁵⁶, M Zinser⁸⁵, M Ziolkowski¹⁴², L Živković¹⁴, G Zobernig¹⁷³, A Zoccoli^{22a,22b}, M zur Nedden¹⁷, G Zurzolo^{105a,105b} and L Zwalinski³²

¹ Department of Physics, University of Adelaide, Adelaide, Australia

² Physics Department, SUNY Albany, Albany NY, USA

³ Department of Physics, University of Alberta, Edmonton AB, Canada

^{4a} Department of Physics, Ankara University, Ankara

^{4b} Istanbul Aydin University, Istanbul

^{4c} 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, USA

⁷ Department of Physics, University of Arizona, Tucson AZ, USA

⁸ Department of Physics, The University of Texas at Arlington, Arlington TX, USA

⁹ Physics Department, 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, USA

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, USA

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, UK

^{20a} Department of Physics, Bogazici University, Istanbul

^{20b} Department of Physics Engineering, Gaziantep University, Gaziantep, Turkey

^{20d} Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey

^{20e} Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey

²¹ Centro de Investigaciones, Universidad Antonio Narino, Bogota, Colombia

^{22a} INFN Sezione di Bologna, Italy

^{22b} 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, USA

²⁵ Department of Physics, Brandeis University, Waltham MA, USA

^{26a} Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro, Brazil

^{26b} Electrical Circuits Department, Federal University of Juiz de Fora (UFJF), Juiz de Fora, Brazil

^{26c} Federal University of Sao Joao del Rei (UFSJ), Sao Joao del Rei, Brazil

^{26d} Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil

²⁷ Physics Department, Brookhaven National Laboratory, Upton NY, USA

^{28a} Transilvania University of Brasov, Brasov, Romania

- ^{28b} National Institute of Physics and Nuclear Engineering, Bucharest, Romania
- ^{28c} National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj Napoca, Romania
- ^{28d} University Politehnica Bucharest, Bucharest, Romania
- ^{28e} West University in Timisoara, Timisoara, Romania
- ²⁹ Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina
- ³⁰ Cavendish Laboratory, University of Cambridge, Cambridge, UK
- ³¹ Department of Physics, Carleton University, Ottawa ON, Canada
- ³² CERN, Geneva, Switzerland
- ³³ Enrico Fermi Institute, University of Chicago, Chicago IL, USA
- ^{34a} Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile
- ^{34b} Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
- ^{35a} Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, People's Republic of China
- ^{35b} Department of Modern Physics, University of Science and Technology of China, Anhui, People's Republic of China
- ^{35c} Department of Physics, Nanjing University, Jiangsu, People's Republic of China
- ^{35d} School of Physics, Shandong University, Shandong, People's Republic of China
- ^{35e} Department of Physics and Astronomy, Shanghai Key Laboratory for Particle Physics and Cosmology, Shanghai Jiao Tong University, Shanghai, People's Republic of China
- ^{35f} Also affiliated with PKU-CHEP
- ^{35g} Physics Department, Tsinghua University, Beijing 100084, People's Republic of China
- ³⁶ Laboratoire de Physique Corpusculaire, Clermont Université and Université Blaise Pascal and CNRS/IN2P3, Clermont-Ferrand, France
- ³⁷ Nevis Laboratory, Columbia University, Irvington NY, USA
- ³⁸ Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
- ^{39a} INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Italy
- ^{39b} Dipartimento di Fisica, Università della Calabria, Rende, Italy
- ^{40a} AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland
- ^{40b} Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
- ⁴¹ Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
- ⁴² Physics Department, Southern Methodist University, Dallas TX, USA
- ⁴³ Physics Department, University of Texas at Dallas, Richardson TX, USA
- ⁴⁴ DESY, Hamburg and Zeuthen, Germany
- ⁴⁵ Institut für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
- ⁴⁶ Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
- ⁴⁷ Department of Physics, Duke University, Durham NC, USA
- ⁴⁸ SUPA—School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK
- ⁴⁹ INFN Laboratori Nazionali di Frascati, Frascati, Italy
- ⁵⁰ Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
- ⁵¹ Section de Physique, Université de Genève, Geneva, Switzerland
- ^{52a} INFN Sezione di Genova, Italy
- ^{52b} Dipartimento di Fisica, Università di Genova, Genova, Italy
- ^{53a} E. Andronikashvili Institute of Physics, Iv. Javakishvili Tbilisi State University, Tbilisi, Georgia
- ^{53b} High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
- ⁵⁴ II Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
- ⁵⁵ SUPA—School of Physics and Astronomy, University of Glasgow, Glasgow, UK
- ⁵⁶ II Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
- ⁵⁷ Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France
- ⁵⁸ Department of Physics, Hampton University, Hampton VA, USA
- ⁵⁹ Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge MA, USA
- ^{60a} Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
- ^{60b} Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
- ^{60c} ZITI Institut für technische Informatik, Ruprecht-Karls-Universität Heidelberg, Mannheim, Germany
- ⁶¹ Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
- ^{62a} Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, People's Republic of China
- ^{62b} Department of Physics, The University of Hong Kong, Hong Kong, People's Republic of China
- ^{62c} Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, People's Republic of China
- ⁶³ Department of Physics, Indiana University, Bloomington IN, USA
- ⁶⁴ Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria
- ⁶⁵ University of Iowa, Iowa City IA, USA
- ⁶⁶ Department of Physics and Astronomy, Iowa State University, Ames IA, USA
- ⁶⁷ Joint Institute for Nuclear Research, JINR Dubna, Dubna, Russia
- ⁶⁸ KEK, High Energy Accelerator Research Organization, Tsukuba, Japan
- ⁶⁹ Graduate School of Science, Kobe University, Kobe, Japan
- ⁷⁰ Faculty of Science, Kyoto University, Kyoto, Japan
- ⁷¹ Kyoto University of Education, Kyoto, Japan
- ⁷² Department of Physics, Kyushu University, Fukuoka, Japan
- ⁷³ Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina
- ⁷⁴ Physics Department, Lancaster University, Lancaster, UK
- ^{75a} INFN Sezione di Lecce, Italy
- ^{75b} Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy
- ⁷⁶ Oliver Lodge Laboratory, University of Liverpool, Liverpool, UK
- ⁷⁷ Department of Physics, Jožef Stefan Institute and University of Ljubljana, Ljubljana, Slovenia
- ⁷⁸ School of Physics and Astronomy, Queen Mary University of London, London, UK
- ⁷⁹ Department of Physics, Royal Holloway University of London, Surrey, UK

