



Dijet resonance search with weak supervision using $\sqrt{s} = 13$ TeV pp collisions in the ATLAS detector

The ATLAS Collaboration

This Letter describes a search for resonant new physics using a machine-learning anomaly detection procedure that does not rely on a signal model hypothesis. Weakly supervised learning is used to train classifiers directly on data to enhance potential signals. The targeted topology is dijet events and the features used for machine learning are the masses of the two jets. The resulting analysis is essentially a three-dimensional search $A \rightarrow BC$, for $m_A \sim \mathcal{O}(\text{TeV})$, $m_B, m_C \sim \mathcal{O}(100 \text{ GeV})$ and B, C are reconstructed as large-radius jets, without paying a penalty associated with a large trials factor in the scan of the masses of the two jets. The full Run 2 $\sqrt{s} = 13$ TeV pp collision data set of 139 fb^{-1} recorded by the ATLAS detector at the Large Hadron Collider is used for the search. There is no significant evidence of a localized excess in the dijet invariant mass spectrum between 1.8 and 8.2 TeV. Cross-section limits for narrow-width A , B , and C particles vary with m_A , m_B , and m_C . For example, when $m_A = 3$ TeV and $m_B \gtrsim 200$ GeV, a production cross section between 1 and 5 fb is excluded at 95% confidence level, depending on m_C . For certain masses, these limits are up to 10 times more sensitive than those obtained by the inclusive dijet search.

A search for dijet resonances is one of the first analyses performed when a hadron collider reaches a new center-of-mass energy [1–8]. While such searches are sensitive to nearly all resonance decays $A \rightarrow BC$, dedicated searches for particular decays will always be more sensitive. This is the motivation for dedicated resonance searches for the case where B and C are τ -leptons [9, 10], b -quarks [11–13], top quarks [14, 15], vector bosons [16, 17], Higgs bosons [18–23], and more, including asymmetric combinations. In all cases, a selection on the structure of the energy flow from each side of the decay is used to enhance events with the targeted topology. Searches for any combination of Standard Model (SM) particles can be well-motivated by one or more theory frameworks beyond the SM (BSM), but not all combinations are currently covered by dedicated searches [24]. Furthermore, there are only a small number of searches [25–39] that cover the vast set of possibilities where at least one of B or C is itself a BSM particle [40]. There is no previous search where all of A , B and C are BSM particles and can have different masses.

While it is crucial to continue searching for particular dijet topologies, the fact that not all SM and BSM possibilities are covered suggests that a complementary generic search effort is required. What is needed is a method for searching for many topologies all at once that ideally does not pay a large statistical trials factor. A variety of existing and proposed model-agnostic searches range from nearly signal model-independent but fully background model-dependent [41–56] (because they compare data with SM simulation) to varying degrees of partial signal-model and background-model independence [57–72]. The method used for this analysis employs a machine-learning-based anomaly detection procedure to perform a dijet search in which the jets from a potential signal have a nontrivial but unknown structure [70, 71]. Simply stated, classifiers are trained to distinguish particular dijet invariant mass bins from their neighbors. Localized resonances will be enhanced with a selection based on the classifier.

This Letter presents a search for a generic $A \rightarrow BC$ resonance, in which all of A , B and C could be BSM particles and the decay products of B and C can be contained within single large-radius jets. The search uses events collected by the ATLAS detector [73, 74] using the full 139 fb^{-1} Run 2 $\sqrt{s} = 13 \text{ TeV}$ pp collision data set. Weakly supervised classifiers are used to enhance potential signals without using simulations of any particular signal models.

Events with at least two jets are considered, and the invariant mass distribution of the two leading jets is used to perform a ‘bump hunt’. Jets are formed [75, 76] from locally calibrated calorimeter cell-clusters [77] using the anti- k_t algorithm [78] with a radius parameter of $R = 1.0$. These jets are trimmed [79] by reclustering the jet constituents with the k_t algorithm using $R = 0.2$ and removing the constituents with transverse momentum (p_T) less than 5% of the original jet p_T . The jet four-vectors are then calibrated as detailed in Ref. [80]. The two jets are required to each have $p_T > 200 \text{ GeV}$ and pseudorapidity¹ $|\eta| < 2.0$. In order to be broadly sensitive to hadronically decaying resonant particles, events are required to have at least one jet with $p_T > 500 \text{ GeV}$ and two leading jets with a rapidity difference of $|\Delta y_{JJ}| < 1.2$. The p_T threshold is chosen so that the online trigger system is fully efficient [81, 82]. Furthermore, both jets must have jet mass $30 \text{ GeV} < m_J < 500 \text{ GeV}$ for stability of the neural network (NN) training described below. The upper threshold reduces the m_{JJ} -dependence of the m_J distribution. The bump hunt is performed for dijet invariant masses in the range $2.28 \text{ TeV} < m_{JJ} < 6.81 \text{ TeV}$.

The masses of the two leading jets are used for classification. As the first application of fully data-driven machine-learning anomaly detection, this restricted feature set is used to establish the procedure and is already sensitive to a wide range of BSM possibilities. Weakly supervised classifiers for high-energy physics [83–86] aim to distinguish signal from background without having labeled examples for training. In particular, the classification without labels method [83] calls for two mixed samples that are statistically identical aside

¹ Pseudorapidity is defined in terms of the angle θ relative to the beam line as $\eta = -\ln(\tan(\theta/2))$.

from different class proportions. For this search, the two samples are constructed using signal regions in m_{JJ} with width $20\% \times m_{JJ}$, chosen to correspond to the detector resolution for a narrow resonance. The signal regions are labeled 0–7 and have boundaries: [1.90, 2.28, 2.74, 3.28, 3.94, 4.73, 5.68, 6.81, 8.17] TeV.

The jet mass probability density varies slowly with m_{JJ} , so neighboring regions in m_{JJ} can be used to construct the mixed event samples required for weak supervision. In particular, a network is trained to distinguish between a given m_{JJ} *signal* region and the two neighboring *sideband* regions. For the case in which some signal is present in the signal region, the network will learn to tag that signal and enhance a bump in the m_{JJ} spectrum, while for the case in which there is no signal in the signal region, the tagging of the network will be essentially random, and the m_{JJ} spectrum will remain smooth after tagging. Since every signal region requires two neighboring sidebands, the m_{JJ} regions 1–6 are chosen, and the entire process outlined below is repeated for each signal region. In order to reduce existing correlations between jet mass and m_{JJ} ,² the jet masses (m_1, m_2) , with $m_1 \geq m_2$, in each m_{JJ} region are each mapped to be between 0 and 1. This mapping is accomplished with the empirical cumulative distribution function of the marginal distribution over both jets, each of mass m_j : $m \mapsto \frac{1}{n_{\text{jets}}} \sum_{i=1}^{n_{\text{jets}}} \mathbb{I}[m > m_i]$. The indicator function $\mathbb{I}[\cdot]$ is unity if its argument is true and zero otherwise, and the resulting marginal distribution is uniform in each m_{JJ} bin. Additional decorrelation is achieved by assigning the same total weight to each sideband. The NNs performing the weakly supervised classification using m_1 and m_2 are fully connected networks built from four hidden layers with sizes 64, 32, 8, and 1. Rectified linear units connect each intermediate hidden layer and the final activation function is sigmoidal. Networks are implemented in Keras [98] with the Tensorflow back end [99] and minimize the binary cross-entropy using the Adam optimizer [100].

In order to eliminate a trial factor associated with (m_1, m_2) , the NN identifies a region of interest, and no event is used to train the NN that is applied to it. A k -fold cross-validation procedure is employed in which the full data set is divided randomly into k parts of equal size. Among these, $k - 2$ parts are used for training n classifiers (the training set) with different initializations, and the $(k - 1)^{\text{th}}$ part is used to decide, based on the loss, which of these n networks to select (the validation set). The selected network is then mapped to an efficiency ϵ in the k^{th} part (the test set) so that the meaning of the network output can be compared across data sets and trainings. The efficiency ϵ is defined as the fraction of events with a given NN value or higher. This output is averaged across the $k - 1$ other permutations of the training and validation parts. The entire procedure is then repeated k times, where each part is a test set exactly once. For this analysis, $k = 5$ and $n = 3$, so there are $3 \times 4 \times 5 = 60$ NNs trained for each signal region. Two event selections from thresholds imposed on the NN outputs are used: one that keeps the 10% most signal-region-like events ($\epsilon = 0.1$) and one that keeps the 1% most signal-region-like events ($\epsilon = 0.01$).

As the classifier-based event selection depends on the data, and in particular on the possible presence of true signals, it is not possible to directly define control regions to validate the method. The entire procedure was validated using simulated events as well as a validation region with $|\Delta y_{JJ}| > 1.2$. For s -channel resonances, it is expected that this inverted rapidity-difference requirement reduces the signal efficiency while enhancing the dijet background by over an order of magnitude.

Following the validation, first, the performance of the NNs on data is studied with and without injected signals. Since the NNs are two-dimensional functions, they can be visualized directly as images. Figure 1 presents the network output from a representative signal region in the absence of signal and also in the presence of injected signals. By construction, there must be a region of low efficiency and the data are the same in all four plots. In the absence of a signal, regions of low efficiency are located randomly throughout the (m_1, m_2) plane. The signals are $W' \rightarrow WZ$, for a new vector boson W' [102], and the W and Z boson

² This is similar to the method used in Ref. [87]; additional decorrelation techniques are described in Refs. [88–97].

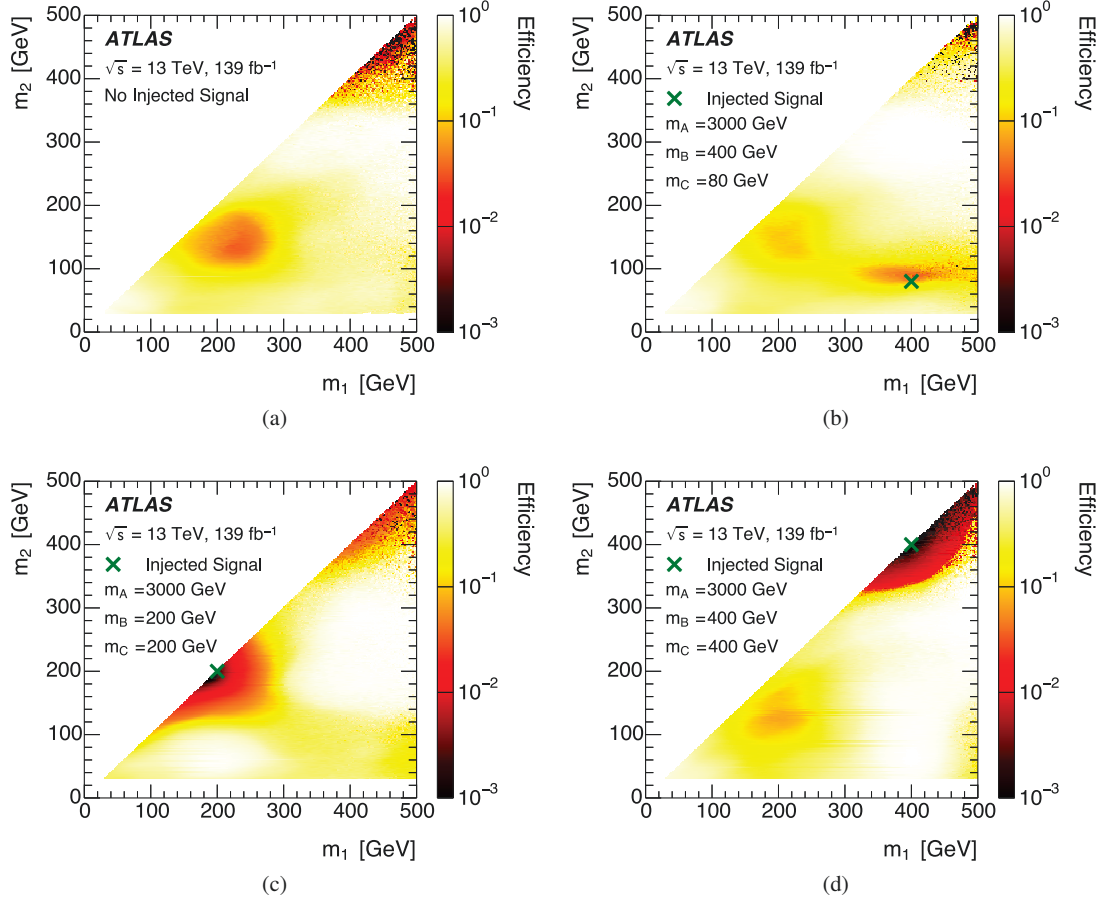


Figure 1: The efficiency mapped output of the NN versus the input variables for the events in signal region 2 for four cases: (a) there is no injected signal; (b) there is an injected signal of $m_A = 3$ TeV, and $m_B = 400$ GeV and $m_C = 80$ GeV, (c) there is an injected signal of $m_A = 3$ TeV, and $m_B = 200$ GeV and $m_C = 200$ GeV, and (d) there is an injected signal of $m_A = 3$ TeV, and $m_B = 400$ GeV and $m_C = 400$ GeV. The location of (m_B, m_C) for the given injected signal is marked with a green $\times$. The injected cross section is just below the limit at low m_B and m_C from the inclusive dijet search [101].

masses are varied, with widths set close to zero. These signals were simulated using PYTHIA 8.2 [103–105] with the A14 set of tuned parameters [106] and NNPDF 2.3 parton distribution function [107]. All samples of simulated data were processed using the full ATLAS detector simulation [108] based on GEANT4 [109]. The amount of signal injected in all cases is about the same as, or less than, the level already excluded by the all-inclusive dijet search [101]. In all cases, the low-efficiency (signal-like) regions of the NN are localized near the injected signal. Some signals are easier to find than others; the difficulty is set both by the relative size of the signal and by the total number of events available for training in the signal vicinity.

After applying an event selection based on the NN trained on a particular signal region, the m_{JJ} spectra are fit with a parametric function. The entire m_{JJ} spectrum between 1.8 and 8.2 TeV is fit with a binning of 100 GeV; however, a *fit signal region* and *fit sideband region* are defined for evaluating the quality of the fit. The fit signal regions are defined as the m_{JJ} signal regions the NN used for training, combined with the

adjacent halves of the left and right neighboring regions; the fit sidebands are defined as the complement of the fit signal regions. An iterative procedure is applied until the p -value from the fit sideband χ^2 is greater than 0.05. Since the NN is trained to distinguish the signal region from its neighboring regions, it is expected that the m_{JJ} spectrum is smooth in the fit sideband region in the presence or absence of a true signal. First, the data are fit to $dn/dx = p_1(1-x)^{p_2-\xi_1 p_3} x^{-p_3}$, where $x = m_{JJ}/\sqrt{s}$, p_i are fit parameters, and the ξ_i are chosen to ensure that the p_i are uncorrelated. If the fit quality is insufficient, an extended function is used instead [101]: $dn/dx = p_1(1-x)^{p_2-\xi_1 p_3} x^{-p_3+(p_4-\xi_2 p_3-\xi_3 p_2)\log(x)}$. If the fit quality remains insufficient, a variation of the UA2 [2] fit function is tested: $dn/dx = p_1 x^{p_2-\xi_3} e^{-p_3 x+(p_4-\xi_2 p_3-\xi_3 p_2)x^2}$. If the fit quality is still insufficient, the fit sidebands are reduced by 400 GeV on both sides and the three functions are tried again in order. This procedure is then iterated until the fit is successful. The fit results in the signal regions for the $\epsilon = 0.1$ and $\epsilon = 0.01$ NN efficiency selections are presented in Figure 2. The largest positive deviation from the fit model is 3.0σ in signal region 1, around 2500 GeV, at $\epsilon = 0.1$. Globally, the positive tail of the signal region significance distribution is consistent with a standard normal distribution at the 1.5σ level.

The W' signal models can be used to set limits on the production cross section of specific new particles. To illustrate the sensitivity of the analysis to the full three-dimensional parameter space (m_A, m_B, m_C) , two m_A points and multiple (m_B, m_C) points are selected. As the NN performance depends on the data, new networks are trained every time a new signal model and signal cross section are injected into the data. In order to reduce statistical fluctuations related to the shape of the signal, for each signal cross section the network is retrained with five random samplings from the signal simulation, and the network with the median performance is chosen. A profile-likelihood-ratio test with asymptotic formulae [110] is used to determine 95% confidence intervals for the excluded signal cross section. The excluded cross section is reported as $\max(\sigma_{\text{CL}}, \sigma_{\text{injected}})$, where σ_{CL} is the cross section determined from the profile-likelihood-ratio test and σ_{injected} is the injected cross section. This procedure is chosen because the network's performance may not be as good if there were truly less signal than was injected. The resulting exclusion limits are presented in Figure 3. As the background expectation is determined entirely from data, the only systematic uncertainty associated with the background is the statistical uncertainty from the fit. The only other relevant uncertainties are those related to the signal m_{JJ} and m_J modeling; experimental uncertainties in the reconstructed jet kinematics account for about a 10% uncertainty in the excluded cross section.

The limits on W' production vary with m_A , m_B , and m_C . For $m_B = m_C = 400$ GeV, the excluded cross section is about 1 fb, a significant improvement over existing limits. Lower m_B and m_C result in weaker limits because of the larger SM background in those regions; it is therefore difficult for the NN to learn to tag these signals. For some models, such as $(m_A, m_B, m_C) = (5000, 80, 80)$ GeV, the NN is not able to identify the signal effectively, resulting in limits weaker than those from previous searches. For comparison, the sensitivities of the ATLAS inclusive dijet search (recast with signals from this paper) [111] and the all-hadronic diboson resonance search [101] are also shown in Figure 3. The inclusive dijet search sensitivity decreases for high m_B and m_C masses due to the use of small-radius jets that do not capture all of the B and C decay products. The diboson resonance search has greater sensitivity when $m_B, m_C \approx m_W, m_Z$, but it has no sensitivity away from these points. Direct searches for B and C that trigger on initial-state radiation are also sensitive to these signal models [34–39], but the sensitivity is much weaker than 10 fb.

