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Letter

Angular analysis of the $B^0 \to K^*(892)^0\mu^+\mu^-$ decay in proton-proton collisions at $\sqrt{s} = 13\,\text{TeV}$

The CMS Collaboration ⋆

CERN, Geneva, Switzerland

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ABSTRACT

A full set of optimized observables is measured in an angular analysis of the decay $B^0 \to K^*(892)^0\mu^+\mu^-$ using a sample of proton-proton collisions at $\sqrt{s} = 13\,\text{TeV}$, collected with the CMS detector at the LHC, corresponding to an integrated luminosity of $140\,\text{fb}^{-1}$. The analysis is performed in six bins of the squared invariant mass of the dimuon system, q^2, over the range $1.1 < q^2 < 16\,\text{GeV}^2$. The results are among the most precise experimental measurements of the angular observables for this decay and are compared to a variety of predictions based on the standard model. Some of these predictions exhibit tension with the measurements.

1. Introduction

The $b \to s\ell^+\ell^-$ flavor-changing neutral-current processes are strongly suppressed according to the standard model (SM) of particle physics, since they only proceed through electroweak loop-level diagrams. Since virtual contributions of physics beyond the SM could occur with comparable amplitudes and alter the decay properties, these transitions are an excellent environment for indirect new physics searches. Among these processes, the $B^0 \to K^{*0}(K^+\pi^-)\mu^+\mu^-$ decay, where K^{*0} indicates the $K^*(892)^0$ meson, has long been considered a promising channel, thanks to its rich kinematical structure defined by the angular momenta of the final state particles. Compared to other well known decay modes, as for example $B^0_s \to \mu^+\mu^-$, where only the branching ratio and mean life are measured [1–4], it provides access to a larger set of observables with high sensitivity to deviations from SM expectations. An extensive program of measuring angular observables from this decay has been carried out by the BaBar [5], Belle [6,7], and CDF [8] Collaborations. The data collected during Run 1 of the CERN LHC (2011–2012) were used by the LHCb [9–11], CMS [12–14], and ATLAS [15] Collaborations to investigate this decay mode. Since the outcomes of those measurements were statistically limited, the additional data collected during Run 2 (2015–2018) can be used to significantly reduce the experimental uncertainties. The most recent model-independent result from the LHCb Collaboration [16], as well as two alternative analyses [17,18], confirm their previous measurement and appear to exhibit tension with some of the predictions based on the SM. These predictions, while all based on the SM, yield different values with varying uncertainties. The largest differences in the calculations arise from the estimation of the non-local hadronic matrix elements and the evaluation of the corresponding uncertainty [19–21].

This Letter contains the first CMS measurement of a complete set of optimized observables averaged over charge-conjugation and parity (*CP*) of the $B^0 \to K^{*0}\mu^+\mu^-$ decay. The results are obtained from the Run 2 data set collected in 2016–2018 at a center-of-mass energy of 13 TeV, corresponding to an integrated luminosity of $140\,\text{fb}^{-1}$. The analysis is performed in bins of the invariant mass squared of the dimuon system, q^2, ranging from 1.1 to $16\,\text{GeV}^2$. The previous CMS analyses of this decay mode utilized smaller data sets from $\sqrt{s} = 7$–$8\,\text{TeV}$ collisions and measured only a partial set of the angular observables. Tabulated results are provided in the HEPData record for this analysis [22]. Throughout this Letter, charge-conjugate states are implied unless explicitly stated otherwise.

2. Decay rate and angular analysis observables

The decay $B^0 \to K^{*0}\mu^+\mu^-$, where the K^{*0} meson decays to $K^+\pi^-$, can be described by q^2 and three decay angles: θ_l, θ_K, and ϕ. The definition of the angles is consistent with the one used in experimental publications and detailed in Ref. [9]. A sketch representing the definition of the angles is shown in Fig. 1. The angle θ_l is defined as the angle between the positive (negative) muon momentum and the direction opposite to the B^0 $(\overline{B}^0)$ momentum in the dimuon rest frame; the angle

⋆ *E-mail address:* cms-publication-committee-chair@cern.ch.

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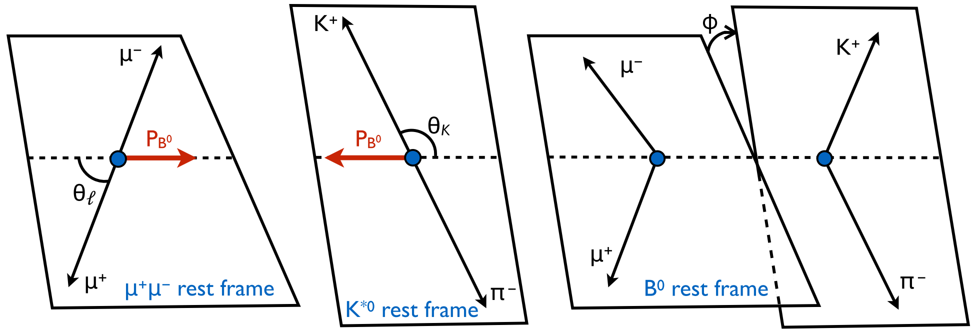

Fig. 1. Sketch representing the definition of the angles θ_l (left), θ_K (center), and ϕ (right).

θ_K is defined as the angle between the kaon momentum and the direction opposite to the B^0 $(\overline{B}^0)$ momentum in the K^{*0} $(\overline{K}^{*0})$ rest frame; the angle ϕ is the angle between the plane containing the μ^+ and μ^- and the plane containing the kaon and the pion from the K^{*0} decay in the B^0 rest frame.

Following the notation of Ref. [23] and the approach further proposed in Refs. [24,25], the *CP*-averaged angular decay rate of the $B^0 \to K^{*0}\mu^+\mu^-$ decay can be written as:

$$
\begin{aligned}
\Gamma_P \equiv \frac{1}{\mathrm{d}\Gamma/\mathrm{d}q^2}\frac{\mathrm{d}^4\Gamma}{\mathrm{d}q^2\mathrm{d}\cos\theta_l\mathrm{d}\cos\theta_K\mathrm{d}\phi} = \\
\frac{9}{32\pi}\Bigg[\frac{3}{4}(1-F_L)\sin^2\theta_K + F_L\cos^2\theta_K \\
+\left(\frac{1}{4}(1-F_L)\sin^2\theta_K - F_L\cos^2\theta_K\right)\cos 2\theta_l \\
+\frac{1}{2}P_1(1-F_L)\sin^2\theta_K\sin^2\theta_l\cos 2\phi \\
+\sqrt{(1-F_L)F_L}\Bigg(\frac{1}{2}P_4'\sin 2\theta_K\sin 2\theta_l\cos\phi \\
+P_5'\sin 2\theta_K\sin\theta_l\cos\phi\Bigg) \\
-\sqrt{(1-F_L)F_L}\Bigg(P_6'\sin 2\theta_K\sin\theta_l\sin\phi \\
+\frac{1}{2}P_8'\sin 2\theta_K\sin 2\theta_l\sin\phi\Bigg) \\
+2P_2(1-F_L)\sin^2\theta_K\cos\theta_l \\
-P_3(1-F_L)\sin^2\theta_K\sin^2\theta_l\sin 2\phi\Bigg],
\end{aligned}
\tag{1}
$$

where F_L is the fraction of longitudinal polarization of the K^{*0} meson, and $P_{1,2,3}$ and $P'_{4,5,6,8}$ are observables that have been optimized to reduce their dependence on the values and uncertainties of the form factors [24]. These observables are functions of the decay amplitudes, which themselves depend on the Wilson coefficients contained in the relevant effective Hamiltonian [23]. In the publications of the LHCb Collaboration [11,16] the definition of some of the $P_i^{(\prime)}$ observables is different, namely $P_4'^{\mathrm{CMS}} = 2P_4'^{\mathrm{LHCb}}$, $P_6'^{\mathrm{CMS}} = -P_6'^{\mathrm{LHCb}}$, and $P_8'^{\mathrm{CMS}} = -2P_8'^{\mathrm{LHCb}}$.

In order to also describe $B^0 \to K^+\pi^-\mu^+\mu^-$ events in which the $K^+\pi^-$ system can be in an *S*-wave instead of *P*-wave configuration, the following extension of the angular decay rate (as in Eq. (7.8) of Ref. [25]) is used:

$$
\begin{aligned}
\frac{1}{\mathrm{d}\Gamma/\mathrm{d}q^2}\frac{\mathrm{d}^4\Gamma}{\mathrm{d}q^2\mathrm{d}\cos\theta_l\mathrm{d}\cos\theta_K\mathrm{d}\phi} = (1-F_S)\Gamma_P \\
+\frac{3}{16\pi}(F_S\sin^2\theta_l + A_S\sin^2\theta_l\cos\theta_K \\
+A_S^4\sin\theta_K\sin 2\theta_l\cos\phi + A_S^5\sin\theta_K\sin\theta_l\cos\phi \\
+A_S^7\sin\theta_K\sin\theta_l\sin\phi + A_S^8\sin\theta_K\sin 2\theta_l\sin\phi),
\end{aligned}
\tag{2}
$$

where the term proportional to F_S is the *S*-wave component, and the terms proportional to the A_S and $A_S^{4,5,7,8}$ coefficients describe the interference between the *S*- and *P*-wave terms.

3. The CMS detector and event samples

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter, and a brass and scintillator hadron calorimeter, each composed of a barrel and two endcap sections. Forward calorimeters extend the pseudorapidity (η) coverage provided by the barrel and endcap detectors. Muons are measured in the range $|\eta| < 2.4$, with detection planes made using three technologies: drift tubes, cathode strip chambers, and resistive-plate chambers. The single-muon trigger efficiency exceeds 90% over the full η range, and the efficiency to reconstruct and identify muons is greater than 96%. Matching muons to tracks measured in the silicon tracker results in a relative transverse momentum (p_T) resolution, for muons with p_T up to 100 GeV, of 1% in the barrel and 3% in the endcaps [26]. The silicon tracker used in 2016 measured charged particles within the range $|\eta| < 2.5$. For nonisolated particles of $1 < p_T < 10$ GeV and $|\eta| < 1.4$, the track resolutions were typically 1.5% in p_T and 25–90 (45–150) μm in the transverse (longitudinal) impact parameter [27]. At the start of 2017, a new pixel detector was installed [28]; the upgraded tracker measured particles up to $|\eta| = 3.0$ with typical resolutions of 1.5% in p_T and 20–75 μm in the transverse impact parameter [29] for nonisolated particles of $1 < p_T < 10$ GeV. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Ref. [30].

Events of interest are selected using a two-tiered trigger system. The first level, composed of custom hardware processors, uses information from the calorimeters and muon detectors to select events at a rate of around 100 kHz within a fixed latency of about 4 μs [31]. The second level, known as the high-level trigger, consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing, and reduces the event rate to around 1 kHz before data storage [32]. All events used in this analysis are selected by a set of triggers demanding two identified muons of opposite charges and an additional track to form a common vertex, displaced from the region of the proton-proton interactions (beamspot). The trigger required each muon to have $p_T > 4$ GeV, $|\eta| < 2.5$, and to pass within 2 cm of the beam axis. The dimuon system was required to have $p_T > 6.9$ GeV, a vertex fit χ^2 probability larger than 10%, a separation of the vertex relative to the beamspot in the transverse plane larger than 3 times the uncertainty of the separation, and the cosine of the angle in the transverse plane between the dimuon momentum vector and the vector from the beamspot to the dimuon vertex greater than 0.9. The additional track was required to have $p_T > 0.8\,(1.2)\,\mathrm{GeV}$ and a minimum distance of closest approach from the beamspot greater than 0 (2) times the uncertainty for data collected in 2016 (2017–2018). As the trigger configuration was restricted in the q^2 range, the analysis is limited to events with $q^2 < 16\,\mathrm{GeV}^2$.

Monte Carlo (MC) simulations are used to determine the impact of the detector geometry, trigger, reconstruction, and selection on the angular distribution of the signal, and to validate the analysis procedure. Simulated events are generated with PYTHIA 8.230 [33], decays of particles containing b or c quarks are simulated with EVTGEN 1.6.0 [34], and final-state radiation is included via PHOTOS 3.61 [35,36]. Events are passed through the CMS detector simulation based on GEANT4 [37] and simulated minimum bias events are added to mimic the number of multiple vertices per event as seen in the data.

4. Event reconstruction, selection, and efficiency modeling

The offline reconstruction requires two oppositely charged muons and two oppositely charged tracks. Muons must satisfy general identification (soft muon) criteria [26] and match the muons used in the trigger. The p_T and η requirements applied by the trigger must be satisfied by the offline muons as well. The two tracks are required to pass the standard high-quality [27] identification criteria, have $|\eta| < 2.4$ and $p_T > 0.8\,\mathrm{GeV}$ to ensure well-measured tracks and match the trigger requirements, and have a distance of closest approach to the beamspot greater than 0.8 times the uncertainty to preferentially select tracks originating from a displaced vertex. One of the two tracks must match the track used in the trigger. In the 2017 and 2018 data sets, the trigger-matched track is required to have $p_T > 1.2\,\mathrm{GeV}$ and the distance of the closest approach to the beamspot greater than twice the uncertainty. A veto is applied to reject tracks that are also reconstructed and identified as muons. The two tracks are fitted to a common vertex to form the K^{*0} candidate. The K^{*0} meson invariant mass is computed for both the $\mathrm{K}^+\pi^-$ and $\mathrm{K}^-\pi^+$ mass hypotheses, and at least one of the two combinations is required to lie within 150 MeV of the nominal K^{*0} meson mass [38]. A $\phi(1020)$ veto is applied, demanding that the invariant mass of the two-track system, when assigning the kaon mass to both, is larger than 1.035 GeV.

The B^0 candidates are formed by combining the two oppositely charged muons with a K^{*0} candidate. The four daughter tracks of the B^0 candidate must originate from a common vertex, with vertex fit χ^2 probability greater than 1%. The momenta of the four tracks are then refitted using the common vertex as a constraint to improve the resolution of the track parameters. The flavor of the B^0 and K^{*0} candidates, and hence the mass assigned to the two hadronic tracks, is determined by the mass assignment that gives a K^{*0} meson mass closest to its nominal value. Based on simulation studies, this criterion results in incorrect flavor assignment for 12–14% of the candidates, depending on the data-taking year and with an increasing trend as a function of q^2.

A multivariate analysis is used to optimize the background rejection. A boosted decision tree is trained on background data events from the mass sidebands and simulated signal events, separately for each year of data-taking. The input variables of the discriminator are: the χ^2 probability of the B^0 candidate decay vertex; the transverse distance between the B^0 candidate decay vertex and the beamspot divided by its uncertainty; the cosine of the angle between the B^0 candidate momentum and the distance vector from the beamspot to the B^0 candidate decay vertex, in the transverse plane; the transverse B^0 candidate impact parameter with respect to the beamspot divided by its uncertainty; the transverse impact parameter of each hadronic track with respect to the beamspot divided by its uncertainty; the K^{*0} candidate invariant mass; and the sum of the final-state particles relative isolation, defined as the sum of the p_T of all the high-quality [27] tracks having $p_T > 0.8\,\mathrm{GeV}$ within a cone of $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2} < 0.4$ centered on the particle, divided by the p_T of the particle. Candidates with a decision tree score above a threshold are retained for analysis, with the threshold set to optimize the expected signal significance.

