


***CP* Properties of Higgs Boson Interactions with Top Quarks in the $t\bar{t}H$ and tH Processes Using $H \rightarrow \gamma\gamma$ with the ATLAS Detector**

G. Aad *et al.**
(ATLAS Collaboration)

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A study of the charge conjugation and parity (*CP*) properties of the interaction between the Higgs boson and top quarks is presented. Higgs bosons are identified via the diphoton decay channel ($H \rightarrow \gamma\gamma$), and their production in association with a top quark pair ($t\bar{t}H$) or single top quark (tH) is studied. The analysis uses 139 fb^{-1} of proton–proton collision data recorded at a center-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$ with the ATLAS detector at the Large Hadron Collider. Assuming a *CP*-even coupling, the $t\bar{t}H$ process is observed with a significance of 5.2 standard deviations. The measured cross section times $H \rightarrow \gamma\gamma$ branching ratio is $1.64^{+0.38}_{-0.36}(\text{stat})^{+0.17}_{-0.14}(\text{sys}) \text{ fb}$, and the measured rate for $t\bar{t}H$ is $1.43^{+0.33}_{-0.31}(\text{stat})^{+0.21}_{-0.15}(\text{sys})$ times the Standard Model expectation. The tH production process is not observed and an upper limit on its rate of 12 times the Standard Model expectation is set. A *CP*-mixing angle greater (less) than 43 (-43)° is excluded at 95% confidence level.

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The observation of Higgs boson production in association with top quarks at the LHC [1,2] provides an opportunity to probe the charge conjugation and parity (*CP*) properties of the Yukawa coupling of the Higgs boson to the top quark. The Standard Model (SM) of particle physics predicts the Higgs boson to be a scalar particle ($J^{CP} = 0^{++}$) with a prescribed coupling to the top quark. However, the presence of a $J^{CP} = 0^{+-}$ pseudoscalar admixture, which introduces a second coupling to the top quark, has not yet been excluded. Any measured *CP*-odd contribution would be a sign of physics beyond the SM and could account for the explanation of the observed baryon asymmetry of the universe. This Letter presents a search for *CP* violation in this coupling and measurements of the production rate of the Higgs boson, via its decay into two photons, in association with top quarks. Recently, the CMS Collaboration performed a similar study [3].

Studies of *CP* properties of the Higgs boson interactions with gauge bosons have been performed by the ATLAS and CMS experiments [4–9]; the results show no deviations from the SM predictions. However, these measurements probe the bosonic couplings in which *CP*-odd contributions enter only via higher-order operators that are suppressed by powers of $1/\Lambda^2$ [10], where Λ is the scale of the new physics in an effective field theory (EFT). In the case

of the Yukawa couplings, the *CP*-odd contributions are not suppressed by powers of $1/\Lambda^2$.

The *CP* properties of the top Yukawa coupling can be probed directly using Higgs boson production in association with top quarks: $t\bar{t}H$ and tH processes. The couplings impact the production rates [11–14] and some kinematic distributions. The tH rate is particularly sensitive to deviations from SM couplings due to destructive interference in the SM between diagrams where the Higgs boson radiates from a top quark and from a W boson. The presence of *CP*-mixing in the top Yukawa coupling also modifies the gluon–gluon fusion (ggF) production rate and the $H \rightarrow \gamma\gamma$ decay rate.

This analysis is performed using 139 fb^{-1} of $\sqrt{s} = 13 \text{ TeV}$ proton–proton (pp) collision data recorded from 2015 to 2018 with the ATLAS detector. The ATLAS detector [15–17] is a multipurpose particle detector with a forward-backward symmetric cylindrical geometry and near 4π coverage in solid angle [18]. The trigger system consists of a hardware-based first-level trigger and a software-based high-level trigger [19]. Events used in this analysis were triggered by requiring two photons with a *loose* identification requirement [20] in the 2015–2016 data-taking period and transverse energies of at least 25 GeV and 35 GeV for the subleading and leading photons, respectively. Due to the greater instantaneous luminosity, the photon trigger identification requirement was tightened in the 2017–2018 data-taking period. The average trigger efficiency is over 98% for events passing the full diphoton event selection for this analysis.

The EFT definition used in this Letter is provided by the Higgs characterization model [21], which is implemented in the MADGRAPH5_AMC@NLO generator [22]. Within

*Full author list given at the end of the article.

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this model, the term in the effective Lagrangian that describes the top Yukawa coupling is

$$\mathcal{L} = -\frac{m_t}{v} \{\bar{\psi}_i \kappa_i [\cos(\alpha) + i \sin(\alpha) \gamma_5] \psi_i\} H$$

where m_t is the top quark mass, v is the Higgs vacuum expectation value, κ_i (> 0) is the top Yukawa coupling parameter, and α is the CP -mixing angle. The SM corresponds to a CP -even coupling with $\alpha = 0$ and $\kappa_t = 1$, while a CP -odd coupling is realized when $\alpha = 90^\circ$.

Simulated $t\bar{t}H$ and tH samples were generated using MADGRAPH5_AMC@NLO 2.6.2 at next-to-leading order in QCD for different α and κ_t (for tH) values, with the NNPDF30NLO [23] parton distribution function (PDF) set used for the matrix element (ME) evaluation, and interfaced to PYTHIA 8 [24] using the NNPDF23LO [25] PDF set for parton showering (PS). The A14 parameter set [26], tuned to data, was used for both PS and underlying event (UE). From these samples, the yields for $t\bar{t}H$ and tH are parameterized as functions of α and κ_t , which are used in the statistical interpretations. Samples for other Higgs boson production processes, ggF [27], vector-boson fusion (VBF) [28], and vector-boson associated production (VH) [29,30] were produced with POWHEG-BOX v2 generator [31] using the PDF4LHC15 PDF set [32] for ME, with the AZNLO set of tuned parameters [33] and PYTHIA 8 for PS using the CTEQ6L1 [34] PDF set. Samples generated with Herwig 7 [35] are used for systematic uncertainty studies that involve modeling of the PS, hadronization and UE. The simulated Higgs boson samples are normalized to the SM cross sections (Refs. [36–54]) times the SM branching ratio (BR) to diphotons (Refs. [36,55–58]) with a Higgs boson mass of 125.09 GeV [59], and specifically for $t\bar{t}H$, the SM predicted cross section times the $H \rightarrow \gamma\gamma$ BR is $\sigma_{t\bar{t}H} \times B_{\gamma\gamma} = 1.15^{+0.09}_{-0.12}$ fb.

Although this analysis relies on a data-driven approach for background estimations, a simulated background sample for the $t\bar{t}\gamma\gamma$ process was generated to optimize the event selection and develop the background model. This sample was generated using the MADGRAPH5_AMC@NLO generator, with the NNPDF23LO PDF set and showered with PYTHIA 8.

All generated Higgs boson events were passed through a full simulation of the ATLAS detector response [60] using GEANT 4 [61]. The $t\bar{t}\gamma\gamma$ events were processed with a fast simulation in which the full simulation of the calorimeter is replaced with a parameterization of the calorimeter response [62]. The effects of multiple pp interactions in the same or neighboring bunch crossings are included using events generated with PYTHIA 8. Events are weighted such that the distribution of the average number of interactions per bunch crossing matches that observed in data, which is typically around 30 to 40.

Events are selected by requiring two isolated photon candidates with transverse momenta p_T greater than

35 GeV and 25 GeV. Both photons must satisfy the *tight* identification requirement [20]. The identification is constructed from a cut-based selection using the electromagnetic shower shape variables. The leading (subleading) photon must have $p_T/m_{\gamma\gamma} > 0.35$ (0.25), and the diphoton invariant mass $m_{\gamma\gamma}$ is required to be in the range $m_{\gamma\gamma} \in [105, 160]$ GeV. Jets are reconstructed using the anti- k_t algorithm [63] with a radius parameter of $R = 0.4$. Events are required to have at least one jet with $p_T > 25$ GeV containing a b -hadron (b -jet), identified using a b -tagging algorithm with an efficiency of 77% and a mistagging rate of 0.9% for light-flavor jets [64].

Selected events are sorted into two $t\bar{t}H$ -enriched regions. The ‘‘Lep’’ region, targeting top quark decays in which at least one of the resulting W bosons decays leptonically, requires events to have at least one isolated lepton (muon or electron) candidate with $p_T > 15$ GeV passing *medium* identification requirements (Refs. [20,65]). The ‘‘Had’’ region targets hadronic top quark decays (as well as top quark decays to both hadronically decaying τ leptons and unreconstructed leptons) and requires events to have at least two additional jets with $p_T > 25$ GeV and no selected lepton.

A boosted decision tree (BDT) used for the top quark reconstruction, denoted by ‘‘Top Reco BDT,’’ is trained with the $t\bar{t}H$ sample by using the XGBOOST package [66] to extract the three-jet (triplet) combination best matching the hadronic decay products of a top quark. This BDT uses p_T , η , ϕ , and the energy E of W boson and b jet (where the W boson candidate is formed by a pair of jets). Furthermore, this BDT uses the angular distance ΔR_{Wb} between the W boson and b jet, ΔR_{jj} between the two jets composing the W boson candidate, and b -tagging information about all three jets in the triplet and the invariant mass of the triplet. For events in the Had region, the triplet with the highest Top Reco BDT score is taken as the primary top quark candidate (t_1). In the Lep region, for events containing only one lepton, a W boson candidate is first constructed from the lepton and missing transverse momentum E_T^{miss} . Then t_1 is reconstructed from this leptonic W boson candidate and the jet giving the highest Top Reco BDT score. No top quark candidate is reconstructed for events containing more than one lepton. After t_1 is selected, if there are at least three additional jets, a second top quark candidate (t_2) is reconstructed by selecting the triplet with the highest BDT score from the remaining jets; if there is only one or two additional jets, then t_2 is taken as the sum of the remaining jets; otherwise no t_2 is reconstructed.

To improve the analysis sensitivity, selected events are categorized using partitions of a two-dimensional BDT space. Two independent BDTs are trained using the XGBOOST algorithm: ‘‘Background Rejection BDT’’ and ‘‘ CP BDT,’’ and each of them is trained separately in the Had and Lep regions. The Background Rejection BDT is trained to separate $t\bar{t}H$ -like events from background that

are mainly nonresonant diphoton production processes, including $\gamma\gamma + \text{jets}$ and $t\bar{t}\gamma\gamma$. A detailed discussion of this methodology is given in Ref. [1]. The CP BDT is trained to separate CP -even from CP -odd couplings using $t\bar{t}H$ and tH processes. The CP BDT uses p_T and η of the diphoton system, p_T and η of t_1 and t_2 , their azimuthal angles calculated relative to the diphoton system $\phi_{\gamma\gamma,t_1}$, $\phi_{\gamma\gamma,t_2}$, as well as their Top Reco BDT scores. It also uses differences in pseudorapidity and azimuthal angle $\Delta\eta_{t_1,t_2}$ and $\Delta\phi_{t_1,t_2}$ between the two top quark candidates, the invariant mass of the diphoton and primary top quark system $m_{\gamma\gamma,t_1}$, the invariant mass of the two top quark candidates m_{t_1,t_2} , the scalar p_T sum of jets H_T , the E_T^{miss} divided by $\sqrt{H_T}$, the number of jets and b -tagged jets, and the minimum and second smallest angular differences $\Delta R_{\gamma j}$ between a photon and a jet.

Figure 1 shows the BDT discriminant distributions in the data as well as those expected from CP -even and CP -odd Higgs boson signals in the Had region. The discriminating power can be seen by comparing the CP -even, CP -odd, and data shapes. Events with low values of the Background Rejection BDT response are removed, and the remaining events are categorized. The number of categories and the boundary locations are chosen to optimize the $t\bar{t}H$ significance and the discriminating power between the CP -even and CP -odd cases. There are 20 categories in total: 12 in the Had region and 8 in the Lep region.

The results are impacted by three distinct types of uncertainties: the statistical uncertainty associated with the data, theoretical modeling systematic uncertainties, and experimental systematic uncertainties. The first

dominates. Theoretical uncertainties for $t\bar{t}H$ and tH rates in the various categories are assessed. The following effects are considered: the value of the strong coupling constant; alternative generator for the PS, hadronization, and UE; and PDF uncertainty. In the three (two) most CP -even sensitive Had (Lep) categories, each of these uncertainties is less than 10%. The background from ggF is less than 0.25 events in each of the most sensitive categories; conservative uncertainties, including a 100% theoretical uncertainty in the modeling of the radiation of additional heavy-flavor jets, are assigned to it in the Had region. The same heavy-flavor uncertainty is also assigned to the VBF and VH processes.

Experimental uncertainties arise from identification and isolation criteria for photons, electrons, and muons and from their energy scale and resolution [20,65]. Jets have uncertainties from b tagging [64] and vertex identification [67] in addition to the energy scale and resolution [68]. Uncertainties in the measurement of E_T^{miss} [69], which is used in the leptonic categories, are also included. These experimental effects impact the expected event yield in each category and can cause events to migrate between the categories. The overall uncertainty is less than 20% in each category. In addition, uncertainties in the luminosity [70] obtained using the LUCID-2 detector [71] and trigger efficiency [19] are responsible for uncertainties in the overall event yield of 1.7% and 0.4%, respectively.

A simultaneous maximum-likelihood fit is performed to the $m_{\gamma\gamma}$ spectra in all the categories. Signal and background shapes are modeled by analytic functions using the strategy discussed in Ref. [6]. The chosen background function is

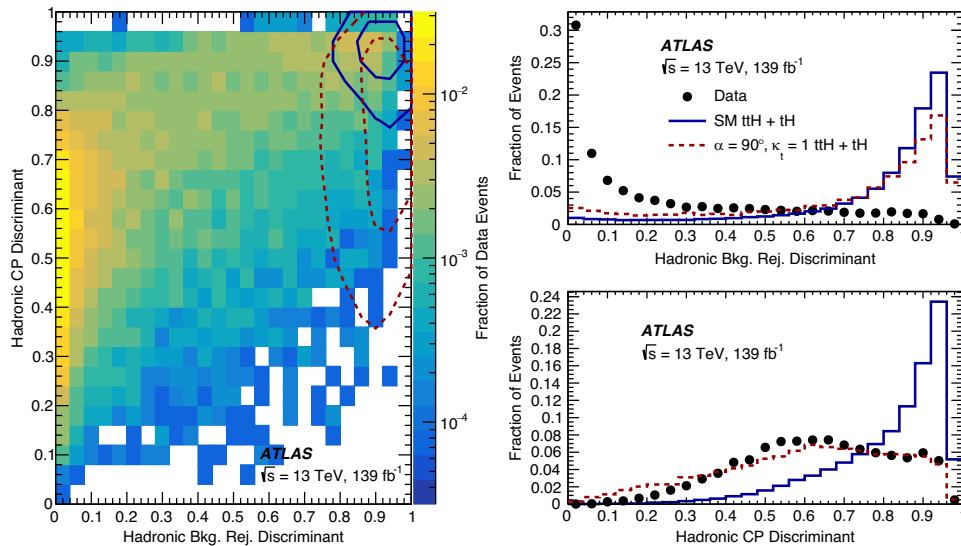


FIG. 1. Left: two-dimensional BDT distribution in the selected data events ($m_{\gamma\gamma} \in [105, 160]$ GeV) from the Had region showing the Background Rejection BDT and CP BDT. The inner (outer) contours capture 25% (50%) of the $t\bar{t}H$ and tH signal events for CP -even (blue) and CP -odd (red) hypotheses. Right: projections onto the background rejection and CP BDT axes. Contributions from CP -even (blue) and CP -odd (red) $t\bar{t}H/tH$ processes and the data (black) are shown and normalized to unit area. The error bars on data are statistical.

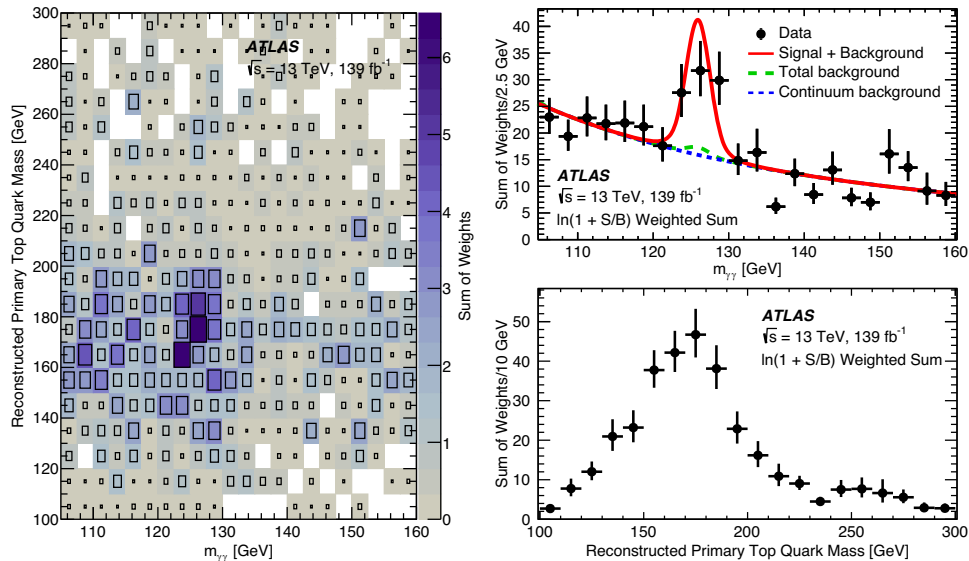


FIG. 2. Distribution of reconstructed primary top quark mass versus reconstructed Higgs boson mass in the data events. The right panels show the projections onto the Higgs boson mass and primary top quark mass axes. In the upper panel, the fitted continuum background (blue), the total background including non- $t\bar{t}H/tH$ Higgs boson production (green), and the total fitted signal plus background (red) are shown. The error bars on data are statistical.

based on the simulated $t\bar{t}\gamma\gamma$ events following the procedure in Ref. [1], which imposes stringent conditions on potential biases in the extracted signal yield to avoid losses in sensitivity. The parameters of the background model and background normalization in each category are left free in the fit. The profile likelihood ratio is used as the test statistic, and the asymptotic approximation [72] is used for statistical interpretations. Yields from $t\bar{t}H$ and tH are extracted after subtracting the very small contribution from other Higgs boson production modes using their SM expected values. Figure 2 shows the distributions of the reconstructed masses for the diphoton system and primary top quark. The events are weighted by $\ln(1 + S/B)$ with S and B being the fitted signal and background yields in the smallest $m_{\gamma\gamma}$ interval containing 90% of the signal in each category. The p value associated with the compatibility between the observed spectra and the fit model using the goodness-of-fit test method described in Ref. [73] is 35%. Assuming a CP -even coupling, the $\sigma_{t\bar{t}H} \times B_{\gamma\gamma}$ is derived by constraining all the non- $t\bar{t}H$ Higgs boson processes to their SM predictions and measured to be $1.64^{+0.38}_{-0.36}(\text{stat})^{+0.17}_{-0.14}(\text{sys})$ fb. The measured rate for $t\bar{t}H$ is $1.43^{+0.33}_{-0.31}(\text{stat})^{+0.21}_{-0.15}(\text{sys})$ times the SM expectation. The background-only hypothesis is rejected with an observed (expected) significance of 5.2σ (4.4σ). The rate for tH is derived by constraining all the non- $t\bar{t}H/tH$ Higgs boson processes to their SM prediction without prior constraint on the rate of $t\bar{t}H$. Using the CLs method [74], this yields a 95% confidence level (CL) upper limit of 12 times the SM prediction, the same as expected assuming the presence of SM tH signal. This is stricter than the previous best limit of 25 times the SM prediction on tH from the CMS analysis

performed using 35.9 fb^{-1} of data at $\sqrt{s} = 13 \text{ TeV}$ [75] with the $t\bar{t}H$ process constrained to the SM prediction.