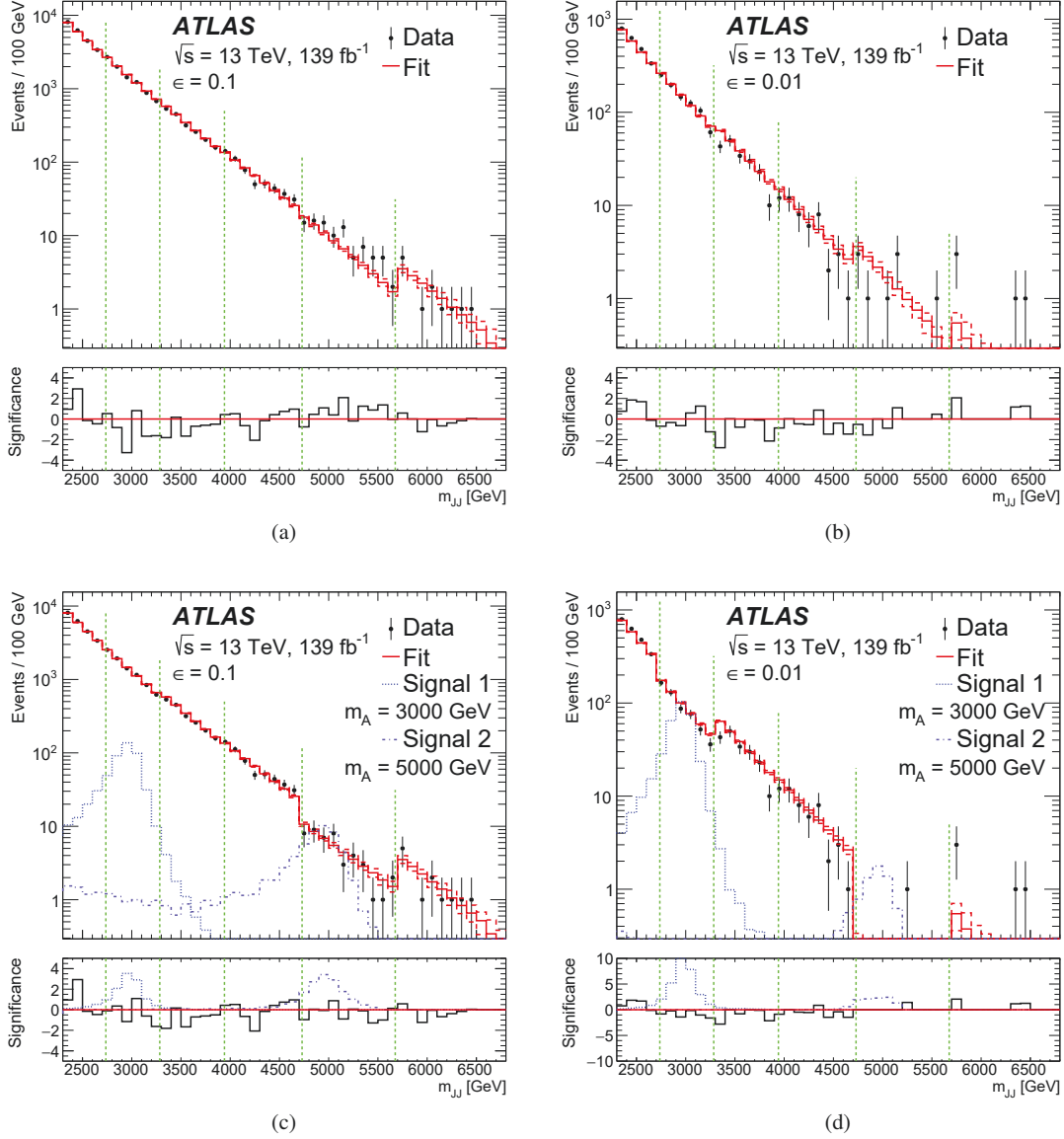


Figure 2: A comparison of the fitted background and the data in all six signal regions, indicated by vertical dashed lines, and for (a,c) $\epsilon = 0.1$ and (b,d) $\epsilon = 0.01$. Dashed histograms represent the fit uncertainty. The lower panel is the Gaussian-equivalent significance of the deviation between the fit and data. The fits are performed including the sidebands, but only the signal region predictions and observations in each region are shown. As the NN is different for each signal region, the presented spectrum is not necessarily smooth. The top plots (a,b) show the result without injected signal, and the bottom plots (c,d) present the same results but with signals injected only for the NN training at $m_A = 3$ TeV (Signal 1) and $m_A = 5$ TeV (Signal 2), each with $m_B = m_C = 200$ GeV. The injected cross section for each signal is just below the limit from the inclusive dijet search [101].

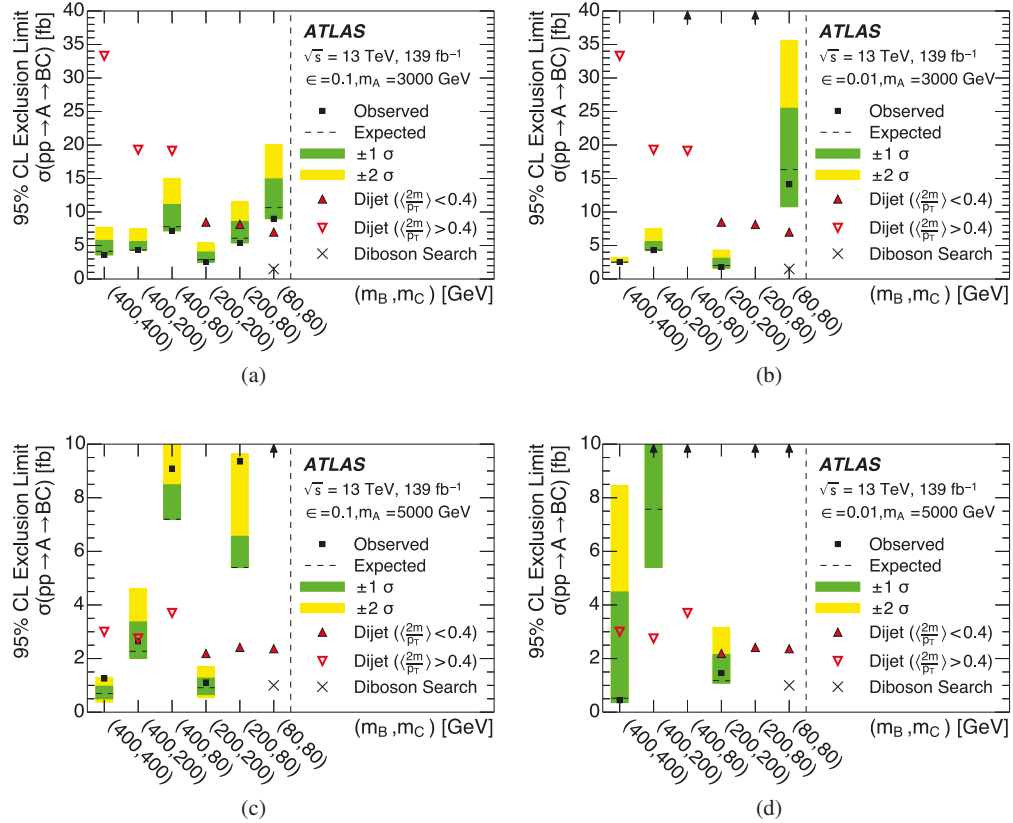


Figure 3: 95% confidence level upper limits on the cross section for a variety of signal models, labeled by (m_B, m_C) , in GeV. The limits are shown for signal models with (a,b) $m_A = 3000$ GeV and NN trained on signal region 2; and (c,d) $m_A = 5000$ GeV and NN trained on signal region 5. The limits are broken down between the analyses with (a,c) $\epsilon = 0.1$ and (b,d) $\epsilon = 0.01$. Also shown are the limits from the ATLAS dijet search [101] and the ATLAS all-hadronic diboson search [111]. The inclusive dijet limits are calculated using the W' signals from this paper and the full analysis pipeline of Ref. [101]; the diboson search limits are computed using the Heavy Vector Triplet [112] W' signal from Ref. [111]. The acceptance for the W' in this paper, compared to the W' acceptance in Ref. [111], is 86% and 54% for $m_{W'} = 3$ and 5 TeV, respectively. Missing observed markers are higher than the plotted range. Poor limits occur when the NN fails to tag the signal.

In conclusion, this Letter presents a model-agnostic resonance search in the all-hadronic final state using the full LHC Run 2 pp data set of the ATLAS experiment. Weakly supervised classification NNs are used to identify the presence of potential signals without training on simulations of any particular signal models. For jets produced from Lorentz-boosted heavy-particle decays, this search is more sensitive than the inclusive dijet search and extends the coverage of the all-hadronic diboson search to regions away from the SM boson masses. This is the first search that covers $A \rightarrow BC$ production where all of A , B and C are BSM particles that can have different masses. The feature space used by the NNs is only two-dimensional, so there is great potential to extend this method to include additional features and more final states in order to ensure broad coverage of unanticipated scenarios.

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The ATLAS Collaboration

G. Aad¹⁰², B. Abbott¹²⁸, D.C. Abbott¹⁰³, A. Abed Abud³⁶, K. Abeling⁵³, D.K. Abhayasinghe⁹⁴, S.H. Abidi¹⁶⁶, O.S. AbouZeid⁴⁰, N.L. Abraham¹⁵⁵, H. Abramowicz¹⁶⁰, H. Abreu¹⁵⁹, Y. Abulaiti⁶, B.S. Acharya^{67a,67b,n}, B. Achkar⁵³, L. Adam¹⁰⁰, C. Adam Bourdarios⁵, L. Adamczyk^{84a}, L. Adamek¹⁶⁶, J. Adelman¹²¹, M. Adersberger¹¹⁴, A. Adiguzel^{12c}, S. Adorni⁵⁴, T. Adye¹⁴³, A.A. Affolder¹⁴⁵, Y. Afik¹⁵⁹, C. Agapopoulou⁶⁵, M.N. Agaras³⁸, A. Aggarwal¹¹⁹, C. Agheorghiesei^{27c}, J.A. Aguilar-Saavedra^{139f,139a,ac}, A. Ahmad³⁶, F. Ahmadov⁸⁰, W.S. Ahmed¹⁰⁴, X. Ai¹⁸, G. Aielli^{74a,74b}, S. Akatsuka⁸⁶, M. Akbiyik¹⁰⁰, T.P.A. Åkesson⁹⁷, E. Akilli⁵⁴, A.V. Akimov¹¹¹, K. Al Khoury⁶⁵, G.L. Alberghi^{23b,23a}, J. Albert¹⁷⁵, M.J. Alconada Verzini¹⁶⁰, S. Alderweireldt³⁶, M. Aleksa³⁶, I.N. Aleksandrov⁸⁰, C. Alexa^{27b}, T. Alexopoulos¹⁰, A. Alfonsi¹²⁰, F. Alfonsi^{23b,23a}, M. Alhroob¹²⁸, B. Ali¹⁴¹, S. Ali¹⁵⁷, M. Aliev¹⁶⁵, G. Alimonti^{69a}, C. Allaire³⁶, B.M.M. Allbrooke¹⁵⁵, B.W. Allen¹³¹, P.P. Allport²¹, A. Aloisio^{70a,70b}, F. Alonso⁸⁹, C. Alpigiani¹⁴⁷, E. Alunno Camelia^{74a,74b}, M. Alvarez Estevez⁹⁹, M.G. Alviggi^{70a,70b}, Y. Amaral Coutinho^{81b}, A. Ambler¹⁰⁴, L. Ambroz¹³⁴, C. Amelung²⁶, D. Amidei¹⁰⁶, S.P. Amor Dos Santos^{139a}, S. Amoroso⁴⁶, C.S. Amrouche⁵⁴, F. An⁷⁹, C. Anastopoulos¹⁴⁸, N. Andari¹⁴⁴, T. Andeen¹¹, J.K. Anders²⁰, S.Y. Andrean^{45a,45b}, A. Andreazza^{69a,69b}, V. Andrei^{61a}, C.R. Anelli¹⁷⁵, S. Angelidakis⁹, A. Angerami³⁹, A.V. Anisenkov^{122b,122a}, A. Annovi^{72a}, C. Antel⁵⁴, M.T. Anthony¹⁴⁸, E. Antipov¹²⁹, M. Antonelli⁵¹, D.J.A. Antrim¹⁷⁰, F. Anulli^{73a}, M. Aoki⁸², J.A. Aparisi Pozo¹⁷³, M.A. Aparo¹⁵⁵, L. Aperio Bella⁴⁶, N. Aranzabal Barrio³⁶, V. Araujo Ferraz^{81a}, R. Araujo Pereira^{81b}, C. Arcangeletti⁵¹, A.T.H. Arce⁴⁹, F.A. Arduh⁸⁹, J-F. Arguin¹¹⁰, S. Argyropoulos⁵², J.-H. Arling⁴⁶, A.J. Armbruster³⁶, A. Armstrong¹⁷⁰, O. Arnaez¹⁶⁶, H. Arnold¹²⁰, Z.P. Arrubarrena Tame¹¹⁴, G. Artoni¹³⁴, K. Asai¹²⁶, S. Asai¹⁶², T. Asawatavonvanich¹⁶⁴, N. Asbah⁵⁹, E.M. Asimakopoulou¹⁷¹, L. Asquith¹⁵⁵, J. Assahsah^{35d}, K. Assamagan²⁹, R. Astalos^{28a}, R.J. Atkin^{33a}, M. Atkinson¹⁷², N.B. Atlay¹⁹, H. Atmani⁶⁵, K. Augsten¹⁴¹, V.A. Austrup¹⁸¹, G. Avolio³⁶, M.K. Ayoub^{15a}, G. Azuelos^{110,ak}, H. Bachacou¹⁴⁴, K. Bachas¹⁶¹, M. Backes¹³⁴, F. Backman^{45a,45b}, P. Bagnaia^{73a,73b}, M. Bahmani⁸⁵, H. Bahrasemani¹⁵¹, A.J. Bailey¹⁷³, V.R. Bailey¹⁷², J.T. Baines¹⁴³, C. Bakalis¹⁰, O.K. Baker¹⁸², P.J. Bakker¹²⁰, E. Bakos¹⁶, D. Bakshi Gupta⁸, S. Balaji¹⁵⁶, E.M. Baldin^{122b,122a}, P. Balek¹⁷⁹, F. Balli¹⁴⁴, W.K. Balunas¹³⁴, J. Balz¹⁰⁰, E. Banas⁸⁵, M. Bandieramonte¹³⁸, A. Bandyopadhyay²⁴, Sw. Banerjee^{180,i}, L. Barak¹⁶⁰, W.M. Barbe³⁸, E.L. Barberio¹⁰⁵, D. Barberis^{55b,55a}, M. Barbero¹⁰², G. Barbour⁹⁵, T. Barillari¹¹⁵, M-S. Barisits³⁶, J. Barkeloo¹³¹, T. Barklow¹⁵², R. Barnea¹⁵⁹, B.M. Barnett¹⁴³, R.M. Barnett¹⁸, Z. Barnovska-Blenessy^{60a}, A. Baroncelli^{60a}, G. Barone²⁹, A.J. Barr¹³⁴, L. Barranco Navarro^{45a,45b}, F. Barreiro⁹⁹, J. Barreiro Guimarães da Costa^{15a}, U. Barron¹⁶⁰, S. Barsov¹³⁷, F. Bartels^{61a}, R. Bartoldus¹⁵², G. Bartolini¹⁰², A.E. Barton⁹⁰, P. Bartos^{28a}, A. Basalaev⁴⁶, A. Basan¹⁰⁰, A. Bassalat^{65,ah}, M.J. Basso¹⁶⁶, R.L. Bates⁵⁷, S. Batlamous^{35e}, J.R. Batley³², B. Batool¹⁵⁰, M. Battaglia¹⁴⁵, M. Bause^{73a,73b}, F. Bauer¹⁴⁴, K.T. Bauer¹⁷⁰, H.S. Bawa³¹, A. Bayirli^{12c}, J.B. Beacham⁴⁹, T. Beau¹³⁵, P.H. Beauchemin¹⁶⁹, F. Becherer⁵², P. Bechtel²⁴, H.C. Beck⁵³, H.P. Beck^{20,p}, K. Becker¹⁷⁷, C. Becot⁴⁶, A. Beddall^{12d}, A.J. Beddall^{12a}, V.A. Bednyakov⁸⁰, M. Bedognetti¹²⁰, C.P. Bee¹⁵⁴, T.A. Beermann¹⁸¹, M. Begalli^{81b}, M. Begel²⁹, A. Behera¹⁵⁴, J.K. Behr⁴⁶, F. Beisiegel²⁴, M. Belfkir⁵, A.S. Bell⁹⁵, G. Bella¹⁶⁰, L. Bellagamba^{23b}, A. Bellerive³⁴, P. Bellos⁹, K. Beloborodov^{122b,122a}, K. Belotskiy¹¹², N.L. Belyaev¹¹², D. Benchevkroun^{35a}, N. Benekos¹⁰, Y. Benhammou¹⁶⁰, D.P. Benjamin⁶, M. Benoit⁵⁴, J.R. Bensinger²⁶, S. Bentvelsen¹²⁰, L. Beresford¹³⁴, M. Beretta⁵¹, D. Berge¹⁹, E. Bergeas Kuutmann¹⁷¹, N. Berger⁵, B. Bergmann¹⁴¹, L.J. Bergsten²⁶, J. Beringer¹⁸, S. Berlendis⁷, G. Bernardi¹³⁵, C. Bernius¹⁵², F.U. Bernlochner²⁴, T. Berry⁹⁴, P. Berta¹⁰⁰, C. Bertella^{15a}, A. Berthold⁴⁸, I.A. Bertram⁹⁰, O. Bessidskaia Bylund¹⁸¹, N. Besson¹⁴⁴, A. Bethani¹⁰¹, S. Bethke¹¹⁵, A. Betti⁴², A.J. Bevan⁹³, J. Beyer¹¹⁵, D.S. Bhattacharya¹⁷⁶, P. Bhattarai²⁶, V.S. Bhopatkar⁶, R. Bi¹³⁸, R.M. Bianchi¹³⁸, O. Biebel¹¹⁴, D. Biedermann¹⁹, R. Bielski³⁶, K. Bierwagen¹⁰⁰, N.V. Biesuz^{72a,72b}, M. Biglietti^{75a}, T.R.V. Billoud¹¹⁰, M. Bindi⁵³, A. Bingul^{12d}, C. Bini^{73a,73b},

