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Aad, G. orcid.org/0000-0002-6665-4934, Aakvaag, E. orcid.org/0000-0001-7616-1554, Abbott, B. orcid.org/0000-0002-5888-2734 et al. (2920 more authors) (2024) Search for light long-lived particles in pp collisions at \sqrt{s} p=13 TeV using displaced vertices in the ATLAS inner detector. Physical Review Letters, 133. 161803. ISSN 0031-9007

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Search for Light Long-Lived Particles in pp Collisions at $\sqrt{s} = 13$ TeV Using Displaced Vertices in the ATLAS Inner Detector

G. Aad *et al.*^{*} (ATLAS Collaboration)

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A search for long-lived particles (LLPs) using 140 fb⁻¹ of pp collision data with $\sqrt{s} = 13$ TeV recorded by the ATLAS experiment at the LHC is presented. The search targets LLPs with masses between 5 and 55 GeV that decay hadronically in the ATLAS inner detector. Benchmark models with LLP pair production from exotic decays of the Higgs boson and models featuring long-lived axionlike particles (ALPs) are considered. No significant excess above the expected background is observed. Upper limits are placed on the branching ratio of the Higgs boson to pairs of LLPs, the cross section for ALPs produced in association with a vector boson, and, for the first time, on the branching ratio of the top quark to an ALP and a u/c quark.

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The majority of experimental searches for dark matter (DM) have concentrated on weakly interacting massive particles (WIMPs) that interact directly with standard model (SM) particles with a strength comparable to that of the weak interaction. However, constraints on WIMPlike DM from both direct [1-9] and indirect detection experiments [10] are becoming increasingly stringent. One compelling alternative to the WIMP paradigm is that DM particles belong to a "dark sector" (DS) that is neutral under the SM gauge group and interacts with the SM only via one or more beyond the SM mediator particles [11-15]. If decays of the mediator to DS particles are kinematically forbidden, its decay back into SM particles will be suppressed by the small coupling between the SM and the mediator, giving rise to potentially macroscopic proper decay lengths ($c\tau \gtrsim 100 \ \mu m$). These so-called long-lived particles (LLPs) are also predicted in scenarios in which the mediator particle couples to the SM via a higher-dimensional operator, such as in models featuring axionlike particles (ALPs) [16,17].

This Letter presents a search for neutral LLPs that decay hadronically, giving a distinct signature of one or more hadronic jets originating at a significantly displaced position from the proton–proton (pp) collision point, referred to as a displaced vertex (DV). Three benchmark models are explored, motivated by different interactions between the SM and DS states. The first benchmark considers the "Higgs portal," in which the SM Higgs boson mediates interactions with the DS through its coupling to a neutral spin-0 boson, s [18,19]. This benchmark gives rise to exotic decays of the Higgs boson to a pair of long-lived s particles that decay back to SM particles with Yukawa-ordered branching ratios. The search targets Higgs boson production either in association with a vector boson (W/Z) or via the vector boson fusion (VBF) process in which a quark from each of the incoming protons radiates a heavy vector boson, which then fuse to produce a Higgs boson [20]. The second benchmark considers extending the SM with an ALP, a, which couples to gluons and W/Z bosons through effective dimension-5 operators, while couplings to photons are suppressed. These interactions are characterized by a scale f_a and Wilson coefficients $C_{\tilde{G}}$ and $C_{\tilde{W}}$, respectively [21]. These operators give rise to the production of a in association with a vector boson (W/Z) and its subsequent decay exclusively into gluons. The third benchmark considers an ALP, a, which couples to up-type quarks [22,23], giving rise to exotic decays of the top quark $t \rightarrow ac/au$ in $t\bar{t}$ events. In this model the *a* boson decays predominantly into charm quark pairs or gluons, with branching ratios that depend on m_a . Example Feynman diagrams of the three benchmark processes can be found in Appendix A.

This search was performed with 140 fb⁻¹ of 13 TeV pp collision data collected by the ATLAS experiment at the Large Hadron Collider (LHC) [24] from 2015 to 2018. Several previous searches for Higgs boson decays to LLPs have been performed that in combination exclude branching ratios BR($H \rightarrow ss$) > 10% for *s* masses above 40 GeV and proper decay lengths between 10⁻³ and 10 m [25–32]. However, for masses below 40 GeV, Higgs boson decays to LLPs with proper decay lengths below 100 mm are unconstrained beyond the limit of 12% on the branching

^{*}Full author list given at the end of the Letter.

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ratio of the Higgs boson to undetected states [33]. A limiting factor in probing this region of phase space with the ATLAS experiment has been the reconstruction of displaced tracks in the inner tracking detector (ID). In 2022, an improved version of the track reconstruction pass for large-impact parameter tracks was deployed in ATLAS [34]. This upgrade significantly reduced the rate of reconstructing so-called fake tracks due to random hit combinations, thereby enhancing computational efficiency and enabling the application of this reconstruction to every recorded data event. This Letter reports the first direct application of this new track reconstruction, which significantly expands the reach of this search with respect to previous ATLAS results and allows for sensitivity to previously unexplored phase space. Notably, this is the first search for Higgs boson decays to hadronically decaying LLPs in the ID to probe the VBF topology, and the first search to probe hadronically decaying longlived ALPs produced in association with a vector boson and via exotic decays of the top quark.

The ATLAS detector [35,36] is a cylindrical detector with forward-backward symmetry and nearly 4π solidangle coverage [37]. It consists of the ID surrounded by a thin superconducting solenoid, electromagnetic and hadronic calorimeters, and a muon spectrometer. The ID covers the pseudorapidity range $|\eta| < 2.5$ and consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors. An extensive software suite [38] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

A primary charged particle (track) reconstruction pass is used to reconstruct charged-particle trajectories with transverse impact parameter (d_0) with respect to the pp interaction point (IP) of $|d_0| < 5$ mm. A large-impact parameter pass, using leftover hits from the primary pass, is used to increase tracking acceptance up to $|d_0| < 300$ mm [34]. The pp interaction vertex with the highest sum of squared transverse momenta of associated tracks is taken as the primary interaction vertex (PV). Hadronic jets are reconstructed from topological clusters of energy deposits in the calorimeters [39] using the anti- k_t algorithm [40,41] with a radius parameter of R = 0.4. The matching of tracks with the calorimeter-based jets is performed via the ghostassociation technique [42]. Jets with transverse momentum $p_T > 20$ GeV are considered in the analysis.

Electron candidates are reconstructed from energy deposits in the calorimeters associated to an ID track, and are required to be within the fiducial region $|\eta| < 2.47$, and outside of $1.37 < |\eta| < 1.52$. Muons are reconstructed by combining tracks reconstructed in the ID with tracks or track segments found in the muon spectrometer (MS) and are required to have $|\eta| < 2.5$. Electrons and muons are required to have $p_T > 10$ GeV and satisfy the *medium* identification criterion [43,44]. To ensure that the selected

electrons (muons) originate from the PV, they must satisfy $|d_0/\sigma(d_0)| < 5(3)$, and $|(z_0 - z_{\rm PV})\sin\theta| < 0.5$ mm, where z_0 is the track's longitudinal impact parameter and z_{PV} is the z coordinate of the PV. In this Letter, electrons and muons satisfying the above criteria will collectively be referred to as leptons. Photon candidates are reconstructed from clustered energy deposits in the electromagnetic calorimeter either without any matching ID track or with a matching photon conversion vertex in the ID material. The loose identification criterion is required [43]. The missing transverse momentum (E_T^{miss}) is defined as the magnitude of the negative vector sum of the transverse momenta of all reconstructed and calibrated electrons, muons, photons, jets, and remaining unclustered energy. The latter is estimated from $low-p_T$ tracks associated with the PV but not assigned to a reconstructed object [45].

Samples of Monte Carlo (MC) simulated events are used to study the three benchmark scenarios. Signal samples were generated assuming mean proper decay lengths of the LLP (either s or a) of 1, 10, 100, and 1000 mm and masses of $m_s = 5$, 16, 40, 55 and $m_a = 40$, 55 GeV for the Higgs portal and ALP benchmarks, respectively. In all samples, the LLP is taken to be a pseudoscalar, although the analysis does not explicitly exploit the CP properties of the LLPs. In the Higgs portal benchmark, the decays of the s particles are simulated assuming a 100% branching ratio to the heaviest quark-antiquark pair that is kinematically allowed. To quantify the dependence of the analysis on the flavor of the final state quarks, additional samples are generated assuming a 100% branching ratio to $u\bar{u}$. In the W/Z plus ALP benchmark, the decay of the *a* particle is simulated assuming a 100% branching ratio to gg. In the exotic top decay benchmark, the *a* particle can decay into either $c\bar{c}$ or gg. For the values of m_a considered in this analysis, the branching ratios to $c\bar{c}$ and gg are approximately 75% and 25%, respectively [23]. Samples of simulated $t\bar{t}$ and V + jets background events are used to optimize the event selections and evaluate systematic uncertainties. Details about the event simulation configurations used can be found in Appendix A.

Events are categorized into three search regions, each targeting a different Higgs boson or ALP production mode. The *1-lepton* region is defined by the presence of exactly one lepton (e/μ) with $p_T > 27$ and $E_T^{\text{miss}} > 30$ GeV. These criteria target signal processes containing a leptonically decaying W boson including WH, Wa, and $t\bar{t}, t \rightarrow ac/au$ production. The 2-lepton region is defined by the presence of exactly two leptons, with the same flavor and opposite charge. The highest p_T lepton is required to have $p_T > 27$ GeV, and the invariant mass of the dilepton system is required to fall between 76 and 106 GeV. These criteria target signal events containing a leptonically decaying Z boson, including ZH and Za production. Events in the 1- and 2-lepton regions are collected with a combination of single and dilepton triggers [46–48].

A matching requirement is applied between the selected leptons and the corresponding leptons reconstructed by the trigger. In both regions, events are required to have at least two jets with $|\eta| < 2.5$. The VBF enriched region targets the Higgs portal benchmark in the VBF production mode. Events are collected with an inclusive VBF trigger [49] enabled during the 2018 data-taking period that is designed to select events with a pair of jets consistent with the VBF process. The data collected with this trigger correspond to a total integrated luminosity of 37.5 fb⁻¹. The VBF enriched region is defined by the absence of any lepton, and the presence of a pair of jets with invariant mass $m_{ii} > 1200 \text{ GeV}$ and angular separation $|\Delta \eta_{ii}| > 4$ and $|\Delta \phi_{jj}| < 2$. The leading (subleading) jet in this pair is required to have transverse momentum $p_{\rm T} > 100(80)$ GeV and $|\eta| < 3.2(4.9)$. These selections ensure that the trigger selection efficiency is approximately 100%. In addition to the pair of jets used to select the VBF topology, events are required to have at least two additional jets with $|\eta| < 2.5$.

The jets emerging from the decay products of an LLP, referred to as *displaced jets*, exhibit a distinct topology compared to *prompt jets* that originate from a *pp* interaction vertex. To distinguish displaced jets from prompt jets, a per-jet boosted decision tree (BDT) is trained using the XGBOOST framework [50]. The output of this classifier is a displaced jet BDT score between zero and one, where a higher score indicates that the jet is more likely to have originated from a displaced decay. This BDT is trained on five jet-level features that discriminate between displaced and prompt jets. The first feature is the fraction of the total jet $p_{\rm T}$ carried by tracks with $|d_0| < 0.5$ mm, which is expected to be smaller for displaced jets than for prompt jets. Similarly, the fraction of the total jet $p_{\rm T}$ carried by tracks with $|d_0| > 0.5$ mm is used, which provides additional information about the contribution from displaced charged particles to the total jet momentum. Third, the fractional value of jet track $p_{\rm T}$ originating from tracks with $|d_0| < 0.5$ and $|(z_0 - z_{\text{vertex}}) \sin \theta| < 0.3$ mm is calculated for each reconstructed pp interaction vertex, and the maximum value of this set is taken. Finally, the maximum $|d_0|$ among tracks in the jet, and the median of the logarithmic transverse impact parameter significance of tracks associated to the jet are used. The BDT is trained on a mixed signal sample comprised of $VH, H \rightarrow ss$ events with $m_s \in \{16, 55\}$ GeV and $c\tau_s \in \{10, 100\}$ mm, and a mixed background sample comprised of simulated $t\bar{t}$, W + jets, and Z + jets events in equal parts. Distributions of the BDT score for jets in selected signal samples and in data can be found in the Supplemental Material [51].

To reconstruct the origin of the hadronic jets produced from the decay of the LLPs, a DV reconstruction algorithm [52] is run on the combined collection of tracks from both the primary and the large-impact parameter tracking passes. Following Ref. [28], selections are placed on the reconstructed vertices to reject DVs from SM processes and random combinations of tracks. DVs are required to have a track multiplicity $n_{\text{track}} \ge 3$ and vertex goodness of fit $\chi^2_{\text{DV}}/n_{\text{DoF}} < 5$. The radial and longitudinal coordinates of the DV position are each required to be less than 300 mm, and a material veto is applied to reject DVs from interactions between high-momentum hadrons and known detector elements [53]. Furthermore, the minimum $|d_0|$ among all tracks associated to a DV ($|d_{0,\min}|$) must satisfy $|d_{0,\min}| > 0.1$ mm, and DVs must contain at least one track with $|d_0| > 3$ mm.

To compute the kinematic properties of DVs, the parameters of the tracks associated to each DV are recalculated after extrapolating their trajectories to the DV position. The resulting track four-momentum vectors, measured with respect to the DV, are then summed together to yield the DV's four-momentum. The ratio of the DV invariant mass $(m_{\rm DV})$ and the maximum angular distance between any two tracks in the DV (ΔR_{max}) is then required to satisfy $m_{\rm DV}/\Delta R_{\rm max} > 4$ GeV, and the scalar sum of the transverse momentum of tracks associated to a DV is required to be above 10 GeV. To associate DVs to displaced jets, the DV momentum vector is required to be within $\Delta R < 0.6$ of a jet with a BDT score greater than 0.5. If multiple DVs are matched to a given jet, only the DV with the smallest ΔR to the jet axis is considered. DVs that satisfy all of the selections above and are matched to a displaced jet are used to count the DV multiplicity in the event $(n_{\rm DV})$.

All events considered in the analysis are required to have at least two jets with a BDT score greater than 0.5. An eventlevel discriminant (BDT_{j0} × BDT_{j1}) is computed by taking the product of the BDT scores of the two jets in the event with the largest BDT scores. From each of the three search regions, two signal regions (SRs) are defined based on the candidate DV multiplicity in the event, $n_{\rm DV} = 1$ or $n_{\rm DV} \ge 2$, resulting in a total of six SRs. Events in the $n_{\rm DV} = 1$ SRs are required to have BDT_{j0} × BDT_{j1} > 0.9. This condition is relaxed to BDT_{j0} × BDT_{j1} > 0.7 in the $n_{\rm DV} \ge 2$ SRs. Example distributions of the event-level discriminant can be found in the Supplemental Material [51].

The dominant sources of background are $t\bar{t}$ and W + jets, Z + jets, and multijet production in the 1-lepton, 2-lepton, and VBF enriched SRs, respectively. The background contribution is estimated using a fully data-driven approach, following the method developed in Ref. [28]. In each of the three search regions, a control region (CR) is defined by requiring BDT_{j0} × BDT_{j1} < 0.7. Assuming a 12% branching ratio of $H \rightarrow ss$ from Ref. [33], the fractional signal contribution in the CRs is expected to be less than 1%. The probability that a jet is matched to a DV is computed separately in each of the three CRs and encoded in a three-dimensional map parametrized in jet $p_{\rm T}$, the jet flavor tagging score (DL1r) [54] that separates light and heavy flavor jets, and BDT score. The map is divided evenly in the BDT dimension using a bin width of 0.01 in

the 1-lepton region, and 0.025 in the 2-lepton and VBF enriched regions, where fewer events are selected. The three probability maps are shown in Fig. 4 of the Supplemental Material [51] as two-dimensional projections. The per-jet probabilities are then used to compute the probability that each event contains exactly one, or greater than one DV based on the $p_{\rm T}$, DL1r, and BDT scores of the jets in the event. The per-event probability weights are applied inclusively to data in the search regions to predict the distributions of BDT_{j0} × BDT_{j1} in events with $n_{\rm DV} = 1$ and $n_{\rm DV} \ge 2$.

Two uncertainties in the background prediction are considered. First, the statistical uncertainty in the background estimate due to the finite number of events in the CR used to derive the maps is computed using ensembles of background estimates from a set of statistically varied perjet probability maps [28]. The standard deviation of this ensemble of estimates is used to define the up and down statistical variations on the nominal prediction. Second, in the 2-lepton and VBF enriched regions, where a coarser binning is used in the BDT dimension of the per-jet probability map, an uncertainty in the background estimate from the binning choice is quantified. In this regard, the difference between the nominal estimate and an alternate estimate computed from a map with a BDT bin width of 0.01 is taken as a systematic uncertainty. The total uncertainty in the background predictions varies from 10%-50%, depending on the signal region. The largest uncertainties are present in the $n_{\rm DV} \ge 2$ regions, especially in the 2-lepton and VBF regions, where the statistical uncertainty is dominant due to the finite number of jets available for deriving the per-jet probability maps.

The background estimate is validated in a subset of the $n_{\rm DV} = 1$ events defined by $0.7 < {\rm BDT}_{j_0} \times {\rm BDT}_{j_1} < 0.9$ within each of the three search regions, and in a dedicated event selection requiring the presence of a single photon with $p_{\rm T} > 160$ GeV and $|\eta| < 2.47$, zero leptons, and two jets with $p_{\rm T} > 20$ GeV. The distributions of data events are found to be well modeled by the predicted background in all regions, validating the extrapolation of the background estimate from the CR to larger values of ${\rm BDT}_{j_0} \times {\rm BDT}_{j_1}$ and to events with $n_{\rm DV} \ge 2$. A more detailed description of the background validation is given in Appendix B.

Instrumental and theoretical uncertainties are assigned on the modeling of the simulated signal samples. The dominant systematic uncertainty is due to the modeling of the BDT score, which is derived as a per-jet uncertainty by comparing the shape of the BDT score between data and the simulated Z + jets sample in the 2-lepton preselection, and then propagated to the final event yield. The impact of this uncertainty is approximately 15%. In the VBF selection, the dominant systematic uncertainty is on the jet energy scale and resolution, reaching values of up to 20% due to the increased uncertainty associated with calibrating jets which have large pseudorapidity [39]. Subleading sources of instrumental uncertainty include those on the primary and large-impact parameter track reconstruction efficiencies (2%-9%) [34]; lepton trigger, reconstruction, and identification efficiencies (0%-2%) [55]; lepton energy scale and resolution (0%-1%) [56]; modeling of the pileup in simulation (2%-4%) [57]; and the total integrated luminosity of the measurement (0.8%) [58,59]. Theoretical uncertainties are considered to account for variations due to the renormalization and factorization scales, parton distribution functions, and parton showering (2%-8%).

For each signal model considered, a binned maximumlikelihood fit to the BDT_{*j*₀} × BDT_{*j*₁} distributions in the SRs is performed. For the Higgs portal model, all six SRs are fitted simultaneously, while in the Wa and $t \rightarrow aq$ (Za) model, only the 1-lepton (2-lepton) $n_{\rm DV} = 1$ SR is considered. Systematic and MC statistical uncertainties are included as nuisance parameters and are constrained in the fit. Systematic uncertainties on the signal efficiency are correlated across the six signal regions, while the systematic and statistical uncertainties on the background are treated as uncorrelated. In the 1-lepton region where there is no systematic uncertainty on the background prediction, a shape uncertainty is included as an additional degree of freedom to the fit. This uncertainty varies linearly across the $n_{\rm DV} = 1$ and $n_{\rm DV} \ge 2$ SRs and allows for the value of the fitted statistical uncertainty to vary from bin to bin.

The distributions of $BDT_{j_0} \times BDT_{j_1}$ for the observed data and the background prediction after the background-only fit to data in the six SRs are shown in Fig. 1. No significant deviation from the SM expectation is observed.



FIG. 1. Distributions of BDT_{j0} × BDT_{j1} for the observed data (black points) and the estimated background (filled histogram) with its uncertainty after the background-only fit to data in the six SRs described in the text. The signal expectation for the Higgs portal model with $m_s = 55$ GeV and $c\tau_s = 100$ mm is shown in the solid line, scaled to BR($H \rightarrow ss \rightarrow 4b$) = 1%. The signal expectation for ALP production in association with a Z boson scaled to $\sigma(qq \rightarrow Za) = 5 \times 10^{-3}$ pb, and for $t \rightarrow aq$ scaled to BR($t \rightarrow aq$) = 0.1% are shown in the dashed and dotted lines, respectively, for $m_a = 55$ GeV and $c\tau_a = 100$ mm. The observed data in the 1- and 2-lepton (VBF) regions corresponds to an integrated luminosity of 140 (37.5) fb⁻¹. The ratio between the data and estimated background is shown in the bottom panel.

The absence of a data excess is translated into exclusion limits at 95% confidence level (CL) on BR($H \rightarrow ss \rightarrow 4b$), $\sigma(qq \rightarrow Va)$, and BR($t \rightarrow aq$). The CLs prescription [60] is used to compute the limits using asymptotic formulae for



FIG. 2. The 95% confidence level limits on the (upper) Higgs boson branching ratio $H \rightarrow ss \rightarrow 4q$, (middle) $q\bar{q} \rightarrow Va$ crosssection where V = W or Z, and (lower) $t \rightarrow aq$ branching ratio shown as a function of the mean proper decay length $c\tau$ of the long-lived particle. The observed limits are shown with a solid line. The expected limits and corresponding $\pm 1\sigma$ uncertainty bands for $m_{s/a} = 55$ GeV are shown with dashed lines and shaded bands, respectively. In the upper plot, the limits shown are on the Higgs boson branching ratio $H \rightarrow ss \rightarrow 4b$ for $m_s = 16$, 40, 55 GeV, and $H \rightarrow ss \rightarrow 4c$ for $m_s = 5$ GeV. In the upper plot, the observed limits for the Higgs portal model from the previous ATLAS search [28] are shown with the dot-dashed lines.

the profile likelihood ratio [61]. The signal yields at different lifetimes are computed by reweighting the exponential LLP decay distributions from the generated values to each target lifetime, following the procedure described in Ref. [28]. The expected and observed exclusion limits are shown in Fig. 2. A comparison of the observed exclusion limits for light and heavy-flavor quark final states can be found in the Supplemental Material [51] for $H \rightarrow ss \rightarrow 4q$, as well as an interpretation of the limits on $\sigma(qq \rightarrow Va)$ in terms of the Wilson coefficients $C_{\tilde{W}}$ and $C_{\tilde{G}}$ parametrizing the effective aVV and agg vertices [21]. For the Higgs portal benchmark, the limits set by this search are considerably stronger than previous ATLAS results [28] using the same dataset, with improvements by as much as a factor of 20 for $m_s = 55$ GeV and $c\tau_s < 10$ mm. These improvements are driven by the updated large-impact parameter track reconstruction, the addition of the 1-lepton and VBF search regions, and the inclusion of $n_{\rm DV} = 1$ signal regions. In particular, the VBF enriched region contributes a similar level of sensitivity as the other two search regions despite having a considerably smaller integrated luminosity.

In summary, this Letter reports the results of a search for LLPs with masses between 5 and 55 GeV that decay hadronically in the ATLAS inner detector. No significant excess beyond the SM prediction is observed. The reported constraints on the Higgs boson branching ratio are the most stringent to date for $m_s < 40$ GeV and $1 < c\tau_s < 100$ mm. For $H \rightarrow ss \rightarrow 4b$, branching ratios greater than 1% are excluded for $m_s = 55$ GeV and $5.4 < c\tau_s < 72$ mm. The exclusion limits are stronger for light-quark final states, with $H \rightarrow ss \rightarrow 4u$ branching ratios greater than 1% excluded for $m_s = 55$ GeV and $4.2 < c\tau_s < 110$ mm. For the first time at the LHC, branching ratios beyond the limit of 12% imposed on Higgs boson decays to undetected states are probed for $m_s < 16 \text{ GeV}$ and $c\tau_s < 100$ mm, with BR $(H \rightarrow ss \rightarrow 4c) > 10\%$ excluded for $m_s = 5$ GeV and 2.9 < $c\tau_s < 21$ mm. The first limits on long-lived ALP models with suppressed coupling to photons are set, excluding cross sections for $qq \rightarrow Va$ greater than 0.1 pb for $40 < m_a < 55$ GeV and $1.0 < c\tau_a < 220$ mm. Long-lived ALPs produced via $t \rightarrow aq$ are probed for the first time, excluding $t \rightarrow aq$ branching ratios greater than 0.1% between $1.6 < c\tau_a <$ 130 mm for $40 < m_a < 55$ GeV.

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End Matter

Appendix A: Simulated data samples-Samples of MC simulated events are used to study the three benchmark scenarios. Higgs boson production in association with a vector boson and via vector-boson fusion (VBF) was simulated using POWHEG BOX V2 [63-66] and interfaced with PYTHIA8.2 [67] to simulate the $H \rightarrow ss$ decay and the subsequent decay of the s. PYTHIA8.2 is also used for simulating parton shower and nonperturbative effects, with parameters set according to the AZNLO tune [68]. The POWHEG BOX prediction is accurate to next-to-leadingorder (NLO) for VH boson plus one-jet production. The loop-induced $gg \rightarrow ZH$ process was generated separately at leading-order (LO). Samples of $pp \rightarrow Va$ and $pp \rightarrow t\bar{t}$ with $t \rightarrow ac/au$ were simulated using MADGRAPH [69] v2.9.9 and interfaced with PYTHIA8.307. The effect of multiple *pp* interactions in the same or neighboring bunches (pileup) was modeled by overlaying the hardscatter process with simulated inelastic pp scattering events. Example Feynman diagrams of the simulated signal processes are shown in Fig. 3.

The production of $t\bar{t}$ events was modeled using the POWHEG BOX V2 generator at NLO and interfaced with



FIG. 3. Example Feynman diagrams for the three benchmark models considered in the analysis. (a) An example diagram for the Higgs portal model, in which the Higgs boson is produced via vector boson fusion, and the long-lived *s* particles decay to pairs of *b* quarks. (b) An example of the *Va* ALP production mode, in which the ALP *a* is produced in association with a *Z* boson, with $a \rightarrow gg$ and $Z \rightarrow \ell^+ \ell^-$. (c) An example diagram of ALP production via the exotic top-quark decay, with $t \rightarrow ac$ and $a \rightarrow c\bar{c}$.

PYTHIA8.230 with parameters set according to the A14 tune [70]. The production of V + jets was simulated with the SHERPA2.2.1 [71] generator using NLO matrix elements for up to two partons, and LO matrix elements for up to four partons calculated with the Comix [72] and OPENLOOPS [73–75] libraries. They were matched with the SHERPA parton shower [76] using the MEPS@NLO prescription [77–80]. The samples were normalized to a next-to-next-to-leading-order prediction [81].

Appendix B: Validation of background estimate—The method of estimating the distributions of events with $n_{\rm DV} = 1$ from the per-jet probabilities is validated by performing closure tests in the CRs. The weighted distributions of BDT_{j0} × BDT_{j1} in the three CRs are found to reproduce the observed distributions of events with $n_{\rm DV} = 1$ within uncertainties. The distributions of the leading and subleading jet $p_{\rm T}$, DL1r, and BDT scores are also found to be well modeled by the estimate in CR events with $n_{\rm DV} = 1$.



FIG. 4. Distributions of $BDT_{j_0} \times BDT_{j_1}$ for the observed data (black points) and the background prediction (teal colored histogram) with its uncertainty in the three $n_{DV} = 1$ validation regions with $0.7 < BDT_{j_0} \times BDT_{j_1} < 0.9$. The ratio between the data and predicted background is shown in the bottom panel. The background estimates are computed using events in the three CRs with $BDT_{j_0} \times BDT_{j_1} < 0.7$.

The extrapolation of the background estimate from the CR to larger values of $BDT_{j_0} \times BDT_{j_1}$ is validated in a subset of the $n_{DV} = 1$ events defined by $0.7 < BDT_{j_0} \times BDT_{j_1} < 0.9$, within the 1-lepton, 2-lepton, and VBF enriched search regions. The observed data in these three validation regions (VRs) are found to agree with the predicted background within uncertainties, as shown in Fig. 4. The largest discrepancy is observed in the 2-lepton VR, with 590 events observed compared to a predicted yield of $676 \pm 193(\text{stat}) \pm 106(\text{syst})$.

To validate the extrapolation to higher values of $BDT_{j_0} \times BDT_{j_1}$ and to events with $n_{DV} \ge 2$, a dedicated *photon VR* is used defined by the presence of a single photon with $p_T > 160$ GeV and $|\eta| < 2.47$, zero leptons, and two jets with $p_T > 20$ GeV. This selection effectively rejects events from all signal models considered and provides an independent set of data events on which to test the background estimation method. The same background estimation strategy is applied to this region as in the three search regions, using a dedicated map computed from events in the photon VR with $BDT_{j_0} \times BDT_{j_1} < 0.7$. The distributions of data events with $n_{DV} \ge 1$ and $BDT_{j_0} \times BDT_{j_1} > 0.7$ and data events with $n_{DV} \ge 2$ are found to be well modeled by the predicted background, as shown in Fig. 5.



FIG. 5. Distributions of $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$ for the observed data (black points) and the background prediction (blue) with its uncertainty in the photon validation region for events with $n_{\text{DV}} = 1$ and $n_{\text{DV}} \ge 2$. The ratio between the data and predicted background is shown in the bottom panel. The background estimate is computed using events in the photon VR with $\text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.7$.

G. Aado, ¹⁰⁴ E. Aakvaago, ¹⁷ B. Abbotto, ¹²³ S. Abdelhameedo, ^{119a} K. Abelingo, ⁵⁶ N. J. Abichto, ⁵⁰ S. H. Abidio, ³⁰ M. Aboelelao, ⁴⁵ A. Aboulhormao, ^{36c} H. Abramowiczo, ¹⁵⁴ H. Abreuo, ¹⁵³ Y. Abulaitio, ¹²⁰ B. S. Acharyao, ^{70a,70b,b} A. Ackermanno, ^{64a} C. Adam Bourdarioso, ⁴ L. Adamczyko, ^{87a} S. V. Addepallio, ²⁷ M. J. Addisono, ¹⁰³ J. Adelmano, ¹¹⁸ A. Adiguzelo, ^{22c} T. Adyeo, ¹³⁷ A. A. Affoldero, ¹³⁹ Y. Afiko, ⁴⁰ M. N. Agaraso, ¹³ J. Agarwalao, ^{74a,74b} A. Aggarwalo, ¹⁰² C. Agheorghiescio, ^{28c} A. Ahmado, ³⁷ F. Ahmadovo, ^{39c} W. S. Ahmedo, ¹⁰⁶ S. Ahujao, ⁹⁷ X. Aio, ^{63e} G. Aiellio, ^{77a,77b} A. Aikoto, ¹⁶⁶ M. Ait Tamlihato, ^{36e} B. Aitbenchikho, ^{36a} M. Akbiyiko, ¹⁰² T. P. A. Åkesson, ¹⁰⁰ A. V. Akimovo, ³⁸
D. Akiyamao, ¹⁷¹ N. N. Akolkaro, ²⁵ S. Aktaso, ^{22a} K. Al Khouryo, ⁴² G. L. Albergin, ^{24b} J. Alberto, ¹⁶⁸ P. Albicocco, ⁵⁴ G. L. Albouyo, ⁶¹ S. Alderweireldto, ⁵³ Z. L. Alegriao, ¹²⁴ M. Aleksa, ³⁷ I. N. Aleksandrovo, ³⁹ C. Alexao, ^{28b} T. Alexopouloso, ¹⁰ F. Alfonsio, ^{24b} M. Algreno, ⁵⁷ M. Alhrobob, ¹⁷⁰ B. Alio, ¹³⁵ H. M. J. Alie, ⁹³ S. Alie, ³² S. W. Alibocuso, ⁴⁴ M. Alizovo, ^{34c} G. Alimontio, ^{72a} W. Alkakhio, ⁵⁶ C. Allaire, ⁶⁷ B. M. M. Albrookee, ¹⁴⁹ J. F. Alleno, ⁵³ C. A. Allendes Floreso, ¹⁴⁰ P. P. Allporto, ²¹ A. Aloisioo, ^{73a,73b} F. Alonsoo, ⁹² C. Alpigianio, ¹⁴¹ Z. M. K. Alsolamio, ⁹³ M. Alvarez Estevezo, ¹⁰¹ A. Alvarez Fernandezo, ¹⁰² M. Alves Cardosoo, ⁵⁷ M. G. Alviggio, ^{73a,73b} M. Alyo, ¹⁰³ Y. Amaral Coutinhoø, ^{84b} A. Amblero, ¹⁰⁶ C. Amelung, ³⁷ M. Amerlo, ¹⁰³ C. G. Ameso, ¹¹¹ D. Amideio, ¹⁰⁸ K. J. Amirieo, ¹⁵⁸ S. P. Amor Dos Santoso, ¹⁵³ G. C. Antello, ⁵⁷ E. Antipovo, ¹⁴⁸ M. Antonellio, ⁵⁴ F. Anullio, ^{76a} M. Aokie, ⁵⁵ T. Antipovo, ¹⁴⁸ M. Antonello, ⁵⁴ F. Anullio, ^{76a} M. Aokie, ⁵⁵ A. Angerami, ^{42,d} A. V. Anisenkovo, ³⁸ A. Annovie, ⁵⁵ C. Angelo, ⁴⁹ A. Anperao, ^{48,48b} A. Andreazzao, ^{72a,72b} S. An

P. Bagnaia[®], ^{76a,76b} M. Bahmani[®], ¹⁹ D. Bahner[®], ⁵⁵ K. Bai[®], ¹²⁶ J. T. Baines[®], ¹³⁷ L. Baines[®], ⁹⁶ O. K. Baker[®], ¹⁷⁵ E. Bakos[®], ¹⁶ D. Bakshi Gupta[®], ⁸ L. E. Balabram Filho[®], ^{84b} V. Balakrishnan[®], ¹²³ R. Balasubramanian[®], ¹¹⁷ E. M. Baldin[®], ³⁸ P. Balek[®], ^{87a} E. Ballabene[®], ^{24b,24a} F. Balli[®], ¹³⁸ L. M. Baltes[®], ^{64a} W. K. Balunas[®], ³³ J. Balz[®], ¹⁰² E. M. Baldin³⁸ P. Balek^{87a} E. Ballabene⁹,^{24b,24a} F. Balli⁹,¹³⁸ L. M. Baltes⁹,^{64a} W. K. Balunas⁹,³³ J. Balz⁹,¹⁰² I. Barnwidhi⁹,^{119b} E. Banas⁹,⁸⁸ M. Bandieramonte⁹,¹³² A. Bandyopadhyay²⁵ S. Bansal⁹,²⁵ L. Barak⁹,¹⁵⁴ M. Barakat^{9,49} E. L. Barberio⁹,¹⁰⁷ D. Barberis⁹,^{58b,58a} M. Barbero⁹,¹⁰⁴ M. Z. Barel⁹,¹¹⁷ K. N. Barends⁹,^{34a} T. Barillari⁹,¹¹² M-S. Barisits^{9,37} T. Barklow^{9,146} P. Baron¹²⁵ D. A. Baron Moreno^{9,103} A. Baroncelli⁹,^{63a} G. Barone^{9,30} A. J. Barr⁹,¹²⁹ J. D. Barr^{9,98} F. Barreiro^{9,101} J. Barreiro Guimarães da Costa^{9,14} U. Barron^{9,154} M. G. Barros Teixeira^{9,133} S. Barsov^{9,38} F. Bartels^{64a} R. Bartolus^{9,146} A. E. Barton^{9,39} P. Bartos^{9,29a} A. Basan^{9,102} M. Baselga^{9,50} A. Bassalat^{67,2} M. J. Basso^{9,159a} S. Bataju^{9,45} R. Bate^{9,167} R. L. Bates^{9,60} S. Batlamous,¹⁰¹ B. Batoolo^{1,144} M. Battaglia^{9,139} D. Battulga^{9,19} M. Bauce^{9,76a,76b} M. Bauer^{9,80} P. Bauer^{9,25} L. T. Bazzano Hurrell^{9,31} J. B. Beacham^{6,52} T. Beau¹³⁰ J. Y. Beaucamp^{9,92} P. H. Beauchemin¹⁶¹ P. Bechtle^{9,25} H. P. Beck^{9,20,h} K. Becker^{9,170} A. J. Beddall^{9,³³} V. A. Bednyakov^{9,39} C. P. Bee^{9,148} L. J. Beemster^{6,16} T. A. Beermann^{9,37} M. Begalli^{9,84d} M. Begel^{9,30} A. Behera^{9,15} P. Bellos^{9,21} K. Beloborodov³⁸ D. Benchekroun^{36a} F. Bendebba^{36a} Y. Benhammou^{9,154} K. C. Benkendorfer^{6,22} L. Beresford^{9,49} M. Beretta^{9,54} E. Bergeaas Kuutmann¹⁶⁴ N. Berger^{9,4} B. Bergmann^{1,154} J. Berry^{9,97} P. Berta^{9,18} G. Bernardi^{9,5} S. Bethke^{9,112} A. Betti^{9,76} A. J. Bevan^{9,96} N. K. Bhalla^{9,55} S. Bhatta^{1,18} J. S. Bethke^{9,112} A. Betti^{7,6a,76b} A. J. Bevan^{9,96} N. K. Bhalla^{9,55} S. Bhatta^{1,18} J. Berry^{9,97} P. Berta^{9,18} G. Bernardi^{9,146} K. D. Bhide^{9,55} V. S. Bhopatkar^{9,124} R. M. Bianchi^{9,132} G. Bianco^{9,24b,24a} T. Berry[®], ⁹⁷ P. Berta[®], ¹³⁶ A. Berthold[®], ⁵¹ S. Bethke[®], ¹¹² A. Betti[®], ^{70a,76b} A. J. Bevan[®], ⁹⁶ N. K. Bhalla[®], ⁵⁵ S. Bhatta⁹, ¹⁴⁸ D. S. Bhattacharya[®], ¹⁶⁹ P. Bhattarai[®], ¹⁴⁶ K. D. Bhide[®], ⁵⁵ V. S. Bhopatkar[®], ¹²⁴ R. M. Bianchi[®], ¹³² G. Bianco[®], ^{24b,24a} O. Biebel[®], ¹¹¹ R. Bielski[®], ¹²⁶ M. Biglietti[®], ^{78a} C. S. Billingsley, ⁴⁵ M. Bindi[®], ⁵⁶ A. Bingul[®], ^{22b} C. Bini[®], ^{76a,76b} A. Biondini[®], ⁹⁴ G. A. Bird[®], ³³ M. Birman[®], ¹⁷² M. Biros[®], ¹³⁶ S. Biryukov[®], ¹⁴⁹ T. Bisanz[®], ⁵⁰ E. Bisceglie[®], ^{44b,44a} J. P. Biswal[®], ¹³⁷ D. Biswas[®], ¹⁴⁴ I. Bloch[®], ⁴⁹ A. Blue[®], ⁶⁰ U. Blumenschein[®], ⁹⁶ J. Blumenthal[®], ¹⁰² V. S. Bobrovnikov[®], ³⁸ M. Boehler[®], ⁵⁵ B. Boehm[®], ¹⁶⁹ D. Bogavac[®], ³⁷ A. G. Bogdanchikov[®], ³⁸ C. Bohm[®], ^{48a} V. Boisvert[®], ⁹⁷ P. Bokan[®], ³⁷ T. Bold[®], ^{87a} M. Bomben^{9,5} M. Bona[®], ⁹⁶ M. Boonekamp[®], ¹³⁸ C. D. Booth^{9,97} A. G. Borbély[®], ⁶⁰ I. S. Bordulev[®], ³⁸ H. M. Borecka-Bielska[®], ¹¹⁰ G. Borissov[®], ⁹³ D. Bortoletto[®], ¹²⁹ D. Boscherini[®], ^{24b} M. Bosman[®], ¹³ J. D. Bossio Sola[®], ³⁷ K. Bouaouda[®], ^{36a} N. Bouchar[®], ¹⁶⁶ L. Boudet[®], ⁴ J. Boudreau[®], ³³ E. V. Bouhova-Thacker^{9,93} D. Bortoletto[®], ³⁰ I. R. Boyko[®], ³⁹ L. Bozianu^{9,57} J. Bracinik[®], ²¹ N. Brahimi^{9,48} G. Brandt^(©), ¹⁷⁴ O. Brandt^(©), ³³ F. Braren^(©), ⁴⁹ B. Brau^(©), ¹⁰⁵ J. E. Brau^(©), ¹²⁶ R. Brener^(©), ¹⁷² L. Brenner^(©), ¹¹⁷ R. Brenner^(©), ¹⁶⁴ S. Bressler^(©), ¹⁷² G. Brianti^(©), ^{79a,79b} D. Britton^(©), ⁶⁰ D. Britzger^(©), ¹¹² I. Brock^(©), ²⁵ G. Brooijmans^(©), ⁴² E. M. Brooks, ^{159b} S. Bressler[®], ¹⁷² G. Brianti[®], ^{193,199} D. Britton[®], ⁶⁰ D. Britzger[®], ¹¹² I. Brock[®], ²⁷ G. Brooijmans[®], ⁷² E. M. Brooks, ²⁴⁹ E. Brost[®], ³⁰ L. M. Brown[®], ¹⁶⁸ L. E. Bruce[®], ⁶² T. L. Bruckler[®], ¹²⁹ P. A. Bruckman de Renstrom[®], ⁸⁸ B. Brüers[®], ⁴⁹ A. Bruni[®], ^{24b} G. Bruni[®], ^{24b} M. Bruschi[®], ^{24b} N. Bruscin[®], ^{76a,76b} T. Buanes[®], ¹⁷ Q. Buat[®], ¹⁴¹ D. Buchi[®], ¹¹² A. G. Buckley[®], ⁶⁰ O. Bulekov[®], ³⁸ B. A. Bullard[®], ¹⁴⁶ S. Burdi[®], ⁹⁴ C. D. Burgard[®], ⁵⁰ A. M. Burger[®], ³⁷ B. Burghgrave[®], ⁸ O. Burlayenko[®], ⁵⁵ J. T. P. Burr[®], ³³ J. C. Burzynski[®], ¹⁴⁵ E. L. Busch[®], ⁴² V. Büscher[®], ¹⁰² P. J. Bussey[®], ⁶⁰ J. M. Butler[®], ²⁶ C. M. Buttar[®], ⁶⁰ J. M. Butterworth[®], ⁹⁸ W. Buttinger[®], ¹³⁷ C. J. Buxo Vazquez[®], ¹⁰⁹ A. R. Buzykaev[®], ³⁸ S. Cabrera Urbán[®], ¹⁶⁶ L. Cadamuro[®], ⁶⁷ D. Caforio[®], ⁵⁹ H. Cai[®], ¹³² Y. Cai[®], ^{14,114c} Y. Cai[®], ^{114a} V. M. M. Cairo[®], ³⁷ O. Cakir⁹, ^{3a} N. Calace[®], ³⁷ P. Calafiura[®], ^{18a} G. Calderini[®], ¹³⁰ P. Calfayan[®], ⁶⁹ G. Callea[®], ⁶⁰ L. P. Caloba, ^{84b} D. Calvet[®], ⁴¹ S. Calvet[®], ⁴¹ M. Calvetti[®], ^{75a,75b} R. Camacho Toro[®], ¹³⁰ S. Camarda[®], ³⁷ D. Camarero Munoz[®], ²⁷ P. Camarri[®], ^{77a,77b} M. T. Camari⁹, ^{73a,73b} D. Camarca[®], ³⁷ C. Camircher[®], ¹⁶⁸ M. Campanelli[®], ⁹⁸ A. Camplani[®], ⁴³ V. Canale[®], ^{73a,73b} P. S. Calveto, ⁴¹ M. Calvettio, ^{75a,75b} R. Camacho Toroo, ¹³⁰ S. Camardao, ³⁷ D. Camarero Munozo, ²⁷ P. Camarrio, ^{77a,77b} M. T. Camerlingoo, ^{73a,73b} D. Camerono, ³⁷ C. Caminchero, ¹⁶⁸ M. Campanellio, ⁹⁸ A. Camplanio, ⁴³ V. Canaleo, ^{72a,72b} A. C. Canbayo, ^{3a} E. Canoneroo, ⁹⁷ J. Canteroo, ¹⁶⁶ Y. Caoo, ¹⁶⁵ F. Capocasao, ²⁷ M. Capuao, ^{44b,44a} A. Carboneo, ^{72a,72b} R. Cardarellio, ^{77a} J. C. J. Cardenaso, ⁸ G. Carduccio, ^{44b,44a} T. Carlio, ³⁷ G. Carlinoo, ^{73a} J. I. Carlottoo, ¹³
B. T. Carlsono, ^{132,1} E. M. Carlsono, ^{168,159a} J. Carmignanio, ⁹⁴ L. Carminatio, ^{72a,72b} A. Carnellio, ¹³⁸ M. Carnesaleo, ^{76a,76b} S. Carono, ¹¹⁶ E. Carquino, ^{140f} S. Carráo, ^{72a} G. Carrattao, ^{24b,24a} A. M. Carrollo, ¹²⁶ T. M. Cartero, ⁵³ M. P. Casadoo, ^{13,1}
M. Casparo, ⁴⁹ F. L. Castillo, ⁴ L. Castillo Garciao, ¹³ V. Castillo Gimenezo, ¹⁶⁶ N. F. Castroo, ^{133a,133e} A. Catinaccioo, ³⁷ J. R. Catmoreo, ¹²⁸ T. Cavaliereo, ⁴ V. Cavaliereo, ³⁰ N. Cavallio, ^{24b,24a} L. J. Caviedes Betancourt, ^{23b}
Y. C. Cekmeceliogluo, ⁴⁹ E. Celebio, ⁸³ S. Cellao, ³⁷ F. Cellio, ¹²⁹ M. S. Centonzeo, ^{71a,71b} V. Cepaitiso, ⁵⁷ K. Cernyo, ¹²⁵ A. S. Cerqueirao, ^{84a} A. Cerrio, ¹⁴⁹ L. Cerritoo, ^{71a,77b} F. Ceruttio, ^{18a} B. Cervatoo, ¹⁴⁴ A. Cervellio, ^{24b} G. Cesarinio, ⁵⁴ S. A. Cetino, ⁸³ D. Chakrabortyo, ¹¹⁸ J. Chano, ^{18a} W. Y. Chano, ¹⁵⁶ J. D. Chapmano, ³³ E. Chapono, ¹³⁸ B. Chargeishvilio, ^{152b} D. G. Charltono, ²¹ M. Chatterjeeo, ²⁰ C. Chauhano, ¹⁵⁶ H. Cheno, ¹¹⁴ H. Cheno, ³⁰ J. Cheno, ^{63c} J. Cheno, ¹⁴⁵ M. Cheno, ¹²⁹ S. Cheno, ¹⁵⁶ S. J. Cheno, ¹⁴⁴ A. Cheno, ¹⁵⁴ H. Cheno, ^{63a} J. Cheno, ^{63a} J. Cheno, ¹⁵⁵ S. J. Cheno, ¹⁵⁶ S. J. Cheno, ^{63c,138} X. Cheno, ¹⁵¹ Y. Cheno, ^{63a} J. Cheno, ^{63a} J. Cheno, ¹⁴⁴ A. Cheno, ¹⁵⁴ H. Cheno, ¹⁵⁵ J. Y. Cheno, ⁶⁵⁴ J. Cheno, ⁶⁵⁴ J. Cheno, ⁶⁵⁴ J. Cheno, ⁶⁵⁴ C. L. Cheng[®],¹⁷³ H. C. Cheng[®],^{65a} S. Cheong[®],¹⁴⁶ A. Cheplakov[®],³⁹ E. Cheremushkina[®],⁴⁹ E. Cherepanova[®],¹¹⁷ R. Cherkaoui El Moursli[®],³⁶ E. Cheu[®],⁷ K. Cheung[®],⁶⁶ L. Chevalier[®],¹³⁸ V. Chiarella[®],⁵⁴ G. Chiarelli[®],^{75a} N. Chiedde[®],¹⁰⁴ G. Chiodini[®],^{71a} A. S. Chisholm[®],²¹ A. Chitan⁹,^{28b} M. Chitishvili[®],¹⁶⁶ M. V. Chizhov[®],³⁹ K. Choi[®],¹¹ Y. Chou[®],¹⁴¹ E. Y. S. Chow[®],¹¹⁶ K. L. Chu[®],¹⁷² M. C. Chu[®],^{65a} X. Chu[®],^{14,114c} Z. Chubinidze[®],⁵⁴ J. Chudoba[®],¹³⁴ J. J. Chwastowski[®],⁸⁸ D. Cieri[®],¹¹² K. M. Ciesla[®],^{87a} V. Cindro⁹,⁹⁵ A. Ciocio[®],^{18a} F. Cirotto[®],^{73a,73b} Z. H. Citron[®],¹⁷² M. Citterio[®],^{72a} D. A. Ciubotaru,^{28b} A. Clark[®],⁵⁷ P. J. Clark[®],⁵³ N. Clarke Hall[®],⁹⁸ C. Clarry[®],¹⁵⁸ J. M. Clavijo Columbie[®],⁴⁹ S. E. Clawson[®],⁴⁹ C. Clement[•],^{48a,48b} J. Clercx[®],⁴⁹ Y. Coadou[®],¹⁰⁴ M. Cobal[®],^{70a,70c} A. Coccaro[®],^{58b} R. F. Coelho Barrue[®],^{133a} R. Coelho Lopes De Sa[®],¹⁰⁵ S. Coelli[®],^{72a} B. Cole[®],⁴² J. Collot[®],⁶¹ P. Conde Muiño[®],^{133a,133g} M. P. Connell[®],^{34c} S. H. Connell[®],^{34c} E. I. Conroy[®],¹²⁹ F. Conventi[®],^{73a,m} H. G. Cooke[®],²¹ A. M. Cooper-Sarkar[®],¹²⁹ F. A. Corchia⁹,^{24b,24a} A. Cordeiro Oudot Choi[®],¹³⁰ L. D. Corpe⁹,⁴¹ M. Corradie^{76a,76b} F. Corriveau[®],^{106,n} A. Cortes-Gonzalez[®],¹⁹ M. J. Costa¹⁶⁶ F. Costanza⁹,⁴ D. Costanzo[®],¹⁴² B. M. Cote⁹,¹²² J. Couthures[®],⁴ G. Cowan^{9,97} K. Cranmer^{9,173} D. Cremonini⁹,^{24b,24a} S. Crépé-Renaudin^{9,61} F. Crescioli⁹,¹³⁰ M. Cristoforetti⁹,^{79a,79b} V. Croft⁹,¹¹⁷ J. E. Crosby⁹,¹²⁴ G. Crosetti⁹,^{44b,44a} A. Cueto⁹,¹⁰¹ H. Cui^{9,98} Z. Cui^{9,7} W. R. Cunningham^{9,60} F. Curcio^{9,166} J. R. Curran^{9,53} P. Czodrowski^{9,37} M. M. Czurylo^{9,37} M. Cristinzianio, M. Cristororettio, V. Croito, J. E. Crosbye, G. Crosettie, A. Cuctoe, H. Cure, Z. Cuio, ⁷ W. R. Cunningham⁶, ⁶⁰ F. Curcio⁶, ¹⁶⁶ J. R. Curran⁶, ⁵³ P. Czodrowski⁶, ³⁷ M. M. Czurylo⁶, ³⁷
M. J. Da Cunha Sargedas De Sousa⁶, ^{58b,58a} J. V. Da Fonseca Pinto⁶, ^{84b} C. Da Via⁶, ¹⁰³ W. Dabrowski⁶, ^{87a} T. Dado⁶, ⁵⁰ S. Dahbi⁶, ¹⁵¹ T. Dai⁶, ¹⁰⁸ D. Dal Santo⁶, ²⁰ C. Dallapiccola⁶, ¹⁰⁵ M. Dam⁶, ⁴³ G. D'amen⁶, ³⁰ V. D'Amico⁶, ¹¹¹ J. Damp⁶, ¹⁰² J. R. Dandoy⁶, ³⁵ D. Dannheim⁶, ³⁷ M. Danninger⁶, ¹⁴⁵ V. Dao⁶, ¹⁴⁸ G. Darbo⁶, ^{58b} S. J. Das⁶, ^{30,0} J. Dannje, J. K. Dandoye, D. Dannienne, M. Dannigere, V. Daoe, G. Darote, S. J. Dase,
F. Dattola⁶, ⁴⁹ S. D'Auria⁶, ^{72a,72b} A. D'avanzo⁶, ^{73a,73b} C. David⁶, ^{34a} T. Davidek⁶, ¹³⁶ I. Dawson⁶, ⁹⁶ H. A. Day-hall⁶, ¹³⁵
K. De⁶, ⁸ R. De Asmundis⁶, ^{73a} N. De Biase⁶, ⁴⁹ S. De Castro⁶, ^{24b,24a} N. De Groot⁶, ¹¹⁶ P. de Jong⁶, ¹¹⁷ H. De la Torre⁶, ¹¹⁸
A. De Maria⁶, ^{114a} A. De Salvo⁶, ^{76a} U. De Sanctis⁶, ^{77a,77b} F. De Santis⁶, ^{71a,71b} A. De Santo⁶, ¹⁴⁹
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R. Joshi^{6,122} J. Jovicevic^{6,16} X. Ju^{6,18a} J. J. Junggeburth^{6,105} T. Junkermann^{6,64a} A. Juste Rozas^{9,13t} M. K. Juzek^{8,88} S. Kabana[®], ¹⁴⁰e A. Kaczmarska[®], ⁸⁸ M. Kado[®], ¹¹² H. Kagan[®], ¹²² M. Kagan[®], ¹⁴⁶ A. Kahn[®], ¹³¹ C. Kahra[®], ¹⁰² T. Kaji[®], ¹⁵⁶
E. Kajomovitz[®], ¹⁵³ N. Kakati[®], ¹⁷² I. Kalaitzidou[®], ⁵⁵ C. W. Kalderon[®], ³⁰ N. J. Karg[®], ¹³⁹ D. Kar[®], ^{34g} K. Karava[®], ¹²⁹
M. J. Kareem[®], ^{159b} E. Karentzos[®], ⁵⁵ O. Karkout[®], ¹¹⁷ S. N. Karpov[®], ³⁹ Z. M. Karpova[®], ³⁹ V. Kartvelishvili[®], ⁹³ A. N. Karyukhin[®], ³⁸ E. Kasimi[®], ¹⁵⁵ J. Katzy[®], ⁴⁹ S. Kaur[®], ³⁵ K. Kawade[®], ¹⁴³ M. P. Kawale[®], ¹²³ C. Kawamoto[®], ⁸⁹ T. Kawamoto[®], ^{63a} E. F. Kay[®], ³⁷ F. I. Kaya[®], ¹⁶¹ S. Kazakos[®], ¹⁰⁹ V. F. Kazanin[®], ³⁸ Y. Ke[®], ¹⁴⁸ J. M. Keaveney[®], ^{34a} R. Kavamotow, E. F. Kayw, F. I. Kayaw, S. Kazakosw, V. F. Kazanino, Y. Kew, N. J. M. Keaveney, ³⁴
R. Keeler¹, ¹⁶⁸ G. V. Kehris⁶, ⁶² J. S. Keller⁶, ³⁵ A. S. Kelly, ⁹⁸ J. J. Kempster⁶, ¹⁴⁹ P. D. Kennedy⁶, ¹⁰² O. Kepka⁶, ¹³⁴
B. P. Kerridge⁶, ¹³⁷ S. Kersten⁶, ¹⁷⁴ B. P. Kerševan⁶, ⁹⁵ L. Keszeghova⁶, ^{29a} S. Ketabchi Haghighat⁶, ¹⁵⁸ R. A. Khan⁶, ¹³²
A. Khanov⁶, ¹²⁴ A. G. Kharlamov⁶, ³⁸ T. Kharlamova⁶, ³⁸ E. E. Khoda⁶, ¹⁴¹ M. Kholodenko⁶, ³⁸ T. J. Khoo⁶, ¹⁹
G. Khoriauli⁶, ¹⁶⁹ J. Khubua⁶, ^{152b} Y. A. R. Khwaira⁶, ¹³⁰ B. Kibirige, ^{34g} D. W. Kim⁶, ^{48a,48b} Y. K. Kim⁶, ⁴⁰ N. Kimura⁶, ⁹⁸
M. K. Kingston⁶, ⁵⁶ A. Kirchhoff⁶, ⁵⁶ C. Kirfel⁶, ²⁵ F. Kirfel⁶, ²⁵ J. Kirk⁶, ¹³⁷ A. E. Kiryunin⁶, ¹¹² C. Kitsaki⁶, ¹⁰
O. Kinwara⁶, ²⁵ M. Kharawa⁶, ¹⁶¹ G. Khiri e³⁵ J. Khi⁵ e¹⁶⁹ M. H. Khi⁵ e⁴⁵ G. D. W. ⁵⁷ H. Kit⁵ e⁹⁴ D. W. ⁵⁷ O. Kivernyk[®], ²⁵ M. Klassen[®], ¹⁶¹ C. Klein[®], ³⁵ L. Klein[®], ¹⁶⁹ M. H. Klein[®], ⁴⁵ S. B. Klein[®], ⁵⁷ U. Klein[®], ⁹⁴ P. Klimek[®], ³⁷ A. Klimentov[®], ³⁰ T. Klioutchnikova[®], ³⁷ P. Kluit[®], ¹¹⁷ S. Kluth[®], ¹¹² E. Kneringer[®], ⁸⁰ T. M. Knight[®], ¹⁵⁸ A. Knue[®], ⁵⁰ R. Kobayashi[®], ⁸⁹ D. Kobylianskii[®], ¹⁷² S. F. Koch[®], ¹²⁹ M. Kocian[®], ¹⁴⁶ P. Kodyš[®], ¹³⁶ D. M. Koeck[®], ¹²⁶ P. T. Koenig[®], ²⁵ T. Koffas[®], ³⁵ O. Kolay[®], ⁵¹ I. Koletsou[®], ⁴ T. Komarek[®], ⁸⁸ K. Köneke[®], ⁵⁵ A. X. Y. Kong[®], ¹ T. Kono[®], ¹²¹ N. Konstantinidis[®], ⁹⁸ P. Kontaxakis[®], ⁵⁷ B. Konya[®], ¹⁰⁰ R. Kopeliansky[®], ⁴² S. Koperny[®], ^{87a} K. Korcyl[®], ⁸⁸ K. Kordas^(b), ^{155,y} A. Korn^(b), ⁸⁸ S. Korn^(b), ⁵⁶ I. Korolkov^(b), ¹³ N. Korotkova^(b), ³⁸ B. Kortman^(b), ¹¹⁷ O. Kortner^(b), ¹¹² S. Kortner^(b), ¹¹² W. H. Kostecka^(b), ¹¹⁸ V. V. Kostyukhin^(b), ¹⁴⁴ A. Kotsokechagia^(b), ¹³⁸ A. Kotwal^(b), ⁵² A. Koulouris^(b), ³⁷ A. Kourkoumeli-Charalampidi^(b), ^{74a,74b} C. Kourkoumelis^(b), ⁹ E. Kourlitis^(b), ^{112,u} O. Kovanda^(b), ¹²⁶ R. Kowalewski^(b), ¹⁶⁸ K. Kowalewsk^(b), ¹⁶⁸ K. W. Kozanecki[®],¹³⁸ A. S. Kozhin[®],³⁸ V. A. Kramarenko[®],³⁸ G. Kramberger[®],⁹⁵ P. Kramer[®],¹⁰² M. W. Krasny[®],¹³⁰ W. Kozanecki, W. A. S. Koznino, W. A. Kramarenkoo, "G. Krambergero, "P. Kramero, "M. W. Krasnyo, A. Krasnyo, "A. S. Koznino, "V. A. Kramarenkoo, "G. Krambergero, "P. Kramero, "M. W. Krasnyo, "A. S. Koznino, "Interpretent of the state of the st Y. Kulchitsky⁰, ^{38,K} S. Kuleshov⁰, ¹⁴⁰⁰, ¹⁴⁰⁰ M. Kumar⁰, ^{34g} N. Kumari⁰, ⁴⁹ P. Kumari⁰, ¹⁵⁹⁶ A. Kupco⁰, ¹³⁴ T. Kupfer, ⁵⁰ A. Kupich⁰, ³⁸ O. Kuprash⁰, ⁵⁵ H. Kurashige⁰, ⁸⁶ L. L. Kurchaninov⁰, ^{159a} O. Kurdysh⁰, ⁶⁷ Y. A. Kurochkin⁰, ³⁸ A. Kuroca⁰, ³⁸ M. Kuze⁰, ¹⁵⁷ A. K. Kvam⁰, ¹⁰⁵ J. Kvita⁰, ¹²⁵ T. Kwan⁰, ¹⁰⁶ N. G. Kyriacou⁰, ¹⁰⁸ L. A. O. Laatu⁰, ¹⁰⁴ C. Lacasta⁰, ¹⁶⁶ F. Lacava⁰, ^{76a,76b} H. Lacker⁰, ¹⁹ D. Lacour⁰, ¹³⁰ N. N. Lad⁰, ⁹⁸ E. Ladygin⁰, ³⁹ A. Lafarge⁰, ⁴¹ B. Laforge⁰, ¹³⁰ T. Lagouri⁰, ¹⁷⁵ F. Z. Lahbabi⁰, ^{36a} S. Lai⁰, ⁵⁶ J. E. Lambert⁰, ¹⁶⁸ S. Lammers⁰, ⁶⁹ W. Lampl⁰, ⁷ C. Lampoudis⁰, ^{155,y} G. Lamprinoudis, ¹⁰² A. N. Lancaster⁰, ¹¹⁸ E. Lançon⁰, ³⁰ U. Landgraf⁰, ⁵⁵ M. P. J. Landon⁹⁶ V. S. Lang⁰, ⁵⁵ O. K. B. Langrekken⁰, ¹²⁸ A. J. Lankford⁰, ¹⁶² F. Lanni⁰, ³⁷ K. Lantzsch⁰, ²⁵ A. Lanza⁰, ^{74a} J. F. Laporte⁰, ¹³⁸ T. Lari⁰, ^{72a} F. Lasagni Manghi⁰, ^{24b} M. Lassnig⁰, ³⁷ V. Latonova⁰, ¹³⁴ A. Laudrain⁰, ¹⁰² A. Laurier⁰, ¹⁵³ S. D. Lawlor⁰, ¹⁴² Z. Lawrence⁰, ¹⁰³ R. Lazaridou, ¹⁷⁰ M. Lazzaroni⁰, ^{72a,72b} B. Le, ¹⁰³ E. M. Le Boulicaut^{9,51} S. Lee⁰, ^{48a,48b} T. F. Lee⁰, ^{48a} B. Leban⁰, ^{24b,24a} A. Lebedev⁰, ⁸² M. LeBlanc⁰, ¹⁰³ F. Ledroit-Guillon⁰, ⁶¹ S. C. Lee⁰, ¹⁵¹ S. Lee⁰, ^{48a,48b} T. F. Lee⁰, ⁹⁴

L. L. Leeuw[®],^{34c} H. P. Lefebvre[®],⁹⁷ M. Lefebvre[®],¹⁶⁸ C. Leggett[®],^{18a} G. Lehmann Miotto[®],³⁷ M. Leigh[®],⁵⁷ W. A. Leight[®],¹⁰⁵ W. Leinone[®],¹¹⁶ A. Leisos[®],^{155,z} M. A. L. Leite[®],^{84c} C. E. Leitgeb[®],¹⁹ R. Leitner[®],¹³⁶ W. A. Leight⁶, ¹⁰⁵ W. Leinonen⁶, ¹¹⁶ A. Leisos⁶, ^{153,2} M. A. L. Leite⁶, ^{84c} C. E. Leitgeb⁶, ¹⁹ R. Leitner⁶, ¹³⁶ K. J. C. Leny⁶, ⁴⁵ T. Lenz⁶, ²⁵ S. Leone⁶, ^{75a} C. Leonidopoulos⁶, ⁵³ A. Leopold⁶, ¹⁴⁷ C. Leroy⁶, ¹¹⁰ R. Les⁶, ¹⁰⁹ C. G. Lester⁶, ³³ M. Levchenko⁷⁸, ³⁸ J. Levêque⁶, ⁴ L. J. Levinson⁶, ¹⁷² G. Levrini⁶, ^{24b,24a} M. P. Lewicki⁶, ⁸⁸ C. Lewis⁶, ¹⁴¹ D. J. Lewis⁶, ⁴ A. Li⁶, ⁵ B. Li⁶, ^{63b} C. Li, ^{63a} C-Q. Li⁶, ¹¹² H. Li⁶, ^{63a} H. Li⁶, ^{63b} H. Li⁶, ¹¹⁴ H. Li⁶, ¹⁵ H. Li⁶, ^{63b} J. Li⁶, ^{63c} K. Li⁶, ^{63b} C. Li^{6,3a} C-Q. Li⁶, ¹¹² H. Li⁶, ^{63a} H. Li⁶, ^{63b} H. Li⁶, ¹²⁹ Z. Li⁶, ¹⁵⁶ Z. Li⁶, ^{14,114c} S. Li⁶, ^{63d,63c} T. Li⁶, ⁵ X. Li⁶, ¹⁰⁶ Z. Li⁶, ¹²⁹ Z. Li⁶, ¹⁵⁶ Z. Li⁶, ^{14,114c} S. Li⁶, ^{63d,63c} T. Li⁶, ⁵⁵ J. Lieber Marin⁶, ^{84e} H. Lien⁶⁹ H. Lin⁶, ¹⁰⁸ H. Lin⁶, ¹⁰⁸ H. Lin⁶, ¹⁰⁸ H. Lin⁶, ⁶⁹ H. Lin⁶, ⁶³ J. Li⁶, ^{63a} X. Liu⁶, ^{63a} M. Liu⁶, ^{63a} H. Li⁶, ^{63a} H. Li⁶, ^{63a} K. Liu⁶, ^{63b} Y. Liu⁶, ^{114b} J. Long^{63a}, ¹⁴¹ Q. Liu⁶, ^{63d,141,63c} X. Liu⁶, ^{63a} X. Liu⁶, ^{63b} Y. Liu⁶, ^{114b,114c} Y. L. Liu⁶, ^{63b} Y. Liu⁶, ^{63a} J. Llorente Merino⁸, ¹⁴² S. L. Lloyd⁹, ⁶⁶ E. M. Lobodzinska⁹, ⁴⁹ P. Loch⁹, ⁷ T. Lohse⁹, ¹⁹ K. Lohwasser⁹, ¹⁴² F. Loiscon⁹, ⁴⁹ M. Lok³¹³, ¹⁴⁴ L. D. Lom⁶³, ²¹ L. D. Long⁶⁵, ¹⁴⁵ L. Long⁶⁶⁸, ¹⁴² F. Long⁶⁶⁸, ¹⁴⁵ L. Ong⁶⁷, ¹⁴⁵ L. Ong⁶⁷ K. Eldo, J. Elorente Merinoo, S. E. Eloydo, E. M. Lobodzińskao, P. Locho, T. Lonseo, K. Lonwassero,
E. Loiaconoo, ⁴⁹ M. Lokajiceko, ^{134,a} J. D. Lomaso, ²¹ J. D. Longo, ¹⁶⁵ I. Longarinio, ¹⁶² R. Longoo, ¹⁶⁵ I. Lopez Pazo, ⁶⁸
A. Lopez Soliso, ⁴⁹ N. Lorenzo Martinezo, ⁴ A. M. Loryo, ¹¹¹ M. Losadao, ^{119a} G. Löschcke Centenoo, ¹⁴⁹ O. Losevao, ³⁸
X. Louo, ^{48a,48b} X. Louo, ^{14,114c} A. Louniso, ⁶⁷ P. A. Loveo, ⁹³ G. Luo, ^{14,114c} M. Luo, ⁶⁷ S. Luo, ¹³¹ Y. J. Luo, ⁶⁶
H. J. Lubattio, ¹⁴¹ C. Lucio, ^{76a,76b} F. L. Lucio Alveso, ^{114a} F. Luehringo, ⁶⁹ I. Luiseo, ¹⁴⁸ O. Lukianchuko, ⁶⁷
O. Lundbergo, ¹⁴⁷ B. Lund-Jenseno, ^{147a} N. A. Luongoo, ⁶ M. S. Lutzo, ³⁷ A. B. Luxo, ²⁶ D. Lynno, ³⁰ R. Lysako, ¹³⁴ E. Lytken[®],¹⁰⁰ V. Lyubushkin[®],³⁹ T. Lyubushkina[®],³⁹ M. M. Lyukova[®],¹⁴⁸ M. Firdaus M. Soberi[®],⁵³ H. Ma[®],³⁰ E. Lytkene, V. Lytbushkine, T. Lytbushkine, M. M. Lytkovae, M. Firdaus M. Soberte, H. Mae,
K. Mae, ^{63a} L. L. Mae, ^{63b} W. Mae, ^{63a} Y. Mae, ¹²⁴ J. C. MacDonalde, ¹⁰² P. C. Machado De Abreu Fariase, ^{84e} R. Madare, ⁴¹ T. Madulae, ⁹⁸ J. Maedae, ⁸⁶ T. Maenoe, ³⁰ H. Maguiree, ¹⁴² V. Maiborodae, ¹³⁸ A. Maioe, ^{133a,133b,133d} K. Maje, ^{87a} O. Majerskye, ⁴⁹ S. Majewskie, ¹²⁶ N. Makovece, ⁶⁷ V. Maksimovice, ¹⁶ B. Malaescue, ¹³⁰ Pa. Maleckie, ⁸⁸ V. P. Maleeve, ³⁸ F. Maleke, ^{61,aa} M. Malie, ⁹⁵ D. Malitoe, ⁹⁷ U. Mallike, ⁸¹ S. Maltezos, ¹⁰ S. Malyukov, ³⁹ J. Mamuzice, ¹³ G. Mancinie, ⁵⁴ M. N. Mancinie, ²⁷ G. Mancoe, ^{74a,74b} J. P. Mandaliae, ⁹⁶ S. S. Mandarrye, ¹⁴⁹ I. Mandiće, ⁹⁵ L. Manchile, M. N. Malchile, G. Marcole, J. T. Mandanae, S. S. Mandariye, T. Mandae, L. Mandae, M. M. Marcole, M. M. Marcole, J. T. Mandanae, S. S. Mandariye, T. Mandae, J. L. Mandae, J. L. Mandae, M. Marcole, M. Mandae, M. Marcole, J. J. Mandae, M. Marcole, J. S. Mandae, J. C. Mankae, J. K. Mandae, J. K. Mandae, J. S. S. Mandae, J. C. Mankae, J. K. Mandae, J. S. Marcole, J. Mandae, J. S. Marcole, J. Mandae, J. S. Marcole, J. Mandae, J. S. S. Mandariye, T. Mandae, J. K. Mandae, J. S. S. Mandae, J. K. Mandae, J. K. Mandae, J. S. S. Mandae, J. K. Mandae, J. K. Marcole, J. Marcole, L. Martinelli[®], ^{76a,76b} M. Martinez[®], ^{13,t} P. Martinez Agullo[®], ¹⁶⁶ V. I. Martinez Outschoorn[®], ¹⁰⁵ P. Martinez Suarez[®], ¹³ S. Martin-Haugh⁰, ¹³⁷ G. Martinovicova⁰, ¹³⁶ V. S. Martoiu⁰, ^{28b} A. C. Martyniuk⁰, ⁹⁸ A. Marzin⁰, ³⁷ D. Mascione⁰, ^{79a,79b} L. Masetti⁰, ¹⁰² T. Mashimo⁰, ¹⁵⁶ J. Masik⁰, ¹⁰³ A. L. Maslennikov⁰, ³⁸ P. Massarotti⁰, ^{73a,73b} P. Mastrandrea⁰, ^{75a,75b} A. Mastroberardino⁶, ^{44b,44a} T. Masubuchi⁶, ¹⁵⁶ T. Mathisen⁶, ¹⁶⁴ J. Matousek⁶, ¹³⁶ N. Matsuzawa, ¹⁵⁶ J. Maurer⁶, ^{28b} A. J. Maury⁶, ⁶⁷ B. Maček⁶, ⁹⁵ D. A. Maximov⁶, ³⁸ A. E. May⁶, ¹⁰³ R. Mazini⁶, ¹⁵¹ I. Maznas⁶, ¹¹⁸ M. Mazza⁶, ¹⁰⁹ S. M. Mazza⁶, ¹³⁹ E. Mazzeo⁶, ^{72a,72b} C. Mc Ginn⁶, ³⁰ J. P. Mc Gowan⁶, ¹⁶⁸ S. P. Mc Kee⁶, ¹⁰⁸ C. C. McCracken⁶, ¹⁶⁷ E. F. McDonald⁶, ¹⁰⁷ A. E. McDougall⁶, ¹¹⁷ J. A. Mcfayden⁶, ¹⁴⁹ R. P. McGovern⁶, ¹³¹ R. P. Mckenzie⁶, ^{34g} T. C. Mclachlan⁽⁹⁾, D. J. Mclaughlin⁽⁹⁾, S. J. McMahon⁽⁹⁾, ¹³⁷ C. M. Mcpartland⁽⁹⁾, ⁹⁴ R. A. McPherson⁽⁹⁾, ^{168,n} T. C. Mclachlan⁹,⁴⁹ D. J. Mclaughlin⁹,⁹⁸ S. J. McMahon⁹,¹³⁷ C. M. Mcpartland⁹,⁹⁴ R. A. McPherson⁹,^{168,n} S. Mehlhase⁹,¹¹¹ A. Mehta⁹⁴ D. Melini⁹,¹⁶⁶ B. R. Mellado Garcia⁹,^{34g} A. H. Melo⁹,⁵⁶ F. Meloni⁹,⁴⁹
A. M. Mendes Jacques Da Costa⁹,¹⁰³ H. Y. Meng⁹,¹⁵⁸ L. Meng⁹,⁹³ S. Menke⁹,¹¹² M. Mentink⁹,³⁷ E. Meoni⁹,^{44b,44a} G. Mercado⁹,¹¹⁸ S. Merianos⁹,¹⁵⁵ C. Merlassino⁹,^{70a,70c} L. Merola⁹,^{73a,73b} C. Meroni⁹,^{72a,72b} J. Metcalfe⁹,⁶
A. S. Mete⁹,⁶ E. Meuser⁹,¹⁰² C. Meyer⁹,⁶⁹ J-P. Meyer⁹,¹³⁸ R. P. Middleton^{9,137} L. Mijović^{9,53} G. Mikenberg^{9,172}
M. Mikestikova^{9,134} M. Mikuž^{9,95} H. Mildner^{9,102} A. Milic^{9,37} D. W. Miller^{9,40} E. H. Miller^{9,146} L. S. Miller^{9,35}
A. Milov^{9,172} D. A. Milstead,^{48a,48b} T. Min,^{114a} A. A. Minaenko^{9,38} I. A. Minashvili⁹,^{152b} L. Mince^{9,60} A. I. Mincer^{9,120}
B. Mindur^{9,87a} M. Mineev^{9,39} Y. Mino^{9,89} L. M. Mir^{9,13} M. Miralles Lopez⁶⁰ M. Mironova^{9,18a} A. Mishima,¹⁵⁶
M. C. Missio^{9,116} A. Mitra^{9,170} V. A. Mitsou^{9,166} Y. Mitsumori^{9,113} O. Miu^{9,158} P.S. Miyagawa^{9,66} T. Mkrtchyan^{9,64a}
M. Mlinarevic^{9,98} T. Mlinarevic^{9,98} M. Mlynarikova^{9,37} S. Mobius^{9,20} P. Mogg^{9,111} M. H. Mohamed Farook^{9,113}
K. Mönig^{9,49} E. Monnier^{9,104} L. Monsonis Romero,¹⁶⁶ J. Montejo Berlingen^{9,13} M. Montella^{9,124} F. Montereali^{9,78a,78b}
F. Monticelli^{9,92} S. Monzani^{9,70a,70c} N. Morange^{9,67} A. L. Moreira De Carvalho^{9,49} M. Moreno Llácer^{9,166}
C. Moreno Martinez^{9,57} P. Morettini^{9,58b} S. Morgenstern^{9,37} M. Morii^{9,62} M. Morinaga^{9,156} F. Morodei^{9,76a,76b} C. Moreno Martinez[®],⁵⁷ P. Morettini[®],^{58b} S. Morgenstern[®],³⁷ M. Morii[®],⁶² M. Morinaga[®],¹⁵⁶ F. Morodei[®],^{76a,76b} L. Morvaj[®],³⁷ P. Moschovakos[®],³⁷ B. Moser[®],³⁷ M. Mosidze[®],^{152b} T. Moskalets[®],⁴⁵ P. Moskvitina[®],¹¹⁶ J. Moss[®],^{32,bb} P. Moszkowicz[®],^{87a} A. Moussa[®],^{36d} E. J. W. Moyse[®],¹⁰⁵ O. Mtintsilana[®],^{34g} S. Muanza[®],¹⁰⁴ J. Mueller[®],¹³²

D. Muenstermann[®],⁹³ R. Müller[®],³⁷ G. A. Mullier[®],¹⁶⁴ A. J. Mullin,³³ J. J. Mullin,¹³¹ D. P. Mungo[®],¹⁵⁸ D. Munoz Perez[®],¹⁶⁶ F. J. Munoz Sanchez[®],¹⁰³ M. Murin[®],¹⁰³ W. J. Murray[®],^{170,137} M. Muškinja[®],⁹⁵ C. Mwewa[®],³⁰ A. G. Myagkov[®],^{38,k} A. J. Myers[®],⁸ G. Myers[®],¹⁰⁸ M. Myska[®],¹³⁵ B. P. Nachman[®],^{18a} O. Nackenhorst[®],⁵⁰ K. Nagai[®],¹²⁹ A. G. Myagkov⁹, ^{38,k} A. J. Myers⁹, ⁸ G. Myers⁹, ¹⁰⁸ M. Myska⁹, ¹³⁵ B. P. Nachman⁹, ^{18a} O. Nackenhorst⁹, ⁵⁰ K. Nagai⁹, ¹²⁹ K. Nagano⁹, ⁸⁵ J. L. Nagle⁹, ^{30,0} E. Nagy⁹, ¹⁰⁴ A. M. Nairz⁹, ³⁷ Y. Nakahama⁹, ⁸⁵ K. Nakamura⁹, ⁸⁵ K. Nakakill⁹, ⁵ H. Nanjo⁹, ¹²⁷ E. A. Narayanan⁹, ¹¹⁵ I. Naryshkin⁹, ³⁸ L. Nasella⁹, ^{72a,72b} M. Naseri⁹, ³⁵ S. Nasri⁹, ^{119b} C. Nass²⁴, ^{24a} G. Navarro⁹, ^{23a} J. Navarro-Gonzalez⁹, ¹⁶⁶ R. Nayak⁹, ¹⁵⁴ A. Nayaz⁹, ¹⁹ P. Y. Nechaeva⁹, ³⁸ S. Nechaeva⁹, ^{24b,24a} F. Nechansky⁹, ⁴⁹ L. Nedic⁹, ¹²⁷ T. J. Neep⁹, ²¹ A. Negri⁹, ^{74a,74b} M. Negrini⁹, ^{24b} C. Nellist⁹, ¹¹⁷ C. Nelson⁹, ¹⁰⁶ K. Nelson⁹, ¹⁰⁸ S. Nemceek⁹, ¹³⁴ M. Nessi⁹, ^{37,ce} M. S. Neubauer⁹, ¹⁶⁵ F. Neuhaus⁹, ¹⁰² J. Neundorf⁹, ⁴⁹ P. R. Newman⁹, ²¹ C. W. Ng⁹, ¹³² Y. W. Y. Ng⁹, ⁴⁹ B. Ngair⁹, ^{119a} H. D. N. Nguyen⁹, ¹¹⁰ R. B. Nickerson⁹, ¹²⁹ R. Nicolaidou⁹, ¹³⁸ J. Nielsen⁹, ¹³⁰ M. Niemeyer⁹, ⁵⁶ J. Niermann^{9,56} N. Nikiforou^{9,37} V. Nikolaenko^{9,38,k} I. Nikolic-Audit⁹, ¹³⁰ K. Nikolopoulos^{9,21} P. Nilsson^{9,30} I. Ninca^{9,49} G. Ninio¹⁵⁴ A. Nisati^{9,76a} N. Nishu^{9,2} R. Nisius^{9,112} J-E. Nitschke^{5,11} E. K. Nkadimeng^{9,34g} T. Nobe^{9,55} L. Novotny^{9,135} R. Novotny^{9,115} L. Nozka^{9,125} K. Ntekas¹⁶² N. M. J. Nunes De Moura Junior^{9,84b} J. Ocariz^{9,130} A. Ochi^{9,85} R. Oishi^{9,156} M. L. Ojeda⁴⁹ Y. Okumura^{9,156} L. F. Oleiro Seabra^{9,133} I. Oleksiyuk^{9,57} S. A. Olivares Pino^{9,1404} G. Oliveira Correa^{9,134} J. Oliveira Damazio^{9,30} D. Oliveira Damazio^{9,30} D. Oliveira Goncalves^{9,84a} J. L. Oliver^{9,162} O. O. Öncel^{9,55} A. P. O'Neill^{9,20} A. Onofre^{9,133} L. M. Osojnak^{9,11} M. J. Oreglia^{6,40} G. E. Orellana^{9,92} D. Orestano^{9,78a,78b} N. Orlando^{9,13} R. S. Orr^{9,158} L. M. Osojnak^{9,131} L. F. Olcino Seabra⁶, ¹³⁵ L. Oleksiyuk⁶, ⁵⁷ S. A. Olivares Pino⁶, ¹⁴⁰⁶ G. Olivein⁶ Correa⁶, ¹³ D. Oliveira Damazio⁶, ³⁰ D. Oliveira Jonazio⁶, ³⁰ D. Oliveira Jonazio⁶, ³¹ D. S. L. Mospiak⁶, ³¹ D. Oregiao⁶, ³² D. S. L. Mondo¹³ R. S. Ort⁶, ³¹ L. D. Nosipak⁶, ³¹ D. Ospian⁶, ³² A. Paccheco Pagese¹³ C. Pado¹³ D. S. Darados P. Davosano⁶, ³² D. S. Dardinio¹¹⁷ J. G. Panduro Vazquez⁶, ³⁷ J. P. Para⁶, ³⁵ D. K. Panchal⁶, ¹¹ C. E. Pandinie¹¹⁷ J. G. Panduro Vazquez⁶, ³⁵ J. A. Parken³, ³ L. Parkuro³, ³⁵ F. Patslo⁶, ³⁵ D. Paredes Hernandez⁶, ⁵⁰ A. Paretie, ^{74*i*-74} K. R. Park⁶⁴ T. H. Park⁶⁵ B. Parcel⁶⁵ S. P. Passaggio⁵ ³⁵ F. Patslo⁸⁵ P. Patslo⁸⁵ B. W. Varish⁶, ³¹ J. A. Parsons⁴² U. Parzefallo⁵⁵ S. Peraku⁸⁴ J. Parke¹⁴ T. H. Park⁶¹ S. U. N. Parke¹⁶, ³⁵ J. R. Parke¹⁷ H. Park⁶¹ S. V. Peleganchuk⁶³, ⁶³ O. Pence⁷⁷ F. P. Patel⁶³ B. Pastore⁷⁷ D. Patel⁶³ S. V. Peleganchuk⁶³, ⁶³ O. Pence⁷⁷ J. P. Patel⁶³ D. Perce⁷⁷ J. P. Patel⁶³ S. V. Peleganchuk⁶³, ⁶³ O. Pence⁷⁷ J. P. Patel⁶³ D. Perce⁷⁹ P. Patel⁶³ S. V. Peleganchuk⁶³, ⁶³ O. Pence⁷⁷ J. P. Patel⁶⁴ D. V. Perepelista^{3,00} G. Perera⁶¹, ¹⁶ H. Perze, Zodina⁶, ¹⁵⁸ M. Petterse¹⁷ T. C. Peterse⁶⁴ J. P. Petio⁶⁴ J. Petrov¹⁶⁴ D. V. Perepelista^{3,10} G. Perra⁶¹, ¹⁵⁸ H. Patklin⁶⁴ H. N. Peterse¹⁷ T. C. Peterse⁶⁴ J. P. Pitel⁶⁴ A. Petio¹⁹¹ H. Perepuda³⁰ G. Perra^{61,16} J. P PHYSICAL REVIEW LETTERS 133, 161803 (2024)
 A. L. Rescia, ⁴⁹ S. Resconie, ^{72a} M. Ressegotti, ^{58b,58a} S. Rettie, ³⁷ J. G. Reyes Rivera, ¹⁰⁹ E. Reynolds, ^{18a}
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 A. Rocchi, ^{77a,77b} C. Roda, ^{75a,75b} S. Rodriguez Boscae, ³⁷ Y. Rodriguez Garcia, ^{23a} A. Rodriguez Rodriguez, ⁵⁵ A. M. Rodríguez Vera, ¹¹⁸ S. Re, ³⁷ J. T. Roemero, ³⁷ A. R. Roepe-Giere, ¹³⁹ J. Roggel, ¹⁷⁴ O. Røhne, ¹²⁸ R. A. Rojas, ¹⁰⁵ C. P. A. Rolando, ¹³⁰ J. Roloff, ³⁰ A. Romaniouk, ³⁸ E. Romano, ^{74a,74b} M. Romano, ^{24b}
 A. C. Romero Hernandez, ¹⁶⁵ N. Rompotis, ⁹⁴ L. Roos, ¹³⁰ S. Rosatio, ^{76a} B. J. Rossero, ⁴⁰ E. Rossi, ¹²⁹ E. Rossi, ^{72a,73b} L. P. Rossi, ⁶² L. Rossini, ⁶⁵ S. Roy-Garando, ¹³⁸ A. Rozanov, ¹⁰⁴ Z. M. A. Rozgire, ¹¹⁰ D. Rousseau, ⁶⁷ D. Rousseau, ⁶⁷ D. Rousseau, ⁶⁷ A. Rubino Jimenez, ¹⁶⁶ A. J. Ruby, ⁹⁴ V. H. Ruelas Rivera, ¹²⁸ A. Ryzhov, ⁴⁵ J. A. Sabater Iglesias, ⁵⁷ P. Sabatini, ¹⁵⁶ T. Saito, ¹⁵⁶ A. Salav, ¹²⁸ A. Ryzhov, ⁴⁵ J. A. Sabater Iglesias, ⁵⁷ P. Sabatini, ¹⁶⁶ H. Sautore, ¹⁴⁹ A. Ruye, ¹⁵⁶ A. Salavatore, ^{44b,44a} F. Salvatore, ¹⁴⁹ A. Salvatore, ¹⁴⁹ A. Salburger, ³⁷ J. Sannel, ⁵⁵ K. Sanoo, ³³ J. Sander, ⁴⁹ J. A. Sandsei, ⁵⁵ P. Santolo, ¹⁵⁶ T. Saito, ¹⁵⁶ A. Salav, ¹²⁸ A. Salavatore, ¹⁶⁴ H. Sandsker, ¹²⁸ C. O. Sander, ⁴⁹ J. A. Sandesia, J. G. Saraiva, "Jost Adamé, O. Sasaki,", K. Satoe, W. C. Sauer, W. E. Sauvano, "P. Savarde, Jost R. Sawada, J. Sardaine, O. Sasaki, "P. K. Satoe, W. C. Sauer, W. E. Sauvano, "P. Savarde, Jost R. Sawada, Jost C. Sawyere, J¹³ L. Sawyere, "P. C. Schaile, "Junct Schaile, "Juncterim, "Junct Schaile, "Junct Schaile, "Junct Schaile, "Junct A. Sopczak^(b), ¹³⁵ A. L. Sopio^(b), ⁹⁸ F. Sopkova^(b), ^{29b} J. D. Sorenson^(b), ¹¹⁵ I. R. Sotarriva Alvarez^(b), ¹⁵⁷ V. Sothilingam, ^{64a}
O. J. Soto Sandoval^(b), ^{140c,140b} S. Sottocornola^(b), ⁶⁹ R. Soualah^(b), ¹⁶³ Z. Soumaimi^(b), ^{36e} D. South^(b), ⁴⁹ N. Soybelman^(b), ¹⁷²
S. Spagnolo^(b), ^{71a,71b} M. Spalla^(b), ¹¹² D. Sperlich^(b), ⁵⁵ G. Spigo^(b), ³⁷ S. Spinali^(b), ⁹³ B. Spisso^(b), ^{73a,73b} D. P. Spiteri^(b), ⁶⁰

M. Spousta[®],¹³⁶ E. J. Staats[®],³⁵ R. Stamen[®],^{64a} A. Stampekis[®],²¹ M. Standke[®],²⁵ E. Stanecka[®],⁸⁸ W. Stanek-Maslouska[®],⁴⁹ M. V. Stange[®],⁵¹ B. Stanislaus[®],^{18a} M. M. Stanitzki[®],⁴⁹ B. Stapf[®],⁴⁹ E. A. Starchenko[®],³⁸ W. Stanek-Maslouska⁹, ⁴⁹ M. V. Stange⁵, ⁵¹ B. Stanislaus^{18a} M. M. Stanitzki⁹, ⁴⁹ B. Stapf⁹, ⁴⁹ E. A. Starchenko³⁸ G. H. Stark⁹, ¹³ J. Stark⁹, ¹⁹ P. Staroba⁹, ¹³⁴ P. Starovoitov⁶, ^{64a} S. Stärz⁹, ¹⁰⁶ R. Staszewski⁹, ⁸⁸ G. Stavropoulos⁴⁷ J. Steentoft⁹, ¹⁶⁴ P. Steinberg⁹, ³⁰ B. Stelzer⁹, ^{145,159a} H. J. Stelzer⁹, ¹³² O. Stelzer-Chilton⁹, ^{159a} H. Stenzel⁹, ⁵⁹ T. J. Stevenson⁹, ¹⁴⁹ G. A. Stewart⁹, ³⁷ J. R. Stewart⁹, ¹²⁴ M. C. Stockton^{9, 37} G. Stoicea^{9, 28b} M. Stolarski⁹, ^{133a} S. Stonjek⁹, ¹¹² A. Straessner^{9, 51} J. Strandberg¹⁴⁷ S. Strandberg<sup>9, ^{48a,48b} M. Stratmann^{9, 174} M. Strauss¹²³ T. Strebler^{9, 104} P. Strizenec^{9, 29b} R. Ströhmer^{9, 169} D. M. Strom¹²⁶ R. Stroynowski^{9, 45} A. Strubig^{9, 48a,48b}
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N. Viaux Maira[®], ¹⁴⁰ T. Vickey[®], ¹⁴² O. E. Vickey Boeriu[®], ¹⁴² G. H. A. Viehhauser[®], ¹²⁹ L. Vigani[®], ^{64b} M. Villa[®], ^{24b,24a} N. Viaux Maira⁶, ¹⁴² T. Vickey⁶, ¹⁴² O. E. Vickey Boeriu⁶, ¹⁴² G. H. A. Viehhauser⁶, ¹²⁹ L. Vigani⁶, ⁰⁴⁰ M. Villa⁶, ^{240,24a} M. Villa⁶, ^{240,24a} M. Villa⁶, ^{240,24a} E. Viluchi⁶, ⁵³ E. Vilucchi⁶, ⁵⁴ M. G. Vincter⁶, ³⁵ A. Visibile, ¹¹⁷ C. Vittori⁶, ³⁷
I. Vivarelli⁶, ^{24b,24a} E. Voevodina⁶, ¹¹² F. Vogel⁶, ¹¹¹ J. C. Voigt⁶, ⁵¹ P. Vokac⁶, ¹³⁵ Yu. Volkotrub⁶, ^{87b} J. Von Ahnen⁶, ⁴⁹ E. Von Toerne⁶, ²⁵ B. Vormwald⁶, ³⁷ V. Vorobel⁶, ¹³⁶ K. Vorobev⁶, ³⁸ M. Vos⁶, ¹⁶⁶ K. Voss⁶, ¹⁴⁴ M. Vozak⁶, ¹¹⁷
L. Vozdecky⁶, ¹²³ N. Vranjes⁶, ¹⁶ M. Vranjes Milosavljevic⁶, ¹⁶ M. Vreeswijk⁶, ¹¹⁷ N. K. Vu⁶, ^{63d,63c} R. Vuillermet⁶, ³⁷ O. Vujinovic⁶, ¹⁰² I. Vukotic⁶, ⁴⁰ S. Wada⁶, ¹⁶⁰ C. Wagner, ¹⁰⁵ J. M. Wagner⁶, ^{18a} W. Wagner⁶, ¹⁷⁴ S. Wahda⁶, ¹⁷⁴ H. Wahlberg⁶, ⁹² M. Wakida⁶, ¹¹³ J. Walder⁶, ¹³⁷ R. Walker⁶, ¹¹¹ W. Walkowiak⁶, ¹⁴⁴ A. Wall⁶, ¹³¹ E. J. Wallin⁶, ¹⁰⁰ T. Wamorkar⁶, ⁶ A. Z. Wang⁶, ¹³⁹ C. Wang⁶, ¹⁰² C. Wang⁶, ¹¹¹ H. Wang⁶, ^{63a} W. T. Wang⁶, ^{65c} P. Wang⁶, ⁸ R. Wang⁶, ⁶² R. Wang⁶, ^{63b} S. Wang⁶, ^{63b} S. Wang⁶, ¹⁴ T. Wang⁶, ^{63a} W. T. Wang⁶, ⁸¹ W. Wang⁶, ¹⁴ X. Wang⁶, ¹¹⁴ A. Wang⁶, ¹¹⁴ X. Wang⁶, ¹¹⁴ X.

X. Wang[®],¹⁶⁵ X. Wang[®],^{63c} Y. Wang[®],^{63d} Y. Wang[®],^{114a} Z. Wang[®],¹⁰⁸ Z. Wang[®],^{63d,52,63c} Z. Wang[®],¹⁰⁸ A. Warburton[®],¹⁰⁶ R. J. Ward[®],²¹ N. Warrack[®],⁶⁰ S. Waterhouse[®],⁹⁷ A. T. Watson[®],²¹ H. Watson[®],⁶⁰ M. F. Watson[®],²¹ E. Watton[©], ^{60,137} G. Watts[©], ¹⁴¹ B. M. Waugh[©], ⁹⁸ J. M. Webb[©], ⁵⁵ C. Weber[©], ³⁰ H. A. Weber[©], ¹⁹ M. S. Weber[©], ²⁰ S. M. Weber[©], ^{64a} C. Wei[©], ^{63a} Y. Wei[©], ⁵⁵ A. R. Weidberg[©], ¹²⁹ E. J. Weik[©], ¹²⁰ J. Weingarten[©], ⁵⁰ C. Weiser[©], ⁵⁵ (1) C. J. Wells⁽⁹⁾, ⁴⁹ T. Wenaus⁽⁹⁾, ³⁰ B. Wendland⁽⁶⁾, ⁵⁰ T. Wengler⁽⁶⁾, ³⁷ N. S. Wenke, ¹¹² N. Wermes⁽⁶⁾, ²⁵ M. Wessels⁽⁶⁾, ^{64a} A. M. Wharton^{9,3} A. S. White^{9,6} A. White^{9,8} M. J. White^{9,1} D. Whiteson^{9,162} L. Wickremasinghe^{9,127}
W. Wiedenmann^{9,173} M. Wielers^{9,137} C. Wiglesworth^{9,43} D. J. Wilbern,¹²³ H. G. Wilkens^{9,37} J. J. H. Wilkinson^{9,33}
D. M. Williams^{9,42} H. H. Williams,¹³¹ S. Williams^{9,33} S. Willocq^{9,105} B. J. Wilson^{9,103} P. J. Windischhofer^{9,40}
F. I. Winkel^{9,31} F. Winklmeier^{9,126} B. T. Winter^{9,55} J. K. Winter^{9,103} M. Wittgen,¹⁴⁶ M. Wobisch^{9,99} T. Wojtkowski,⁶¹ F. I. Winkele,³¹ F. Winklmeiere,¹²⁶ B. T. Wintere,⁵⁵ J. K. Wintere,¹⁰³ M. Wittgen,¹⁴⁶ M. Wobische,⁹⁹ T. Wojtkowski,⁶¹ Z. Wolffse,¹¹⁷ J. Wollrath,¹⁶² M. W. Woltere,⁸⁸ H. Wolterse,^{133a,133c} M. C. Wong,¹³⁹ E. L. Woodwarde,⁴² S. D. Worme,⁴⁹ B. K. Wosieke,⁸⁸ K. W. Woźniake,⁸⁸ S. Wozniewski,⁵⁶ K. Wraighte,⁶⁰ C. Wue,²¹ M. Wue,^{114b} M. Wue,¹¹⁶ S. L. Wue,¹⁷³ X. Wue,⁵⁷ Y. Wue,^{63a} Z. Wue,⁴ J. Wuerzingere,^{112,u} T. R. Wyatte,¹⁰³ B. M. Wynnee,⁵³ S. Xellae,⁴³ L. Xiae,^{114a} M. Xiae,¹⁵ J. Xiange,^{65c} M. Xiee,^{63a} S. Xine,^{14,114c} A. Xionge,¹²⁶ J. Xionge,^{18a} D. Xue,¹⁴ H. Xue,^{63a} L. Xue,^{63a} R. Xue,¹³¹ T. Xue,¹⁰⁸ Y. Xue,¹⁵ Z. Xue,⁵³ Z. Xu,^{114a} B. Yabsleye,¹⁵⁰ S. Yacoobe,^{34a} Y. Yamaguchie,¹⁵⁷ E. Yamashitae,¹⁵⁶ H. Yamauchie,¹⁶⁰ T. Yamazakie,^{18a} Y. Yamazakie,⁸⁶ J. Yan,^{63c} S. Yane,⁶⁰ Z. Yane,¹⁰⁵ H. J. Yange,^{63a} S. Yange,^{63a} T. Yange,^{65c} X. Yange,³⁷ X. Yange,¹⁴ Y. Yange,⁴⁵ Y. Yang,^{63a} Z. Yange,^{63a} T. Yange,^{65c} X. Yange,³⁷ X. Yange,¹⁴ Y. Yange,⁴⁵ Y. Yang,^{63a} Z. Yange,^{63a} T. Yange,^{65c} J. Yee,¹⁴ S. Yee,³⁰ X. Yee,^{63a} Y. Yehe,⁹⁸ I. Yeletskikhe,³⁹ B. K. Yeoe,^{18b} M. R. Yexleye,⁹⁸ T. P. Yildirime,¹²⁹ P. Yine,⁴² K. Yoritae,¹⁷¹ S. Younase,^{28b} C. J. S. Younge,³⁷ C. Younge,¹⁴⁶ C. Yue,^{14,114c} Y. Yue,^{63a} J. Yuane,^{14,114c} M. Yuane,¹⁰⁸ R. Yuane,^{63d,63c} L. Yuee,⁹⁸ M. Zaazouae,^{63a} B. Zabinskie,⁸⁸ E. Zaid,⁵³ Z. K. Zake,⁸⁸ T. Zakareishvilie,¹⁶⁶ N. Zakharchuke,³⁵ S. Zambitoe,⁵⁷ J. A. Zamora Saa^(b), ^{140d,140b} J. Zang^(b), ¹⁵⁶ D. Zanzi^(b), ⁵⁵ O. Zaplatilek^(b), ¹³⁵ C. Zeitnitz^(b), ¹⁷⁴ H. Zeng^(b), ¹⁴ J. C. Zeng^(b), ¹⁶⁵ D. T. Zenger Jr.^(b), ²⁷ O. Zenin^(b), ³⁸ T. Ženiš^(b), ^{29a} S. Zenz^(b), ⁹⁶ S. Zerradi^(b), ^{36a} D. Zerwas^(b), ⁶⁷ M. Zhai^(b), ^{14,114c} D. F. Zhang^(b), ¹⁴² D. I. Zenger Jr., O. Zenino, T. Zeniso, S. Zenzo, S. Zenzo, S. Zerradio, D. Zerwaso, M. Zhaio, D. F. Zhango,
J. Zhango, ^{63b} J. Zhango, ⁶ K. Zhango, ^{14,114c} L. Zhango, ^{63a} L. Zhango, ^{114a} P. Zhango, ^{14,114c} R. Zhango, ¹⁷³ S. Zhango, ¹⁰⁸
S. Zhango, ⁹¹ T. Zhango, ¹⁵⁶ X. Zhango, ^{63c} X. Zhango, ^{63b} Y. Zhango, ^{63c} Y. Zhango, ⁹⁸ Y. Zhango, ^{114a} Z. Zhango, ^{18a}
Z. Zhango, ^{63b} Z. Zhango, ⁶⁷ H. Zhaoo, ¹⁴¹ T. Zhaoo, ^{63b} Y. Zhaoo, ¹³⁹ Z. Zhaoo, ^{63a} Z. Zhaoo, ^{63a} A. Zhemchugovo, ³⁹
J. Zhengo, ^{114a} K. Zhengo, ¹⁶⁵ X. Zhengo, ^{63a} Z. Zhengo, ¹⁴⁶ D. Zhongo, ¹⁶⁵ B. Zhouo, ¹⁰⁸ H. Zhouo, ⁷ N. Zhouo, ^{63c}
Y. Zhou, ¹⁵ Y. Zhouo, ^{114a} Y. Zhou, ⁷ C. G. Zhuo, ^{63b} J. Zhuo, ¹⁰⁸ X. Zhuo, ^{63c} Y. Zhuo, ^{63c} Y. Zhuo, ^{63a} X. Zhuango, ¹⁴ K. Zhukov[®], ³⁸ N. I. Zimine[®], ³⁹ J. Zinsser[®], ^{64b} M. Ziolkowski[®], ¹⁴⁴ L. Živković[®], ¹⁶ A. Zoccoli[®], ^{24b,24a} K. Zoch[®], ⁶² T. G. Zorbas[®], ¹⁴² O. Zormpa[®], ⁴⁷ W. Zou[®], ⁴² and L. Zwalinski[®]³⁷

(ATLAS Collaboration)

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

²Department of Physics, University of Alberta, Edmonton, Alberta, Canada

^{3a}Department of Physics, Ankara University, Ankara, Türkiye

^{3b}Division of Physics, TOBB University of Economics and Technology, Ankara, Türkiye

⁴LAPP, Université Savoie Mont Blanc, CNRS/IN2P3, Annecy, France

⁶High Energy Physics Division, Argonne National Laboratory, Argonne, Illinois, USA

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

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

⁹Physics Department, National and Kapodistrian University of Athens, Athens, Greece

¹⁰Physics Department, National Technical University of Athens, Zografou, Greece

¹Department of Physics, University of Texas at Austin, Austin, Texas, USA

¹²Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan

¹³Institut de Física d'Altes Energies (IFAE), Barcelona Institute of Science and Technology, Barcelona, Spain

¹⁴Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China ¹⁵Physics Department, Tsinghua University, Beijing, China

¹⁶Institute of Physics, University of Belgrade, Belgrade, Serbia

¹⁷Department for Physics and Technology, University of Bergen, Bergen, Norway

^{18a}Physics Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA ^{18b}University of California, Berkeley, California, USA

⁵APC, Université Paris Cité, CNRS/IN2P3, Paris, France

¹⁹Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany

²⁰Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern,

Bern, Switzerland

²¹School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom

^{22a}Department of Physics, Bogazici University, Istanbul, Türkiye

^{22b}Department of Physics Engineering, Gaziantep University, Gaziantep, Türkiye

^{22c}Department of Physics, Istanbul University, Istanbul, Türkiye

^{23a}Facultad de Ciencias y Centro de Investigaciónes, Universidad Antonio Nariño, Bogotá, Colombia

^{23b}Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia

^{24a}Dipartimento di Fisica e Astronomia A. Righi, Università di Bologna, Bologna, Italy ^{24b}INFN Sezione di Bologna, Italy

²⁵Physikalisches Institut, Universität Bonn, Bonn, Germany

²⁶Department of Physics, Boston University, Boston, Massachusetts, USA

²⁷Department of Physics, Brandeis University, Waltham, Massachusetts, USA

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

^{28b}Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania

^{28c}Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi, Romania

^{28d}National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department,

Cluj-Napoca, Romania

^{28e}National University of Science and Technology Politechnica, Bucharest, Romania

^{28f}West University in Timisoara, Timisoara, Romania

^{28g}Faculty of Physics, University of Bucharest, Bucharest, Romania

^{29a}Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovak Republic

²⁹⁶Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic

³⁰Physics Department, Brookhaven National Laboratory, Upton, New York, USA

³¹Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física, y CONICET,

Instituto de Física de Buenos Aires (IFIBA), Buenos Aires, Argentina

³²California State University, California, USA

³³Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

^{34a}Department of Physics, University of Cape Town, Cape Town, South Africa ^{34b}iThemba Labs, Western Cape, South Africa

^{34c}Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa

^{34d}National Institute of Physics, University of the Philippines Diliman (Philippines), Philippines

³⁴^cUniversity of South Africa, Department of Physics, Pretoria, South Africa ^{34f}University of Zululand, KwaDlangezwa, South Africa

^{34g}School of Physics, University of the Witwatersrand, Johannesburg, South Africa

³⁵Department of Physics, Carleton University, Ottawa, Ontario, Canada

^{36a}Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies - Université Hassan II,

Casablanca, Morocco

^{36b}Faculté des Sciences, Université Ibn-Tofail, Kénitra, Morocco

^{36c}Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech, Morocco

^{36d}LPMR, Faculté des Sciences, Université Mohamed Premier, Oujda, Morocco

^{36e}Faculté des sciences, Université Mohammed V, Rabat, Morocco

^{36f}Institute of Applied Physics, Mohammed VI Polytechnic University, Ben Guerir, Morocco