Extraction of values for the top Yukawa coupling requires additional information. In particular, the BR of $H \rightarrow \gamma\gamma$ is needed to recover the total Higgs boson production rate, and the Higgs boson coupling to gluons is needed to account for the small ggF background. The corresponding Higgs boson coupling modifiers κ_γ and κ_g are measured in the Run 2 Higgs boson coupling combination [76]. This combination includes the first 80 fb^{-1} of data used in this paper, and $t\bar{t}H$ and tH analyses from other decay channels. The combination analysis is repeated without the $t\bar{t}H$ and tH inputs, and this result is used to constrain κ_g and κ_γ . The impact on κ_g and κ_γ of removing input $t\bar{t}H$ and tH analyses from the combination is small. The correlation of the systematic uncertainties between the Higgs boson coupling combination and this analysis is neglected. The correlation has a small impact on α , and a similar effect on κ_t , as on signal strength reported in Ref. [76]. This analysis is insensitive to the potential modifications of ggF kinematics due to CP mixing, which is therefore neglected. The results of the fit for $\kappa_t \cos(\alpha)$ and $\kappa_t \sin(\alpha)$ are shown as contours in Fig. 3. A limit on α is set without prior constraint on κ_t in the fit: $|\alpha| > 43^\circ$ is excluded at 95% CL. The expected exclusion is $|\alpha| > 63^\circ$ under the CP -even hypothesis. A value of $\alpha = 90$ (180) $^\circ$ is excluded at 3.9σ (2.5σ). A comparable study from the CMS experiment excluded $\alpha = 90^\circ$ at 3.2σ [3]. If κ_γ and κ_g are parameterized using α and κ_t [11], the observed (expected) exclusion is $|\alpha| > 43$ (56) $^\circ$ without prior constraint on κ_t in the fit. The impact of the systematic uncertainties is negligible.

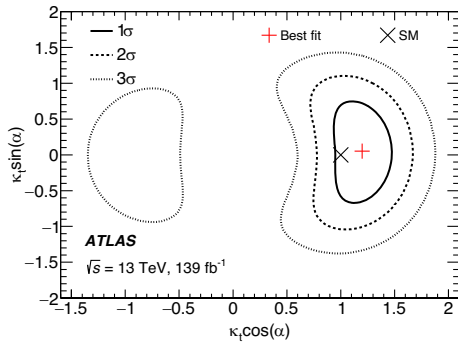


FIG. 3. Two-dimensional likelihood contours for $\kappa_t \cos(\alpha)$ and $\kappa_t \sin(\alpha)$ with ggF and $H \rightarrow \gamma\gamma$ constrained by the Higgs boson coupling combination.

In summary, the production rate of the Higgs boson in association with top quarks is measured, and the CP property of the top Yukawa coupling is studied. The $\text{no-}\tilde{t}\tilde{t}H$ hypothesis is rejected with a significance of 5.2σ , and the measured $\sigma_{\tilde{t}\tilde{t}H} \times B_{\gamma\gamma}$ is $1.64^{+0.38}_{-0.36}(\text{stat})^{+0.17}_{-0.14}(\text{sys})$ fb. The measured rate for $\tilde{t}\tilde{t}H$ is $1.43^{+0.33}_{-0.31}(\text{stat})^{+0.21}_{-0.15}(\text{sys})$ times the SM expectation. The tH process is not observed, and an upper limit of 12 times the SM expectation is set on its rate at 95% CL. All measurements are consistent with the SM expectations, and the possibility of CP -odd couplings between the Higgs boson and top quark is severely constrained. A pure CP -odd coupling is excluded at 3.9σ , and $|\alpha| > 43^\circ$ is excluded at 95% CL.

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 S. Adorni,⁵⁴ T. Adye,¹⁴³ A. A. Affolder,¹⁴⁵ Y. Afik,¹⁵⁹ C. Agapopoulou,⁶⁵ M. N. Agaras,³⁸ A. Aggarwal,¹¹⁹
 C. Agheorghiesei,^{27c} J. A. Aguilar-Saavedra,^{139f,139a,c} A. Ahmad,³⁶ F. Ahmadov,⁸⁰ W. S. Ahmed,¹⁰⁴ X. Ai,¹⁸ G. Aielli,^{74a,74b}
 S. Akatsuka,⁸⁶ M. Akbiyik,¹⁰⁰ T. P. A. Åkesson,⁹⁷ E. Akilli,⁵⁴ A. V. Akimov,¹¹¹ K. Al Khoury,⁶⁵ G. L. Alberghi,^{23b,23a}
 J. Albert,¹⁷⁵ M. J. Alconada Verzini,¹⁶⁰ S. Alderweireldt,³⁶ M. Aleksa,³⁶ I. N. Aleksandrov,⁸⁰ C. Alexa,^{27b} T. Alexopoulos,¹⁰
 A. Alfonsi,¹²⁰ F. Alfonsi,^{23b,23a} M. Alhroob,¹²⁸ B. Ali,¹⁴¹ S. Ali,¹⁵⁷ M. Aliev,¹⁶⁵ G. Alimonti,^{69a} C. Allaire,³⁶
 B. M. M. Allbrooke,¹⁵⁵ B. W. Allen,¹³¹ P. P. Allport,²¹ A. Aloisio,^{70a,70b} F. Alonso,⁸⁹ C. Alpigiani,¹⁴⁷
 E. Alunno Camelia,^{74a,74b} M. Alvarez Estevez,⁹⁹ M. G. Alviggi,^{70a,70b} Y. Amaral Coutinho,^{81b} A. Ambler,¹⁰⁴ L. Ambroz,¹³⁴
 C. Amelung,²⁶ D. Amidei,¹⁰⁶ S. P. Amor Dos Santos,^{139a} S. Amoroso,⁴⁶ C. S. Amrouche,⁵⁴ F. An,⁷⁹ C. Anastopoulos,¹⁴⁸
 N. Andari,¹⁴⁴ T. Andeen,¹¹ J. K. Anders,²⁰ S. Y. Andreev,^{45a,45b} A. Andreatta,^{69a,69b} V. Andrei,^{61a} C. R. Anelli,¹⁷⁵
 S. Angelidakis,⁹ A. Angerami,³⁹ A. V. Anisenkov,^{122b,122a} A. Annovi,^{72a} C. Antel,⁵⁴ M. T. Anthony,¹⁴⁸ E. Antipov,¹²⁹
 M. Antonelli,⁵¹ D. J. A. Antrim,¹⁷⁰ F. Anulli,^{73a} M. Aoki,⁸² J. A. Aparisi Pozo,¹⁷³ M. A. Aparo,¹⁵⁵ L. Aperio Bella,⁴⁶
 N. Aranzabal Barrio,³⁶ V. Araujo Ferraz,^{81a} R. Araujo Pereira,^{81b} C. Arcangeletti,⁵¹ A. T. H. Arce,⁴⁹ F. A. Arduh,⁸⁹
 J-F. Arguin,¹¹⁰ S. Argyropoulos,⁵² J.-H. Arling,⁴⁶ A. J. Armbruster,³⁶ A. Armstrong,¹⁷⁰ O. Arnaez,¹⁶⁶ H. Arnold,¹²⁰
 Z. P. Arrubarrena Tame,¹¹⁴ G. Artoni,¹³⁴ K. Asai,¹²⁶ S. Asai,¹⁶² T. Asawatavonvanich,¹⁶⁴ N. Asbah,⁵⁹
 E. M. Asimakopoulou,¹⁷¹ L. Asquith,¹⁵⁵ J. Assahsah,^{35d} K. Assamagan,²⁹ R. Aсталos,^{28a} R. J. Atkin,^{33a} M. Atkinson,¹⁷²
 N. B. Atlay,¹⁹ H. Atmani,⁶⁵ K. Augsten,¹⁴¹ V. A. Austrup,¹⁸¹ G. Avolio,³⁶ M. K. Ayoub,^{15a} G. Azuelos,^{110,d} H. Bachacou,¹⁴⁴
 K. Bachas,¹⁶¹ M. Backes,¹³⁴ F. Backman,^{45a,45b} P. Bagnaia,^{73a,73b} M. Bahmani,⁸⁵ H. Bahrasemani,¹⁵¹ A. J. Bailey,¹⁷³
 V. R. Bailey,¹⁷² J. T. Baines,¹⁴³ C. Bakalis,¹⁰ O. K. Baker,¹⁸² P. J. Bakker,¹²⁰ E. Bakos,¹⁶ D. Bakshi Gupta,⁸ S. Balaji,¹⁵⁶
 E. M. Baldin,^{122b,122a} P. Balek,¹⁷⁹ F. Balli,¹⁴⁴ W. K. Balunas,¹³⁴ J. Balz,¹⁰⁰ E. Banas,⁸⁵ M. Bandieramonte,¹³⁸
 A. Bandyopadhyay,²⁴ Sw. Banerjee,^{180,e} L. Barak,¹⁶⁰ W. M. Barbe,³⁸ E. L. Barberio,¹⁰⁵ D. Barberis,^{55b,55a} M. Barbero,¹⁰²
 G. Barbour,⁹⁵ T. Barillari,¹¹⁵ M.-S. Barisits,³⁶ J. Barkeloo,¹³¹ T. Barklow,¹⁵² R. Barnea,¹⁵⁹ B. M. Barnett,¹⁴³ R. M. Barnett,¹⁸
 Z. Barnovska-Blenessy,^{60a} A. Baroncelli,^{60a} G. Barone,²⁹ A. J. Barr,¹³⁴ L. Barranco Navarro,^{45a,45b} F. Barreiro,⁹⁹
 J. Barreiro Guimarães da Costa,^{15a} U. Barron,¹⁶⁰ S. Barsov,¹³⁷ F. Bartels,^{61a} R. Bartoldus,¹⁵² G. Bartolini,¹⁰² A. E. Barton,⁹⁰
 P. Bartos,^{28a} A. Basalaev,⁴⁶ A. Basan,¹⁰⁰ A. Bassalat,^{65,f} M. J. Basso,¹⁶⁶ R. L. Bates,⁵⁷ S. Batlamous,^{35e} J. R. Batley,³²
 B. Batool,¹⁵⁰ M. Battaglia,¹⁴⁵ M. Bause,^{73a,73b} F. Bauer,¹⁴⁴ K. T. Bauer,¹⁷⁰ P. Bauer,²⁴ H. S. Bawa,³¹ A. Bayirli,^{12c}
 J. B. Beacham,⁴⁹ T. Beau,¹³⁵ P. H. Beauchemin,¹⁶⁹ F. Becherer,⁵² P. Bechtel,²⁴ H. C. Beck,⁵³ H. P. Beck,^{20,g} K. Becker,¹⁷⁷
 C. Becot,⁴⁶ A. Beddall,^{12d} A. J. Beddall,^{12a} V. A. Bednyakov,⁸⁰ M. Bedognetti,¹²⁰ C. P. Bee,¹⁵⁴ T. A. Beermann,¹⁸¹
 M. Begalli,^{81b} M. Begel,²⁹ A. Behera,¹⁵⁴ J. K. Behr,⁴⁶ F. Beisiegel,²⁴ M. Belfkir,⁵ A. S. Bell,⁹⁵ G. Bella,¹⁶⁰ L. Bellagamba,^{23b}
 A. Bellerive,³⁴ P. Bellos,⁹ K. Beloborodov,^{122b,122a} K. Belotskiy,¹¹² N. L. Belyaev,¹¹² D. Benckekroun,^{35a} N. Benekos,¹⁰
 Y. Benhammou,¹⁶⁰ D. P. Benjamin,⁶ M. Benoit,⁵⁴ J. R. Bensinger,²⁶ S. Bentvelsen,¹²⁰ L. Beresford,¹³⁴ M. Beretta,⁵¹
 D. Berge,¹⁹ E. Bergeaas Kuutmann,¹⁷¹ N. Berger,⁵ B. Bergmann,¹⁴¹ L. J. Bergsten,²⁶ J. Beringer,¹⁸ S. Berlendis,⁷
 G. Bernardi,¹³⁵ C. Bernius,¹⁵² F. U. Bernlochner,²⁴ T. Berry,⁹⁴ P. Berta,¹⁰⁰ C. Bertella,^{15a} A. Berthold,⁴⁸ I. A. Bertram,⁹⁰
 O. Bessidskaia Bylund,¹⁸¹ N. Besson,¹⁴⁴ A. Bethani,¹⁰¹ S. Bethke,¹¹⁵ A. Betti,⁴² A. J. Bevan,⁹³ J. Beyer,¹¹⁵
 D. S. Bhattacharya,¹⁷⁶ P. Bhattarai,²⁶ V. S. Bhopatkar,⁶ R. Bi,¹³⁸ R. M. Bianchi,¹³⁸ O. Biebel,¹¹⁴ D. Biedermann,¹⁹
 R. Bielski,³⁶ K. Bierwagen,¹⁰⁰ N. V. Biesuz,^{72a,72b} M. Biglietti,^{75a} T. R. V. Billoud,¹¹⁰ M. Bindi,⁵³ A. Bingul,^{12d} C. Bini,^{73a,73b}
 S. Biondi,^{23b,23a} C. J. Birch-sykes,¹⁰¹ M. Birman,¹⁷⁹ T. Bisanz,⁵³ J. P. Biswal,³ D. Biswas,^{180,e} A. Bitadze,¹⁰¹ C. Bittrich,⁴⁸
 K. Bjørke,¹³³ T. Blazek,^{28a} I. Bloch,⁴⁶ C. Blocker,²⁶ A. Blue,⁵⁷ U. Blumenschein,⁹³ G. J. Bobbink,¹²⁰
 V. S. Bobrovnikov,^{122b,122a} S. S. Bocchetta,⁹⁷ D. Boerner,⁴⁶ D. Bogavac,¹⁴ A. G. Bogdanchikov,^{122b,122a} C. Bohm,^{45a}
 V. Boisvert,⁹⁴ P. Bokan,^{53,171} T. Bold,^{84a} A. E. Bolz,^{61b} M. Bomben,¹³⁵ M. Bona,⁹³ J. S. Bonilla,¹³¹ M. Boonekamp,¹⁴⁴
 C. D. Booth,⁹⁴ A. G. Borbély,⁵⁷ H. M. Borecka-Bielska,⁹¹ L. S. Borgna,⁹⁵ A. Borisov,¹²³ G. Borisso,⁹⁰ D. Bortoletto,¹³⁴
 D. Boscherini,^{23b} M. Bosman,¹⁴ J. D. Bossio Sola,¹⁰⁴ K. Bouaouda,^{35a} J. Boudreau,¹³⁸ E. V. Bouhova-Thacker,⁹⁰
 D. Boumediene,³⁸ S. K. Boutle,⁵⁷ A. Boveia,¹²⁷ J. Boyd,³⁶ D. Boye,^{33c} I. R. Boyko,⁸⁰ A. J. Bozson,⁹⁴ J. Bracinik,²¹
 N. Brahimi,^{60d} G. Brandt,¹⁸¹ O. Brandt,³² F. Braren,⁴⁶ B. Brau,¹⁰³ J. E. Brau,¹³¹ W. D. Breaden Madden,⁵⁷ K. Brendlinger,⁴⁶
 R. Brenner,¹⁵⁹ L. Brenner,³⁶ R. Brenner,¹⁷¹ S. Bressler,¹⁷⁹ B. Brickwedde,¹⁰⁰ D. L. Briglin,²¹ D. Britton,⁵⁷ D. Britzger,¹¹⁵
 I. Brock,²⁴ R. Brock,¹⁰⁷ G. Brooijmans,³⁹ W. K. Brooks,^{146d} E. Brost,²⁹ P. A. Bruckman de Renstrom,⁸⁵ B. Brüers,⁴⁶
 D. Bruncko,^{28b} A. Bruni,^{23b} G. Bruni,^{23b} L. S. Bruni,¹²⁰ S. Bruno,^{74a,74b} M. Bruschi,^{23b} N. Brusino,^{73a,73b} L. Bryngemark,¹⁵²
 T. Buanes,¹⁷ Q. Buat,¹⁵⁴ P. Buchholz,¹⁵⁰ A. G. Buckley,⁵⁷ I. A. Budagov,⁸⁰ M. K. Bugge,¹³³ F. Bühner,⁵² O. Bulekov,¹¹²
 B. A. Bullard,⁵⁹ T. J. Burch,¹²¹ S. Burdin,⁹¹ C. D. Burgard,¹²⁰ A. M. Burger,¹²⁹ B. Burghgrave,⁸ J. T. P. Burr,⁴⁶