S. Biondi^{23b,23a}, C.J. Birch-sykes¹⁰¹, M. Birman¹⁷⁹, T. Bisanz⁵³, J.P. Biswal³, D. Biswas^{180,i}, A. Bitadze¹⁰¹, C. Bittrich⁴⁸, K. Björke¹³³, T. Blazek^{28a}, I. Bloch⁴⁶, C. Blocker²⁶, A. Blue⁵⁷, U. Blumenschein⁹³, G.J. Bobbink¹²⁰, V.S. Bobrovnikov^{122b,122a}, S.S. Bocchetta⁹⁷, D. Boerner⁴⁶, D. Bogavac¹⁴, A.G. Bogdanchikov^{122b,122a}, C. Bohm^{45a}, V. Boisvert⁹⁴, P. Bokan^{53,171}, T. Bold^{84a}, A.E. Bolz^{61b}, M. Bomben¹³⁵, M. Bona⁹³, J.S. Bonilla¹³¹, M. Boonekamp¹⁴⁴, C.D. Booth⁹⁴, A.G. Borbély⁵⁷, H.M. Borecka-Bielska⁹¹, L.S. Borgna⁹⁵, A. Borisov¹²³, G. Borissov⁹⁰, D. Bortoletto¹³⁴, D. Boscherini^{23b}, M. Bosman¹⁴, J.D. Bossio Sola¹⁰⁴, K. Bouaouda^{35a}, J. Boudreau¹³⁸, E.V. Bouhova-Thacker⁹⁰, D. Boumediene³⁸, S.K. Boutle⁵⁷, A. Boveia¹²⁷, J. Boyd³⁶, D. Boye^{33c}, I.R. Boyko⁸⁰, A.J. Bozson⁹⁴, J. Bracinik²¹, N. Brahimi^{60d}, G. Brandt¹⁸¹, O. Brandt³², F. Braren⁴⁶, B. Brau¹⁰³, J.E. Brau¹³¹, W.D. Brearden Madden⁵⁷, K. Brendlinger⁴⁶, R. Brenner¹⁵⁹, L. Brenner³⁶, R. Brenner¹⁷¹, S. Bressler¹⁷⁹, B. Brickwedde¹⁰⁰, D.L. Briglin²¹, D. Britton⁵⁷, D. Britzger¹¹⁵, I. Brock²⁴, R. Brock¹⁰⁷, G. Brooijmans³⁹, W.K. Brooks^{146d}, E. Brost²⁹, P.A. Bruckman de Renstrom⁸⁵, B. Brüers⁴⁶, D. Bruncko^{28b}, A. Bruni^{23b}, G. Bruni^{23b}, L.S. Bruni¹²⁰, S. Bruno^{74a,74b}, M. Bruschi^{23b}, N. Bruscino^{73a,73b}, L. Bryngemark¹⁵², T. Buanes¹⁷, Q. Buat¹⁵⁴, P. Buchholz¹⁵⁰, A.G. Buckley⁵⁷, I.A. Budagov⁸⁰, M.K. Bugge¹³³, F. Bühner⁵², O. Bulekov¹¹², B.A. Bullard⁵⁹, T.J. Burch¹²¹, S. Burdin⁹¹, C.D. Burgard¹²⁰, A.M. Burger¹²⁹, B. Burghgrave⁸, J.T.P. Burr⁴⁶, C.D. Burton¹¹, J.C. Burzynski¹⁰³, V. Büscher¹⁰⁰, E. Buschmann⁵³, P.J. Bussey⁵⁷, J.M. Butler²⁵, C.M. Buttar⁵⁷, J.M. Butterworth⁹⁵, P. Butti³⁶, W. Buttinger³⁶, C.J. Buxo Vazquez¹⁰⁷, A. Buzatu¹⁵⁷, A.R. Buzykaev^{122b,122a}, G. Cabras^{23b,23a}, S. Cabrera Urbán¹⁷³, D. Caforio⁵⁶, H. Cai¹³⁸, V.M.M. Cairo¹⁵², O. Cakir^{4a}, N. Calace³⁶, P. Calafiura¹⁸, G. Calderini¹³⁵, P. Calfayan⁶⁶, G. Callea⁵⁷, L.P. Caloba^{81b}, A. Caltabiano^{74a,74b}, S. Calvente Lopez⁹⁹, D. Calvet³⁸, S. Calvet³⁸, T.P. Calvet¹⁰², M. Calvetti^{72a,72b}, R. Camacho Toro¹³⁵, S. Camarda³⁶, D. Camarero Munoz⁹⁹, P. Camarri^{74a,74b}, M.T. Camerlingo^{75a,75b}, D. Cameron¹³³, C. Camincher³⁶, S. Campana³⁶, M. Campanelli⁹⁵, A. Camplani⁴⁰, V. Canale^{70a,70b}, A. Canesse¹⁰⁴, M. Cano Bret^{60c}, J. Cantero¹²⁹, T. Cao¹⁶⁰, Y. Cao¹⁷², M.D.M. Capeans Garrido³⁶, M. Capua^{41b,41a}, R. Cardarelli^{74a}, F. Cardillo¹⁴⁸, G. Carducci^{41b,41a}, I. Carli¹⁴², T. Carli³⁶, G. Carlino^{70a}, B.T. Carlson¹³⁸, E.M. Carlson^{175,167a}, L. Carminati^{69a,69b}, R.M.D. Carney¹⁵², S. Caron¹¹⁹, E. Carquin^{146d}, S. Carrá⁴⁶, G.C. Carratta^{23b,23a}, J.W.S. Carter¹⁶⁶, T.M. Carter⁵⁰, M.P. Casado^{14,f}, A.F. Casha¹⁶⁶, F.L. Castillo¹⁷³, L. Castillo Garcia¹⁴, V. Castillo Gimenez¹⁷³, N.F. Castro^{139a,139e}, A. Catinaccio³⁶, J.R. Catmore¹³³, A. Cattai³⁶, V. Cavaliere²⁹, V. Cavasinni^{72a,72b}, E. Celebi^{12b}, F. Celli¹³⁴, K. Cerny¹³⁰, A.S. Cerqueira^{81a}, A. Cerri¹⁵⁵, L. Cerrito^{74a,74b}, F. Cerutti¹⁸, A. Cervelli^{23b,23a}, S.A. Cetin^{12b}, Z. Chadi^{35a}, D. Chakraborty¹²¹, J. Chan¹⁸⁰, W.S. Chan¹²⁰, W.Y. Chan⁹¹, J.D. Chapman³², B. Chargeishvili^{158b}, D.G. Charlton²¹, T.P. Charman⁹³, C.C. Chau³⁴, S. Che¹²⁷, S. Chekanov⁶, S.V. Chekulaev^{167a}, G.A. Chelkov^{80,af}, B. Chen⁷⁹, C. Chen^{60a}, C.H. Chen⁷⁹, H. Chen²⁹, J. Chen^{60a}, J. Chen³⁹, J. Chen²⁶, S. Chen¹³⁶, S.J. Chen^{15c}, X. Chen^{15b}, Y. Chen^{60a}, Y-H. Chen⁴⁶, H.C. Cheng^{63a}, H.J. Cheng^{15a}, A. Cheplakov⁸⁰, E. Cheremushkina¹²³, R. Cherkaoui El Moursli^{35e}, E. Cheu⁷, K. Cheung⁶⁴, T.J.A. Chevalérias¹⁴⁴, L. Chevalier¹⁴⁴, V. Chiarella⁵¹, G. Chiarelli^{72a}, G. Chiodini^{68a}, A.S. Chisholm²¹, A. Chitan^{27b}, I. Chiu¹⁶², Y.H. Chiu¹⁷⁵, M.V. Chizhov⁸⁰, K. Choi¹¹, A.R. Chomont^{73a,73b}, Y.S. Chow¹²⁰, L.D. Christopher^{33e}, M.C. Chu^{63a}, X. Chu^{15a,15d}, J. Chudoba¹⁴⁰, J.J. Chwastowski⁸⁵, L. Chytka¹³⁰, D. Cieri¹¹⁵, K.M. Ciesla⁸⁵, D. Cinca⁴⁷, V. Cindro⁹², I.A. Cioară^{27b}, A. Ciocio¹⁸, F. Ciotto^{70a,70b}, Z.H. Citron^{179j}, M. Citterio^{69a}, D.A. Ciubotaru^{27b}, B.M. Ciungu¹⁶⁶, A. Clark⁵⁴, M.R. Clark³⁹, P.J. Clark⁵⁰, S.E. Clawson¹⁰¹, C. Clement^{45a,45b}, Y. Coadou¹⁰², M. Cobal^{167a,67c}, A. Coccaro^{55b}, J. Cochran⁷⁹, R. Coelho Lopes De Sa¹⁰³, H. Cohen¹⁶⁰, A.E.C. Coimbra³⁶, B. Cole³⁹, A.P. Colijn¹²⁰, J. Collot⁵⁸, P. Conde Muiño^{139a,139h}, S.H. Connell^{33c}, I.A. Connelly⁵⁷, S. Constantinescu^{27b}, F. Conventi^{70a,al}, A.M. Cooper-Sarkar¹³⁴, F. Cormier¹⁷⁴, K.J.R. Cormier¹⁶⁶, L.D. Corpe⁹⁵, M. Corradi^{73a,73b}, E.E. Corrigan⁹⁷, F. Corriveau^{104,aa}, A. Cortes-Gonzalez³⁶, M.J. Costa¹⁷³, F. Costanza⁵, D. Costanzo¹⁴⁸, G. Cowan⁹⁴, J.W. Cowley³², J. Crane¹⁰¹, K. Cranmer¹²⁵, R.A. Creager¹³⁶, S. Crépe-Renaudin⁵⁸, F. Crescioli¹³⁵, M. Cristinziani²⁴, V. Croft¹⁶⁹, G. Crosetti^{41b,41a}, A. Cueto⁵, T. Cuhadar Donszelmann¹⁷⁰, H. Cui^{15a,15d}, A.R. Cukierman¹⁵², W.R. Cunningham⁵⁷, S. Czekierda⁸⁵,

P. Czodrowski³⁶, M.M. Czurylo^{61b}, M.J. Da Cunha Sargedas De Sousa^{60b}, J.V. Da Fonseca Pinto^{81b}, C. Da Via¹⁰¹, W. Dabrowski^{84a}, F. Dachs³⁶, T. Dado⁴⁷, S. Dahbi^{33e}, T. Dai¹⁰⁶, C. Dallapiccola¹⁰³, M. Dam⁴⁰, G. D'amen²⁹, V. D'Amico^{75a,75b}, J. Damp¹⁰⁰, J.R. Dandoy¹³⁶, M.F. Daneri³⁰, M. Danninger¹⁵¹, V. Dao³⁶, G. Darbo^{55b}, O. Dartsis⁵, A. Dattagupta¹³¹, T. Daubney⁴⁶, S. D'Auria^{69a,69b}, C. David^{167b}, T. Davidek¹⁴², D.R. Davis⁴⁹, I. Dawson¹⁴⁸, K. De⁸, R. De Asmundis^{70a}, M. De Beurs¹²⁰, S. De Castro^{23b,23a}, N. De Groot¹¹⁹, P. de Jong¹²⁰, H. De la Torre¹⁰⁷, A. De Maria^{15c}, D. De Pedis^{73a}, A. De Salvo^{73a}, U. De Sanctis^{74a,74b}, M. De Santis^{74a,74b}, A. De Santo¹⁵⁵, J.B. De Vivie De Regie⁶⁵, C. Debenedetti¹⁴⁵, D.V. Dedovich⁸⁰, A.M. Deiana⁴², J. Del Peso⁹⁹, Y. Delabat Diaz⁴⁶, D. Delgove⁶⁵, F. Deliot¹⁴⁴, C.M. Delitzsch⁷, M. Della Pietra^{70a,70b}, D. Della Volpe⁵⁴, A. Dell'Acqua³⁶, L. Dell'Asta^{74a,74b}, M. Delmastro⁵, C. Delporte⁶⁵, P.A. Delsart⁵⁸, D.A. DeMarco¹⁶⁶, S. Demers¹⁸², M. Demichev⁸⁰, G. Demontigny¹¹⁰, S.P. Denisov¹²³, L. D'Eramo¹²¹, D. Derendarz⁸⁵, J.E. Derkaoui^{35d}, F. Derue¹³⁵, P. Dervan⁹¹, K. Desch²⁴, K. Dette¹⁶⁶, C. Deutsch²⁴, M.R. Devesa³⁰, P.O. Deviveiros³⁶, F.A. Di Bello^{73a,73b}, A. Di Ciaccio^{74a,74b}, L. Di Ciaccio⁵, W.K. Di Clemente¹³⁶, C. Di Donato^{70a,70b}, A. Di Girolamo³⁶, G. Di Gregorio^{72a,72b}, B. Di Micco^{75a,75b}, R. Di Nardo^{75a,75b}, K.F. Di Petrillo⁵⁹, R. Di Sipio¹⁶⁶, C. Diaconu¹⁰², F.A. Dias¹²⁰, T. Dias Do Vale^{139a}, M.A. Diaz^{146a}, F.G. Diaz Capriles²⁴, J. Dickinson¹⁸, M. Didenko¹⁶⁵, E.B. Diehl¹⁰⁶, J. Dietrich¹⁹, S. Díez Cornell⁴⁶, C. Díez Pardos¹⁵⁰, A. Dimitrievska¹⁸, W. Ding^{15b}, J. Dingfelder²⁴, S.J. Dittmeier^{61b}, F. Dittus³⁶, F. Djama¹⁰², T. Djobava^{158b}, J.I. Djuvslund¹⁷, M.A.B. Do Vale^{81c}, M. Dobre^{27b}, D. Dodsworth²⁶, C. Doglioni⁹⁷, J. Dolejsi¹⁴², Z. Dolezal¹⁴², M. Donadelli^{81d}, B. Dong^{60c}, J. Donini³⁸, A. D'onofrio^{15c}, M. D'Onofrio⁹¹, J. Dopke¹⁴³, A. Doria^{70a}, M.T. Dova⁸⁹, A.T. Doyle⁵⁷, E. Drechsler¹⁵¹, E. Dreyer¹⁵¹, T. Dreyer⁵³, A.S. Drobac¹⁶⁹, D. Du^{60b}, T.A. du Pree¹²⁰, Y. Duan^{60d}, F. Dubinin¹¹¹, M. Dubovsky^{28a}, A. Dubreuil⁵⁴, E. Duchovni¹⁷⁹, G. Duckeck¹¹⁴, O.A. Ducu³⁶, D. Duda¹¹⁵, A. Dudarev³⁶, A.C. Dudder¹⁰⁰, E.M. Duffield¹⁸, M. D'uffizi¹⁰¹, L. Duflo⁶⁵, M. Dührssen³⁶, C. Dülsen¹⁸¹, M. Dumancic¹⁷⁹, A.E. Dumitriu^{27b}, M. Dunford^{61a}, A. Duperrin¹⁰², H. Duran Yildiz^{4a}, M. Düren⁵⁶, A. Durglishvili^{158b}, D. Duschinger⁴⁸, B. Dutta⁴⁶, D. Duvnjak¹, G.I. Dyckes¹³⁶, M. Dyndal³⁶, S. Dysch¹⁰¹, B.S. Dziedzic⁸⁵, M.G. Eggleston⁴⁹, T. Eifert⁸, G. Eigen¹⁷, K. Einsweiler¹⁸, T. Ekelof¹⁷¹, H. El Jarrari^{35e}, V. Ellajosyula¹⁷¹, M. Ellert¹⁷¹, F. Ellinghaus¹⁸¹, A.A. Elliot⁹³, N. Ellis³⁶, J. Elmsheuser²⁹, M. Elsing³⁶, D. Emeliyanov¹⁴³, A. Emerman³⁹, Y. Enari¹⁶², M.B. Epland⁴⁹, J. Erdmann⁴⁷, A. Ereditato²⁰, P.A. Erland⁸⁵, M. Errenst¹⁸¹, M. Escalier⁶⁵, C. Escobar¹⁷³, O. Estrada Pastor¹⁷³, E. Etzion¹⁶⁰, H. Evans⁶⁶, M.O. Evans¹⁵⁵, A. Ezhilov¹³⁷, F. Fabbri⁵⁷, L. Fabbri^{23b,23a}, V. Fabiani¹¹⁹, G. Facini¹⁷⁷, R.M. Fakhruddinov¹²³, S. Falciano^{73a}, P.J. Falke²⁴, S. Falke³⁶, J. Faltova¹⁴², Y. Fang^{15a}, Y. Fang^{15a}, G. Fanourakis⁴⁴, M. Fanti^{69a,69b}, M. Faraj^{67a,67c,q}, A. Farbin⁸, A. Farilla^{75a}, E.M. Farina^{71a,71b}, T. Farooque¹⁰⁷, S.M. Farrington⁵⁰, P. Farthouat³⁶, F. Fassi^{35e}, P. Fassnacht³⁶, D. Fassoulitis⁹, M. Fauci Giannelli⁵⁰, W.J. Fawcett³², L. Fayard⁶⁵, O.L. Fedin^{137,o}, W. Fedorko¹⁷⁴, A. Fehr²⁰, M. Feickert¹⁷², L. Feligioni¹⁰², A. Fell¹⁴⁸, C. Feng^{60b}, M. Feng⁴⁹, M.J. Fenton¹⁷⁰, A.B. Fenyuk¹²³, S.W. Ferguson⁴³, J. Ferrando⁴⁶, A. Ferrante¹⁷², A. Ferrari¹⁷¹, P. Ferrari¹²⁰, R. Ferrari^{71a}, D.E. Ferreira de Lima^{61b}, A. Ferrer¹⁷³, D. Ferrere⁵⁴, C. Ferretti¹⁰⁶, F. Fiedler¹⁰⁰, A. Filipčič⁹², F. Filthaut¹¹⁹, K.D. Finelli²⁵, M.C.N. Fiolhais^{139a,139c,a}, L. Fiorini¹⁷³, F. Fischer¹¹⁴, J. Fischer¹⁰⁰, W.C. Fisher¹⁰⁷, T. Fitschen⁶⁵, I. Fleck¹⁵⁰, P. Fleischmann¹⁰⁶, T. Flick¹⁸¹, B.M. Flierl¹¹⁴, L. Flores¹³⁶, L.R. Flores Castillo^{63a}, F.M. Follega^{76a,76b}, N. Fomin¹⁷, J.H. Foo¹⁶⁶, G.T. Forcolin^{76a,76b}, B.C. Forland⁶⁶, A. Formica¹⁴⁴, F.A. Förster¹⁴, A.C. Forti¹⁰¹, E. Fortin¹⁰², M.G. Foti¹³⁴, D. Fournier⁶⁵, H. Fox⁹⁰, P. Francavilla^{72a,72b}, S. Francescato^{73a,73b}, M. Franchini^{23b,23a}, S. Franchino^{61a}, D. Francis³⁶, L. Franco⁵, L. Franconi²⁰, M. Franklin⁵⁹, G. Frattari^{73a,73b}, A.N. Fray⁹³, P.M. Freeman²¹, B. Freund¹¹⁰, W.S. Freund^{81b}, E.M. Freundlich⁴⁷, D.C. Frizzell¹²⁸, D. Froidevaux³⁶, J.A. Frost¹³⁴, M. Fujimoto¹²⁶, C. Fukunaga¹⁶³, E. Fullana Torregrosa¹⁷³, T. Fusayasu¹¹⁶, J. Fuster¹⁷³, A. Gabrielli^{23b,23a}, A. Gabrielli³⁶, S. Gadatsch⁵⁴, P. Gadow¹¹⁵, G. Gagliardi^{55b,55a}, L.G. Gagnon¹¹⁰, G.E. Gallardo¹³⁴, E.J. Gallas¹³⁴, B.J. Gallop¹⁴³, R. Gamboa Goni⁹³, K.K. Gan¹²⁷, S. Ganguly¹⁷⁹, J. Gao^{60a}, Y. Gao⁵⁰, Y.S. Gao^{31,l}, F.M. Garay Walls^{146a}, C. García¹⁷³, J.E. García Navarro¹⁷³, J.A. García Pascual^{15a}, C. Garcia-Argos⁵²,