To reduce the contamination from $\mathrm{B}^+ \to \mathrm{K}^+\mu^+\mu^-$, including the dimuon decays of J/ψ and $\psi(2\mathrm{S})$ mesons, a veto is imposed on the invariant mass of the two possible $\mathrm{K}^+\mu^+\mu^-$ triplets, where K^+ is, in turn, one of the two hadronic tracks from the $\mathrm{K}^+\pi^-\mu^+\mu^-$ candidate, with the charged kaon mass assigned. The event is discarded if the mass of either $\mathrm{K}^+\mu^+\mu^-$ combination is within a region corresponding to three times the $\mathrm{K}^+\mu^+\mu^-$ mass resolution around the B^+ meson mass. This selection suppresses the contamination from these decays to a negligible level.

The J/ψ and $\psi(2\mathrm{S})$ meson control samples are defined by the ranges of the dedicated q^2 bins, 8.68–10.09 GeV^2 and 12.86–14.18 GeV^2, and the requirement $|q - m_{\mathrm{J}/\psi}| < 3\sigma_q$ and $|q - m_{\psi(2\mathrm{S})}| < 3\sigma_q$, respectively. Here σ_q is the per-event uncertainty in the dimuon invariant mass q, and m represents the nominal mass of the charmonium state. Events satisfying these requirements are excluded from the signal q^2 bins. However, a fraction of events from the resonant channels still appears in the adjoining q^2 bins, mainly due to an unreconstructed photon from the charmonium decay. This contamination is reduced by applying combined requirements on q and the B^0 candidate invariant mass, which are tuned independently for the dimuon mass regions below the J/ψ meson mass, between the J/ψ and the $\psi(2\mathrm{S})$ meson masses, and above the $\psi(2\mathrm{S})$ meson mass. These requirements are set so that less than 10% of the background events originate from the resonant channels, by using simulated events to measure the remaining resonant contamination. For $q < m_{\mathrm{J}/\psi}$ ($q > m_{\mathrm{J}/\psi}$), candidates must satisfy the condition $|(m - m_{\mathrm{B}^0}) - (q - m_{\mathrm{J}/\psi})| > 190\,(90)\,\mathrm{MeV}$, where m is the invariant mass of the B^0 candidate. For $q < m_{\psi(2\mathrm{S})}$ ($q > m_{\psi(2\mathrm{S})}$), candidates must satisfy the condition $|(m - m_{\mathrm{B}^0}) - (q - m_{\psi(2\mathrm{S})})| > 70\,(80)\,\mathrm{MeV}$. These requirements are tightened to 200, 100, 80, and 110 MeV in the 2016 data sample, as a consequence of the different detector configuration, trigger conditions, and offline selection criteria. In addition, B^0 candidates formed by the final-state particles from the $\mathrm{B}^0 \to \mathrm{J}/\psi\mathrm{K}^{*0}$ decay, where the identification of a muon and a hadron track is inverted, are rejected with dedicated requirements obtained from simulation. Two alternative B^0 candidates, denoted as "alt", are formed by reversing the identification of the same-sign muon and hadron track pairs, and the one giving a K^{*0} mass closest to its nominal value is selected ($\mathrm{B}^0_{\mathrm{alt}}$). Requirements on $m(\mathrm{K}^{*0}_{\mathrm{alt}})$, q_{alt}, $m(\mathrm{B}^0_{\mathrm{alt}})$, $\Delta R(\mu, \mathrm{track})$, and $\Delta p_T(\mu, \mathrm{track})$ are placed so that 90% of the reversed candidates are rejected, with less than 1% impact on the signal efficiency. Peaking backgrounds from $\mathrm{B}^0_\mathrm{s} \to \mu^+\mu^-\phi(1020)$, $\mathrm{B}^0_\mathrm{s} \to \mu^+\mu^-\mathrm{K}^{*0}$ and $\mathrm{B}^0_\mathrm{s} \to \mu^+\mu^-\mathrm{K}^+\mathrm{K}^-$ decays are studied in simulation, using their equivalent decays with intermediate J/ψ and $\psi(2\mathrm{S})$ resonances. After the full reconstruction and selection chain, their contribution is negligible compared to the J/ψ resonant channel decay.

The contamination from $\Lambda^0_\mathrm{b} \to \mathrm{pK}^-\mu^+\mu^-$ decays is investigated directly with data by assigning the proton and kaon masses to the hadronic tracks of the $\mathrm{K}^+\pi^-\mu^+\mu^-$ candidates, and searching for a peak at the nominal Λ^0_b mass in the candidate invariant mass distribution. No evidence of such contamination is found.

Finally, partially reconstructed decays $\mathrm{B}^+ \to \mathrm{K}^+\psi(2S)(\to \mathrm{J}/\psi\pi^+\pi^-)$ contribute to the low-mass sideband of the J/ψ control sample and present a narrow peak in the $\cos\theta_\mathrm{K}$ distribution in the region $0.6 < \cos\theta_\mathrm{K} < 0.8$. To reject this background, a selection is applied on $m(\mu\mu\mathrm{K})$, $m(\mu\mu\pi)$, $m(\mu\mu\mathrm{K}_\pi\pi_\mathrm{K})$, and $m(\mathrm{K}_\pi\pi_\mathrm{K})$ invariant masses in the events with $p_T(\mathrm{K}) > p_T(\pi)$, where K_π and π_K are given the kaon and pion flavor assignment, respectively, based on which combination is closest to the K^{*0} mass, but are assigned the charged pion and kaon mass, respectively, in the invariant mass calculations.

The acceptance, as well as the efficiency to trigger, reconstruct, and select the signal and control channel events, are modeled with a function of the three angular variables, using simulated event samples, individually for each year of data-taking and q^2 bin. These functions are obtained by applying the nonparametric kernel density estimator method [39,40] to the unbinned distributions of simulated events before and after imposing the acceptance and selection criteria previously described, and computing their ratio. Studies of this method using simulated events find that it reproduces important features of the efficiency and remains robust in regions of the phase space that are poorly populated by simulated events. Efficiencies are determined for both correctly identified (the kaon and pion have the correct charge) and misidentified (the kaon and pion charges are reversed) candidates, with both contributing as signal in the fit described below. Corrections derived from the data are applied to the simulated events to improve the modeling of the additional proton-proton interactions within the same or nearby bunch crossings and of those variables correlated with the decay angles. The latter are evaluated by training a classifier on the difference between simulation and data from the $B^0 \to J/\psi K^{*0}$ control sample. The background-subtracted data distributions have been obtained via the $_s\mathcal{P}$lot technique [41], where the reconstructed B^0 candidate invariant mass is used as the discriminating variable. The inputs to the classifier are the transverse momenta of the final-state particles, the B^0 candidate η, and the topological variables that are correlated to the angular ones. The output score of the classifier is used to reweight the simulation. The effectiveness of the method has been validated assessing the compatibility of the distributions of the input features in data and in the corrected simulation, on an independent sample of $B^0 \to J/\psi K^{*0}$ events, as well as on a sample of $B^0 \to \psi(2S)K^{*0}$ events.

5. Fit procedure

The angular observables are measured in each q^2 bin by performing an unbinned maximum-likelihood fit to the four-dimensional distribution of the invariant mass of the B^0 candidate, m, and the three angular variables: $\cos\theta_K$, $\cos\theta_l$, and ϕ. The bin definition is the same as in Ref. [14], except that the first bin starts from $1.1\,\text{GeV}^2$ rather than $1.0\,\text{GeV}^2$ to exclude the contamination from the $\phi(1020)$ resonance. The exact bin definition is reported in Table 2. All B^0 candidates with the invariant mass in the range $5 < m < 5.6\,\text{GeV}$ are included and a simultaneous fit is performed to data sets collected in 2016, 2017, and 2018.

The probability density function (PDF) used to fit each of these three data sets is:

$$\begin{aligned}
&P(m, \cos\theta_K, \cos\theta_l, \phi) = \\
&\quad Y_S \Big[S^C(m)\, S^a(\cos\theta_K, \cos\theta_l, \phi)\, \epsilon^C(\cos\theta_K, \cos\theta_l, \phi) \\
&\quad + R S^M(m) \\
&\quad \times S^a(-\cos\theta_K, -\cos\theta_l, -\phi) \epsilon^M(\cos\theta_K, \cos\theta_l, \phi) \Big] \\
&\quad + Y_B\, B^m(m) B^a(\cos\theta_K, \cos\theta_l, \phi),
\end{aligned} \tag{3}$$

where the first and second terms represent the contributions of the signal events for which the flavor has been correctly and wrongly identified, respectively, while the third term describes the background contribution. The Y_S and Y_B parameters represent the yield of signal and background events, respectively. The functions S^C and S^M describe the mass distribution of correctly identified and misidentified signal candidates, respectively, and they are parametrized, depending on the q^2 bin, by a Crystal Ball function [42] plus a Gaussian or a double Crystal Ball function [43] (with a single or double Gaussian kernel and two power-law tails in opposite directions). The function S^a is the angular decay rate as written in Eq. (2). The functions ϵ^C and ϵ^M represent the efficiency for correctly and misidentified events, respectively, as a function of the angular variables. The parameter R represents the ratio of the relative amount of misidentified events in data and the same value as computed on MC samples; the information of the latter value is contained in the relative value of ϵ^M with respect to ϵ^C, while R is introduced to account for differences between data and simulation. The function B^m represents the mass distribution of the combinatorial background events and consists of an exponential function; in the ranges $6 < q^2 < 8.68\,\text{GeV}^2$ and $10.09 < q^2 < 12.86\,\text{GeV}^2$, the exponential is multiplied by a function describing the reduction of background events from the requirements used to reduce the J/ψ and $\psi(2S)$ meson contamination. The function B^a represents the angular distribution of the background, which is modeled by a three-dimensional Bernstein polynomial determined from the data sidebands. The sidebands are regions of the $K^+\pi^-\mu^+\mu^-$ mass spectrum that do not contain the signal peak. Their range is defined to minimize the contamination from signal events, while providing a sufficiently large sample to ensure a good fit of the angular distribution. This approach results in signal contamination below 6% for the events within the sideband regions. The Bernstein polynomial degree is chosen as the lowest value that produces a p-value larger than 5%: the degree varies between 2 and 6 for $\cos\theta_K$, between 1 and 5 for $\cos\theta_l$, and between 2 and 5 for ϕ, depending on the data-taking year and q^2 bin. The functions ϵ^C, ϵ^M, and B^a are constrained to have the same value at $\phi = \pm\pi$.

In the simultaneous fit, the parameters of the PDF corresponding to the angular observables are shared among the three data sets, while other parameters are independent to account for the effects of different data-taking conditions on the efficiency and resolution. The coefficients of the S-wave and its interference with the P-wave are treated as nuisance parameters and are shared among the three data sets. All parameters are free, except those of the background angular shape, which are fixed to the values obtained from the data sidebands as described above. The parameters of the signal mass shapes are constrained to the results of the fit to the $K^+\pi^-\mu^+\mu^-$ mass distribution of simulated signal events through Gaussian likelihood factors. An additional Gaussian constraint is applied to the parameter R, with a mean equal to one and a width corresponding to the expected statistical fluctuation of R in the data, which varies from 5 to 20% depending on the data-taking year and the q^2 bin. The fit strategy comprises a procedure relying on the penalization of the likelihood function to ensure that the resulting angular observables lie in the physical region of the parameter space, i.e. provide a non-negative decay rate.

The best fit value of the parameters and approximate 68% CL confidence intervals are extracted using scans of the profile likelihood ratio, following the procedure described in Section 3.2 of Ref. [44]. The validity of this method and its robustness to the presence of nonphysical regions of the parameter space have been proven by an extensive study of its statistical coverage. The fit procedure and results are validated through fits to pseudo-experiments, MC simulation samples, and control samples.

6. Systematic uncertainties

Several sources of systematic uncertainties are evaluated to account for possible biases introduced by the analysis procedure, differences between the signal features in data and simulation, and any unaccounted minor background sources.

The possible bias introduced by mismodeling the efficiency shape is evaluated using simulated events as the difference between the results from fitting the generated angular variable distribution of generated events and fitting the reconstructed angular variable distributions of reconstructed events incorporating the efficiency. Additionally, a systematic uncertainty is estimated to account for possible biases in the fit results when the fit procedure is performed in realistic conditions (presence of background, limited number of available events). A set of 100 independent samples is created with the signal obtained from MC simulation and the background generated from the corresponding PDF, with signal and background yields matched to the respective values estimated from the data. Each of the samples is fit with the standard procedure and the average value over all 100 samples is calculated for each parameter. The systematic uncertainty is obtained by subtracting the average value from the value measured in the fit to the full signal-only MC simulation sample.

To evaluate the uncertainty due to the misidentification fraction being measured using simulated samples, the Gaussian constraint on the

Table 1
The uncertainties considered in the analysis on the various angular observables. For each source of uncertainty, the range covers the absolute variation observed across the q^2 bins.

Source	F_L ($\times 10^{-3}$)	P_1 ($\times 10^{-3}$)	P_2 ($\times 10^{-3}$)	P_3 ($\times 10^{-3}$)
Efficiency modeling	1–9	7–44	3–11	0–46
Fit bias	1–2	0–6	2–62	1–12
Misidentification fraction	0–2	1–4	1–3	0–14
Signal mass resolution	1–10	1–12	2–11	1–21
Signal mass shape	0–9	1–22	0–10	3–70
Background mass shape	0–5	1–16	1–13	0–8
Efficiency (statistical)	1–10	5–31	1–64	4–45
Background (statistical)	2–6	4–20	1–21	2–16
Data/simulation differences	8	0–23	0–16	0–13
Partially reco background	1	1	0	1
Resonant background	0–1	0–6	0–5	0–2
Source	P'_4 ($\times 10^{-3}$)	P'_5 ($\times 10^{-3}$)	P'_6 ($\times 10^{-3}$)	P'_8 ($\times 10^{-3}$)
Efficiency modeling	3–87	2–13	5–16	6–28
Fit bias	9–54	0–8	0–3	0–24
Misidentification fraction	1–5	1–10	0–4	0–12
Signal mass resolution	4–23	0–12	0–5	0–16
Signal mass shape	2–16	1–15	0–7	0–91
Background mass shape	6–30	1–13	0–7	1–10
Efficiency (statistical)	5–47	4–22	4–13	10–59
Background (statistical)	6–37	4–24	3–9	5–23
Data/simulation differences	0–11	0–13	0–3	0–30
Partially reco background	25	0	0	2
Resonant background	0–30	0–11	0–5	0–12

parameter R is removed in the fit to the $B^0 \to J/\psi K^{*0}$ control sample, yielding an unconstrained measurement of R. Then, a set of alternative fits is performed, using the measured R values (1.07, 1.02, and 1.02 for 2016, 2017, and 2018, respectively) as the means for the Gaussian constraints in the signal fits.

The systematic uncertainty associated with possible differences in the mass resolution between data and simulation is evaluated by first measuring a resolution scale factor with the $B^0 \to J/\psi K^{*0}$ control sample and then applying the same scale factor in the fit to the signal bins. The difference with respect to the nominal result is taken as a systematic uncertainty.

Systematic uncertainties are assessed for the signal and background mass shapes. To evaluate the uncertainty related to the choice of the signal mass model, a fit is performed to the data using the correctly identified and misidentified mass spectra from MC simulation as templates for the S^C and S^M components of the PDF. To evaluate the uncertainty related to the choice of the background mass model, a fit is performed to the data using Bernstein polynomials. For the highest q^2 bin only, the exponential function corrected for the threshold effect at the low edge of the mass range was also used as an alternative function.

The efficiency is evaluated on a finite sample of simulated events. A set of efficiency functions reflecting the statistical variation of the simulated event sample is generated, and used to fit the data. The standard deviation of the results obtained on each angular parameter is included as a systematic uncertainty. As the angular parameters of the background function are fixed in the fit, the statistical uncertainty related to the background parameters is evaluated separately. This is done by varying the parameters using the covariance matrix of the fit to the sidebands to generate 100 different background functions. The uncertainty is obtained by taking the standard deviation of the results obtained by fitting the data with each of the alternative background functions.

The effect of data-to-simulation differences on the angular efficiency and resolution is assessed by performing a fit on the J/ψ control sample and calculating the difference ($\Delta F_L^{J/\psi}$) between the F_L value obtained from this fit and its current world average [38]. This difference is then used to fit the signal sample, with the F_L parameter fixed to $F_L^{\text{nom}} + \Delta F_L^{J/\psi}$, where F_L^{nom} is the value of F_L obtained from the nominal fit to the signal sample. The value of $\Delta F_L^{J/\psi}$ and the deviation of the other fit parameters from their nominal values are assigned as systematic uncertainties.

The bias introduced by the contamination from partially reconstructed background sources in the lower-mass sideband on the background angular shape is evaluated in the J/ψ control sample, excluding from the mass sidebands events with the B^0 candidate mass lower than 5.1 GeV to define the background angular shape. The difference between the new results and the nominal ones is considered as a systematic uncertainty. Finally, the uncertainty due to the possible contamination of events from the two resonant channels in the adjoining q^2 bins is evaluated by adding a component with a simulation-based shape to the PDF to describe the contribution of the resonant channels, and using the difference of the results as the systematic uncertainty.

The systematic uncertainties are determined for each q^2 bin, and in cases where the systematic uncertainty is obtained as the difference between a nominal and alternative configuration, the systematic uncertainty is symmetrized. Their impact on the various angular parameters is summarized in Table 1. The individual systematic uncertainties are considered independent and added in quadrature.

7. Results

The projections of the fitted PDF on the mass and angular distributions are shown in Fig. 2 for all q^2 bins. The fit quality has been verified in all q^2 bins by assessing the agreement between the PDF projections and the data.

Table 2 and Fig. 3 provide the measured values of the *CP*-averaged observables in bins of q^2 along with the corresponding uncertainties. The size of the uncertainties varies between different $P_i^{(\prime)}$ observables, based on their dependence on F_L and, more generally, on the formula defining the observable. Fig. 3 also contains four predictions based on the SM. The q^2 range of validity of the predictions varies depending on the methods used to estimate the form factors. The ABCDMN predictions are obtained using the theoretical framework discussed in Ref. [20], which combines local form factors derived from lattice quantum chromodynamics [45,46] and light-cone sum rules [47], and non-local form factors from Ref. [48]. The EOS predictions are obtained using the procedure described in Ref. [49] and the EOS [50] software package, using the same sources as ABCDMN for the form-factor calculations, but with

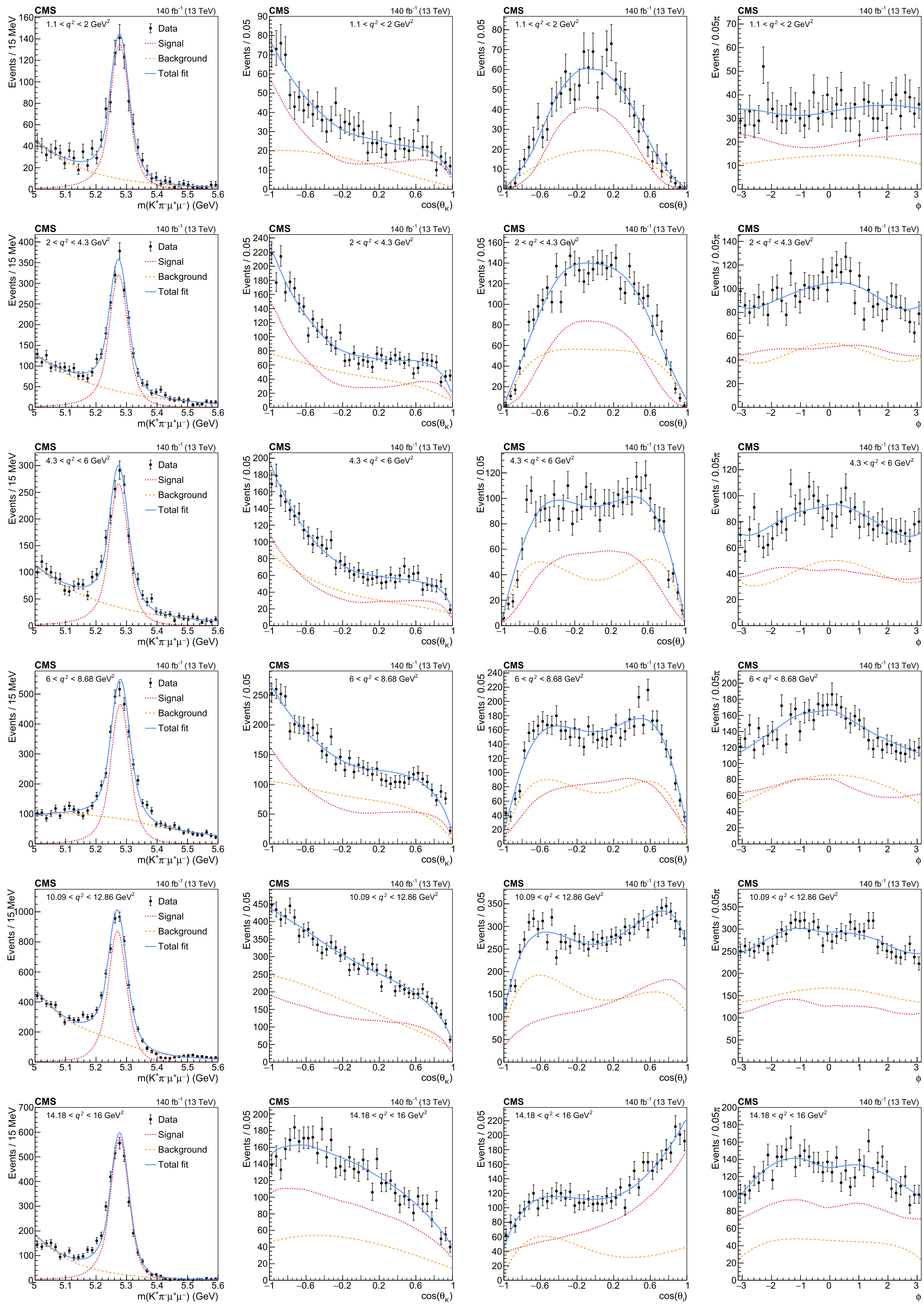

Fig. 2. Mass and angular distributions for the six q^2 bins (one bin per row). The projections of the total fitted distribution (blue solid line) and its different components are overlaid. The signal is shown by the red dotted line, and the background by the orange dashed line.

Table 2
The measured *CP*-averaged angular observables, in the corresponding q^2 bins. The first uncertainty is statistical and the second is systematic.

	$1.1 < q^2 < 2\,\text{GeV}^2$	$2 < q^2 < 4.3\,\text{GeV}^2$	$4.3 < q^2 < 6\,\text{GeV}^2$
F_L	$0.709\ ^{+0.073}_{-0.054} \pm 0.021$	$0.810\ ^{+0.036}_{-0.030} \pm 0.016$	$0.714\ ^{+0.032}_{-0.030} \pm 0.012$
P_1	$0.09\ ^{+0.23}_{-0.20} \pm 0.04$	$-0.29\ ^{+0.19}_{-0.21} \pm 0.05$	$-0.30\ ^{+0.15}_{-0.17} \pm 0.04$
P_2	$-0.37\ ^{+0.17}_{-0.13} \pm 0.10$	$-0.244\ ^{+0.094}_{-0.077} \pm 0.039$	$0.121\ ^{+0.080}_{-0.076} \pm 0.030$
P_3	$-0.05\ ^{+0.21}_{-0.22} \pm 0.04$	$-0.19\ ^{+0.20}_{-0.22} \pm 0.09$	$-0.03 \pm 0.14 \pm 0.08$
P'_4	$-0.44\ ^{+0.29}_{-0.32} \pm 0.11$	$-0.43\ ^{+0.16}_{-0.19} \pm 0.08$	$-0.72\ ^{+0.15}_{-0.16} \pm 0.07$
P'_5	$0.36\ ^{+0.17}_{-0.13} \pm 0.03$	$-0.14\ ^{+0.10}_{-0.09} \pm 0.04$	$-0.44 \pm 0.10 \pm 0.03$
P'_6	$0.000\ ^{+0.094}_{-0.097} \pm 0.021$	$0.108\ ^{+0.075}_{-0.071} \pm 0.018$	$0.129\ ^{+0.074}_{-0.071} \pm 0.011$
P'_8	$0.16 \pm 0.37 \pm 0.11$	$0.73\ ^{+0.18}_{-0.19} \pm 0.06$	$-0.01 \pm 0.22 \pm 0.04$
	$6 < q^2 < 8.68\,\text{GeV}^2$	$10.09 < q^2 < 12.86\,\text{GeV}^2$	$14.18 < q^2 < 16\,\text{GeV}^2$
F_L	$0.627 \pm 0.016 \pm 0.011$	$0.474\ ^{+0.011}_{-0.013} \pm 0.009$	$0.394 \pm 0.012 \pm 0.009$
P_1	$-0.06 \pm 0.10 \pm 0.05$	$-0.439\ ^{+0.051}_{-0.047} \pm 0.030$	$-0.465 \pm 0.037 \pm 0.025$
P_2	$0.188\ ^{+0.039}_{-0.040} \pm 0.014$	$0.386\ ^{+0.021}_{-0.019} \pm 0.018$	$0.440\ ^{+0.008}_{-0.010} \pm 0.008$
P_3	$0.099\ ^{+0.092}_{-0.090} \pm 0.014$	$0.013\ ^{+0.041}_{-0.043} \pm 0.007$	$-0.034\ ^{+0.037}_{-0.038} \pm 0.010$
P'_4	$-0.95 \pm 0.10 \pm 0.06$	$-1.025\ ^{+0.064}_{-0.066} \pm 0.059$	$-1.159\ ^{+0.042}_{-0.038} \pm 0.041$
P'_5	$-0.495 \pm 0.067 \pm 0.023$	$-0.746\ ^{+0.033}_{-0.032} \pm 0.014$	$-0.688\ ^{+0.038}_{-0.036} \pm 0.021$
P'_6	$0.010 \pm 0.052 \pm 0.016$	$0.080\ ^{+0.037}_{-0.041} \pm 0.011$	$0.121\ ^{+0.040}_{-0.039} \pm 0.011$
P'_8	$0.06 \pm 0.14 \pm 0.04$	$0.09\ ^{+0.09}_{-0.10} \pm 0.03$	$0.011\ ^{+0.089}_{-0.086} \pm 0.022$

a different approach to combining them. Additional predictions are calculated using the `flavio` [51] software package, which combines local form factors from lattice quantum chromodynamics [45,46] and light-cone sum rules [52], and quantum chromodynamics factorization for nonlocal form factors [53,54]. The predictions calculated with the `HEP-fit` [55] software package adopt a conservative estimation of non-local hadronic matrix elements and their uncertainties, to account for a possible large impact from charm-loop penguin diagrams [19,56].

The HEPfit predictions, given the large uncertainties, are compatible with the measurements. The EOS and ABCDMN predictions, while showing compatibility with the analysis results for most of the observables, present tensions with the measured values of P_2 and P'_5, in the region of q^2 below the J/ψ resonance. The deviation for P'_5 is at a level of 3.2 (2.2) and 4.9 (3.0) standard deviations for EOS (ABCDMN) predictions in the regions $4.3 < q^2 < 6\,\text{GeV}^2$ and $6 < q^2 < 8.68\,\text{GeV}^2$, respectively, while for P_2 the difference corresponds to 2.2 (1.5) and 6.4 (4.1) standard deviations for EOS (ABCDMN) predictions, in the same q^2 ranges. The flavio predictions show similar tensions for the P'_5 parameter, at the level of 2.6 standard deviations in the regions $4.3 < q^2 < 6\,\text{GeV}^2$. The value of P'_8 in the second bin of q^2 disagrees with the predictions, with a significance that ranges between 1.5 and 3.5 standard deviations. The current measurements are compatible with those presented in previous analyses from the CMS Collaboration [13,14] and other experiments [7,11,15,16], as shown for P_2 and P'_5 in Fig. 4. The statistical uncertainty has significantly improved compared to previous CMS publications.