C. D. Burton,¹¹ J. C. Burzynski,¹⁰³ V. Büscher,¹⁰⁰ E. Buschmann,⁵³ P. J. Bussey,⁵⁷ J. M. Butler,²⁵ C. M. Buttar,⁵⁷
 J. M. Butterworth,⁹⁵ P. Butti,³⁶ W. Buttinger,³⁶ C. J. Buxo Vazquez,¹⁰⁷ A. Buzatu,¹⁵⁷ A. R. Buzykaev,^{122b,122a}
 G. Cabras,^{23b,23a} S. Cabrera Urbán,¹⁷³ D. Caforio,⁵⁶ H. Cai,¹³⁸ V. M. M. Cairo,¹⁵² O. Cakir,^{4a} N. Calace,³⁶ P. Calafiura,¹⁸
 G. Calderini,¹³⁵ P. Calfayan,⁶⁶ G. Callea,⁵⁷ L. P. Caloba,^{81b} A. Caltabiano,^{74a,74b} S. Calvente Lopez,⁹⁹ D. Calvet,³⁸
 S. Calvet,³⁸ T. P. Calvet,¹⁰² M. Calvetti,^{72a,72b} R. Camacho Toro,¹³⁵ S. Camarda,³⁶ D. Camarero Munoz,⁹⁹ P. Camarri,^{74a,74b}
 M. T. Camerlingo,^{75a,75b} D. Cameron,¹³³ C. Camincher,³⁶ S. Campana,³⁶ M. Campanelli,⁹⁵ A. Camplani,⁴⁰ V. Canale,^{70a,70b}
 A. Canesse,¹⁰⁴ M. Cano Bret,⁷⁸ J. Cantero,¹²⁹ T. Cao,¹⁶⁰ Y. Cao,¹⁷² M. D. M. Capeans Garrido,³⁶ M. Capua,^{41b,41a}
 R. Cardarelli,^{74a} F. Cardillo,¹⁴⁸ G. Carducci,^{41b,41a} I. Carli,¹⁴² T. Carli,³⁶ G. Carlino,^{70a} B. T. Carlson,¹³⁸ E. M. Carlson,^{175,167a}
 L. Carminati,^{69a,69b} R. M. D. Carney,¹⁵² S. Caron,¹¹⁹ E. Carquin,^{146d} S. Carrá,⁴⁶ G. Carratta,^{23b,23a} J. W. S. Carter,¹⁶⁶
 T. M. Carter,⁵⁰ M. P. Casado,^{14,h} A. F. Casha,¹⁶⁶ F. L. Castillo,¹⁷³ L. Castillo Garcia,¹⁴ V. Castillo Gimenez,¹⁷³
 N. F. Castro,^{139a,139e} A. Catinaccio,³⁶ J. R. Catmore,¹³³ A. Cattai,³⁶ V. Cavaliere,²⁹ V. Cavasinni,^{72a,72b} E. Celebi,^{12b}
 F. Celli,¹³⁴ K. Cerny,¹³⁰ A. S. Cerqueira,^{81a} A. Cerri,¹⁵⁵ L. Cerrito,^{74a,74b} F. Cerutti,¹⁸ A. Cervelli,^{23b,23a} S. A. Cetin,^{12b}
 Z. Chadi,^{35a} D. Chakraborty,¹²¹ J. Chan,¹⁸⁰ W. S. Chan,¹²⁰ W. Y. Chan,⁹¹ J. D. Chapman,³² B. Chargeishvili,^{158b}
 D. G. Charlton,²¹ T. P. Charman,⁹³ C. C. Chau,³⁴ S. Che,¹²⁷ S. Chekanov,⁶ S. V. Chekulaev,^{167a} G. A. Chelkov,^{80,i} B. Chen,⁷⁹
 C. Chen,^{60a} C. H. Chen,⁷⁹ H. Chen,²⁹ J. Chen,^{60a} J. Chen,³⁹ J. Chen,²⁶ S. Chen,¹³⁶ S. J. Chen,^{15c} X. Chen,^{15b} Y. Chen,^{60a}
 Y-H. Chen,⁴⁶ H. C. Cheng,^{63a} H. J. Cheng,^{15a} A. Cheplakov,⁸⁰ E. Cheremushkina,¹²³ R. Cherkaoui El Moursli,^{35e} E. Cheu,⁷
 K. Cheung,⁶⁴ T. J. A. Chevalérias,¹⁴⁴ L. Chevalier,¹⁴⁴ V. Chiarella,⁵¹ G. Chiarelli,^{72a} G. Chiodini,^{68a} A. S. Chisholm,²¹
 A. Chitan,^{27b} I. Chiu,¹⁶² Y. H. Chiu,¹⁷⁵ M. V. Chizhov,⁸⁰ K. Choi,¹¹ A. R. Chomont,^{73a,73b} Y. S. Chow,¹²⁰
 L. D. Christopher,^{33e} M. C. Chu,^{63a} X. Chu,^{15a,15d} J. Chudoba,¹⁴⁰ J. J. Chwastowski,⁸⁵ L. Chytka,¹³⁰ D. Cieri,¹¹⁵
 K. M. Ciesla,⁸⁵ D. Cinca,⁴⁷ V. Cindro,⁹² I. A. Cioară,^{27b} A. Ciocio,¹⁸ F. Ciotto,^{70a,70b} Z. H. Citron,^{179,j} M. Citterio,^{69a}
 D. A. Ciubotaru,^{27b} B. M. Ciungu,¹⁶⁶ A. Clark,⁵⁴ M. R. Clark,³⁹ P. J. Clark,⁵⁰ S. E. Clawson,¹⁰¹ C. Clement,^{45a,45b}
 Y. Coadou,¹⁰² M. Cobal,^{67a,67c} A. Coccaro,^{55b} J. Cochran,⁷⁹ R. Coelho Lopes De Sa,¹⁰³ H. Cohen,¹⁶⁰ A. E. C. Coimbra,³⁶
 B. Cole,³⁹ A. P. Colijn,¹²⁰ J. Collot,⁵⁸ P. Conde Muiño,^{139a,139h} S. H. Connell,^{33c} I. A. Connelly,⁵⁷ S. Constantinescu,^{27b}
 F. Conventi,^{70a,k} A. M. Cooper-Sarkar,¹³⁴ F. Cormier,¹⁷⁴ K. J. R. Cormier,¹⁶⁶ L. D. Corpe,⁹⁵ M. Corradi,^{73a,73b}
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 A. Cueto,⁵ T. Cuhadar Donszelmann,¹⁷⁰ H. Cui,^{15a,15d} A. R. Cukierman,¹⁵² W. R. Cunningham,⁵⁷ S. Czekierda,⁸⁵
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 A. Dattagupta,¹³¹ T. Daubney,⁴⁶ S. D'Auria,^{69a,69b} C. David,^{167b} T. Davidek,¹⁴² D. R. Davis,⁴⁹ I. Dawson,¹⁴⁸ K. De,⁸
 R. De Asmundis,^{70a} M. De Beurs,¹²⁰ S. De Castro,^{23b,23a} N. De Groot,¹¹⁹ P. de Jong,¹²⁰ H. De la Torre,¹⁰⁷ A. De Maria,^{15c}
 D. De Pedis,^{73a} A. De Salvo,^{73a} U. De Sanctis,^{74a,74b} M. De Santis,^{74a,74b} A. De Santo,¹⁵⁵ J. B. De Vivie De Regie,⁶⁵
 C. Debenedetti,¹⁴⁵ D. V. Dedovich,⁸⁰ A. M. Deiana,⁴² J. Del Peso,⁹⁹ Y. Delabat Diaz,⁴⁶ D. Delgove,⁶⁵ F. Deliot,¹⁴⁴
 C. M. Delitzsch,⁷ M. Della Pietra,^{70a,70b} D. Della Volpe,⁵⁴ A. Dell'Acqua,³⁶ L. Dell'Asta,^{74a,74b} M. Delmastro,⁵
 C. Delporte,⁶⁵ P. A. Delsart,⁵⁸ D. A. DeMarco,¹⁶⁶ S. Demers,¹⁸² M. Demichev,⁸⁰ G. Demontigny,¹¹⁰ S. P. Denisov,¹²³
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 C. Di Donato,^{70a,70b} A. Di Girolamo,³⁶ G. Di Gregorio,^{72a,72b} B. Di Micco,^{75a,75b} R. Di Nardo,^{75a,75b} K. F. Di Petrillo,⁵⁹
 R. Di Sipio,¹⁶⁶ C. Diaconu,¹⁰² F. A. Dias,¹²⁰ T. Dias Do Vale,^{139a} M. A. Diaz,^{146a} F. G. Diaz Capriles,²⁴ J. Dickinson,¹⁸
 M. Didenko,¹⁶⁵ E. B. Diehl,¹⁰⁶ J. Dietrich,¹⁹ S. Díez Cornell,⁴⁶ C. Diez Pardos,¹⁵⁰ A. Dimitrievska,¹⁸ W. Ding,^{15b}
 J. Dingfelder,²⁴ S. J. Dittmeier,^{61b} F. Dittus,³⁶ F. Djama,¹⁰² T. Djobava,^{158b} J. I. Djuvsland,¹⁷ M. A. B. Do Vale,^{81c}
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 T. Dreyer,⁵³ A. S. Drobac,¹⁶⁹ D. Du,^{60b} T. A. du Pree,¹²⁰ Y. Duan,^{60d} F. Dubinin,¹¹¹ M. Dubovsky,^{28a} A. Dubreuil,⁵⁴
 E. Duchovni,¹⁷⁹ G. Duckeck,¹¹⁴ O. A. Ducu,³⁶ D. Duda,¹¹⁵ A. Dudarev,³⁶ A. C. Dudder,¹⁰⁰ E. M. Duffield,¹⁸ M. D'uffizi,¹⁰¹
 L. Duflot,⁶⁵ M. Dührssen,³⁶ C. Dülsen,¹⁸¹ M. Dumancic,¹⁷⁹ A. E. Dumitriu,^{27b} M. Dunford,^{61a} A. Duperrin,¹⁰²
 H. Duran Yildiz,^{4a} M. Düren,⁵⁶ A. Durglishvili,^{158b} D. Duschinger,⁴⁸ B. Dutta,⁴⁶ D. Duvnjak,¹ G. I. Dyckes,¹³⁶ M. Dyndal,³⁶
 S. Dysch,¹⁰¹ B. S. Dziedzic,⁸⁵ M. G. Eggleston,⁴⁹ T. Eifert,⁸ G. Eigen,¹⁷ K. Einsweiler,¹⁸ T. Ekelof,¹⁷¹ H. El Jarrari,^{35e}

V. Ellajosyula,¹⁷¹ M. Ellert,¹⁷¹ F. Ellinghaus,¹⁸¹ A. A. Elliot,⁹³ N. Ellis,³⁶ J. Elmsheuser,²⁹ M. Elsing,³⁶ D. Emelianov,¹⁴³ A. Emerman,³⁹ Y. Enari,¹⁶² M. B. Epland,⁴⁹ J. Erdmann,⁴⁷ A. Ereditato,²⁰ P. A. Erland,⁸⁵ M. Errenst,¹⁸¹ M. Escalier,⁶⁵ C. Escobar,¹⁷³ O. Estrada Pastor,¹⁷³ E. Etzion,¹⁶⁰ H. Evans,⁶⁶ M. O. Evans,¹⁵⁵ A. Ezhilov,¹³⁷ F. Fabbri,⁵⁷ L. Fabbri,^{23b,23a} V. Fabiani,¹¹⁹ G. Facini,¹⁷⁷ R. M. Fakhruddinov,¹²³ S. Falciano,^{73a} P. J. Falke,²⁴ S. Falke,³⁶ J. Faltova,¹⁴² Y. Fang,^{15a} Y. Fang,^{15a} G. Fanourakis,⁴⁴ M. Fanti,^{69a,69b} M. Faraj,^{67a,67c,m} A. Farbin,⁸ A. Farilla,^{75a} E. M. Farina,^{71a,71b} T. Farooque,¹⁰⁷ S. M. Farrington,⁵⁰ P. Farthouat,³⁶ F. Fassi,^{35e} P. Fassnacht,³⁶ D. Fassouliotis,⁹ M. Faucci Giannelli,⁵⁰ W. J. Fawcett,³² L. Fayard,⁶⁵ O. L. Fedin,^{137,n} W. Fedorko,¹⁷⁴ A. Fehr,²⁰ M. Feickert,¹⁷² L. Feligioni,¹⁰² A. Fell,¹⁴⁸ C. Feng,^{60b} M. Feng,⁴⁹ M. J. Fenton,¹⁷⁰ A. B. Fenyuk,¹²³ S. W. Ferguson,⁴³ J. Ferrando,⁴⁶ A. Ferrante,¹⁷² A. Ferrari,¹⁷¹ P. Ferrari,¹²⁰ R. Ferrari,^{71a} D. E. Ferreira de Lima,^{61b} A. Ferrer,¹⁷³ D. Ferrere,⁵⁴ C. Ferretti,¹⁰⁶ F. Fiedler,¹⁰⁰ A. Filipčič,⁹² F. Filthaut,¹¹⁹ K. D. Finelli,²⁵ M. C. N. Fiolhais,^{139a,139c,o} L. Fiorini,¹⁷³ F. Fischer,¹¹⁴ J. Fischer,¹⁰⁰ W. C. Fisher,¹⁰⁷ T. Fitschen,²¹ I. Fleck,¹⁵⁰ P. Fleischmann,¹⁰⁶ T. Flick,¹⁸¹ B. M. Flierl,¹¹⁴ L. Flores,¹³⁶ L. R. Flores Castillo,^{63a} F. M. Follega,^{76a,76b} N. Fomin,¹⁷ J. H. Foo,¹⁶⁶ G. T. Forcolin,^{76a,76b} B. C. Forland,⁶⁶ A. Formica,¹⁴⁴ F. A. Förster,¹⁴ A. C. Forti,¹⁰¹ E. Fortin,¹⁰² M. G. Foti,¹³⁴ D. Fournier,⁶⁵ H. Fox,⁹⁰ P. Francavilla,^{72a,72b} S. Francescato,^{73a,73b} M. Franchini,^{23b,23a} S. Franchino,^{61a} D. Francis,³⁶ L. Franco,⁵ L. Franconi,²⁰ M. Franklin,⁵⁹ G. Frattari,^{73a,73b} A. N. Fray,⁹³ P. M. Freeman,²¹ B. Freund,¹¹⁰ W. S. Freund,^{81b} E. M. Freundlich,⁴⁷ D. C. Frizzell,¹²⁸ D. Froidevaux,³⁶ J. A. Frost,¹³⁴ M. Fujimoto,¹²⁶ C. Fukunaga,¹⁶³ E. Fullana Torregrosa,¹⁷³ T. Fusayasu,¹¹⁶ J. Fuster,¹⁷³ A. Gabrielli,^{23b,23a} A. Gabrielli,³⁶ S. Gadatsch,⁵⁴ P. Gadow,¹¹⁵ G. Gagliardi,^{55b,55a} L. G. Gagnon,¹¹⁰ G. E. Gallardo,¹³⁴ E. J. Gallas,¹³⁴ B. J. Gallop,¹⁴³ R. Gamboa Goni,⁹³ K. K. Gan,¹²⁷ S. Ganguly,¹⁷⁹ J. Gao,^{60a} Y. Gao,⁵⁰ Y. S. Gao,^{31,p} F. M. Garay Walls,^{146a} C. García,¹⁷³ J. E. García Navarro,¹⁷³ J. A. García Pascual,^{15a} C. Garcia-Argos,⁵² M. Garcia-Sciveres,¹⁸ R. W. Gardner,³⁷ N. Garelli,¹⁵² S. Gargiulo,⁵² C. A. Garner,¹⁶⁶ V. Garonne,¹³³ S. J. Gasiorowski,¹⁴⁷ P. Gaspar,^{81b} A. Gaudiello,^{55b,55a} G. Gaudio,^{71a} I. L. Gavrilenko,¹¹¹ A. Gavriluk,¹²⁴ C. Gay,¹⁷⁴ G. Gaycken,⁴⁶ E. N. Gazis,¹⁰ A. A. Geanta,^{27b} C. M. Gee,¹⁴⁵ C. N. P. Gee,¹⁴³ J. Geisen,⁹⁷ M. Geisen,¹⁰⁰ C. Gemme,^{55b} M. H. Genest,⁵⁸ C. Geng,¹⁰⁶ S. Gentile,^{73a,73b} S. George,⁹⁴ T. Gerialis,⁴⁴ L. O. Gerlach,⁵³ P. Gessinger-Befurt,¹⁰⁰ G. Gessner,⁴⁷ S. Ghasemi,¹⁵⁰ M. Ghasemi Bostanabad,¹⁷⁵ M. Ghneimat,¹⁵⁰ A. Ghosh,⁶⁵ A. Ghosh,⁷⁸ B. Giacobbe,^{23b} S. Giagu,^{73a,73b} N. Giangiacomi,^{23b,23a} P. Giannetti,^{72a} A. Giannini,^{70a,70b} G. Giannini,¹⁴ S. M. Gibson,⁹⁴ M. Gignac,¹⁴⁵ D. T. Gil,^{84b} B. J. Gilbert,³⁹ D. Gillberg,³⁴ G. Gilles,¹⁸¹ D. M. Gingrich,^{3,d} M. P. Giordani,^{67a,67c} P. F. Giraud,¹⁴⁴ G. Giugliarelli,^{67a,67c} D. Giugni,^{69a} F. Giuli,^{74a,74b} S. Gkaitatzis,¹⁶¹ I. Gkialas,^{9,q} E. L. Gkoukousis,¹⁴ P. Gkoutoumis,¹⁰ L. K. Gladilin,¹¹³ C. Glasman,⁹⁹ J. Glatzer,¹⁴ P. C. F. Glaysheer,⁴⁶ A. Glazov,⁴⁶ G. R. Gledhill,¹³¹ I. Gnesi,^{41b,r} M. Goblirsch-Kolb,²⁶ D. Godin,¹¹⁰ S. Goldfarb,¹⁰⁵ T. Golling,⁵⁴ D. Golubkov,¹²³ A. Gomes,^{139a,139b} R. Goncalves Gama,⁵³ R. Gonçalo,^{139a,139c} G. Gonella,¹³¹ L. Gonella,²¹ A. Gongadze,⁸⁰ F. Gonnella,²¹ J. L. Gonski,³⁹ S. González de la Hoz,¹⁷³ S. Gonzalez Fernandez,¹⁴ R. Gonzalez Lopez,⁹¹ C. Gonzalez Renteria,¹⁸ R. Gonzalez Suarez,¹⁷¹ S. Gonzalez-Sevilla,⁵⁴ G. R. Gonzalvo Rodriguez,¹⁷³ L. Goossens,³⁶ N. A. Gorasia,²¹ P. A. Gorbounov,¹²⁴ H. A. Gordon,²⁹ B. Gorini,³⁶ E. Gorini,^{68a,68b} A. Gorišek,⁹² A. T. Goshaw,⁴⁹ M. I. Gostkin,⁸⁰ C. A. Gottardo,¹¹⁹ M. Goughri,^{35b} A. G. Goussiou,¹⁴⁷ N. Govender,^{33c} C. Goy,⁵ I. Grabowska-Bold,^{84a} E. C. Graham,⁹¹ J. Gramling,¹⁷⁰ E. Gramstad,¹³³ S. Grancagnolo,¹⁹ M. Grandi,¹⁵⁵ V. Gratchev,¹³⁷ P. M. Gravila,^{27f} F. G. Gravili,^{68a,68b} C. Gray,⁵⁷ H. M. Gray,¹⁸ C. Grefe,²⁴ K. Gregersen,⁹⁷ I. M. Gregor,⁴⁶ P. Grenier,¹⁵² K. Grevtsov,⁴⁶ C. Grieco,¹⁴ N. A. Grieser,¹²⁸ A. A. Grillo,¹⁴⁵ K. Grimm,^{31,s} S. Grinstein,^{14,t} J.-F. Grivaz,⁶⁵ S. Groh,¹⁰⁰ E. Gross,¹⁷⁹ J. Grosse-Knetter,⁵³ Z. J. Grout,⁹⁵ C. Grud,¹⁰⁶ A. Grummer,¹¹⁸ J. C. Grundy,¹³⁴ L. Guan,¹⁰⁶ W. Guan,¹⁸⁰ C. Gubbels,¹⁷⁴ J. Guenther,³⁶ A. Guerguichon,⁶⁵ J. G. R. Guerrero Rojas,¹⁷³ F. Guescini,¹¹⁵ D. Guest,¹⁷⁰ R. Gugel,¹⁰⁰ A. Guida,⁴⁶ T. Guillemin,⁵ S. Guindon,³⁶ U. Gul,⁵⁷ J. Guo,^{60c} W. Guo,¹⁰⁶ Y. Guo,^{60a} Z. Guo,¹⁰² R. Gupta,⁴⁶ S. Gurbuz,^{12c} G. Gustavino,¹²⁸ M. Guth,⁵² P. Gutierrez,¹²⁸ C. Gutschow,⁹⁵ C. Guyot,¹⁴⁴ C. Gwenlan,¹³⁴ C. B. Gwilliam,⁹¹ E. S. Haaland,¹³³ A. Haas,¹²⁵ C. Haber,¹⁸ H. K. Hadavand,⁸ A. Hadeif,^{60a} M. Haleem,¹⁷⁶ J. Haley,¹²⁹ J. J. Hall,¹⁴⁸ G. Halladjian,¹⁰⁷ G. D. Hallewell,¹⁰² K. Hamano,¹⁷⁵ H. Hamdaoui,^{35e} M. Hamer,²⁴ G. N. Hamity,⁵⁰ K. Han,^{60a,u} L. Han,^{60a} S. Han,¹⁸ Y. F. Han,¹⁶⁶ K. Hanagaki,^{82,v} M. Hance,¹⁴⁵ D. M. Handl,¹¹⁴ M. D. Hank,³⁷ R. Hankache,¹³⁵ E. Hansen,⁹⁷ J. B. Hansen,⁴⁰ J. D. Hansen,⁴⁰ M. C. Hansen,²⁴ P. H. Hansen,⁴⁰ E. C. Hanson,¹⁰¹ K. Hara,¹⁶⁸ T. Harenberg,¹⁸¹ S. Harkusha,¹⁰⁸ P. F. Harrison,¹⁷⁷ N. M. Hartman,¹⁵² N. M. Hartmann,¹¹⁴ Y. Hasegawa,¹⁴⁹ A. Hasib,⁵⁰ S. Hassani,¹⁴⁴ S. Haug,²⁰ R. Hauser,¹⁰⁷ L. B. Havener,³⁹ M. Havranek,¹⁴¹ C. M. Hawkes,²¹ R. J. Hawkings,³⁶ S. Hayashida,¹¹⁷ D. Hayden,¹⁰⁷ C. Hayes,¹⁰⁶ R. L. Hayes,¹⁷⁴ C. P. Hays,¹³⁴ J. M. Hays,⁹³ H. S. Hayward,⁹¹ S. J. Haywood,¹⁴³ F. He,^{60a} Y. He,¹⁶⁴ M. P. Heath,⁵⁰ V. Hedberg,⁹⁷ S. Heer,²⁴ A. L. Heggelund,¹³³ C. Heidegger,⁵² K. K. Heidegger,⁵² W. D. Heidorn,⁷⁹ J. Heilman,³⁴ S. Heim,⁴⁶ T. Heim,¹⁸ B. Heinemann,^{46,w} J. J. Heinrich,¹³¹ L. Heinrich,³⁶ J. Hejbal,¹⁴⁰ L. Helary,⁴⁶ A. Held,¹²⁵ S. Hellesund,¹³³ C. M. Helling,¹⁴⁵ S. Hellman,^{45a,45b} C. Helsen,³⁶ R. C. W. Henderson,⁹⁰ Y. Heng,¹⁸⁰ L. Henkelmann,³²