M. Garcia-Sciveres¹⁸, R.W. Gardner³⁷, N. Garelli¹⁵², S. Gargiulo⁵², C.A. Garner¹⁶⁶, V. Garonne¹³³, S.J. Gasirowski¹⁴⁷, P. Gaspar^{81b}, A. Gaudiello^{55b,55a}, G. Gaudio^{71a}, I.L. Gavrilenko¹¹¹, A. Gavriluk¹²⁴, C. Gay¹⁷⁴, G. Gaycken⁴⁶, E.N. Gazis¹⁰, A.A. Geanta^{27b}, C.M. Gee¹⁴⁵, C.N.P. Gee¹⁴³, J. Geisen⁹⁷, M. Geisen¹⁰⁰, C. Gemme^{55b}, M.H. Genest⁵⁸, C. Geng¹⁰⁶, S. Gentile^{73a,73b}, S. George⁹⁴, T. Gerasis⁴⁴, L.O. Gerlach⁵³, P. Gessinger-Befurt¹⁰⁰, G. Gessner⁴⁷, S. Ghasemi¹⁵⁰, M. Ghasemi Bostanabad¹⁷⁵, M. Ghneimat¹⁵⁰, A. Ghosh⁶⁵, A. Ghosh⁷⁸, B. Giacobbe^{23b}, S. Giagu^{73a,73b}, N. Giangiacomi^{23b,23a}, P. Giannetti^{72a}, A. Giannini^{70a,70b}, G. Giannini¹⁴, S.M. Gibson⁹⁴, M. Gignac¹⁴⁵, D.T. Gil^{84b}, B.J. Gilbert³⁹, D. Gillberg³⁴, G. Gilles¹⁸¹, D.M. Gingrich^{3,ak}, M.P. Giordani^{67a,67c}, P.F. Giraud¹⁴⁴, G. Giugliarelli^{67a,67c}, D. Giugni^{69a}, F. Giuli^{74a,74b}, S. Gkaitatzis¹⁶¹, I. Gkialas^{9,g}, E.L. Gkoukousis¹⁴, P. Gkoutoumis¹⁰, L.K. Gladilin¹¹³, C. Glasman⁹⁹, J. Glatzer¹⁴, P.C.F. Glaysheer⁴⁶, A. Glazov⁴⁶, G.R. Gledhill¹³¹, I. Gnesi^{41b,b}, M. Goblirsch-Kolb²⁶, D. Godin¹¹⁰, S. Goldfarb¹⁰⁵, T. Golling⁵⁴, D. Golubkov¹²³, A. Gomes^{139a,139b}, R. Goncalves Gama⁵³, R. Gonçalo^{139a,139c}, G. Gonella¹³¹, L. Gonella²¹, A. Gongadze⁸⁰, F. Gonnella²¹, J.L. Gonski³⁹, S. González de la Hoz¹⁷³, S. Gonzalez Fernandez¹⁴, R. Gonzalez Lopez⁹¹, C. Gonzalez Renteria¹⁸, R. Gonzalez Suarez¹⁷¹, S. Gonzalez-Sevilla⁵⁴, G.R. Gonzalvo Rodriguez¹⁷³, L. Goossens³⁶, N.A. Gorasia²¹, P.A. Gorbounov¹²⁴, H.A. Gordon²⁹, B. Gorini³⁶, E. Gorini^{68a,68b}, A. Gorišek⁹², A.T. Goshaw⁴⁹, M.I. Gostkin⁸⁰, C.A. Gottardo¹¹⁹, M. Goughri^{35b}, A.G. Goussiou¹⁴⁷, N. Govender^{33c}, C. Goy⁵, I. Grabowska-Bold^{84a}, E.C. Graham⁹¹, J. Gramling¹⁷⁰, E. Gramstad¹³³, S. Grancagnolo¹⁹, M. Grandi¹⁵⁵, V. Gratchev¹³⁷, P.M. Gravila^{27f}, F.G. Gravili^{68a,68b}, C. Gray⁵⁷, H.M. Gray¹⁸, C. Grefe²⁴, K. Gregersen⁹⁷, I.M. Gregor⁴⁶, P. Grenier¹⁵², K. Grevtsov⁴⁶, C. Grieco¹⁴, N.A. Grieser¹²⁸, A.A. Grillo¹⁴⁵, K. Grimm^{31,k}, S. Grinstein^{14,v}, J.-F. Grivaz⁶⁵, S. Groh¹⁰⁰, E. Gross¹⁷⁹, J. Grosse-Knetter⁵³, Z.J. Grout⁹⁵, C. Grud¹⁰⁶, A. Grummer¹¹⁸, J.C. Grundy¹³⁴, L. Guan¹⁰⁶, W. Guan¹⁸⁰, C. Gubbels¹⁷⁴, J. Guenther³⁶, A. Guerguichon⁶⁵, J.G.R. Guerrero Rojas¹⁷³, F. Guescini¹¹⁵, D. Guest¹⁷⁰, R. Gugel¹⁰⁰, A. Guida⁴⁶, T. Guillemin⁵, S. Guindon³⁶, U. Gul⁵⁷, J. Guo^{60c}, W. Guo¹⁰⁶, Y. Guo^{60a}, Z. Guo¹⁰², R. Gupta⁴⁶, S. Gurbuz^{12c}, G. Gustavino¹²⁸, M. Guth⁵², P. Gutierrez¹²⁸, C. Gutsche⁹⁵, C. Guyot¹⁴⁴, C. Gwenlan¹³⁴, C.B. Gwilliam⁹¹, E.S. Haaland¹³³, A. Haas¹²⁵, C. Haber¹⁸, H.K. Hadavand⁸, A. Hadei^{60a}, M. Haleem¹⁷⁶, J. Haley¹²⁹, J.J. Hall¹⁴⁸, G. Halladjian¹⁰⁷, G.D. Hallowell¹⁰², K. Hamano¹⁷⁵, H. Hamdaoui^{35e}, M. Hamer²⁴, G.N. Hamity⁵⁰, K. Han^{60a,u}, L. Han^{60a}, S. Han¹⁸, Y.F. Han¹⁶⁶, K. Hanagaki^{82,s}, M. Hance¹⁴⁵, D.M. Handl¹¹⁴, M.D. Hank³⁷, R. Hankache¹³⁵, E. Hansen⁹⁷, J.B. Hansen⁴⁰, J.D. Hansen⁴⁰, M.C. Hansen²⁴, P.H. Hansen⁴⁰, E.C. Hanson¹⁰¹, K. Hara¹⁶⁸, T. Harenberg¹⁸¹, S. Harkusha¹⁰⁸, P.F. Harrison¹⁷⁷, N.M. Hartman¹⁵², N.M. Hartmann¹¹⁴, Y. Hasegawa¹⁴⁹, A. Hasib⁵⁰, S. Hassani¹⁴⁴, S. Haug²⁰, R. Hauser¹⁰⁷, L.B. Havener³⁹, M. Havranek¹⁴¹, C.M. Hawkes²¹, R.J. Hawkins³⁶, S. Hayashida¹¹⁷, D. Hayden¹⁰⁷, C. Hayes¹⁰⁶, R.L. Hayes¹⁷⁴, C.P. Hays¹³⁴, J.M. Hays⁹³, H.S. Hayward⁹¹, S.J. Haywood¹⁴³, F. He^{60a}, Y. He¹⁶⁴, M.P. Heath⁵⁰, V. Hedberg⁹⁷, S. Heer²⁴, A.L. Heggelund¹³³, C. Heidegger⁵², K.K. Heidegger⁵², W.D. Heidorn⁷⁹, J. Heilman³⁴, S. Heim⁴⁶, T. Heim¹⁸, B. Heinemann^{46,ai}, J.J. Heinrich¹³¹, L. Heinrich³⁶, J. Hejbal¹⁴⁰, L. Helary⁴⁶, A. Held¹²⁵, S. Hellesund¹³³, C.M. Helling¹⁴⁵, S. Hellman^{45a,45b}, C. Helsens³⁶, R.C.W. Henderson⁹⁰, Y. Heng¹⁸⁰, L. Henkelmann³², A.M. Henriques Correia³⁶, H. Herde²⁶, Y. Hernández Jiménez^{33e}, H. Herr¹⁰⁰, M.G. Herrmann¹¹⁴, T. Herrmann⁴⁸, G. Herten⁵², R. Hertenberger¹¹⁴, L. Hervas³⁶, T.C. Herwig¹³⁶, G.G. Hesketh⁹⁵, N.P. Hessey^{167a}, H. Hibi⁸³, A. Higashida¹⁶², S. Higashino⁸², E. Higón-Rodríguez¹⁷³, K. Hildebrand³⁷, J.C. Hill³², K.K. Hill²⁹, K.H. Hiller⁴⁶, S.J. Hillier²¹, M. Hils⁴⁸, I. Hinchliffe¹⁸, F. Hinterkeuser²⁴, M. Hirose¹³², S. Hirose⁵², D. Hirschbuehl¹⁸¹, B. Hiti⁹², O. Hladik¹⁴⁰, D.R. Hlaluku^{33e}, J. Hobbs¹⁵⁴, N. Hod¹⁷⁹, M.C. Hodgkinson¹⁴⁸, A. Hoecker³⁶, D. Hohn⁵², D. Hohov⁶⁵, T. Holm²⁴, T.R. Holmes³⁷, M. Holzbock¹¹⁴, L.B.A.H. Hommels³², T.M. Hong¹³⁸, J.C. Honig⁵², A. Hönle¹¹⁵, B.H. Hooberman¹⁷², W.H. Hopkins⁶, Y. Horii¹¹⁷, P. Horn⁴⁸, L.A. Horyn³⁷, S. Hou¹⁵⁷, A. Hoummada^{35a}, J. Howarth⁵⁷, J. Hoya⁸⁹, M. Hrabovsky¹³⁰, J. Hrdinka⁷⁷, J. Hrivnac⁶⁵, A. Hrynevich¹⁰⁹, T. Hryn'ova⁵, P.J. Hsu⁶⁴, S.-C. Hsu¹⁴⁷, Q. Hu²⁹, S. Hu^{60c}, Y.F. Hu^{15a,15d,am}, D.P. Huang⁹⁵, Y. Huang^{60a}, Y. Huang^{15a}, Z. Hubacek¹⁴¹, F. Hubaut¹⁰², M. Huebner²⁴, F. Huegging²⁴, T.B. Huffman¹³⁴, M. Huhtinen³⁶,

R. Hulsken⁵⁸, R.F.H. Hunter³⁴, P. Huo¹⁵⁴, N. Huseynov^{80,ab}, J. Huston¹⁰⁷, J. Huth⁵⁹, R. Hyneman¹⁰⁶, S. Hyrych^{28a}, G. Iacobucci⁵⁴, G. Iakovidis²⁹, I. Ibragimov¹⁵⁰, L. Iconomidou-Fayard⁶⁵, P. Iengo³⁶, R. Ignazzi⁴⁰, O. Igonkina^{120,x,*}, R. Iguchi¹⁶², T. Iizawa⁵⁴, Y. Ikegami⁸², M. Ikeno⁸², N. Ilic^{119,166,aa}, F. Iltzsche⁴⁸, H. Imam^{35a}, G. Introzzi^{71a,71b}, M. Iodice^{75a}, K. Iordanidou^{167a}, V. Ippolito^{73a,73b}, M.F. Isacson¹⁷¹, M. Ishino¹⁶², W. Islam¹²⁹, C. Issever^{19,46}, S. Istin¹⁵⁹, F. Ito¹⁶⁸, J.M. Iturbe Ponce^{63a}, R. Iuppa^{76a,76b}, A. Ivina¹⁷⁹, H. Iwasaki⁸², J.M. Izen⁴³, V. Izzo^{70a}, P. Jacka¹⁴⁰, P. Jackson¹, R.M. Jacobs⁴⁶, B.P. Jaeger¹⁵¹, V. Jain², G. Jäkel¹⁸¹, K.B. Jakobi¹⁰⁰, K. Jakobs⁵², T. Jakoubek¹⁷⁹, J. Jamieson⁵⁷, K.W. Janas^{84a}, R. Jansky⁵⁴, M. Janus⁵³, P.A. Janus^{84a}, G. Jarlskog⁹⁷, A.E. Jaspán⁹¹, N. Javadov^{80,ab}, T. Javůrek³⁶, M. Javůrková¹⁰³, F. Jeanneau¹⁴⁴, L. Jeanty¹³¹, J. Jejelava^{158a}, P. Jenni^{52,c}, N. Jeong⁴⁶, S. Jézéquel⁵, H. Ji¹⁸⁰, J. Jia¹⁵⁴, H. Jiang⁷⁹, Y. Jiang^{60a}, Z. Jiang¹⁵², S. Jiggins⁵², F.A. Jimenez Morales³⁸, J. Jimenez Pena¹¹⁵, S. Jin^{15c}, A. Jinaru^{27b}, O. Jinnouchi¹⁶⁴, H. Jivan^{33e}, P. Johansson¹⁴⁸, K.A. Johns⁷, C.A. Johnson⁶⁶, R.W.L. Jones⁹⁰, S.D. Jones¹⁵⁵, T.J. Jones⁹¹, J. Jongmanns^{61a}, J. Jovicevic³⁶, X. Ju¹⁸, J.J. Junggeburth¹¹⁵, A. Juste Rozas^{14,v}, A. Kaczmarek⁸⁵, M. Kado^{73a,73b}, H. Kagan¹²⁷, M. Kagan¹⁵², A. Kahn³⁹, C. Kahra¹⁰⁰, T. Kaji¹⁷⁸, E. Kajomovitz¹⁵⁹, C.W. Kalderon²⁹, A. Kaluza¹⁰⁰, A. Kamenshchikov¹²³, M. Kaneda¹⁶², N.J. Kang¹⁴⁵, S. Kang⁷⁹, Y. Kano¹¹⁷, J. Kanzaki⁸², L.S. Kaplan¹⁸⁰, D. Kar^{33e}, K. Karava¹³⁴, M.J. Kareem^{167b}, I. Karkanas¹⁶¹, S.N. Karpov⁸⁰, Z.M. Karpova⁸⁰, V. Kartvelishvili⁹⁰, A.N. Karyukhin¹²³, E. Kasimi¹⁶¹, A. Kastanas^{45a,45b}, C. Kato^{60d,60c}, J. Katzy⁴⁶, K. Kawade¹⁴⁹, K. Kawagoe⁸⁸, T. Kawaguchi¹¹⁷, T. Kawamoto¹⁴⁴, G. Kawamura⁵³, E.F. Kay¹⁷⁵, S. Kazakos¹⁴, V.F. Kazanin^{122b,122a}, R. Keeler¹⁷⁵, R. Kehoe⁴², J.S. Keller³⁴, E. Kellermann⁹⁷, D. Kelsey¹⁵⁵, J.J. Kempster²¹, J. Kendrick²¹, K.E. Kennedy³⁹, O. Kepka¹⁴⁰, S. Kersten¹⁸¹, B.P. Kerševan⁹², S. Ketabchi Haghighat¹⁶⁶, M. Khader¹⁷², F. Khalil-Zada¹³, M. Khandoga¹⁴⁴, A. Khanov¹²⁹, A.G. Kharlamov^{122b,122a}, T. Kharlamova^{122b,122a}, E.E. Khoda¹⁷⁴, A. Khodinov¹⁶⁵, T.J. Khoo⁵⁴, G. Khorauli¹⁷⁶, E. Khramov⁸⁰, J. Khubua^{158b}, S. Kido⁸³, M. Kiehn⁵⁴, C.R. Kilby⁹⁴, E. Kim¹⁶⁴, Y.K. Kim³⁷, N. Kimura⁹⁵, A. Kirchhoff⁵³, D. Kirchmeier⁴⁸, J. Kirk¹⁴³, A.E. Kiryunin¹¹⁵, T. Kishimoto¹⁶², D.P. Kisliuk¹⁶⁶, V. Kitali⁴⁶, C. Kitsaki¹⁰, O. Kivernyk²⁴, T. Klapdor-Kleingrothaus⁵², M. Klassen^{61a}, C. Klein³⁴, M.H. Klein¹⁰⁶, M. Klein⁹¹, U. Klein⁹¹, K. Kleinknecht¹⁰⁰, P. Klimek¹²¹, A. Klimentov²⁹, T. Klingl²⁴, T. Klioutchnikova³⁶, F.F. Klitzner¹¹⁴, P. Kluit¹²⁰, S. Kluth¹¹⁵, E. Kneringer⁷⁷, E.B.F.G. Knoops¹⁰², A. Knue⁵², D. Kobayashi⁸⁸, M. Kobel⁴⁸, M. Kocian¹⁵², T. Kodama¹⁶², P. Kodys¹⁴², D.M. Koeck¹⁵⁵, P.T. Koenig²⁴, T. Koffas³⁴, N.M. Köhler³⁶, M. Kolb¹⁴⁴, I. Koletsou⁵, T. Komarek¹³⁰, T. Kondo⁸², K. Köneke⁵², A.X.Y. Kong¹, A.C. König¹¹⁹, T. Kono¹²⁶, V. Konstantinides⁹⁵, N. Konstantinidis⁹⁵, B. Konya⁹⁷, R. Kopeliānsky⁶⁶, S. Koperny^{84a}, K. Korcyl⁸⁵, K. Kordas¹⁶¹, G. Koren¹⁶⁰, A. Korn⁹⁵, I. Korolkov¹⁴, E.V. Korolkova¹⁴⁸, N. Korotkova¹¹³, O. Kortner¹¹⁵, S. Kortner¹¹⁵, V.V. Kostyukhin^{148,165}, A. Kotskechagia⁶⁵, A. Kotwal⁴⁹, A. Koulouris¹⁰, A. Kourkumeli-Charalampidi^{71a,71b}, C. Kourkumelis⁹, E. Kourlitis⁶, V. Kouskoura²⁹, R. Kowalewski¹⁷⁵, W. Kozanecki¹⁰¹, A.S. Kozhin¹²³, V.A. Kramarenko¹¹³, G. Kramberger⁹², D. Krasnopevtsev^{60a}, M.W. Krasny¹³⁵, A. Krasznahorkay³⁶, D. Krauss¹¹⁵, J.A. Kremer¹⁰⁰, J. Kretzschmar⁹¹, P. Krieger¹⁶⁶, F. Krieter¹¹⁴, A. Krishnan^{61b}, M. Krivos¹⁴², K. Krizka¹⁸, K. Kroeninger⁴⁷, H. Kroha¹¹⁵, J. Kroll¹⁴⁰, J. Kroll¹³⁶, K.S. Krowpman¹⁰⁷, U. Kruchonak⁸⁰, H. Krüger²⁴, N. Krumnack⁷⁹, M.C. Kruse⁴⁹, J.A. Krzysiak⁸⁵, A. Kubota¹⁶⁴, O. Kuchinskaia¹⁶⁵, S. Kудay^{4b}, J.T. Kuechler⁴⁶, S. Kuehn³⁶, T. Kuhl⁴⁶, V. Kukhtin⁸⁰, Y. Kulchitsky^{108,ad}, S. Kuleshov^{146b}, Y.P. Kulinich¹⁷², M. Kuna⁵⁸, T. Kunigo⁸⁶, A. Kupco¹⁴⁰, T. Kupfer⁴⁷, O. Kuprash⁵², H. Kurashige⁸³, L.L. Kurchaninov^{167a}, Y.A. Kurochkin¹⁰⁸, A. Kurova¹¹², M.G. Kurth^{15a,15d}, E.S. Kuwertz³⁶, M. Kuze¹⁶⁴, A.K. Kvam¹⁴⁷, J. Kvita¹³⁰, T. Kwan¹⁰⁴, F. La Ruffa^{41b,41a}, C. Lacasta¹⁷³, F. Lacava^{73a,73b}, D.P.J. Lack¹⁰¹, H. Lacker¹⁹, D. Lacour¹³⁵, E. Ladygin⁸⁰, R. Lafaye⁵, B. Laforge¹³⁵, T. Lagouri^{146c}, S. Lai⁵³, I.K. Lakomic^{84a}, J.E. Lambert¹²⁸, S. Lammers⁶⁶, W. Lampl⁷, C. Lampoudis¹⁶¹, E. Lançon²⁹, U. Landgraf⁵², M.P.J. Landon⁹³, M.C. Lanfermann⁵⁴, V.S. Lang⁵², J.C. Lange⁵³, R.J. Langenberg¹⁰³, A.J. Lankford¹⁷⁰, F. Lanni²⁹, K. Lantzsch²⁴, A. Lanza^{71a}, A. Lapertosa^{55b,55a}, J.F. Laporte¹⁴⁴, T. Lari^{69a}, F. Lasagni Manghi^{23b,23a}, M. Lassnig³⁶, T.S. Lau^{63a},

