

Properties of $g \rightarrow b\bar{b}$ at small opening angles in pp collisions with the ATLAS detector at $\sqrt{s} = 13$ TeV

M. Aaboud *et al.**
(ATLAS Collaboration)

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The fragmentation of high-energy gluons at small opening angles is largely unconstrained by present measurements. Gluon splitting to b -quark pairs is a unique probe into the properties of gluon fragmentation because identified b -tagged jets provide a proxy for the quark daughters of the initial gluon. In this study, key differential distributions related to the $g \rightarrow b\bar{b}$ process are measured using 33 fb^{-1} of $\sqrt{s} = 13$ TeV pp collision data recorded by the ATLAS experiment at the LHC in 2016. Jets constructed from charged-particle tracks, clustered with the anti- k_r jet algorithm with radius parameter $R = 0.2$, are used to probe angular scales below the $R = 0.4$ jet radius. The observables are unfolded to particle level in order to facilitate direct comparisons with predictions from present and future simulations. Multiple significant differences are observed between the data and parton shower Monte Carlo predictions, providing input to improve these predictions of the main source of background events in analyses involving boosted Higgs bosons decaying into b -quarks.

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I. INTRODUCTION

The search for highly Lorentz-boosted Higgs bosons produced by Standard Model (SM) processes [1] or by beyond-the-SM (BSM) processes [2–7] is of crucial importance at the Large Hadron Collider (LHC). As the branching ratio for the Higgs boson to decay into bottom quark pairs dominates the total decay rate, the boosted $H \rightarrow b\bar{b}$ channel can be the most sensitive to BSM effects entering at high Higgs boost. Algorithms for identifying jets resulting from bottom quark fragmentation are very powerful, so the main background for searches with boosted Higgs bosons contains b -quarks. The main contribution to this background is gluon splitting to $b\bar{b}$ pairs at small opening angles since the angle between the b -quarks in $H \rightarrow b\bar{b}$ scales with the Higgs boson mass (m_H) and momentum (p_H) as m_H/p_H . The $g \rightarrow b\bar{b}$ process also contributes to many other important SM measurements and searches by providing a source of additional real b -quark jets that can fake a signal for b -quarks originating from other processes (see e.g., Refs. [8–12]).

The modeling of $g \rightarrow b\bar{b}$ fragmentation is complex and provides a useful probe of quantum chromodynamics (QCD). The large mass of the b -quark introduces a

significant modification to the massless QCD splitting functions by screening the soft-emission singularity. Trijet measurements from LEP [13–15] and SLD [16] provide valuable information about the rate of $g \rightarrow b\bar{b}$, but have not explored the differential properties of the fragmentation in the small opening-angle regime. Previous measurements that include the $b\bar{b}$ final state at the $Spp\bar{p}S$, Tevatron, and LHC using inclusive [17–36], multijet [37–39], and associated production [40–49] topologies have focused on well-separated quark pairs (dominated by fixed-order instead of parton-splitting effects) and were limited in their kinematic reach due in part to small datasets and low momentum transfers.

The high transverse momentum and low angular separation regime for $g \rightarrow b\bar{b}$ can be probed at the LHC using b -tagged small-radius jets within large-radius jets. This topology is used to calibrate b -tagging in dense environments [50–52] and is studied phenomenologically [53,54]. The measurement shown in this paper builds on these studies by using data collected by the ATLAS detector from $\sqrt{s} = 13$ TeV pp collisions in order to perform a differential cross-section measurement of $g \rightarrow b\bar{b}$ inside jets at high transverse momentum—see Fig. 1 for a representative Feynman diagram. Small-radius jets built from charged-particle tracks are used as proxies for b -quarks and can be used as precision probes of the small opening-angle regime.

This paper is organized as follows. After a brief introduction to the ATLAS detector in Sec. II, the data and simulations used for the measurement are documented in Sec. III. Section IV describes the event selection and

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

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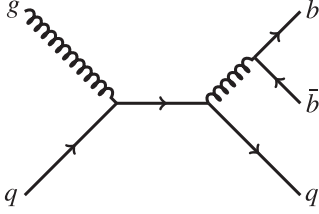


FIG. 1. A representative diagram for the high- p_T $g \rightarrow b\bar{b}$ process studied in this paper.

Sec. V lists and motivates the observables to be measured. The key challenge in the measurement is the estimation of background processes, which is performed using a data-driven approach illustrated in Sec. VI. The data are unfolded to correct for detector effects to allow direct comparisons to particle-level predictions. This procedure is explained in Sec. VII and the associated systematic uncertainties are detailed in Sec. VIII. The results are presented in Sec. IX and the paper concludes with Sec. X.

II. ATLAS DETECTOR

The ATLAS detector [55] is a multipurpose particle detector with a forward/backward-symmetric cylindrical geometry. The detector has a nearly 4π coverage in solid angle¹ and consists of an inner tracking detector, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner detector (ID) is surrounded by a superconducting solenoid providing a 2 T magnetic field and covers a pseudorapidity range of $|\eta| < 2.5$. The ID is composed of silicon pixel and microstrip detectors as well as a transition radiation tracker. For the LHC $\sqrt{s} = 13$ TeV run, the silicon pixel detector has been upgraded to include an additional layer close to the beam interaction point [56]. The lead/liquid-argon electromagnetic sampling calorimeters measure electromagnetic energies with high granularity for the pseudorapidity region of $|\eta| < 3.2$. Hadron energies are measured by a hadronic (steel/scintillator tile) calorimeter with $|\eta| < 1.7$. The forward and end cap regions between $1.5 < |\eta| < 4.9$ are instrumented with liquid-argon calorimeters for both the electromagnetic and hadronic measurements. Surrounding the calorimeters, the muon spectrometer includes three large superconducting toroidal magnets with eight coils each. The muon spectrometer has a system of precision tracking chambers covering $|\eta| < 2.7$ and fast trigger chambers covering $|\eta| < 2.4$. A two-level trigger system is used to select events for further analysis [57]. The first-level trigger is implemented in hardware and

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

utilizes partial detector information to reduce the accepted event rate to 100 kHz. The high-level trigger is based on software and accepts events at a rate of 1 kHz.

III. DATASETS

This measurement uses the dataset of pp collisions recorded by the ATLAS detector in 2016, corresponding to an integrated luminosity of 33 fb^{-1} at a center-of-mass energy of $\sqrt{s} = 13$ TeV. Events are considered only if they were collected during stable beam conditions and satisfy data quality requirements. Due to the high instantaneous luminosity and the large total inelastic proton-proton scattering cross section, on average there are about 25 simultaneous (pileup) collisions in each bunch crossing.

The measurement presented in this paper uses a variety of Monte Carlo (MC) simulated event samples to correct for detector effects as well as for direct comparisons with the unfolded data. Inclusive jet events were generated at leading order in the strong coupling constant, α_s , with PYTHIA 8.1 [58] using a $2 \rightarrow 2$ matrix element, the NNPDF2.3LO parton distribution function (PDF) set [59], and a set of generator parameter values called the A14 tune [60]. The EVTGEN [61] program was used to model the heavy-flavor decays to agree with experimental data. Additional inclusive jet events were simulated using a different generator in order to study the impact of modeling uncertainties related to both the perturbative and nonperturbative aspects of fragmentation. SHERPA 2.1 [62] generates events using multileg $2 \rightarrow 2$ and $2 \rightarrow 3$ matrix elements, which are matched to parton showers following the Catani-Krauss-Kuhn-Webber (CKKW) prescription [63]. These SHERPA events were simulated using the CT10 PDF set [64] and the default parameter tune in SHERPA.

Energy depositions from particles in MC event samples interacting with the detector and the subsequent detector readout were modeled using a full simulation of the ATLAS detector [65] implemented in Geant4 [66]. The effects of pileup were simulated with unbiased pp collisions using PYTHIA 8.1 and overlaid on the nominal inclusive jet events.

IV. OBJECT AND EVENT SELECTION

Section IV A describes the definition of collision vertices, charged-particle tracks, jets, and b -jets. Following the discussion of objects, Section IV B describes the particle-level definition of the measurement phase space and the detector-level selections used to create an enriched sample of jets resulting from $g \rightarrow b\bar{b}$.

A. Object reconstruction, identification and association

Collision vertices are reconstructed from ID tracks. Each vertex is required to be associated with at least two tracks with $p_T > 0.4$ GeV. The primary hard-scattering vertex of the event is chosen to be the vertex having the highest $\sum p_T^2$ calculated using all associated tracks. Particle-level events

in simulation are considered before the addition of pileup and therefore there is no ambiguity in selecting the collision vertex.

Calorimeter jets are built from calibrated topological calorimeter-cell clusters [67] using the anti- k_t [68] algorithm with radius parameter $R = 1.0$ as implemented in FastJet [69]. Jets are groomed using a trimming procedure [70]. This procedure reclusters the constituents of a jet into subjets with a smaller radius of size $R_{\text{sub}} = 0.2$ and removes those subjets with a low fraction of the full jet momentum $f_{\text{cut}} = 0.05$. Following jet grooming, the mass and momentum of the resulting jets are corrected so that the detector-level values match the particle-level values on average [71]. These large-radius jets are proxies for the gluons.

Smaller-radius jets are used as proxies for the b -quarks originating from the gluons. For this purpose, jets are clustered using tracks as inputs (*track-jets*). Track-jets clustered from tracks with $p_T > 500$ MeV that have been well matched to the primary vertex² and are composed of at least one pixel detector hit and at least six hits in the silicon tracker [72] are constructed using the anti- k_t algorithm with $R = 0.2$. Track-jets are required to have at least two tracks. Four-vectors are calculated for each track, assuming the mass of the charged pion. Small-radius jets are matched to large-radius jets via ghost association [73]. This matching procedure creates ghost versions of the small-radius jets with the same direction but infinitesimal p_T . Jet clustering is repeated and small-radius jets are assigned to the large-radius jet that contains their ghosted version. Since the jet finding algorithm is infrared safe, the four-momenta of the jets are unaffected by the addition of ghosts.

Particle-level jets are clustered using the same algorithms as for detector-level jets, except the inputs to jet finding are all stable particles ($c\tau > 10$ mm) excluding all muons and neutrinos. The same trimming algorithm applied to calorimeter jets is also applied to the large-radius particle-level jets. Particle-level track-jets are formed from all stable charged particles that have $p_T > 500$ MeV and $|\eta| < 2.5$, excluding muons.

Track-jets that are likely to have originated from the fragmentation of a b -quark (b -jet) are identified using the MV2c10 algorithm [74,75], which is a combination of three baseline algorithms IP3D, SV, and JetFitter. The IP3D algorithm uses log-likelihood ratios of the three-dimensional signed impact parameter significance of tracks associated with jets. The SV tagger reconstructs the secondary decay vertices of b -hadrons. The JetFitter algorithm reconstructs the topology of detached vertices along the b -hadron decay axis. Finally, the MV2c10 algorithm combines the outputs of the baseline algorithms with a boosted decision tree and assigns a probability of a jet

²The transverse impact parameter must be less than 2 mm and the longitudinal impact parameter multiplied by the sine of the polar angle must be less than 3 mm.

being a b -jet, c -jet, or light-flavor jet. The selected working point corresponds to a b -jet efficiency, a c -jet efficiency, and a light-flavor-jet rejection of $\epsilon_b = 60\%$, $\epsilon_c = 15\%$, and $1/\epsilon_{\text{light}} = 480$, respectively, as measured in $t\bar{t}$ events for jets with $p_T > 10$ GeV and $|\eta| < 2.5$. A p_T - and η -dependent scale factor is applied to MC events to account for the measured efficiency difference between data and MC events at the chosen working point [76]. This scale factor is consistent with unity for b -jets with uncertainties ranging from a few to 10% and the scale factor for light-flavor jets is between 1.5 and 2 with an uncertainty that ranges from about 30%–50%.

Particle-level track-jets are tagged as b -jets if there is a b -hadron from the simulated event record with $p_T > 5$ GeV that is ghost-associated with the jet. If instead a hadron containing a c -quark from the event record with $p_T > 5$ GeV can be matched to the jet by ghost-association, it is declared a c -jet. All other jets are declared to be light-flavor jets.

B. Event selection

At detector level events are selected using single-jet triggers. In the first-level trigger, a sliding-window algorithm based on low-granularity calorimeter towers records events with transverse energy greater than 100 GeV. In the high-level trigger, $R = 1.0$ anti- k_t jets are formed from calibrated calorimeter-cell clusters and the p_T threshold is 420 GeV. This trigger scheme is fully efficient for calibrated offline jets with $p_T > 450$ GeV and $|\eta| < 2$ and therefore these kinematic requirements are used to select jets for the measurement. The offline analysis requires the highest- p_T calorimeter jet to have at least two associated track-jets with $p_T > 10$ GeV and $|\eta| < 2.5$. If there are more than two track-jets, only the leading two are used for subsequent analysis. In order to enhance the $g \rightarrow b\bar{b}$ purity, the leading track-jet associated with the selected calorimeter jet must be b -tagged by the MV2c10 algorithm at the 60% efficiency working point. Requiring both track-jets to be b -tagged increases the purity but degrades the precision of the background fit described in Sec. VI and so only one is required.

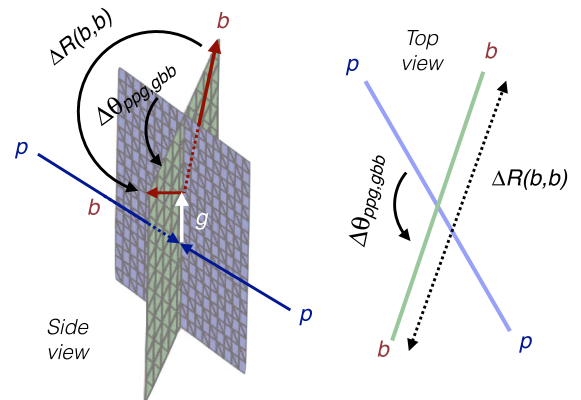


FIG. 2. Schematic diagrams illustrating the $\Delta R(b, b)$ and $\Delta\theta_{\text{ppg}, \text{gbb}}$ observables. In this example, the gluon is emitted at $\eta = 0$.

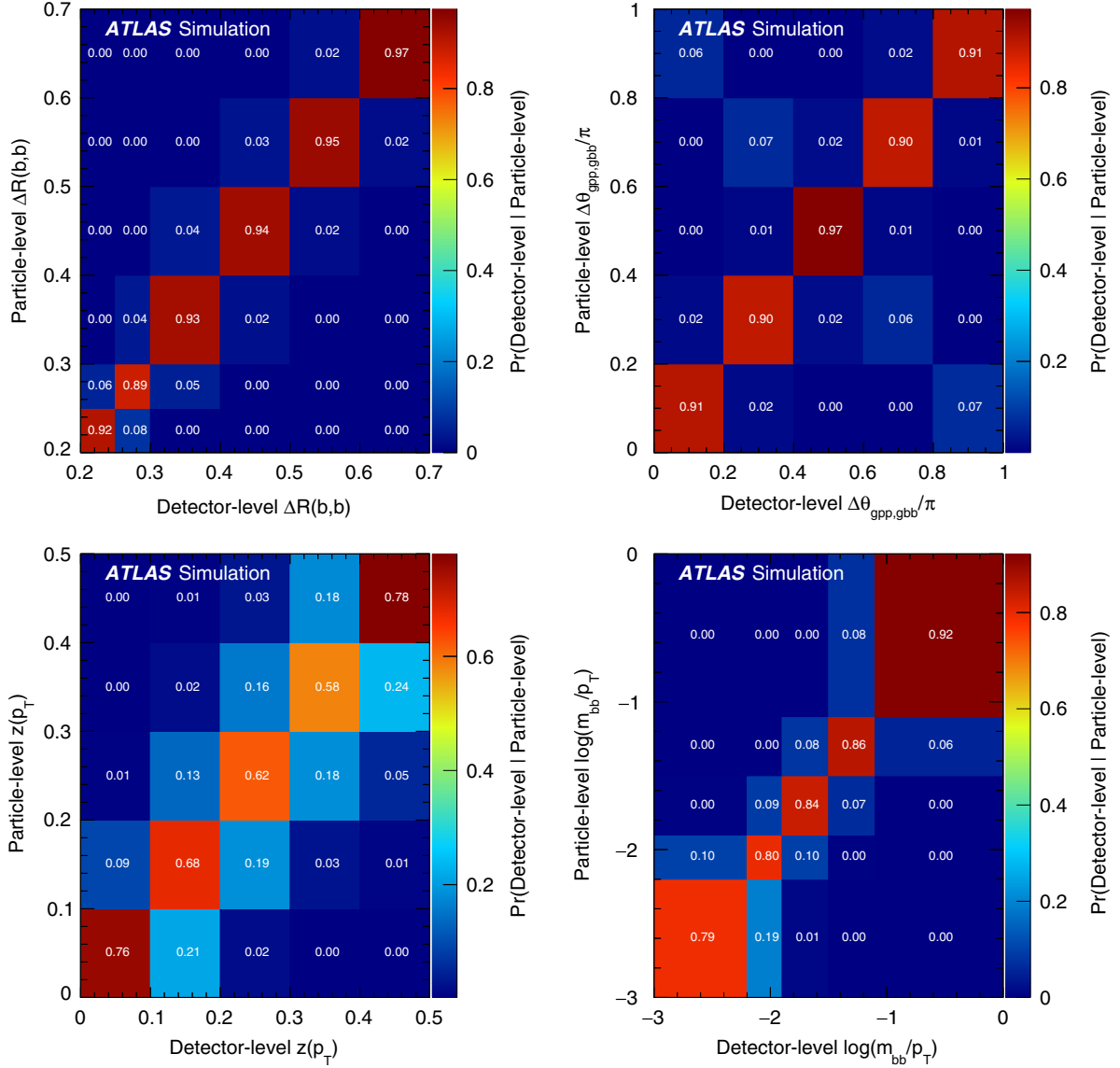


FIG. 3. The detector response is represented as the conditional probability of the detector-level quantity given the particle-level quantity, written as $\text{Pr}(\text{detector-level}|\text{particle-level})$, in simulation for $\Delta R(b,b)$ (top left), $\Delta\theta_{\text{ppg,gb}\bar{b}}$ (top right), $z(p_T)$ (bottom left), and $\log(m_{bb}/p_T)$ (bottom right). The small antidiagonal component for $\Delta\theta_{\text{ppg,gb}\bar{b}}$ is due to cases where the leading and subleading track-jets are swapped between detector level and particle level so $\Delta\theta_{\text{ppg,gb}\bar{b}} \mapsto \pi - \Delta\theta_{\text{ppg,gb}\bar{b}}$.

At particle level events are required to have at least one large-radius jet with $p_T > 450$ GeV. The leading jet needs to have at least two associated particle-level track-jets with $p_T > 10$ GeV. Both of the associated small-radius jets must be tagged as b -jets.

This inclusive event selection produces a sample where QCD scattering processes dominate.

V. OBSERVABLES

The kinematic properties of the $g \rightarrow b\bar{b}$ process are characterized by three quantities: the opening angle between the b -quarks, the momentum sharing between

the b -quarks, and the orientation of the gluon splitting relative to the gluon production plane. The first of these quantities is probed by measuring the $\Delta R(b,b) = \sqrt{\Delta\phi(b,b)^2 + \Delta\eta(b,b)^2}$ between track-jets. Momentum sharing is explored using the quantity $z(p_T) = p_{T,2}/(p_{T,1} + p_{T,2})$, where $p_{T,1}$ and $p_{T,2}$ are the transverse momenta of the leading and subleading track-jets, respectively. A quantity sensitive to the relative orientation of the gluon splitting is $\Delta\theta_{\text{ppg,gb}\bar{b}}$, which is the angle between the plane spanned by the beam line and the vector sum of the two track-jets and the plane spanned by the two track-jets. The angular quantities $\Delta R(b,b)$ and $\Delta\theta_{\text{ppg,gb}\bar{b}}$ are depicted in Fig. 2.

In addition to these quantities, the dimensionless mass $\log(m_{b\bar{b}}/p_T)$ is also measured, where the mass and p_T in the logarithm are computed from the four-vector sum of the two track-jets. The $b\bar{b}$ mass is an important observable for measurements and searches with Higgs and Z bosons. Track-jets, in contrast to the calorimeter-based subjects from trimming, are used due to their excellent angular resolution; in simulation, there is little difference between using the directions from the track-jets, the full jets (including neutrals), or the b -hadrons from the b -quark fragmentation. There is some discrepancy between these different objects for the energy-dependent observables, but the track-jets are still useful due to their excellent momentum resolution in the gluon p_T range probed in this measurement. The excellent angular and momentum resolutions are presented in Fig. 3, which shows the detector response for all four observables targeted with this measurement.