A. M. Henriques Correia,³⁶ H. Herde,²⁶ Y. Hernández Jiménez,^{33e} H. Herr,¹⁰⁰ M. G. Herrmann,¹¹⁴ T. Herrmann,⁴⁸
 G. Herten,⁵² R. Hertenberger,¹¹⁴ L. Hervás,³⁶ T. C. Herwig,¹³⁶ G. G. Hesketh,⁹⁵ N. P. Hessey,^{167a} H. Hibi,⁸³ A. Higashida,¹⁶²
 S. Higashino,⁸² E. Higón-Rodríguez,¹⁷³ K. Hildebrand,³⁷ J. C. Hill,³² K. K. Hill,²⁹ K. H. Hiller,⁴⁶ S. J. Hillier,²¹ M. Hils,⁴⁸
 I. Hinchliffe,¹⁸ F. Hinterkeuser,²⁴ M. Hirose,¹³² S. Hirose,⁵² D. Hirschbuehl,¹⁸¹ B. Hiti,⁹² O. Hladik,¹⁴⁰ D. R. Hlaluku,^{33e}
 J. Hobbs,¹⁵⁴ N. Hod,¹⁷⁹ M. C. Hodgkinson,¹⁴⁸ A. Hoecker,³⁶ D. Hohn,⁵² D. Hohov,⁶⁵ T. Holm,²⁴ T. R. Holmes,³⁷
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 J. Hrivnac,⁶⁵ A. Hrynevich,¹⁰⁹ T. Hryn'ova,⁵ P. J. Hsu,⁶⁴ S.-C. Hsu,¹⁴⁷ Q. Hu,²⁹ S. Hu,^{60c} Y. F. Hu,^{15a,15d,x} D. P. Huang,⁹⁵
 Y. Huang,^{60a} Y. Huang,^{15a} Z. Hubacek,¹⁴¹ F. Hubaut,¹⁰² M. Huebner,²⁴ F. Huegging,²⁴ T. B. Huffman,¹³⁴ M. Huhtinen,³⁶
 R. Hulsken,⁵⁸ R. F. H. Hunter,³⁴ P. Huo,¹⁵⁴ N. Huseynov,^{80,y} J. Huston,¹⁰⁷ J. Huth,⁵⁹ R. Hyneman,¹⁰⁶ S. Hyrych,^{28a}
 G. Iacobucci,⁵⁴ G. Iakovidis,²⁹ I. Ibragimov,¹⁵⁰ L. Iconomidou-Fayard,⁶⁵ P. Iengo,³⁶ R. Ignazzi,⁴⁰ O. Igonkina,^{120,a,z}
 R. Iguchi,¹⁶² T. Iizawa,⁵⁴ Y. Ikegami,⁸² M. Ikeno,⁸² N. Ilic,^{119,166,l} F. Iltzsche,⁴⁸ H. Imam,^{35a} G. Introzzi,^{71a,71b} M. Iodice,^{75a}
 K. Iordanidou,^{167a} V. Ippolito,^{73a,73b} M. F. Isacson,¹⁷¹ M. Ishino,¹⁶² W. Islam,¹²⁹ C. Issever,^{19,46} S. Istin,¹⁵⁹ F. Ito,¹⁶⁸
 J. M. Iturbe Ponce,^{63a} R. Iuppa,^{76a,76b} A. Ivina,¹⁷⁹ H. Iwasaki,⁸² J. M. Izen,⁴³ V. Izzo,^{70a} P. Jacka,¹⁴⁰ P. Jackson,¹
 R. M. Jacobs,⁴⁶ B. P. Jaeger,¹⁵¹ V. Jain,² G. Jäkel,¹⁸¹ K. B. Jakobi,¹⁰⁰ K. Jakobs,⁵² T. Jakoubek,¹⁷⁹ J. Jamieson,⁵⁷
 K. W. Janas,^{84a} R. Jansky,⁵⁴ M. Janus,⁵³ P. A. Janus,^{84a} G. Jarlskog,⁹⁷ A. E. Jaspan,⁹¹ N. Javadov,^{80,y} T. Javůrek,³⁶
 M. Javurkova,¹⁰³ F. Jeanneau,¹⁴⁴ L. Jeanty,¹³¹ J. Jejelava,^{158a} P. Jenni,^{52,aa} N. Jeong,⁴⁶ S. Jézéquel,⁵ H. Ji,¹⁸⁰ J. Jia,¹⁵⁴
 H. Jiang,⁷⁹ Y. Jiang,^{60a} Z. Jiang,¹⁵² S. Jiggins,⁵² F. A. Jimenez Morales,³⁸ J. Jimenez Pena,¹¹⁵ S. Jin,^{15c} A. Jinaru,^{27b}
 O. Jinnouchi,¹⁶⁴ H. Jivan,^{33e} P. Johansson,¹⁴⁸ K. A. Johns,⁷ C. A. Johnson,⁶⁶ R. W. L. Jones,⁹⁰ S. D. Jones,¹⁵⁵ T. J. Jones,⁹¹
 J. Jongmanns,^{61a} J. Jovicevic,³⁶ X. Ju,¹⁸ J. J. Junggeburth,¹¹⁵ A. Juste Rozas,^{14,t} A. Kaczmarska,⁸⁵ M. Kado,^{73a,73b}
 H. Kagan,¹²⁷ M. Kagan,¹⁵² A. Kahn,³⁹ C. Kahra,¹⁰⁰ T. Kaji,¹⁷⁸ E. Kajomovitz,¹⁵⁹ C. W. Kalderon,²⁹ A. Kaluza,¹⁰⁰
 A. Kamenshchikov,¹²³ M. Kaneda,¹⁶² N. J. Kang,¹⁴⁵ S. Kang,⁷⁹ Y. Kano,¹¹⁷ J. Kanzaki,⁸² L. S. Kaplan,¹⁸⁰ D. Kar,^{33e}
 K. Karava,¹³⁴ M. J. Kareem,^{167b} I. Karkanas,¹⁶¹ S. N. Karpov,⁸⁰ Z. M. Karpova,⁸⁰ V. Kartvelishvili,⁹⁰ A. N. Karyukhin,¹²³
 E. Kasimi,¹⁶¹ A. Kastanas,^{45a,45b} C. Kato,^{60d,60c} J. Katzy,⁴⁶ K. Kawade,¹⁴⁹ K. Kawagoe,⁸⁸ T. Kawaguchi,¹¹⁷ T. Kawamoto,¹⁴⁴
 G. Kawamura,⁵³ E. F. Kay,¹⁷⁵ S. Kazakos,¹⁴ V. F. Kazanin,^{122b,122a} R. Keeler,¹⁷⁵ R. Kehoe,⁴² J. S. Keller,³⁴ E. Kellermann,⁹⁷
 D. Kelsey,¹⁵⁵ J. J. Kempster,²¹ J. Kendrick,²¹ K. E. Kennedy,³⁹ O. Kepka,¹⁴⁰ S. Kersten,¹⁸¹ B. P. Kerševan,⁹²
 S. Ketabchi Haghighat,¹⁶⁶ M. Khader,¹⁷² F. Khalil-Zada,¹³ M. Khandoga,¹⁴⁴ A. Khanov,¹²⁹ A. G. Kharlamov,^{122b,122a}
 T. Kharlamova,^{122b,122a} E. E. Khoda,¹⁷⁴ A. Khodinov,¹⁶⁵ T. J. Khoo,⁵⁴ G. Khoriauli,¹⁷⁶ E. Khramov,⁸⁰ J. Khubua,^{158b}
 S. Kido,⁸³ M. Kiehn,³⁶ C. R. Kilby,⁹⁴ E. Kim,¹⁶⁴ Y. K. Kim,³⁷ N. Kimura,⁹⁵ A. Kirchhoff,⁵³ D. Kirchmeier,⁴⁸ J. Kirk,¹⁴³
 A. E. Kiryunin,¹¹⁵ T. Kishimoto,¹⁶² D. P. Kisliuk,¹⁶⁶ V. Kitali,⁴⁶ C. Kitsaki,¹⁰ O. Kivernyk,²⁴ T. Klapdor-Kleingrothaus,⁵²
 M. Klassen,^{61a} C. Klein,³⁴ M. H. Klein,¹⁰⁶ M. Klein,⁹¹ U. Klein,⁹¹ K. Kleinknecht,¹⁰⁰ P. Klimek,¹²¹ A. Klimentov,²⁹
 T. Klingl,²⁴ T. Klioutchnikova,³⁶ F. F. Klitzner,¹¹⁴ P. Kluit,¹²⁰ S. Kluth,¹¹⁵ E. Kneringer,⁷⁷ E. B. F. G. Knoops,¹⁰² A. Knue,⁵²
 D. Kobayashi,⁸⁸ M. Kobel,⁴⁸ M. Kocian,¹⁵² T. Kodama,¹⁶² P. Kodys,¹⁴² D. M. Koeck,¹⁵⁵ P. T. Koenig,²⁴ T. Koffas,³⁴
 N. M. Köhler,³⁶ M. Kolb,¹⁴⁴ I. Koletsou,⁵ T. Komarek,¹³⁰ T. Kondo,⁸² K. Köneke,⁵² A. X. Y. Kong,¹ A. C. König,¹¹⁹
 T. Kono,¹²⁶ V. Konstantinides,⁹⁵ N. Konstantinidis,⁹⁵ B. Konya,⁹⁷ R. Kopeliansky,⁶⁶ S. Koperny,^{84a} K. Korcyl,⁸⁵
 K. Kordas,¹⁶¹ G. Koren,¹⁶⁰ A. Korn,⁹⁵ I. Korolkov,¹⁴ E. V. Korolkova,¹⁴⁸ N. Korotkova,¹¹³ O. Kortner,¹¹⁵ S. Kortner,¹¹⁵
 V. V. Kostyukhin,^{148,165} A. Kotskechagia,⁶⁵ A. Kotwal,⁴⁹ A. Koulouris,¹⁰ A. Kourkoumeli-Charalampidi,^{71a,71b}
 C. Kourkoumelis,⁹ E. Kourlitis,⁶ V. Kouskoura,²⁹ R. Kowalewski,¹⁷⁵ W. Kozanecki,¹⁰¹ A. S. Kozhin,¹²³
 V. A. Kramarenko,¹¹³ G. Kramberger,⁹² D. Krasnopevtsev,^{60a} M. W. Krasny,¹³⁵ A. Krasznahorkay,³⁶ D. Krauss,¹¹⁵
 J. A. Kremer,¹⁰⁰ J. Kretschmar,⁹¹ P. Krieger,¹⁶⁶ F. Krieter,¹¹⁴ A. Krishnan,^{61b} M. Krivos,¹⁴² K. Krizka,¹⁸ K. Kroeninger,⁴⁷
 H. Kroha,¹¹⁵ J. Kroll,¹⁴⁰ J. Kroll,¹³⁶ K. S. Krowpman,¹⁰⁷ U. Kruchonak,⁸⁰ H. Krüger,²⁴ N. Krumnack,⁷⁹ M. C. Kruse,⁴⁹
 J. A. Krzysiak,⁸⁵ A. Kubota,¹⁶⁴ O. Kuchinskaia,¹⁶⁵ S. Kuday,^{4b} J. T. Kuechler,⁴⁶ S. Kuehn,³⁶ T. Kuhl,⁴⁶ V. Kukhtin,⁸⁰
 Y. Kulchitsky,^{108,bb} S. Kuleshov,^{146b} Y. P. Kulinich,¹⁷² M. Kuna,⁵⁸ T. Kunigo,⁸⁶ A. Kupco,¹⁴⁰ T. Kupfer,⁴⁷ O. Kuprash,⁵²
 H. Kurashige,⁸³ L. L. Kurchaninov,^{167a} Y. A. Kurochkin,¹⁰⁸ A. Kurova,¹¹² M. G. Kurth,^{15a,15d} E. S. Kuwertz,³⁶ M. Kuze,¹⁶⁴
 A. K. Kvam,¹⁴⁷ J. Kvita,¹³⁰ T. Kwan,¹⁰⁴ F. La Ruffa,^{41b,41a} C. Lacasta,¹⁷³ F. Lacava,^{73a,73b} D. P. J. Lack,¹⁰¹ H. Lacker,¹⁹
 D. Lacour,¹³⁵ E. Ladygin,⁸⁰ R. Lafaye,⁵ B. Laforge,¹³⁵ T. Lagouri,^{146c} S. Lai,⁵³ I. K. Lakomic,^{84a} J. E. Lambert,¹²⁸
 S. Lammers,⁶⁶ W. Lampl,⁷ C. Lampoudis,¹⁶¹ E. Lançon,²⁹ U. Landgraf,⁵² M. P. J. Landon,⁹³ M. C. Lanfermann,⁵⁴
 V. S. Lang,⁵² J. C. Lange,⁵³ R. J. Langenberg,¹⁰³ A. J. Lankford,¹⁷⁰ F. Lanni,²⁹ K. Lantzsck,²⁴ A. Lanza,^{71a}
 A. Lapertosa,^{55b,55a} J. F. Laporte,¹⁴⁴ T. Lari,^{69a} F. Lasagni Manghi,^{23b,23a} M. Lassnig,³⁶ T. S. Lau,^{63a} A. Laudrain,⁶⁵