A. Laudrain⁶⁵, A. Laurier³⁴, M. Lavorgna^{70a,70b}, S.D. Lawlor⁹⁴, M. Lazzaroni^{69a,69b}, B. Le¹⁰¹,
 E. Le Guirrec¹⁰², A. Lebedev⁷⁹, M. LeBlanc⁷, T. LeCompte⁶, F. Ledroit-Guillon⁵⁸, A.C.A. Lee⁹⁵,
 C.A. Lee²⁹, G.R. Lee¹⁷, L. Lee⁵⁹, S.C. Lee¹⁵⁷, S. Lee⁷⁹, B. Lefebvre^{167a}, H.P. Lefebvre⁹⁴, M. Lefebvre¹⁷⁵,
 C. Leggett¹⁸, K. Lehmann¹⁵¹, N. Lehmann²⁰, G. Lehmann Miotto³⁶, W.A. Leight⁴⁶, A. Leisos^{161,t},
 M.A.L. Leite^{81d}, C.E. Leitgeb¹¹⁴, R. Leitner¹⁴², D. Lellouch^{179,*}, K.J.C. Leney⁴², T. Lenz²⁴, S. Leone^{72a},
 C. Leonidopoulos⁵⁰, A. Leopold¹³⁵, C. Leroy¹¹⁰, R. Les¹⁰⁷, C.G. Lester³², M. Levchenko¹³⁷, J. Levêque⁵,
 D. Levin¹⁰⁶, L.J. Levinson¹⁷⁹, D.J. Lewis²¹, B. Li^{15b}, B. Li¹⁰⁶, C-Q. Li^{60a}, F. Li^{60c}, H. Li^{60a}, H. Li^{60b},
 J. Li^{60c}, K. Li¹⁴⁷, L. Li^{60c}, M. Li^{15a,15d}, Q. Li^{15a,15d}, Q.Y. Li^{60a}, S. Li^{60d,60c}, X. Li⁴⁶, Y. Li⁴⁶, Z. Li^{60b},
 Z. Li¹³⁴, Z. Li¹⁰⁴, Z. Liang^{15a}, M. Liberatore⁴⁶, B. Liberti^{74a}, A. Liblong¹⁶⁶, K. Lie^{63c}, S. Lim²⁹,
 C.Y. Lin³², K. Lin¹⁰⁷, R.A. Linck⁶⁶, R.E. Lindley⁷, J.H. Lindon²¹, A. Linss⁴⁶, A.L. Lioni⁵⁴, E. Lipeles¹³⁶,
 A. Lipniacka¹⁷, T.M. Liss^{172,aj}, A. Lister¹⁷⁴, J.D. Little⁸, B. Liu⁷⁹, B.L. Liu⁶, H.B. Liu²⁹, J.B. Liu^{60a},
 J.K.K. Liu³⁷, K. Liu^{60d}, M. Liu^{60a}, P. Liu^{15a}, X. Liu^{60a}, Y. Liu⁴⁶, Y. Liu^{15a,15d}, Y.L. Liu¹⁰⁶, Y.W. Liu^{60a},
 M. Livan^{71a,71b}, A. Lleres⁵⁸, J. Llorente Merino¹⁵¹, S.L. Lloyd⁹³, C.Y. Lo^{63b}, E.M. Lobodzinska⁴⁶,
 P. Loch⁷, S. Loffredo^{74a,74b}, T. Lohse¹⁹, K. Lohwasser¹⁴⁸, M. Lokajicek¹⁴⁰, J.D. Long¹⁷², R.E. Long⁹⁰,
 I. Longarini^{73a,73b}, L. Longo³⁶, K.A. Looper¹²⁷, I. Lopez Paz¹⁰¹, A. Lopez Solis¹⁴⁸, J. Lorenz¹¹⁴,
 N. Lorenzo Martinez⁵, A.M. Lory¹¹⁴, P.J. Lösel¹¹⁴, A. Lösle⁵², X. Lou⁴⁶, X. Lou^{15a}, A. Lounis⁶⁵, J. Love⁶,
 P.A. Love⁹⁰, J.J. Lozano Bahilo¹⁷³, M. Lu^{60a}, Y.J. Lu⁶⁴, H.J. Lubatti¹⁴⁷, C. Luci^{73a,73b},
 F.L. Lucio Alves^{15c}, A. Lucotte⁵⁸, F. Luehring⁶⁶, I. Luise¹³⁵, L. Luminari^{73a}, B. Lund-Jensen¹⁵³,
 M.S. Lutz¹⁶⁰, D. Lynn²⁹, H. Lyons⁹¹, R. Lysak¹⁴⁰, E. Lytken⁹⁷, F. Lyu^{15a}, V. Lyubushkin⁸⁰,
 T. Lyubushkina⁸⁰, H. Ma²⁹, L.L. Ma^{60b}, Y. Ma⁹⁵, D.M. Mac Donell¹⁷⁵, G. Maccarrone⁵¹,
 A. Macchiolo¹¹⁵, C.M. Macdonald¹⁴⁸, J.C. Macdonald¹⁴⁸, J. Machado Miguens¹³⁶, D. Madaffari¹⁷³,
 R. Madar³⁸, W.F. Mader⁴⁸, M. Madugoda Ralalage Don¹²⁹, N. Madysa⁴⁸, J. Maeda⁸³, T. Maeno²⁹,
 M. Maerker⁴⁸, V. Magerl⁵², N. Magini⁷⁹, J. Magro^{67a,67c,q}, D.J. Mahon³⁹, C. Maidantchik^{81b}, T. Maier¹¹⁴,
 A. Maio^{139a,139b,139d}, K. Maj^{84a}, O. Majersky^{28a}, S. Majewski¹³¹, Y. Makida⁸², N. Makovec⁶⁵,
 B. Malaescu¹³⁵, Pa. Malecki⁸⁵, V.P. Maleev¹³⁷, F. Malek⁵⁸, D. Malito^{41b,41a}, U. Mallik⁷⁸, D. Malon⁶,
 C. Malone³², S. Maltezos¹⁰, S. Malyukov⁸⁰, J. Mamuzic¹⁷³, G. Mancini^{70a,70b}, I. Mandić⁹²,
 L. Manhaes de Andrade Filho^{81a}, I.M. Maniatis¹⁶¹, J. Manjarres Ramos⁴⁸, K.H. Mankinen⁹⁷, A. Mann¹¹⁴,
 A. Manousos⁷⁷, B. Mansoulie¹⁴⁴, I. Manthos¹⁶¹, S. Manzoni¹²⁰, A. Marantis¹⁶¹, G. Marceca³⁰,
 L. Marchese¹³⁴, G. Marchiori¹³⁵, M. Marcisovsky¹⁴⁰, L. Marcoccia^{74a,74b}, C. Marcon⁹⁷,
 C.A. Marin Tobon³⁶, M. Marjanovic¹²⁸, Z. Marshall¹⁸, M.U.F. Martensson¹⁷¹, S. Marti-Garcia¹⁷³,
 C.B. Martin¹²⁷, T.A. Martin¹⁷⁷, V.J. Martin⁵⁰, B. Martin dit Latour¹⁷, L. Martinelli^{75a,75b}, M. Martinez^{14,v},
 P. Martinez Agullo¹⁷³, V.I. Martinez Outschoorn¹⁰³, S. Martin-Haugh¹⁴³, V.S. Martoiu^{27b},
 A.C. Martyniuk⁹⁵, A. Marzin³⁶, S.R. Maschek¹¹⁵, L. Masetti¹⁰⁰, T. Mashimo¹⁶², R. Mashinistov¹¹¹,
 J. Masik¹⁰¹, A.L. Maslennikov^{122b,122a}, L. Massa^{23b,23a}, P. Massarotti^{70a,70b}, P. Mastrandrea^{72a,72b},
 A. Mastroberardino^{41b,41a}, T. Masubuchi¹⁶², D. Matakias²⁹, A. Matic¹¹⁴, N. Matsuzawa¹⁶², P. Mättig²⁴,
 J. Maurer^{27b}, B. Maček⁹², D.A. Maximov^{122b,122a}, R. Mazini¹⁵⁷, I. Maznas¹⁶¹, S.M. Mazza¹⁴⁵,
 J.P. Mc Gowan¹⁰⁴, S.P. Mc Kee¹⁰⁶, T.G. McCarthy¹¹⁵, W.P. McCormack¹⁸, E.F. McDonald¹⁰⁵,
 J.A. Mcfayden³⁶, G. Mchedlidze^{158b}, M.A. McKay⁴², K.D. McLean¹⁷⁵, S.J. McMahon¹⁴³,
 P.C. McNamara¹⁰⁵, C.J. McNicol¹⁷⁷, R.A. McPherson^{175,aa}, J.E. Mdhuli^{33e}, Z.A. Meadows¹⁰³,
 S. Meehan³⁶, T. Megy³⁸, S. Mehlhase¹¹⁴, A. Mehta⁹¹, B. Meirose⁴³, D. Melini¹⁵⁹, B.R. Mellado Garcia^{33e},
 J.D. Mellenthin⁵³, M. Melo^{28a}, F. Meloni⁴⁶, A. Melzer²⁴, E.D. Mendes Gouveia^{139a,139e}, L. Meng³⁶,
 X.T. Meng¹⁰⁶, S. Menke¹¹⁵, E. Meoni^{41b,41a}, S. Mergelmeyer¹⁹, S.A.M. Merkt¹³⁸, C. Merlassino¹³⁴,
 P. Mermod⁵⁴, L. Merola^{70a,70b}, C. Meroni^{69a}, G. Merz¹⁰⁶, O. Meshkov^{113,111}, J.K.R. Meshreki¹⁵⁰,
 J. Metcalfe⁶, A.S. Mete⁶, C. Meyer⁶⁶, J-P. Meyer¹⁴⁴, M. Michetti¹⁹, R.P. Middleton¹⁴³, L. Mijović⁵⁰,
 G. Mikenberg¹⁷⁹, M. Mikesikova¹⁴⁰, M. Mikuž⁹², H. Mildner¹⁴⁸, A. Milic¹⁶⁶, C.D. Milke⁴²,
 D.W. Miller³⁷, A. Milov¹⁷⁹, D.A. Milstead^{45a,45b}, R.A. Mina¹⁵², A.A. Minaenko¹²³, I.A. Minashvili^{158b},
 A.I. Mincer¹²⁵, B. Mindur^{84a}, M. Mineev⁸⁰, Y. Minegishi¹⁶², L.M. Mir¹⁴, M. Mironova¹³⁴, A. Mirto^{68a,68b},

K.P. Mistry¹³⁶, T. Mitani¹⁷⁸, J. Mitrevski¹¹⁴, V.A. Mitsou¹⁷³, M. Mittal^{60c}, O. Miu¹⁶⁶, A. Miucci²⁰, P.S. Miyagawa⁹³, A. Mizukami⁸², J.U. Mjörnmark⁹⁷, T. Mkrtchyan^{61a}, M. Mlynarikova¹⁴², T. Moa^{45a,45b}, S. Mobius⁵³, K. Mochizuki¹¹⁰, P. Mogg¹¹⁴, S. Mohapatra³⁹, R. Moles-Valls²⁴, K. Mönig⁴⁶, E. Monnier¹⁰², A. Montalbano¹⁵¹, J. Montejo Berlingen³⁶, M. Montella⁹⁵, F. Monticelli⁸⁹, S. Monzani^{69a}, N. Morange⁶⁵, A.L. Moreira De Carvalho^{139a}, D. Moreno^{22a}, M. Moreno Llácer¹⁷³, C. Moreno Martinez¹⁴, P. Morettini^{55b}, M. Morgenstern¹⁵⁹, S. Morgenstern⁴⁸, D. Mori¹⁵¹, M. Morii⁵⁹, M. Morinaga¹⁷⁸, V. Morisbak¹³³, A.K. Morley³⁶, G. Mornacchi³⁶, A.P. Morris⁹⁵, L. Morvaj¹⁵⁴, P. Moschovakos³⁶, B. Moser¹²⁰, M. Mosidze^{158b}, T. Moskalets¹⁴⁴, J. Moss^{31,m}, E.J.W. Moyse¹⁰³, S. Muanza¹⁰², J. Mueller¹³⁸, R.S.P. Mueller¹¹⁴, D. Muenstermann⁹⁰, G.A. Mullier⁹⁷, D.P. Mungo^{69a,69b}, J.L. Munoz Martinez¹⁴, F.J. Munoz Sanchez¹⁰¹, P. Murin^{28b}, W.J. Murray^{177,143}, A. Murrone^{69a,69b}, J.M. Muse¹²⁸, M. Muškinja¹⁸, C. Mwewa^{33a}, A.G. Myagkov^{123,af}, A.A. Myers¹³⁸, G. Myers⁶⁶, J. Myers¹³¹, M. Myska¹⁴¹, B.P. Nachman¹⁸, O. Nackenhorst⁴⁷, A. Nag Nag⁴⁸, K. Nagai¹³⁴, K. Nagano⁸², Y. Nagasaka⁶², J.L. Nagle²⁹, E. Nagy¹⁰², A.M. Nairz³⁶, Y. Nakahama¹¹⁷, K. Nakamura⁸², T. Nakamura¹⁶², H. Nanjo¹³², F. Napolitano^{61a}, R.F. Naranjo Garcia⁴⁶, R. Narayan⁴², I. Naryshkin¹³⁷, T. Naumann⁴⁶, G. Navarro^{22a}, P.Y. Nechaeva¹¹¹, F. Nechansky⁴⁶, T.J. Neepe²¹, A. Negri^{71a,71b}, M. Negrini^{23b}, C. Nellist¹¹⁹, C. Nelson¹⁰⁴, M.E. Nelson^{45a,45b}, S. Nemecek¹⁴⁰, M. Nessi^{36,e}, M.S. Neubauer¹⁷², F. Neuhaus¹⁰⁰, M. Neumann¹⁸¹, R. Newhouse¹⁷⁴, P.R. Newman²¹, C.W. Ng¹³⁸, Y.S. Ng¹⁹, Y.W.Y. Ng¹⁷⁰, B. Ngair^{35e}, H.D.N. Nguyen¹⁰², T. Nguyen Manh¹¹⁰, E. Nibigira³⁸, R.B. Nickerson¹³⁴, R. Nicolaidou¹⁴⁴, D.S. Nielsen⁴⁰, J. Nielsen¹⁴⁵, M. Niemeyer⁵³, N. Nikiforou¹¹, V. Nikolaenko^{123,af}, I. Nikolic-Audit¹³⁵, K. Nikolopoulos²¹, P. Nilsson²⁹, H.R. Nindhito⁵⁴, Y. Ninomiya⁸², A. Nisati^{73a}, N. Nishu^{60c}, R. Nisius¹¹⁵, I. Nitsche⁴⁷, T. Nitta¹⁷⁸, T. Nobe¹⁶², D.L. Noel³², Y. Noguchi⁸⁶, I. Nomidis¹³⁵, M.A. Nomura²⁹, M. Nordberg³⁶, J. Novak⁹², T. Novak⁹², O. Novgorodova⁴⁸, R. Novotny¹⁴¹, L. Nozka¹³⁰, K. Ntekas¹⁷⁰, E. Nurse⁹⁵, F.G. Oakham^{34,ak}, H. Oberlack¹¹⁵, J. Ocariz¹³⁵, A. Ochi⁸³, I. Ochoa³⁹, J.P. Ochoa-Ricoux^{146a}, K. O'Connor²⁶, S. Oda⁸⁸, S. Odaka⁸², S. Oerdek⁵³, A. Ogrodnik^{84a}, A. Oh¹⁰¹, C.C. Ohm¹⁵³, H. Oide¹⁶⁴, M.L. Ojeda¹⁶⁶, H. Okawa¹⁶⁸, Y. Okazaki⁸⁶, M.W. O'Keefe⁹¹, Y. Okumura¹⁶², T. Okuyama⁸², A. Olariu^{27b}, L.F. Oleiro Seabra^{139a}, S.A. Olivares Pino^{146a}, D. Oliveira Damazio²⁹, J.L. Oliver¹, M.J.R. Olsson¹⁷⁰, A. Olszewski⁸⁵, J. Olszowska⁸⁵, OÖ. Öncel²⁴, D.C. O'Neil¹⁵¹, A.P. O'Neill¹³⁴, A. Onofre^{139a,139e}, P.U.E. Onyisi¹¹, H. Oppen¹³³, R.G. Oreamuno Madriz¹²¹, M.J. Oreglia³⁷, G.E. Orellana⁸⁹, D. Orestano^{75a,75b}, N. Orlando¹⁴, R.S. Orr¹⁶⁶, V. O'Shea⁵⁷, R. Ospanov^{60a}, G. Otero y Garzon³⁰, H. Otono⁸⁸, P.S. Ott^{61a}, G.J. Ottino¹⁸, M. Ouchrif^{35d}, J. Ouellette²⁹, F. Ould-Saada¹³³, A. Ouraou¹⁴⁴, Q. Ouyang^{15a}, M. Owen⁵⁷, R.E. Owen¹⁴³, V.E. Ozcan^{12c}, N. Ozturk⁸, J. Pacalt¹³⁰, H.A. Pacey³², K. Pachal⁴⁹, A. Pacheco Pages¹⁴, C. Padilla Aranda¹⁴, S. Pagan Griso¹⁸, G. Palacino⁶⁶, S. Palazzo⁵⁰, S. Palestini³⁶, M. Palka^{84b}, P. Palni^{84a}, C.E. Pandini⁵⁴, J.G. Panduro Vazquez⁹⁴, P. Pani⁴⁶, G. Panizzo^{67a,67c}, L. Paolozzi⁵⁴, C. Papadatos¹¹⁰, K. Papageorgiou^{9g}, S. Parajuli⁴², A. Paramonov⁶, C. Paraskevopoulos¹⁰, D. Paredes Hernandez^{63b}, S.R. Paredes Saenz¹³⁴, B. Parida¹⁷⁹, T.H. Park¹⁶⁶, A.J. Parker³¹, M.A. Parker³², F. Parodi^{55b,55a}, E.W. Parrish¹²¹, J.A. Parsons³⁹, U. Parzefall⁵², L. Pascual Dominguez¹³⁵, V.R. Pascuzzi¹⁸, J.M.P. Pasner¹⁴⁵, F. Pasquali¹²⁰, E. Pasqualucci^{73a}, S. Passaggio^{55b}, F. Pastore⁹⁴, P. Pasuwan^{45a,45b}, S. Patariaia¹⁰⁰, J.R. Pater¹⁰¹, A. Pathak^{180,i}, J. Patton⁹¹, T. Pauly³⁶, J. Pearkes¹⁵², B. Pearson¹¹⁵, M. Pedersen¹³³, L. Pedraza Diaz¹¹⁹, R. Pedro^{139a}, T. Peiffer⁵³, S.V. Peleganchuk^{122b,122a}, O. Penc¹⁴⁰, H. Peng^{60a}, B.S. Peralva^{81a}, M.M. Perego⁶⁵, A.P. Pereira Peixoto^{139a}, L. Pereira Sanchez^{45a,45b}, D.V. Perepelitsa²⁹, E. Perez Codina^{167a}, F. Peri¹⁹, L. Perini^{69a,69b}, H. Pernegger³⁶, S. Perrella³⁶, A. Perrevoort¹²⁰, K. Peters⁴⁶, R.F.Y. Peters¹⁰¹, B.A. Petersen³⁶, T.C. Petersen⁴⁰, E. Petit¹⁰², V. Petousis¹⁴¹, A. Petridis¹, C. Petridou¹⁶¹, P. Petroff⁶⁵, F. Petrucci^{75a,75b}, M. Pettee¹⁸², N.E. Pettersson¹⁰³, K. Petukhova¹⁴², A. Peyaud¹⁴⁴, R. Pezoa^{146d}, L. Pezzotti^{71a,71b}, T. Pham¹⁰⁵, F.H. Phillips¹⁰⁷, P.W. Phillips¹⁴³, M.W. Phipps¹⁷², G. Piacquadio¹⁵⁴, E. Pianori¹⁸, A. Picazio¹⁰³, R.H. Pickles¹⁰¹, R. Piegaia³⁰, D. Pietreanu^{27b}, J.E. Pilcher³⁷, A.D. Pilkington¹⁰¹, M. Pinamonti^{67a,67c}, J.L. Pinfold³, C. Pitman Donaldson⁹⁵, M. Pitt¹⁶⁰, L. Pizzimento^{74a,74b}, A. Pizzini¹²⁰, M.-A. Pleier²⁹, V. Plesanovs⁵²,