VI. BACKGROUND ESTIMATION

After the event selection, the contribution from large-radius jets that do not have two associated track-jets containing b -hadron is subtracted from data, as described below, before correcting for detector effects. The fraction of background events may not be well modeled by the simulation, so correction factors are determined from data template fits to the impact parameter distribution and applied for each bin of the four target observables of the analysis prior to subtraction.³ In each bin of the target observable distributions, the distribution of the signed impact parameter significance s_{d_0} is fitted to data using templates from simulation while letting the fraction of each flavor component float in the fit [50,51]. For a given track, $s_{d_0} = s_j |d_0| / \sigma(d_0)$, where d_0 is the transverse impact parameter relative to the beam line and $\sigma(d_0)$ is the uncertainty in d_0 from the track fit and the variable s_j is the sign of d_0 with respect to the jet axis: $s_j = +1$ if $\sin(\phi_{\text{jet}} - \phi_{\text{track}}) \cdot d_0 > 0$ and $s_j = -1$ otherwise. The transverse impact parameter itself is signed, with $\text{sign}(d_0) = \text{sign}(\vec{p}_{T,\text{track}} \times (\vec{r}_{\text{IP},xy} - \vec{r}_{\text{PV},xy}))$, where $\vec{r}_{\text{IP},xy}$ and $\vec{r}_{\text{PV},xy}$ are the locations of the track impact parameter and primary vertex, respectively, in the transverse plane.

Due to the long lifetime of b -hadrons, the values of s_{d_0} for tracks in b -jets tend to be larger than those for tracks in c -jets and light-flavor jets. Therefore, the distribution of s_{d_0} can be used to extract the fractions of b -jets, c -jets, and light-flavor jets using templates from simulation. For each track-jet j_i , the s_{d_0} from the track with the second largest $|s_{d_0}|$, called $s_{d_0}^{\text{sub}}(j_i)$, is used for the extraction. The leading and third-leading s_{d_0} values (ordered by $|s_{d_0}|$) are used as a validation of the flavor-fraction fitting procedure and

produce consistent results. The leading s_{d_0} is not as well modeled as $s_{d_0}^{\text{sub}}$ and therefore the χ^2 resulting from the fit procedure described below is slightly worse. The value of $s_{d_0}^{\text{sub}}$ does not have a strong dependence on jet p_T , so the fit is performed inclusively. This choice was validated by using p_T -binned fits, which produce results consistent with the inclusive approach.

A binned maximum-likelihood fit to $s_{d_0}^{\text{sub}}(j_1)$ and $s_{d_0}^{\text{sub}}(j_2)$ is performed to extract the flavor fractions. Given the flavors of track-jets j_1 and j_2 ($p_{T,1} \geq p_{T,2}$), $s_{d_0}^{\text{sub}}(j_1)$ and $s_{d_0}^{\text{sub}}(j_2)$ are well approximated as being statistically independent (linear correlation is less than 5%). Therefore, the probability distribution $p(s_{d_0}^{\text{sub}}(j_1), s_{d_0}^{\text{sub}}(j_2))$ can be approximated by the product of marginals $p(s_{d_0}^{\text{sub}}(j_1)) \times p(s_{d_0}^{\text{sub}}(j_2))$. This approximation reduces a two-dimensional fit to a simultaneous fit of two one-dimensional distributions. In order to increase the robustness of the fit, flavor combinations with similar templates are merged. The three templates used for each bin of the target observable are BB (signal), B, and L + C. The BB template only includes events where both jets are labeled as b -jets using MC particle-level flavor labeling. The B template is an aggregation of bl and bc events in which the leading track-jets are labeled as b and the subleading track-jets are labeled as light-flavor or c in particle-level flavor labeling. This template also includes cases in which a $g \rightarrow b\bar{b}$ splitting was fully contained inside one small-radius track-jet and the second track-jet is due to a light quark or gluon. The rest of the events are merged into the L + C template. The nominal results use fits from PYTHIA templates. Uncertainties in the templates, in particular resulting from the template merging scheme and from the choice of generator, are described in Sec. VIII A.

Examples of the flavor-fraction determination fits are shown in Fig. 4 for one bin of $\Delta R(b, b)$. The template binning was chosen to have enough sensitivity in the tails while also having sufficient simulation statistics to populate the templates; for reference, the MC statistical uncertainty is shown in the error bands. Since the leading track-jet is required to be b -tagged, the distribution of $s_{d_0}^{\text{sub}}(j_1)$ is broader and shifted toward more positive values than the distribution of $s_{d_0}^{\text{sub}}(j_2)$. In contrast, the subleading jet is most often a light-flavor jet for both the B and L + C categories and therefore $s_{d_0}^{\text{sub}}(j_2)$ is nearly symmetric about zero. The BB template is similar in shape for the leading and subleading track-jets. For this particular fit, the χ^2 per degree of freedom improves from 72/22 (prefit) to 13.5/22 (postfit). As a result of the fit, the background fraction changes from 79.6% to 82.8%. A comparison of the prefit and postfit flavor fractions for all bins of ΔR as well as the other observables is presented in Fig. 5. Except for $\Delta\theta_{\text{ppg,gb}}^{\text{bb}}$ and the highest bin of $z(p_T)$ the PYTHIA simulation prediction for the shape of the flavor-fraction

³As these fits are performed at detector level, there is no statistical correlation between bins. Therefore, the fits are performed independently for each observable bin.

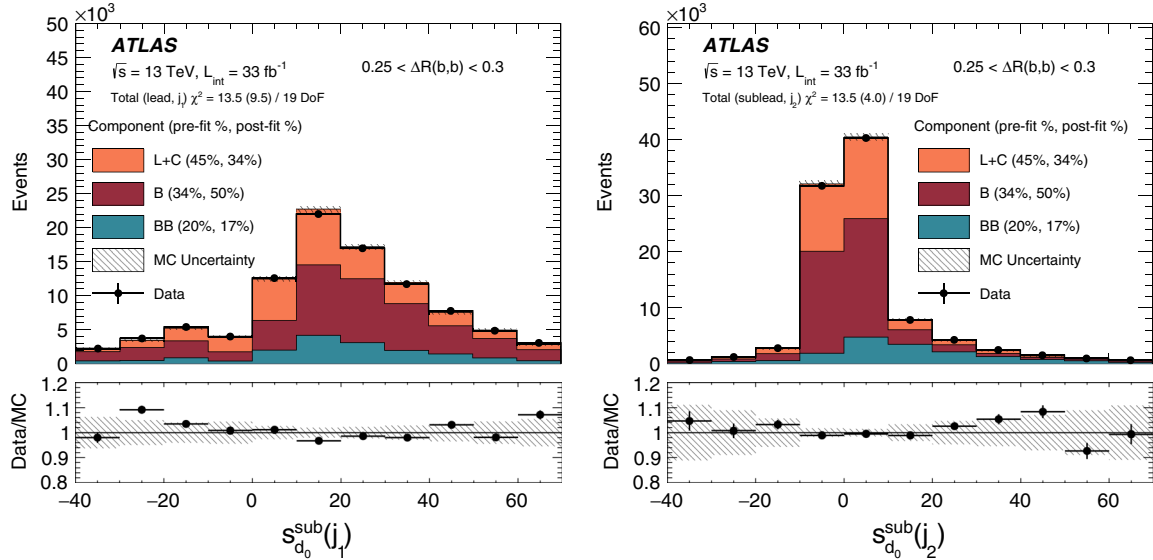


FIG. 4. The distribution of $S_{d_0}^{sub}$ in data and in simulation, postfit, for the higher- p_T track-jet (left) and for the lower- p_T track-jet (right) in the bin $0.25 < \Delta R(b, b) < 0.3$. The three components are the signal double- b (BB), the background single b (B), and the background non- b components (L + C). Percentages reported in the legend indicate the prefit and postfit fraction of each component. Only data and MC statistical uncertainties are shown. The lower panel shows the ratio between data and the postfit simulation.

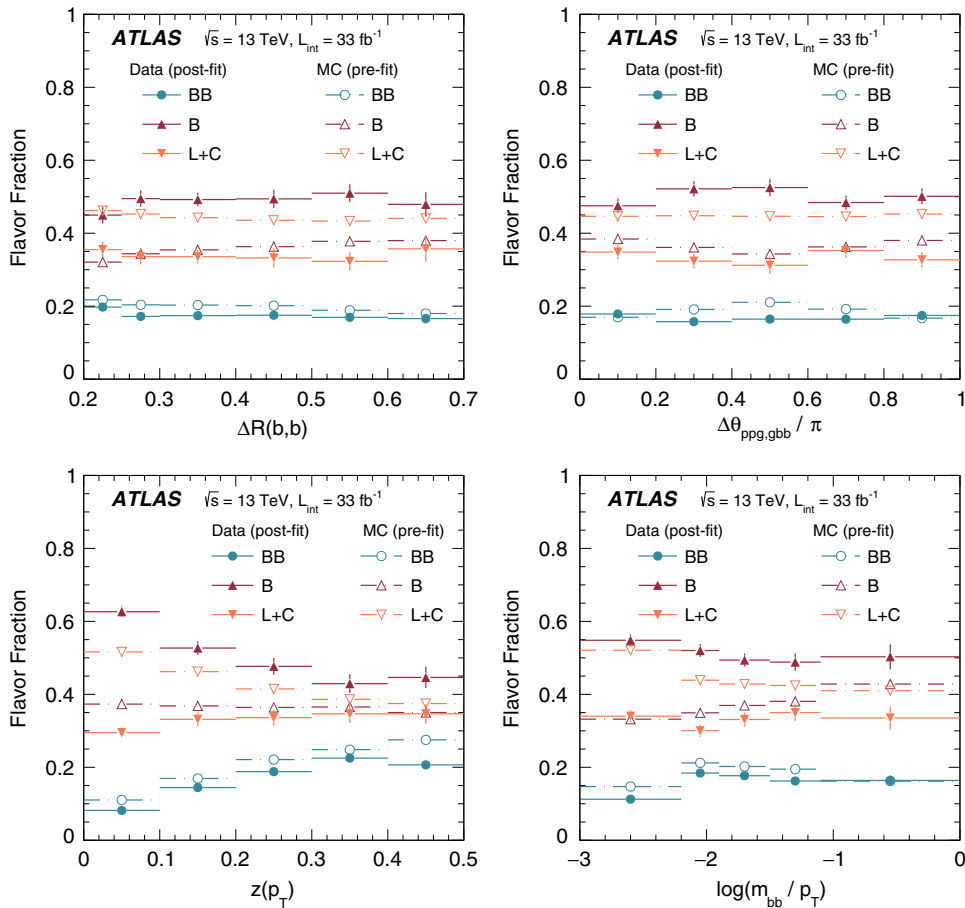


FIG. 5. The prefit (MC) and postfit (data) flavor fractions for $\Delta R(b, b)$ (top left), $\Delta\theta_{ppg, gbb}$ (top right), $z(p_T)$ (bottom left), and $\log(m_{bb}/p_T)$ (bottom right) are indicated with open and solid markers respectively. The error bars include only statistical uncertainties from the flavor-fraction fit. The fit’s systematic uncertainties are comparable in magnitude, but correlated across the bins. The impact of both the flavor-fraction fit’s statistical and systematic uncertainties on the final results is presented in Table I.

distribution is accurate for the BB fraction. In all cases the BB yield is slightly overestimated. The flavor fractions from B and L + C are inverted between PYTHIA and data.

VII. UNFOLDING

After subtracting the background from the detector-level distributions, as described in Sec. VI, the data are corrected for resolution and acceptance effects. The fiducial volume of the measurement is described by the particle-level object and event selection in Sec. IV. First, the data are corrected for events that pass the detector-level selection but not the particle-level selection using the simulations introduced in Sec. III. Then, the iterative Bayes (IB) unfolding technique [77] is used to correct for the detector resolution in events that pass both the detector-level and particle-level selections. The IB method is applied with four iterations implemented in the RooUnfold framework [78]. After the application of the response matrix, a final correction is applied to account for events that pass the particle-level but not detector-level selection. Uncertainties in the unfolding procedure are described in Sec. VIII.

VIII. UNCERTAINTIES

Systematic and statistical uncertainties were assessed for each aspect of the analysis, including the background subtraction, acceptance and efficiency correction factors, response matrix, and unfolding method. For each uncertainty, a component of the analysis chain is varied and then the entire procedure including the background subtraction is repeated. Table I provides a summary of the systematic uncertainties for each observable. The jet energy scale, the unfolding, and the theoretical modeling uncertainties dominate. Further details about each category are provided in Sec. VIII A for the uncertainties associated with each analysis object, in Sec. VIII B for the background fit procedure uncertainty, and in Sec. VIII C for the unfolding method and theoretical modeling uncertainties.

TABLE I. Summary of systematic uncertainty sizes for each observable for the normalized differential cross sections.

	$\Delta R(b, b)$	$\Delta\theta_{\text{ppg, gbb}}$	$z(p_T)$	$\log(m_{bb}/p_T)$
Calorimeter jet energy	2–3%	2–5%	3–6%	2–4%
Flavor tagging	1–2%	<1%	<1%	1–2%
Tracking	1–2%	2–3%	2–4%	1–2%
Background fit	3–6%	1%	2–9%	2–5%
Unfolding method	<1%	<1%	1–4%	1%
Theoretical modeling	2–11%	2–14%	3–9%	4–12%
Statistical	1%	1%	1%	1%
Total	5–13%	5–15%	7–13%	6–13%

A. Object reconstruction

Each object used in the analysis has an associated uncertainty. These uncertainties affect the acceptance factors and the response matrix, as well as the background fit templates.

1. Calorimeter jets

The energies of large-radius jets are shifted and smeared to account for uncertainties in both the bias and variance of the reconstructed energy. Jet energy scale uncertainties are determined by comparing calorimeter-based and tracker-based jet energy measurements in inclusive dijet events, and range from 2% to 6% [79].

2. Flavor tagging

Data/MC corrections (“scale factors”) and uncertainties in the b -tagging efficiencies and c -jet misidentification rates are determined from $t\bar{t}$ events [80]. Light-flavor misidentification rates are studied using dijet events. The b -jet uncertainties are 5%–10%, while the c -jet uncertainties are 20% and light-flavor jet uncertainties are about 50%. Uncertainties for track-jets with $p_T > 300$ GeV are extrapolated from low- p_T jets as there are too few events with high- p_T jets for a proper calibration. Extrapolation uncertainties are evaluated by varying quantities such as impact parameter resolutions and descriptions of the detector material. The extrapolated uncertainties are added in quadrature on top of the data-based p_T - and η -dependent uncertainties and range from 20% to 100% depending on the p_T and the flavor of the jet. As the flavor fractions are constrained *in situ*, there is a significant reduction from the prior flavor-tagging uncertainty values described above. In particular, there is little sensitivity to the background scale factors and there is no sensitivity to inclusive flavor-tagging scale factors for b -jets. Residual $\Delta R(b, b)$ -dependent scale factor uncertainties that account for differences in the modeling of isolated versus nonisolated b -jets are derived from dedicated performance studies [50,51].

3. Tracking

Systematic uncertainties are estimated for the track reconstruction efficiency, fake rate, and track parameter scales and resolutions. The main source of inclusive tracking inefficiency is multiple scattering in the ID, so the uncertainty is set by the accuracy with which the ID material is simulated [81]. This leads to a 0.5% uncertainty for $|\eta| < 0.1$, which grows to 2.7% at the end of the ID acceptance. An additional source of inefficiency arises inside the high-multiplicity environment in the cores of jets due to silicon pixel and microstrip cluster merging. The uncertainty in the modeling of this density-induced inefficiency is about 0.8% [82,83]. Fake tracks are due to combinations from multiple charged particles. The track selection described in Sec. IV reduces the contribution of

fake tracks to much less than 1% with a relative uncertainty that is about 30% [84]. The track parameters that are most relevant for this analysis are p_T and d_0 . Weak modes in the ID alignment cause a bias in the track sagitta that is corrected for using a dedicated calibration and the calibration uncertainty is propagated through to the measurement [72]. The modeling of the d_0 scale and resolution was studied in $Z \rightarrow \mu^+\mu^-$ events at low p_T and in dijet events at high p_T [72] and is used to assign an uncertainty to the modeling of these important track properties.

B. Background fit

In addition to the fit validations described in Sec. VI, several aspects of the fit are varied in order to assess the uncertainty in the extracted flavor fractions.

1. Fit range

The nominal flavor fraction fit is performed for $s_{d_0}^{\text{sub}} \in [-40, 70]$. In order to assess the impact of this choice and the sensitivity to the $s_{d_0}^{\text{sub}}$ tails, the fit is repeated while excluding the left and right tails of the distributions, corresponding to $s_{d_0}^{\text{sub}} \in [-30, 70]$ and $s_{d_0}^{\text{sub}} \in [-40, 60]$.

2. Template merging scheme

Merging background components to form three aggregated templates fixes the relative fractions of the template subcomponents. The sensitivity of the fitted flavor fractions to this choice is estimated by varying each merged background component up or down by a factor of 2. The fit range has a bigger impact on the uncertainty than the merging variations of the flavor fractions.

C. Unfolding method and theoretical modeling

An uncertainty resulting from the unfolding method described in Sec. VII is determined by unfolding the prediction from a different simulation with the nominal procedure. The alternative simulation is constructed by reweighting the nominal particle-level spectrum so that the simulated detector-level spectrum, obtained by propagating the reweighted particle-level spectrum through the response matrix, agrees well with the data. The modified detector-level distribution is unfolded with the nominal response matrix and the difference between this and the reweighted particle-level spectrum is an indication of the bias due to the unfolding method (in particular, the choice of prior) [85].

The unfolded result can depend on the modeling of jet fragmentation through the background fit, the prior, the response matrix, and the correction factors. The s_{d_0} distribution does not strongly depend on the properties of the jet radiation pattern, but an uncertainty is determined by taking the fitted background using templates from SHERPA instead of PYTHIA. Variations in the prior are already accounted for in the data-driven nonclosure uncertainty

described above. The rest of the contributions are evaluated by comparing the result using PYTHIA with the result using the alternative SHERPA sample described in Sec. VI. This comparison is decomposed into components corresponding to varying only the response matrix or only the initial/final correction factors. Varying only one component at a time is possible by reweighting a component of the PYTHIA simulation to match the SHERPA simulation and then evaluating the relative difference in the unfolded result. All of the components are added in quadrature to determine the total uncertainty due to fragmentation modeling. Each component is treated as uncorrelated because the uncertainty is based on only two fragmentation models and therefore a potential reduced uncertainty from exploiting potentially unphysical correlations between kinematic properties impacting acceptance and substructure attributes impacting the response is avoided.

IX. RESULTS

The unfolded results along with multiple parton shower MC predictions are presented in Fig. 6. By construction, $0.2 \leq \Delta R \leq 1.0$ and the peak around 0.3 is due to the radius of the track-jets. Furthermore, $0 \leq z(p_T) \leq 0.5$, with some distortions to the natural distribution at low values due to the p_T threshold applied to the small-radius track-jets.

The SHERPA predictions are generally more accurate than those from PYTHIA, although there are significant differences between both generators and the data at low mass, low $z(p_T)$ and for all $\Delta\theta_{\text{ppg,gb}}^{\text{bb}}$. The $\Delta\theta_{\text{ppg,gb}}^{\text{bb}}$ distribution in data appears to be inverted with respect to the one from PYTHIA (with a minimum instead of maximum at $\pi/2$) while SHERPA predicts a relatively uniform distribution. For comparison, the figure contains a version of PYTHIA⁴ with the azimuthal asymmetries induced by gluon polarization turned off.⁵ This sample appears to be closer to SHERPA and also to the data, consistent with the studies in Ref. [86], which also suggest a good agreement with simulations that include higher-order effects. In general, the properties of gluon polarization inside unpolarized hadrons are largely unconstrained by experimental data (see e.g., Ref. [87] and references therein). This and future measurements of $\Delta\theta_{\text{ppg,gb}}^{\text{bb}}$ may provide a new way to extract p_T -dependent parton distributions in order to better understand proton structure and further improve the precision of various cross-section calculations [88].

In addition to studying gluon production properties, $g \rightarrow b\bar{b}$ provides a handle on gluon fragmentation. Due to the large b -quark mass and in general the large m_{bb} mass that is

⁴Due to the available settings in PYTHIA, different versions were used for these comparisons. It was checked that there is no significant difference in $\Delta\theta_{\text{ppg,gb}}^{\text{bb}}$ between PYTHIA versions 8.186 and 8.230.

⁵TimeShower:phiPolAsym=off and TimeShower:phiPolAsymHard=off.