- 80 Department of Physics and Astronomy, University College London, London, UK
- 81 Louisiana Tech University, Ruston LA, USA
- 82 Laboratoire de Physique Nucléaire et de Hautes Energies, UPMC and Université Paris-Diderot and CNRS/IN2P3, Paris, France
- 83 Fysiska institutionen, Lunds universitet, Lund, Sweden
- 84 Departamento de Física Teórica C-15, Universidad Autónoma de Madrid, Madrid, Spain
- 85 Institut für Physik, Universität Mainz, Mainz, Germany
- 86 School of Physics and Astronomy, University of Manchester, Manchester, UK
- 87 CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
- 88 Department of Physics, University of Massachusetts, Amherst MA, USA
- 89 Department of Physics, McGill University, Montreal QC, Canada
- 90 School of Physics, University of Melbourne, Victoria, Australia
- 91 Department of Physics, The University of Michigan, Ann Arbor MI, USA
- 92 Department of Physics and Astronomy, Michigan State University, East Lansing MI, USA
- 93a INFN Sezione di Milano, Italy
- 93b Dipartimento di Fisica, Università di Milano, Milano, Italy
- 94 B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Republic of Belarus
- 95 National Scientific and Educational Centre for Particle and High Energy Physics, Minsk, Republic of Belarus
- 96 Group of Particle Physics, University of Montreal, Montreal QC, Canada
- 97 P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia
- 98 Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia
- 99 National Research Nuclear University MEPhI, Moscow, Russia
- 100 D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia
- 101 Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany
- 102 Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany
- 103 Nagasaki Institute of Applied Science, Nagasaki, Japan
- 104 Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan
- 105a INFN Sezione di Napoli, Italy
- 105b Dipartimento di Fisica, Università di Napoli, Napoli, Italy
- 106 Department of Physics and Astronomy, University of New Mexico, Albuquerque NM, USA
- 107 Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, The Netherlands
- 108 Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, The Netherlands
- 109 Department of Physics, Northern Illinois University, DeKalb IL, USA
- 110 Budker Institute of Nuclear Physics, SB RAS, Novosibirsk, Russia
- 111 Department of Physics, New York University, New York NY, USA
- 112 Ohio State University, Columbus OH, USA
- 113 Faculty of Science, Okayama University, Okayama, Japan
- 114 Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman OK, USA
- 115 Department of Physics, Oklahoma State University, Stillwater OK, USA
- 116 Palacký University, RCPTM, Olomouc, Czech Republic
- 117 Center for High Energy Physics, University of Oregon, Eugene OR, USA
- 118 LAL, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France
- 119 Graduate School of Science, Osaka University, Osaka, Japan
- 120 Department of Physics, University of Oslo, Oslo, Norway
- 121 Department of Physics, Oxford University, Oxford, UK
- 122a INFN Sezione di Pavia, Italy
- 122b Dipartimento di Fisica, Università di Pavia, Pavia, Italy
- 123 Department of Physics, University of Pennsylvania, Philadelphia PA, USA
- 124 National Research Centre 'Kurchatov Institute' B.P. Konstantinov Petersburg Nuclear Physics Institute, St. Petersburg, Russia
- 125a INFN Sezione di Pisa, Italy
- 125b Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy
- 126 Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh PA, USA
- 127a Laboratório de Instrumentação e Física Experimental de Partículas—LIP, Lisboa, Portugal
- 127b Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal
- 127c Department of Physics, University of Coimbra, Coimbra, Portugal
- 127d Centro de Física Nuclear da Universidade de Lisboa, Lisboa, Portugal
- 127e Departamento de Física, Universidade do Minho, Braga, Portugal
- 127f Departamento de Física Teórica y del Cosmos and CAFPE, Universidad de Granada, Granada, Spain
- 127g Dep Física and CEFITEC de Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal
- 128 Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic
- 129 Czech Technical University in Prague, Praha, Czech Republic
- 130 Faculty of Mathematics and Physics, Charles University in Prague, Praha, Czech Republic
- 131 State Research Center Institute for High Energy Physics (Protvino), NRC KI, Russia
- 132 Particle Physics Department, Rutherford Appleton Laboratory, Didcot, UK
- 133a INFN Sezione di Roma, Italy
- 133b Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy
- 134a INFN Sezione di Roma Tor Vergata, Italy
- 134b Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy
- 135a INFN Sezione di Roma Tre, Italy
- 135b Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy
- 136a Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies—Université Hassan II, Casablanca, Morocco
- 136b Centre National de l'Energie des Sciences Techniques Nucleaires, Rabat, Morocco
- 136c Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech, Morocco
- 136d Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda, Morocco

- ^{136e} Faculté des sciences, Université Mohammed V, Rabat, Morocco
- ¹³⁷ 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
- ¹³⁸ Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA, USA
- ¹³⁹ Department of Physics, University of Washington, Seattle WA, USA
- ¹⁴⁰ Department of Physics and Astronomy, University of Sheffield, Sheffield, UK
- ¹⁴¹ Department of Physics, Shinshu University, Nagano, Japan
- ¹⁴² Fachbereich Physik, Universität Siegen, Siegen, Germany
- ¹⁴³ Department of Physics, Simon Fraser University, Burnaby BC, Canada
- ¹⁴⁴ SLAC National Accelerator Laboratory, Stanford CA, USA
- ^{145a} Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava, Slovakia
- ^{145b} Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic, Slovakia
- ^{146a} Department of Physics, University of Cape Town, Cape Town, South Africa
- ^{146b} Department of Physics, University of Johannesburg, Johannesburg, South Africa
- ^{146c} School of Physics, University of the Witwatersrand, Johannesburg, South Africa
- ^{147a} Department of Physics, Stockholm University, Sweden
- ^{147b} The Oskar Klein Centre, Stockholm, Sweden
- ¹⁴⁸ Physics Department, Royal Institute of Technology, Stockholm, Sweden
- ¹⁴⁹ Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook NY, USA
- ¹⁵⁰ Department of Physics and Astronomy, University of Sussex, Brighton, UK
- ¹⁵¹ School of Physics, University of Sydney, Sydney, Australia
- ¹⁵² Institute of Physics, Academia Sinica, Taipei, Taiwan
- ¹⁵³ Department of Physics, Technion: Israel Institute of Technology, Haifa, Israel
- ¹⁵⁴ Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel
- ¹⁵⁵ Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
- ¹⁵⁶ International Center for Elementary Particle Physics and Department of Physics, The University of Tokyo, Tokyo, Japan
- ¹⁵⁷ Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan
- ¹⁵⁸ Department of Physics, Tokyo Institute of Technology, Tokyo, Japan
- ¹⁵⁹ Department of Physics, University of Toronto, Toronto ON, Canada
- ^{160a} TRIUMF, Vancouver BC, Canada
- ^{160b} Department of Physics and Astronomy, York University, Toronto ON, Canada
- ¹⁶¹ Faculty of Pure and Applied Sciences, and Center for Integrated Research in Fundamental Science and Engineering, University of Tsukuba, Tsukuba, Japan
- ¹⁶² Department of Physics and Astronomy, Tufts University, Medford MA, USA
- ¹⁶³ Department of Physics and Astronomy, University of California Irvine, Irvine CA, USA
- ^{164a} INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine, Italy
- ^{164b} ICTP, Trieste, Italy
- ^{164c} Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy
- ¹⁶⁵ Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden
- ¹⁶⁶ Department of Physics, University of Illinois, Urbana IL, USA
- ¹⁶⁷ Instituto de Física Corpuscular (IFIC) and Departamento de Física Atomica, Molecular y Nuclear and Departamento de Ingeniería Electrónica and Instituto de Microelectrónica de Barcelona (IMB-CNM), University of Valencia and CSIC, Valencia, Spain
- ¹⁶⁸ Department of Physics, University of British Columbia, Vancouver BC, Canada
- ¹⁶⁹ Department of Physics and Astronomy, University of Victoria, Victoria BC, Canada
- ¹⁷⁰ Department of Physics, University of Warwick, Coventry, UK
- ¹⁷¹ Waseda University, Tokyo, Japan
- ¹⁷² Department of Particle Physics, The Weizmann Institute of Science, Rehovot, Israel
- ¹⁷³ Department of Physics, University of Wisconsin, Madison WI, USA
- ¹⁷⁴ Fakultät für Physik und Astronomie, Julius-Maximilians-Universität, Würzburg, Germany
- ¹⁷⁵ Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany
- ¹⁷⁶ Department of Physics, Yale University, New Haven CT, USA
- ¹⁷⁷ Yerevan Physics Institute, Yerevan, Armenia
- ¹⁷⁸ Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France
- ¹⁷⁹ Also at Department of Physics, King's College London, London, UK
- ¹⁸⁰ Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan
- ¹⁸¹ Also at Novosibirsk State University, Novosibirsk, Russia
- ¹⁸² Also at TRIUMF, Vancouver BC, Canada
- ¹⁸³ Also at Department of Physics & Astronomy, University of Louisville, Louisville, KY, USA
- ¹⁸⁴ Also at Department of Physics, California State University, Fresno CA, USA
- ¹⁸⁵ Also at Department of Physics, University of Fribourg, Fribourg, Switzerland
- ¹⁸⁶ Also at Departament de Física de la Universitat Autònoma de Barcelona, Barcelona, Spain
- ¹⁸⁷ Also at Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, Portugal
- ¹⁸⁸ Also at Tomsk State University, Tomsk, Russia
- ¹⁸⁹ Also at Università di Napoli Parthenope, Napoli, Italy
- ¹⁹⁰ Also at Institute of Particle Physics (IPP), Canada
- ¹⁹¹ Also at National Institute of Physics and Nuclear Engineering, Bucharest, Romania
- ¹⁹² Also at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg, Russia
- ¹⁹³ Also at Department of Physics, The University of Michigan, Ann Arbor MI, USA
- ¹⁹⁴ Also at Centre for High Performance Computing, CSIR Campus, Rosebank, Cape Town, South Africa
- ¹⁹⁵ Also at Louisiana Tech University, Ruston LA, USA
- ¹⁹⁶ Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain
- ¹⁹⁷ Also at Graduate School of Science, Osaka University, Osaka, Japan