V. Pleskot¹⁴², E. Plotnikova⁸⁰, P. Podberezko^{122b,122a}, R. Poettgen⁹⁷, R. Poggi⁵⁴, L. Poggioli¹³⁵, I. Pogrebnyak¹⁰⁷, D. Pohl²⁴, I. Pokharel⁵³, G. Polesello^{71a}, A. Poley^{151,167a}, A. Policicchio^{73a,73b}, R. Polifka¹⁴², A. Polini^{23b}, C.S. Pollard⁴⁶, V. Polychronakos²⁹, D. Ponomarenko¹¹², L. Pontecorvo³⁶, S. Popa^{27a}, G.A. Popeneciu^{27d}, L. Portales⁵, D.M. Portillo Quintero⁵⁸, S. Pospisil¹⁴¹, K. Potamianos⁴⁶, I.N. Potrap⁸⁰, C.J. Potter³², H. Potti¹¹, T. Poulsen⁹⁷, J. Poveda¹⁷³, T.D. Powell¹⁴⁸, G. Pownall⁴⁶, M.E. Pozo Astigarraga³⁶, P. Pralavorio¹⁰², S. Prell⁷⁹, D. Price¹⁰¹, M. Primavera^{68a}, M.L. Proffitt¹⁴⁷, N. Proklova¹¹², K. Prokofiev^{63c}, F. Prokoshin⁸⁰, S. Protopopescu²⁹, J. Proudfoot⁶, M. Przybycien^{84a}, D. Pudzha¹³⁷, A. Puri¹⁷², P. Puzo⁶⁵, D. Pyatiizbyantseva¹¹², J. Qian¹⁰⁶, Y. Qin¹⁰¹, A. Quadt⁵³, M. Queitsch-Maitland³⁶, M. Racko^{28a}, F. Ragusa^{69a,69b}, G. Rahal⁹⁸, J.A. Raine⁵⁴, S. Rajagopalan²⁹, A. Ramirez Morales⁹³, K. Ran^{15a,15d}, D.M. Rauch⁴⁶, F. Rauscher¹¹⁴, S. Rave¹⁰⁰, B. Ravina¹⁴⁸, I. Ravinovich¹⁷⁹, J.H. Rawling¹⁰¹, M. Raymond³⁶, A.L. Read¹³³, N.P. Readioff¹⁴⁸, M. Reale^{68a,68b}, D.M. Rebuzzi^{71a,71b}, G. Redlinger²⁹, K. Reeves⁴³, J. Reichert¹³⁶, D. Reikher¹⁶⁰, A. Reiss¹⁰⁰, A. Rej¹⁵⁰, C. Rembser³⁶, A. Renardi⁴⁶, M. Renda^{27b}, M.B. Rendel¹¹⁵, A.G. Rennie⁵⁷, S. Resconi^{69a}, E.D. Resseguie¹⁸, S. Rettie⁹⁵, B. Reynolds¹²⁷, E. Reynolds²¹, O.L. Rezanova^{122b,122a}, P. Reznicek¹⁴², E. Ricci^{76a,76b}, R. Richter¹¹⁵, S. Richter⁴⁶, E. Richter-Was^{84b}, M. Ridel¹³⁵, P. Rieck¹¹⁵, O. Rifki⁴⁶, M. Rijssenbeek¹⁵⁴, A. Rimoldi^{71a,71b}, M. Rimoldi⁴⁶, L. Rinaldi^{23b}, T.T. Rinn¹⁷², G. Ripellino¹⁵³, I. Riu¹⁴, P. Rivadeneira⁴⁶, J.C. Rivera Vergara¹⁷⁵, F. Rizatdinova¹²⁹, E. Rizvi⁹³, C. Rizzi³⁶, S.H. Robertson^{104,aa}, M. Robin⁴⁶, D. Robinson³², C.M. Robles Gajardo^{146d}, M. Robles Manzano¹⁰⁰, A. Robson⁵⁷, A. Rocchi^{74a,74b}, E. Rocco¹⁰⁰, C. Roda^{72a,72b}, S. Rodriguez Bosca¹⁷³, A.M. Rodríguez Vera^{167b}, S. Roe³⁶, J. Roggel¹⁸¹, O. Røhne¹³³, R. Röhrig¹¹⁵, R.A. Rojas^{146d}, B. Roland⁵², C.P.A. Roland⁶⁶, J. Roloff²⁹, A. Romaniouk¹¹², M. Romano^{23b,23a}, N. Rompotis⁹¹, M. Ronzani¹²⁵, L. Roos¹³⁵, S. Rosati^{73a}, G. Rosin¹⁰³, B.J. Rosser¹³⁶, E. Rossi⁴⁶, E. Rossi^{75a,75b}, E. Rossi^{70a,70b}, L.P. Rossi^{55b}, L. Rossini⁴⁶, R. Rosten¹⁴, M. Rotaru^{27b}, B. Rottler⁵², D. Rousseau⁶⁵, G. Rovelli^{71a,71b}, A. Roy¹¹, D. Roy^{33e}, A. Rozanov¹⁰², Y. Rozen¹⁵⁹, X. Ruan^{33e}, T.A. Ruggeri¹, F. Rühr⁵², A. Ruiz-Martinez¹⁷³, A. Rummeler³⁶, Z. Rurikova⁵², N.A. Rusakovich⁸⁰, H.L. Russell¹⁰⁴, L. Rustige^{38,47}, J.P. Rutherford⁷, E.M. Rüttinger¹⁴⁸, M. Rybar³⁹, G. Rybkin⁶⁵, E.B. Rye¹³³, A. Ryzhov¹²³, J.A. Sabater Iglesias⁴⁶, P. Sabatini⁵³, L. Sabetta^{73a,73b}, S. Sacerdoti⁶⁵, H.F.W. Sadrozinski¹⁴⁵, R. Sadykov⁸⁰, F. Safai Tehrani^{73a}, B. Safarzadeh Samani¹⁵⁵, M. Safdari¹⁵², P. Saha¹²¹, S. Saha¹⁰⁴, M. Sahinsoy¹¹⁵, A. Sahu¹⁸¹, M. Saimpert³⁶, M. Saito¹⁶², T. Saito¹⁶², H. Sakamoto¹⁶², D. Salamani⁵⁴, G. Salamanna^{75a,75b}, A. Salnikov¹⁵², J. Salt¹⁷³, A. Salvador Salas¹⁴, D. Salvatore^{41b,41a}, F. Salvatore¹⁵⁵, A. Salvucci^{63a,63b,63c}, A. Salzburger³⁶, J. Samarati³⁶, D. Sammel⁵², D. Sampsonidis¹⁶¹, D. Sampsonidou¹⁶¹, J. Sánchez¹⁷³, A. Sanchez Pineda^{67a,36,67c}, H. Sandaker¹³³, C.O. Sander⁴⁶, I.G. Sanderswood⁹⁰, M. Sandhoff¹⁸¹, C. Sandoval^{22b}, D.P.C. Sankey¹⁴³, M. Sannino^{55b,55a}, Y. Sano¹¹⁷, A. Sansoni⁵¹, C. Santoni³⁸, H. Santos^{139a,139b}, S.N. Santpur¹⁸, A. Santra¹⁷³, K.A. Saoucha¹⁴⁸, A. Saproinov⁸⁰, J.G. Saraiva^{139a,139d}, O. Sasaki⁸², K. Sato¹⁶⁸, F. Sauerburger⁵², E. Sauvan⁵, P. Savard^{166,ak}, R. Sawada¹⁶², C. Sawyer¹⁴³, L. Sawyer^{96,ae}, I. Sayago Galvan¹⁷³, C. Sbarra^{23b}, A. Sbrizzi^{67a,67c}, T. Scanlon⁹⁵, J. Schaarschmidt¹⁴⁷, P. Schacht¹¹⁵, D. Schaefer³⁷, L. Schaefer¹³⁶, S. Schaepe³⁶, U. Schäfer¹⁰⁰, A.C. Schaffer⁶⁵, D. Schaile¹¹⁴, R.D. Schamberger¹⁵⁴, E. Schanet¹¹⁴, C. Scharf¹⁹, N. Scharmberg¹⁰¹, V.A. Schegelsky¹³⁷, D. Scheirich¹⁴², F. Schenck¹⁹, M. Schernau¹⁷⁰, C. Schiavi^{55b,55a}, L.K. Schildgen²⁴, Z.M. Schillaci²⁶, E.J. Schioppa^{68a,68b}, M. Schioppa^{41b,41a}, K.E. Schleicher⁵², S. Schlenker³⁶, K.R. Schmidt-Sommerfeld¹¹⁵, K. Schmieden³⁶, C. Schmitt¹⁰⁰, S. Schmitt⁴⁶, J.C. Schmoeckel⁴⁶, L. Schoeffel¹⁴⁴, A. Schoening^{61b}, P.G. Scholer⁵², E. Schopf¹³⁴, M. Schott¹⁰⁰, J.F.P. Schouwenberg¹¹⁹, J. Schovancova³⁶, S. Schramm⁵⁴, F. Schroeder¹⁸¹, A. Schulte¹⁰⁰, H-C. Schultz-Coulon^{61a}, M. Schumacher⁵², B.A. Schumm¹⁴⁵, Ph. Schune¹⁴⁴, A. Schwartzman¹⁵², T.A. Schwarz¹⁰⁶, Ph. Schwemling¹⁴⁴, R. Schwienhorst¹⁰⁷, A. Sciandra¹⁴⁵, G. Sciolla²⁶, M. Scornajenghi^{41b,41a}, F. Scuri^{72a}, F. Scutti¹⁰⁵, L.M. Scyboz¹¹⁵, C.D. Sebastiani⁹¹, P. Seema¹⁹, S.C. Seidel¹¹⁸, A. Seiden¹⁴⁵, B.D. Seidlitz²⁹, T. Seiss³⁷, C. Seitz⁴⁶, J.M. Seixas^{81b}, G. Sekhniaidze^{70a}, S.J. Sekula⁴², N. Semprini-Cesari^{23b,23a}, S. Sen⁴⁹, C. Serfon²⁹, L. Serin⁶⁵, L. Serkin^{67a,67b}, M. Sessa^{60a}, H. Severini¹²⁸, S. Sevova¹⁵², F. Sforza^{55b,55a},