8. Summary

In summary, the study of the full angular distribution of the flavor-changing neutral-current $B^0 \to K^{*0}\mu^+\mu^-$ decay has been performed using $140\,\text{fb}^{-1}$ of proton-proton collision data recorded by the CMS detector at the LHC at $\sqrt{s} = 13\,\text{TeV}$. A complete set of observables has been measured via unbinned maximum likelihood fits to the B^0 candidate mass and angular variables, in bins of the squared invariant mass of the dimuon system ranging from 1.1 to $16\,\text{GeV}^2$. The measurements are compared to a variety of predictions based on the standard model, with tension in a few of the angular observables seen for some of the predictions, as is also reported by other experiments. These results are among the most precise experimental measurements of the angular observables of this decay, and provide a valuable contribution to the understanding of the $b \to s\ell^+\ell^-$ processes.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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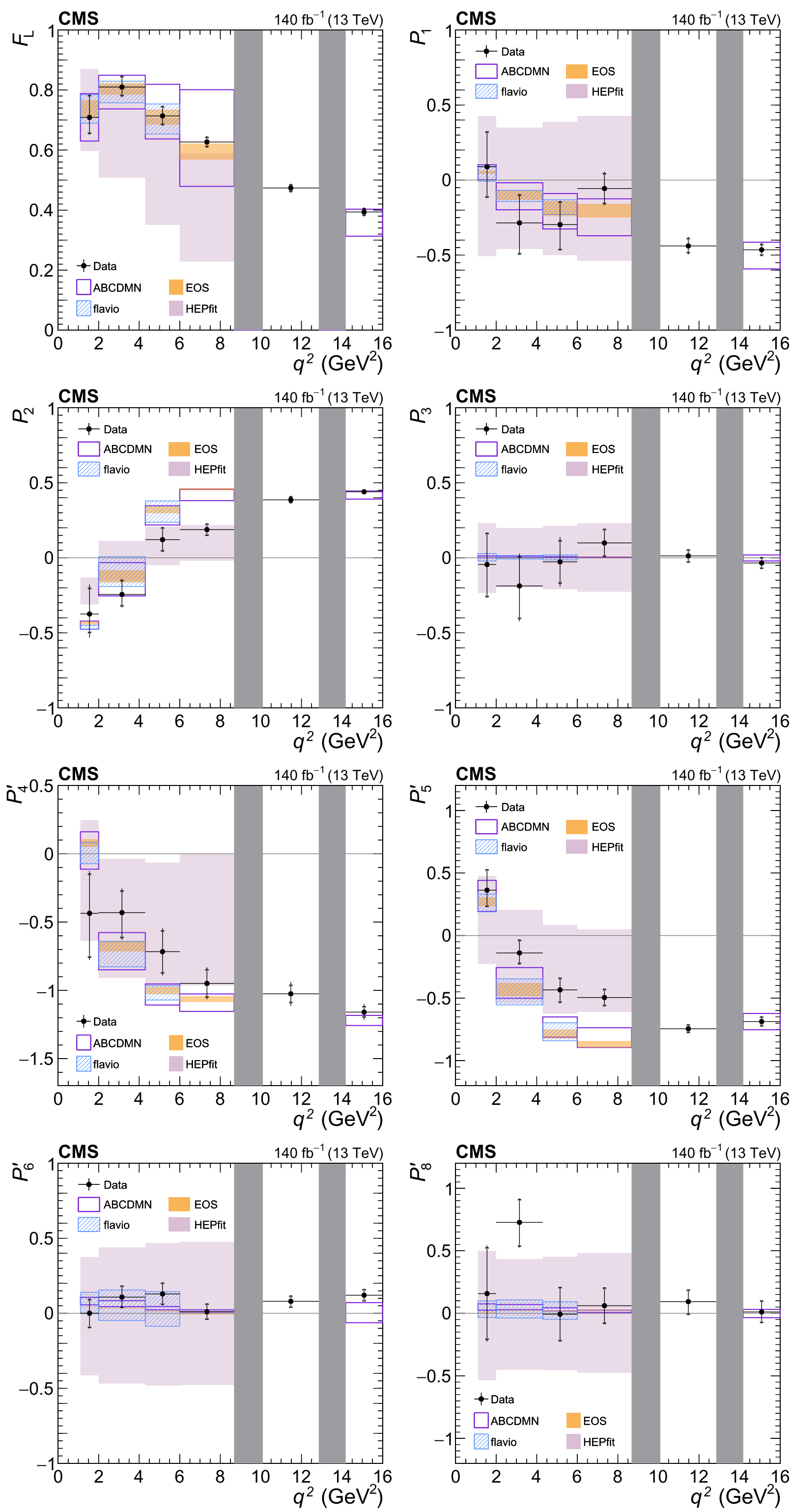

Fig. 3. Measurements of the angular observables versus q^2. The inner vertical bars represent the statistical uncertainties, while the outer vertical bars give the total uncertainties. The horizontal bars show the bin widths. The vertical shaded regions correspond to the J/ψ and ψ(2S) resonances. Predictions are shown, averaged in each bin, from Ref. [20] (labeled ABCDMN), and the `EOS` [50], `flavio` [51], and `HEPfit` [55] libraries.

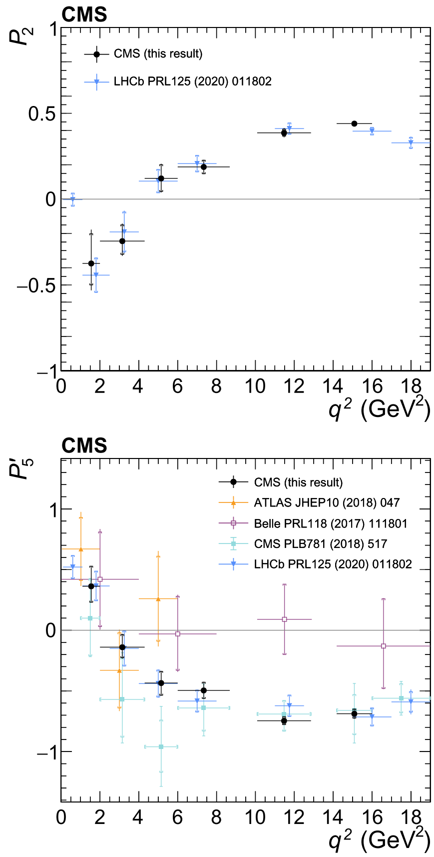

Fig. 4. Comparison of current measurements of P_2 and P_5' to a previous P_2 measurement by LHCb [16] and previous P_5' results from ATLAS [15], Belle [7], CMS [14], and LHCb [16]. The inner vertical bars represent the statistical uncertainties, while the outer vertical bars give the total uncertainties. The horizontal bars show the bin widths.

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Data availability

Release and preservation of data used by the CMS Collaboration as the basis for publications is guided by the CMS data preservation, re-use and open access policy.

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The CMS collaboration

A. Hayrapetyan, A. Tumasyan [1]

Yerevan Physics Institute, Yerevan, Armenia

W. Adam, J.W. Andrejkovic, L. Benato, T. Bergauer, S. Chatterjee, K. Damanakis, M. Dragicevic, P.S. Hussain, M. Jeitler [2], N. Krammer, A. Li, D. Liko, I. Mikulec, J. Schieck [2], R. Schöfbeck [2], D. Schwarz, M. Sonawane, W. Waltenberger, C.-E. Wulz [2]

Institut für Hochenergiephysik, Vienna, Austria

T. Janssen, T. Van Laer, P. Van Mechelen

Universiteit Antwerpen, Antwerpen, Belgium

N. Breugelmans, J. D'Hondt, S. Dansana, A. De Moor, M. Delcourt, F. Heyen, S. Lowette, I. Makarenko, D. Müller, S. Tavernier, M. Tytgat [3], G.P. Van Onsem, S. Van Putte, D. Vannerom

Vrije Universiteit Brussel, Brussel, Belgium

B. Bilin, B. Clerbaux, A.K. Das, I. De Bruyn, G. De Lentdecker, H. Evard, L. Favart, P. Gianneios, J. Jaramillo, A. Khalilzadeh, F.A. Khan, K. Lee, A. Malara, S. Paredes, M.A. Shahzad, L. Thomas, M. Vanden Bemden, C. Vander Velde, P. Vanlaer

Université Libre de Bruxelles, Bruxelles, Belgium

M. De Coen, D. Dobur, G. Gokbulut, Y. Hong, J. Knolle, L. Lambrecht, D. Marckx, K. Mota Amarilo, K. Skovpen, N. Van Den Bossche, J. van der Linden, L. Wezenbeek

Ghent University, Ghent, Belgium

A. Benecke, A. Bethani, G. Bruno, C. Caputo, J. De Favereau De Jeneret, C. Delaere, I.S. Donertas, A. Giammanco, A.O. Guzel, Sa. Jain, V. Lemaitre, J. Lidrych, P. Mastrapasqua, T.T. Tran

Université Catholique de Louvain, Louvain-la-Neuve, Belgium

G.A. Alves, E. Coelho, G. Correia Silva, C. Hensel, T. Menezes De Oliveira, C. Mora Herrera [4], P. Rebello Teles, M. Soeiro, A. Vilela Pereira [4]

Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

W.L. Aldá Júnior, M. Barroso Ferreira Filho, H. Brandao Malbouisson, W. Carvalho, J. Chinellato [5], E.M. Da Costa, G.G. Da Silveira [6], D. De Jesus Damiao, S. Fonseca De Souza, R. Gomes De Souza, T. Laux Kuhn [6], M. Macedo, J. Martins, L. Mundim, H. Nogima, J.P. Pinheiro, A. Santoro, A. Sznajder, M. Thiel

Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil

C.A. Bernardes [6], L. Calligaris, T.R. Fernandez Perez Tomei, E.M. Gregores, I. Maietto Silverio, P.G. Mercadante, S.F. Novaes, B. Orzari, Sandra S. Padula

Universidade Estadual Paulista, Universidade Federal do ABC, São Paulo, Brazil

A. Aleksandrov, G. Antchev, R. Hadjiiska, P. Iaydjiev, M. Misheva, M. Shopova, G. Sultanov

Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria

A. Dimitrov, L. Litov, B. Pavlov, P. Petkov, A. Petrov, E. Shumka

University of Sofia, Sofia, Bulgaria

S. Keshri, D. Laroze, S. Thakur

Instituto De Alta Investigación, Universidad de Tarapacá, Casilla 7 D, Arica, Chile

T. Cheng, T. Javaid, L. Yuan

Beihang University, Beijing, China

Z. Hu, Z. Liang, J. Liu

Department of Physics, Tsinghua University, Beijing, China

G.M. Chen [7], H.S. Chen [7], M. Chen [7], F. Iemmi, C.H. Jiang, A. Kapoor [8], H. Liao, Z.-A. Liu [9], R. Sharma [10], J.N. Song [9], J. Tao, C. Wang [7], J. Wang, Z. Wang [7], H. Zhang, J. Zhao

Institute of High Energy Physics, Beijing, China

A. Agapitos, Y. Ban, A. Carvalho Antunes De Oliveira, S. Deng, B. Guo, C. Jiang, A. Levin, C. Li, Q. Li, Y. Mao, S. Qian, S.J. Qian, X. Qin, X. Sun, D. Wang, H. Yang, L. Zhang, Y. Zhao, C. Zhou

State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing, China

S. Yang

Guangdong Provincial Key Laboratory of Nuclear Science and Guangdong-Hong Kong Joint Laboratory of Quantum Matter, South China Normal University, Guangzhou, China

Z. You

Sun Yat-Sen University, Guangzhou, China

K. Jaffel, N. Lu

University of Science and Technology of China, Hefei, China

G. Bauer [11], B. Li [12], K. Yi [13], J. Zhang

Nanjing Normal University, Nanjing, China

Y. Li

Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) - Fudan University, Shanghai, China

Z. Lin, C. Lu, M. Xiao

Zhejiang University, Hangzhou, Zhejiang, China

C. Avila, D.A. Barbosa Trujillo, A. Cabrera, C. Florez, J. Fraga, J.A. Reyes Vega

Universidad de Los Andes, Bogota, Colombia

F. Ramirez, C. Rendón, M. Rodriguez, A.A. Ruales Barbosa, J.D. Ruiz Alvarez

Universidad de Antioquia, Medellin, Colombia

D. Giljanovic, N. Godinovic, D. Lelas, A. Sculac

University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia

M. Kovac, A. Petkovic, T. Sculac

University of Split, Faculty of Science, Split, Croatia

P. Bargassa, V. Brigljevic, B.K. Chitroda, D. Ferencek, K. Jakovcic, A. Starodumov [14], T. Susa

Institute Rudjer Boskovic, Zagreb, Croatia

A. Attikis, K. Christoforou, A. Hadjiagapiou, C. Leonidou, J. Mousa, C. Nicolaou, L. Paizanos, F. Ptochos, P.A. Razis, H. Rykaczewski, H. Saka, A. Stepennov

University of Cyprus, Nicosia, Cyprus

M. Finger, M. Finger Jr., A. Kveton

Charles University, Prague, Czech Republic

E. Ayala

Escuela Politecnica Nacional, Quito, Ecuador

E. Carrera Jarrin

Universidad San Francisco de Quito, Quito, Ecuador

H. Abdalla [15], Y. Assran [16,17], B. El-mahdy

Academy of Scientific Research and Technology of the Arab Republic of Egypt, Egyptian Network of High Energy Physics, Cairo, Egypt

M.A. Mahmoud, Y. Mohammed

Center for High Energy Physics (CHEP-FU), Fayoum University, El-Fayoum, Egypt

K. Ehataht, M. Kadastik, T. Lange, S. Nandan, C. Nielsen, J. Pata, M. Raidal, L. Tani, C. Veelken

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

H. Kirschenmann, K. Osterberg, M. Voutilainen

Department of Physics, University of Helsinki, Helsinki, Finland

S. Bharthuar, N. Bin Norjoharuddeen, E. Brücken, F. Garcia, P. Inkaew, K.T.S. Kallonen, T. Lampén, K. Lassila-Perini, S. Lehti, T. Lindén, M. Myllymäki, M.m. Rantanen, H. Siikonen, J. Tuominiemi

Helsinki Institute of Physics, Helsinki, Finland

P. Luukka, H. Petrow

Lappeenranta-Lahti University of Technology, Lappeenranta, Finland

M. Besancon, F. Couderc, M. Dejardin, D. Denegri, J.L. Faure, F. Ferri, S. Ganjour, P. Gras, G. Hamel de Monchenault, M. Kumar, V. Lohezic, J. Malcles, F. Orlandi, L. Portales, A. Rosowsky, M.Ö. Sahin, A. Savoy-Navarro[18], P. Simkina, M. Titov, M. Tornago

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

F. Beaudette, G. Boldrini, P. Busson, A. Cappati, C. Charlot, M. Chiusi, T.D. Cuisset, F. Damas, O. Davignon, A. De Wit, I.T. Ehle, B.A. Fontana Santos Alves, S. Ghosh, A. Gilbert, R. Granier de Cassagnac, A. Hakimi, B. Harikrishnan, L. Kalipoliti, G. Liu, M. Nguyen, C. Ochando, R. Salerno, J.B. Sauvan, Y. Sirois, L. Urda Gómez, E. Vernazza, A. Zabi, A. Zghiche

Laboratoire Leprince-Ringuet, CNRS/IN2P3, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France

J.-L. Agram[19], J. Andrea, D. Apparu, D. Bloch, J.-M. Brom, E.C. Chabert, C. Collard, S. Falke, U. Goerlach, R. Haeberle, A.-C. Le Bihan, M. Meena, O. Poncet, G. Saha, M.A. Sessini, P. Van Hove, P. Vaucelle

Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France

A. Di Florio

Centre de Calcul de l'Institut National de Physique Nucleaire et de Physique des Particules, CNRS/IN2P3, Villeurbanne, France

D. Amram, S. Beauceron, B. Blancon, G. Boudoul, N. Chanon, D. Contardo, P. Depasse, C. Dozen[20], H. El Mamouni, J. Fay, S. Gascon, M. Gouzevitch, C. Greenberg, G. Grenier, B. Ille, E. Jourd'huy, I.B. Laktineh, M. Lethuillier, L. Mirabito, S. Perries, A. Purohit, M. Vander Donckt, P. Verdier, J. Xiao

Institut de Physique des 2 Infinis de Lyon (IP2I), Villeurbanne, France

I. Lomidze, T. Toriashvili[21], Z. Tsamalaidze[14]

Georgian Technical University, Tbilisi, Georgia

V. Botta, S. Consuegra Rodríguez, L. Feld, K. Klein, M. Lipinski, D. Meuser, A. Pauls, D. Pérez Adán, N. Röwert, M. Teroerde

RWTH Aachen University, I. Physikalisches Institut, Aachen, Germany

S. Diekmann, A. Dodonova, N. Eich, D. Eliseev, F. Engelke, J. Erdmann, M. Erdmann, P. Fackeldey, B. Fischer, T. Hebbeker, K. Hoepfner, F. Ivone, A. Jung, M.y. Lee, F. Mausolf, M. Merschmeyer, A. Meyer, S. Mukherjee, D. Noll, F. Nowotny, A. Pozdnyakov, Y. Rath,

W. Redjeb, F. Rehm, H. Reithler, V. Sarkisovi, A. Schmidt, C. Seth, A. Sharma, J.L. Spah, A. Stein, F. Torres Da Silva De Araujo [22], S. Wiedenbeck, S. Zaleski

RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany

C. Dziwok, G. Flügge, T. Kress, A. Nowack, O. Pooth, A. Stahl, T. Ziemons, A. Zotz

RWTH Aachen University, III. Physikalisches Institut B, Aachen, Germany

H. Aarup Petersen, M. Aldaya Martin, J. Alimena, S. Amoroso, Y. An, J. Bach, S. Baxter, M. Bayatmakou, H. Becerril Gonzalez, O. Behnke, A. Belvedere, F. Blekman [23], K. Borras [24], A. Campbell, A. Cardini, C. Cheng, F. Colombina, G. Eckerlin, D. Eckstein, L.I. Estevez Banos, E. Gallo [23], A. Geiser, V. Guglielmi, M. Guthoff, A. Hinzmann, L. Jeppe, B. Kaech, M. Kasemann, C. Kleinwort, R. Kogler, M. Komm, D. Krücker, W. Lange, D. Leyva Pernia, K. Lipka [25], W. Lohmann [26], F. Lorkowski, R. Mankel, I.-A. Melzer-Pellmann, M. Mendizabal Morentin, A.B. Meyer, G. Milella, K. Moral Figueroa, A. Mussgiller, L.P. Nair, J. Niedziela, A. Nürnberg, Y. Otarid, J. Park, E. Ranken, A. Raspereza, D. Rastorguev, J. Rübenach, L. Rygaard, A. Saggio, M. Scham [27,24], S. Schnake [24], P. Schütze, C. Schwanenberger [23], D. Selivanova, K. Sharko, M. Shchedrolosiev, D. Stafford, F. Vazzoler, A. Ventura Barroso, R. Walsh, D. Wang, Q. Wang, K. Wichmann, L. Wiens [24], C. Wissing, Y. Yang, A. Zimermmane Castro Santos

Deutsches Elektronen-Synchrotron, Hamburg, Germany

A. Albrecht, S. Albrecht, M. Antonello, S. Bein, S. Bollweg, M. Bonanomi, P. Connor, K. El Morabit, Y. Fischer, E. Garutti, A. Grohsjean, J. Haller, D. Hundhausen, H.R. Jabusch, G. Kasieczka, P. Keicher, R. Klanner, W. Korcari, T. Kramer, C.c. Kuo, V. Kutzner, F. Labe, J. Lange, A. Lobanov, C. Matthies, L. Moureaux, M. Mrowietz, A. Nigamova, Y. Nissan, A. Paasch, K.J. Pena Rodriguez, T. Quadfasel, B. Raciti, M. Rieger, D. Savoiu, J. Schindler, P. Schleper, M. Schröder, J. Schwandt, M. Sommerhalder, H. Stadie, G. Steinbrück, A. Tews, B. Wiederspan, M. Wolf

University of Hamburg, Hamburg, Germany

S. Brommer, E. Butz, T. Chwalek, A. Dierlamm, A. Droll, U. Elicabuk, N. Faltermann, M. Giffels, A. Gottmann, F. Hartmann [28], R. Hofsaess, M. Horzela, U. Husemann, J. Kieseler, M. Klute, R. Koppenhöfer, O. Lavoryk, J.M. Lawhorn, M. Link, A. Lintuluoto, S. Maier, S. Mitra, M. Mormile, Th. Müller, M. Neukum, M. Oh, E. Pfeffer, M. Presilla, G. Quast, K. Rabbertz, B. Regnery, N. Shadskiy, I. Shvetsov, H.J. Simonis, L. Sowa, L. Stockmeier, K. Tauqeer, M. Toms, N. Trevisani, R.F. Von Cube, M. Wassmer, S. Wieland, F. Wittig, R. Wolf, X. Zuo

Karlsruher Institut fuer Technologie, Karlsruhe, Germany

G. Anagnostou, G. Daskalakis, A. Kyriakis, A. Papadopoulos [28], A. Stakia

Institute of Nuclear and Particle Physics (INPP), NCSR Demokritos, Aghia Paraskevi, Greece

P. Kontaxakis, G. Melachroinos, Z. Painesis, I. Papavergou, I. Paraskevas, N. Saoulidou, K. Theofilatos, E. Tziaferi, K. Vellidis, I. Zisopoulos

National and Kapodistrian University of Athens, Athens, Greece

G. Bakas, T. Chatzistavrou, G. Karapostoli, K. Kousouris, I. Papakrivopoulos, E. Siamarkou, G. Tsipolitis, A. Zacharopoulou

National Technical University of Athens, Athens, Greece

I. Bestintzanos, I. Evangelou, C. Foudas, C. Kamtsikis, P. Katsoulis, P. Kokkas, P.G. Kosmoglou Kioseoglou, N. Manthos, I. Papadopoulos, J. Strologas

University of Ioánnina, Ioánnina, Greece

C. Hajdu, D. Horvath[29,30], K. Márton, A.J. Rádl[31], F. Sikler, V. Veszpremi

HUN-REN Wigner Research Centre for Physics, Budapest, Hungary

M. Csanád, K. Farkas, A. Fehérkuti[32], M.M.A. Gadallah[33], Á. Kadlecsik, P. Major, G. Pásztor, G.I. Veres

MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary

L. Olah, G. Zilizi

Faculty of Informatics, University of Debrecen, Debrecen, Hungary

G. Bencze, S. Czellar, J. Molnar, Z. Szillasi

HUN-REN ATOMKI - Institute of Nuclear Research, Debrecen, Hungary

T. Csorgo[32], F. Nemes[32], T. Novak

Karoly Robert Campus, MATE Institute of Technology, Gyongyos, Hungary

S. Bansal, S.B. Beri, V. Bhatnagar, G. Chaudhary, S. Chauhan, N. Dhingra[34], A. Kaur, A. Kaur, H. Kaur, M. Kaur, S. Kumar, T. Sheokand, J.B. Singh, A. Singla

Panjab University, Chandigarh, India

A. Ahmed, A. Bhardwaj, A. Chhetri, B.C. Choudhary, A. Kumar, A. Kumar, M. Naimuddin, K. Ranjan, M.K. Saini, S. Saumya

University of Delhi, Delhi, India

S. Baradia, S. Barman[35], S. Bhattacharya, S. Das Gupta, S. Dutta, S. Dutta, S. Sarkar

Saha Institute of Nuclear Physics, HBNI, Kolkata, India

M.M. Ameen, P.K. Behera, S.C. Behera, S. Chatterjee, G. Dash, P. Jana, P. Kalbhor, S. Kamble, J.R. Komaragiri[36], D. Kumar[36], T. Mishra, B. Parida[37], P.R. Pujahari, N.R. Saha, A. Sharma, A.K. Sikdar, R.K. Singh, P. Verma, S. Verma, A. Vijay

Indian Institute of Technology Madras, Madras, India

S. Dugad, G.B. Mohanty, M. Shelake, P. Suryadevara

Tata Institute of Fundamental Research-A, Mumbai, India

A. Bala, S. Banerjee, R.M. Chatterjee, M. Guchait, Sh. Jain, A. Jaiswal, S. Kumar, G. Majumder, K. Mazumdar, S. Parolia, A. Thachayath

Tata Institute of Fundamental Research-B, Mumbai, India

S. Bahinipati[38], C. Kar, D. Maity[39], P. Mal, V.K. Muraleedharan Nair Bindhu[39], K. Naskar[39], A. Nayak[39], S. Nayak, K. Pal, P. Sadangi, S.K. Swain, S. Varghese[39], D. Vats[39]

National Institute of Science Education and Research, An OCC of Homi Bhabha National Institute, Bhubaneswar, Odisha, India

S. Acharya[40], A. Alpana, S. Dube, B. Gomber[40], P. Hazarika, B. Kansal, A. Laha, B. Sahu[40], S. Sharma, K.Y. Vaish

Indian Institute of Science Education and Research (IISER), Pune, India

H. Bakhshiansohi[41], A. Jafari[42], M. Zeinali[43]

Isfahan University of Technology, Isfahan, Iran

S. Bashiri, S. Chenarani [44], S.M. Etesami, Y. Hosseini, M. Khakzad, E. Khazaie, M. Mohammadi Najafabadi, S. Tizchang [45]

Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

M. Felcini, M. Grunewald

University College Dublin, Dublin, Ireland

M. Abbrescia [a,b], A. Colaleo [a,b], D. Creanza [a,c], B. D'Anzi [a,b], N. De Filippis [a,c], M. De Palma [a,b], W. Elmetenawee [a,b,46], N. Ferrara [a,b], L. Fiore [a], G. Iaselli [a,c], L. Longo [a], M. Louka [a,b], G. Maggi [a,c], M. Maggi [a], I. Margjeka [a], V. Mastrapasqua [a,b], S. My [a,b], S. Nuzzo [a,b], A. Pellecchia [a,b], A. Pompili [a,b], G. Pugliese [a,c], R. Radogna [a,b], D. Ramos [a], A. Ranieri [a], L. Silvestris [a], F.M. Simone [a,c], Ü. Sözbilir [a], A. Stamerra [a,b], D. Troiano [a,b], R. Venditti [a,b], P. Verwilligen [a], A. Zaza [a,b]

[a] *INFN Sezione di Bari, Bari, Italy*
[b] *Università di Bari, Bari, Italy*
[c] *Politecnico di Bari, Bari, Italy*

G. Abbiendi [a], C. Battilana [a,b], D. Bonacorsi [a,b], P. Capiluppi [a,b], A. Castro [a,b,†], F.R. Cavallo [a], M. Cuffiani [a,b], G.M. Dallavalle [a], T. Diotalevi [a,b], F. Fabbri [a], A. Fanfani [a,b], D. Fasanella [a], P. Giacomelli [a], L. Giommi [a,b], C. Grandi [a], L. Guiducci [a,b], S. Lo Meo [a,47], M. Lorusso [a,b], L. Lunerti [a], S. Marcellini [a], G. Masetti [a], F.L. Navarria [a,b], G. Paggi [a,b], A. Perrotta [a], F. Primavera [a,b], A.M. Rossi [a,b], S. Rossi Tisbeni [a,b], T. Rovelli [a,b], G.P. Siroli [a,b]

[a] *INFN Sezione di Bologna, Bologna, Italy*
[b] *Università di Bologna, Bologna, Italy*

S. Costa [a,b,48], A. Di Mattia [a], A. Lapertosa [a], R. Potenza [a,b], A. Tricomi [a,b,48], C. Tuve [a,b]

[a] *INFN Sezione di Catania, Catania, Italy*
[b] *Università di Catania, Catania, Italy*

P. Assiouras [a], G. Barbagli [a], G. Bardelli [a,b], B. Camaiani [a,b], A. Cassese [a], R. Ceccarelli [a], V. Ciulli [a,b], C. Civinini [a], R. D'Alessandro [a,b], E. Focardi [a,b], T. Kello [a], G. Latino [a,b], P. Lenzi [a,b], M. Lizzo [a], M. Meschini [a], S. Paoletti [a], A. Papanastassiou [a,b], G. Sguazzoni [a], L. Viliani [a]

[a] *INFN Sezione di Firenze, Firenze, Italy*
[b] *Università di Firenze, Firenze, Italy*

L. Benussi, S. Bianco, S. Meola [49], D. Piccolo

INFN Laboratori Nazionali di Frascati, Frascati, Italy

M. Alves Gallo Pereira [a], F. Ferro [a], E. Robutti [a], S. Tosi [a,b]

[a] *INFN Sezione di Genova, Genova, Italy*
[b] *Università di Genova, Genova, Italy*

A. Benaglia [a], F. Brivio [a], F. Cetorelli [a,b], F. De Guio [a,b], M.E. Dinardo [a,b], P. Dini [a], S. Gennai [a], R. Gerosa [a,b], A. Ghezzi [a,b], P. Govoni [a,b], L. Guzzi [a], M.T. Lucchini [a,b], M. Malberti [a], S. Malvezzi [a], A. Massironi [a], D. Menasce [a], L. Moroni [a], M. Paganoni [a,b], S. Palluotto [a,b], D. Pedrini [a], A. Perego [a,b], B.S. Pinolini [a], G. Pizzati [a,b], S. Ragazzi [a,b], T. Tabarelli de Fatis [a,b]

[a] *INFN Sezione di Milano-Bicocca, Milano, Italy*
[b] *Università di Milano-Bicocca, Milano, Italy*

S. Buontempo [a], A. Cagnotta [a,b], F. Carnevali [a,b], N. Cavallo [a,c], F. Fabozzi [a,c], A.O.M. Iorio [a,b], L. Lista [a,b,50], P. Paolucci [a,28], B. Rossi [a]

[a] *INFN Sezione di Napoli, Napoli, Italy*
[b] *Università di Napoli 'Federico II', Napoli, Italy*
[c] *Università della Basilicata, Potenza, Italy*

[d] Scuola Superiore Meridionale (SSM), Napoli, Italy

R. Ardino [a], P. Azzi [a], N. Bacchetta [a,51], D. Bisello [a,b], P. Bortignon [a], G. Bortolato [a,b], A. Bragagnolo [a,b], A.C.M. Bulla [a], R. Carlin [a,b], T. Dorigo [a,52], F. Gasparini [a,b], U. Gasparini [a,b], S. Giorgetti [a], M. Gulmini [a,53], E. Lusiani [a], M. Margoni [a,b], G. Maron [a,53], A.T. Meneguzzo [a,b], M. Migliorini [a,b], J. Pazzini [a,b], P. Ronchese [a,b], R. Rossin [a,b], F. Simonetto [a,b], M. Tosi [a,b], A. Triossi [a,b], M. Zanetti [a,b], P. Zotto [a,b], A. Zucchetta [a,b], G. Zumerle [a,b]

[a] INFN Sezione di Padova, Padova, Italy
[b] Università di Padova, Padova, Italy
[c] Università di Trento, Trento, Italy

A. Braghieri [a], S. Calzaferri [a], D. Fiorina [a], P. Montagna [a,b], V. Re [a], C. Riccardi [a,b], P. Salvini [a], I. Vai [a,b], P. Vitulo [a,b]

[a] INFN Sezione di Pavia, Pavia, Italy
[b] Università di Pavia, Pavia, Italy

S. Ajmal [a,b], M.E. Ascioti [a,b], G.M. Bilei [a], C. Carrivale [a,b], D. Ciangottini [a,b], L. Fanò [a,b], M. Magherini [a,b], V. Mariani [a,b], M. Menichelli [a], F. Moscatelli [a,54], A. Rossi [a,b], A. Santocchia [a,b], D. Spiga [a], T. Tedeschi [a,b]

[a] INFN Sezione di Perugia, Perugia, Italy
[b] Università di Perugia, Perugia, Italy

C. Aimè [a], C.A. Alexe [a,c], P. Asenov [a,b], P. Azzurri [a], G. Bagliesi [a], R. Bhattacharya [a], L. Bianchini [a,b], T. Boccali [a], E. Bossini [a], D. Bruschini [a,c], R. Castaldi [a], M.A. Ciocci [a,b], M. Cipriani [a,b], V. D'Amante [a,d], R. Dell'Orso [a], S. Donato [a], A. Giassi [a], F. Ligabue [a,c], A.C. Marini [a], D. Matos Figueiredo [a], A. Messineo [a,b], S. Mishra [a], M. Musich [a,b], F. Palla [a], A. Rizzi [a,b], G. Rolandi [a,c], S. Roy Chowdhury [a], T. Sarkar [a], A. Scribano [a], P. Spagnolo [a], R. Tenchini [a], G. Tonelli [a,b], N. Turini [a,d], F. Vaselli [a,c], A. Venturi [a], P.G. Verdini [a]

[a] INFN Sezione di Pisa, Pisa, Italy
[b] Università di Pisa, Pisa, Italy
[c] Scuola Normale Superiore di Pisa, Pisa, Italy
[d] Università di Siena, Siena, Italy

C. Baldenegro Barrera [a,b], P. Barria [a], C. Basile [a,b], F. Cavallari [a], L. Cunqueiro Mendez [a,b], D. Del Re [a,b], E. Di Marco [a,b], M. Diemoz [a], F. Errico [a,b], R. Gargiulo [a,b], E. Longo [a,b], L. Martikainen [a,b], J. Mijuskovic [a,b], G. Organtini [a,b], F. Pandolfi [a], R. Paramatti [a,b], C. Quaranta [a,b], S. Rahatlou [a,b], C. Rovelli [a], F. Santanastasio [a,b], L. Soffi [a], V. Vladimirov [a,b]

[a] INFN Sezione di Roma, Roma, Italy
[b] Sapienza Università di Roma, Roma, Italy

N. Amapane [a,b], R. Arcidiacono [a,c], S. Argiro [a,b], M. Arneodo [a,c], N. Bartosik [a], R. Bellan [a,b], A. Bellora [a,b], C. Biino [a], C. Borca [a,b], N. Cartiglia [a], M. Costa [a,b], R. Covarelli [a,b], N. Demaria [a], L. Finco [a], M. Grippo [a,b], B. Kiani [a,b], F. Legger [a], F. Luongo [a,b], C. Mariotti [a], L. Markovic [a,b], S. Maselli [a], A. Mecca [a,b], L. Menzio [a,b], P. Meridiani [a], E. Migliore [a,b], M. Monteno [a], R. Mulargia [a], M.M. Obertino [a,b], G. Ortona [a], L. Pacher [a,b], N. Pastrone [a], M. Pelliccioni [a], M. Ruspa [a,c], F. Siviero [a,b], V. Sola [a,b], A. Solano [a,b], A. Staiano [a], C. Tarricone [a,b], D. Trocino [a], G. Umoret [a,b], R. White [a,b]

[a] INFN Sezione di Torino, Torino, Italy
[b] Università di Torino, Torino, Italy
[c] Università del Piemonte Orientale, Novara, Italy

J. Babbar [a,b], S. Belforte [a], V. Candelise [a,b], M. Casarsa [a], F. Cossutti [a], K. De Leo [a], G. Della Ricca [a,b]

[a] INFN Sezione di Trieste, Trieste, Italy
[b] Università di Trieste, Trieste, Italy

S. Dogra, J. Hong, B. Kim, J. Kim, D. Lee, H. Lee, S.W. Lee, C.S. Moon, Y.D. Oh, M.S. Ryu, S. Sekmen, B. Tae, Y.C. Yang

Kyungpook National University, Daegu, Korea

M.S. Kim

Department of Mathematics and Physics - GWNU, Gangneung, Korea

G. Bak, P. Gwak, H. Kim, D.H. Moon

Chonnam National University, Institute for Universe and Elementary Particles, Kwangju, Korea

E. Asilar, J. Choi[55], D. Kim, T.J. Kim, J.A. Merlin, Y. Ryou

Hanyang University, Seoul, Korea

S. Choi, S. Han, B. Hong, K. Lee, K.S. Lee, S. Lee, J. Yoo

Korea University, Seoul, Korea

J. Goh, S. Yang

Kyung Hee University, Department of Physics, Seoul, Korea

H.S. Kim, Y. Kim, S. Lee

Sejong University, Seoul, Korea

J. Almond, J.H. Bhyun, J. Choi, J. Choi, W. Jun, J. Kim, Y.W. Kim, S. Ko, H. Kwon, H. Lee, J. Lee, J. Lee, B.H. Oh, S.B. Oh, H. Seo, U.K. Yang, I. Yoon

Seoul National University, Seoul, Korea

W. Jang, D.Y. Kang, Y. Kang, S. Kim, B. Ko, J.S.H. Lee, Y. Lee, I.C. Park, Y. Roh, I.J. Watson

University of Seoul, Seoul, Korea

S. Ha, K. Hwang, H.D. Yoo

Yonsei University, Department of Physics, Seoul, Korea

M. Choi, M.R. Kim, H. Lee, Y. Lee, I. Yu

Sungkyunkwan University, Suwon, Korea

T. Beyrouthy, Y. Gharbia

College of Engineering and Technology, American University of the Middle East (AUM), Dasman, Kuwait

F. Alazemi

Kuwait University - College of Science - Department of Physics, Safat, Kuwait

K. Dreimanis, A. Gaile, C. Munoz Diaz, D. Osite, G. Pikurs, A. Potrebko, M. Seidel, D. Sidiropoulos Kontos

Riga Technical University, Riga, Latvia

N.R. Strautnieks

University of Latvia (LU), Riga, Latvia

M. Ambrozas, A. Juodagalvis, A. Rinkevicius, G. Tamulaitis

Vilnius University, Vilnius, Lithuania

I. Yusuff[56], Z. Zolkapli

National Centre for Particle Physics, Universiti Malaya, Kuala Lumpur, Malaysia

J.F. Benitez, A. Castaneda Hernandez, H.A. Encinas Acosta, L.G. Gallegos Maríñez, M. León Coello, J.A. Murillo Quijada, A. Sehrawat, L. Valencia Palomo

Universidad de Sonora (UNISON), Hermosillo, Mexico

G. Ayala, H. Castilla-Valdez, H. Crotte Ledesma, E. De La Cruz-Burelo, I. Heredia-De La Cruz [57], R. Lopez-Fernandez, J. Mejia Guisao, C.A. Mondragon Herrera, A. Sánchez Hernández

Centro de Investigacion y de Estudios Avanzados del IPN, Mexico City, Mexico

C. Oropeza Barrera, D.L. Ramirez Guadarrama, M. Ramírez García

Universidad Iberoamericana, Mexico City, Mexico

I. Bautista, I. Pedraza, H.A. Salazar Ibarguen, C. Uribe Estrada

Benemerita Universidad Autonoma de Puebla, Puebla, Mexico

I. Bubanja, N. Raicevic

University of Montenegro, Podgorica, Montenegro

P.H. Butler

University of Canterbury, Christchurch, New Zealand

A. Ahmad, M.I. Asghar, A. Awais, M.I.M. Awan, H.R. Hoorani, W.A. Khan

National Centre for Physics, Quaid-I-Azam University, Islamabad, Pakistan

V. Avati, L. Grzanka, M. Malawski

AGH University of Krakow, Krakow, Poland

H. Bialkowska, M. Bluj, M. Górski, M. Kazana, M. Szleper, P. Zalewski

National Centre for Nuclear Research, Swierk, Poland

K. Bunkowski, K. Doroba, A. Kalinowski, M. Konecki, J. Krolikowski, A. Muhammad

Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

P. Fokow, K. Pozniak, W. Zabolotny

Warsaw University of Technology, Warsaw, Poland

M. Araujo, D. Bastos, C. Beirão Da Cruz E Silva, A. Boletti, M. Bozzo, T. Camporesi, G. Da Molin, P. Faccioli, M. Gallinaro, J. Hollar, N. Leonardo, G.B. Marozzo, A. Petrilli, M. Pisano, J. Seixas, J. Varela, J.W. Wulff

Laboratório de Instrumentação e Física Experimental de Partículas, Lisboa, Portugal

P. Adzic, P. Milenovic

Faculty of Physics, University of Belgrade, Belgrade, Serbia

D. Devetak, M. Dordevic, J. Milosevic, L. Nadderd, V. Rekovic

VINCA Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

J. Alcaraz Maestre, Cristina F. Bedoya, J.A. Brochero Cifuentes, Oliver M. Carretero, M. Cepeda, M. Cerrada, N. Colino, B. De La Cruz, A. Delgado Peris, A. Escalante Del Valle, D. Fernández Del Val, J.P. Fernández Ramos, J. Flix, M.C. Fouz, O. Gonzalez Lopez, S. Goy Lopez, J.M. Hernandez, M.I. Josa, J. Llorente Merino, C. Martin Perez, E. Martin Viscasillas, D. Moran, C.M. Morcillo Perez, Á. Navarro Tobar, C. Perez Dengra, A. Pérez-Calero Yzquierdo, J. Puerta Pelayo, I. Redondo, S. Sánchez Navas, J. Sastre, J. Vazquez Escobar

Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain

J.F. de Trocóniz

Universidad Autónoma de Madrid, Madrid, Spain

B. Alvarez Gonzalez, J. Cuevas, J. Fernandez Menendez, S. Folgueras, I. Gonzalez Caballero, P. Leguina, E. Palencia Cortezon, J. Prado Pico, C. Ramón Álvarez, V. Rodríguez Bouza, A. Soto Rodríguez, A. Trapote, C. Vico Villalba, P. Vischia

Universidad de Oviedo, Instituto Universitario de Ciencias y Tecnologías Espaciales de Asturias (ICTEA), Oviedo, Spain

S. Bhowmik, S. Blanco Fernández, I.J. Cabrillo, A. Calderon, J. Duarte Campderros, M. Fernandez, G. Gomez, C. Lasaosa García, R. Lopez Ruiz, C. Martinez Rivero, P. Martinez Ruiz del Arbol, F. Matorras, P. Matorras Cuevas, E. Navarrete Ramos, J. Piedra Gomez, L. Scodellaro, I. Vila, J.M. Vizan Garcia

Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain

B. Kailasapathy[58], D.D.C. Wickramarathna

University of Colombo, Colombo, Sri Lanka

W.G.D. Dharmaratna[59], K. Liyanage, N. Perera

University of Ruhuna, Department of Physics, Matara, Sri Lanka

D. Abbaneo, C. Amendola, E. Auffray, G. Auzinger, J. Baechler, D. Barney, A. Bermúdez Martínez, M. Bianco, A.A. Bin Anuar, A. Bocci, L. Borgonovi, C. Botta, E. Brondolin, C. Caillol, G. Cerminara, N. Chernyavskaya, D. d'Enterria, A. Dabrowski, A. David, A. De Roeck, M.M. Defranchis, M. Deile, M. Dobson, G. Franzoni, W. Funk, S. Giani, D. Gigi, K. Gill, F. Glege, J. Hegeman, J.K. Heikkilä, B. Huber, V. Innocente, T. James, P. Janot, O. Kaluzinska, O. Karacheban[26], S. Laurila, P. Lecoq, E. Leutgeb, C. Lourenço, L. Malgeri, M. Mannelli, M. Matthewman, A. Mehta, F. Meijers, S. Mersi, E. Meschi, V. Milosevic, F. Monti, F. Moortgat, M. Mulders, I. Neutelings, S. Orfanelli, F. Pantaleo, G. Petrucciani, A. Pfeiffer, M. Pierini, H. Qu, D. Rabady, B. Ribeiro Lopes, F. Riti, M. Rovere, H. Sakulin, R. Salvatico, S. Sanchez Cruz, S. Scarfi, C. Schwick, M. Selvaggi, A. Sharma, K. Shchelina, P. Silva, P. Sphicas[60], A.G. Stahl Leiton, A. Steen, S. Summers, D. Treille, P. Tropea, D. Walter, J. Wanczyk[61], J. Wang, K.A. Wozniak[62], S. Wuchterl, P. Zehetner, P. Zejdl, W.D. Zeuner

CERN, European Organization for Nuclear Research, Geneva, Switzerland

T. Bevilacqua[63], L. Caminada[63], A. Ebrahimi, W. Erdmann, R. Horisberger, Q. Ingram, H.C. Kaestli, D. Kotlinski, C. Lange, M. Missiroli[63], L. Noehte[63], T. Rohe, A. Samalan

PSI Center for Neutron and Muon Sciences, Villigen, Switzerland

T.K. Aarrestad, M. Backhaus, G. Bonomelli, A. Calandri, C. Cazzaniga, K. Datta, P. De Bryas Dexmiers D'archiac[61], A. De Cosa, G. Dissertori, M. Dittmar, M. Donegà, F. Eble, M. Galli, K. Gedia, F. Glessgen, C. Grab, N. Härringer, T.G. Harte, D. Hits, W. Lustermann, A.-M. Lyon, R.A. Manzoni, M. Marchegiani, L. Marchese, A. Mascellani[61], F. Nessi-Tedaldi, F. Pauss, V. Perovic, S. Pigazzini, B. Ristic, R. Seidita, J. Steggemann[61], A. Tarabini, D. Valsecchi, R. Wallny

ETH Zurich - Institute for Particle Physics and Astrophysics (IPA), Zurich, Switzerland

C. Amsler[64], P. Bärtschi, M.F. Canelli, K. Cormier, M. Huwiler, W. Jin, A. Jofrehei, B. Kilminster, S. Leontsinis, S.P. Liechti, A. Macchiolo, P. Meiring, F. Meng, J. Motta, A. Reimers, P. Robmann, M. Senger, E. Shokr, F. Stäger, R. Tramontano