³⁷CERN, Geneva, Switzerland

³⁸Affiliated with an institute covered by a cooperation agreement with CERN

³⁹Affiliated with an international laboratory covered by a cooperation agreement with CERN

⁴⁰Enrico Fermi Institute, University of Chicago, Chicago, Illinois, USA

⁴¹LPC, Université Clermont Auvergne, CNRS/IN2P3, Clermont-Ferrand, France

⁴²Nevis Laboratory, Columbia University, Irvington, New York, USA

⁴³Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

^{44a}Dipartimento di Fisica, Università della Calabria, Rende, Italy

44b INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Italy

⁴⁵Physics Department, Southern Methodist University, Dallas, Texas, USA

⁴⁶Physics Department, University of Texas at Dallas, Richardson, Texas, USA

⁴⁷National Centre for Scientific Research "Demokritos", Agia Paraskevi, Greece

^{48a}Department of Physics, Stockholm University, Sweden

48bOskar Klein Centre, Stockholm, Sweden

⁴⁹Deutsches Elektronen-Synchrotron DESY, Hamburg and Zeuthen, Germany

⁵⁰Fakultät Physik, Technische Universität Dortmund, Dortmund, Germany

⁵¹Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany

²Department of Physics, Duke University, Durham, North Carolina, USA

⁵³SUPA - School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom

⁵⁴INFN e Laboratori Nazionali di Frascati, Frascati, Italy

⁵⁵Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

⁵⁶II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

⁵⁷Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland

^{58a}Dipartimento di Fisica, Università di Genova, Genova, Italy

^{58b}INFN Sezione di Genova, Italy

⁵⁹II. Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany

⁶⁰SUPA - School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom

⁶¹LPSC, Université Grenoble Alpes, CNRS/IN2P3, Grenoble INP, Grenoble, France

⁶²Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, Massachusetts, USA

^aDepartment of Modern Physics and State Key Laboratory of Particle Detection and Electronics,

University of Science and Technology of China, Hefei, China

^{63b}Institute of Frontier and Interdisciplinary Science and Key Laboratory of Particle Physics and Particle Irradiation (MOE),

Shandong University, Qingdao, China

63c School of Physics and Astronomy, Shanghai Jiao Tong University, Key Laboratory for Particle Astrophysics and Cosmology (MOE),

SKLPPC, Shanghai, China

63dTsung-Dao Lee Institute, Shanghai, China

^{63e}School of Physics and Microelectronics, Zhengzhou University, China

^{64a}Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany

^{64b}Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany

^{65a}Department of Physics, Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China

^{65b}Department of Physics, University of Hong Kong, Hong Kong, China

⁶⁵C Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology,

Clear Water Bay, Kowloon, Hong Kong, China

⁶⁶Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

⁶⁷IJCLab, Université Paris-Saclay, CNRS/IN2P3, 91405, Orsay, France

⁶⁸Centro Nacional de Microelectrónica (IMB-CNM-CSIC), Barcelona, Spain

Department of Physics, Indiana University, Bloomington, Indiana, USA

^{70a}INFN Gruppo Collegato di Udine, Sezione di Trieste, Udine, Italy

^{70b}ICTP, Trieste, Italy

⁷⁰CDipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine, Italy ⁷¹aINFN Sezione di Lecce, Italy

^{71b}Dipartimento di Matematica e Fisica, Università del Salento, Lecce, Italy

^{72a}INFN Sezione di Milano, Italy

^{72b}Dipartimento di Fisica, Università di Milano, Milano, Italy

^{73a}INFN Sezione di Napoli, Italy

^{73b}Dipartimento di Fisica, Università di Napoli, Napoli, Italy

^{74a}INFN Sezione di Pavia, Italy

^{74b}Dipartimento di Fisica, Università di Pavia, Pavia, Italy

^{75a}INFN Sezione di Pisa, Italy

^{75b}Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy

^{76a}INFN Sezione di Roma, Italy

^{76b}Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy

^{7a}INFN Sezione di Roma Tor Vergata, Italy

^{77b}Dipartimento di Fisica, Università di Roma Tor Vergata, Roma, Italy

^{78a}INFN Sezione di Roma Tre, Italy

^{78b}Dipartimento di Matematica e Fisica, Università Roma Tre, Roma, Italy

^{79a}INFN-TIFPA, Italy

^{79b}Università degli Studi di Trento, Trento, Italy

⁸⁰Universität Innsbruck, Department of Astro and Particle Physics, Innsbruck, Austria

⁸¹University of Iowa, Iowa City, Iowa, USA

⁸²Department of Physics and Astronomy, Iowa State University, Ames, Iowa, USA

⁸³Istinye University, Sariyer, Istanbul, Türkiye

^{84a}Departamento de Engenharia Elétrica, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, Brazil

⁸⁴⁶Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro, Brazil

^{84c}Instituto de Física, Universidade de São Paulo, São Paulo, Brazil

^{34d}Rio de Janeiro State University, Rio de Janeiro, Brazil

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^{84e}Federal University of Bahia, Bahia, Brazil

⁸⁵KEK, High Energy Accelerator Research Organization, Tsukuba, Japan ⁸⁶Graduate School of Science, Kobe University, Kobe, Japan ^{87a}AGH University of Krakow, Faculty of Physics and Applied Computer Science, Krakow, Poland ^{87b}Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland ⁸⁸Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland

⁸⁹Faculty of Science, Kyoto University, Kyoto, Japan

⁹⁰Research Center for Advanced Particle Physics and Department of Physics, Kyushu University, Fukuoka, Japan ⁹¹L2IT, Université de Toulouse, CNRS/IN2P3, UPS, Toulouse, France

⁹²Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, La Plata, Argentina

³Physics Department, Lancaster University, Lancaster, United Kingdom

⁹⁴Oliver Lodge Laboratory, University of Liverpool, Liverpool, United Kingdom

⁹⁵Department of Experimental Particle Physics, Jožef Stefan Institute and Department of Physics, University of Ljubljana,

Ljubljana, Slovenia

⁹⁶School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom

⁷Department of Physics, Royal Holloway University of London, Egham, United Kingdom

⁹⁸Department of Physics and Astronomy, University College London, London, United Kingdom

⁹⁹Louisiana Tech University, Ruston, Los Angeles, USA

¹⁰⁰Fysiska institutionen, Lunds universitet, Lund, Sweden

¹⁰¹Departamento de Física Teorica C-15 and CIAFF, Universidad Autónoma de Madrid, Madrid, Spain

¹⁰²Institut für Physik, Universität Mainz, Mainz, Germany

¹⁰³School of Physics and Astronomy, University of Manchester, Manchester, United Kingdom ¹⁰⁴CPPM, Aix-Marseille Université, CNRS/IN2P3, Marseille, France

¹⁰⁵Department of Physics, University of Massachusetts, Amherst, Massachusetts, USA

¹⁰⁶Department of Physics, McGill University, Montreal, Quebec, Canada

School of Physics, University of Melbourne, Victoria, Australia

¹⁰⁸Department of Physics, University of Michigan, Ann Arbor, Michigan, USA

¹⁰⁹Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA

¹¹⁰Group of Particle Physics, University of Montreal, Montreal, Quebec, Canada

¹¹¹Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany

¹¹²Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany

¹¹³Graduate School of Science and Kobayashi-Maskawa Institute, Nagoya University, Nagoya, Japan ^{114a}Department of Physics, Nanjing University, Nanjing, China

^{114b}School of Science, Shenzhen Campus of Sun Yat-sen University, China

^{114c}University of Chinese Academy of Science (UCAS), Beijing, China

¹¹⁵Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico, USA

¹¹⁶Institute for Mathematics, Astrophysics and Particle Physics, Radboud University/Nikhef, Nijmegen, Netherlands

¹Nikhef National Institute for Subatomic Physics and University of Amsterdam, Amsterdam, Netherlands

¹¹⁸Department of Physics, Northern Illinois University, DeKalb, Illinois, USA

^aNew York University Abu Dhabi, Abu Dhabi, United Arab Emirates

^{119b}United Arab Emirates University, Al Ain, United Arab Emirates

¹²⁰Department of Physics, New York University, New York, New York, USA

¹²¹Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo, Japan

¹²²Ohio State University, Columbus, Ohio, USA

¹²³Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, Oklahoma, USA

¹²⁴Department of Physics, Oklahoma State University, Stillwater, Oklahoma, USA

¹²⁵Palacký University, Joint Laboratory of Optics, Olomouc, Czech Republic

¹²⁶Institute for Fundamental Science, University of Oregon, Eugene, Oregon, USA

Graduate School of Science, Osaka University, Osaka, Japan

¹²⁸Department of Physics, University of Oslo, Oslo, Norway

¹²⁹Department of Physics, Oxford University, Oxford, United Kingdom

¹³⁰LPNHE. Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France

¹³¹Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania, USA

¹³²Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania, USA

^{133a}Laboratório de Instrumentação e Física Experimental de Partículas - LIP, Lisboa, Portugal

^{133b}Departamento de Física, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

^{133c}Departamento de Física, Universidade de Coimbra, Coimbra, Portugal

^{133d}Centro de Física Nuclear da Universidade de Lisboa, Lisboa, Portugal

^{133e}Departamento de Física, Universidade do Minho, Braga, Portugal

^{133f}Departamento de Física Teórica y del Cosmos, Universidad de Granada, Granada (Spain), Spain

^{133g}Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal

⁴Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

¹³⁵Czech Technical University in Prague, Prague, Czech Republic

¹³⁶Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

¹³⁷Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom

¹³⁸IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France

¹³⁹Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, California, USA

^{140a}Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile

^{140b}Millennium Institute for Subatomic physics at high energy frontier (SAPHIR), Santiago, Chile

¹⁴⁰^cInstituto de Investigación Multidisciplinario en Ciencia y Tecnología, y Departamento de Física,

Universidad de La Serena, Chile

^{140d}Universidad Andres Bello, Department of Physics, Santiago, Chile

^{140e}Instituto de Alta Investigación, Universidad de Tarapacá, Arica, Chile

^{140f}Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

¹¹Department of Physics, University of Washington, Seattle, Washington, USA

¹⁴²Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

⁴³Department of Physics, Shinshu University, Nagano, Japan

¹⁴⁴Department Physik, Universität Siegen, Siegen, Germany

¹⁴⁵Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada

¹⁴⁶SLAC National Accelerator Laboratory, Stanford, California, USA

¹⁴⁷Department of Physics, Royal Institute of Technology, Stockholm, Sweden

¹⁴⁸Departments of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA

Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom

School of Physics, University of Sydney, Sydney, Australia

¹⁵¹Institute of Physics, Academia Sinica, Taipei, Taiwan

^{152a}E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi, Georgia

^{152b}High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia

^{152c}University of Georgia, Tbilisi, Georgia

¹⁵³Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel

¹⁵⁴Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel

¹⁵⁵Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

¹⁵⁶International Center for Elementary Particle Physics and Department of Physics, University of Tokyo, Tokyo, Japan

¹⁵⁷Department of Physics, Tokyo Institute of Technology, Tokyo, Japan

¹⁵⁸Department of Physics, University of Toronto, Toronto, Ontario, Canada ^{159a}TRIUMF, Vancouver, British Columbia, Canada

^{159b}Department of Physics and Astronomy, York University, Toronto, Ontario, Canada

¹⁶⁰Division of Physics and Tomonaga Center for the History of the Universe, Faculty of Pure and Applied Sciences,

University of Tsukuba, Tsukuba, Japan

¹⁶¹Department of Physics and Astronomy, Tufts University, Medford, Massachusetts, USA

¹⁶²Department of Physics and Astronomy, University of California Irvine, Irvine, California, USA

¹⁶³University of Sharjah, Sharjah, United Arab Emirates

¹⁶⁴Department of Physics and Astronomy, University of Uppsala, Uppsala, Sweden

¹⁶⁵Department of Physics, University of Illinois, Urbana, Illinois, USA

¹⁶⁶Instituto de Física Corpuscular (IFIC), Centro Mixto Universidad de Valencia - CSIC, Valencia, Spain

⁶⁷Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada

¹⁶⁸Department of Physics and Astronomy, University of Victoria, Victoria, British Columbia, Canada

¹⁶⁹Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

¹⁷⁰Department of Physics, University of Warwick, Coventry, United Kingdom

¹⁷¹Waseda University, Tokyo, Japan

¹⁷²Department of Particle Physics and Astrophysics, Weizmann Institute of Science, Rehovot, Israel

¹⁷³Department of Physics, University of Wisconsin, Madison, Wisconsin, USA

¹⁷⁴Fakultät für Mathematik und Naturwissenschaften, Fachgruppe Physik, Bergische Universität Wuppertal, Wuppertal, Germany

¹⁷⁵Department of Physics, Yale University, New Haven, Connecticut, USA

^aDeceased.

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

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

^dAlso at Lawrence Livermore National Laboratory, Livermore, USA.

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

^fAlso at Department of Physics, University of Thessaly, Greece.

- ^gAlso at An-Najah National University, Nablus, Palestine.
- ^hAlso at Department of Physics, University of Fribourg, Fribourg, Switzerland.
- ⁱAlso at Department of Physics, Westmont College, Santa Barbara, USA.
- ^jAlso at Departament de Fisica de la Universitat Autonoma de Barcelona, Barcelona, Spain.
- ^kAlso at Affiliated with an institute covered by a cooperation agreement with CERN.
- ¹Also at The Collaborative Innovation Center of Quantum Matter (CICQM), Beijing, China.
- ^mAlso at Università di Napoli Parthenope, Napoli, Italy.
- ⁿAlso at Institute of Particle Physics (IPP), Canada.
- ^oAlso at University of Colorado Boulder, Department of Physics, Colorado, USA.
- ^PAlso at Borough of Manhattan Community College, City University of New York, New York, New York, USA.
- ^qAlso at National Institute of Physics, University of the Philippines Diliman (Philippines), Philippines.
- ^rAlso at Department of Financial and Management Engineering, University of the Aegean, Chios, Greece.
- ^sAlso at Centro Studi e Ricerche Enrico Fermi, Italy.
- ^tAlso at Institucio Catalana de Recerca i Estudis Avancats, ICREA, Barcelona, Spain.
- ^uAlso at Technical University of Munich, Munich, Germany.
- ^vAlso at Yeditepe University, Physics Department, Istanbul, Türkiye.
- ^wAlso at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia.
- ^xAlso at CERN, Geneva, Switzerland.
- ^yAlso at Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, Greece.
- ^zAlso at Hellenic Open University, Patras, Greece.
- ^{aa}Also at Department of Physics, Stellenbosch University, South Africa.
- ^{bb}Also at Department of Physics, California State University, Sacramento, USA.
- ^{cc}Also at Département de Physique Nucléaire et Corpusculaire, Université de Genève, Genève, Switzerland.
- ^{dd}Also at Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany.
- ee Also at Department of Physics, Stanford University, Stanford, California, USA.
- ^{ff}Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria.
- ^{gg}Also at Washington College, Chestertown, Maryland, USA.
- ^{hh}Also at Institute of Applied Physics, Mohammed VI Polytechnic University, Ben Guerir, Morocco.
- ⁱⁱAlso at Institute of Physics and Technology, Mongolian Academy of Sciences, Ulaanbaatar, Mongolia.