A. Sfyrila⁵⁴, E. Shabalina⁵³, J.D. Shahinian¹⁴⁵, N.W. Shaikh^{45a,45b}, D. Shaked Renous¹⁷⁹, L.Y. Shan^{15a},
 M. Shapiro¹⁸, A. Sharma¹³⁴, A.S. Sharma¹, P.B. Shatalov¹²⁴, K. Shaw¹⁵⁵, S.M. Shaw¹⁰¹, M. Shehade¹⁷⁹,
 Y. Shen¹²⁸, A.D. Sherman²⁵, P. Sherwood⁹⁵, L. Shi⁹⁵, S. Shimizu⁸², C.O. Shimmin¹⁸², Y. Shimogama¹⁷⁸,
 M. Shimojima¹¹⁶, I.P.J. Shipsey¹³⁴, S. Shirabe¹⁶⁴, M. Shiyakova^{80,y}, J. Shlomi¹⁷⁹, A. Shmeleva¹¹¹,
 M.J. Shochet³⁷, J. Shojaii¹⁰⁵, D.R. Shope¹⁵³, S. Shrestha¹²⁷, E.M. Shrif^{33e}, E. Shulga¹⁷⁹, P. Sicho¹⁴⁰,
 A.M. Sickles¹⁷², E. Sideras Haddad^{33e}, O. Sidiropoulou³⁶, A. Sidoti^{23b,23a}, F. Siegert⁴⁸, Dj. Sijacki¹⁶,
 M.Jr. Silva¹⁸⁰, M.V. Silva Oliveira³⁶, S.B. Silverstein^{45a}, S. Simion⁶⁵, R. Simoniello¹⁰⁰,
 C.J. Simpson-allso²¹, S. Simsek^{12b}, P. Sinervo¹⁶⁶, V. Sinetckii¹¹³, S. Singh¹⁵¹, M. Sioli^{23b,23a}, I. Siral¹³¹,
 S.Yu. Sivoklov¹¹³, J. Sjölin^{45a,45b}, A. Skaf⁵³, E. Skorda⁹⁷, P. Skubic¹²⁸, M. Slawinska⁸⁵, K. Sliwa¹⁶⁹,
 R. Slovak¹⁴², V. Smakhtin¹⁷⁹, B.H. Smart¹⁴³, J. Smiesko^{28b}, N. Smirnov¹¹², S.Yu. Smirnov¹¹²,
 Y. Smirnov¹¹², L.N. Smirnova^{113,r}, O. Smirnova⁹⁷, E.A. Smith³⁷, H.A. Smith¹³⁴, M. Smizanska⁹⁰,
 K. Smolek¹⁴¹, A. Smykiewicz⁸⁵, A.A. Snesarev¹¹¹, H.L. Snoek¹²⁰, I.M. Snyder¹³¹, S. Snyder²⁹,
 R. Sobie^{175,aa}, A. Soffer¹⁶⁰, A. Søgaaard⁵⁰, F. Sohns⁵³, C.A. Solans Sanchez³⁶, E.Yu. Soldatov¹¹²,
 U. Soldevila¹⁷³, A.A. Solodkov¹²³, A. Soloshenko⁸⁰, O.V. Solovyanov¹²³, V. Solovyev¹³⁷, P. Sommer¹⁴⁸,
 H. Son¹⁶⁹, W. Song¹⁴³, W.Y. Song^{167b}, A. Sopczak¹⁴¹, A.L. Sopio⁹⁵, F. Sopkova^{28b}, S. Sottocornola^{71a,71b},
 R. Soualah^{67a,67c}, A.M. Soukharev^{122b,122a}, D. South⁴⁶, S. Spagnolo^{68a,68b}, M. Spalla¹¹⁵,
 M. Spangenberg¹⁷⁷, F. Spanò⁹⁴, D. Sperlich⁵², T.M. Spieker^{61a}, G. Spigo³⁶, M. Spina¹⁵⁵, D.P. Spiteri⁵⁷,
 M. Spousta¹⁴², A. Stabile^{69a,69b}, B.L. Stamas¹²¹, R. Stamen^{61a}, M. Stamenkovic¹²⁰, E. Stanecka⁸⁵,
 B. Stanislaus¹³⁴, M.M. Stanitzki⁴⁶, M. Stankaityte¹³⁴, B. Stapf¹²⁰, E.A. Starchenko¹²³, G.H. Stark¹⁴⁵,
 J. Stark⁵⁸, P. Staroba¹⁴⁰, P. Starovoitov^{61a}, S. Stärz¹⁰⁴, R. Staszewski⁸⁵, G. Stavropoulos⁴⁴, M. Stegler⁴⁶,
 P. Steinberg²⁹, A.L. Steinhebel¹³¹, B. Stelzer^{151,167a}, H.J. Stelzer¹³⁸, O. Stelzer-Chilton^{167a}, H. Stenzel⁵⁶,
 T.J. Stevenson¹⁵⁵, G.A. Stewart³⁶, M.C. Stockton³⁶, G. Stoicea^{27b}, M. Stolarski^{139a}, S. Stonjek¹¹⁵,
 A. Straessner⁴⁸, J. Strandberg¹⁵³, S. Strandberg^{45a,45b}, M. Strauss¹²⁸, T. Strebler¹⁰², P. Strizenec^{28b},
 R. Ströhmer¹⁷⁶, D.M. Strom¹³¹, R. Stroynowski⁴², A. Strubig⁵⁰, S.A. Stucci²⁹, B. Stugu¹⁷, J. Stupak¹²⁸,
 N.A. Styles⁴⁶, D. Su¹⁵², W. Su^{60c}, X. Su^{60a}, V.V. Sulin¹¹¹, M.J. Sullivan⁹¹, D.M.S. Sultan⁵⁴,
 S. Sultansoy^{4c}, T. Sumida⁸⁶, S. Sun¹⁰⁶, X. Sun¹⁰¹, K. Suruliz¹⁵⁵, C.J.E. Suster¹⁵⁶, M.R. Sutton¹⁵⁵,
 S. Suzuki⁸², M. Svatos¹⁴⁰, M. Swiatlowski^{167a}, S.P. Swift², T. Swirski¹⁷⁶, A. Sydorenko¹⁰⁰, I. Sykora^{28a},
 M. Sykora¹⁴², T. Sykora¹⁴², D. Ta¹⁰⁰, K. Tackmann^{46,w}, J. Taenzer¹⁶⁰, A. Taffard¹⁷⁰, R. Tafirout^{167a},
 E. Tagiev¹²³, R. Takashima⁸⁷, K. Takeda⁸³, T. Takeshita¹⁴⁹, E.P. Takeva⁵⁰, Y. Takubo⁸², M. Talby¹⁰²,
 A.A. Talyshev^{122b,122a}, K.C. Tam^{63b}, N.M. Tamir¹⁶⁰, J. Tanaka¹⁶², R. Tanaka⁶⁵, S. Tapia Araya¹⁷²,
 S. Tapprogge¹⁰⁰, A. Tarek Abouelfadl Mohamed¹⁰⁷, S. Tarem¹⁵⁹, K. Tariq^{60b}, G. Tarna^{27b,d},
 G.F. Tartarelli^{69a}, P. Tas¹⁴², M. Tasevsky¹⁴⁰, T. Tashiro⁸⁶, E. Tassi^{41b,41a}, A. Tavares Delgado^{139a},
 Y. Tayalati^{35e}, A.J. Taylor⁵⁰, G.N. Taylor¹⁰⁵, W. Taylor^{167b}, H. Teagle⁹¹, A.S. Tee⁹⁰,
 R. Teixeira De Lima¹⁵², P. Teixeira-Dias⁹⁴, H. Ten Kate³⁶, J.J. Teoh¹²⁰, S. Terada⁸², K. Terashi¹⁶²,
 J. Terron⁹⁹, S. Terzo¹⁴, M. Testa⁵¹, R.J. Teuscher^{166,aa}, S.J. Thais¹⁸², N. Themistokleous⁵⁰,
 T. Theveneaux-Pelzer⁴⁶, F. Thiele⁴⁰, D.W. Thomas⁹⁴, J.O. Thomas⁴², J.P. Thomas²¹, E.A. Thompson⁴⁶,
 P.D. Thompson²¹, E. Thomson¹³⁶, E.J. Thorpe⁹³, R.E. Ticse Torres⁵³, V.O. Tikhomirov^{111,ag},
 Yu.A. Tikhonov^{122b,122a}, S. Timoshenko¹¹², P. Tipton¹⁸², S. Tisserant¹⁰², K. Todome^{23b,23a},
 S. Todorova-Nova¹⁴², S. Todt⁴⁸, J. Tojo⁸⁸, S. Tokár^{28a}, K. Tokushuku⁸², E. Tolley¹²⁷, R. Tombs³²,
 K.G. Tomiwa^{33e}, M. Tomoto¹¹⁷, L. Tompkins¹⁵², P. Tornambe¹⁰³, E. Torrence¹³¹, H. Torres⁴⁸,
 E. Torró Pastor¹⁴⁷, C. Toscirri¹³⁴, J. Toth^{102,z}, D.R. Tovey¹⁴⁸, A. Traeet¹⁷, C.J. Treado¹²⁵, T. Trefzger¹⁷⁶,
 F. Tresoldi¹⁵⁵, A. Tricoli²⁹, I.M. Trigger^{167a}, S. Trincas-Duvold¹³⁵, D.A. Trischuk¹⁷⁴, W. Trischuk¹⁶⁶,
 B. Trocme⁵⁸, A. Trofymov⁶⁵, C. Troncon^{69a}, F. Trovato¹⁵⁵, L. Truong^{33c}, M. Trzebinski⁸⁵, A. Trzupek⁸⁵,
 F. Tsai⁴⁶, J.C.-L. Tseng¹³⁴, P.V. Tsiarehsha^{108,ad}, A. Tsirigotis^{161,t}, V. Tsiskaridze¹⁵⁴, E.G. Tskhadadze^{158a},
 M. Tsopoulou¹⁶¹, I.I. Tsukerman¹²⁴, V. Tsulaia¹⁸, S. Tsuno⁸², D. Tsybychev¹⁵⁴, Y. Tu^{63b}, A. Tudorache^{27b},
 V. Tudorache^{27b}, T.T. Tulbure^{27a}, A.N. Tuna⁵⁹, S. Turchikhin⁸⁰, D. Turgeman¹⁷⁹, I. Turk Cakir^{4b},
 R.J. Turner²¹, R.T. Turra^{69a}, P.M. Tuts³⁹, S. Tzamarias¹⁶¹, E. Tzovara¹⁰⁰, K. Uchida¹⁶², F. Ukegawa¹⁶⁸,

G. Unal³⁶, M. Unal¹¹, A. Undrus²⁹, G. Unel¹⁷⁰, F.C. Ungaro¹⁰⁵, Y. Unno⁸², K. Uno¹⁶², J. Urban^{28b}, P. Urquijo¹⁰⁵, G. Usai⁸, Z. Uysal^{12d}, V. Vacek¹⁴¹, B. Vachon¹⁰⁴, K.O.H. Vadla¹³³, T. Vafeiadis³⁶, A. Vaidya⁹⁵, C. Valderanis¹¹⁴, E. Valdes Santurio^{45a,45b}, M. Valente⁵⁴, S. Valentinetti^{23b,23a}, A. Valero¹⁷³, L. Valéry⁴⁶, R.A. Vallance²¹, A. Vallier³⁶, J.A. Valls Ferrer¹⁷³, T.R. Van Daalen¹⁴, P. Van Gemmeren⁶, S. Van Stroud⁹⁵, I. Van Vulpen¹²⁰, M. Vanadia^{74a,74b}, W. Vandelli³⁶, M. Vandenbroucke¹⁴⁴, E.R. Vandewall¹²⁹, A. Vaniachine¹⁶⁵, D. Vannicola^{73a,73b}, R. Vari^{73a}, E.W. Varnes⁷, C. Varni^{55b,55a}, T. Varol¹⁵⁷, D. Varouchas⁶⁵, K.E. Varvell¹⁵⁶, M.E. Vasile^{27b}, G.A. Vasquez¹⁷⁵, F. Vazeille³⁸, D. Vazquez Furelos¹⁴, T. Vazquez Schroeder³⁶, J. Veatch⁵³, V. Vecchio¹⁰¹, M.J. Veen¹²⁰, L.M. Veloce¹⁶⁶, F. Veloso^{139a,139c}, S. Veneziano^{73a}, A. Ventura^{68a,68b}, A. Verbytskyi¹¹⁵, V. Vercesi^{71a}, M. Verducci^{72a,72b}, C.M. Vergel Infante⁷⁹, C. Vergis²⁴, W. Verkerke¹²⁰, A.T. Vermeulen¹²⁰, J.C. Vermeulen¹²⁰, C. Vernieri¹⁵², M.C. Vetterli^{151,ak}, N. Viaux Maira^{146d}, T. Vickey¹⁴⁸, O.E. Vickey Boeriu¹⁴⁸, G.H.A. Viehhauser¹³⁴, L. Vigani^{61b}, M. Villa^{23b,23a}, M. Villaplana Perez³, E.M. Villhauer⁵⁰, E. Vilucchi⁵¹, M.G. Vinciter³⁴, G.S. Virdee²¹, A. Vishwakarma⁵⁰, C. Vittori^{23b,23a}, I. Vivarelli¹⁵⁵, M. Vogel¹⁸¹, P. Vokac¹⁴¹, S.E. von Buddenbrock^{33e}, E. Von Toerne²⁴, V. Vorobel¹⁴², K. Vorobev¹¹², M. Vos¹⁷³, J.H. Vosseveld⁹¹, M. Vozak¹⁰¹, N. Vranjes¹⁶, M. Vranjes Milosavljevic¹⁶, V. Vrba¹⁴¹, M. Vreeswijk¹²⁰, R. Vuillermet³⁶, I. Vukotic³⁷, S. Wada¹⁶⁸, P. Wagner²⁴, W. Wagner¹⁸¹, J. Wagner-Kuhr¹¹⁴, S. Wahdan¹⁸¹, H. Wahlberg⁸⁹, R. Wakasa¹⁶⁸, V.M. Walbrecht¹¹⁵, J. Walder¹⁴³, R. Walker¹¹⁴, S.D. Walker⁹⁴, W. Walkowiak¹⁵⁰, V. Wallangen^{45a,45b}, A.M. Wang⁵⁹, A.Z. Wang¹⁸⁰, C. Wang^{60a}, C. Wang^{60c}, F. Wang¹⁸⁰, H. Wang¹⁸, H. Wang³, J. Wang^{63a}, P. Wang⁴², Q. Wang¹²⁸, R.-J. Wang¹⁰⁰, R. Wang^{60a}, R. Wang⁶, S.M. Wang¹⁵⁷, W.T. Wang^{60a}, W. Wang^{15c}, W.X. Wang^{60a}, Y. Wang^{60a}, Z. Wang¹⁰⁶, C. Wanotayaroj⁴⁶, A. Warburton¹⁰⁴, C.P. Ward³², D.R. Wardrope⁹⁵, N. Warrack⁵⁷, A.T. Watson²¹, M.F. Watson²¹, G. Watts¹⁴⁷, B.M. Waugh⁹⁵, A.F. Webb¹¹, C. Weber²⁹, M.S. Weber²⁰, S.A. Weber³⁴, S.M. Weber^{61a}, A.R. Weidberg¹³⁴, J. Weingarten⁴⁷, M. Weirich¹⁰⁰, C. Weiser⁵², P.S. Wells³⁶, T. Wenaus²⁹, B. Wendland⁴⁷, T. Wengler³⁶, S. Wenig³⁶, N. Wermes²⁴, M. Wessels^{61a}, T.D. Weston²⁰, K. Whalen¹³¹, A.M. Wharton⁹⁰, A.S. White¹⁰⁶, A. White⁸, M.J. White¹, D. Whiteson¹⁷⁰, B.W. Whitmore⁹⁰, W. Wiedenmann¹⁸⁰, C. Wiel⁴⁸, M. Wielers¹⁴³, N. Wieseotte¹⁰⁰, C. Wiglesworth⁴⁰, L.A.M. Wiik-Fuchs⁵², H.G. Wilkens³⁶, L.J. Wilkins⁹⁴, H.H. Williams¹³⁶, S. Williams³², S. Willocq¹⁰³, P.J. Windischhofer¹³⁴, I. Wingerter-Seez⁵, E. Winkels¹⁵⁵, F. Winklmeier¹³¹, B.T. Winter⁵², M. Wittgen¹⁵², M. Wobisch⁹⁶, A. Wolf¹⁰⁰, R. Wölker¹³⁴, J. Wollrath⁵², M.W. Wolter⁸⁵, H. Wolters^{139a,139c}, V.W.S. Wong¹⁷⁴, N.L. Woods¹⁴⁵, S.D. Worm⁴⁶, B.K. Wosiek⁸⁵, K.W. Woźniak⁸⁵, K. Wraight⁵⁷, S.L. Wu¹⁸⁰, X. Wu⁵⁴, Y. Wu^{60a}, J. Wuerzinger¹³⁴, T.R. Wyatt¹⁰¹, B.M. Wynne⁵⁰, S. Xella⁴⁰, L. Xia¹⁷⁷, J. Xiang^{63c}, X. Xiao¹⁰⁶, X. Xie^{60a}, I. Xiotidis¹⁵⁵, D. Xu^{15a}, H. Xu^{60a}, H. Xu^{60a}, L. Xu²⁹, T. Xu¹⁴⁴, W. Xu¹⁰⁶, Z. Xu^{60b}, Z. Xu¹⁵², B. Yabsley¹⁵⁶, S. Yacoob^{33a}, K. Yajima¹³², D.P. Yallup⁹⁵, N. Yamaguchi⁸⁸, Y. Yamaguchi¹⁶⁴, A. Yamamoto⁸², M. Yamatani¹⁶², T. Yamazaki¹⁶², Y. Yamazaki⁸³, J. Yan^{60c}, Z. Yan²⁵, H.J. Yang^{60c,60d}, H.T. Yang¹⁸, S. Yang^{60a}, T. Yang^{63c}, X. Yang^{60b,58}, Y. Yang¹⁶², Z. Yang^{60a}, W.-M. Yao¹⁸, Y.C. Yap⁴⁶, Y. Yasu⁸², E. Yatsenko^{60c}, H. Ye^{15c}, J. Ye⁴², S. Ye²⁹, I. Yeletsikh⁸⁰, M.R. Yexley⁹⁰, E. Yigitbasi²⁵, P. Yin³⁹, K. Yorita¹⁷⁸, K. Yoshihara⁷⁹, C.J.S. Young³⁶, C. Young¹⁵², J. Yu⁷⁹, R. Yuan^{60b,h}, X. Yue^{61a}, M. Zaazoua^{35e}, B. Zabinski⁸⁵, G. Zacharis¹⁰, E. Zaffaroni⁵⁴, J. Zahreddine¹³⁵, A.M. Zaitsev^{123,af}, T. Zakareishvili^{158b}, N. Zakharchuk³⁴, S. Zambito³⁶, D. Zanzi³⁶, D.R. Zaripovas⁵⁷, S.V. Zeißner⁴⁷, C. Zeitnitz¹⁸¹, G. Zemaityte¹³⁴, J.C. Zeng¹⁷², O. Zenin¹²³, T. Ženiš^{28a}, D. Zerwas⁶⁵, M. Zgubić¹³⁴, B. Zhang^{15c}, D.F. Zhang^{15b}, G. Zhang^{15b}, J. Zhang⁶, Kaili. Zhang^{15a}, L. Zhang^{15c}, L. Zhang^{60a}, M. Zhang¹⁷², R. Zhang¹⁸⁰, S. Zhang¹⁰⁶, X. Zhang^{60c}, X. Zhang^{60b}, Y. Zhang^{15a,15d}, Z. Zhang^{63a}, Z. Zhang⁶⁵, P. Zhao⁴⁹, Z. Zhao^{60a}, A. Zhemchugov⁸⁰, Z. Zheng¹⁰⁶, D. Zhong¹⁷², B. Zhou¹⁰⁶, C. Zhou¹⁸⁰, H. Zhou⁷, M.S. Zhou^{15a,15d}, M. Zhou¹⁵⁴, N. Zhou^{60c}, Y. Zhou⁷, C.G. Zhu^{60b}, C. Zhu^{15a,15d}, H.L. Zhu^{60a}, H. Zhu^{15a}, J. Zhu¹⁰⁶, Y. Zhu^{60a}, X. Zhuang^{15a}, K. Zhukov¹¹¹, V. Zhulanov^{122b,122a}, D. Zieminska⁶⁶, N.I. Zimine⁸⁰, S. Zimmermann⁵², Z. Zinonos¹¹⁵, M. Ziolkowski¹⁵⁰, L. Živković¹⁶, G. Zobernig¹⁸⁰, A. Zoccoli^{23b,23a}, K. Zoch⁵³, T.G. Zorbass¹⁴⁸, R. Zou³⁷, L. Zwalinski³⁶.