A. Laurier,³⁴ M. Lavorgna,^{70a,70b} S. D. Lawlor,⁹⁴ M. Lazzaroni,^{69a,69b} B. Le,¹⁰¹ E. Le Guirriec,¹⁰² A. Lebedev,⁷⁹ M. LeBlanc,⁷ T. LeCompte,⁶ F. Ledroit-Guillon,⁵⁸ A. C. A. Lee,⁹⁵ C. A. Lee,²⁹ G. R. Lee,¹⁷ L. Lee,⁵⁹ S. C. Lee,¹⁵⁷ S. Lee,⁷⁹ B. Lefebvre,^{167a} H. P. Lefebvre,⁹⁴ M. Lefebvre,¹⁷⁵ C. Leggett,¹⁸ K. Lehmann,¹⁵¹ N. Lehmann,²⁰ G. Lehmann Miotto,³⁶ W. A. Leight,⁴⁶ A. Leisos,^{161,cc} M. A. L. Leite,^{81d} C. E. Leitgeb,¹¹⁴ R. Leitner,¹⁴² D. Lellouch,^{179,a} K. J. C. Leney,⁴² T. Lenz,²⁴ S. Leone,^{72a} C. Leonidopoulos,⁵⁰ A. Leopold,¹³⁵ C. Leroy,¹¹⁰ R. Les,¹⁰⁷ C. G. Lester,³² M. Levchenko,¹³⁷ J. Levêque,⁵ D. Levin,¹⁰⁶ L. J. Levinson,¹⁷⁹ D. J. Lewis,²¹ B. Li,^{15b} B. Li,¹⁰⁶ C-Q. Li,^{60a} F. Li,^{60c} H. Li,^{60a} H. Li,^{60b} J. Li,^{60c} K. Li,¹⁴⁷ L. Li,^{60c} M. Li,^{15a,15d} Q. Li,^{15a,15d} Q. Y. Li,^{60a} S. Li,^{60d,60c} X. Li,⁴⁶ Y. Li,⁴⁶ Z. Li,^{60b} Z. Li,¹³⁴ Z. Li,¹⁰⁴ Z. Liang,^{15a} M. Liberatore,⁴⁶ B. Liberti,^{74a} A. Liblong,¹⁶⁶ K. Lie,^{63c} S. Lim,²⁹ C. Y. Lin,³² K. Lin,¹⁰⁷ R. A. Linck,⁶⁶ R. E. Lindley,⁷ J. H. Lindon,²¹ A. Linss,⁴⁶ A. L. Lioni,⁵⁴ E. Lipeles,¹³⁶ A. Lipniacka,¹⁷ T. M. Liss,^{172,dd} A. Lister,¹⁷⁴ J. D. Little,⁸ B. Liu,⁷⁹ B. L. Liu,⁶ H. B. Liu,²⁹ J. B. Liu,^{60a} J. K. K. Liu,³⁷ K. Liu,^{60d} M. Liu,^{60a} P. Liu,^{15a} X. Liu,^{60a} Y. Liu,⁴⁶ Y. Liu,^{15a,15d} Y. L. Liu,¹⁰⁶ Y. W. Liu,^{60a} M. Livan,^{71a,71b} A. Lleres,⁵⁸ J. Llorente Merino,¹⁵¹ S. L. Lloyd,⁹³ C. Y. Lo,^{63b} E. M. Lobodzinska,⁴⁶ P. Loch,⁷ S. Loffredo,^{74a,74b} T. Lohse,¹⁹ K. Lohwasser,¹⁴⁸ M. Lokajicek,¹⁴⁰ J. D. Long,¹⁷² R. E. Long,⁹⁰ I. Longarini,^{73a,73b} L. Longo,³⁶ K. A. Looper,¹²⁷ I. Lopez Paz,¹⁰¹ A. Lopez Solis,¹⁴⁸ J. Lorenz,¹¹⁴ N. Lorenzo Martinez,⁵ A. M. Lory,¹¹⁴ P. J. Lösel,¹¹⁴ A. Lösle,⁵² X. Lou,⁴⁶ X. Lou,^{15a} A. Lounis,⁶⁵ J. Love,⁶ P. A. Love,⁹⁰ J. J. Lozano Bahilo,¹⁷³ M. Lu,^{60a} Y. J. Lu,⁶⁴ H. J. Lubatti,¹⁴⁷ C. Luci,^{73a,73b} F. L. Lucio Alves,^{15c} A. Lucotte,⁵⁸ F. Luehring,⁶⁶ I. Luise,¹³⁵ L. Luminari,^{73a} B. Lund-Jensen,¹⁵³ M. S. Lutz,¹⁶⁰ D. Lynn,²⁹ H. Lyons,⁹¹ R. Lysak,¹⁴⁰ E. Lytken,⁹⁷ F. Lyu,^{15a} V. Lyubushkin,⁸⁰ T. Lyubushkina,⁸⁰ H. Ma,²⁹ L. L. Ma,^{60b} Y. Ma,⁹⁵ D. M. Mac Donell,¹⁷⁵ G. Maccarrone,⁵¹ A. Macchiolo,¹¹⁵ C. M. Macdonald,¹⁴⁸ J. C. Macdonald,¹⁴⁸ J. Machado Miguens,¹³⁶ D. Madaffari,¹⁷³ R. Madar,³⁸ W. F. Mader,⁴⁸ M. Madugoda Ralalage Don,¹²⁹ N. Madysa,⁴⁸ J. Maeda,⁸³ T. Maeno,²⁹ M. Maerker,⁴⁸ V. Magerl,⁵² N. Magini,⁷⁹ J. Magro,^{67a,67c,m} D. J. Mahon,³⁹ C. Maidantchik,^{81b} T. Maier,¹¹⁴ A. Maio,^{139a,139b,139d} K. Maj,^{84a} O. Majersky,^{28a} S. Majewski,¹³¹ Y. Makida,⁸² N. Makovec,⁶⁵ B. Malaescu,¹³⁵ Pa. Malecki,⁸⁵ V. P. Maleev,¹³⁷ F. Malek,⁵⁸ D. Malito,^{41b,41a} U. Mallik,⁷⁸ D. Malon,⁶ C. Malone,³² S. Maltezos,¹⁰ S. Malyukov,⁸⁰ J. Mamuzic,¹⁷³ G. Mancini,^{70a,70b} I. Mandić,⁹² L. Manhaes de Andrade Filho,^{81a} I. M. Maniatis,¹⁶¹ J. Manjarres Ramos,⁴⁸ K. H. Mankinen,⁹⁷ A. Mann,¹¹⁴ A. Manousos,⁷⁷ B. Mansoulie,¹⁴⁴ I. Manthos,¹⁶¹ S. Manzoni,¹²⁰ A. Marantis,¹⁶¹ G. Marceca,³⁰ L. Marchese,¹³⁴ G. Marchiori,¹³⁵ M. Marcisovsky,¹⁴⁰ L. Marcoccia,^{74a,74b} C. Marcon,⁹⁷ C. A. Marin Tobon,³⁶ M. Marjanovic,¹²⁸ Z. Marshall,¹⁸ M. U. F. Martensson,¹⁷¹ S. Marti-Garcia,¹⁷³ C. B. Martin,¹²⁷ T. A. Martin,¹⁷⁷ V. J. Martin,⁵⁰ B. Martin dit Latour,¹⁷ L. Martinelli,^{75a,75b} M. Martinez,^{14,t} P. Martinez Agullo,¹⁷³ V. I. Martinez Outschoorn,¹⁰³ S. Martin-Haugh,¹⁴³ V. S. Martoiu,^{27b} A. C. Martyniuk,⁹⁵ A. Marzin,³⁶ S. R. Maschek,¹¹⁵ L. Masetti,¹⁰⁰ T. Mashimo,¹⁶² R. Mashinistov,¹¹¹ J. Masik,¹⁰¹ A. L. Maslennikov,^{122b,122a} L. Massa,^{23b,23a} P. Massarotti,^{70a,70b} P. Mastrandrea,^{72a,72b} A. Mastroberardino,^{41b,41a} T. Masubuchi,¹⁶² D. Matakias,²⁹ A. Matic,¹¹⁴ N. Matsuzawa,¹⁶² P. Mättig,²⁴ J. Maurer,^{27b} B. Maček,⁹² D. A. Maximov,^{122b,122a} R. Mazini,¹⁵⁷ I. Maznas,¹⁶¹ S. M. Mazza,¹⁴⁵ J. P. Mc Gowan,¹⁰⁴ S. P. Mc Kee,¹⁰⁶ T. G. McCarthy,¹¹⁵ W. P. McCormack,¹⁸ E. F. McDonald,¹⁰⁵ J. A. Mcfayden,³⁶ G. Mchedlidze,^{158b} M. A. McKay,⁴² K. D. McLean,¹⁷⁵ S. J. McMahon,¹⁴³ P. C. McNamara,¹⁰⁵ C. J. McNicol,¹⁷⁷ R. A. McPherson,^{175,1} J. E. Mdhului,^{33e} Z. A. Meadows,¹⁰³ S. Meehan,³⁶ T. Megy,³⁸ S. Mehlhase,¹¹⁴ A. Mehta,⁹¹ B. Meirose,⁴³ D. Melini,¹⁵⁹ B. R. Mellado Garcia,^{33e} J. D. Mellenthin,⁵³ M. Melo,^{28a} F. Meloni,⁴⁶ A. Melzer,²⁴ E. D. Mendes Gouveia,^{139a,139e} L. Meng,³⁶ X. T. Meng,¹⁰⁶ S. Menke,¹¹⁵ E. Meoni,^{41b,41a} S. Mergelmeyer,¹⁹ S. A. M. Merkt,¹³⁸ C. Merlassino,¹³⁴ P. Mermod,⁵⁴ L. Merola,^{70a,70b} C. Meroni,^{69a} G. Merz,¹⁰⁶ O. Meshkov,^{113,111} J. K. R. Meshreki,¹⁵⁰ J. Metcalfe,⁶ A. S. Mete,⁶ C. Meyer,⁶⁶ J-P. Meyer,¹⁴⁴ M. Michetti,¹⁹ R. P. Middleton,¹⁴³ L. Mijović,⁵⁰ G. Mikenberg,¹⁷⁹ M. Mikestikova,¹⁴⁰ M. Mikuž,⁹² H. Mildner,¹⁴⁸ A. Milic,¹⁶⁶ C. D. Milke,⁴² D. W. Miller,³⁷ A. Milov,¹⁷⁹ D. A. Milstead,^{45a,45b} R. A. Mina,¹⁵² A. A. Minaenko,¹²³ I. A. Minashvili,^{158b} A. I. Mincer,¹²⁵ B. Mindur,^{84a} M. Mineev,⁸⁰ Y. Minegishi,¹⁶² L. M. Mir,¹⁴ M. Miralles Lopez,¹⁷³ M. Mironova,¹³⁴ A. Mirto,^{68a,68b} K. P. Mistry,¹³⁶ T. Mitani,¹⁷⁸ J. Mitrevski,¹¹⁴ V. A. Mitsou,¹⁷³ M. Mittal,^{60c} O. Miu,¹⁶⁶ A. Miucci,²⁰ P. S. Miyagawa,⁹³ A. Mizukami,⁸² J. U. Mjörnmark,⁹⁷ T. Mkrtychyan,^{61a} M. Mlynarikova,¹⁴² T. Moa,^{45a,45b} S. Mobius,⁵³ K. Mochizuki,¹¹⁰ P. Mogg,¹¹⁴ S. Mohapatra,³⁹ R. Moles-Valls,²⁴ K. Mönig,⁴⁶ E. Monnier,¹⁰² A. Montalbano,¹⁵¹ J. Montejo Berlingen,³⁶ M. Montella,⁹⁵ F. Monticelli,⁸⁹ S. Monzani,^{69a} N. Morange,⁶⁵ A. L. Moreira De Carvalho,^{139a} D. Moreno,^{22a} M. Moreno Llácer,¹⁷³ C. Moreno Martinez,¹⁴ P. Morettini,^{55b} M. Morgenstern,¹⁵⁹ S. Morgenstern,⁴⁸ D. Mori,¹⁵¹ M. Morii,⁵⁹ M. Morinaga,¹⁷⁸ V. Morisbak,¹³³ A. K. Morley,³⁶ G. Mornacchi,³⁶ A. P. Morris,⁹⁵ L. Morvaj,¹⁵⁴ P. Moschovakos,³⁶ B. Moser,¹²⁰ M. Mosidze,^{158b} T. Moskalets,¹⁴⁴ J. Moss,^{31,ee} E. J. W. Moyse,¹⁰³ S. Muanza,¹⁰² J. Mueller,¹³⁸ R. S. P. Mueller,¹¹⁴ D. Muenstermann,⁹⁰ G. A. Mullier,⁹⁷ D. P. Mungo,^{69a,69b} J. L. Munoz Martinez,¹⁴ F. J. Munoz Sanchez,¹⁰¹ P. Murin,^{28b} W. J. Murray,^{177,143} A. Murrone,^{69a,69b} J. M. Muse,¹²⁸ M. Muškinja,¹⁸ C. Mwewa,^{33a}