Universität Zürich, Zurich, Switzerland

C. Adloff[65], D. Bhowmik, C.M. Kuo, W. Lin, P.K. Rout, P.C. Tiwari[36]

National Central University, Chung-Li, Taiwan

L. Ceard, K.F. Chen, Z.g. Chen, A. De Iorio, W.-S. Hou, T.h. Hsu, Y.w. Kao, S. Karmakar, G. Kole, Y.y. Li, R.-S. Lu, E. Paganis, X.f. Su, J. Thomas-Wilsker, L.s. Tsai, D. Tsionou, H.y. Wu, E. Yazgan

National Taiwan University (NTU), Taipei, Taiwan

C. Asawatangtrakuldee, N. Srimanobhas, V. Wachirapusitanand

High Energy Physics Research Unit, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

D. Agyel, F. Boran, F. Dolek, I. Dumanoglu[66], E. Eskut, Y. Guler[67], E. Gurpinar Guler[67], C. Isik, O. Kara, A. Kayis Topaksu, U. Kiminsu, Y. Komurcu, G. Onengut, K. Ozdemir[68], A. Polatoz, B. Tali[69], U.G. Tok, S. Turkcapar, E. Uslan, I.S. Zorbakir

Çukurova University, Physics Department, Science and Art Faculty, Adana, Turkey

G. Sokmen, M. Yalvac[70]

Middle East Technical University, Physics Department, Ankara, Turkey

B. Akgun, I.O. Atakisi, E. Gülmez, M. Kaya[71], O. Kaya[72], S. Tekten[73]

Bogazici University, Istanbul, Turkey

A. Cakir, K. Cankocak[66,74], G.G. Dincer[66], S. Sen[75]

Istanbul Technical University, Istanbul, Turkey

O. Aydilek[76], B. Hacisahinoglu, I. Hos[77], B. Kaynak, S. Ozkorucuklu, O. Potok, H. Sert, C. Simsek, C. Zorbilmez

Istanbul University, Istanbul, Turkey

S. Cerci, B. Isildak[78], D. Sunar Cerci, T. Yetkin

Yildiz Technical University, Istanbul, Turkey

A. Boyaryntsev, B. Grynyov

Institute for Scintillation Materials of National Academy of Science of Ukraine, Kharkiv, Ukraine

L. Levchuk

National Science Centre, Kharkiv Institute of Physics and Technology, Kharkiv, Ukraine

D. Anthony, J.J. Brooke, A. Bundock, F. Bury, E. Clement, D. Cussans, H. Flacher, M. Glowacki, J. Goldstein, H.F. Heath, M.-L. Holmberg, L. Kreczko, S. Paramesvaran, L. Robertshaw, V.J. Smith, K. Walkingshaw Pass

University of Bristol, Bristol, United Kingdom

A.H. Ball, K.W. Bell, A. Belyaev[79], C. Brew, R.M. Brown, D.J.A. Cockerill, C. Cooke, A. Elliot, K.V. Ellis, K. Harder, S. Harper, J. Linacre, K. Manolopoulos, D.M. Newbold, E. Olaiya, D. Petyt, T. Reis, A.R. Sahasransu, G. Salvi, T. Schuh, C.H. Shepherd-Themistocleous, I.R. Tomalin, K.C. Whalen, T. Williams

Rutherford Appleton Laboratory, Didcot, United Kingdom

I. Andreou, R. Bainbridge, P. Bloch, C.E. Brown, O. Buchmuller, C.A. Carrillo Montoya, G.S. Chahal[80], D. Colling, J.S. Dancu, I. Das, P. Dauncey, G. Davies, M. Della Negra, S. Fayer, G. Fedi, G. Hall, A. Howard, G. Iles, C.R. Knight, P. Krueper, J. Langford, K.H. Law, J. León Holgado, L. Lyons, A.-M. Magnan, B. Maier, S. Mallios, M. Mieskolainen, J. Nash[81], M. Pesaresi, P.B. Pradeep, B.C. Radburn-Smith, A. Richards, A. Rose, K. Savva, C. Seez, R. Shukla, A. Tapper, K. Uchida, G.P. Uttley, T. Virdee[28], M. Vojinovic, N. Wardle, D. Winterbottom

Imperial College, London, United Kingdom

J.E. Cole, A. Khan, P. Kyberd, I.D. Reid

Brunel University, Uxbridge, United Kingdom

S. Abdullin, A. Brinkerhoff, E. Collins, M.R. Darwish, J. Dittmann, K. Hatakeyama, J. Hiltbrand, B. McMaster, J. Samudio, S. Sawant, C. Sutantawibul, J. Wilson

Baylor University, Waco, TX, USA

R. Bartek, A. Dominguez, A.E. Simsek, S.S. Yu

Catholic University of America, Washington, DC, USA

B. Bam, A. Buchot Perraguin, R. Chudasama, S.I. Cooper, C. Crovella, S.V. Gleyzer, E. Pearson, C.U. Perez, P. Rumerio[82], E. Usai, R. Yi

The University of Alabama, Tuscaloosa, AL, USA

A. Akpinar, C. Cosby, G. De Castro, Z. Demiragli, C. Erice, C. Fangmeier, C. Fernandez Madrazo, E. Fontanesi, D. Gastler, F. Golf, S. Jeon, J. O'cain, I. Reed, J. Rohlf, K. Salyer, D. Sperka, D. Spitzbart, I. Suarez, A. Tsatsos, A.G. Zecchinelli

Boston University, Boston, MA, USA

G. Barone, G. Benelli, D. Cutts, L. Gouskos, M. Hadley, U. Heintz, J.M. Hogan[83], T. Kwon, G. Landsberg, K.T. Lau, D. Li, J. Luo, S. Mondal, T. Russell, S. Sagir[84], X. Shen, F. Simpson, M. Stamenkovic, N. Venkatasubramanian, X. Yan

Brown University, Providence, RI, USA

S. Abbott, B. Barton, C. Brainerd, R. Breedon, H. Cai, M. Calderon De La Barca Sanchez, M. Chertok, M. Citron, J. Conway, P.T. Cox, R. Erbacher, F. Jensen, O. Kukral, G. Mocellin, M. Mulhearn, S. Ostrom, W. Wei, S. Yoo, F. Zhang

University of California, Davis, Davis, CA, USA

K. Adamidis, M. Bachtis, D. Campos, R. Cousins, A. Datta, G. Flores Avila, J. Hauser, M. Ignatenko, M.A. Iqbal, T. Lam, Y.f. Lo, E. Manca, A. Nunez Del Prado, D. Saltzberg, V. Valuev

University of California, Los Angeles, CA, USA

R. Clare, J.W. Gary, G. Hanson

University of California, Riverside, Riverside, CA, USA

A. Aportela, A. Arora, J.G. Branson, S. Cittolin, S. Cooperstein, D. Diaz, J. Duarte, L. Giannini, Y. Gu, J. Guiang, R. Kansal, V. Krutelyov, R. Lee, J. Letts, M. Masciovecchio, F. Mokhtar, S. Mukherjee, M. Pieri, M. Quinnan, B.V. Sathia Narayanan, V. Sharma, M. Tadel, E. Vourliotis, F. Würthwein, Y. Xiang, A. Yagil

University of California, San Diego, La Jolla, CA, USA

A. Barzdukas, L. Brennan, C. Campagnari, K. Downham, C. Grieco, J. Incandela, J. Kim, A.J. Li, P. Masterson, H. Mei, J. Richman, S.N. Santpur, U. Sarica, R. Schmitz, F. Setti, J. Sheplock, D. Stuart, T.Á. Vámi, S. Wang, D. Zhang

University of California, Santa Barbara - Department of Physics, Santa Barbara, CA, USA

S. Bhattacharya, A. Bornheim, O. Cerri, A. Latorre, J. Mao, H.B. Newman, G. Reales Gutiérrez, M. Spiropulu, J.R. Vlimant, C. Wang, S. Xie, R.Y. Zhu

California Institute of Technology, Pasadena, CA, USA

J. Alison, S. An, P. Bryant, M. Cremonesi, V. Dutta, T. Ferguson, T.A. Gómez Espinosa, A. Harilal, A. Kallil Tharayil, C. Liu, T. Mudholkar, S. Murthy, P. Palit, K. Park, M. Paulini, A. Roberts, A. Sanchez, W. Terrill

Carnegie Mellon University, Pittsburgh, PA, USA

J.P. Cumalat, W.T. Ford, A. Hart, A. Hassani, G. Karathanasis, N. Manganelli, J. Pearkes, C. Savard, N. Schonbeck, K. Stenson, K.A. Ulmer, S.R. Wagner, N. Zipper, D. Zuolo

University of Colorado Boulder, Boulder, CO, USA

J. Alexander, S. Bright-Thonney, X. Chen, D.J. Cranshaw, J. Fan, X. Fan, S. Hogan, P. Kotamnives, J. Monroy, M. Oshiro, J.R. Patterson, M. Reid, A. Ryd, J. Thom, P. Wittich, R. Zou

Cornell University, Ithaca, NY, USA

M. Albrow, M. Alyari, O. Amram, G. Apollinari, A. Apresyan, L.A.T. Bauerdick, D. Berry, J. Berryhill, P.C. Bhat, K. Burkett, J.N. Butler, A. Canepa, G.B. Cerati, H.W.K. Cheung, F. Chlebana, G. Cummings, J. Dickinson, I. Dutta, V.D. Elvira, Y. Feng, J. Freeman, A. Gandrakota, Z. Gecse, L. Gray, D. Green, A. Grummer, S. Grünendahl, D. Guerrero, O. Gutsche, R.M. Harris, R. Heller, T.C. Herwig, J. Hirschauer, B. Jayatilaka, S. Jindariani, M. Johnson, U. Joshi, T. Klijnsma, B. Klima, K.H.M. Kwok, S. Lammel, C. Lee, D. Lincoln, R. Lipton, T. Liu, C. Madrid, K. Maeshima, C. Mantilla, D. Mason, P. McBride, P. Merkel, S. Mrenna, S. Nahn, J. Ngadiuba, D. Noonan, S. Norberg, V. Papadimitriou, N. Pastika, K. Pedro, C. Pena[85], F. Ravera, A. Reinsvold Hall[86], L. Ristori, M. Safdari, E. Sexton-Kennedy, N. Smith, A. Soha, L. Spiegel, S. Stoynev, J. Strait, L. Taylor, S. Tkaczyk, N.V. Tran, L. Uplegger, E.W. Vaandering, I. Zoi

Fermi National Accelerator Laboratory, Batavia, IL, USA

C. Aruta, P. Avery, D. Bourilkov, P. Chang, V. Cherepanov, R.D. Field, C. Huh, E. Koenig, M. Kolosova, J. Konigsberg, A. Korytov, K. Matchev, N. Menendez, G. Mitselmakher, K. Mohrman, A. Muthirakalayil Madhu, N. Rawal, S. Rosenzweig, Y. Takahashi, J. Wang

University of Florida, Gainesville, FL, USA

T. Adams, A. Al Kadhim, A. Askew, S. Bower, R. Hashmi, R.S. Kim, S. Kim, T. Kolberg, G. Martinez, H. Prosper, P.R. Prova, M. Wulansatiti, R. Yohay, J. Zhang

Florida State University, Tallahassee, FL, USA

B. Alsufyani, M.M. Baarmand, S. Butalla, S. Das, T. Elkafrawy[87], M. Hohlmann, E. Yanes

Florida Institute of Technology, Melbourne, FL, USA

M.R. Adams, A. Baty, C. Bennett, R. Cavanaugh, R. Escobar Franco, O. Evdokimov, C.E. Gerber, M. Hawksworth, A. Hingrajiya, D.J. Hofman, J.h. Lee, D.S. Lemos, A.H. Merrit, C. Mills, S. Nanda, G. Oh, B. Ozek, D. Pilipovic, R. Pradhan, E. Prifti, T. Roy, S. Rudrabhatla, N. Singh, M.B. Tonjes, N. Varelas, M.A. Wadud, Z. Ye, J. Yoo

University of Illinois Chicago, Chicago, IL, USA

M. Alhusseini, D. Blend, K. Dilsiz [88], L. Emediato, G. Karaman, O.K. Köseyan, J.-P. Merlo, A. Mestvirishvili [89], O. Neogi, H. Ogul [90], Y. Onel, A. Penzo, C. Snyder, E. Tiras [91]

The University of Iowa, Iowa City, IA, USA

B. Blumenfeld, L. Corcodilos, J. Davis, A.V. Gritsan, L. Kang, S. Kyriacou, P. Maksimovic, M. Roguljic, J. Roskes, S. Sekhar, M. Swartz

Johns Hopkins University, Baltimore, MD, USA

A. Abreu, L.F. Alcerro Alcerro, J. Anguiano, S. Arteaga Escatel, P. Baringer, A. Bean, Z. Flowers, D. Grove, J. King, G. Krintiras, M. Lazarovits, C. Le Mahieu, J. Marquez, M. Murray, M. Nickel, M. Pitt, S. Popescu [92], C. Rogan, C. Royon, S. Sanders, C. Smith, G. Wilson

The University of Kansas, Lawrence, KS, USA

B. Allmond, R. Gujju Gurunadha, A. Ivanov, K. Kaadze, Y. Maravin, J. Natoli, D. Roy, G. Sorrentino

Kansas State University, Manhattan, KS, USA

A. Baden, A. Belloni, J. Bistany-riebman, Y.M. Chen, S.C. Eno, N.J. Hadley, S. Jabeen, R.G. Kellogg, T. Koeth, B. Kronheim, Y. Lai, S. Lascio, A.C. Mignerey, S. Nabili, C. Palmer, C. Papageorgakis, M.M. Paranjpe, E. Popova [93], A. Shevelev, L. Wang

University of Maryland, College Park, MD, USA

J. Bendavid, I.A. Cali, P.c. Chou, M. D'Alfonso, J. Eysermans, C. Freer, G. Gomez-Ceballos, M. Goncharov, G. Grosso, P. Harris, D. Hoang, D. Kovalskyi, J. Krupa, L. Lavezzo, Y.-J. Lee, K. Long, C. Mcginn, A. Novak, M.I. Park, C. Paus, C. Reissel, C. Roland, G. Roland, S. Rothman, G.S.F. Stephans, Z. Wang, B. Wyslouch, T.J. Yang

Massachusetts Institute of Technology, Cambridge, MA, USA

B. Crossman, B.M. Joshi, C. Kapsiak, M. Krohn, D. Mahon, J. Mans, B. Marzocchi, M. Revering, R. Rusack, R. Saradhy, N. Strobbe

University of Minnesota, Minneapolis, MN, USA

K. Bloom, D.R. Claes, G. Haza, J. Hossain, C. Joo, I. Kravchenko, J.E. Siado, W. Tabb, A. Vagnerini, A. Wightman, F. Yan, D. Yu

University of Nebraska-Lincoln, Lincoln, NE, USA

H. Bandyopadhyay, L. Hay, H.w. Hsia, I. Iashvili, A. Kalogeropoulos, A. Kharchilava, M. Morris, D. Nguyen, S. Rappoccio, H. Rejeb Sfar, A. Williams, P. Young

State University of New York at Buffalo, Buffalo, NY, USA

G. Alverson, E. Barberis, J. Bonilla, B. Bylsma, M. Campana, J. Dervan, Y. Haddad, Y. Han, I. Israr, A. Krishna, J. Li, M. Lu, G. Madigan, R. Mccarthy, D.M. Morse, V. Nguyen, T. Orimoto, A. Parker, L. Skinnari, D. Wood

Northeastern University, Boston, MA, USA

J. Bueghly, S. Dittmer, K.A. Hahn, Y. Liu, M. Mcginnis, Y. Miao, D.G. Monk, M.H. Schmitt, A. Taliercio, M. Velasco

Northwestern University, Evanston, IL, USA

G. Agarwal, R. Band, R. Bucci, S. Castells, A. Das, R. Goldouzian, M. Hildreth, K.W. Ho, K. Hurtado Anampa, T. Ivanov, C. Jessop, K. Lannon, J. Lawrence, N. Loukas, L. Lutton, J. Mariano, N. Marinelli, I. Mcalister, T. McCauley, C. Mcgrady, C. Moore, Y. Musienko[14], H. Nelson, M. Osherson, A. Piccinelli, R. Ruchti, A. Townsend, Y. Wan, M. Wayne, H. Yockey, M. Zarucki, L. Zygala

University of Notre Dame, Notre Dame, IN, USA

A. Basnet, M. Carrigan, L.S. Durkin, C. Hill, M. Joyce, M. Nunez Ornelas, K. Wei, D.A. Wenzl, B.L. Winer, B.R. Yates

The Ohio State University, Columbus, OH, USA

H. Bouchamaoui, K. Coldham, P. Das, G. Dezoort, P. Elmer, A. Frankenthal, B. Greenberg, N. Haubrich, K. Kennedy, G. Kopp, S. Kwan, D. Lange, A. Loeliger, D. Marlow, I. Ojalvo, J. Olsen, D. Stickland, C. Tully, L.H. Vage

Princeton University, Princeton, NJ, USA

S. Malik, R. Sharma

University of Puerto Rico, Mayaguez, PR, USA

A.S. Bakshi, S. Chandra, R. Chawla, A. Gu, L. Gutay, M. Jones, A.W. Jung, A.M. Koshy, M. Liu, G. Negro, N. Neumeister, G. Paspalaki, S. Piperov, V. Scheurer, J.F. Schulte, M. Stojanovic, J. Thieman, A.K. Virdi, F. Wang, A. Wildridge, W. Xie, Y. Yao

Purdue University, West Lafayette, IN, USA

J. Dolen, N. Parashar, A. Pathak

Purdue University Northwest, Hammond, IN, USA

D. Acosta, T. Carnahan, K.M. Ecklund, P.J. Fernández Manteca, S. Freed, P. Gardner, F.J.M. Geurts, I. Krommydas, W. Li, J. Lin, O. Miguel Colin, B.P. Padley, R. Redjimi, J. Rotter, E. Yigitbasi, Y. Zhang

Rice University, Houston, TX, USA

A. Bodek, P. de Barbaro, R. Demina, J.L. Dulemba, A. Garcia-Bellido, O. Hindrichs, A. Khukhunaishvili, N. Parmar, P. Parygin[93], R. Taus

University of Rochester, Rochester, NY, USA

B. Chiarito, J.P. Chou, S.V. Clark, D. Gadkari, Y. Gershtein, E. Halkiadakis, M. Heindl, C. Houghton, D. Jaroslawski, S. Konstantinou, I. Laflotte, A. Lath, R. Montalvo, K. Nash, J. Reichert, H. Routray, P. Saha, S. Salur, S. Schnetzer, S. Somalwar, R. Stone, S.A. Thayil, S. Thomas, J. Vora, H. Wang

Rutgers, The State University of New Jersey, Piscataway, NJ, USA

D. Ally, A.G. Delannoy, S. Fiorendi, S. Higginbotham, T. Holmes, A.R. Kanuganti, N. Karunarathna, L. Lee, E. Nibigira, S. Spanier

University of Tennessee, Knoxville, TN, USA

D. Aebi, M. Ahmad, T. Akhter, K. Androsov[61], O. Bouhali[94], R. Eusebi, J. Gilmore, T. Huang, T. Kamon[95], H. Kim, S. Luo, R. Mueller, D. Overton, D. Rathjens, A. Safonov

Texas A&M University, College Station, TX, USA

N. Akchurin, J. Damgov, N. Gogate, V. Hegde, A. Hussain, Y. Kazhykarim, K. Lamichhane, S.W. Lee, A. Mankel, T. Peltola, I. Volobouev

Texas Tech University, Lubbock, TX, USA

E. Appelt, Y. Chen, S. Greene, A. Gurrola, W. Johns, R. Kunnawalkam Elayavalli, A. Melo, F. Romeo, P. Sheldon, S. Tuo, J. Velkovska, J. Viinikainen

Vanderbilt University, Nashville, TN, USA

B. Cardwell, H. Chung, B. Cox, J. Hakala, R. Hirosky, A. Ledovskoy, C. Neu

University of Virginia, Charlottesville, VA, USA

S. Bhattacharya, P.E. Karchin

Wayne State University, Detroit, MI, USA

A. Aravind, S. Banerjee, K. Black, T. Bose, E. Chavez, S. Dasu, P. Everaerts, C. Galloni, H. He, M. Herndon, A. Herve, C.K. Koraka, A. Lanaro, R. Loveless, J. Madhusudanan Sreekala, A. Mallampalli, A. Mohammadi, S. Mondal, G. Parida, L. Pétré, D. Pinna, A. Savin, V. Shang, V. Sharma, W.H. Smith, D. Teague, H.F. Tsoi, W. Vetens, A. Warden

University of Wisconsin - Madison, Madison, WI, USA

S. Afanasiev, V. Alexakhin, D. Budkouski, I. Golutvin[†], I. Gorbunov, V. Karjavine, V. Korenkov, A. Lanev, A. Malakhov, V. Matveev[96], V. Palichik, V. Perelygin, M. Savina, V. Shalaev, S. Shmatov, S. Shulha, V. Smirnov, O. Teryaev, N. Voytishin, B.S. Yuldashev[97], A. Zarubin, I. Zhizhin, G. Gavrilov, V. Golovtcov, Y. Ivanov, V. Kim[96], P. Levchenko[98], V. Murzin, V. Oreshkin, D. Sosnov, V. Sulimov, L. Uvarov, A. Vorobyev[†], Yu. Andreev, A. Dermenev, S. Gninenko, N. Golubev, A. Karneyeu, D. Kirpichnikov, M. Kirsanov, N. Krasnikov, I. Tlisova, A. Toropin, T. Aushev, K. Ivanov, V. Gavrilov, N. Lychkovskaya, A. Nikitenko[99,100], V. Popov, A. Zhokin, R. Chistov[96], M. Danilov[96], S. Polikarpov[96], V. Andreev, M. Azarkin, M. Kirakosyan, A. Terkulov, E. Boos, V. Bunichev, M. Dubinin[85], L. Dudko, A. Ershov, A. Gribushin, V. Klyukhin, O. Kodolova[100], S. Obraztsov, S. Petrushanko, V. Savrin, A. Snigirev, V. Blinov[96], T. Dimova[96], A. Kozyrev[96], O. Radchenko[96], Y. Skovpen[96], V. Kachanov, D. Konstantinov, S. Slabospitskii, A. Uzunian, A. Babaev, V. Borshch, D. Druzhkin[101]

Authors affiliated with an institute or an international laboratory covered by a cooperation agreement with CERN

[†] Deceased.
[1] Also at Yerevan State University, Yerevan, Armenia.
[2] Also at TU Wien, Vienna, Austria.
[3] Also at Ghent University, Ghent, Belgium.
[4] Also at Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil.
[5] Also at Universidade Estadual de Campinas, Campinas, Brazil.
[6] Also at Federal University of Rio Grande do Sul, Porto Alegre, Brazil.
[7] Also at University of Chinese Academy of Sciences, Beijing, China.
[8] Also at China Center of Advanced Science and Technology, Beijing, China.
[9] Also at University of Chinese Academy of Sciences, Beijing, China.
[10] Also at China Spallation Neutron Source, Guangdong, China.
[11] Now at Henan Normal University, Xinxiang, China.
[12] Also at University of Shanghai for Science and Technology, Shanghai, China.
[13] Now at The University of Iowa, Iowa City, Iowa, USA.
[14] Also at an institute or an international laboratory covered by a cooperation agreement with CERN.
[15] Also at Cairo University, Cairo, Egypt.

[16] Also at Suez University, Suez, Egypt.
[17] Now at British University in Egypt, Cairo, Egypt.
[18] Also at Purdue University, West Lafayette, Indiana, USA.
[19] Also at Université de Haute Alsace, Mulhouse, France.
[20] Also at Istinye University, Istanbul, Turkey.
[21] Also at Tbilisi State University, Tbilisi, Georgia.
[22] Also at The University of the State of Amazonas, Manaus, Brazil.
[23] Also at University of Hamburg, Hamburg, Germany.
[24] Also at RWTH Aachen University, III. Physikalisches Institut A, Aachen, Germany.
[25] Also at Bergische University Wuppertal (BUW), Wuppertal, Germany.
[26] Also at Brandenburg University of Technology, Cottbus, Germany.
[27] Also at Forschungszentrum Jülich, Juelich, Germany.
[28] Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
[29] Also at HUN-REN ATOMKI - Institute of Nuclear Research, Debrecen, Hungary.
[30] Now at Universitatea Babes-Bolyai - Facultatea de Fizica, Cluj-Napoca, Romania.
[31] Also at MTA-ELTE Lendület CMS Particle and Nuclear Physics Group, Eötvös Loránd University, Budapest, Hungary.
[32] Also at HUN-REN Wigner Research Centre for Physics, Budapest, Hungary.
[33] Also at Physics Department, Faculty of Science, Assiut University, Assiut, Egypt.
[34] Also at Punjab Agricultural University, Ludhiana, India.
[35] Also at University of Visva-Bharati, Santiniketan, India.
[36] Also at Indian Institute of Science (IISc), Bangalore, India.
[37] Also at Amity University Uttar Pradesh, Noida, India.
[38] Also at IIT Bhubaneswar, Bhubaneswar, India.
[39] Also at Institute of Physics, Bhubaneswar, India.
[40] Also at University of Hyderabad, Hyderabad, India.
[41] Also at Deutsches Elektronen-Synchrotron, Hamburg, Germany.
[42] Also at Isfahan University of Technology, Isfahan, Iran.
[43] Also at Sharif University of Technology, Tehran, Iran.
[44] Also at Department of Physics, University of Science and Technology of Mazandaran, Behshahr, Iran.
[45] Also at Department of Physics, Faculty of Science, Arak University, ARAK, Iran.
[46] Also at Helwan University, Cairo, Egypt.
[47] Also at Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Bologna, Italy.
[48] Also at Centro Siciliano di Fisica Nucleare e di Struttura Della Materia, Catania, Italy.
[49] Also at Università degli Studi Guglielmo Marconi, Roma, Italy.
[50] Also at Scuola Superiore Meridionale, Università di Napoli 'Federico II', Napoli, Italy.
[51] Also at Fermi National Accelerator Laboratory, Batavia, Illinois, USA.
[52] Also at Lulea University of Technology, Lulea, Sweden.
[53] Also at Laboratori Nazionali di Legnaro dell'INFN, Legnaro, Italy.
[54] Also at Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, Perugia, Italy.
[55] Also at Institut de Physique des 2 Infinis de Lyon (IP2I), Villeurbanne, France.
[56] Also at Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, Bangi, Malaysia.
[57] Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico.
[58] Also at Trincomalee Campus, Eastern University, Sri Lanka, Nilaveli, Sri Lanka.
[59] Also at Saegis Campus, Nugegoda, Sri Lanka.
[60] Also at National and Kapodistrian University of Athens, Athens, Greece.
[61] Also at Ecole Polytechnique Fédérale Lausanne, Lausanne, Switzerland.
[62] Also at University of Vienna, Vienna, Austria.
[63] Also at Universität Zürich, Zurich, Switzerland.
[64] Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria.
[65] Also at Laboratoire d'Annecy-le-Vieux de Physique des Particules, IN2P3-CNRS, Annecy-le-Vieux, France.
[66] Also at Near East University, Research Center of Experimental Health Science, Mersin, Turkey.
[67] Also at Konya Technical University, Konya, Turkey.
[68] Also at Izmir Bakircay University, Izmir, Turkey.
[69] Also at Adiyaman University, Adiyaman, Turkey.
[70] Also at Bozok Universitetesi Rektörlügü, Yozgat, Turkey.
[71] Also at Marmara University, Istanbul, Turkey.
[72] Also at Milli Savunma University, Istanbul, Turkey.
[73] Also at Kafkas University, Kars, Turkey.
[74] Now at Istanbul Okan University, Istanbul, Turkey.
[75] Also at Hacettepe University, Ankara, Turkey.
[76] Also at Erzincan Binali Yildirim University, Erzincan, Turkey.
[77] Also at Istanbul University - Cerrahpasa, Faculty of Engineering, Istanbul, Turkey.
[78] Also at Yildiz Technical University, Istanbul, Turkey.
[79] Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.
[80] Also at IPPP Durham University, Durham, United Kingdom.
[81] Also at Monash University, Faculty of Science, Clayton, Australia.
[82] Also at Università di Torino, Torino, Italy.
[83] Also at Bethel University, St. Paul, Minnesota, USA.
[84] Also at Karamanoğlu Mehmetbey University, Karaman, Turkey.
[85] Also at California Institute of Technology, Pasadena, California, USA.
[86] Also at United States Naval Academy, Annapolis, Maryland, USA.
[87] Also at Ain Shams University, Cairo, Egypt.
[88] Also at Bingol University, Bingol, Turkey.
[89] Also at Georgian Technical University, Tbilisi, Georgia.
[90] Also at Sinop University, Sinop, Turkey.
[91] Also at Erciyes University, Kayseri, Turkey.
[92] Also at Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Bucharest, Romania.
[93] Now at another institute or international laboratory covered by a cooperation agreement with CERN.
[94] Also at Texas A&M University at Qatar, Doha, Qatar.
[95] Also at Kyungpook National University, Daegu, Korea.

[96] Also at another institute or international laboratory covered by a cooperation agreement with CERN.
[97] Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan.
[98] Also at Northeastern University, Boston, Massachusetts, USA.
[99] Also at Imperial College, London, United Kingdom.
[100] Now at Yerevan Physics Institute, Yerevan, Armenia.
[101] Also at Universiteit Antwerpen, Antwerpen, Belgium.