- ¹Department of Physics, University of Adelaide, Adelaide; Australia.
- ²Physics Department, SUNY Albany, Albany NY; United States of America.
- ³Department of Physics, University of Alberta, Edmonton AB; Canada.
- ⁴(^a)Department of Physics, Ankara University, Ankara; (^b)Istanbul Aydin University, Istanbul; (^c)Division of Physics, TOBB University of Economics and Technology, Ankara; Turkey.
- ⁵LAPP, Université Grenoble Alpes, Université Savoie Mont Blanc, CNRS/IN2P3, Annecy; France.
- ⁶High Energy Physics Division, Argonne National Laboratory, Argonne IL; United States of America.
- ⁷Department of Physics, University of Arizona, Tucson AZ; United States of America.
- ⁸Department of Physics, University of Texas at Arlington, Arlington TX; United States of America.
- ⁹Physics Department, National and Kapodistrian University of Athens, Athens; Greece.
- ¹⁰Physics Department, National Technical University of Athens, Zografou; Greece.
- ¹¹Department of Physics, University of Texas at Austin, Austin TX; United States of America.
- ¹²(^a)Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul; (^b)Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul; (^c)Department of Physics, Bogazici University, Istanbul; (^d)Department of Physics Engineering, Gaziantep University, Gaziantep; Turkey.
- ¹³Institute of Physics, Azerbaijan Academy of Sciences, Baku; Azerbaijan.
- ¹⁴Institut de Física d'Altes Energies (IFAE), Barcelona Institute of Science and Technology, Barcelona; Spain.
- ¹⁵(^a)Institute of High Energy Physics, Chinese Academy of Sciences, Beijing; (^b)Physics Department, Tsinghua University, Beijing; (^c)Department of Physics, Nanjing University, Nanjing; (^d)University of Chinese Academy of Science (UCAS), Beijing; China.
- ¹⁶Institute of Physics, University of Belgrade, Belgrade; Serbia.
- ¹⁷Department for Physics and Technology, University of Bergen, Bergen; Norway.
- ¹⁸Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley CA; United States of America.
- ¹⁹Institut für Physik, Humboldt Universität zu Berlin, Berlin; Germany.
- ²⁰Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern; Switzerland.
- ²¹School of Physics and Astronomy, University of Birmingham, Birmingham; United Kingdom.
- ²²(^a)Facultad de Ciencias y Centro de Investigaciones, Universidad Antonio Nariño, Bogotá; (^b)Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia; Colombia.
- ²³(^a)INFN Bologna and Università di Bologna, Dipartimento di Fisica; (^b)INFN Sezione di Bologna; Italy.
- ²⁴Physikalisches Institut, Universität Bonn, Bonn; Germany.
- ²⁵Department of Physics, Boston University, Boston MA; United States of America.
- ²⁶Department of Physics, Brandeis University, Waltham MA; United States of America.
- ²⁷(^a)Transilvania University of Brasov, Brasov; (^b)Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest; (^c)Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi; (^d)National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj-Napoca; (^e)University Politehnica Bucharest, Bucharest; (^f)West University in Timisoara, Timisoara; Romania.
- ²⁸(^a)Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava; (^b)Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice; Slovak Republic.
- ²⁹Physics Department, Brookhaven National Laboratory, Upton NY; United States of America.
- ³⁰Departamento de Física, Universidad de Buenos Aires, Buenos Aires; Argentina.
- ³¹California State University, CA; United States of America.
- ³²Cavendish Laboratory, University of Cambridge, Cambridge; United Kingdom.

- ^{33(a)}Department of Physics, University of Cape Town, Cape Town;^(b)iThemba Labs, Western Cape;^(c)Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg;^(d)University of South Africa, Department of Physics, Pretoria;^(e)School of Physics, University of the Witwatersrand, Johannesburg; South Africa.
- ³⁴Department of Physics, Carleton University, Ottawa ON; Canada.
- ^{35(a)}Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies - Université Hassan II, Casablanca;^(b)Faculté des Sciences, Université Ibn-Tofail, Kénitra;^(c)Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech;^(d)Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda;^(e)Faculté des sciences, Université Mohammed V, Rabat; Morocco.
- ³⁶CERN, Geneva; Switzerland.
- ³⁷Enrico Fermi Institute, University of Chicago, Chicago IL; United States of America.
- ³⁸LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand; France.
- ³⁹Nevis Laboratory, Columbia University, Irvington NY; United States of America.
- ⁴⁰Niels Bohr Institute, University of Copenhagen, Copenhagen; Denmark.
- ^{41(a)}Dipartimento di Fisica, Università della Calabria, Rende;^(b)INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati; Italy.
- ⁴²Physics Department, Southern Methodist University, Dallas TX; United States of America.
- ⁴³Physics Department, University of Texas at Dallas, Richardson TX; United States of America.
- ⁴⁴National Centre for Scientific Research "Demokritos", Agia Paraskevi; Greece.
- ^{45(a)}Department of Physics, Stockholm University;^(b)Oskar Klein Centre, Stockholm; Sweden.
- ⁴⁶Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen; Germany.
- ⁴⁷Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund; Germany.
- ⁴⁸Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden; Germany.
- ⁴⁹Department of Physics, Duke University, Durham NC; United States of America.
- ⁵⁰SUPA - School of Physics and Astronomy, University of Edinburgh, Edinburgh; United Kingdom.
- ⁵¹INFN e Laboratori Nazionali di Frascati, Frascati; Italy.
- ⁵²Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg; Germany.
- ⁵³II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen; Germany.
- ⁵⁴Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève; Switzerland.
- ^{55(a)}Dipartimento di Fisica, Università di Genova, Genova;^(b)INFN Sezione di Genova; Italy.
- ⁵⁶II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen; Germany.
- ⁵⁷SUPA - School of Physics and Astronomy, University of Glasgow, Glasgow; United Kingdom.
- ⁵⁸LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble; France.
- ⁵⁹Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge MA; United States of America.
- ^{60(a)}Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Hefei;^(b)Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE), Shandong University, Qingdao;^(c)School of Physics and Astronomy, Shanghai Jiao Tong University, KLPPAC-MoE, SKLPPC, Shanghai;^(d)Tsung-Dao Lee Institute, Shanghai; China.
- ^{61(a)}Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg;^(b)Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg; Germany.
- ⁶²Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima; Japan.
- ^{63(a)}Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong;^(b)Department of Physics, University of Hong Kong, Hong Kong;^(c)Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong; China.
- ⁶⁴Department of Physics, National Tsing Hua University, Hsinchu; Taiwan.

- ⁶⁵IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay; France.
- ⁶⁶Department of Physics, Indiana University, Bloomington IN; United States of America.
- ^{67(a)}INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine; ^(b)ICTP, Trieste; ^(c)Dipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine; Italy.
- ^{68(a)}INFN Sezione di Lecce; ^(b)Dipartimento di Matematica e Fisica, Università del Salento, Lecce; Italy.
- ^{69(a)}INFN Sezione di Milano; ^(b)Dipartimento di Fisica, Università di Milano, Milano; Italy.
- ^{70(a)}INFN Sezione di Napoli; ^(b)Dipartimento di Fisica, Università di Napoli, Napoli; Italy.
- ^{71(a)}INFN Sezione di Pavia; ^(b)Dipartimento di Fisica, Università di Pavia, Pavia; Italy.
- ^{72(a)}INFN Sezione di Pisa; ^(b)Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa; Italy.
- ^{73(a)}INFN Sezione di Roma; ^(b)Dipartimento di Fisica, Sapienza Università di Roma, Roma; Italy.
- ^{74(a)}INFN Sezione di Roma Tor Vergata; ^(b)Dipartimento di Fisica, Università di Roma Tor Vergata, Roma; Italy.
- ^{75(a)}INFN Sezione di Roma Tre; ^(b)Dipartimento di Matematica e Fisica, Università Roma Tre, Roma; Italy.
- ^{76(a)}INFN-TIFPA; ^(b)Università degli Studi di Trento, Trento; Italy.
- ⁷⁷Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck; Austria.
- ⁷⁸University of Iowa, Iowa City IA; United States of America.
- ⁷⁹Department of Physics and Astronomy, Iowa State University, Ames IA; United States of America.
- ⁸⁰Joint Institute for Nuclear Research, Dubna; Russia.
- ^{81(a)}Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora; ^(b)Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro; ^(c)Universidade Federal de São João del Rei (UFSJ), São João del Rei; ^(d)Instituto de Física, Universidade de São Paulo, São Paulo; Brazil.
- ⁸²KEK, High Energy Accelerator Research Organization, Tsukuba; Japan.
- ⁸³Graduate School of Science, Kobe University, Kobe; Japan.
- ^{84(a)}AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow; ^(b)Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow; Poland.
- ⁸⁵Institute of Nuclear Physics Polish Academy of Sciences, Krakow; Poland.
- ⁸⁶Faculty of Science, Kyoto University, Kyoto; Japan.
- ⁸⁷Kyoto University of Education, Kyoto; Japan.
- ⁸⁸Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka ; Japan.
- ⁸⁹Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata; Argentina.
- ⁹⁰Physics Department, Lancaster University, Lancaster; United Kingdom.
- ⁹¹Oliver Lodge Laboratory, University of Liverpool, Liverpool; United Kingdom.
- ⁹²Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana; Slovenia.
- ⁹³School of Physics and Astronomy, Queen Mary University of London, London; United Kingdom.
- ⁹⁴Department of Physics, Royal Holloway University of London, Egham; United Kingdom.
- ⁹⁵Department of Physics and Astronomy, University College London, London; United Kingdom.
- ⁹⁶Louisiana Tech University, Ruston LA; United States of America.
- ⁹⁷Fysiska institutionen, Lunds universitet, Lund; Sweden.
- ⁹⁸Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne; France.
- ⁹⁹Departamento de Física Teórica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid; Spain.
- ¹⁰⁰Institut für Physik, Universität Mainz, Mainz; Germany.
- ¹⁰¹School of Physics and Astronomy, University of Manchester, Manchester; United Kingdom.
- ¹⁰²CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille; France.

- ¹⁰³Department of Physics, University of Massachusetts, Amherst MA; United States of America.
- ¹⁰⁴Department of Physics, McGill University, Montreal QC; Canada.
- ¹⁰⁵School of Physics, University of Melbourne, Victoria; Australia.
- ¹⁰⁶Department of Physics, University of Michigan, Ann Arbor MI; United States of America.
- ¹⁰⁷Department of Physics and Astronomy, Michigan State University, East Lansing MI; United States of America.
- ¹⁰⁸B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk; Belarus.
- ¹⁰⁹Research Institute for Nuclear Problems of Byelorussian State University, Minsk; Belarus.
- ¹¹⁰Group of Particle Physics, University of Montreal, Montreal QC; Canada.
- ¹¹¹P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow; Russia.
- ¹¹²National Research Nuclear University MEPhI, Moscow; Russia.
- ¹¹³D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow; Russia.
- ¹¹⁴Fakultät für Physik, Ludwig-Maximilians-Universität München, München; Germany.
- ¹¹⁵Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München; Germany.
- ¹¹⁶Nagasaki Institute of Applied Science, Nagasaki; Japan.
- ¹¹⁷Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya; Japan.
- ¹¹⁸Department of Physics and Astronomy, University of New Mexico, Albuquerque NM; United States of America.
- ¹¹⁹Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen; Netherlands.
- ¹²⁰Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam; Netherlands.
- ¹²¹Department of Physics, Northern Illinois University, DeKalb IL; United States of America.
- ^{122(a)}Budker Institute of Nuclear Physics and NSU, SB RAS, Novosibirsk;^(b)Novosibirsk State University Novosibirsk; Russia.
- ¹²³Institute for High Energy Physics of the National Research Centre Kurchatov Institute, Protvino; Russia.
- ¹²⁴Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of National Research Centre "Kurchatov Institute", Moscow; Russia.
- ¹²⁵Department of Physics, New York University, New York NY; United States of America.
- ¹²⁶Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo; Japan.
- ¹²⁷Ohio State University, Columbus OH; United States of America.
- ¹²⁸Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman OK; United States of America.
- ¹²⁹Department of Physics, Oklahoma State University, Stillwater OK; United States of America.
- ¹³⁰Palacký University, RCPTM, Joint Laboratory of Optics, Olomouc; Czech Republic.
- ¹³¹Institute for Fundamental Science, University of Oregon, Eugene, OR; United States of America.
- ¹³²Graduate School of Science, Osaka University, Osaka; Japan.
- ¹³³Department of Physics, University of Oslo, Oslo; Norway.
- ¹³⁴Department of Physics, Oxford University, Oxford; United Kingdom.
- ¹³⁵LPNHE, Sorbonne Université, Université de Paris, CNRS/IN2P3, Paris; France.
- ¹³⁶Department of Physics, University of Pennsylvania, Philadelphia PA; United States of America.
- ¹³⁷Konstantinov Nuclear Physics Institute of National Research Centre "Kurchatov Institute", PNPI, St. Petersburg; Russia.
- ¹³⁸Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh PA; United States of America.
- ^{139(a)}Laboratório de Instrumentação e Física Experimental de Partículas - LIP, Lisboa;^(b)Departamento de

Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa;^(c)Departamento de Física, Universidade de Coimbra, Coimbra;^(d)Centro de Física Nuclear da Universidade de Lisboa, Lisboa;^(e)Departamento de Física, Universidade do Minho, Braga;^(f)Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada (Spain);^(g)Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica;^(h)Instituto Superior Técnico, Universidade de Lisboa, Lisboa; Portugal.

¹⁴⁰Institute of Physics of the Czech Academy of Sciences, Prague; Czech Republic.

¹⁴¹Czech Technical University in Prague, Prague; Czech Republic.

¹⁴²Charles University, Faculty of Mathematics and Physics, Prague; Czech Republic.

¹⁴³Particle Physics Department, Rutherford Appleton Laboratory, Didcot; United Kingdom.

¹⁴⁴IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette; France.

¹⁴⁵Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz CA; United States of America.

^{146(a)}Departamento de Física, Pontificia Universidad Católica de Chile, Santiago;^(b)Universidad Andres Bello, Department of Physics, Santiago;^(c)Instituto de Alta Investigación, Universidad de Tarapacá;^(d)Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso; Chile.

¹⁴⁷Department of Physics, University of Washington, Seattle WA; United States of America.

¹⁴⁸Department of Physics and Astronomy, University of Sheffield, Sheffield; United Kingdom.

¹⁴⁹Department of Physics, Shinshu University, Nagano; Japan.

¹⁵⁰Department Physik, Universität Siegen, Siegen; Germany.

¹⁵¹Department of Physics, Simon Fraser University, Burnaby BC; Canada.

¹⁵²SLAC National Accelerator Laboratory, Stanford CA; United States of America.

¹⁵³Physics Department, Royal Institute of Technology, Stockholm; Sweden.

¹⁵⁴Departments of Physics and Astronomy, Stony Brook University, Stony Brook NY; United States of America.

¹⁵⁵Department of Physics and Astronomy, University of Sussex, Brighton; United Kingdom.

¹⁵⁶School of Physics, University of Sydney, Sydney; Australia.

¹⁵⁷Institute of Physics, Academia Sinica, Taipei; Taiwan.

^{158(a)}E. Andronikashvili Institute of Physics, Iv. Javakishvili Tbilisi State University, Tbilisi;^(b)High Energy Physics Institute, Tbilisi State University, Tbilisi; Georgia.

¹⁵⁹Department of Physics, Technion, Israel Institute of Technology, Haifa; Israel.

¹⁶⁰Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv; Israel.

¹⁶¹Department of Physics, Aristotle University of Thessaloniki, Thessaloniki; Greece.

¹⁶²International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo; Japan.

¹⁶³Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo; Japan.

¹⁶⁴Department of Physics, Tokyo Institute of Technology, Tokyo; Japan.

¹⁶⁵Tomsk State University, Tomsk; Russia.

¹⁶⁶Department of Physics, University of Toronto, Toronto ON; Canada.

^{167(a)}TRIUMF, Vancouver BC;^(b)Department of Physics and Astronomy, York University, Toronto ON; Canada.

¹⁶⁸Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba; Japan.

¹⁶⁹Department of Physics and Astronomy, Tufts University, Medford MA; United States of America.

¹⁷⁰Department of Physics and Astronomy, University of California Irvine, Irvine CA; United States of America.

¹⁷¹Department of Physics and Astronomy, University of Uppsala, Uppsala; Sweden.

- ¹⁷²Department of Physics, University of Illinois, Urbana IL; United States of America.
- ¹⁷³Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia - CSIC, Valencia; Spain.
- ¹⁷⁴Department of Physics, University of British Columbia, Vancouver BC; Canada.
- ¹⁷⁵Department of Physics and Astronomy, University of Victoria, Victoria BC; Canada.
- ¹⁷⁶Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg; Germany.
- ¹⁷⁷Department of Physics, University of Warwick, Coventry; United Kingdom.
- ¹⁷⁸Waseda University, Tokyo; Japan.
- ¹⁷⁹Department of Particle Physics, Weizmann Institute of Science, Rehovot; Israel.
- ¹⁸⁰Department of Physics, University of Wisconsin, Madison WI; United States of America.
- ¹⁸¹Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal; Germany.
- ¹⁸²Department of Physics, Yale University, New Haven CT; United States of America.
- ^a Also at Borough of Manhattan Community College, City University of New York, New York NY; United States of America.
- ^b Also at Centro Studi e Ricerche Enrico Fermi; Italy.
- ^c Also at CERN, Geneva; Switzerland.
- ^d Also at CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille; France.
- ^e Also at Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève; Switzerland.
- ^f Also at Departament de Física de la Universitat Autònoma de Barcelona, Barcelona; Spain.
- ^g Also at Department of Financial and Management Engineering, University of the Aegean, Chios; Greece.
- ^h Also at Department of Physics and Astronomy, Michigan State University, East Lansing MI; United States of America.
- ⁱ Also at Department of Physics and Astronomy, University of Louisville, Louisville, KY; United States of America.
- ^j Also at Department of Physics, Ben Gurion University of the Negev, Beer Sheva; Israel.
- ^k Also at Department of Physics, California State University, East Bay; United States of America.
- ^l Also at Department of Physics, California State University, Fresno; United States of America.
- ^m Also at Department of Physics, California State University, Sacramento; United States of America.
- ⁿ Also at Department of Physics, King's College London, London; United Kingdom.
- ^o Also at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg; Russia.
- ^p Also at Department of Physics, University of Fribourg, Fribourg; Switzerland.
- ^q Also at Dipartimento di Matematica, Informatica e Fisica, Università di Udine, Udine; Italy.
- ^r Also at Faculty of Physics, M.V. Lomonosov Moscow State University, Moscow; Russia.
- ^s Also at Graduate School of Science, Osaka University, Osaka; Japan.
- ^t Also at Hellenic Open University, Patras; Greece.
- ^u Also at IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay; France.
- ^v Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona; Spain.
- ^w Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg; Germany.
- ^x Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen; Netherlands.
- ^y Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia; Bulgaria.
- ^z Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest; Hungary.
- ^{aa} Also at Institute of Particle Physics (IPP), Vancouver; Canada.
- ^{ab} Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku; Azerbaijan.

- ac* Also at Instituto de Fisica Teorica, IFT-UAM/CSIC, Madrid; Spain.
- ad* Also at Joint Institute for Nuclear Research, Dubna; Russia.
- ae* Also at Louisiana Tech University, Ruston LA; United States of America.
- af* Also at Moscow Institute of Physics and Technology State University, Dolgoprudny; Russia.
- ag* Also at National Research Nuclear University MEPhI, Moscow; Russia.
- ah* Also at Physics Department, An-Najah National University, Nablus; Palestine.
- ai* Also at Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg; Germany.
- aj* Also at The City College of New York, New York NY; United States of America.
- ak* Also at TRIUMF, Vancouver BC; Canada.
- al* Also at Università di Napoli Parthenope, Napoli; Italy.
- am* Also at University of Chinese Academy of Sciences (UCAS), Beijing; China.
- * Deceased