A. G. Myagkov,^{123,i} A. A. Myers,¹³⁸ G. Myers,⁶⁶ J. Myers,¹³¹ M. Myska,¹⁴¹ B. P. Nachman,¹⁸ O. Nackenhörst,⁴⁷
 A. Nag Nag,⁴⁸ K. Nagai,¹³⁴ K. Nagano,⁸² Y. Nagasaka,⁶² J. L. Nagle,²⁹ E. Nagy,¹⁰² A. M. Nairz,³⁶ Y. Nakahama,¹¹⁷
 K. Nakamura,⁸² T. Nakamura,¹⁶² H. Nanjo,¹³² F. Napolitano,^{61a} R. F. Naranjo Garcia,⁴⁶ R. Narayan,⁴² I. Naryshkin,¹³⁷
 T. Naumann,⁴⁶ G. Navarro,^{22a} P. Y. Nechaeva,¹¹¹ F. Nechansky,⁴⁶ T. J. Neep,²¹ A. Negri,^{71a,71b} M. Negrini,^{23b} C. Nellist,¹¹⁹
 C. Nelson,¹⁰⁴ M. E. Nelson,^{45a,45b} S. Nemecek,¹⁴⁰ M. Nessi,^{36,ff} M. S. Neubauer,¹⁷² F. Neuhaus,¹⁰⁰ M. Neumann,¹⁸¹
 R. Newhouse,¹⁷⁴ P. R. Newman,²¹ C. W. Ng,¹³⁸ Y. S. Ng,¹⁹ Y. W. Y. Ng,¹⁷⁰ B. Ngair,^{35e} H. D. N. Nguyen,¹⁰²
 T. Nguyen Manh,¹¹⁰ E. Nibigira,³⁸ R. B. Nickerson,¹³⁴ R. Nicolaidou,¹⁴⁴ D. S. Nielsen,⁴⁰ J. Nielsen,¹⁴⁵ M. Niemeyer,⁵³
 N. Nikiforou,¹¹ V. Nikolaenko,^{123,i} I. Nikolic-Audit,¹³⁵ K. Nikolopoulos,²¹ P. Nilsson,²⁹ H. R. Nindhito,⁵⁴ Y. Ninomiya,⁸²
 A. Nisati,^{73a} N. Nishu,^{60c} R. Nisius,¹¹⁵ I. Nitsche,⁴⁷ T. Nitta,¹⁷⁸ T. Nobe,¹⁶² D. L. Noel,³² Y. Noguchi,⁸⁶ I. Nomidis,¹³⁵
 M. A. Nomura,²⁹ M. Nordberg,³⁶ J. Novak,⁹² T. Novak,⁹² O. Novgorodova,⁴⁸ R. Novotny,¹⁴¹ L. Nozka,¹³⁰ K. Ntekas,¹⁷⁰
 E. Nurse,⁹⁵ F. G. Oakham,^{34,d} H. Oberlack,¹¹⁵ J. Ocariz,¹³⁵ A. Ochi,⁸³ I. Ochoa,³⁹ J. P. Ochoa-Ricoux,^{146a} K. O'Connor,²⁶
 S. Oda,⁸⁸ S. Odaka,⁸² S. Oerdek,⁵³ A. Ogrodnik,^{84a} A. Oh,¹⁰¹ C. C. Ohm,¹⁵³ H. Oide,¹⁶⁴ M. L. Ojeda,¹⁶⁶ H. Okawa,¹⁶⁸
 Y. Okazaki,⁸⁶ M. W. O'Keefe,⁹¹ Y. Okumura,¹⁶² T. Okuyama,⁸² A. Olariu,^{27b} L. F. Oleiro Seabra,^{139a} S. A. Olivares Pino,^{146a}
 D. Oliveira Damazio,²⁹ J. L. Oliver,¹ M. J. R. Olsson,¹⁷⁰ A. Olszewski,⁸⁵ J. Olszowska,⁸⁵ Ö. O. Öncel,²⁴ D. C. O'Neil,¹⁵¹
 A. P. O'Neill,¹³⁴ A. Onofre,^{139a,139e} P. U. E. Onyisi,¹¹ H. Oppen,¹³³ R. G. Oreamuno Madriz,¹²¹ M. J. Oreglia,³⁷
 G. E. Orellana,⁸⁹ D. Orestano,^{75a,75b} N. Orlando,¹⁴ R. S. Orr,¹⁶⁶ V. O'Shea,⁵⁷ R. Ospanov,^{60a} G. Otero y Garzon,³⁰
 H. Otono,⁸⁸ P. S. Ott,^{61a} G. J. Ottino,¹⁸ M. Ouchrif,^{35d} J. Ouellette,²⁹ F. Ould-Saada,¹³³ A. Ouraou,¹⁴⁴ Q. Ouyang,^{15a}
 M. Owen,⁵⁷ R. E. Owen,¹⁴³ V. E. Ozcan,^{12c} N. Ozturk,⁸ J. Pacalt,¹³⁰ H. A. Pacey,³² K. Pachal,⁴⁹ A. Pacheco Pages,¹⁴
 C. Padilla Aranda,¹⁴ S. Pagan Griso,¹⁸ G. Palacino,⁶⁶ S. Palazzo,⁵⁰ S. Palestini,³⁶ M. Palka,^{84b} P. Palni,^{84a} C. E. Pandini,⁵⁴
 J. G. Panduro Vazquez,⁹⁴ P. Pani,⁴⁶ G. Panizzo,^{67a,67c} L. Paolozzi,⁵⁴ C. Papadatos,¹¹⁰ K. Papageorgiou,^{9,q} S. Parajuli,⁴²
 A. Paramonov,⁶ C. Paraskevopoulos,¹⁰ D. Paredes Hernandez,^{63b} S. R. Paredes Saenz,¹³⁴ B. Parida,¹⁷⁹ T. H. Park,¹⁶⁶
 A. J. Parker,³¹ M. A. Parker,³² F. Parodi,^{55b,55a} E. W. Parrish,¹²¹ J. A. Parsons,³⁹ U. Parzefall,⁵² L. Pascual Dominguez,¹³⁵
 V. R. Pascuzzi,¹⁸ J. M. P. Pasner,¹⁴⁵ F. Pasquali,¹²⁰ E. Pasqualucci,^{73a} S. Passaggio,^{55b} F. Pastore,⁹⁴ P. Pasuwan,^{45a,45b}
 S. Patariaia,¹⁰⁰ J. R. Pater,¹⁰¹ A. Pathak,^{180,e} J. Patton,⁹¹ T. Pauly,³⁶ J. Pearkes,¹⁵² B. Pearson,¹¹⁵ M. Pedersen,¹³³
 L. Pedraza Diaz,¹¹⁹ R. Pedro,^{139a} T. Peiffer,⁵³ S. V. Peleganchuk,^{122b,122a} O. Penc,¹⁴⁰ H. Peng,^{60a} B. S. Peralva,^{81a}
 M. M. Perego,⁶⁵ A. P. Pereira Peixoto,^{139a} L. Pereira Sanchez,^{45a,45b} D. V. Perepelitsa,²⁹ E. Perez Codina,^{167a} F. Peri,¹⁹
 L. Perini,^{69a,69b} H. Pernegger,³⁶ S. Perrella,³⁶ A. Perrevoort,¹²⁰ K. Peters,⁴⁶ R. F. Y. Peters,¹⁰¹ B. A. Petersen,³⁶
 T. C. Petersen,⁴⁰ E. Petit,¹⁰² V. Petousis,¹⁴¹ A. Petridis,¹ C. Petridou,¹⁶¹ P. Petroff,⁶⁵ F. Petrucci,^{75a,75b} M. Pettee,¹⁸²
 N. E. Pettersson,¹⁰³ K. Petukhova,¹⁴² A. Peyaud,¹⁴⁴ R. Pezoa,^{146d} L. Pezzotti,^{71a,71b} T. Pham,¹⁰⁵ F. H. Phillips,¹⁰⁷
 P. W. Phillips,¹⁴³ M. W. Phipps,¹⁷² G. Piacquadio,¹⁵⁴ E. Pianori,¹⁸ A. Picazio,¹⁰³ R. H. Pickles,¹⁰¹ R. Piegaiia,³⁰
 D. Pietreanu,^{27b} J. E. Pilcher,³⁷ A. D. Pilkington,¹⁰¹ M. Pinamonti,^{67a,67c} J. L. Pinfold,³ C. Pitman Donaldson,⁹⁵ M. Pitt,¹⁶⁰
 L. Pizzimento,^{74a,74b} A. Pizzini,¹²⁰ M.-A. Pleier,²⁹ V. Plesanovs,⁵² V. Pleskot,¹⁴² E. Plotnikova,⁸⁰ P. Podberezko,^{122b,122a}
 R. Poettgen,⁹⁷ R. Poggi,⁵⁴ L. Poggioli,¹³⁵ I. Pogrebnyak,¹⁰⁷ D. Pohl,²⁴ I. Pokharel,⁵³ G. Polesello,^{71a} A. Poley,^{151,167a}
 A. Policicchio,^{73a,73b} R. Polifka,¹⁴² A. Polini,^{23b} C. S. Pollard,⁴⁶ V. Polychronakos,²⁹ D. Ponomarenko,¹¹² L. Pontecorvo,³⁶
 S. Popa,^{27a} G. A. Popeneciu,^{27d} L. Portales,⁵ D. M. Portillo Quintero,⁵⁸ S. Pospisil,¹⁴¹ K. Potamianos,⁴⁶ I. N. Potrap,⁸⁰
 C. J. Potter,³² H. Potti,¹¹ T. Poulsen,⁹⁷ J. Poveda,¹⁷³ T. D. Powell,¹⁴⁸ G. Pownall,⁴⁶ M. E. Pozo Astigarraga,³⁶ P. Pralavorio,¹⁰²
 S. Prell,⁷⁹ D. Price,¹⁰¹ M. Primavera,^{68a} M. L. Proffitt,¹⁴⁷ N. Proklova,¹¹² K. Prokofiev,^{63c} F. Prokoshin,⁸⁰ S. Protopopescu,²⁹
 J. Proudfoot,⁶ M. Przybycien,^{84a} D. Pudzha,¹³⁷ A. Puri,¹⁷² P. Puzo,⁶⁵ D. Pyatizbyantseva,¹¹² J. Qian,¹⁰⁶ Y. Qin,¹⁰¹
 A. Quadt,⁵³ M. Queitsch-Maitland,³⁶ M. Racko,^{28a} F. Ragusa,^{69a,69b} G. Rahal,⁹⁸ J. A. Raine,⁵⁴ S. Rajagopalan,²⁹
 A. Ramirez Morales,⁹³ K. Ran,^{15a,15d} D. M. Rauch,⁴⁶ F. Rauscher,¹¹⁴ S. Rave,¹⁰⁰ B. Ravina,¹⁴⁸ I. Ravinovich,¹⁷⁹
 J. H. Rawling,¹⁰¹ M. Raymond,³⁶ A. L. Read,¹³³ N. P. Readioff,¹⁴⁸ M. Reale,^{68a,68b} D. M. Rebuffi,^{71a,71b} G. Redlinger,²⁹
 K. Reeves,⁴³ J. Reichert,¹³⁶ D. Reikher,¹⁶⁰ A. Reiss,¹⁰⁰ A. Rej,¹⁵⁰ C. Rembser,³⁶ A. Renardi,⁴⁶ M. Renda,^{27b} M. B. Rendel,¹¹⁵
 A. G. Rennie,⁵⁷ S. Resconi,^{69a} E. D. Resseguie,¹⁸ S. Rettie,⁹⁵ B. Reynolds,¹²⁷ E. Reynolds,²¹ O. L. Rezanova,^{122b,122a}
 P. Reznicek,¹⁴² E. Ricci,^{76a,76b} R. Richter,¹¹⁵ S. Richter,⁴⁶ E. Richter-Was,^{84b} M. Ridel,¹³⁵ P. Rieck,¹¹⁵ O. Rifki,⁴⁶
 M. Rijssenbeek,¹⁵⁴ A. Rimoldi,^{71a,71b} M. Rimoldi,⁴⁶ L. Rinaldi,^{23b} T. T. Rinn,¹⁷² G. Ripellino,¹⁵³ I. Riu,¹⁴ P. Rivadeneira,⁴⁶
 J. C. Rivera Vergara,¹⁷⁵ F. Rizatdinova,¹²⁹ E. Rizvi,⁹³ C. Rizzi,³⁶ B. R. Roberts,¹⁸ S. H. Robertson,^{104,l} M. Robin,⁴⁶
 D. Robinson,³² C. M. Robles Gajardo,^{146d} M. Robles Manzano,¹⁰⁰ A. Robson,⁵⁷ A. Rocchi,^{74a,74b} E. Rocco,¹⁰⁰
 C. Roda,^{72a,72b} S. Rodriguez Bosca,¹⁷³ A. M. Rodríguez Vera,^{167b} S. Roe,³⁶ J. Roggel,¹⁸¹ O. Röhne,¹³³ R. Röhrig,¹¹⁵
 R. A. Rojas,^{146d} B. Roland,⁵² C. P. A. Roland,⁶⁶ J. Roloff,²⁹ A. Romaniouk,¹¹² M. Romano,^{23b,23a} N. Rompotis,⁹¹

M. Ronzani,¹²⁵ L. Roos,¹³⁵ S. Rosati,^{73a} G. Rosin,¹⁰³ B. J. Rosser,¹³⁶ E. Rossi,⁴⁶ E. Rossi,^{75a,75b} E. Rossi,^{70a,70b} L. P. Rossi,^{55b}
 L. Rossini,⁴⁶ R. Rosten,¹⁴ M. Rotaru,^{27b} B. Rottler,⁵² D. Rousseau,⁶⁵ G. Rovelli,^{71a,71b} A. Roy,¹¹ D. Roy,^{33e} A. Rozanov,¹⁰²
 Y. Rozen,¹⁵⁹ X. Ruan,^{33e} T. A. Ruggeri,¹ F. Rühr,⁵² A. Ruiz-Martinez,¹⁷³ A. Rummler,³⁶ Z. Rurikova,⁵² N. A. Rusakovich,⁸⁰
 H. L. Russell,¹⁰⁴ L. Rustige,^{38,47} J. P. Rutherford,⁷ E. M. Rüttinger,¹⁴⁸ M. Rybar,³⁹ G. Rybkin,⁶⁵ E. B. Rye,¹³³ A. Ryzhov,¹²³
 J. A. Sabater Iglesias,⁴⁶ P. Sabatini,⁵³ L. Sabetta,^{73a,73b} S. Sacerdoti,⁶⁵ H. F-W. Sadrozinski,¹⁴⁵ R. Sadykov,⁸⁰
 F. Safai Tehrani,^{73a} B. Safarzadeh Samani,¹⁵⁵ M. Safdari,¹⁵² P. Saha,¹²¹ S. Saha,¹⁰⁴ M. Sahinsoy,¹¹⁵ A. Sahu,¹⁸¹
 M. Saimpert,³⁶ M. Saito,¹⁶² T. Saito,¹⁶² H. Sakamoto,¹⁶² D. Salamani,⁵⁴ G. Salamanna,^{75a,75b} A. Salnikov,¹⁵² J. Salt,¹⁷³
 A. Salvador Salas,¹⁴ D. Salvatore,^{41b,41a} F. Salvatore,¹⁵⁵ A. Salvucci,^{63a,63b,63c} A. Salzburger,³⁶ J. Samarati,³⁶ D. Sammel,⁵²
 D. Sampsonidis,¹⁶¹ D. Sampsonidou,¹⁶¹ J. Sánchez,¹⁷³ A. Sanchez Pineda,^{67a,36,67c} H. Sandaker,¹³³ C. O. Sander,⁴⁶
 I. G. Sanderswood,⁹⁰ M. Sandhoff,¹⁸¹ C. Sandoval,^{22b} D. P. C. Sankey,¹⁴³ M. Sannino,^{55b,55a} Y. Sano,¹¹⁷ A. Sansoni,⁵¹
 C. Santoni,³⁸ H. Santos,^{139a,139b} S. N. Santpur,¹⁸ A. Santra,¹⁷³ K. A. Saoucha,¹⁴⁸ A. Sapronov,⁸⁰ J. G. Saraiva,^{139a,139d}
 O. Sasaki,⁸² K. Sato,¹⁶⁸ F. Sauerburger,⁵² E. Sauvan,⁵ P. Savard,^{166,d} R. Sawada,¹⁶² C. Sawyer,¹⁴³ L. Sawyer,^{96,gg}
 I. Sayago Galvan,¹⁷³ C. Sbarra,^{23b} A. Sbrizzi,^{67a,67c} T. Scanlon,⁹⁵ J. Schaarschmidt,¹⁴⁷ P. Schacht,¹¹⁵ D. Schaefer,³⁷
 L. Schaefer,¹³⁶ S. Schaepe,³⁶ U. Schäfer,¹⁰⁰ A. C. Schaffer,⁶⁵ D. Schaile,¹¹⁴ R. D. Schamberger,¹⁵⁴ E. Schanet,¹¹⁴ C. Scharf,¹⁹
 N. Scharmberg,¹⁰¹ V. A. Schegelsky,¹³⁷ D. Scheirich,¹⁴² F. Schenck,¹⁹ M. Schernau,¹⁷⁰ C. Schiavi,^{55b,55a} L. K. Schildgen,²⁴
 Z. M. Schillaci,²⁶ E. J. Schioppa,^{68a,68b} M. Schioppa,^{41b,41a} K. E. Schleicher,⁵² S. Schlenker,³⁶ K. R. Schmidt-Sommerfeld,¹¹⁵
 K. Schmieden,³⁶ C. Schmitt,¹⁰⁰ S. Schmitt,⁴⁶ J. C. Schmoeckel,⁴⁶ L. Schoeffel,¹⁴⁴ A. Schoening,^{61b} P. G. Scholer,⁵²
 E. Schopf,¹³⁴ M. Schott,¹⁰⁰ J. F. P. Schouwenberg,¹¹⁹ J. Schovancova,³⁶ S. Schramm,⁵⁴ F. Schroeder,¹⁸¹ A. Schulte,¹⁰⁰
 H-C. Schultz-Coulon,^{61a} M. Schumacher,⁵² B. A. Schumm,¹⁴⁵ Ph. Schune,¹⁴⁴ A. Schwartzman,¹⁵² T. A. Schwarz,¹⁰⁶
 Ph. Schwemling,¹⁴⁴ R. Schwienhorst,¹⁰⁷ A. Sciandra,¹⁴⁵ G. Sciolla,²⁶ M. Scornajenghi,^{41b,41a} F. Scuri,^{72a} F. Scutti,¹⁰⁵
 L. M. Scyboz,¹¹⁵ C. D. Sebastiani,⁹¹ P. Seema,¹⁹ S. C. Seidel,¹¹⁸ A. Seiden,¹⁴⁵ B. D. Seidlitz,²⁹ T. Seiss,³⁷ C. Seitz,⁴⁶
 J. M. Seixas,^{81b} G. Sekhniaidze,^{70a} S. J. Sekula,⁴² N. Semprini-Cesari,^{23b,23a} S. Sen,⁴⁹ C. Serfon,²⁹ L. Serin,⁶⁵ L. Serkin,^{67a,67b}
 M. Sessa,^{60a} H. Severini,¹²⁸ S. Sevova,¹⁵² F. Sforza,^{55b,55a} A. Sfyrta,⁵⁴ E. Shabalina,⁵³ J. D. Shahinian,¹⁴⁵ N. W. Shaikh,^{45a,45b}
 D. Shaked Renous,¹⁷⁹ L. Y. Shan,^{15a} M. Shapiro,¹⁸ A. Sharma,¹³⁴ A. S. Sharma,¹ P. B. Shatalov,¹²⁴ K. Shaw,¹⁵⁵
 S. M. Shaw,¹⁰¹ M. Shehade,¹⁷⁹ Y. Shen,¹²⁸ A. D. Sherman,²⁵ P. Sherwood,⁹⁵ L. Shi,⁹⁵ S. Shimizu,⁸² C. O. Shimmin,¹⁸²
 Y. Shimogama,¹⁷⁸ M. Shimojima,¹¹⁶ I. P. J. Shipsey,¹³⁴ S. Shirabe,¹⁶⁴ M. Shiyakova,^{80,hh} J. Shlomi,¹⁷⁹ A. Shmeleva,¹¹¹
 M. J. Shochet,³⁷ J. Shojaii,¹⁰⁵ D. R. Shope,¹⁵³ S. Shrestha,¹²⁷ E. M. Shrif,^{33e} E. Shulga,¹⁷⁹ P. Sicho,¹⁴⁰ A. M. Sickles,¹⁷²
 E. Sideras Haddad,^{33e} O. Sidiropoulou,³⁶ A. Sidoti,^{23b,23a} F. Siegert,⁴⁸ Dj. Sijacki,¹⁶ M. Jr. Silva,¹⁸⁰ M. V. Silva Oliveira,³⁶
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 S. Singh,¹⁵¹ M. Sioli,^{23b,23a} I. Siral,¹³¹ S. Yu. Sivoklov,¹¹³ J. Sjölin,^{45a,45b} A. Skaf,⁵³ E. Skorda,⁹⁷ P. Skubic,¹²⁸
 M. Slawinska,⁸⁵ K. Sliwa,¹⁶⁹ R. Slovak,¹⁴² V. Smakhtin,¹⁷⁹ B. H. Smart,¹⁴³ J. Smiesko,^{28b} N. Smirnov,¹¹² S. Yu. Smirnov,¹¹²
 Y. Smirnov,¹¹² L. N. Smirnova,^{113,ii} O. Smirnova,⁹⁷ E. A. Smith,³⁷ H. A. Smith,¹³⁴ M. Smizanska,⁹⁰ K. Smolek,¹⁴¹
 A. Smykiewicz,⁸⁵ A. A. Snesarev,¹¹¹ H. L. Snoek,¹²⁰ I. M. Snyder,¹³¹ S. Snyder,²⁹ R. Sobie,^{175,1} A. Soffer,¹⁶⁰ A. Søggaard,⁵⁰
 F. Sohns,⁵³ C. A. Solans Sanchez,³⁶ E. Yu. Soldatov,¹¹² U. Soldevila,¹⁷³ A. A. Solodkov,¹²³ A. Soloshenko,⁸⁰
 O. V. Solovyanov,¹²³ V. Solovyev,¹³⁷ P. Sommer,¹⁴⁸ H. Son,¹⁶⁹ W. Song,¹⁴³ W. Y. Song,^{167b} A. Sopczak,¹⁴¹ A. L. Soppio,⁹⁵
 F. Sopkova,^{28b} S. Sottocornola,^{71a,71b} R. Soualah,^{67a,67c} A. M. Soukharev,^{122b,122a} D. South,⁴⁶ S. Spagnolo,^{68a,68b} M. Spalla,¹¹⁵
 M. Spangenberg,¹⁷⁷ F. Spanò,⁹⁴ D. Sperlich,⁵² T. M. Spieker,^{61a} G. Spigo,³⁶ M. Spina,¹⁵⁵ D. P. Spiteri,⁵⁷ M. Spousta,¹⁴²
 A. Stabile,^{69a,69b} B. L. Stamas,¹²¹ R. Stamen,^{61a} M. Stamenkovic,¹²⁰ E. Stanecka,⁸⁵ B. Stanislaus,¹³⁴ M. M. Stanitzki,⁴⁶
 M. Stankaityte,¹³⁴ B. Stapf,¹²⁰ E. A. Starchenko,¹²³ G. H. Stark,¹⁴⁵ J. Stark,⁵⁸ P. Staroba,¹⁴⁰ P. Starovoitov,^{61a} S. Stärz,¹⁰⁴
 R. Staszewski,⁸⁵ G. Stavropoulos,⁴⁴ M. Stegler,⁴⁶ P. Steinberg,²⁹ A. L. Steinhebel,¹³¹ B. Stelzer,^{151,167a} H. J. Stelzer,¹³⁸
 O. Stelzer-Chilton,^{167a} H. Stenzel,⁵⁶ T. J. Stevenson,¹⁵⁵ G. A. Stewart,³⁶ M. C. Stockton,³⁶ G. Stoicea,^{27b} M. Stolarski,^{139a}
 S. Stonjek,¹¹⁵ A. Straessner,⁴⁸ J. Strandberg,¹⁵³ S. Strandberg,^{45a,45b} M. Strauss,¹²⁸ T. Strebler,¹⁰² P. Strizenec,^{28b}
 R. Ströhmer,¹⁷⁶ D. M. Strom,¹³¹ R. Stroynowski,⁴² A. Strubig,⁵⁰ S. A. Stucci,²⁹ B. Stugu,¹⁷ J. Stupak,¹²⁸ N. A. Styles,⁴⁶
 D. Su,¹⁵² W. Su,^{60c} X. Su,^{60a} V. V. Sulin,¹¹¹ M. J. Sullivan,⁹¹ D. M. S. Sultan,⁵⁴ S. Sultansoy,^{4c} T. Sumida,⁸⁶ S. Sun,¹⁰⁶
 X. Sun,¹⁰¹ K. Suruliz,¹⁵⁵ C. J. E. Suster,¹⁵⁶ M. R. Sutton,¹⁵⁵ S. Suzuki,⁸² M. Svatos,¹⁴⁰ M. Swiatlowski,^{167a} S. P. Swift,²
 T. Swirski,¹⁷⁶ A. Sydorenko,¹⁰⁰ I. Sykora,^{28a} M. Sykora,¹⁴² T. Sykora,¹⁴² D. Ta,¹⁰⁰ K. Tackmann,^{46,ij} J. Taenzer,¹⁶⁰
 A. Taffard,¹⁷⁰ R. Tafirout,^{167a} E. Tagiev,¹²³ R. Takashima,⁸⁷ K. Takeda,⁸³ T. Takeshita,¹⁴⁹ E. P. Takeva,⁵⁰ Y. Takubo,⁸²
 M. Talby,¹⁰² A. A. Talyshev,^{122b,122a} K. C. Tam,^{63b} N. M. Tamir,¹⁶⁰ J. Tanaka,¹⁶² R. Tanaka,⁶⁵ S. Tapia Araya,¹⁷²
 S. Tapprogge,¹⁰⁰ A. Tarek Abouelfadl Mohamed,¹⁰⁷ S. Tarem,¹⁵⁹ K. Tariq,^{60b} G. Tarna,^{27b,kk} G. F. Tartarelli,^{69a} P. Tas,¹⁴²