- ¹⁹⁸ Also at Department of Physics, National Tsing Hua University, Taiwan
- ¹⁹⁹ Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, The Netherlands
- ²⁰⁰ Also at Department of Physics, The University of Texas at Austin, Austin TX, USA
- ²⁰¹ Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia
- ²⁰² Also at CERN, Geneva, Switzerland
- ²⁰³ Also at Georgian Technical University (GTU), Tbilisi, Georgia
- ²⁰⁴ Also at Ochadai Academic Production, Ochanomizu University, Tokyo, Japan
- ²⁰⁵ Also at Manhattan College, New York NY, USA
- ²⁰⁶ Also at Hellenic Open University, Patras, Greece
- ²⁰⁷ Also at Academia Sinica Grid Computing, Institute of Physics, Academia Sinica, Taipei, Taiwan
- ²⁰⁸ Also at School of Physics, Shandong University, Shandong, People's Republic of China
- ²⁰⁹ Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia
- ²¹⁰ Also at section de Physique, Université de Genève, Geneva, Switzerland
- ²¹¹ Also at Eotvos Lorand University, Budapest, Hungary
- ²¹² Also at International School for Advanced Studies (SISSA), Trieste, Italy
- ²¹³ Also at Department of Physics and Astronomy, University of South Carolina, Columbia SC, USA
- ²¹⁴ Also at School of Physics and Engineering, Sun Yat-sen University, Guangzhou, People's Republic of China
- ²¹⁵ Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria
- ²¹⁶ Also at Faculty of Physics, M.V.Lomonosov Moscow State University, Moscow, Russia
- ²¹⁷ Also at Institute of Physics, Academia Sinica, Taipei, Taiwan
- ²¹⁸ Also at National Research Nuclear University MEPhI, Moscow, Russia
- ²¹⁹ Also at Department of Physics, Stanford University, Stanford CA, USA
- ²²⁰ Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary
- ²²¹ Also at Flensburg University of Applied Sciences, Flensburg, Germany
- ²²² Also at University of Malaya, Department of Physics, Kuala Lumpur, Malaysia
- ²²³ Also at CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France
- ²²⁴ Deceased