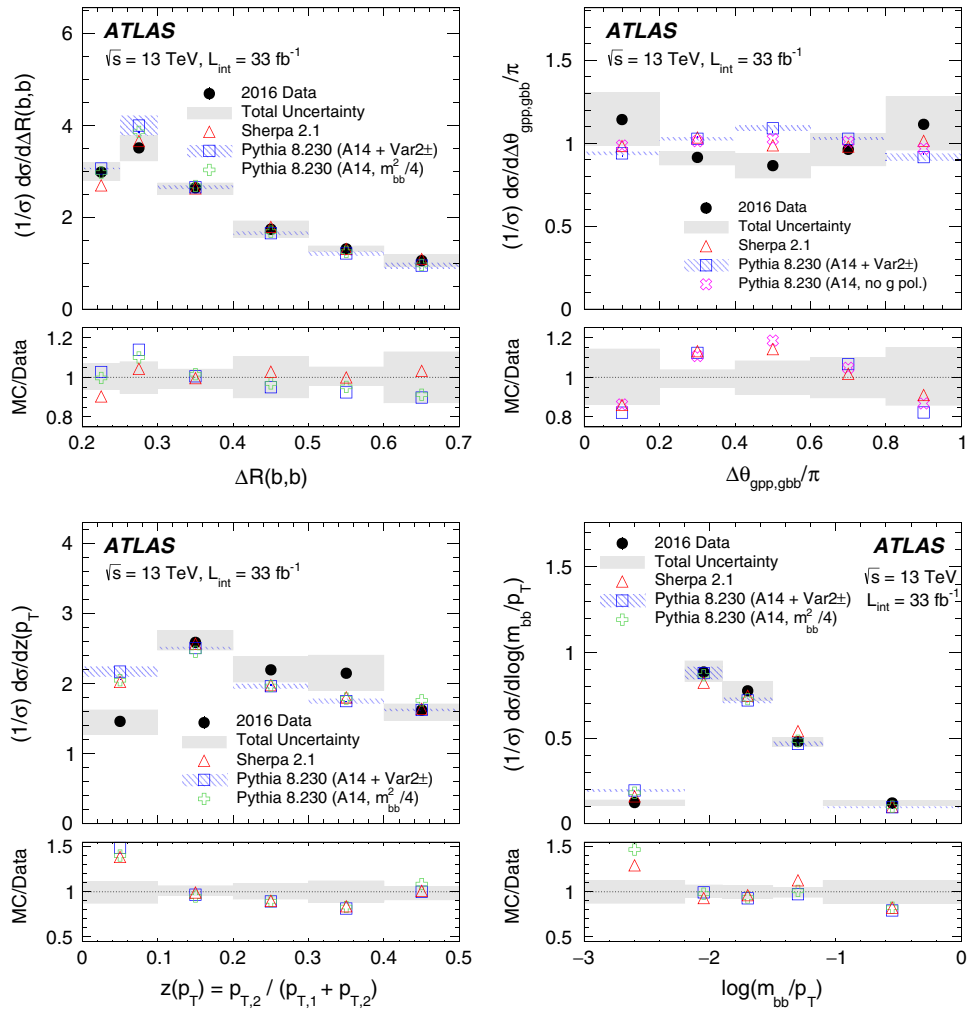


FIG. 6. The unfolded distribution of $\Delta R(b, b)$ (top left), $\Delta\theta_{\text{ppg,gb}}$ (top right), $z(p_T)$ (bottom left), and $\log(m_{bb}/p_T)$ (bottom right). Error bands represent the sum in quadrature of statistical and systematic uncertainties (see Sec. VIII). These data are compared with predictions from the PYTHIA and SHERPA MC simulations. The bands for the PYTHIA prediction represented by a square indicate the $\text{Var}2\pm$ variations (dominated by a $\pm 10\%$ variation in the final-state shower α_s). The additional set of PYTHIA markers use $m_{bb}^2/4$ for the renormalization scale.

possible after splitting, there are many formally equivalent model choices in describing gluon fragmentation. For example, the scale at which the strong coupling constant acts (renormalization scale) may be better described as scaling with m_{bb}^2 instead of the PYTHIA default $p_{T,bb}^2$. To illustrate the sensitivity of $\Delta R(b, b)$, $z(p_T)$ and $\log(m/p_T)$ to fragmentation settings in PYTHIA, the plots of Fig. 6 show the final-state radiation variations of the A14 tune (indicated as an uncertainty band in the plot) as well as a different way to treat the b -quark mass in the QCD splitting kernels indicated by the $m_{bb}^2/4$ variation ($m_{bb}^2/4$ instead of $p_{T,bb}^2$ for the renormalization scale).⁶ No variation describes all of the data, but some variations are worse than others.

⁶TimeShower:weightGluonToQuark=5 and TimeShower:scaleGluonToQuark=0.25.

For example, the $\text{Var}2 + \text{A14}$ variation, which increases the final-state shower $\alpha_s(M_Z)$ value to 0.139, moves the prediction further from the data in nearly all measurement bins. Related variations (not shown) such as using m_{bb}^2 instead of $p_{T,bb}^2$ as the renormalization scale, adding additional phase-space factors, or suppressing high-mass $b\bar{b}$ pairs, are not significantly different from the nominal PYTHIA setup.⁷

⁷Variations of TimeShower:weightGluonToQuark and TimeShower:scaleGluonToQuark; when TimeShower:weightGluonToQuark=1, then the $g \rightarrow b\bar{b}$ kernel is weighted by an extra β phase-space factor; when TimeShower:weightGluonToQuark=5, this kernel is reweighted to $\alpha_s(m_{bb}^2)$ instead of $\alpha_s(p_T^2)$; when TimeShower:weightGluonToQuark=8, there is an additional factor that suppresses the rate of high-mass $b\bar{b}$ pairs.

X. CONCLUSION

This paper presents a measurement of various properties of $g \rightarrow b\bar{b}$ at high p_T and low $\Delta R(b, b)$ from 33 fb^{-1} of $\sqrt{s} = 13 \text{ TeV}$ pp collisions recorded by the ATLAS detector at the LHC. A flavor-fraction fit is used to remove contributions from processes other than $g \rightarrow b\bar{b}$. The fitted fractions significantly disagree with the prefit PYTHIA predictions and suggest that further studies could improve the modeling of analyses sensitive to these fractions. The measured properties are unfolded to correct for the detector acceptance and resolution for direct comparison with particle-level models. Comparisons are made at the particle level between the distributions and various models of jet formation. Simulations from the SHERPA event generator generally provide a better model than PYTHIA, especially for the $\Delta\theta_{\text{ppg, gbb}}$ observable, which is sensitive to the modeling of the gluon polarization. The particle-level spectra are publicly available [89] for further interpretation and can be used to validate QCD MC predictions and tune their models' free parameters.

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M. Aaboud,^{34d} G. Aad,⁹⁹ B. Abbott,¹²⁵ D. C. Abbott,¹⁰⁰ O. Abidinov,^{13,†} B. Abeloos,¹²⁹ D. K. Abhayasinghe,⁹¹ S. H. Abidi,¹⁶⁴ O. S. AbouZeid,³⁹ N. L. Abraham,¹⁵³ H. Abramowicz,¹⁵⁸ H. Abreu,¹⁵⁷ Y. Abulaiti,⁶ B. S. Acharya,^{64a,64b,p} S. Adachi,¹⁶⁰ L. Adam,⁹⁷ L. Adamczyk,^{81a} L. Adamek,¹⁶⁴ J. Adelman,¹¹⁹ M. Adersberger,¹¹² A. Adiguzel,^{12c,ah} T. Adye,¹⁴¹ A. A. Affolder,¹⁴³ Y. Afik,¹⁵⁷ C. Agapopoulou,¹²⁹ C. Agheorghiesei,^{27c} J. A. Aguilar-Saavedra,^{137f,137a,ag} F. Ahmadov,^{77,ae} G. Aielli,^{71a,71b} S. Akatsuka,⁸³ T. P. A. Åkesson,⁹⁴ E. Akilli,⁵² A. V. Akimov,¹⁰⁸ G. L. Alberghi,^{23b,23a} J. Albert,¹⁷³ P. Albicocco,⁴⁹ M. J. Alconada Verzini,⁸⁶ S. Alderweireldt,¹¹⁷ M. Aleksa,³⁵ I. N. Aleksandrov,⁷⁷ C. Alexa,^{27b} D. Alexandre,¹⁹ T. Alexopoulos,¹⁰ M. Alhroob,¹²⁵ B. Ali,¹³⁹ G. Alimonti,^{66a} J. Alison,³⁶ S. P. Alkire,¹⁴⁵ C. Allaire,¹²⁹ B. M. M. Allbrooke,¹⁵³ B. W. Allen,¹²⁸ P. P. Allport,²¹ A. Aloisio,^{67a,67b} A. Alonso,³⁹ F. Alonso,⁸⁶ C. Alpigiani,¹⁴⁵ A. A. Alshehri,⁵⁵ M. I. Alstary,⁹⁹ B. Alvarez Gonzalez,³⁵ D. Álvarez Piqueras,¹⁷¹ M. G. Alvigi,^{67a,67b} B. T. Amadio,¹⁸ Y. Amaral Coutinho,^{78b} A. Ambler,¹⁰¹ L. Ambroz,¹³² C. Amelung,²⁶ D. Amidei,¹⁰³ S. P. Amor Dos Santos,^{137a,137c} S. Amoroso,⁴⁴ C. S. Amrouche,⁵² F. An,⁷⁶ C. Anastopoulos,¹⁴⁶ N. Andari,¹⁴² T. Andeen,¹¹ C. F. Anders,^{59b} J. K. Anders,²⁰ A. Andreazza,^{66a,66b} V. Andrei,^{59a} C. R. Anelli,¹⁷³ S. Angelidakis,³⁷ I. Angelozzi,¹¹⁸ A. Angerami,³⁸ A. V. Anisenkov,^{120b,120a} A. Annovi,^{69a} C. Antel,^{59a} M. T. Anthony,¹⁴⁶ M. Antonelli,⁴⁹ D. J. A. Antrim,¹⁶⁸ F. Anulli,^{70a} M. Aoki,⁷⁹ J. A. Aparisi Pozo,¹⁷¹ L. Aperio Bella,³⁵ G. Arabidze,¹⁰⁴ J. P. Araque,^{137a} V. Araujo Ferraz,^{78b} R. Araujo Pereira,^{78b} A. T. H. Arce,⁴⁷ F. A. Arduh,⁸⁶ J-F. Arguin,¹⁰⁷ S. Argyropoulos,⁷⁵ J.-H. Arling,⁴⁴ A. J. Armbruster,³⁵ L. J. Armitage,⁹⁰ A. Armstrong,¹⁶⁸ O. Arnaez,¹⁶⁴ H. Arnold,¹¹⁸ A. Artamonov,^{109,†} G. Artoni,¹³² S. Artz,⁹⁷ S. Asai,¹⁶⁰ N. Asbah,⁵⁷ E. M. Asimakopoulou,¹⁶⁹ L. Asquith,¹⁵³ K. Assamagan,²⁹ R. Astalos,^{28a} R. J. Atkin,^{32a} M. Atkinson,¹⁷⁰ N. B. Atlay,¹⁴⁸ K. Augsten,¹³⁹ G. Avolio,³⁵ R. Avramidou,^{58a} M. K. Ayoub,^{15a} A. M. Azoulay,^{165b} G. Azuelos,^{107,av} A. E. Baas,^{59a} M. J. Baca,²¹ H. Bachacou,¹⁴² K. Bachas,^{65a,65b} M. Backes,¹³² P. Bagnaia,^{70a,70b} M. Bahmani,⁸² H. Bahrasemani,¹⁴⁹ A. J. Bailey,¹⁷¹ V. R. Bailey,¹⁷⁰ J. T. Baines,¹⁴¹ M. Bajic,³⁹ C. Bakalis,¹⁰ O. K. Baker,¹⁸⁰ P. J. Bakker,¹¹⁸ D. Bakshi Gupta,⁸ S. Balaji,¹⁵⁴ E. M. Baldin,^{120b,120a} P. Balek,¹⁷⁷ F. Balli,¹⁴² W. K. Balunas,¹³² J. Balz,⁹⁷ E. Banas,⁸² A. Bandyopadhyay,²⁴ S. Banerjee,^{178,1} A. A. E. Bannoura,¹⁷⁹ L. Barak,¹⁵⁸ W. M. Barbe,³⁷ E. L. Barberio,¹⁰² D. Barberis,^{53b,53a} M. Barbero,⁹⁹ T. Barillari,¹¹³ M.-S. Barisits,³⁵ J. Barkeloo,¹²⁸ T. Barklow,¹⁵⁰ R. Barnea,¹⁵⁷ S. L. Barnes,^{58c} B. M. Barnett,¹⁴¹ R. M. Barnett,¹⁸ Z. Barnovska-Blenessy,^{58a} A. Baroncelli,^{72a} G. Barone,²⁹ A. J. Barr,¹³² L. Barranco Navarro,¹⁷¹ F. Barreiro,⁹⁶ J. Barreiro Guimarães da Costa,^{15a} R. Bartoldus,¹⁵⁰ A. E. Barton,⁸⁷ P. Bartos,^{28a} A. Basalaeu,⁴⁴ A. Bassalat,¹²⁹ R. L. Bates,⁵⁵ S. J. Batista,¹⁶⁴ S. Batlamous,^{34e} J. R. Batley,³¹ M. Battaglia,¹⁴³ M. Bause,^{70a,70b} F. Bauer,¹⁴² K. T. Bauer,¹⁶⁸ H. S. Bawa,¹⁵⁰ J. B. Beacham,¹²³ T. Beau,¹³³ P. H. Beauchemin,¹⁶⁷ P. Bechtel,²⁴ H. C. Beck,⁵¹ H. P. Beck,^{20,s} K. Becker,⁵⁰ M. Becker,⁹⁷ C. Becot,⁴⁴ A. Beddall,^{12d} A. J. Beddall,^{12a} V. A. Bednyakov,⁷⁷ M. Bedognetti,¹¹⁸ C. P. Bee,¹⁵² T. A. Beermann,⁷⁴ M. Begalli,^{78b} M. Begel,²⁹ A. Behera,¹⁵² J. K. Behr,⁴⁴ F. Beisiegel,²⁴ A. S. Bell,⁹² G. Bella,¹⁵⁸ L. Bellagamba,^{23b} A. Bellerive,³³ M. Bellomo,¹⁵⁷ P. Bellos,⁹ K. Beloborodov,^{120b,120a} K. Belotskiy,¹¹⁰ N. L. Belyaev,¹¹⁰ O. Benary,^{158,†} D. Benchekroun,^{34a} N. Benekos,¹⁰ Y. Benhamou,¹⁵⁸ E. Benhar Noccioli,¹⁸⁰ J. Benitez,⁷⁵ D. P. Benjamin,⁶ M. Benoit,⁵² J. R. Bensinger,²⁶ S. Bentvelsen,¹¹⁸ L. Beresford,¹³² M. Beretta,⁴⁹ D. Berge,⁴⁴ E. Bergeas Kuutmann,¹⁶⁹ N. Berger,⁵ B. Bergmann,¹³⁹ L. J. Bergsten,²⁶ J. Beringer,¹⁸ S. Berlendis,⁷ N. R. Bernard,¹⁰⁰ G. Bernardi,¹³³ C. Bernius,¹⁵⁰ F. U. Bernlochner,²⁴ T. Berry,⁹¹ P. Berta,⁹⁷ C. Bertella,^{15a} G. Bertoli,^{43a,43b} I. A. Bertram,⁸⁷ G. J. Besjes,³⁹ O. Bessidskaia Bylund,¹⁷⁹ N. Besson,¹⁴² A. Bethani,⁹⁸ S. Bethke,¹¹³ A. Betti,²⁴ A. J. Bevan,⁹⁰ J. Beyer,¹¹³ R. Bi,¹³⁶ R. M. Bianchi,¹³⁶ O. Biebel,¹¹² D. Biedermann,¹⁹ R. Bielski,³⁵ K. Bierwagen,⁹⁷ N. V. Biesuz,^{69a,69b} M. Biglietti,^{72a} T. R. V. Billoud,¹⁰⁷ M. Bindi,⁵¹ A. Bingul,^{12d} C. Bini,^{70a,70b} S. Biondi,^{23b,23a} M. Birman,¹⁷⁷ T. Bisanz,⁵¹ J. P. Biswal,¹⁵⁸ A. Bitadze,⁹⁸ C. Bittrich,⁴⁶ D. M. Bjergaard,⁴⁷ J. E. Black,¹⁵⁰ K. M. Black,²⁵ T. Blazek,^{28a} I. Bloch,⁴⁴ C. Blocker,²⁶ A. Blue,⁵⁵ U. Blumenschein,⁹⁰ Dr. Blunier,^{144a} G. J. Bobbink,¹¹⁸ V. S. Bobrovnikov,^{120b,120a} S. S. Bocchetta,⁹⁴ A. Bocci,⁴⁷ D. Boerner,⁴⁴ D. Bogavac,¹¹² A. G. Bogdanchikov,^{120b,120a} C. Bohm,^{43a} V. Boisvert,⁹¹ P. Bokan,^{51,169} T. Bold,^{81a} A. S. Boldyrev,¹¹¹

A. E. Bolz,^{59b} M. Bomben,¹³³ M. Bona,⁹⁰ J. S. Bonilla,¹²⁸ M. Boonekamp,¹⁴² H. M. Borecka-Bielska,⁸⁸ A. Borisov,¹²¹ G. Borissoy,⁸⁷ J. Bortfeldt,³⁵ D. Bortoletto,¹³² V. Bortolotto,^{71a,71b} D. Boscherini,^{23b} M. Bosman,¹⁴ J. D. Bossio Sola,³⁰ K. Bouaouda,^{34a} J. Boudreau,¹³⁶ E. V. Bouhova-Thacker,⁸⁷ D. Boumediene,³⁷ C. Bourdarios,¹²⁹ S. K. Boutle,⁵⁵ A. Boveia,¹²³ J. Boyd,³⁵ D. Boye,^{32b,ap} I. R. Boyko,⁷⁷ A. J. Bozson,⁹¹ J. Bracinik,²¹ N. Brahimi,⁹⁹ G. Brandt,¹⁷⁹ O. Brandt,^{59a} F. Braren,⁴⁴ U. Bratzler,¹⁶¹ B. Brau,¹⁰⁰ J. E. Brau,¹²⁸ W. D. Breaden Madden,⁵⁵ K. Brendlinger,⁴⁴ L. Brenner,⁴⁴ R. Brenner,¹⁶⁹ S. Bressler,¹⁷⁷ B. Brickwedde,⁹⁷ D. L. Briglin,²¹ D. Britton,⁵⁵ D. Britzger,¹¹³ I. Brock,²⁴ R. Brock,¹⁰⁴ G. Brooijmans,³⁸ T. Brooks,⁹¹ W. K. Brooks,^{144b} E. Brost,¹¹⁹ J. H. Broughton,²¹ P. A. Bruckman de Renstrom,⁸² D. Bruncko,^{28b} A. Bruni,^{23b} G. Bruni,^{23b} L. S. Bruni,¹¹⁸ S. Bruno,^{71a,71b} B. H. Brunt,³¹ M. Bruschi,^{23b} N. Bruscano,¹³⁶ P. Bryant,³⁶ L. Bryngemark,⁹⁴ T. Buanes,¹⁷ Q. Buat,³⁵ P. Buchholz,¹⁴⁸ A. G. Buckley,⁵⁵ I. A. Budagov,⁷⁷ M. K. Bugge,¹³¹ F. Bühner,⁵⁰ O. Bulekov,¹¹⁰ T. J. Burch,¹¹⁹ S. Burdin,⁸⁸ C. D. Burgard,¹¹⁸ A. M. Burger,⁵ B. Burghgrave,⁸ K. Burka,⁸² I. Burmeister,⁴⁵ J. T. P. Burr,¹³² V. Büscher,⁹⁷ E. Buschmann,⁵¹ P. Bussey,⁵⁵ J. M. Butler,²⁵ C. M. Buttar,⁵⁵ J. M. Butterworth,⁹² P. Butti,³⁵ W. Buttinger,³⁵ A. Buzatu,¹⁵⁵ A. R. Buzykaev,^{120b,120a} G. Cabras,^{23b,23a} S. Cabrera Urbán,¹⁷¹ D. Caforio,¹³⁹ H. Cai,¹⁷⁰ V. M. M. Cairo,² O. Cakir,^{4a} N. Calace,³⁵ P. Calafiura,¹⁸ A. Calandri,⁹⁹ G. Calderini,¹³³ P. Calfayan,⁶³ G. Callea,⁵⁵ L. P. Caloba,^{78b} S. Calvente Lopez,⁹⁶ D. Calvet,³⁷ S. Calvet,³⁷ T. P. Calvet,¹⁵² M. Calvetti,^{69a,69b} R. Camacho Toro,¹³³ S. Camarda,³⁵ D. Camarero Munoz,⁹⁶ P. Camarri,^{71a,71b} D. Cameron,¹³¹ R. Caminal Armadans,¹⁰⁰ C. Camincher,³⁵ S. Campana,³⁵ M. Campanelli,⁹² A. Camplani,³⁹ A. Campoverde,¹⁴⁸ V. Canale,^{67a,67b} M. Cano Bret,^{58c} J. Cantero,¹²⁶ T. Cao,¹⁵⁸ Y. Cao,¹⁷⁰ M. D. M. Capeans Garrido,³⁵ M. Capua,^{40b,40a} R. M. Carbone,³⁸ R. Cardarelli,^{71a} F. C. Cardillo,¹⁴⁶ I. Carli,¹⁴⁰ T. Carli,³⁵ G. Carlino,^{67a} B. T. Carlson,¹³⁶ L. Carminati,^{66a,66b} R. M. D. Carney,^{43a,43b} S. Caron,¹¹⁷ E. Carquin,^{144b} S. Carrá,^{66a,66b} J. W. S. Carter,¹⁶⁴ M. P. Casado,^{14g} A. F. Casha,¹⁶⁴ D. W. Casper,¹⁶⁸ R. Castelijns,¹¹⁸ F. L. Castillo,¹⁷¹ V. Castillo Gimenez,¹⁷¹ N. F. Castro,^{137a,137e} A. Catinaccio,³⁵ J. R. Catmore,¹³¹ A. Cattai,³⁵ J. Caudron,²⁴ V. Cavaliere,²⁹ E. Cavallaro,¹⁴ D. Cavalli,^{66a} M. Cavalli-Sforza,¹⁴ V. Cavasinni,^{69a,69b} E. Celebi,^{12b} L. Cerda Alberich,¹⁷¹ A. S. Cerqueira,^{78a} A. Cerri,¹⁵³ L. Cerrito,^{71a,71b} F. Cerutti,¹⁸ A. Cervelli,^{23b,23a} S. A. Cetin,^{12b} A. Chafaq,^{34a} D. Chakraborty,¹¹⁹ S. K. Chan,⁵⁷ W. S. Chan,¹¹⁸ W. Y. Chan,⁸⁸ J. D. Chapman,³¹ B. Chargeishvili,^{156b} D. G. Charlton,²¹ C. C. Chau,³³ C. A. Chavez Barajas,¹⁵³ S. Che,¹²³ A. Chegwiddden,¹⁰⁴ S. Chekanov,⁶ S. V. Chekulaev,^{165a} G. A. Chelkov,^{77,au} M. A. Chelstowska,³⁵ B. Chen,⁷⁶ C. Chen,^{58a} C. H. Chen,⁷⁶ H. Chen,²⁹ J. Chen,^{58a} J. Chen,³⁸ S. Chen,¹³⁴ S. J. Chen,^{15c} X. Chen,^{15b,at} Y. Chen,⁸⁰ Y-H. Chen,⁴⁴ H. C. Cheng,^{61a} H. J. Cheng,^{15d} A. Cheplakov,⁷⁷ E. Cheremushkina,¹²¹ R. Cherkaoui El Moursli,^{34e} E. Cheu,⁷ K. Cheung,⁶² T. J. A. Chevalérias,¹⁴² L. Chevalier,¹⁴² V. Chiarella,⁴⁹ G. Chiarelli,^{69a} G. Chiodini,^{65a} A. S. Chisholm,^{35,21} A. Chitan,^{27b} I. Chiu,¹⁶⁰ Y. H. Chiu,¹⁷³ M. V. Chizhov,⁷⁷ K. Choi,⁶³ A. R. Chomont,¹²⁹ S. Chouridou,¹⁵⁹ Y. S. Chow,¹¹⁸ V. Christodoulou,⁹² M. C. Chu,^{61a} J. Chudoba,¹³⁸ A. J. Chuinard,¹⁰¹ J. J. Chwastowski,⁸² L. Chytka,¹²⁷ D. Cinca,⁴⁵ V. Cindro,⁸⁹ I. A. Cioară,²⁴ A. Ciocio,¹⁸ F. Ciotto,^{67a,67b} Z. H. Citron,¹⁷⁷ M. Citterio,^{66a} A. Clark,⁵² M. R. Clark,³⁸ P. J. Clark,⁴⁸ C. Clement,^{43a,43b} Y. Coadou,⁹⁹ M. Cobal,^{64a,64c} A. Coccaro,^{53b} J. Cochran,⁷⁶ H. Cohen,¹⁵⁸ A. E. C. Coimbra,¹⁷⁷ L. Colasurdo,¹¹⁷ B. Cole,³⁸ A. P. Colijn,¹¹⁸ J. Collot,⁵⁶ P. Conde Muiño,^{137a,i} E. Coniavitis,⁵⁰ S. H. Connell,^{32b} I. A. Connelly,⁹⁸ S. Constantinescu,^{27b} F. Conventi,^{67a,aw} A. M. Cooper-Sarkar,¹³² F. Cormier,¹⁷² K. J. R. Cormier,¹⁶⁴ L. D. Corpe,⁹² M. Corradi,^{70a,70b} E. E. Corrigan,⁹⁴ F. Corriveau,^{101,ac} A. Cortes-Gonzalez,³⁵ M. J. Costa,¹⁷¹ F. Costanza,⁵ D. Costanzo,¹⁴⁶ G. Cowan,⁹¹ J. W. Cowley,³¹ B. E. Cox,⁹⁸ J. Crane,⁹⁸ K. Cranmer,¹²² S. J. Crawley,⁵⁵ R. A. Creager,¹³⁴ S. Crépe-Renaudin,⁵⁶ F. Crescioli,¹³³ M. Cristinziani,²⁴ V. Croft,¹²² G. Crosetti,^{40b,40a} A. Cueto,⁹⁶ T. Cuhadar Donszelmann,¹⁴⁶ A. R. Cukierman,¹⁵⁰ S. Czekierda,⁸² P. Czodrowski,³⁵ M. J. Da Cunha Sargedas De Sousa,^{58b} C. Da Via,⁹⁸ W. Dabrowski,^{81a} T. Dado,^{28a} S. Dahbi,^{34e} T. Dai,¹⁰³ F. Dallaire,¹⁰⁷ C. Dallapiccola,¹⁰⁰ M. Dam,³⁹ G. D'amen,^{23b,23a} J. Damp,⁹⁷ J. R. Dandoy,¹³⁴ M. F. Daneri,³⁰ N. P. Dang,^{178,1} N. D. Dann,⁹⁸ M. Danninger,¹⁷² V. Dao,³⁵ G. Darbo,^{53b} O. Dartsis,⁵ A. Dattagupta,¹²⁸ T. Daubney,⁴⁴ S. D'Auria,^{66a,66b} W. Davey,²⁴ C. David,⁴⁴ T. Davidek,¹⁴⁰ D. R. Davis,⁴⁷ E. Dawe,¹⁰² I. Dawson,¹⁴⁶ K. De,⁸ R. De Asmundis,^{67a} A. De Benedetti,¹²⁵ M. De Beurs,¹¹⁸ S. De Castro,^{23b,23a} S. De Cecco,^{70a,70b} N. De Groot,¹¹⁷ P. de Jong,¹¹⁸ H. De la Torre,¹⁰⁴ A. De Maria,^{69a,69b} D. De Pedis,^{70a} A. De Salvo,^{70a} U. De Sanctis,^{71a,71b} M. De Santis,^{71a,71b} A. De Santo,¹⁵³ K. De Vasconcelos Corga,⁹⁹ J. B. De Vivie De Regie,¹²⁹ C. Debenedetti,¹⁴³ D. V. Dedovich,⁷⁷ M. Del Gaudio,^{40b,40a} J. Del Peso,⁹⁶ Y. Delabat Diaz,⁴⁴ D. Delgove,¹²⁹ F. Deliot,¹⁴² C. M. Delitzsch,⁷ M. Della Pietra,^{67a,67b} D. Della Volpe,⁵² A. Dell'Acqua,³⁵ L. Dell'Asta,²⁵ M. Delmastro,⁵ C. Delporte,¹²⁹ P. A. Delsart,⁵⁶ D. A. DeMarco,¹⁶⁴ S. Demers,¹⁸⁰ M. Demichev,⁷⁷ S. P. Denisov,¹²¹ D. Denysiuk,¹¹⁸ L. D'Eramo,¹³³ D. Derendarz,⁸² J. E. Derkaoui,^{34d} F. Derue,¹³³ P. Dervan,⁸⁸ K. Desch,²⁴ C. Deterre,⁴⁴ K. Dette,¹⁶⁴ M. R. Devesa,³⁰ P. O. Deviveiros,³⁵ A. Dewhurst,¹⁴¹ S. Dhaliwal,²⁶ F. A. Di Bello,⁵² A. Di Ciaccio,^{71a,71b} L. Di Ciaccio,⁵ W. K. Di Clemente,¹³⁴ C. Di Donato,^{67a,67b} A. Di Girolamo,³⁵ G. Di Gregorio,^{69a,69b} B. Di Micco,^{72a,72b}

R. Di Nardo,¹⁰⁰ K. F. Di Petrillo,⁵⁷ R. Di Sipio,¹⁶⁴ D. Di Valentino,³³ C. Diaconu,⁹⁹ M. Diamond,¹⁶⁴ F. A. Dias,³⁹ T. Dias Do Vale,^{137a} M. A. Diaz,^{144a} J. Dickinson,¹⁸ E. B. Diehl,¹⁰³ J. Dietrich,¹⁹ S. Díez Cornell,⁴⁴ A. Dimitrievska,¹⁸ J. Dingfelder,²⁴ F. Dittus,³⁵ F. Djama,⁹⁹ T. Djobava,^{156b} J. I. Djuvsland,¹⁷ M. A. B. Do Vale,^{78c} M. Dobre,^{27b} D. Dodsworth,²⁶ C. Doglioni,⁹⁴ J. Dolejsi,¹⁴⁰ Z. Dolezal,¹⁴⁰ M. Donadelli,^{78d} J. Donini,³⁷ A. D'Onofrio,⁹⁰ M. D'Onofrio,⁸⁸ J. Dopke,¹⁴¹ A. Doria,^{67a} M. T. Dova,⁸⁶ A. T. Doyle,⁵⁵ E. Drechsler,¹⁴⁹ E. Dreyer,¹⁴⁹ T. Dreyer,⁵¹ Y. Du,^{58b} F. Dubinin,¹⁰⁸ M. Dubovsky,^{28a} A. Dubreuil,⁵² E. Duchovni,¹⁷⁷ G. Duckeck,¹¹² A. Ducourthial,¹³³ O. A. Ducu,^{107,x} D. Duda,¹¹³ A. Dudarev,³⁵ A. C. Dudder,⁹⁷ E. M. Duffield,¹⁸ L. Duflot,¹²⁹ M. Dührssen,³⁵ C. Dülsen,¹⁷⁹ M. Dumancic,¹⁷⁷ A. E. Dumitriu,^{27b,e} A. K. Duncan,⁵⁵ M. Dunford,^{59a} A. Duperrin,⁹⁹ H. Duran Yildiz,^{4a} M. Düren,⁵⁴ A. Durglishvili,^{156b} D. Duschinger,⁴⁶ B. Dutta,⁴⁴ D. Duvnjak,¹ G. Dyckes,¹³⁴ M. Dyndal,⁴⁴ S. Dysch,⁹⁸ B. S. Dziedzic,⁸² K. M. Ecker,¹¹³ R. C. Edgar,¹⁰³ T. Eifert,³⁵ G. Eigen,¹⁷ K. Einsweiler,¹⁸ T. Ekelof,¹⁶⁹ M. El Kacimi,^{34c} R. El Kosseifi,⁹⁹ V. Ellajosyula,¹⁶⁹ M. Ellert,¹⁶⁹ F. Ellinghaus,¹⁷⁹ A. A. Elliot,⁹⁰ N. Ellis,³⁵ J. Elmsheuser,²⁹ M. Elsing,³⁵ D. Emelianov,¹⁴¹ A. Emerman,³⁸ Y. Enari,¹⁶⁰ J. S. Ennis,¹⁷⁵ M. B. Epland,⁴⁷ J. Erdmann,⁴⁵ A. Ereditato,²⁰ S. Errede,¹⁷⁰ M. Escalier,¹²⁹ C. Escobar,¹⁷¹ O. Estrada Pastor,¹⁷¹ A. I. Etienne,¹⁴² E. Etzion,¹⁵⁸ H. Evans,⁶³ A. Ezhilov,¹³⁵ M. Ezzi,^{34e} F. Fabbri,⁵⁵ L. Fabbri,^{23b,23a} V. Fabiani,¹¹⁷ G. Facini,⁹² R. M. Faisca Rodrigues Pereira,^{137a} R. M. Fakhruddinov,¹²¹ S. Falciano,^{70a} P. J. Falke,⁵ S. Falke,⁵ J. Faltova,¹⁴⁰ Y. Fang,^{15a} M. Fanti,^{66a,66b} A. Farbin,⁸ A. Farilla,^{72a} E. M. Farina,^{68a,68b} T. Farooque,¹⁰⁴ S. Farrell,¹⁸ S. M. Farrington,¹⁷⁵ P. Farthouat,³⁵ F. Fassi,^{34e} P. Fassnacht,³⁵ D. Fassouliotis,⁹ M. Fauci Giannelli,⁴⁸ W. J. Fawcett,³¹ L. Fayard,¹²⁹ O. L. Fedin,^{135,q} W. Fedorko,¹⁷² M. Feickert,⁴¹ S. Feigl,¹³¹ L. Feligioni,⁹⁹ C. Feng,^{58b} E. J. Feng,³⁵ M. Feng,⁴⁷ M. J. Fenton,⁵⁵ A. B. Fenyuk,¹²¹ J. Ferrando,⁴⁴ A. Ferrari,¹⁶⁹ P. Ferrari,¹¹⁸ R. Ferrari,^{68a} D. E. Ferreira de Lima,^{59b} A. Ferrer,¹⁷¹ D. Ferrere,⁵² C. Ferretti,¹⁰³ F. Fiedler,⁹⁷ A. Filipčič,⁸⁹ F. Filthaut,¹¹⁷ K. D. Finelli,²⁵ M. C. N. Fiolhais,^{137a,137c,a} L. Fiorini,¹⁷¹ C. Fischer,¹⁴ W. C. Fisher,¹⁰⁴ I. Fleck,¹⁴⁸ P. Fleischmann,¹⁰³ R. R. M. Fletcher,¹³⁴ T. Flick,¹⁷⁹ B. M. Flierl,¹¹² L. M. Flores,¹³⁴ L. R. Flores Castillo,^{61a} F. M. Follega,^{73a,73b} N. Fomin,¹⁷ G. T. Forcolin,^{73a,73b} A. Formica,¹⁴² F. A. Förster,¹⁴ A. C. Forti,⁹⁸ A. G. Foster,²¹ D. Fournier,¹²⁹ H. Fox,⁸⁷ S. Fracchia,¹⁴⁶ P. Francavilla,^{69a,69b} M. Franchini,^{23b,23a} S. Franchino,^{59a} D. Francis,³⁵ L. Franconi,¹⁴³ M. Franklin,⁵⁷ M. Frate,¹⁶⁸ A. N. Fray,⁹⁰ D. Freeborn,⁹² B. Freund,¹⁰⁷ W. S. Freund,^{78b} E. M. Freundlich,⁴⁵ D. C. Frizzell,¹²⁵ D. Froidevaux,³⁵ J. A. Frost,¹³² C. Fukunaga,¹⁶¹ E. Fullana Torregrosa,¹⁷¹ E. Fumagalli,^{53b,53a} T. Fusayasu,¹¹⁴ J. Fuster,¹⁷¹ A. Gabrielli,^{23b,23a} A. Gabrielli,¹⁸ G. P. Gach,^{81a} S. Gadatsch,⁵² P. Gadow,¹¹³ G. Gagliardi,^{53b,53a} L. G. Gagnon,¹⁰⁷ C. Galea,^{27b} B. Galhardo,^{137a,137c} E. J. Gallas,¹³² B. J. Gallop,¹⁴¹ P. Gallus,¹³⁹ G. Galster,³⁹ R. Gamboa Goni,⁹⁰ K. K. Gan,¹²³ S. Ganguly,¹⁷⁷ J. Gao,^{58a} Y. Gao,⁸⁸ Y. S. Gao,^{150,n} C. García,¹⁷¹ J. E. García Navarro,¹⁷¹ J. A. García Pascual,^{15a} C. Garcia-Argos,⁵⁰ M. Garcia-Sciveres,¹⁸ R. W. Gardner,³⁶ N. Garelli,¹⁵⁰ S. Gargiulo,⁵⁰ V. Garonne,¹³¹ K. Gasnikova,⁴⁴ A. Gaudiello,^{53b,53a} G. Gaudio,^{68a} I. L. Gavrilenko,¹⁰⁸ A. Gavrilyuk,¹⁰⁹ C. Gay,¹⁷² G. Gaycken,²⁴ E. N. Gazis,¹⁰ C. N. P. Gee,¹⁴¹ J. Geisen,⁵¹ M. Geisen,⁹⁷ M. P. Geisler,^{59a} C. Gemme,^{53b} M. H. Genest,⁵⁶ C. Geng,¹⁰³ S. Gentile,^{70a,70b} S. George,⁹¹ D. Gerbaudo,¹⁴ G. Gessner,⁴⁵ S. Ghasemi,¹⁴⁸ M. Ghasemi Bostanabad,¹⁷³ M. Ghneimat,²⁴ B. Giacobbe,^{23b} S. Giagu,^{70a,70b} N. Giangiacomi,^{23b,23a} P. Giannetti,^{69a} A. Giannini,^{67a,67b} S. M. Gibson,⁹¹ M. Gignac,¹⁴³ D. Gillberg,³³ G. Gilles,¹⁷⁹ D. M. Gingrich,^{3,av} M. P. Giordani,^{64a,64c} F. M. Giorgi,^{23b} P. F. Giraud,¹⁴² P. Giromini,⁵⁷ G. Giugliarelli,^{64a,64c} D. Giugni,^{66a} F. Giuli,¹³² M. Giulini,^{59b} S. Gkaitatzis,¹⁵⁹ I. Gkialas,^{9,k} E. L. Gkoukousis,¹⁴ P. Gkoutoumis,¹⁰ L. K. Gladilin,¹¹¹ C. Glasman,⁹⁶ J. Glatzer,¹⁴ P. C. F. Glaysher,⁴⁴ A. Glazov,⁴⁴ M. Goblirsch-Kolb,²⁶ S. Goldfarb,¹⁰² T. Golling,⁵² D. Golubkov,¹²¹ A. Gomes,^{137a,137b} R. Goncalves Gama,¹⁵¹ R. Gonçalves,^{137a} G. Gonella,⁵⁰ L. Gonella,²¹ A. Gongadze,⁷⁷ F. Gonnella,²¹ J. L. Gonski,⁵⁷ S. González de la Hoz,¹⁷¹ S. Gonzalez-Sevilla,⁵² L. Goossens,³⁵ P. A. Gorbounov,¹⁰⁹ H. A. Gordon,²⁹ B. Gorini,³⁵ E. Gorini,^{65a,65b} A. Gorišek,⁸⁹ A. T. Goshaw,⁴⁷ C. Gössling,⁴⁵ M. I. Gostkin,⁷⁷ C. A. Gottardo,²⁴ C. R. Goudet,¹²⁹ D. Goujdami,^{34c} A. G. Goussiou,¹⁴⁵ N. Govender,^{32b,c} C. Goy,⁵ E. Gozani,¹⁵⁷ I. Grabowska-Bold,^{81a} P. O. J. Gradin,¹⁶⁹ E. C. Graham,⁸⁸ J. Gramling,¹⁶⁸ E. Gramstad,¹³¹ S. Grancagnolo,¹⁹ V. Gratchev,¹³⁵ P. M. Gravila,^{27f} F. G. Gravili,^{65a,65b} C. Gray,⁵⁵ H. M. Gray,¹⁸ Z. D. Greenwood,^{93,ak} C. Greife,²⁴ K. Gregersen,⁹⁴ I. M. Gregor,⁴⁴ P. Grenier,¹⁵⁰ K. Grevtsov,⁴⁴ N. A. Grieser,¹²⁵ J. Griffiths,⁸ A. A. Grillo,¹⁴³ K. Grimm,^{150,b} S. Grinstein,^{14,y} J.-F. Grivaz,¹²⁹ S. Groh,⁹⁷ E. Gross,¹⁷⁷ J. Grosse-Knetter,⁵¹ Z. J. Grout,⁹² C. Grud,¹⁰³ A. Grummer,¹¹⁶ L. Guan,¹⁰³ W. Guan,¹⁷⁸ J. Guenther,³⁵ A. Guerguichon,¹²⁹ F. Guescini,^{165a} D. Guest,¹⁶⁸ R. Gugel,⁵⁰ B. Gui,¹²³ T. Guillemin,⁵ S. Guindon,³⁵ U. Gul,⁵⁵ J. Guo,^{58c} W. Guo,¹⁰³ Y. Guo,^{58a,t} Z. Guo,⁹⁹ R. Gupta,⁴⁴ S. Gurbuz,^{12c} G. Gustavino,¹²⁵ P. Gutierrez,¹²⁵ C. Gutsche,⁹² C. Guyot,¹⁴² M. P. Guzik,^{81a} C. Gwenlan,¹³² C. B. Gwilliam,⁸⁸ A. Haas,¹²² C. Haber,¹⁸ H. K. Hadavand,⁸ N. Haddad,^{34e} A. Hadeef,^{58a} S. Hageböck,³⁵ M. Hagihara,¹⁶⁶ M. Haleem,¹⁷⁴ J. Haley,¹²⁶ G. Halladjian,¹⁰⁴ G. D. Hallewell,⁹⁹ K. Hamacher,¹⁷⁹ P. Hamal,¹²⁷ K. Hamano,¹⁷³ H. Hamdaoui,^{34e} A. Hamilton,^{32a} G. N. Hamity,¹⁴⁶ K. Han,^{58a,aj} L. Han,^{58a} S. Han,^{15d} K. Hanagaki,^{79,v} M. Hance,¹⁴³

D. M. Handl,¹¹² B. Haney,¹³⁴ R. Hankache,¹³³ P. Hanke,^{59a} E. Hansen,⁹⁴ J. B. Hansen,³⁹ J. D. Hansen,³⁹ M. C. Hansen,²⁴ P. H. Hansen,³⁹ K. Hara,¹⁶⁶ A. S. Hard,¹⁷⁸ T. Harenberg,¹⁷⁹ S. Harkusha,¹⁰⁵ P. F. Harrison,¹⁷⁵ N. M. Hartmann,¹¹² Y. Hasegawa,¹⁴⁷ A. Hasib,⁴⁸ S. Hassani,¹⁴² S. Haug,²⁰ R. Hauser,¹⁰⁴ L. Hauswald,⁴⁶ L. B. Havener,³⁸ M. Havranek,¹³⁹ C. M. Hawkes,²¹ R. J. Hawkings,³⁵ D. Hayden,¹⁰⁴ C. Hayes,¹⁵² C. P. Hays,¹³² J. M. Hays,⁹⁰ H. S. Hayward,⁸⁸ S. J. Haywood,¹⁴¹ F. He,^{58a} M. P. Heath,⁴⁸ V. Hedberg,⁹⁴ L. Heelan,⁸ S. Heer,²⁴ K. K. Heidegger,⁵⁰ J. Heilman,³³ S. Heim,⁴⁴ T. Heim,¹⁸ B. Heinemann,^{44,aq} J. J. Heinrich,¹¹² L. Heinrich,¹²² C. Heinz,⁵⁴ J. Hejbal,¹³⁸ L. Helary,^{59b} A. Held,¹⁷² S. Hellesund,¹³¹ C. M. Helling,¹⁴³ S. Hellman,^{43a,43b} C. Helsens,³⁵ R. C. W. Henderson,⁸⁷ Y. Heng,¹⁷⁸ S. Henkelmann,¹⁷² A. M. Henriques Correia,³⁵ G. H. Herbert,¹⁹ H. Herde,²⁶ V. Herget,¹⁷⁴ Y. Hernández Jiménez,^{32c} H. Herr,⁹⁷ M. G. Herrmann,¹¹² T. Herrmann,⁴⁶ G. Herten,⁵⁰ R. Hertenberger,¹¹² L. Hervas,³⁵ T. C. Herwig,¹³⁴ G. G. Hesketh,⁹² N. P. Hessey,^{165a} A. Higashida,¹⁶⁰ S. Higashino,⁷⁹ E. Higón-Rodríguez,¹⁷¹ K. Hildebrand,³⁶ E. Hill,¹⁷³ J. C. Hill,³¹ K. K. Hill,²⁹ K. H. Hiller,⁴⁴ S. J. Hillier,²¹ M. Hils,⁴⁶ I. Hinchliffe,¹⁸ F. Hinterkeuser,²⁴ M. Hirose,¹³⁰ D. Hirschbuehl,¹⁷⁹ B. Hiti,⁸⁹ O. Hladik,¹³⁸ D. R. Hlaluku,^{32c} X. Hoad,⁴⁸ J. Hobbs,¹⁵² N. Hod,¹⁷⁷ M. C. Hodgkinson,¹⁴⁶ A. Hoecker,³⁵ M. R. Hoferkamp,¹¹⁶ F. Hoenig,¹¹² D. Hohn,⁵⁰ D. Hohov,¹²⁹ T. R. Holmes,³⁶ M. Holzbock,¹¹² M. Homann,⁴⁵ B. H. Hommels,³¹ S. Honda,¹⁶⁶ T. Honda,⁷⁹ T. M. Hong,¹³⁶ A. Hönle,¹¹³ B. H. Hooberman,¹⁷⁰ W. H. Hopkins,¹²⁸ Y. Horii,¹¹⁵ P. Horn,⁴⁶ A. J. Horton,¹⁴⁹ L. A. Horyn,³⁶ J.-Y. Hostachy,⁵⁶ A. Hostiuc,¹⁴⁵ S. Hou,¹⁵⁵ A. Houmada,^{34a} J. Howarth,⁹⁸ J. Hoya,⁸⁶ M. Hrabovsky,¹²⁷ J. Hrdinka,³⁵ I. Hristova,¹⁹ J. Hrivnac,¹²⁹ A. Hrynevich,¹⁰⁶ T. Hryn'ova,⁵ P. J. Hsu,⁶² S.-C. Hsu,¹⁴⁵ Q. Hu,²⁹ S. Hu,^{58c} Y. Huang,^{15a} Z. Hubacek,¹³⁹ F. Hubaut,⁹⁹ M. Huebner,²⁴ F. Huegging,²⁴ T. B. Huffman,¹³² M. Huhtinen,³⁵ R. F. H. Hunter,³³ P. Huo,¹⁵² A. M. Hupe,³³ N. Huseynov,^{77,ae} J. Huston,¹⁰⁴ J. Huth,⁵⁷ R. Hyneman,¹⁰³ G. Iacobucci,⁵² G. Iakovidis,²⁹ I. Ibragimov,¹⁴⁸ L. Iconomidou-Fayard,¹²⁹ Z. Idrissi,^{34e} P. Inengo,³⁵ R. Ignazzi,³⁹ O. Igonkina,^{118,aa} R. Iguchi,¹⁶⁰ T. Iizawa,⁵² Y. Ikegami,⁷⁹ M. Ikeno,⁷⁹ D. Iliadis,¹⁵⁹ N. Ilic,¹¹⁷ F. Iltzsche,⁴⁶ G. Introzzi,^{68a,68b} M. Iodice,^{72a} K. Iordanidou,³⁸ V. Ippolito,^{70a,70b} M. F. Isacson,¹⁶⁹ N. Ishijima,¹³⁰ M. Ishino,¹⁶⁰ M. Ishitsuka,¹⁶² W. Islam,¹²⁶ C. Issever,¹³² S. Istin,¹⁵⁷ F. Ito,¹⁶⁶ J. M. Iturbe Ponce,^{61a} R. Iuppa,^{73a,73b} A. Ivina,¹⁷⁷ H. Iwasaki,⁷⁹ J. M. Izen,⁴² V. Izzo,^{67a} P. Jacka,¹³⁸ P. Jackson,¹ R. M. Jacobs,²⁴ V. Jain,² G. Jäkel,¹⁷⁹ K. B. Jakobi,⁹⁷ K. Jakobs,⁵⁰ S. Jakobsen,⁷⁴ T. Jakoubek,¹³⁸ D. O. Jamin,¹²⁶ R. Jansky,⁵² J. Janssen,²⁴ M. Janus,⁵¹ P. A. Janus,^{81a} G. Jarlskog,⁹⁴ N. Javadov,^{77,ae} T. Javůrek,³⁵ M. Javurkova,⁵⁰ F. Jeanneau,¹⁴² L. Jeanty,¹²⁸ J. Jejelava,^{156a,af} A. Jelinskas,¹⁷⁵ P. Jenni,^{50,d} J. Jeong,⁴⁴ N. Jeong,⁴⁴ S. Jézéquel,⁵ H. Ji,¹⁷⁸ J. Jia,¹⁵² H. Jiang,⁷⁶ Y. Jiang,^{58a} Z. Jiang,^{150,r} S. Jiggins,⁵⁰ F. A. Jimenez Morales,³⁷ J. Jimenez Pena,¹⁷¹ S. Jin,^{15c} A. Jinaru,^{27b} O. Jinnouchi,¹⁶² H. Jivan,^{32c} P. Johansson,¹⁴⁶ K. A. Johns,⁷ C. A. Johnson,⁶³ K. Jon-And,^{43a,43b} R. W. L. Jones,⁸⁷ S. D. Jones,¹⁵³ S. Jones,⁷ T. J. Jones,⁸⁸ J. Jongmanns,^{59a} P. M. Jorge,^{137a,137b} J. Jovicevic,^{165a} X. Ju,¹⁸ J. J. Junggeburth,¹¹³ A. Juste Rozas,^{14,y} A. Kaczmarska,⁸² M. Kado,¹²⁹ H. Kagan,¹²³ M. Kagan,¹⁵⁰ T. Kajii,¹⁷⁶ E. Kajomovitz,¹⁵⁷ C. W. Kalderon,⁹⁴ A. Kaluza,⁹⁷ A. Kamenshchikov,¹²¹ L. Kanjir,⁸⁹ Y. Kano,¹⁶⁰ V. A. Kantserov,¹¹⁰ J. Kanzaki,⁷⁹ L. S. Kaplan,¹⁷⁸ D. Kar,^{32c} M. J. Kareem,^{165b} E. Karentzos,¹⁰ S. N. Karpov,⁷⁷ Z. M. Karpova,⁷⁷ V. Kartvelishvili,⁸⁷ A. N. Karyukhin,¹²¹ L. Kashif,¹⁷⁸ R. D. Kass,¹²³ A. Kastanas,^{43a,43b} Y. Kataoka,¹⁶⁰ C. Kato,^{58d,58c} J. Katzy,⁴⁴ K. Kawade,⁸⁰ K. Kawagoe,⁸⁵ T. Kawaguchi,¹¹⁵ T. Kawamoto,¹⁶⁰ G. Kawamura,⁵¹ E. F. Kay,⁸⁸ V. F. Kazanin,^{120b,120a} R. Keeler,¹⁷³ R. Kehoe,⁴¹ J. S. Keller,³³ E. Kellermann,⁹⁴ J. J. Kempster,²¹ J. Kendrick,²¹ O. Kepka,¹³⁸ S. Kersten,¹⁷⁹ B. P. Kerševan,⁸⁹ S. Ketabchi Haghghat,¹⁶⁴ R. A. Keyes,¹⁰¹ M. Khader,¹⁷⁰ F. Khalil-Zada,¹³ A. Khanov,¹²⁶ A. G. Kharlamov,^{120b,120a} T. Kharlamova,^{120b,120a} E. E. Khoda,¹⁷² A. Khodinov,¹⁶³ T. J. Khoo,⁵² E. Khramov,⁷⁷ J. Khubua,^{156b} S. Kido,⁸⁰ M. Kiehn,⁵² C. R. Kilby,⁹¹ Y. K. Kim,³⁶ N. Kimura,^{64a,64c} O. M. Kind,¹⁹ B. T. King,⁸⁸ D. Kirchmeier,⁴⁶ J. Kirk,¹⁴¹ A. E. Kiryunin,¹¹³ T. Kishimoto,¹⁶⁰ V. Kitali,⁴⁴ O. Kivernyk,⁵ E. Kladiva,^{28b,†} T. Klapdor-Kleingrothaus,⁵⁰ M. H. Klein,¹⁰³ M. Klein,⁸⁸ U. Klein,⁸⁸ K. Kleinknecht,⁹⁷ P. Klimek,¹¹⁹ A. Klimentov,²⁹ T. Klingl,²⁴ T. Klioutchnikova,³⁵ F. F. Klitzner,¹¹² P. Kluit,¹¹⁸ S. Kluth,¹¹³ E. Kneringer,⁷⁴ E. B. F. G. Knoop,⁹⁹ A. Knue,⁵⁰ D. Kobayashi,⁸⁵ T. Kobayashi,¹⁶⁰ M. Kobel,⁴⁶ M. Kocian,¹⁵⁰ P. Kodys,¹⁴⁰ P. T. Koenig,²⁴ T. Koffas,³³ E. Koffeman,¹¹⁸ N. M. Köhler,¹¹³ T. Koi,¹⁵⁰ M. Kolb,^{59b} I. Koletsou,⁵ T. Kondo,⁷⁹ N. Kondrashova,^{58c} K. Köneke,⁵⁰ A. C. König,¹¹⁷ T. Kono,⁷⁹ R. Konoplich,^{122,am} V. Konstantinides,⁹² N. Konstantinidis,⁹² B. Konya,⁹⁴ R. Kopeliansky,⁶³ S. Koperny,^{81a} K. Korcyl,⁸² K. Kordas,¹⁵⁹ G. Koren,¹⁵⁸ A. Korn,⁹² I. Korolkov,¹⁴ E. V. Korolkova,¹⁴⁶ N. Korotkova,¹¹¹ O. Kortner,¹¹³ S. Kortner,¹¹³ T. Kosek,¹⁴⁰ V. V. Kostyukhin,²⁴ A. Kotwal,⁴⁷ A. Koulouris,¹⁰ A. Kourkoumeli-Charalampidi,^{68a,68b} C. Kourkoumelis,⁹ E. Kourlitis,¹⁴⁶ V. Kouskoura,²⁹ A. B. Kowalewska,⁸² R. Kowalewski,¹⁷³ C. Kozakai,¹⁶⁰ W. Kozanecki,¹⁴² A. S. Kozhin,¹²¹ V. A. Kramarenko,¹¹¹ G. Kramberger,⁸⁹ D. Krasnopevtsev,^{58a} M. W. Krasny,¹³³ A. Krasznahorkay,³⁵ D. Krauss,¹¹³ J. A. Kremer,^{81a} J. Kretzschmar,⁸⁸ P. Krieger,¹⁶⁴ K. Krizka,¹⁸ K. Kroeninger,⁴⁵ H. Kroha,¹¹³ J. Kroll,¹³⁸ J. Kroll,¹³⁴ J. Krstic,¹⁶ U. Kruchonak,⁷⁷ H. Krüger,²⁴ N. Krumnack,⁷⁶ M. C. Kruse,⁴⁷ T. Kubota,¹⁰²

S. Kudah,^{4b} J. T. Kuechler,⁴⁴ S. Kuehn,³⁵ A. Kugel,^{59a} T. Kuhl,⁴⁴ V. Kukhtin,⁷⁷ R. Kukla,⁹⁹ Y. Kulchitsky,^{105,ai}
 S. Kuleshov,^{144b} Y. P. Kulinich,¹⁷⁰ M. Kuna,⁵⁶ T. Kunigo,⁸³ A. Kupco,¹³⁸ T. Kupfer,⁴⁵ O. Kuprash,⁵⁰ H. Kurashige,⁸⁰
 L. L. Kurchaninov,^{165a} Y. A. Kurochkin,¹⁰⁵ A. Kurova,¹¹⁰ M. G. Kurth,^{15d} E. S. Kuwertz,³⁵ M. Kuze,¹⁶² J. Kvita,¹²⁷
 T. Kwan,¹⁰¹ A. La Rosa,¹¹³ J. L. La Rosa Navarro,^{78d} L. La Rotonda,^{40b,40a} F. La Ruffa,^{40b,40a} C. Lacasta,¹⁷¹ F. Lacava,^{70a,70b}
 J. Lacey,⁴⁴ D. P. J. Lack,⁹⁸ H. Lacker,¹⁹ D. Lacour,¹³³ E. Ladygin,⁷⁷ R. Lafaye,⁵ B. Laforge,¹³³ T. Lagouri,^{32c} S. Lai,⁵¹
 S. Lammers,⁶³ W. Lampl,⁷ E. Lançon,²⁹ U. Landgraf,⁵⁰ M. P. J. Landon,⁹⁰ M. C. Lanfermann,⁵² V. S. Lang,⁴⁴ J. C. Lange,⁵¹
 R. J. Langenberg,³⁵ A. J. Lankford,¹⁶⁸ F. Lanni,²⁹ K. Lantzsche,²⁴ A. Lanza,^{68a} A. Lapertosa,^{53b,53a} S. Laplace,¹³³
 J. F. Laporte,¹⁴² T. Lari,^{66a} F. Lasagni Manghi,^{23b,23a} M. Lassnig,³⁵ T. S. Lau,^{61a} A. Laudrain,¹²⁹ M. Lavorgna,^{67a,67b}
 M. Lazzaroni,^{66a,66b} B. Le,¹⁰² O. Le Dortz,¹³³ E. Le Guirriec,⁹⁹ E. P. Le Quilleuc,¹⁴² M. LeBlanc,⁷ T. LeCompte,⁶
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 F. Legger,¹¹² C. Leggett,¹⁸ K. Lehmann,¹⁴⁹ N. Lehmann,¹⁷⁹ G. Lehmann Miotto,³⁵ W. A. Leight,⁴⁴ A. Leisos,^{159,w}
 M. A. L. Leite,^{78d} R. Leitner,¹⁴⁰ D. Lellouch,¹⁷⁷ K. J. C. Leney,⁹² T. Lenz,²⁴ B. Lenzi,³⁵ R. Leone,⁷ S. Leone,^{69a}
 C. Leonidopoulos,⁴⁸ G. Lerner,¹⁵³ C. Leroy,¹⁰⁷ R. Les,¹⁶⁴ A. A. J. Lesage,¹⁴² C. G. Lester,³¹ M. Levchenko,¹³⁵ J. Levêque,⁵
 D. Levin,¹⁰³ L. J. Levinson,¹⁷⁷ B. Li,^{15b} B. Li,¹⁰³ C-Q. Li,^{58a,al} H. Li,^{58a} H. Li,^{58b} K. Li,¹⁵⁰ L. Li,^{58c} M. Li,^{15a} Q. Li,^{15d}
 Q. Y. Li,^{58a} S. Li,^{58d,58c} X. Li,^{58c} Y. Li,⁴⁴ Z. Liang,^{15a} B. Liberti,^{71a} A. Liblong,¹⁶⁴ K. Lie,^{61c} S. Liem,¹¹⁸ A. Limosani,¹⁵⁴
 C. Y. Lin,³¹ K. Lin,¹⁰⁴ T. H. Lin,⁹⁷ R. A. Linck,⁶³ J. H. Lindon,²¹ A. L. Lioni,⁵² E. Lipeles,¹³⁴ A. Lipniacka,¹⁷ M. Lisovsky,^{59b}
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 J. K. K. Liu,¹³² K. Liu,¹³³ M. Liu,^{58a} P. Liu,¹⁸ Y. Liu,^{15a} Y. L. Liu,^{58a} Y. W. Liu,^{58a} M. Livan,^{68a,68b} A. Lleres,⁵⁶
 J. Llorente Merino,^{15a} S. L. Lloyd,⁹⁰ C. Y. Lo,^{61b} F. Lo Sterzo,⁴¹ E. M. Lobodzinska,⁴⁴ P. Loch,⁷ T. Lohse,¹⁹
 K. Lohwasser,¹⁴⁶ M. Lokajicek,¹³⁸ J. D. Long,¹⁷⁰ R. E. Long,⁸⁷ L. Longo,^{65a,65b} K. A. Looper,¹²³ J. A. Lopez,^{144b}
 I. Lopez Paz,⁹⁸ A. Lopez Solis,¹⁴⁶ J. Lorenz,¹¹² N. Lorenzo Martinez,⁵ M. Losada,²² P. J. Lösel,¹¹² A. Lösle,⁵⁰ X. Lou,⁴⁴
 X. Lou,^{15a} A. Lounis,¹²⁹ J. Love,⁶ P. A. Love,⁸⁷ J. J. Lozano Bahilo,¹⁷¹ H. Lu,^{61a} M. Lu,^{58a} Y. J. Lu,⁶² H. J. Lubatti,¹⁴⁵
 C. Luci,^{70a,70b} A. Lucotte,⁵⁶ C. Luedtke,⁵⁰ F. Luehring,⁶³ I. Luise,¹³³ L. Luminari,^{70a} B. Lund-Jensen,¹⁵¹ M. S. Lutz,¹⁰⁰
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 Y. Ma,^{58b} G. Maccarrone,⁴⁹ A. Macchiolo,¹¹³ C. M. Macdonald,¹⁴⁶ J. Machado Miguens,^{134,137b} D. Madaffari,¹⁷¹ R. Madar,³⁷
 W. F. Mader,⁴⁶ N. Madysa,⁴⁶ J. Maeda,⁸⁰ K. Maekawa,¹⁶⁰ S. Maeland,¹⁷ T. Maeno,²⁹ M. Maerker,⁴⁶ A. S. Maevskiy,¹¹¹
 V. Magerl,⁵⁰ D. J. Mahon,³⁸ C. Maidantchik,^{78b} T. Maier,¹¹² A. Maio,^{137a,137b,a137d} O. Majersky,^{28a} S. Majewski,¹²⁸
 Y. Makida,⁷⁹ N. Makovec,¹²⁹ B. Malaescu,¹³³ Pa. Malecki,⁸² V. P. Maleev,¹³⁵ F. Malek,⁵⁶ U. Mallik,⁷⁵ D. Malon,⁶
 C. Malone,³¹ S. Maltezos,¹⁰ S. Malyukov,³⁵ J. Mamuzic,¹⁷¹ G. Mancini,⁴⁹ I. Mandić,⁸⁹ L. Manhaes de Andrade Filho,^{78a}
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 S. Manzoni,^{66a,66b} A. Marantis,¹⁵⁹ G. Marceca,³⁰ L. Marchese,¹³² G. Marchiori,¹³³ M. Marcisovsky,¹³⁸ C. Marcon,⁹⁴
 C. A. Marin Tobon,³⁵ M. Marjanovic,³⁷ F. Marroquim,^{78b} Z. Marshall,¹⁸ M. U. F. Martensson,¹⁶⁹ S. Marti-Garcia,¹⁷¹
 C. B. Martin,¹²³ T. A. Martin,¹⁷⁵ V. J. Martin,⁴⁸ B. Martin dit Latour,¹⁷ M. Martinez,^{14,y} V. I. Martinez Outschoorn,¹⁰⁰
 S. Martin-Haugh,¹⁴¹ V. S. Martoiu,^{27b} A. C. Martyniuk,⁹² A. Marzin,³⁵ L. Masetti,⁹⁷ T. Mashimo,¹⁶⁰ R. Mashinistov,¹⁰⁸
 J. Masik,⁹⁸ A. L. Maslennikov,^{120b,120a} L. H. Mason,¹⁰² L. Massa,^{71a,71b} P. Massarotti,^{67a,67b} P. Mastrandrea,^{69a,69b}
 A. Mastroberardino,^{40b,40a} T. Masubuchi,¹⁶⁰ P. Mättig,²⁴ J. Maurer,^{27b} B. Maček,⁸⁹ S. J. Maxfield,⁸⁸ D. A. Maximov,^{120b,120a}
 R. Mazini,¹⁵⁵ I. Maznas,¹⁵⁹ S. M. Mazza,¹⁴³ S. P. Mc Kee,¹⁰³ A. McCarn,⁴¹ T. G. McCarthy,¹¹³ L. I. McClymont,⁹²
 W. P. McCormack,¹⁸ E. F. McDonald,¹⁰² J. A. McFayden,³⁵ G. Mchedlidze,⁵¹ M. A. McKay,⁴¹ K. D. McLean,¹⁷³
 S. J. McMahan,¹⁴¹ P. C. McNamara,¹⁰² C. J. McNicol,¹⁷⁵ R. A. McPherson,^{173,ac} J. E. Mdhuli,^{32c} Z. A. Meadows,¹⁰⁰
 S. Meehan,¹⁴⁵ T. M. Megy,⁵⁰ S. Mehlhase,¹¹² A. Mehta,⁸⁸ T. Meideck,⁵⁶ B. Meirose,⁴² D. Melini,^{171,h}
 B. R. Mellado Garcia,^{32c} J. D. Mellenthin,⁵¹ M. Melo,^{28a} F. Meloni,⁴⁴ A. Melzer,²⁴ S. B. Menary,⁹⁸
 E. D. Mendes Gouveia,^{137a} L. Meng,³⁵ X. T. Meng,¹⁰³ S. Menke,¹¹³ E. Meoni,^{40b,40a} S. Mergelmeyer,¹⁹ S. A. M. Merkt,¹³⁶
 C. Merlassino,²⁰ P. Mermod,⁵² L. Merola,^{67a,67b} C. Meroni,^{66a} A. Messina,^{70a,70b} J. Metcalfe,⁶ A. S. Mete,¹⁶⁸ C. Meyer,⁶³
 J. Meyer,¹⁵⁷ J-P. Meyer,¹⁴² H. Meyer Zu Theenhausen,^{59a} F. Miano,¹⁵³ R. P. Middleton,¹⁴¹ L. Mijović,⁴⁸ G. Mikenberg,¹⁷⁷
 M. Mikestikova,¹³⁸ M. Mikuž,⁸⁹ M. Milesi,¹⁰² A. Milic,¹⁶⁴ D. A. Millar,⁹⁰ D. W. Miller,³⁶ A. Milov,¹⁷⁷ D. A. Milstead,^{43a,43b}
 R. A. Mina,^{150,r} A. A. Minaenko,¹²¹ M. Miñano Moya,¹⁷¹ I. A. Minashvili,^{156b} A. I. Mincer,¹²² B. Mindur,^{81a} M. Mineev,⁷⁷
 Y. Minegishi,¹⁶⁰ Y. Ming,¹⁷⁸ L. M. Mir,¹⁴ A. Mirto,^{65a,65b} K. P. Mistry,¹³⁴ T. Mitani,¹⁷⁶ J. Mitrevski,¹¹² V. A. Mitsou,¹⁷¹
 M. Mittal,^{58c} A. Miucci,²⁰ P. S. Miyagawa,¹⁴⁶ A. Mizukami,⁷⁹ J. U. Mjörnmark,⁹⁴ T. Mkrchyan,¹⁸¹ M. Mlynarikova,¹⁴⁰
 T. Moa,^{43a,43b} K. Mochizuki,¹⁰⁷ P. Mogg,⁵⁰ S. Mohapatra,³⁸ S. Molander,^{43a,43b} R. Moles-Valls,²⁴ M. C. Mondragon,¹⁰⁴

K. Mönig,⁴⁴ J. Monk,³⁹ E. Monnier,⁹⁹ A. Montalbano,¹⁴⁹ J. Montejo Berlingen,³⁵ F. Monticelli,⁸⁶ S. Monzani,^{66a} N. Morange,¹²⁹ D. Moreno,²² M. Moreno Llácer,³⁵ P. Morettini,^{53b} M. Morgenstern,¹¹⁸ S. Morgenstern,⁴⁶ D. Mori,¹⁴⁹ M. Morii,⁵⁷ M. Morinaga,¹⁷⁶ V. Morisbak,¹³¹ A. K. Morley,³⁵ G. Mornacchi,³⁵ A. P. Morris,⁹² L. Morvaj,¹⁵² P. Moschovakos,¹⁰ M. Mosidze,^{156b} H. J. Moss,¹⁴⁶ J. Moss,^{150,o} K. Motohashi,¹⁶² R. Mount,¹⁵⁰ E. Mountricha,³⁵ E. J. W. Moyse,¹⁰⁰ S. Muanza,⁹⁹ F. Mueller,¹¹³ J. Mueller,¹³⁶ R. S. P. Mueller,¹¹² D. Muenstermann,⁸⁷ G. A. Mullier,⁹⁴ F. J. Munoz Sanchez,⁹⁸ P. Murin,^{28b} W. J. Murray,^{175,141} A. Murrone,^{66a,66b} M. Muškinja,⁸⁹ C. Mwewa,^{32a} A. G. Myagkov,^{121,an} J. Myers,¹²⁸ M. Myska,¹³⁹ B. P. Nachman,¹⁸ O. Nackenhorst,⁴⁵ K. Nagai,¹³² K. Nagano,⁷⁹ Y. Nagasaka,⁶⁰ M. Nagel,⁵⁰ E. Nagy,⁹⁹ A. M. Nairz,³⁵ Y. Nakahama,¹¹⁵ K. Nakamura,⁷⁹ T. Nakamura,¹⁶⁰ I. Nakano,¹²⁴ H. Nanjo,¹³⁰ F. Napolitano,^{59a} R. F. Naranjo Garcia,⁴⁴ R. Narayan,¹¹ D. I. Narrias Villar,^{59a} I. Naryshkin,¹³⁵ T. Naumann,⁴⁴ G. Navarro,²² H. A. Neal,^{103,†} P. Y. Nechaeva,¹⁰⁸ T. J. Neep,¹⁴² A. Negri,^{68a,68b} M. Negrini,^{23b} S. Nektarijevic,¹¹⁷ C. Nellist,⁵¹ M. E. Nelson,¹³² S. Nemecek,¹³⁸ P. Nemethy,¹²² M. Nessi,^{35,f} M. S. Neubauer,¹⁷⁰ M. Neumann,¹⁷⁹ P. R. Newman,²¹ T. Y. Ng,^{61c} Y. S. Ng,¹⁹ Y. W. Y. Ng,¹⁶⁸ H. D. N. Nguyen,⁹⁹ T. Nguyen Manh,¹⁰⁷ E. Nibigira,³⁷ R. B. Nickerson,¹³² R. Nicolaidou,¹⁴² D. S. Nielsen,³⁹ J. Nielsen,¹⁴³ N. Nikiforou,¹¹ V. Nikolaenko,^{121,an} I. Nikolic-Audit,¹³³ K. Nikolopoulos,²¹ P. Nilsson,²⁹ H. R. Nindhito,⁵² Y. Ninomiya,⁷⁹ A. Nisati,^{70a} N. Nishu,^{58c} R. Nisius,¹¹³ I. Nitsche,⁴⁵ T. Nitta,¹⁷⁶ T. Nobe,¹⁶⁰ Y. Noguchi,⁸³ M. Nomachi,¹³⁰ I. Nomidis,¹³³ M. A. Nomura,²⁹ M. Nordberg,³⁵ N. Norjoharuddeen,¹³² T. Novak,⁸⁹ O. Novgorodova,⁴⁶ R. Novotny,¹³⁹ L. Nozka,¹²⁷ K. Ntekas,¹⁶⁸ E. Nurse,⁹² F. Nuti,¹⁰² F. G. Oakham,^{33,av} H. Oberlack,¹¹³ J. Ocariz,¹³³ A. Ochi,⁸⁰ I. Ochoa,³⁸ J. P. Ochoa-Ricoux,^{144a} K. O'Connor,²⁶ S. Oda,⁸⁵ S. Odaka,⁷⁹ S. Oerdek,⁵¹ A. Oh,⁹⁸ S. H. Oh,⁴⁷ C. C. Ohm,¹⁵¹ H. Oide,^{53b,53a} M. L. Ojeda,¹⁶⁴ H. Okawa,¹⁶⁶ Y. Okazaki,⁸³ Y. Okumura,¹⁶⁰ T. Okuyama,⁷⁹ A. Olariu,^{27b} L. F. Oleiro Seabra,^{137a} S. A. Olivares Pino,^{144a} D. Oliveira Damazio,²⁹ J. L. Oliver,¹ M. J. R. Olsson,³⁶ A. Olszewski,⁸² J. Olszowska,⁸² D. C. O'Neil,¹⁴⁹ A. Onofre,^{137a,137e} K. Onogi,¹¹⁵ P. U. E. Onyisi,¹¹ H. Oppen,¹³¹ M. J. Oreglia,³⁶ G. E. Orellana,⁸⁶ Y. Oren,¹⁵⁸ D. Orestano,^{72a,72b} E. C. Orgill,⁹⁸ N. Orlando,¹⁴ A. A. O'Rourke,⁴⁴ R. S. Orr,¹⁶⁴ B. Osculati,^{53b,53a,†} V. O'Shea,⁵⁵ R. Ospanov,^{58a} G. Otero y Garzon,³⁰ H. Otono,⁸⁵ M. Ouchrif,^{34d} F. Ould-Saada,¹³¹ A. Ouraou,¹⁴² Q. Ouyang,^{15a} M. Owen,⁵⁵ R. E. Owen,²¹ V. E. Ozcan,^{12c} N. Ozturk,⁸ J. Pacalt,¹²⁷ H. A. Pacey,³¹ K. Pachal,¹⁴⁹ A. Pacheco Pages,¹⁴ L. Pacheco Rodriguez,¹⁴² C. Padilla Aranda,¹⁴ S. Pagan Griso,¹⁸ M. Paganini,¹⁸⁰ G. Palacino,⁶³ S. Palazzo,⁴⁸ S. Palestini,³⁵ M. Palka,^{81b} D. Pallin,³⁷ I. Panagoulas,¹⁰ C. E. Pandini,³⁵ J. G. Panduro Vazquez,⁹¹ P. Pani,⁴⁴ G. Panizzo,^{64a,64c} L. Paolozzi,⁵² K. Papageorgiou,^{9,k} A. Paramonov,⁶ D. Paredes Hernandez,^{61b} S. R. Paredes Saenz,¹³² B. Parida,¹⁶³ T. H. Park,³³ A. J. Parker,⁸⁷ M. A. Parker,³¹ F. Parodi,^{53b,53a} E. W. P. Parrish,¹¹⁹ J. A. Parsons,³⁸ U. Parzefall,⁵⁰ V. R. Pascuzzi,¹⁶⁴ J. M. P. Pasner,¹⁴³ E. Pasqualucci,^{70a} S. Passaggio,^{53b} F. Pastore,⁹¹ P. Pasuwan,^{43a,43b} S. Patariaia,⁹⁷ J. R. Pater,⁹⁸ A. Pathak,^{178,1} T. Pauly,³⁵ B. Pearson,¹¹³ M. Pedersen,¹³¹ L. Pedraza Diaz,¹¹⁷ R. Pedro,^{137a,137b} S. V. Peleganchuk,^{120b,120a} O. Penc,¹³⁸ C. Peng,^{15d} H. Peng,^{58a} B. S. Peralva,^{78a} M. M. Perego,¹²⁹ A. P. Pereira Peixoto,^{137a} D. V. Perepelitsa,²⁹ F. Peri,¹⁹ L. Perini,^{66a,66b} H. Pernegger,³⁵ S. Perrella,^{67a,67b} V. D. Peshekhonov,^{77,†} K. Peters,⁴⁴ R. F. Y. Peters,⁹⁸ B. A. Petersen,³⁵ T. C. Petersen,³⁹ E. Petit,⁵⁶ A. Petridis,¹ C. Petridou,¹⁵⁹ P. Petroff,¹²⁹ M. Petrov,¹³² F. Petrucci,^{72a,72b} M. Pettee,¹⁸⁰ N. E. Pettersson,¹⁰⁰ A. Peyaud,¹⁴² R. Pezoa,^{144b} T. Pham,¹⁰² F. H. Phillips,¹⁰⁴ P. W. Phillips,¹⁴¹ M. W. Phipps,¹⁷⁰ G. Piacquadio,¹⁵² E. Pianori,¹⁸ A. Picazio,¹⁰⁰ R. H. Pickles,⁹⁸ R. Piegaia,³⁰ J. E. Pilcher,³⁶ A. D. Pilkington,⁹⁸ M. Pinamonti,^{71a,71b} J. L. Pinfold,³ M. Pitt,¹⁷⁷ L. Pizzimento,^{71a,71b} M.-A. Pleier,²⁹ V. Pleskot,¹⁴⁰ E. Plotnikova,⁷⁷ D. Pluth,⁷⁶ P. Podberezko,^{120b,120a} R. Poettgen,⁹⁴ R. Poggi,⁵² L. Poggioli,¹²⁹ I. Pogrebnyak,¹⁰⁴ D. Pohl,²⁴ I. Pokharel,⁵¹ G. Polesello,^{68a} A. Poley,¹⁸ A. Policicchio,^{70a,70b} R. Polifka,³⁵ A. Polini,^{23b} C. S. Pollard,⁴⁴ V. Polychronakos,²⁹ D. Ponomarenko,¹¹⁰ L. Pontecorvo,³⁵ G. A. Popeneciu,^{27d} D. M. Portillo Quintero,¹³³ S. Pospisil,¹³⁹ K. Potamianos,⁴⁴ I. N. Potrap,⁷⁷ C. J. Potter,³¹ H. Potti,¹¹ T. Poulsen,⁹⁴ J. Poveda,³⁵ T. D. Powell,¹⁴⁶ M. E. Pozo Astigarraga,³⁵ P. Pralavorio,⁹⁹ S. Prell,⁷⁶ D. Price,⁹⁸ M. Primavera,^{65a} S. Prince,¹⁰¹ M. L. Proffitt,¹⁴⁵ N. Proklova,¹¹⁰ K. Prokofiev,^{61c} F. Prokoshin,^{144b} S. Protopopescu,²⁹ J. Proudfoot,⁶ M. Przybycien,^{81a} A. Puri,¹⁷⁰ P. Puzo,¹²⁹ J. Qian,¹⁰³ Y. Qin,⁹⁸ A. Quadt,⁵¹ M. Queitsch-Maitland,⁴⁴ A. Qureshi,¹ P. Rados,¹⁰² F. Ragusa,^{66a,66b} G. Rahal,⁹⁵ J. A. Raine,⁵² S. Rajagopalan,²⁹ A. Ramirez Morales,⁹⁰ K. Ran,^{15a} T. Rashid,¹²⁹ S. Raspopov,⁵ M. G. Ratti,^{66a,66b} D. M. Rauch,⁴⁴ F. Rauscher,¹¹² S. Rave,⁹⁷ B. Ravina,¹⁴⁶ I. Ravinovich,¹⁷⁷ J. H. Rawling,⁹⁸ M. Raymond,³⁵ A. L. Read,¹³¹ N. P. Readioff,⁵⁶ M. Reale,^{65a,65b} D. M. Rebuzzi,^{68a,68b} A. Redelbach,¹⁷⁴ G. Redlinger,²⁹ R. G. Reed,^{32c} K. Reeves,⁴² L. Rehnisch,¹⁹ J. Reichert,¹³⁴ D. Reikher,¹⁵⁸ A. Reiss,⁹⁷ A. Rej,¹⁴⁸ C. Rembser,³⁵ H. Ren,^{15d} M. Rescigno,^{70a} S. Resconi,^{66a} E. D. Resseguie,¹³⁴ S. Rettie,¹⁷² E. Reynolds,²¹ O. L. Rezanova,^{120b,120a} P. Reznicek,¹⁴⁰ E. Ricci,^{73a,73b} R. Richter,¹¹³ S. Richter,⁴⁴ E. Richter-Was,^{81b} O. Ricken,²⁴ M. Ridel,¹³³ P. Rieck,¹¹³ C. J. Riegel,¹⁷⁹ O. Rifki,⁴⁴ M. Rijssenbeek,¹⁵² A. Rimoldi,^{68a,68b} M. Rimoldi,²⁰ L. Rinaldi,^{23b} G. Ripellino,¹⁵¹ B. Ristić,⁸⁷ E. Ritsch,³⁵ I. Riu,¹⁴ J. C. Rivera Vergara,^{144a} F. Rizatdinova,¹²⁶

E. Rizvi,⁹⁰ C. Rizzi,¹⁴ R. T. Roberts,⁹⁸ S. H. Robertson,^{101,ac} D. Robinson,³¹ J. E. M. Robinson,⁴⁴ A. Robson,⁵⁵ E. Rocco,⁹⁷
 C. Roda,^{69a,69b} Y. Rodina,⁹⁹ S. Rodriguez Bosca,¹⁷¹ A. Rodriguez Perez,¹⁴ D. Rodriguez Rodriguez,¹⁷¹
 A. M. Rodríguez Vera,^{165b} S. Roe,³⁵ O. Røhne,¹³¹ R. Röhrig,¹¹³ C. P. A. Roland,⁶³ J. Roloff,⁵⁷ A. Romaniouk,¹¹⁰
 M. Romano,^{23b,23a} N. Rompotis,⁸⁸ M. Ronzani,¹²² L. Roos,¹³³ S. Rosati,^{70a} K. Rosbach,⁵⁰ N-A. Rosien,⁵¹ B. J. Rosser,¹³⁴
 E. Rossi,⁴⁴ E. Rossi,^{72a,72b} E. Rossi,^{67a,67b} L. P. Rossi,^{53b} L. Rossini,^{66a,66b} J. H. N. Rosten,³¹ R. Rosten,¹⁴ M. Rotaru,^{27b}
 J. Rothberg,¹⁴⁵ D. Rousseau,¹²⁹ D. Roy,^{32c} A. Rozanov,⁹⁹ Y. Rozen,¹⁵⁷ X. Ruan,^{32c} F. Rubbo,¹⁵⁰ F. Rühr,⁵⁰
 A. Ruiz-Martinez,¹⁷¹ Z. Rurikova,⁵⁰ N. A. Rusakovich,⁷⁷ H. L. Russell,¹⁰¹ J. P. Rutherford,⁷ E. M. Rüttinger,^{44,m}
 Y. F. Ryabov,¹³⁵ M. Rybar,³⁸ G. Rybkin,¹²⁹ S. Ryu,⁶ A. Ryzhov,¹²¹ G. F. Rzehorz,⁵¹ P. Sabatini,⁵¹ G. Sabato,¹¹⁸
 S. Sacerdoti,¹²⁹ H. F-W. Sadrozinski,¹⁴³ R. Sadykov,⁷⁷ F. Safai Tehrani,^{70a} P. Saha,¹¹⁹ M. Sahinsoy,^{59a} A. Sahu,¹⁷⁹
 M. Saimpert,⁴⁴ M. Saito,¹⁶⁰ T. Saito,¹⁶⁰ H. Sakamoto,¹⁶⁰ A. Sakharov,^{122,am} D. Salamani,⁵² G. Salamanna,^{72a,72b}
 J. E. Salazar Loyola,^{144b} P. H. Sales De Bruin,¹⁶⁹ D. Salihagic,^{113,†} A. Salsnikov,¹⁵⁰ J. Salt,¹⁷¹ D. Salvatore,^{40b,40a}
 F. Salvatore,¹⁵³ A. Salvucci,^{61a,61b,61c} A. Salzburger,³⁵ J. Samarati,³⁵ D. Sammel,⁵⁰ D. Sampsonidis,¹⁵⁹ D. Sampsonidou,¹⁵⁹
 J. Sánchez,¹⁷¹ A. Sanchez Pineda,^{64a,64c} H. Sandaker,¹³¹ C. O. Sander,⁴⁴ M. Sandhoff,¹⁷⁹ C. Sandoval,²² D. P. C. Sankey,¹⁴¹
 M. Sannino,^{53b,53a} Y. Sano,¹¹⁵ A. Sansoni,⁴⁹ C. Santoni,³⁷ H. Santos,^{137a} A. Santra,¹⁷¹ A. Sapronov,⁷⁷ J. G. Saraiva,^{137a,137d}
 O. Sasaki,⁷⁹ K. Sato,¹⁶⁶ E. Sauvan,⁵ P. Savard,^{164,av} N. Savic,¹¹³ R. Sawada,¹⁶⁰ C. Sawyer,¹⁴¹ L. Sawyer,^{93,ak} C. Sbarra,^{23b}
 A. Sbrizzi,^{23a} T. Scanlon,⁹² J. Schaarschmidt,¹⁴⁵ P. Schacht,¹¹³ B. M. Schachtner,¹¹² D. Schaefer,³⁶ L. Schaefer,¹³⁴
 J. Schaeffer,⁹⁷ S. Schaepe,³⁵ U. Schäfer,⁹⁷ A. C. Schaffer,¹²⁹ D. Schaile,¹¹² R. D. Schamberger,¹⁵² N. Scharmberg,⁹⁸
 V. A. Schegelsky,¹³⁵ D. Scheirich,¹⁴⁰ F. Schenck,¹⁹ M. Schernau,¹⁶⁸ C. Schiavi,^{53b,53a} S. Schier,¹⁴³ L. K. Schildgen,²⁴
 Z. M. Schillaci,²⁶ E. J. Schioppa,³⁵ M. Schioppa,^{40b,40a} K. E. Schleicher,⁵⁰ S. Schlenker,³⁵ K. R. Schmidt-Sommerfeld,¹¹³
 K. Schmieden,³⁵ C. Schmitt,⁹⁷ S. Schmitt,⁴⁴ S. Schmitz,⁹⁷ J. C. Schmoeckel,⁴⁴ U. Schnoor,⁵⁰ L. Schoeffel,¹⁴²
 A. Schoening,^{59b} E. Schopf,¹³² M. Schott,⁹⁷ J. F. P. Schouwenberg,¹¹⁷ J. Schovancova,³⁵ S. Schramm,⁵² A. Schulte,⁹⁷
 H-C. Schultz-Coulon,^{59a} M. Schumacher,⁵⁰ B. A. Schumm,¹⁴³ Ph. Schune,¹⁴² A. Schwartzman,¹⁵⁰ T. A. Schwarz,¹⁰³
 Ph. Schwemling,¹⁴² R. Schwienhorst,¹⁰⁴ A. Sciandra,²⁴ G. Sciolla,²⁶ M. Scornajenghi,^{40b,40a} F. Scuri,^{69a} F. Scutti,¹⁰²
 L. M. Scyboz,¹¹³ C. D. Sebastiani,^{70a,70b} P. Seema,¹⁹ S. C. Seidel,¹¹⁶ A. Seiden,¹⁴³ T. Seiss,³⁶ J. M. Seixas,^{78b}
 G. Sekhniaidze,^{67a} K. Sekhon,¹⁰³ S. J. Sekula,⁴¹ N. Semprini-Cesari,^{23b,23a} S. Sen,⁴⁷ S. Senkin,³⁷ C. Serfon,¹³¹ L. Serin,¹²⁹
 L. Serkin,^{64a,64b} M. Sessa,^{58a} H. Severini,¹²⁵ F. Sforza,¹⁶⁷ A. Sfyrla,⁵² E. Shabalina,⁵¹ J. D. Shahinian,¹⁴³ N. W. Shaikh,^{43a,43b}
 D. Shaked Renous,¹⁷⁷ L. Y. Shan,^{15a} R. Shang,¹⁷⁰ J. T. Shank,²⁵ M. Shapiro,¹⁸ A. S. Sharma,¹ A. Sharma,¹³²
 P. B. Shatalov,¹⁰⁹ K. Shaw,¹⁵³ S. M. Shaw,⁹⁸ A. Shcherbakova,¹³⁵ Y. Shen,¹²⁵ N. Sherafati,³³ A. D. Sherman,²⁵
 P. Sherwood,⁹² L. Shi,^{155,ar} S. Shimizu,⁷⁹ C. O. Shimmin,¹⁸⁰ Y. Shimogama,¹⁷⁶ M. Shimojima,¹¹⁴ I. P. J. Shipsey,¹³²
 S. Shirabe,⁸⁵ M. Shiyakova,⁷⁷ J. Shlomi,¹⁷⁷ A. Shmeleva,¹⁰⁸ D. Shoaleh Saadi,¹⁰⁷ M. J. Shochet,³⁶ S. Shojaii,¹⁰²
 D. R. Shope,¹²⁵ S. Shrestha,¹²³ E. Shulga,¹¹⁰ P. Sicho,¹³⁸ A. M. Sickles,¹⁷⁰ P. E. Sidebo,¹⁵¹ E. Sideras Haddad,^{32c}
 O. Sidiropoulou,³⁵ A. Sidoti,^{23b,23a} F. Siegert,⁴⁶ Dj. Sijacki,¹⁶ J. Silva,^{137a} M. Silva Jr.,¹⁷⁸ M. V. Silva Oliveira,^{78a}
 S. B. Silverstein,^{43a} S. Simion,¹²⁹ E. Simioni,⁹⁷ M. Simon,⁹⁷ R. Simoniello,⁹⁷ P. Sinervo,¹⁶⁴ N. B. Sinev,¹²⁸ M. Sioli,^{23b,23a}
 I. Siral,¹⁰³ S. Yu. Sivoklov,¹¹¹ J. Sjölin,^{43a,43b} P. Skubic,¹²⁵ T. Slavicek,¹³⁹ M. Slawinska,⁸² K. Sliwa,¹⁶⁷ R. Slovak,¹⁴⁰
 V. Smakhtin,¹⁷⁷ B. H. Smart,⁵ J. Smiesko,^{28a} N. Smirnov,¹¹⁰ S. Yu. Smirnov,¹¹⁰ Y. Smirnov,¹¹⁰ L. N. Smirnova,¹¹¹
 O. Smirnova,⁹⁴ J. W. Smith,⁵¹ M. Smizanska,⁸⁷ K. Smolek,¹³⁹ A. Smykiewicz,⁸² A. A. Snesarev,¹⁰⁸ I. M. Snyder,¹²⁸
 S. Snyder,²⁹ R. Sobie,^{173,ac} A. M. Soffa,¹⁶⁸ A. Soffer,¹⁵⁸ A. Søgaaard,⁴⁸ F. Sohns,⁵¹ G. Sokhrannyi,⁸⁹ C. A. Solans Sanchez,³⁵
 M. Solar,¹³⁹ E. Yu. Soldatov,¹¹⁰ U. Soldevila,¹⁷¹ A. A. Solodkov,¹²¹ A. Soloshenko,⁷⁷ O. V. Solovyanov,¹²¹ V. Solovyeu,¹³⁵
 P. Sommer,¹⁴⁶ H. Son,¹⁶⁷ W. Song,¹⁴¹ W. Y. Song,^{165b} A. Sopczak,¹³⁹ F. Sopkova,^{28b} C. L. Sotiropoulou,^{69a,69b}
 S. Sottocornola,^{68a,68b} R. Soualah,^{64a,64c,j} A. M. Soukharev,^{120b,120a} D. South,⁴⁴ S. Spagnolo,^{65a,65b} M. Spalla,¹¹³
 M. Spangenberg,¹⁷⁵ F. Spanò,⁹¹ D. Sperlich,¹⁹ T. M. Spieker,^{59a} R. Spighi,^{23b} G. Spigo,³⁵ L. A. Spiller,¹⁰² D. P. Spiteri,⁵⁵
 M. Spousta,¹⁴⁰ A. Stabile,^{66a,66b} B. L. Stamas,¹¹⁹ R. Stamen,^{59a} S. Stamm,¹⁹ E. Stanecka,⁸² R. W. Stanek,⁶ B. Stanislaus,¹³²
 M. M. Stanitzki,⁴⁴ B. Stapf,¹¹⁸ E. A. Starchenko,¹²¹ G. H. Stark,¹⁴³ J. Stark,⁵⁶ S. H. Stark,³⁹ P. Staroba,¹³⁸ P. Starovoitov,^{59a}
 S. Stärz,¹⁰¹ R. Staszewski,⁸² M. Stegler,⁴⁴ P. Steinberg,²⁹ B. Stelzer,¹⁴⁹ H. J. Stelzer,³⁵ O. Stelzer-Chilton,^{165a} H. Stenzel,⁵⁴
 T. J. Stevenson,¹⁵³ G. A. Stewart,³⁵ M. C. Stockton,³⁵ G. Stoicea,^{27b} P. Stolte,⁵¹ S. Stonjek,¹¹³ A. Straessner,⁴⁶
 J. Strandberg,¹⁵¹ S. Strandberg,^{43a,43b} M. Strauss,¹²⁵ P. Strizenec,^{28b} R. Ströhmer,¹⁷⁴ D. M. Strom,¹²⁸ R. Stroynowski,⁴¹
 A. Strubig,⁴⁸ S. A. Stucci,²⁹ B. Stugu,¹⁷ J. Stupak,¹²⁵ N. A. Styles,⁴⁴ D. Su,¹⁵⁰ S. Suchek,^{59a} Y. Sugaya,¹³⁰ M. Suk,¹³⁹
 V. V. Sulín,¹⁰⁸ M. J. Sullivan,⁸⁸ D. M. S. Sultan,⁵² S. Sultansoy,^{4c} T. Sumida,⁸³ S. Sun,¹⁰³ X. Sun,³ K. Suruliz,¹⁵³
 C. J. E. Suster,¹⁵⁴ M. R. Sutton,¹⁵³ S. Suzuki,⁷⁹ M. Svatos,¹³⁸ M. Swiatlowski,³⁶ S. P. Swift,² A. Sydorenko,⁹⁷ I. Sykora,^{28a}

M. Sykora,¹⁴⁰ T. Sykora,¹⁴⁰ D. Ta,⁹⁷ K. Tackmann,^{44,z} J. Taenzer,¹⁵⁸ A. Taffard,¹⁶⁸ R. Tafirout,^{165a} E. Tahirovic,⁹⁰ N. Taiblum,¹⁵⁸ H. Takai,²⁹ R. Takashima,⁸⁴ K. Takeda,⁸⁰ T. Takeshita,¹⁴⁷ Y. Takubo,⁷⁹ M. Talby,⁹⁹ A. A. Talyshev,^{120b,120a} J. Tanaka,¹⁶⁰ M. Tanaka,¹⁶² R. Tanaka,¹²⁹ B. B. Tannenwald,¹²³ S. Tapia Araya,¹⁷⁰ S. Tapprogge,⁹⁷ A. Tarek Abouelfadl Mohamed,¹³³ S. Tarem,¹⁵⁷ G. Tarna,^{27b,e} G. F. Tartarelli,^{66a} P. Tas,¹⁴⁰ M. Tasevsky,¹³⁸ T. Tashiro,⁸³ E. Tassi,^{40b,40a} A. Tavares Delgado,^{137a,137b} Y. Tayalati,^{34e} A. J. Taylor,⁴⁸ G. N. Taylor,¹⁰² P. T. E. Taylor,¹⁰² W. Taylor,^{165b} A. S. Tee,⁸⁷ R. Teixeira De Lima,¹⁵⁰ P. Teixeira-Dias,⁹¹ H. Ten Kate,³⁵ J. J. Teoh,¹¹⁸ S. Terada,⁷⁹ K. Terashi,¹⁶⁰ J. Terron,⁹⁶ S. Terzo,¹⁴ M. Testa,⁴⁹ R. J. Teuscher,^{164,ac} S. J. Thais,¹⁸⁰ T. Theveneaux-Pelzer,⁴⁴ F. Thiele,³⁹ D. W. Thomas,⁹¹ J. P. Thomas,²¹ A. S. Thompson,⁵⁵ P. D. Thompson,²¹ L. A. Thomsen,¹⁸⁰ E. Thomson,¹³⁴ Y. Tian,³⁸ R. E. Tisce Torres,⁵¹ V. O. Tikhomirov,^{108,ao} Yu. A. Tikhonov,^{120b,120a} S. Timoshenko,¹¹⁰ P. Tipton,¹⁸⁰ S. Tisserant,⁹⁹ K. Todome,¹⁶² S. Todorova-Nova,⁵ S. Todt,⁴⁶ J. Tojo,⁸⁵ S. Tokár,^{28a} K. Tokushuku,⁷⁹ E. Tolley,¹²³ K. G. Tomiwa,^{32c} M. Tomoto,¹¹⁵ L. Tompkins,^{150,r} K. Toms,¹¹⁶ B. Tong,⁵⁷ P. Tornambe,⁵⁰ E. Torrence,¹²⁸ H. Torres,⁴⁶ E. Torró Pastor,¹⁴⁵ C. Toscirci,¹³² J. Toth,^{99,ab} F. Touchard,⁹⁹ D. R. Tovey,¹⁴⁶ C. J. Treado,¹²² T. Trefzger,¹⁷⁴ F. Tresoldi,¹⁵³ A. Tricoli,²⁹ I. M. Trigger,^{165a} S. Trincaz-Duvold,¹³³ W. Trischuk,¹⁶⁴ B. Trocmé,⁵⁶ A. Trofymov,¹²⁹ C. Troncon,^{66a} M. Trovatelli,¹⁷³ F. Trovato,¹⁵³ L. Truong,^{32b} M. Trzebinski,⁸² A. Trzupek,⁸² F. Tsai,⁴⁴ J. C.-L. Tseng,¹³² P. V. Tsiarshka,^{105,ai} A. Tsirigotis,¹⁵⁹ N. Tsirintanis,⁹ V. Tsiskaridze,¹⁵² E. G. Tskhadadze,^{156a} I. I. Tsukerman,¹⁰⁹ V. Tsulaia,¹⁸ S. Tsuno,⁷⁹ D. Tsybychev,^{152,163} Y. Tu,^{61b} A. Tudorache,^{27b} V. Tudorache,^{27b} T. T. Tulbure,^{27a} A. N. Tuna,⁵⁷ S. Turchikhin,⁷⁷ D. Turgeman,¹⁷⁷ I. Turk Cakir,^{4b,u} R. J. Turner,²¹ R. T. Turra,^{66a} P. M. Tuts,³⁸ S. Tzamarias,¹⁵⁹ E. Tzovara,⁹⁷ G. Ucchielli,⁴⁵ I. Ueda,⁷⁹ M. Ughetto,^{43a,43b} F. Ukegawa,¹⁶⁶ G. Unal,³⁵ A. Undrus,²⁹ G. Unel,¹⁶⁸ F. C. Ungaro,¹⁰² Y. Unno,⁷⁹ K. Uno,¹⁶⁰ J. Urban,^{28b} P. Urquijo,¹⁰² G. Usai,⁸ J. Usui,⁷⁹ L. Vacavant,⁹⁹ V. Vacek,¹³⁹ B. Vachon,¹⁰¹ K. O. H. Vadla,¹³¹ A. Vaidya,⁹² C. Valderanis,¹¹² E. Valdes Santurio,^{43a,43b} M. Valente,⁵² S. Valentinetti,^{23b,23a} A. Valero,¹⁷¹ L. Valéry,⁴⁴ R. A. Vallance,²¹ A. Vallier,⁵ J. A. Valls Ferrer,¹⁷¹ T. R. Van Daalen,¹⁴ H. Van der Graaf,¹¹⁸ P. Van Gemmeren,⁶ I. Van Vulpen,¹¹⁸ M. Vanadia,^{71a,71b} W. Vandelli,³⁵ A. Vaniachine,¹⁶³ P. Vankov,¹¹⁸ R. Vari,^{70a} E. W. Varnes,⁷ C. Varni,^{53b,53a} T. Varol,⁴¹ D. Varouchas,¹²⁹ K. E. Varvell,¹⁵⁴ G. A. Vasquez,^{144b} J. G. Vasquez,¹⁸⁰ F. Vazeille,³⁷ D. Vazquez Furelos,¹⁴ T. Vazquez Schroeder,³⁵ J. Veatch,⁵¹ V. Vecchio,^{72a,72b} L. M. Veloce,¹⁶⁴ F. Veloso,^{137a,137c} S. Veneziano,^{70a} A. Ventura,^{65a,65b} N. Venturi,³⁵ A. Verbytskyi,¹¹³ V. Vercesi,^{68a} M. Verducci,^{72a,72b} C. M. Vergel Infante,⁷⁶ C. Vergis,²⁴ W. Verkerke,¹¹⁸ A. T. Vermeulen,¹¹⁸ J. C. Vermeulen,¹¹⁸ M. C. Vetterli,^{149,av} N. Viaux Maira,^{144b} M. Vicente Barreto Pinto,⁵² I. Vichou,^{170,†} T. Vickey,¹⁴⁶ O. E. Vickey Boeriu,¹⁴⁶ G. H. A. Viehhauser,¹³² S. Viel,¹⁸ L. Vigani,¹³² M. Villa,^{23b,23a} M. Villaplana Perez,^{66a,66b} E. Vilucchi,⁴⁹ M. G. Vincter,³³ V. B. Vinogradov,⁷⁷ A. Vishwakarma,⁴⁴ C. Vittori,^{23b,23a} I. Vivarelli,¹⁵³ S. Vlachos,¹⁰ M. Vogel,¹⁷⁹ P. Vokac,¹³⁹ G. Volpi,¹⁴ S. E. von Buddenbrock,^{32c} E. Von Toerne,²⁴ V. Vorobel,¹⁴⁰ K. Vorobev,¹¹⁰ M. Vos,¹⁷¹ J. H. Vossebeld,⁸⁸ N. Vranjes,¹⁶ M. Vranjes Milosavljevic,¹⁶ V. Vrba,¹³⁹ M. Vreeswijk,¹¹⁸ T. Šfiligoj,⁸⁹ R. Vuillemermet,³⁵ I. Vukotic,³⁶ T. Ženiš,^{28a} L. Živković,¹⁶ P. Wagner,²⁴ W. Wagner,¹⁷⁹ J. Wagner-Kuhr,¹¹² H. Wahlberg,⁸⁶ S. Wahrenmund,⁴⁶ K. Wakamiya,⁸⁰ V. M. Walbrecht,¹¹³ J. Walder,⁸⁷ R. Walker,¹¹² S. D. Walker,⁹¹ W. Walkowiak,¹⁴⁸ V. Wallangen,^{43a,43b} A. M. Wang,⁵⁷ C. Wang,^{58b} F. Wang,¹⁷⁸ H. Wang,¹⁸ H. Wang,³ J. Wang,¹⁵⁴ J. Wang,^{59b} P. Wang,⁴¹ Q. Wang,¹²⁵ R.-J. Wang,¹³³ R. Wang,^{58a} R. Wang,⁶ S. M. Wang,¹⁵⁵ W. T. Wang,^{58a} W. Wang,^{15c,ad} W. X. Wang,^{58a,ad} Y. Wang,^{58a,al} Z. Wang,^{58c} C. Wanotayaroj,⁴⁴ A. Warburton,¹⁰¹ C. P. Ward,³¹ D. R. Wardrope,⁹² A. Washbrook,⁴⁸ A. T. Watson,²¹ M. F. Watson,²¹ G. Watts,¹⁴⁵ S. Watts,⁹⁸ B. M. Waugh,⁹² A. F. Webb,¹¹ S. Webb,⁹⁷ C. Weber,¹⁸⁰ M. S. Weber,²⁰ S. A. Weber,³³ S. M. Weber,^{59a} A. R. Weidberg,¹³² J. Weingarten,⁴⁵ M. Weirich,⁹⁷ C. Weiser,⁵⁰ P. S. Wells,³⁵ T. Wenaus,²⁹ T. Wengler,³⁵ S. Wenig,³⁵ N. Wermes,²⁴ M. D. Werner,⁷⁶ P. Werner,³⁵ M. Wessels,^{59a} T. D. Weston,²⁰ K. Whalen,¹²⁸ N. L. Whallon,¹⁴⁵ A. M. Wharton,⁸⁷ A. S. White,¹⁰³ A. White,⁸ M. J. White,¹ R. White,^{144b} D. Whiteson,¹⁶⁸ B. W. Whitmore,⁸⁷ F. J. Wickens,¹⁴¹ W. Wiedenmann,¹⁷⁸ M. Wielers,¹⁴¹ C. Wigglesworth,³⁹ L. A. M. Wiik-Fuchs,⁵⁰ F. Wilk,⁹⁸ H. G. Wilkens,³⁵ L. J. Wilkins,⁹¹ H. H. Williams,¹³⁴ S. Williams,³¹ C. Willis,¹⁰⁴ S. Willocq,¹⁰⁰ J. A. Wilson,²¹ I. Wingerter-Seez,⁵ E. Winkels,¹⁵³ F. Winklmeier,¹²⁸ O. J. Winston,¹⁵³ B. T. Winter,⁵⁰ M. Wittgen,¹⁵⁰ M. Wobisch,⁹³ A. Wolf,⁹⁷ T. M. H. Wolf,¹¹⁸ R. Wolff,⁹⁹ J. Wollrath,⁵⁰ M. W. Wolter,⁸² H. Wolters,^{137a,137c} V. W. S. Wong,¹⁷² N. L. Woods,¹⁴³ S. D. Worm,²¹ B. K. Wosiek,⁸² K. W. Woźniak,⁸² K. Wraight,⁵⁵ S. L. Wu,¹⁷⁸ X. Wu,⁵² Y. Wu,^{58a} T. R. Wyatt,⁹⁸ B. M. Wynne,⁴⁸ S. Xella,³⁹ Z. Xi,¹⁰³ L. Xia,¹⁷⁵ D. Xu,^{15a} H. Xu,^{58a,e} L. Xu,²⁹ T. Xu,¹⁴² W. Xu,¹⁰³ Z. Xu,¹⁵⁰ B. Yabsley,¹⁵⁴ S. Yacoob,^{32a} K. Yajima,¹³⁰ D. P. Yallup,⁹² D. Yamaguchi,¹⁶² Y. Yamaguchi,¹⁶² A. Yamamoto,⁷⁹ T. Yamanaka,¹⁶⁰ F. Yamane,⁸⁰ M. Yamatani,¹⁶⁰ T. Yamazaki,¹⁶⁰ Y. Yamazaki,⁸⁰ Z. Yan,²⁵ H. J. Yang,^{58c,58d} H. T. Yang,¹⁸ S. Yang,⁷⁵ Y. Yang,¹⁶⁰ Z. Yang,¹⁷ W.-M. Yao,¹⁸ Y. C. Yap,⁴⁴ Y. Yasu,⁷⁹ E. Yatsenko,^{58c,58d} J. Ye,⁴¹ S. Ye,²⁹ I. Yeletsikh,⁷⁷ E. Yigitbasi,²⁵ E. Yildirim,⁹⁷ K. Yorita,¹⁷⁶ K. Yoshihara,¹³⁴ C. J. S. Young,³⁵ C. Young,¹⁵⁰ J. Yu,⁷⁶ X. Yue,^{59a} S. P. Y. Yuen,²⁴ B. Zabinski,⁸²

G. Zacharis,¹⁰ E. Zaffaroni,⁵² R. Zaidan,¹⁴ A. M. Zaitsev,^{121,an} T. Zakareishvili,^{156b} N. Zakharchuk,³³ S. Zambito,⁵⁷ D. Zanzi,³⁵ D. R. Zariповas,⁵⁵ S. V. Zeiβner,⁴⁵ C. Zeitnitz,¹⁷⁹ G. Zemaityte,¹³² J. C. Zeng,¹⁷⁰ O. Zenin,¹²¹ D. Zerwas,¹²⁹ M. Zgubič,¹³² D. F. Zhang,^{15b} F. Zhang,¹⁷⁸ G. Zhang,^{58a} G. Zhang,^{15b} H. Zhang,^{15c} J. Zhang,⁶ L. Zhang,^{15c} L. Zhang,^{58a} M. Zhang,¹⁷⁰ R. Zhang,^{58a} R. Zhang,²⁴ X. Zhang,^{58b} Y. Zhang,^{15d} Z. Zhang,¹²⁹ P. Zhao,⁴⁷ Y. Zhao,^{58b} Z. Zhao,^{58a} A. Zhemchugov,⁷⁷ Z. Zheng,¹⁰³ D. Zhong,¹⁷⁰ B. Zhou,¹⁰³ C. Zhou,¹⁷⁸ M. S. Zhou,^{15d} M. Zhou,¹⁵² N. Zhou,^{58c} Y. Zhou,⁷ C. G. Zhu,^{58b} H. L. Zhu,^{58a} H. Zhu,^{15a} J. Zhu,¹⁰³ Y. Zhu,^{58a} X. Zhuang,^{15a} K. Zhukov,¹⁰⁸ V. Zhulanov,^{120b,120a} A. Zibell,¹⁷⁴ D. Zieminska,⁶³ N. I. Zimine,⁷⁷ S. Zimmermann,⁵⁰ Z. Zinonos,¹¹³ M. Ziolkowski,¹⁴⁸ G. Zobernig,¹⁷⁸ A. Zoccoli,^{23b,23a} K. Zoch,⁵¹ T. G. Zorbas,¹⁴⁶ R. Zou,³⁶ and L. Zwalinski³⁵

(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, 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*
²²*Centro de Investigaciones, Universidad Antonio Nariño, Bogota, Colombia*
^{23a}*Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy*
^{23b}*INFN Sezione di Bologna, 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*Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom*
- ^{32a}*Department of Physics, University of Cape Town, Cape Town, South Africa*
- ^{32b}*Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa*
- ^{32c}*School of Physics, University of the Witwatersrand, Johannesburg, South Africa*
- ³³*Department of Physics, Carleton University, Ottawa, Ontario, Canada*
- ^{34a}*Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies—Université Hassan II, Casablanca, Morocco*
- ^{34b}*Centre National de l’Energie des Sciences Techniques Nucleaires (CNESTEN), Rabat, Morocco*
- ^{34c}*Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech, Morocco*
- ^{34d}*Faculté des Sciences, Université Mohamed Premier and LTPM, Oujda, Morocco*
- ^{34e}*Faculté des sciences, Université Mohammed V, Rabat, Morocco*
- ³⁵*CERN, Geneva, Switzerland*
- ³⁶*Enrico Fermi Institute, University of Chicago, Chicago, Illinois, USA*
- ³⁷*LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand, France*
- ³⁸*Nevis Laboratory, Columbia University, Irvington, New York, USA*
- ³⁹*Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark*
- ^{40a}*Dipartimento di Fisica, Università della Calabria, Rende, Italy*
- ^{40b}*INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Italy*
- ⁴¹*Physics Department, Southern Methodist University, Dallas, Texas, USA*
- ⁴²*Physics Department, University of Texas at Dallas, Richardson, Texas, USA*
- ^{43a}*Department of Physics, Stockholm University, Stockholm, Sweden*
- ^{43b}*Oskar Klein Centre, Stockholm, Sweden*
- ⁴⁴*Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen, Germany*
- ⁴⁵*Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany*
- ⁴⁶*Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany*
- ⁴⁷*Department of Physics, Duke University, Durham, North Carolina, USA*
- ⁴⁸*SUPA—School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom*
- ⁴⁹*INFN e Laboratori Nazionali di Frascati, Frascati, Italy*
- ⁵⁰*Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany*
- ⁵¹*II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany*
- ⁵²*Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland*
- ^{53a}*Dipartimento di Fisica, Università di Genova, Genova, Italy*
- ^{53b}*INFN Sezione di Genova, Genova, Italy*
- ⁵⁴*II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany*
- ⁵⁵*SUPA—School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom*
- ⁵⁶*LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble, France*
- ⁵⁷*Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, Massachusetts, USA*
- ^{58a}*Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Hefei, China*
- ^{58b}*Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE), Shandong University, Qingdao, China*
- ^{58c}*School of Physics and Astronomy, Shanghai Jiao Tong University, KLPPAC-MoE, SKLPPC, Shanghai, China*
- ^{58d}*Tsung-Dao Lee Institute, Shanghai, China*
- ^{59a}*Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany*
- ^{59b}*Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany*
- ⁶⁰*Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan*
- ^{61a}*Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China*
- ^{61b}*Department of Physics, University of Hong Kong, Hong Kong, China*
- ^{61c}*Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China*
- ⁶²*Department of Physics, National Tsing Hua University, Hsinchu, Taiwan*
- ⁶³*Department of Physics, Indiana University, Bloomington, Indiana, USA*
- ^{64a}*INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine, Italy*
- ^{64b}*ICTP, Trieste, Italy*

- ^{64c}*Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy*
^{65a}*INFN Sezione di Lecce, Lecce, Italy*
- ^{65b}*Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy*
^{66a}*INFN Sezione di Milano, Milano, Italy*
^{66b}*Dipartimento di Fisica, Università di Milano, Milano, Italy*
^{67a}*INFN Sezione di Napoli, Napoli, Italy*
- ^{67b}*Dipartimento di Fisica, Università di Napoli, Napoli, Italy*
^{68a}*INFN Sezione di Pavia, Pavia, Italy*
^{68b}*Dipartimento di Fisica, Università di Pavia, Pavia, Italy*
^{69a}*INFN Sezione di Pisa, Pisa, Italy*
- ^{69b}*Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy*
^{70a}*INFN Sezione di Roma, Roma, Italy*
- ^{70b}*Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy*
^{71a}*INFN Sezione di Roma Tor Vergata, Roma, Italy*
- ^{71b}*Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy*
^{72a}*INFN Sezione di Roma Tre, Roma, Italy*
- ^{72b}*Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy*
^{73a}*INFN-TIFPA, Trento, Italy*
^{73b}*Università degli Studi di Trento, Trento, Italy*
- ⁷⁴*Institut für Astro- und Teilchenphysik, Leopold-Franzens-Universität, Innsbruck, Austria*
⁷⁵*University of Iowa, Iowa City, Iowa, USA*
- ⁷⁶*Department of Physics and Astronomy, Iowa State University, Ames, Iowa, USA*
⁷⁷*Joint Institute for Nuclear Research, Dubna, Russia*
- ^{78a}*Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, Brazil*
^{78b}*Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro, Brazil*
^{78c}*Universidade Federal de São João del Rei (UFSJ), São João del Rei, Brazil*
^{78d}*Instituto de Física, Universidade de São Paulo, São Paulo, Brazil*
- ⁷⁹*KEK, High Energy Accelerator Research Organization, Tsukuba, Japan*
⁸⁰*Graduate School of Science, Kobe University, Kobe, Japan*
- ^{81a}*AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland*
^{81b}*Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland*
⁸²*Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland*
⁸³*Faculty of Science, Kyoto University, Kyoto, Japan*
⁸⁴*Kyoto University of Education, Kyoto, Japan*
- ⁸⁵*Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan*
- ⁸⁶*Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina*
⁸⁷*Physics Department, Lancaster University, Lancaster, United Kingdom*
⁸⁸*Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom*
- ⁸⁹*Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia*
- ⁹⁰*School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom*
⁹¹*Department of Physics, Royal Holloway University of London, Egham, United Kingdom*
⁹²*Department of Physics and Astronomy, University College London, London, United Kingdom*
⁹³*Louisiana Tech University, Ruston, Louisiana, USA*
⁹⁴*Fysiska institutionen, Lunds universitet, Lund, Sweden*
- ⁹⁵*Centre de Calcul de l'Institut National de Physique Nucléaire et de Physique des Particules (IN2P3), Villeurbanne, France*
- ⁹⁶*Departamento de Física Teórica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid, Spain*
⁹⁷*Institut für Physik, Universität Mainz, Mainz, Germany*
- ⁹⁸*School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom*
⁹⁹*CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France*
- ¹⁰⁰*Department of Physics, University of Massachusetts, Amherst, Massachusetts, USA*
¹⁰¹*Department of Physics, McGill University, Montreal Quebec, Canada*
¹⁰²*School of Physics, University of Melbourne, Victoria, Australia*
¹⁰³*Department of Physics, University of Michigan, Ann Arbor, Michigan, USA*
- ¹⁰⁴*Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA*
¹⁰⁵*B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus*

- ¹⁰⁶*Research Institute for Nuclear Problems of Byelorussian State University, Minsk, Belarus*
- ¹⁰⁷*Group of Particle Physics, University of Montreal, Montreal Québec, Canada*
- ¹⁰⁸*P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia*
- ¹⁰⁹*Institute for Theoretical and Experimental Physics of the National Research Centre Kurchatov Institute, Moscow, Russia*
- ¹¹⁰*National Research Nuclear University MEPhI, Moscow, Russia*
- ¹¹¹*D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University, Moscow, Russia*
- ¹¹²*Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany*
- ¹¹³*Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany*
- ¹¹⁴*Nagasaki Institute of Applied Science, Nagasaki, Japan*
- ¹¹⁵*Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan*
- ¹¹⁶*Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico, USA*
- ¹¹⁷*Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands*
- ¹¹⁸*Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands*
- ¹¹⁹*Department of Physics, Northern Illinois University, DeKalb, Illinois, USA*
- ^{120a}*Budker Institute of Nuclear Physics and NSU, SB RAS, Novosibirsk, Russia*
- ^{120b}*Novosibirsk State University Novosibirsk, Novosibirsk, Russia*
- ¹²¹*Institute for High Energy Physics of the National Research Centre Kurchatov Institute, Protvino, Russia*
- ¹²²*Department of Physics, New York University, New York, New York, USA*
- ¹²³*The Ohio State University, Columbus, Ohio, USA*
- ¹²⁴*Faculty of Science, Okayama University, Okayama, Japan*
- ¹²⁵*Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, Oklahoma, USA*
- ¹²⁶*Department of Physics, Oklahoma State University, Stillwater, Oklahoma, USA*
- ¹²⁷*Palacký University, RCPTM, Joint Laboratory of Optics, Olomouc, Czech Republic*
- ¹²⁸*Center for High Energy Physics, University of Oregon, Eugene, Oregon, USA*
- ¹²⁹*LAL, Université Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France*
- ¹³⁰*Graduate School of Science, Osaka University, Osaka, Japan*
- ¹³¹*Department of Physics, University of Oslo, Oslo, Norway*
- ¹³²*Department of Physics, Oxford University, Oxford, United Kingdom*
- ¹³³*LPNHE, Sorbonne Université, Paris Diderot Sorbonne Paris Cité, CNRS/IN2P3, Paris, France*
- ¹³⁴*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania, USA*
- ¹³⁵*Konstantinov Nuclear Physics Institute of National Research Centre “Kurchatov Institute”, PNPI, St. Petersburg, Russia*
- ¹³⁶*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania, USA*
- ^{137a}*Laboratório de Instrumentação e Física Experimental de Partículas—LIP, Lisboa, Spain*
- ^{137b}*Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Spain*
- ^{137c}*Departamento de Física, Universidade de Coimbra, Coimbra, Spain*
- ^{137d}*Centro de Física Nuclear da Universidade de Lisboa, Lisboa, Spain*
- ^{137e}*Departamento de Física, Universidade do Minho, Braga, Spain*
- ^{137f}*Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada, Spain*
- ^{137g}*Dep Física and CEFITEC of Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal*
- ¹³⁸*Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic*
- ¹³⁹*Czech Technical University in Prague, Prague, Czech Republic*
- ¹⁴⁰*Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic*
- ¹⁴¹*Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom*
- ¹⁴²*IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France*
- ¹⁴³*Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, California, USA*
- ^{144a}*Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile*
- ^{144b}*Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile*
- ¹⁴⁵*Department of Physics, University of Washington, Seattle, Washington, USA*
- ¹⁴⁶*Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom*
- ¹⁴⁷*Department of Physics, Shinshu University, Nagano, Japan*
- ¹⁴⁸*Department Physik, Universität Siegen, Siegen, Germany*
- ¹⁴⁹*Department of Physics, Simon Fraser University, Burnaby British Columbia, Canada*
- ¹⁵⁰*SLAC National Accelerator Laboratory, Stanford, California, USA*

- ¹⁵¹*Physics Department, Royal Institute of Technology, Stockholm, Sweden*
- ¹⁵²*Departments of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA*
- ¹⁵³*Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom*
- ¹⁵⁴*School of Physics, University of Sydney, Sydney, Australia*
- ¹⁵⁵*Institute of Physics, Academia Sinica, Taipei, Taiwan*
- ^{156a}*E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi, Georgia*
- ^{156b}*High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia*
- ¹⁵⁷*Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel*
- ¹⁵⁸*Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel*
- ¹⁵⁹*Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece*
- ¹⁶⁰*International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo, Japan*
- ¹⁶¹*Graduate School of Science and Technology, Tokyo Metropolitan University, Tokyo, Japan*
- ¹⁶²*Department of Physics, Tokyo Institute of Technology, Tokyo, Japan*
- ¹⁶³*Tomsk State University, Tomsk, Russia*
- ¹⁶⁴*Department of Physics, University of Toronto, Toronto, Ontario, Canada*
- ^{165a}*TRIUMF, Vancouver, British Columbia, Canada*
- ^{165b}*Department of Physics and Astronomy, York University, Toronto, Ontario, Canada*
- ¹⁶⁶*Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan*
- ¹⁶⁷*Department of Physics and Astronomy, Tufts University, Medford, Massachusetts, USA*
- ¹⁶⁸*Department of Physics and Astronomy, University of California Irvine, Irvine, California, USA*
- ¹⁶⁹*Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden*
- ¹⁷⁰*Department of Physics, University of Illinois, Urbana, Illinois, USA*
- ¹⁷¹*Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia—CSIC, Valencia, Spain*
- ¹⁷²*Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada*
- ¹⁷³*Department of Physics and Astronomy, University of Victoria, Victoria, British Columbia, Canada*
- ¹⁷⁴*Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg, Germany*
- ¹⁷⁵*Department of Physics, University of Warwick, Coventry, United Kingdom*
- ¹⁷⁶*Waseda University, Tokyo, Japan*
- ¹⁷⁷*Department of Particle Physics, Weizmann Institute of Science, Rehovot, Israel*
- ¹⁷⁸*Department of Physics, University of Wisconsin, Madison, Wisconsin, USA*
- ¹⁷⁹*Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany*
- ¹⁸⁰*Department of Physics, Yale University, New Haven, Connecticut, USA*
- ¹⁸¹*Yerevan Physics Institute, Yerevan, Armenia*

[†]Deceased.

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

^bAlso at California State University, East Bay, Hayward, California, USA.

^cAlso at Centre for High Performance Computing, CSIR Campus, Rosebank, Cape Town, South Africa.

^dAlso at CERN, Geneva, Switzerland.

^eAlso at CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France.

^fAlso at Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland.

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

^hAlso at Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada (Spain), Spain.

ⁱAlso at Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal.

^jAlso at Department of Applied Physics and Astronomy, University of Sharjah, Sharjah, United Arab Emirates.

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

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

^mAlso at Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom.

ⁿAlso at Department of Physics, California State University, Fresno, California, USA.

^oAlso at Department of Physics, California State University, Sacramento, California, USA.

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

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

^rAlso at Department of Physics, the Stanford University, USA.

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

^tAlso at Department of Physics, University of Michigan, Ann Arbor, Michigan, USA.

^uAlso at Giresun University, Faculty of Engineering, Giresun, Turkey.

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

- ^w Also at Hellenic Open University, Patras, Greece.
- ^x Also at Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania.
- ^y Also at Institutio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain.
- ^z Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany.
- ^{aa} Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands.
- ^{ab} Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary.
- ^{ac} Also at Institute of Particle Physics (IPP), Canada.
- ^{ad} Also at Institute of Physics, Academia Sinica, Taipei, Taiwan.
- ^{ae} Also at Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan.
- ^{af} Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia.
- ^{ag} Also at Instituto de Física Teórica de la Universidad Autónoma de Madrid, Spain.
- ^{ah} Also at Istanbul University, Department of Physics, Istanbul, Turkey.
- ^{ai} Also at Joint Institute for Nuclear Research, Dubna, Russia.
- ^{aj} Also at LAL, Université Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France.
- ^{ak} Also at Louisiana Tech University, Ruston, Louisiana, USA.
- ^{al} Also at LPNHE, Sorbonne Université, Paris Diderot Sorbonne Paris Cité, CNRS/IN2P3, Paris, France.
- ^{am} Also at Manhattan College, New York New York, USA.
- ^{an} Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia.
- ^{ao} Also at National Research Nuclear University MEPhI, Moscow, Russia.
- ^{ap} Also at Physics Dept. University of South Africa, Pretoria, South Africa.
- ^{aq} Also at Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany.
- ^{ar} Also at School of Physics, Sun Yat-sen University, Guangzhou, China.
- ^{as} Also at The City College of New York, New York, New York, USA.
- ^{at} Also at The Collaborative Innovation Center of Quantum Matter (CICQM), Beijing, China.
- ^{au} Also at Tomsk State University, Tomsk, and Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia.
- ^{av} Also at TRIUMF, Vancouver, British Columbia, Canada.
- ^{aw} Also at Università di Napoli Parthenope, Napoli, Italy.