M. Tasevsky,¹⁴⁰ T. Tashiro,⁸⁶ E. Tassi,^{41b,41a} A. Tavares Delgado,^{139a} Y. Tayalati,^{35e} A. J. Taylor,⁵⁰ G. N. Taylor,¹⁰⁵
 W. Taylor,^{167b} H. Teagle,⁹¹ A. S. Tee,⁹⁰ R. Teixeira De Lima,¹⁵² P. Teixeira-Dias,⁹⁴ H. Ten Kate,³⁶ J. J. Teoh,¹²⁰ S. Terada,⁸²
 K. Terashi,¹⁶² J. Terron,⁹⁹ S. Terzo,¹⁴ M. Testa,⁵¹ R. J. Teuscher,^{166,1} S. J. Thais,¹⁸² N. Themistokleous,⁵⁰
 T. Theveneaux-Pelzer,⁴⁶ F. Thiele,⁴⁰ D. W. Thomas,⁹⁴ J. O. Thomas,⁴² J. P. Thomas,²¹ E. A. Thompson,⁴⁶ P. D. Thompson,²¹
 E. Thomson,¹³⁶ E. J. Thorpe,⁹³ R. E. Ticse Torres,⁵³ V. O. Tikhomirov,^{111,11} Yu. A. Tikhonov,^{122b,122a} S. Timoshenko,¹¹²
 P. Tipton,¹⁸² S. Tisserant,¹⁰² K. Todome,^{23b,23a} S. Todorova-Nova,¹⁴² S. Todt,⁴⁸ J. Tojo,⁸⁸ S. Tokár,^{28a} K. Tokushuku,⁸²
 E. Tolley,¹²⁷ R. Tombs,³² K. G. Tomiwa,^{33e} M. Tomoto,¹¹⁷ L. Tompkins,¹⁵² P. Tornambe,¹⁰³ E. Torrence,¹³¹ H. Torres,⁴⁸
 E. Torró Pastor,¹⁴⁷ C. Tosciri,¹³⁴ J. Toth,^{102,mm} D. R. Tovey,¹⁴⁸ A. Traeet,¹⁷ C. J. Treado,¹²⁵ T. Trefzger,¹⁷⁶ F. Tresoldi,¹⁵⁵
 A. Tricoli,²⁹ I. M. Trigger,^{167a} S. Trincaz-Duvoid,¹³⁵ D. A. Trischuk,¹⁷⁴ W. Trischuk,¹⁶⁶ B. Trocmé,⁵⁸ A. Trofymov,⁶⁵
 C. Troncon,^{69a} F. Trovato,¹⁵⁵ L. Truong,^{33c} M. Trzebinski,⁸⁵ A. Trzuppek,⁸⁵ F. Tsai,⁴⁶ J. C.-L. Tseng,¹³⁴ P. V. Tsiareshka,^{108,bb}
 A. Tsirigotis,^{161,cc} V. Tsiskaridze,¹⁵⁴ E. G. Tskhadadze,^{158a} M. Tsopoulou,¹⁶¹ I. I. Tsukerman,¹²⁴ V. Tsulaia,¹⁸ S. Tsuno,⁸²
 D. Tsybychev,¹⁵⁴ Y. Tu,^{63b} A. Tudorache,^{27b} V. Tudorache,^{27b} T. T. Tulbure,^{27a} A. N. Tuna,⁵⁹ S. Turchikhin,⁸⁰
 D. Turgeman,¹⁷⁹ I. Turk Cakir,^{4b,nn} R. J. Turner,²¹ R. T. Turra,^{69a} P. M. Tuts,³⁹ S. Tzamaris,¹⁶¹ E. Tzovara,¹⁰⁰ K. Uchida,¹⁶²
 F. Ukegawa,¹⁶⁸ G. Unal,³⁶ M. Unal,¹¹ A. Undrus,²⁹ G. Unel,¹⁷⁰ F. C. Ungaro,¹⁰⁵ Y. Unno,⁸² K. Uno,¹⁶² J. Urban,^{28b}
 P. Urquijo,¹⁰⁵ G. Usai,⁸ Z. Uysal,^{12d} V. Vacek,¹⁴¹ B. Vachon,¹⁰⁴ K. O. H. Vadla,¹³³ T. Vafeiadis,³⁶ A. Vaidya,⁹⁵
 C. Valderanis,¹¹⁴ E. Valdes Santurio,^{45a,45b} M. Valente,⁵⁴ S. Valentinetti,^{23b,23a} A. Valero,¹⁷³ L. Valéry,⁴⁶ R. A. Vallance,²¹
 A. Vallier,³⁶ J. A. Valls Ferrer,¹⁷³ T. R. Van Daalen,¹⁴ P. Van Gemmeren,⁶ S. Van Stroud,⁹⁵ I. Van Vulpen,¹²⁰
 M. Vanadia,^{74a,74b} W. Vandelli,³⁶ M. Vandembroucke,¹⁴⁴ E. R. Vandewall,¹²⁹ A. Vaniachine,¹⁶⁵ D. Vannicola,^{73a,73b} R. Vari,^{73a}
 E. W. Varnes,⁷ C. Varni,^{55b,55a} T. Varol,¹⁵⁷ D. Varouchas,⁶⁵ K. E. Varvell,¹⁵⁶ M. E. Vasile,^{27b} G. A. Vasquez,¹⁷⁵ F. Vazeille,³⁸
 D. Vazquez Furelos,¹⁴ T. Vazquez Schroeder,³⁶ J. Veatch,⁵³ V. Vecchio,¹⁰¹ M. J. Veen,¹²⁰ L. M. Veloce,¹⁶⁶ F. Veloso,^{139a,139c}
 S. Veneziano,^{73a} A. Ventura,^{68a,68b} A. Verbytskyi,¹¹⁵ V. Vercesi,^{71a} M. Verducci,^{72a,72b} C. M. Vergel Infante,⁷⁹ C. Vergis,²⁴
 W. Verkerke,¹²⁰ A. T. Vermeulen,¹²⁰ J. C. Vermeulen,¹²⁰ C. Vernieri,¹⁵² M. C. Vetterli,^{151,d} N. Viaux Maira,^{146d} T. Vickey,¹⁴⁸
 O. E. Vickey Boeriu,¹⁴⁸ G. H. A. Viehhauser,¹³⁴ L. Vigani,^{61b} M. Villa,^{23b,23a} M. Villaplana Perez,³ E. M. Villhauer,⁵⁰
 E. Vilucchi,⁵¹ M. G. Vincter,³⁴ G. S. Virdee,²¹ A. Vishwakarma,⁵⁰ C. Vittori,^{23b,23a} I. Vivarelli,¹⁵⁵ M. Vogel,¹⁸¹ P. Vokac,¹⁴¹
 S. E. von Buddenbrock,^{33e} E. Von Toerne,²⁴ V. Vorobel,¹⁴² K. Vorobev,¹¹² M. Vos,¹⁷³ J. H. Vosseveld,⁹¹ M. Vozak,¹⁰¹
 N. Vranjes,¹⁶ M. Vranjes Milosavljevic,¹⁶ V. Vrba,¹⁴¹ M. Vreeswijk,¹²⁰ R. Vuillermet,³⁶ I. Vukotic,³⁷ S. Wada,¹⁶⁸
 P. Wagner,²⁴ W. Wagner,¹⁸¹ J. Wagner-Kuhr,¹¹⁴ S. Wahdan,¹⁸¹ H. Wahlberg,⁸⁹ R. Wakasa,¹⁶⁸ V. M. Walbrecht,¹¹⁵
 J. Walder,¹⁴³ R. Walker,¹¹⁴ S. D. Walker,⁹⁴ W. Walkowiak,¹⁵⁰ V. Wallangen,^{45a,45b} A. M. Wang,⁵⁹ A. Z. Wang,¹⁸⁰ C. Wang,^{60a}
 C. Wang,^{60c} F. Wang,¹⁸⁰ H. Wang,¹⁸ H. Wang,³ J. Wang,^{63a} P. Wang,⁴² Q. Wang,¹²⁸ R.-J. Wang,¹⁰⁰ R. Wang,^{60a} R. Wang,⁶
 S. M. Wang,¹⁵⁷ W. T. Wang,^{60a} W. Wang,^{15c} W. X. Wang,^{60a} Y. Wang,^{60a} Z. Wang,¹⁰⁶ C. Wanotayaroj,⁴⁶ A. Warburton,¹⁰⁴
 C. P. Ward,³² D. R. Wardrope,⁹⁵ N. Warrack,⁵⁷ A. T. Watson,²¹ M. F. Watson,²¹ G. Watts,¹⁴⁷ B. M. Waugh,⁹⁵ A. F. Webb,¹¹
 C. Weber,²⁹ M. S. Weber,²⁰ S. A. Weber,³⁴ S. M. Weber,^{61a} A. R. Weidberg,¹³⁴ J. Weingarten,⁴⁷ M. Weirich,¹⁰⁰ C. Weiser,⁵²
 P. S. Wells,³⁶ T. Wenaus,²⁹ B. Wendland,⁴⁷ T. Wengler,³⁶ S. Wenig,³⁶ N. Wermes,²⁴ M. Wessels,^{61a} T. D. Weston,²⁰
 K. Whalen,¹³¹ A. M. Wharton,⁹⁰ A. S. White,¹⁰⁶ A. White,⁸ M. J. White,¹ D. Whiteson,¹⁷⁰ B. W. Whitmore,⁹⁰
 W. Wiedenmann,¹⁸⁰ C. Wiel,⁴⁸ M. Wielers,¹⁴³ N. Wieseotte,¹⁰⁰ C. Wiglesworth,⁴⁰ L. A. M. Wiik-Fuchs,⁵² H. G. Wilkens,³⁶
 L. J. Wilkins,⁹⁴ H. H. Williams,¹³⁶ S. Williams,³² S. Willocq,¹⁰³ P. J. Windischhofer,¹³⁴ I. Wingerter-Seez,⁵ E. Winkels,¹⁵⁵
 F. Winklmeier,¹³¹ B. T. Winter,⁵² M. Wittgen,¹⁵² M. Wobisch,⁹⁶ A. Wolf,¹⁰⁰ R. Wölker,¹³⁴ J. Wollrath,⁵² M. W. Wolter,⁸⁵
 H. Wolters,^{139a,139c} V. W. S. Wong,¹⁷⁴ N. L. Woods,¹⁴⁵ S. D. Worm,⁴⁶ B. K. Wosiek,⁸⁵ K. W. Woźniak,⁸⁵ K. Wraight,⁵⁷
 S. L. Wu,¹⁸⁰ X. Wu,⁵⁴ Y. Wu,^{60a} J. Wuerzinger,¹³⁴ T. R. Wyatt,¹⁰¹ B. M. Wynne,⁵⁰ S. Xella,⁴⁰ L. Xia,¹⁷⁷ J. Xiang,^{63c}
 X. Xiao,¹⁰⁶ X. Xie,^{60a} I. Xiotidis,¹⁵⁵ D. Xu,^{15a} H. Xu,^{60a} H. Xu,^{60a} L. Xu,²⁹ T. Xu,¹⁴⁴ W. Xu,¹⁰⁶ Z. Xu,^{60b} Z. Xu,¹⁵²
 B. Yabsley,¹⁵⁶ S. Yacoob,^{33a} K. Yajima,¹³² D. P. Yallup,⁹⁵ N. Yamaguchi,⁸⁸ Y. Yamaguchi,¹⁶⁴ A. Yamamoto,⁸²
 M. Yamatani,¹⁶² T. Yamazaki,¹⁶² Y. Yamazaki,⁸³ J. Yan,^{60c} Z. Yan,²⁵ H. J. Yang,^{60c,60d} H. T. Yang,¹⁸ S. Yang,^{60a} T. Yang,^{63c}
 X. Yang,^{60b,58} Y. Yang,¹⁶² Z. Yang,^{60a} W.-M. Yao,¹⁸ Y. C. Yap,⁴⁶ Y. Yasu,⁸² E. Yatsenko,^{60c} H. Ye,^{15c} J. Ye,⁴² S. Ye,²⁹
 I. Yeletsikh,⁸⁰ M. R. Yexley,⁹⁰ E. Yigitbasi,²⁵ P. Yin,³⁹ K. Yorita,¹⁷⁸ K. Yoshihara,⁷⁹ C. J. S. Young,³⁶ C. Young,¹⁵² J. Yu,⁷⁹
 R. Yuan,^{60b,oo} X. Yue,^{61a} M. Zaazoua,^{35e} B. Zabinski,⁸⁵ G. Zacharis,¹⁰ E. Zaffaroni,⁵⁴ J. Zahreddine,¹³⁵ A. M. Zaitsev,^{123,i}
 T. Zakareishvili,^{158b} N. Zakharchuk,³⁴ S. Zambito,³⁶ D. Zanzi,³⁶ D. R. Zaripovas,⁵⁷ S. V. Zeiβner,⁴⁷ C. Zeitnitz,¹⁸¹
 G. Zemaityte,¹³⁴ J. C. Zeng,¹⁷² O. Zenin,¹²³ T. Ženiš,^{28a} D. Zerwas,⁶⁵ M. Zgubič,¹³⁴ B. Zhang,^{15c} D. F. Zhang,^{15b}
 G. Zhang,^{15b} J. Zhang,⁶ K. Zhang,^{15a} L. Zhang,^{15c} L. Zhang,^{60a} M. Zhang,¹⁷² R. Zhang,¹⁸⁰ S. Zhang,¹⁰⁶ X. Zhang,^{60c}
 X. Zhang,^{60b} Y. Zhang,^{15a,15d} Z. Zhang,^{63a} Z. Zhang,⁶⁵ P. Zhao,⁴⁹ Z. Zhao,^{60a} A. Zhemchugov,⁸⁰ Z. Zheng,¹⁰⁶ D. Zhong,¹⁷²

B. Zhou,¹⁰⁶ C. Zhou,¹⁸⁰ H. Zhou,⁷ M. S. Zhou,^{15a,15d} M. Zhou,¹⁵⁴ N. Zhou,^{60c} Y. Zhou,⁷ C. G. Zhu,^{60b} C. Zhu,^{15a,15d}
 H. L. Zhu,^{60a} H. Zhu,^{15a} J. Zhu,¹⁰⁶ Y. Zhu,^{60a} X. Zhuang,^{15a} K. Zhukov,¹¹¹ V. Zhulanov,^{122b,122a} D. Zieminska,⁶⁶
 N. I. Zimine,⁸⁰ S. Zimmermann,⁵² Z. Zinonos,¹¹⁵ M. Ziolkowski,¹⁵⁰ L. Živković,¹⁶ G. Zobernig,¹⁸⁰ A. Zoccoli,^{23b,23a}
 K. Zoch,⁵³ T. G. Zorbas,¹⁴⁸ R. Zou,³⁷ and L. Zwalinski³⁶

(ATLAS Collaboration)

- ¹*Department of Physics, University of Adelaide, Adelaide, Australia*
²*Physics Department, SUNY Albany, Albany, New York, USA*
³*Department of Physics, University of Alberta, Edmonton, Alberta, Canada*
^{4a}*Department of Physics, Ankara University, Ankara, Turkey*
^{4b}*Istanbul Aydin University, Application and Research Center for Advanced Studies, Istanbul, Turkey*
^{4c}*Division of Physics, TOBB University of Economics and Technology, Ankara, Turkey*
⁵*LAPP, Université Grenoble Alpes, Université Savoie Mont Blanc, CNRS/IN2P3, Annecy, France*
⁶*High Energy Physics Division, Argonne National Laboratory, Argonne, Illinois, USA*
⁷*Department of Physics, University of Arizona, Tucson, Arizona, USA*
⁸*Department of Physics, University of Texas at Arlington, Arlington, Texas, USA*
⁹*Physics Department, National and Kapodistrian University of Athens, Athens, Greece*
¹⁰*Physics Department, National Technical University of Athens, Zografou, Greece*
¹¹*Department of Physics, University of Texas at Austin, Austin, Texas, USA*
^{12a}*Bahcesehir University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey*
^{12b}*Istanbul Bilgi University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey*
^{12c}*Department of Physics, Bogazici University, Istanbul, Turkey*
^{12d}*Department of Physics Engineering, Gaziantep University, Gaziantep, Turkey*
¹³*Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan*
¹⁴*Institut de Física d'Altes Energies (IFAE), Barcelona Institute of Science and Technology, Barcelona, Spain*
^{15a}*Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China*
^{15b}*Physics Department, Tsinghua University, Beijing, China*
^{15c}*Department of Physics, Nanjing University, Nanjing, China*
^{15d}*University of Chinese Academy of Science (UCAS), Beijing, China*
¹⁶*Institute of Physics, University of Belgrade, Belgrade, Serbia*
¹⁷*Department for Physics and Technology, University of Bergen, Bergen, Norway*
¹⁸*Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley, California, USA*
¹⁹*Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany*
²⁰*Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland*
²¹*School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom*
^{22a}*Facultad de Ciencias y Centro de Investigaciones, Universidad Antonio Nariño, Bogotá, Colombia*
^{22b}*Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia, Colombia*
^{23a}*INFN Bologna and Università' di Bologna, Dipartimento di Fisica, Italy*
^{23b}*INFN Sezione di Bologna, Italy*
²⁴*Physikalisches Institut, Universität Bonn, Bonn, Germany*
²⁵*Department of Physics, Boston University, Boston, Massachusetts, USA*
²⁶*Department of Physics, Brandeis University, Waltham, Massachusetts, USA*
^{27a}*Transilvania University of Brasov, Brasov, Romania*
^{27b}*Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania*
^{27c}*Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi, Romania*
^{27d}*National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj-Napoca, Romania*
^{27e}*University Politehnica Bucharest, Bucharest, Romania*
^{27f}*West University in Timisoara, Timisoara, Romania*
^{28a}*Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovak Republic*
^{28b}*Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic*
²⁹*Physics Department, Brookhaven National Laboratory, Upton, New York, USA*
³⁰*Departamento de Física, Universidad de Buenos Aires, Buenos Aires, Argentina*
³¹*California State University, California, USA*
³²*Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom*
^{33a}*Department of Physics, University of Cape Town, Cape Town, South Africa*
^{33b}*iThemba Labs, Western Cape, South Africa*

- ^{33c}*Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa*
- ^{33d}*University of South Africa, Department of Physics, Pretoria, South Africa*
- ^{33e}*School of Physics, University of the Witwatersrand, Johannesburg, South Africa*
- ³⁴*Department of Physics, Carleton University, Ottawa, Ontario, Canada*
- ^{35a}*Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies—Université Hassan II, Casablanca, Morocco*
- ^{35b}*Faculté des Sciences, Université Ibn-Tofail, Kénitra, Morocco*
- ^{35c}*Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech, Morocco*
- ^{35d}*Faculté des Sciences, Université Mohamed Premier and LTPM, Oujda, Morocco*
- ^{35e}*Faculté des sciences, Université Mohammed V, Rabat, Morocco*
- ³⁶*CERN, Geneva, Switzerland*
- ³⁷*Enrico Fermi Institute, University of Chicago, Chicago, Illinois, USA*
- ³⁸*LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand, France*
- ³⁹*Nevis Laboratory, Columbia University, Irvington, New York, USA*
- ⁴⁰*Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark*
- ^{41a}*Dipartimento di Fisica, Università della Calabria, Rende, Italy*
- ^{41b}*INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Italy*
- ⁴²*Physics Department, Southern Methodist University, Dallas, Texas, USA*
- ⁴³*Physics Department, University of Texas at Dallas, Richardson, Texas, USA*
- ⁴⁴*National Centre for Scientific Research “Demokritos”, Agia Paraskevi, Greece*
- ^{45a}*Department of Physics, Stockholm University, Sweden*
- ^{45b}*Oskar Klein Centre, Stockholm, Sweden*
- ⁴⁶*Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen, Germany*
- ⁴⁷*Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany*
- ⁴⁸*Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany*
- ⁴⁹*Department of Physics, Duke University, Durham, North Carolina, USA*
- ⁵⁰*SUPA—School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom*
- ⁵¹*INFN e Laboratori Nazionali di Frascati, Frascati, Italy*
- ⁵²*Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany*
- ⁵³*II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany*
- ⁵⁴*Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland*
- ^{55a}*Dipartimento di Fisica, Università di Genova, Genova, Italy*
- ^{55b}*INFN Sezione di Genova, Italy*
- ⁵⁶*II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany*
- ⁵⁷*SUPA—School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom*
- ⁵⁸*LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble, France*
- ⁵⁹*Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, Massachusetts, USA*
- ^{60a}*Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Hefei, China*
- ^{60b}*Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE), Shandong University, Qingdao, China*
- ^{60c}*School of Physics and Astronomy, Shanghai Jiao Tong University, KLPPAC-MoE, SKLPPC, Shanghai, China*
- ^{60d}*Tsung-Dao Lee Institute, Shanghai, China*
- ^{61a}*Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany*
- ^{61b}*Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany*
- ⁶²*Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan*
- ^{63a}*Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*
- ^{63b}*Department of Physics, University of Hong Kong, Hong Kong, China*
- ^{63c}*Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China*
- ⁶⁴*Department of Physics, National Tsing Hua University, Hsinchu, Taiwan*
- ⁶⁵*IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay, France*
- ⁶⁶*Department of Physics, Indiana University, Bloomington, Indiana, USA*
- ^{67a}*INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine, Italy*
- ^{67b}*ICTP, Trieste, Italy*
- ^{67c}*Dipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine, Italy*
- ^{68a}*INFN Sezione di Lecce, Italy*
- ^{68b}*Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy*
- ^{69a}*INFN Sezione di Milano, Italy*
- ^{69b}*Dipartimento di Fisica, Università di Milano, Milano, Italy*

- ^{70a}*INFN Sezione di Napoli, Italy*
^{70b}*Dipartimento di Fisica, Università di Napoli, Napoli, Italy*
^{71a}*INFN Sezione di Pavia, Italy*
^{71b}*Dipartimento di Fisica, Università di Pavia, Pavia, Italy*
^{72a}*INFN Sezione di Pisa, Italy*
^{72b}*Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy*
^{73a}*INFN Sezione di Roma, Italy*
^{73b}*Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy*
^{74a}*INFN Sezione di Roma Tor Vergata, Italy*
^{74b}*Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy*
^{75a}*INFN Sezione di Roma Tre, Italy*
^{75b}*Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy*
^{76a}*INFN-TIFPA, Italy*
^{76b}*Università degli Studi di Trento, Trento, Italy*
⁷⁷*Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria*
⁷⁸*University of Iowa, Iowa City Iowa, USA*
⁷⁹*Department of Physics and Astronomy, Iowa State University, Ames, Iowa, USA*
⁸⁰*Joint Institute for Nuclear Research, Dubna, Russia*
^{81a}*Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, Brazil*
^{81b}*Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro, Brazil*
^{81c}*Universidade Federal de São João del Rei (UFSJ), São João del Rei, Brazil*
^{81d}*Instituto de Física, Universidade de São Paulo, São Paulo, Brazil*
⁸²*KEK, High Energy Accelerator Research Organization, Tsukuba, Japan*
⁸³*Graduate School of Science, Kobe University, Kobe, Japan*
^{84a}*AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland*
^{84b}*Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland*
⁸⁵*Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland*
⁸⁶*Faculty of Science, Kyoto University, Kyoto, Japan*
⁸⁷*Kyoto University of Education, Kyoto, Japan*
⁸⁸*Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan*
⁸⁹*Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina*
⁹⁰*Physics Department, Lancaster University, Lancaster, United Kingdom*
⁹¹*Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom*
⁹²*Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia*
⁹³*School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom*
⁹⁴*Department of Physics, Royal Holloway University of London, Egham, United Kingdom*
⁹⁵*Department of Physics and Astronomy, University College London, London, United Kingdom*
⁹⁶*Louisiana Tech University, Ruston, Louisiana, USA*
⁹⁷*Fysiska institutionen, Lunds universitet, Lund, Sweden*
⁹⁸*Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France*
⁹⁹*Departamento de Física Teórica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid, Spain*
¹⁰⁰*Institut für Physik, Universität Mainz, Mainz, Germany*
¹⁰¹*School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom*
¹⁰²*CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France*
¹⁰³*Department of Physics, University of Massachusetts, Amherst, Massachusetts, USA*
¹⁰⁴*Department of Physics, McGill University, Montreal, Quebec, Canada*
¹⁰⁵*School of Physics, University of Melbourne, Victoria, Australia*
¹⁰⁶*Department of Physics, University of Michigan, Ann Arbor, Michigan, USA*
¹⁰⁷*Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA*
¹⁰⁸*B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus*
¹⁰⁹*Research Institute for Nuclear Problems of Byelorussian State University, Minsk, Belarus*
¹¹⁰*Group of Particle Physics, University of Montreal, Montreal, Quebec, Canada*
¹¹¹*P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia*
¹¹²*National Research Nuclear University MEPhI, Moscow, Russia*
¹¹³*D.V. Skobel'syn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia*
¹¹⁴*Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany*
¹¹⁵*Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany*
¹¹⁶*Nagasaki Institute of Applied Science, Nagasaki, Japan*
¹¹⁷*Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan*

- ¹¹⁸*Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico, USA*
- ¹¹⁹*Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands*
- ¹²⁰*Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands*
- ¹²¹*Department of Physics, Northern Illinois University, DeKalb, Illinois, USA*
- ^{122a}*Budker Institute of Nuclear Physics and NSU, SB RAS, Novosibirsk, Russia*
- ^{122b}*Novosibirsk State University Novosibirsk, Russia*
- ¹²³*Institute for High Energy Physics of the National Research Centre Kurchatov Institute, Protvino, Russia*
- ¹²⁴*Institute for Theoretical and Experimental Physics named by A.I. Alikhanov of National Research Centre “Kurchatov Institute”, Moscow, Russia*
- ¹²⁵*Department of Physics, New York University, New York, New York, USA*
- ¹²⁶*Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo, Japan*
- ¹²⁷*Ohio State University, Columbus, Ohio, USA*
- ¹²⁸*Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman Oklahoma, USA*
- ¹²⁹*Department of Physics, Oklahoma State University, Stillwater, Oklahoma, USA*
- ¹³⁰*Palacký University, RCPTM, Joint Laboratory of Optics, Olomouc, Czech Republic*
- ¹³¹*Institute for Fundamental Science, University of Oregon, Eugene, Oregon, USA*
- ¹³²*Graduate School of Science, Osaka University, Osaka, Japan*
- ¹³³*Department of Physics, University of Oslo, Oslo, Norway*
- ¹³⁴*Department of Physics, Oxford University, Oxford, United Kingdom*
- ¹³⁵*LPNHE, Sorbonne Université, Université de Paris, CNRS/IN2P3, Paris, France*
- ¹³⁶*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania, USA*
- ¹³⁷*Konstantinov Nuclear Physics Institute of National Research Centre “Kurchatov Institute”, PNPI, St. Petersburg, Russia*
- ¹³⁸*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania, USA*
- ^{139a}*Laboratório de Instrumentação e Física Experimental de Partículas—LIP, Lisboa, Portugal*
- ^{139b}*Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal*
- ^{139c}*Departamento de Física, Universidade de Coimbra, Coimbra, Portugal*
- ^{139d}*Centro de Física Nuclear da Universidade de Lisboa, Lisboa, Portugal*
- ^{139e}*Departamento de Física, Universidade do Minho, Braga, Portugal*
- ^{139f}*Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada (Spain), Spain*
- ^{139g}*Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal*
- ^{139h}*Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal*
- ¹⁴⁰*Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic*
- ¹⁴¹*Czech Technical University in Prague, Prague, Czech Republic*
- ¹⁴²*Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic*
- ¹⁴³*Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom*
- ¹⁴⁴*IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France*
- ¹⁴⁵*Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, California, USA*
- ^{146a}*Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile*
- ^{146b}*Universidad Andres Bello, Department of Physics, Santiago, Chile*
- ^{146c}*Instituto de Alta Investigación, Universidad de Tarapacá, Chile*
- ^{146d}*Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile*
- ¹⁴⁷*Department of Physics, University of Washington, Seattle, Washington, USA*
- ¹⁴⁸*Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom*
- ¹⁴⁹*Department of Physics, Shinshu University, Nagano, Japan*
- ¹⁵⁰*Department Physik, Universität Siegen, Siegen, Germany*
- ¹⁵¹*Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada*
- ¹⁵²*SLAC National Accelerator Laboratory, Stanford, California, USA*
- ¹⁵³*Physics Department, Royal Institute of Technology, Stockholm, Sweden*
- ¹⁵⁴*Departments of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA*
- ¹⁵⁵*Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom*
- ¹⁵⁶*School of Physics, University of Sydney, Sydney, Australia*
- ¹⁵⁷*Institute of Physics, Academia Sinica, Taipei, Taiwan*
- ^{158a}*E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi, Georgia*
- ^{158b}*High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia*
- ¹⁵⁹*Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel*
- ¹⁶⁰*Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel*
- ¹⁶¹*Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece*
- ¹⁶²*International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo, Japan*
- ¹⁶³*Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan*
- ¹⁶⁴*Department of Physics, Tokyo Institute of Technology, Tokyo, Japan*

- ¹⁶⁵*Tomsk State University, Tomsk, Russia*
- ¹⁶⁶*Department of Physics, University of Toronto, Toronto, Ontario, Canada*
- ^{167a}*TRIUMF, Vancouver, British Columbia, Canada*
- ^{167b}*Department of Physics and Astronomy, York University, Toronto, Ontario, Canada*
- ¹⁶⁸*Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan*
- ¹⁶⁹*Department of Physics and Astronomy, Tufts University, Medford, Massachusetts, USA*
- ¹⁷⁰*Department of Physics and Astronomy, University of California Irvine, Irvine, California, USA*
- ¹⁷¹*Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden*
- ¹⁷²*Department of Physics, University of Illinois, Urbana, Illinois, USA*
- ¹⁷³*Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia—CSIC, Valencia, Spain*
- ¹⁷⁴*Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada*
- ¹⁷⁵*Department of Physics and Astronomy, University of Victoria, Victoria, British Columbia, Canada*
- ¹⁷⁶*Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg, Germany*
- ¹⁷⁷*Department of Physics, University of Warwick, Coventry, United Kingdom*
- ¹⁷⁸*Waseda University, Tokyo, Japan*
- ¹⁷⁹*Department of Particle Physics, Weizmann Institute of Science, Rehovot, Israel*
- ¹⁸⁰*Department of Physics, University of Wisconsin, Madison, Wisconsin, USA*
- ¹⁸¹*Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany*
- ¹⁸²*Department of Physics, Yale University, New Haven, Connecticut, USA*

^aDeceased.

^bAlso at Department of Physics, King's College London, London, United Kingdom.

^cAlso at Instituto de Física Teórica, IFT-UAM/CSIC, Madrid, Spain.

^dAlso at TRIUMF, Vancouver, British Columbia, Canada.

^eAlso at Department of Physics and Astronomy, University of Louisville, Louisville, Kentucky, USA.

^fAlso at Physics Department, An-Najah National University, Nablus, Palestine.

^gAlso at Department of Physics, University of Fribourg, Fribourg, Switzerland.

^hAlso at Departament de Física de la Universitat Autònoma de Barcelona, Barcelona, Spain.

ⁱAlso at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia.

^jAlso at Department of Physics, Ben Gurion University of the Negev, Beer Sheva, Israel.

^kAlso at Università di Napoli Parthenope, Napoli, Italy.

^lAlso at Institute of Particle Physics (IPP), Vancouver, Canada.

^mAlso at Dipartimento di Matematica, Informatica e Fisica, Università di Udine, Udine, Italy.

ⁿAlso at Department of Physics, St. Petersburg State Polytechnical University, St. Petersburg, Russia.

^oAlso at Borough of Manhattan Community College, City University of New York, New York, New York, USA.

^pAlso at Department of Physics, California State University, Fresno, USA.

^qAlso at Department of Financial and Management Engineering, University of the Aegean, Chios, Greece.

^rAlso at Centro Studi e Ricerche Enrico Fermi, Italy.

^sAlso at Department of Physics, California State University, East Bay, USA.

^tAlso at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain.

^uAlso at IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay, France.

^vAlso at Graduate School of Science, Osaka University, Osaka, Japan.

^wAlso at Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany.

^xAlso at University of Chinese Academy of Sciences (UCAS), Beijing, China.

^yAlso at Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan.

^zAlso at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands.

^{aa}Also at CERN, Geneva, Switzerland.

^{bb}Also at Joint Institute for Nuclear Research, Dubna, Russia.

^{cc}Also at Hellenic Open University, Patras, Greece.

^{dd}Also at The City College of New York, New York, New York, USA.

^{ee}Also at Department of Physics, California State University, Sacramento, USA.

^{ff}Also at Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland.

^{gg}Also at Louisiana Tech University, Ruston, Louisiana, USA.

^{hh}Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria.

ⁱⁱAlso at Faculty of Physics, M.V. Lomonosov Moscow State University, Moscow, Russia.

^{jj}Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany.

^{kk}Also at CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France.

^{ll}Also at National Research Nuclear University MEPhI, Moscow, Russia.

^{mm}Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary.

ⁿⁿAlso at Giresun University, Faculty of Engineering, Giresun, Turkey.

^{oo}Also at Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA.