

# Search for Higgs boson pair production in association with top-quark pairs using $196\text{ fb}^{-1}$ of proton–proton collision data at $\sqrt{s} = 13$ and 13.6 TeV with the ATLAS detector



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**ABSTRACT:** This paper presents the first search for non-resonant Higgs boson pair production in association with a top-quark pair ( $t\bar{t}HH$ ) using proton–proton collision data collected with the ATLAS detector at the Large Hadron Collider. The data sample corresponds to an integrated luminosity of  $196\text{ fb}^{-1}$ , comprising  $140\text{ fb}^{-1}$  at a centre-of-mass energy of  $\sqrt{s} = 13$  TeV and  $56\text{ fb}^{-1}$  at 13.6 TeV. The search targets three distinct final states expected from  $t\bar{t}HH$  decays: (i) one lepton (electron or muon) with at least five  $b$ -quarks, (ii) at least two  $b$ -quarks accompanied by two leptons with the same electric charges or multiple leptons, and (iii) at least three  $b$ -quarks with two photons. The  $t\bar{t}HH$  production cross-section, relative to its Standard Model prediction, is measured to be  $\mu_{t\bar{t}HH} = -3^{+11}_{-12}$ . This result corresponds to a 95% confidence-level upper limit of 20 times the Standard Model prediction for the  $t\bar{t}HH$  production cross-section, with an expected limit of 21. The Higgs effective field theory Wilson coefficient  $c_{t\bar{t}HH}$  is also constrained at the same confidence level to the range of  $-3.9 < c_{t\bar{t}HH} < 3.3$ , compared with the expected range of  $-4.0 < c_{t\bar{t}HH} < 3.5$ .

**KEYWORDS:** Hadron-Hadron Scattering

**ARXIV EPRINT:** [2603.13113](https://arxiv.org/abs/2603.13113)

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**1 Introduction**

The Standard Model of particle physics (SM) has proven to be an immensely successful theory in describing fundamental particles and their interactions. A crucial aspect of this theory is the Brout–Englert–Higgs mechanism [1–3] for the electroweak symmetry breaking (EWSB), which predicts the existence of a neutral scalar particle known as the Higgs boson ( $H$ ). Since its discovery in 2012 by the ATLAS and CMS collaborations [4, 5], substantial progress has been made in understanding the production processes and decay modes of the Higgs boson and its couplings to fermions and gauge bosons [6, 7]. However, the trilinear and quartic self-couplings of the Higgs boson remain only weakly constrained. These self-couplings are linked to the Higgs potential, which drives the EWSB, and can be studied through Higgs boson pair ( $HH$ ) production.

Following the discovery of the Higgs boson, the search for  $HH$  production has become a central focus of the physics programme at the Large Hadron Collider (LHC). Among the

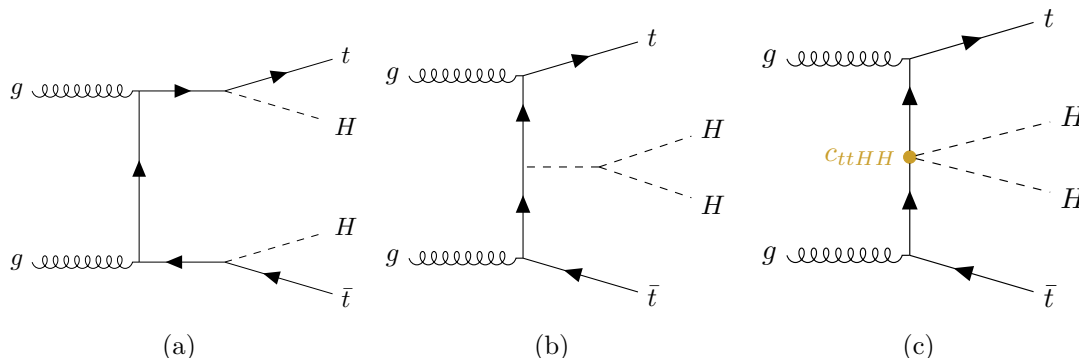


**Figure 1.** Examples of leading-order Feynman diagrams for the non-resonant  $t\bar{t}HH$  process. Each diagram depicts a distinct subprocess arising from different Higgs boson couplings: (a) the Higgs–top Yukawa coupling, (b) the Higgs–top Yukawa coupling and Higgs boson trilinear self-coupling, and (c) the non-SM  $t\bar{t}HH$  quartic coupling (highlighted with a circle), as described by the Higgs effective field theory.

primary  $HH$  production processes in proton–proton ( $pp$ ) collisions at the LHC, gluon–gluon fusion (ggF) and vector-boson fusion (VBF) processes have garnered the most attention due to their higher cross-sections. Various  $HH$  decay channels, such as  $b\bar{b}b\bar{b}$ ,  $b\bar{b}\gamma\gamma$ , and  $b\bar{b}\tau^+\tau^-$ , have been explored [8, 9]. The production of  $HH$  in association with a vector boson, known as the  $VHH$  process, has also been investigated [10, 11]. No evidence for  $HH$  production has been observed at the LHC. The combined 95% confidence level (CL) upper limit on the  $HH$  production cross-section, expressed relative to the SM prediction, is 2.9 from ATLAS [8], 3.5 from CMS [9] and 2.5 from their combination [12].

This paper presents the first search for Higgs boson pair production in association with a top-quark pair ( $t\bar{t}HH$ ), focusing on non-resonant  $HH$  production as predicted by the SM. The  $t\bar{t}HH$  process has the third largest  $HH$  production cross-section in the SM, after the ggF and VBF  $HH$  processes. Examples of the leading Feynman diagrams for the process are shown in figure 1.

In the SM, the  $t\bar{t}HH$  process has a predicted cross-section of  $\sigma_{t\bar{t}HH} = 0.756^{+4.3\%}_{-15.0\%}$  (scale)  $\pm 3.4\%$  (PDF +  $\alpha_s$ ) fb for  $pp$  collisions at  $\sqrt{s} = 13$  TeV and  $0.860^{+4.2\%}_{-14.0\%}$  (scale)  $\pm 3.3\%$  (PDF +  $\alpha_s$ ) fb at 13.6 TeV, calculated at next-to-leading order (NLO) in quantum chromodynamics (QCD) for a top-quark mass of  $m_t = 172.5$  GeV and a Higgs boson mass of  $m_H = 125$  GeV [13, 14]. The “PDF+ $\alpha_s$ ” uncertainty accounts for uncertainties in the parton distribution functions and strong coupling constant, the “scale” uncertainty is due to the finite order of QCD calculations. Approximately 81% of the cross-section arises from the Higgs–top Yukawa coupling diagram shown in figure 1(a), while about 8% originates from the diagram involving the Higgs boson self-coupling shown in figure 1(b). The remaining 11% results from constructive interference between the two diagrams. Although the  $t\bar{t}HH$  cross-section is sensitive to deviations of the Higgs boson self-coupling from its SM value, its dependence on the coupling modifier is considerably weaker than in the ggF and VBF  $HH$  production modes [13].

The analysis utilises the full LHC Run 2 data sample (2015–2018), corresponding to an integrated luminosity of  $140 \text{ fb}^{-1}$  collected with the ATLAS detector at a centre-of-mass energy  $\sqrt{s} = 13 \text{ TeV}$  and a Run 3 data sample (2022–2023) corresponding to  $56 \text{ fb}^{-1}$  at  $\sqrt{s} = 13.6 \text{ TeV}$ . The analysis is performed using the framework documented in ref. [15], developed within the ATLAS Collaboration for collision data analysis. The statistical interpretation is carried out using TREXFITTER framework [16].

Since the top quark decays almost exclusively into a  $W$  boson and a  $b$ -quark,  $t\bar{t}HH$  events can result in a variety of final states with two or more  $b$ -quarks, depending on the decay modes of the  $W$  and Higgs bosons. The search leverages the large branching ratio of the  $H \rightarrow b\bar{b}$  decay and the distinctive experimental signatures of leptons and photons. Three specific final states are considered. The first, labelled as 1L, is characterised by a single lepton ( $\ell = \text{electron or muon}$ ) and at least five  $b$ -quarks, capturing signals primarily from  $W \rightarrow \ell\nu$  and  $HH \rightarrow b\bar{b}b\bar{b}$  decays. The second, referred to as SSML, requires two or more  $b$ -quarks together with two leptons with the same electric charges (same-sign dilepton pair) or more than two leptons. It is designed to select events in which at least one  $W$  boson decays leptonically, with additional leptons potentially arising from Higgs boson decays (e.g.  $H \rightarrow \tau\tau, WW^*, ZZ^*$  decays). The third, referred to as  $b\bar{b}\gamma\gamma$ , consists of at least two  $b$ -quarks together with two photons, targeting  $HH \rightarrow b\bar{b}\gamma\gamma$  decays.

The effect of new physics introduced by a new  $t\bar{t}HH$  quartic interaction, shown in figure 1(c), can be modelled using an effective field theory (EFT) approach. The results are interpreted in the Higgs effective field theory (HEFT) framework [17–22], as it allows the  $t\bar{t}HH$  quartic interaction via the Wilson coefficient  $c_{t\bar{t}HH}$  to be directly targeted without affecting other Higgs boson couplings. Unlike the ggF  $HH$  channel, which includes additional Higgs–gluon couplings, the  $t\bar{t}HH$  channel is only affected by them at higher loop-order in weakly interacting theories, making the interpretation more robust.

This paper is structured as follows: Section 2 provides a brief overview of the ATLAS detector, and section 3 describes the data and Monte Carlo (MC) samples used in the analysis. The reconstruction and identification of the physics objects, along with the event-selection criteria, are summarised in section 4. The definitions of the signal and background regions, together with the background estimation methods, are presented in section 5, while the multivariate techniques employed for signal–background separation are outlined in section 6. Theoretical and experimental uncertainties are discussed in section 7, and the final results and the HEFT interpretation are given in sections 8 and 9, respectively. Finally, section 10 provides the conclusions.

## 2 ATLAS detector

The ATLAS experiment [23, 24] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a near  $4\pi$  coverage in solid angle.<sup>1</sup> It consists of an inner tracking detector surrounded by a thin superconducting solenoid

<sup>1</sup>ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the  $z$ -axis along the beam pipe. The  $x$ -axis points from the IP to the centre of the LHC ring, and the  $y$ -axis points upwards. Polar coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the  $z$ -axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as

providing a 2 T axial magnetic field, electromagnetic (EM) and hadronic calorimeters, and a muon spectrometer. The inner detector (ID) covers the pseudorapidity range  $|\eta| < 2.5$ . It consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors. Lead/liquid-argon (LAr) sampling calorimeters provide EM energy measurements with high granularity within the region  $|\eta| < 3.2$ . A steel/scintillator-tile hadronic calorimeter covers the central pseudorapidity range ( $|\eta| < 1.7$ ). The endcap and forward regions are instrumented with LAr calorimeters for EM and hadronic energy measurements up to  $|\eta| = 4.9$ . The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. The muon spectrometer includes a system of precision tracking chambers up to  $|\eta| = 2.7$  and fast detectors for triggering up to  $|\eta| = 2.4$ . The luminosity is measured mainly by the LUCID-2 detector that is located close to the beampipe. A two-level trigger system was used to select events [25, 26]. The first-level trigger is implemented in hardware and used a subset of the detector information to accept events at a rate close to 100 kHz. This is followed by a software-based trigger that reduced the accepted rate of complete events to 1.25 kHz and 3 kHz on average in Run 2 and Run 3, respectively, depending on the data-taking conditions. A software suite [27] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

### 3 Data and Monte Carlo samples

The data used in the 1L and SSML channels were collected using single-lepton (electron or muon) triggers with varying transverse momentum ( $p_T$ ) thresholds and isolation requirements [26, 28, 29]. The lowest  $p_T$  threshold ranged from 24 to 26 GeV for electrons and from 20 to 26 GeV for muons throughout the data-taking period covered by this search. Events in the  $b\bar{b}\gamma\gamma$  channel were collected with diphoton triggers [26, 28], with nominal transverse momentum of 35 (25) GeV for the leading (sub-leading) photon. Events are included in the search only if all relevant detector subsystems were confirmed to be in optimal operating condition [30], resulting in a total integrated luminosity of  $140.1 \pm 1.2 \text{ fb}^{-1}$  for the Run 2 data sample [31] and  $56.0 \pm 1.1 \text{ fb}^{-1}$  for the Run 3 data sample [32, 33].

MC simulations play a central role in signal modelling, efficiency determination, background estimation, and event selection optimisation. The simulated samples were produced using a variety of event generators, along with different programs for parton showering, hadronisation, and underlying event modelling, collectively referred to as soft-QCD processes below. The decays of bottom and charm hadrons were simulated using the EVTGEN program [34], except for samples generated by SHERPA [35]. Top quarks were decayed at leading order (LO) using MADSPIN [36, 37] to preserve spin correlations. All simulations assumed a top-quark mass of 172.5 GeV, a Higgs boson mass of 125 GeV, and the corresponding decay branching ratios [14]. Simulated processes were normalised to the most accurate theoretical cross-section predictions available.

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$\eta = -\ln \tan(\theta/2)$  and is equal to the rapidity  $y = \frac{1}{2} \ln \left( \frac{E+p_z}{E-p_z} \right)$  in the relativistic limit. Angular distance is measured in units of  $\Delta R \equiv \sqrt{(\Delta y)^2 + (\Delta \phi)^2}$ .

Table 1 summarises the nominal signal and background samples used in this search, and additional details of the signal and major background processes are provided in this section. Alternative samples employing different generators or parton-shower models are also used to evaluate modelling uncertainties. All samples were generated with statistics far exceeding those of the data, in most cases by more than two orders of magnitude. The MC samples were processed through an ATLAS detector simulation program [38], either using GEANT4 [39] or a fast simulation with parameterised calorimeter showers [40]. Pile-up effects, i.e. multiple interactions occurring within the same or nearby bunch crossings, were modelled by overlaying [41] the hard-scatter events with simulated inelastic  $pp$  collisions generated using the EPOS [42] and PYTHIA [43] programs. The distribution of the average number of interactions was matched to that observed in the data for each data-taking period.

For samples generated with POWHEGBOX [44–49], MADGRAPH (MG5) [50], and MADGRAPH5\_AMC@NLO (MG5\_AMC) [51], soft-QCD processes were modelled using PYTHIA with the NNPDF2.31o [52] parton distribution function (PDF) set and the A14 set of tuned parameters (tune) [53]. Samples generated with SHERPA used its native implementation of soft-QCD modelling. Events generated with the HERWIG7 [54–56] generator, together with the MMHT2014 NLO [57] PDF set and H7-UE tune, are used to assess systematic uncertainties associated with the modelling of soft-QCD processes.

The  $t\bar{t}HH$  signal samples were generated to cover all the final states considered in this analysis, with decay filters applied to ensure orthogonality at generator level. For the 1L channel, separate samples were produced for fully hadronic, single-leptonic, and dileptonic decays of the top-quark pairs, with the Higgs boson pair decaying as  $HH \rightarrow b\bar{b}b\bar{b}$ . To target the SSML final state, inclusive samples were generated with all possible top-quark and Higgs boson decays except  $HH \rightarrow b\bar{b}b\bar{b}$ , and were filtered to contain either a same-sign dilepton pair or at least three leptons. In both channels, the ggF and VBF  $HH$  contributions are found to be negligible and therefore are not considered. Dedicated samples with  $HH \rightarrow b\bar{b}\gamma\gamma$  decays were also produced. The signal samples were modelled with version 3.3.1 of the MADGRAPH (MG5) generator [50] at LO using NNPDF2.31o, and were interfaced to PYTHIA8 for parton-shower and underlying-event modelling using the A14 tune. The renormalisation ( $\mu_r$ ) and factorisation ( $\mu_f$ ) scales were set to  $H_T^{\text{scale}}/2$ , where  $H_T^{\text{scale}}$  is defined as the sum of the transverse masses  $\sqrt{p_T^2 + m^2}$  of all final-state partons. The  $t\bar{t}HH$  samples were normalised using the SM cross-section computed at NLO in QCD [13].

The three search channels have distinct background compositions due to their differing signal characteristics. In the 1L channel, the dominant background arises from  $t\bar{t}$  production accompanied by additional heavy-flavour jets. The SSML channel features a complex mixture, including contributions from top-quark pair production in association with a  $W$ ,  $Z$ , or Higgs boson, four top-quark production, and events containing charge-misidentified leptons or leptons originating from heavy-flavour decays. The  $b\bar{b}\gamma\gamma$  channel is affected by both continuum and resonant backgrounds: the former primarily from  $\gamma\gamma + \text{jets}$  processes, and the latter from single-Higgs or non- $t\bar{t}HH$  di-Higgs production. In all channels, MC simulation plays a central role in estimating background contributions, as detailed in section 5. A brief overview of the simulation of the major background processes is provided below.

| Process                              | Generator       | ME order  | Parton Shower | PDF set                 | Tune        |
|--------------------------------------|-----------------|-----------|---------------|-------------------------|-------------|
| $t\bar{t}HH$                         | MG5             | LO        | PYTHIA8       | NNPDF2.31o              | A14         |
| $t\bar{t}$ (5FS)                     | POWHEGBOX       | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $t\bar{t}t\bar{t}$                   | MG5_AMC         | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $t\bar{t}t$                          | MG5_AMC         | LO        | PYTHIA8       | NNPDF2.31o              | A14         |
| $t\bar{t}W$                          | SHERPA          | MEPS@NLO  | SHERPA        | NNPDF3.0nnlo            | SHERPA      |
| $t\bar{t}Z$                          | MG5_AMC         | NLO       | PYTHIA8       | NNPDF3.0nnlo            | A14         |
| $t\bar{t}WW$                         | MG5_AMC (MG5)   | LO        | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $t\bar{t}WZ, t\bar{t}WH, t\bar{t}ZZ$ | MG5             | LO        | PYTHIA8       | NNPDF2.31o              | A14         |
| $tW$                                 | POWHEGBOX       | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $tZ$                                 | MG5_AMC         | LO        | PYTHIA8       | NNPDF3.0NL0nf4          | A14         |
| $t(q)b$ ( $t$ -channel)              | POWHEGBOX       | NLO       | PYTHIA8       | NNPDF3.0NL0nf4          | A14         |
| $t(q)b$ ( $s$ -channel)              | POWHEGBOX       | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $tWZ, tHq, tHW$                      | MG5_AMC         | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |
| $V/VV/VVV + \text{jets}$             | SHERPA          | MEPS@NLO† | SHERPA        | NNPDF3.0nlo             | SHERPA      |
| $\gamma\gamma + \text{jets}$         | SHERPA          | NLO       | SHERPA        | NNPDF3.0nnlo            | A14         |
| $\gamma\gamma + t\bar{t}$            | MG5             | LO        | PYTHIA8       | NNPDF2.31o              | A14         |
| $ggF\ H$                             | NNLOPS [58, 59] | NLO       | PYTHIA8       | PDF4LHC15               | AZNLO (A14) |
| $VBF\ H$                             | POWHEGBOX       | NLO       | PYTHIA8       | PDF4LHC15 (PDF4LHC21)   | AZNLO (A14) |
| $VH$                                 | POWHEGBOX       | NLO       | PYTHIA8       | PDF4LHC15 (PDF4LHC21)   | AZNLO (A14) |
| $t\bar{t}H$                          | POWHEGBOX       | NLO       | PYTHIA8       | NNPDF3.0nlo (PDF4LHC21) | A14         |
| $ggF\ HH$                            | POWHEGBOX       | NLO       | PYTHIA8       | PDF4LHC21               | A14         |
| $VBF\ HH$                            | MG5             | NLO       | PYTHIA8       | NNPDF3.0nlo             | A14         |

† For the subdominant  $gg \rightarrow VV$  contribution, the ME calculation is at leading order.

**Table 1.** List of MC event generators and their associated matrix-element (ME) orders, parton showers, PDFs, and underlying set of tuned parameters used for simulating signal and background processes. When different from the Run 2 configuration, Run 3 settings are indicated in parentheses.

Top-quark pair production ( $t\bar{t}$ ) is a dominant background source in both the 1L and SSML channels. The process was modelled using a  $t\bar{t}$  sample generated in the five-flavour scheme (5FS) with the POWHEGBOX generator at NLO, in which  $b$ -quarks are treated as massless, and the NNPDF3.0nlo [60] PDF set. The  $h_{\text{damp}}$  parameter was set to 1.5 times of the top-quark mass ( $m_t$ ) in POWHEGBOX [61], and the `pThard` parameter was set zero in PYTHIA.<sup>2</sup> The  $\mu_r$  and  $\mu_f$  scales were set to the POWHEGBOX default choice of  $\sqrt{m_t^2 + p_T^2}$ , where  $p_T$  is the top-quark transverse momentum. The simulated sample was normalised to the SM prediction at next-to-next-to-leading order (NNLO) in QCD including next-to-next-to-leading logarithmic (NNLL) resummation, as computed with TOP++2 [62].

Top-quark pair production in association with a  $W$  boson ( $t\bar{t}W$ ) is one of the dominant background processes in the SSML channel. It was simulated using the SHERPA generator [35], which provides matrix-element calculations at NLO accuracy in QCD for up to one additional

<sup>2</sup>The  $h_{\text{damp}}$  parameter regulates the modelling of low- and high- $p_T$  radiation within POWHEGBOX, while `pThard` controls how PYTHIA vetos its own radiation to avoid double-counting emissions already generated by POWHEGBOX.

parton, and at LO accuracy for up to two additional partons [63–65], merged with the SHERPA parton shower through the MEPS@NLO prescription [66]. The  $\mu_r$  and  $\mu_f$  scales were set to be  $H_T^{\text{scale}}/2$  as for the  $t\bar{t}HH$  signal sample. Electroweak corrections up to orders  $\alpha^2\alpha_s^2$  and  $\alpha^3$  [67, 68] were included, along with real-emission contributions from subleading corrections at order  $\alpha^3\alpha_s$  [69]. The process was normalised to the SM cross-section computed at NNLO in QCD [70].

Top-quark pair production in association with a  $Z$  boson ( $t\bar{t}Z$ ) or a Higgs boson ( $t\bar{t}H$ ) constitute two other important background sources in the SSML channel. The  $t\bar{t}Z$  sample was simulated using MG5\_AMC at NLO with the NNPDF3.0nlo PDF set, with  $\mu_r$  and  $\mu_f$  both set to  $H_T^{\text{scale}}/2$ . It was normalised to the SM cross-section calculated at NLO in QCD and electroweak corrections [14, 71]. The  $t\bar{t}H$  sample was simulated using POWHEGBOX at NLO with the PDF set of NNPDF3.0nlo for Run 2 and PDF4LHC21 [72] for Run 3. The  $\mu_r$  and  $\mu_f$  scales were set to the geometric mean of the transverse mass of the three outgoing partons. The process was normalised to the SM cross-section calculated at NLO in QCD and electroweak corrections [14, 73–76].

The four-top-quark production process ( $t\bar{t}t\bar{t}$ ) also contributes significantly in the SSML channel. It was simulated using the MADGRAPH5\_AMC@NLO generator, which incorporates matrix-element calculations at NLO accuracy in QCD. The  $\mu_r$  and  $\mu_f$  scales were set to  $H_T^{\text{scale}}/2$ . The simulated sample was normalised to the SM cross-section computed at NLO in QCD, including electroweak corrections [69]. Together with the three-top-quark process ( $t\bar{t}t$ ), modelled at LO using MADGRAPH5\_AMC@NLO as described in ref. [77], these contributions are collectively referred to as the multi-top background in the following.

In the 1L and SSML channels, additional minor background processes, such as  $V/VV/VVV$  + jets and  $t\bar{t} + VV$ , are modelled using SHERPA at NLO and MADGRAPH at LO, respectively, as detailed in refs. [77–79].

For the  $b\bar{b}\gamma\gamma$  channel, the non-resonant diphoton background arises from processes with two prompt photons and events in which one or both photon candidates originate from misidentified jets. The normalisation of this background is determined entirely from data, while SHERPA MC samples with two prompt photons were used to model its kinematics. The resonant background contributions from single Higgs boson production (primarily ggF  $H$  and VBF  $H$ ) and non- $t\bar{t}HH$  Higgs boson pair production (mainly ggF  $HH$  and VBF  $HH$ ) were modelled using MC samples, most of which were generated with the POWHEGBOX generator as described in ref. [80].

#### 4 Analysis strategy, object identification, and event selection

Although all three channels target  $t\bar{t}HH$  production, their distinct signatures and background compositions require dedicated analysis strategies. The 1L and SSML final states feature relatively high signal and background rates, enabling analyses to be performed both on the combined Run 2 and Run 3 data samples and separately for each data-taking period. In contrast, the  $b\bar{b}\gamma\gamma$  final state offers a cleaner signature but suffers from limited numbers of events, motivating an analysis based solely on the combined data sample.

The 1L and SSML channels adopt similar methodologies, relying on both simulation and data for background estimation and employing transformer-based machine learning

techniques [81] to enhance signal-to-background discrimination. Potential  $t\bar{t}HH$  contributions are extracted through simultaneous fits to the transformer outputs in the signal regions and to selected fit variables in the background control regions. In the  $b\bar{b}\gamma\gamma$  channel, potential signals are identified using a strategy analogous to ref. [80], based on fits to the diphoton invariant-mass spectra. This method leverages the narrow Higgs boson resonance and the excellent diphoton mass resolution of the ATLAS detector, enabling a fully data-driven determination of the continuum background from the resonance sidebands.

The physics objects used in this analysis are summarised in section 4.1, with many shared across the three channels. The event selection criteria specific to each channel are then described in sections 4.2, 4.3, and 4.4. To be considered, an event must have a primary vertex (PV), defined as the vertex reconstructed with at least two ID tracks with  $p_T > 500$  MeV. If multiple PVs are present, the one with the largest sum of  $p_T^2$  of its associated tracks is chosen [82].

## 4.1 Object definition

Electrons are reconstructed by matching topological energy clusters in the EM calorimeter with tracks in the ID and are identified using likelihood-based criteria that incorporate calorimeter shower shape, track-to-cluster matching, and associated track quality requirements [83–85]. Electron candidates must have  $p_T > 15$  GeV and  $|\eta_{\text{cluster}}| < 2.47$ , excluding the transition region between the barrel and endcap calorimeters ( $1.37 < |\eta_{\text{cluster}}| < 1.52$ ). In the 1L channel, they are required to satisfy the *loose* identification likelihood and *loose* isolation criteria [83], whereas the SSML channel requires the *tight* identification likelihood and *tight* isolation criteria. Unless otherwise stated, the isolation criteria are based on combined tracking and calorimeter information.

Muons are reconstructed by combining tracks from the ID with those from the muon spectrometer [86, 87]. Muon candidates must have  $p_T > 15$  GeV and  $|\eta| < 2.5$ . In the 1L channel, they must satisfy the *loose* identification quality and *loose* track-based isolation requirements, while in the SSML channel they are required to meet the *medium* identification quality and *tight* isolation criteria [88].

To select leptons originating from the primary vertex, the transverse impact parameter, normalised by its estimated uncertainty ( $|d_0|/\sigma(d_0)$ ), must be less than five for electrons and three for muons, while the longitudinal impact parameter must satisfy  $|z_0 \sin \theta| < 0.5$  mm for both lepton flavours.

Photons are reconstructed from the topological energy clusters in the EM calorimeter [83–85]. Photon candidates are required to have  $|\eta_{\text{cluster}}| < 1.37$  or  $1.52 < |\eta_{\text{cluster}}| < 2.37$ . Photons are required to satisfy *tight* identification likelihood and *loose* track-based isolation criteria.

Jets are reconstructed using a particle-flow algorithm [89] that combines measurements from the ID and the calorimeters. The anti- $k_t$  algorithm [90] with a radius parameter of  $R = 0.4$  is employed. Jets are required to have  $p_T > 20$  GeV and  $|\eta| < 2.5$  and a calibration procedure is performed as described in refs. [91, 92]. To mitigate pile-up effects, the jet-vertex tagger (JVT) [93] is applied to jets with  $p_T < 60$  GeV and  $|\eta| < 2.4$ .

Jets originating from the hadronisation of  $b$ -quarks are identified (*b-tagged*) using the GN2 algorithm [94], a transformer-based neural network designed to predict the flavour of

reconstructed jets. The network takes as input per-track quantities and their associated uncertainties, along with the jet  $p_T$  and  $\eta$ . Its output scores are combined into a  $b$ -tagging discriminant. Five thresholds, referred to as working points (WP), are defined with average efficiencies of 65%, 70%, 77%, 85%, and 90% for tagging  $b$ -quark jets in simulated  $t\bar{t}$  events. A pseudo-continuous  $b$ -tagging (PCBT) score,  $w_{\text{PCBT}}$ , is assigned to each jet and represents the number of WPs it satisfies. The score starts at one for jets failing to satisfy any WP and increases by one for each successively tighter WP satisfied. It reaches a maximum value of  $w_{\text{PCBT}} = 6$  for jets satisfying the tightest 65% WP. In the following,  $N_b^{90\% (85\%, 77\%)}$  denotes the number of  $b$ -tagged jets satisfying the 90% (85%, 77%) WP. Another relevant variable is  $\sum_{\text{jet}} w_{\text{PCBT}}$ , defined as the sum of the  $w_{\text{PCBT}}$  scores of all jets in the event for which a valid  $w_{\text{PCBT}}$  is assigned.

The missing transverse momentum, with its magnitude denoted by  $E_T^{\text{miss}}$ , is defined as the negative vectorial sum of the  $p_T$  of all reconstructed and calibrated objects in the event. This sum also includes momenta from ID tracks matched to the primary vertex but not associated with any other reconstructed objects (soft term) [95].

A sequential overlap-removal procedure is applied independently in each channel to ensure that the same calorimeter energy deposit or track is not assigned to multiple reconstructed objects. The procedure uses the lepton selection described above for the 1L channel, whereas for the SSML channel the isolation requirements are removed from the lepton selection. For the  $b\bar{b}\gamma\gamma$  channel, the leptons considered in the removal procedure are selected using the *medium* identification requirement together with *loose* isolation criteria. The impact of the overlap-removal procedure on the search is negligible.

Channel-specific event selections are then applied to maximise the sensitivity of each channel.

## 4.2 1L selections

In the 1L channel, candidate events are required to contain exactly one lepton (electron or muon) with transverse momentum  $p_T > 27$  GeV, satisfying *tight* identification and isolation requirements. The selected lepton must be matched to a corresponding trigger-level object.  $E_T^{\text{miss}}$  is required to exceed 20 GeV, consistent with the presence of a neutrino from the leptonic top-quark decay.

Events are required to have at least six jets and at least four  $b$ -tagged jets identified with the GN2 algorithm using the 85% WP,  $N_b^{85\%} \geq 4$ . The nominal misidentification rates for this WP are approximately 20% for  $c$ -jets and 1% for light-flavour jets.

To mitigate the parton-shower limitations in the modelling of high jet multiplicities and low jet transverse momenta, an upper limit of eleven jets is imposed. Since signal  $t\bar{t}HH$  events are expected to exhibit substantial hadronic activity, the scalar sum of jet transverse momenta,  $H_T^{\text{jets}}$ , is required to be greater than 400 GeV.

## 4.3 SSML selections

The event selection for the SSML channel follows the strategy developed for studies of the  $t\bar{t}t\bar{t}$  production process, using the procedures detailed in refs. [96, 97]. Candidate events are required to contain at least two leptons with  $p_T > 15$  GeV, with the leading lepton required

to satisfy  $p_T > 27 \text{ GeV}$  and to be matched to a corresponding trigger-level object. Events are categorised into two sub-channels: same-sign dilepton (SS2L) and trilepton (3L). The SS2L sub-channel includes events with exactly two leptons of the same electric charge, while the 3L sub-channel includes events with three or more leptons.

To reduce background from charge mis-identification in  $Z \rightarrow e^+e^-$  processes, SS2L events with same-sign electrons must satisfy  $|m_{ee} - m_Z| > 10 \text{ GeV}$ . In the 3L sub-channel, all opposite-sign same-flavour lepton pairs are required to meet  $|m_{\ell\ell} - m_Z| > 10 \text{ GeV}$  to suppress contamination from  $Z$  boson decays.

#### 4.4 $b\bar{b}\gamma\gamma$ selections

The  $b\bar{b}\gamma\gamma$  channel targets the  $HH \rightarrow b\bar{b}\gamma\gamma$  decays of  $t\bar{t}HH$  events. The selection of the two photons follows the long-established ATLAS criteria [4, 80]. Events must contain exactly two photons with an invariant mass in the range of  $105 < m_{\gamma\gamma} < 160 \text{ GeV}$ . The leading (subleading) photon is required to satisfy the condition on the relative transverse momentum of  $p_T/m_{\gamma\gamma} > 35\%(25\%)$ , ensuring a uniform acceptance across the  $m_{\gamma\gamma}$  spectrum. This selection guarantees that both photons carry sufficient transverse momentum to be compatible with a Higgs boson decay, while suppressing backgrounds containing photons originating from QCD processes. In addition, events must contain at least two  $b$ -tagged jets selected with the 90% working point,  $N_b^{90\%} \geq 2$ .

### 5 Signal regions, control regions, and background estimation

Background contributions across the three channels are estimated by using one of three approaches: fully simulation-based, hybrid simulation-data, or fully data-driven methods. Processes that are well modelled or negligible are taken directly from MC simulation, while backgrounds that are difficult to simulate reliably use MC to describe their kinematic properties and data control regions (CR) to determine their normalisation. In the  $b\bar{b}\gamma\gamma$  search, where a narrow  $H \rightarrow \gamma\gamma$  resonance is targeted, the continuum background is extracted from the diphoton mass sidebands in data defined as  $105 < m_{\gamma\gamma} < 120 \text{ GeV} \cup 130 < m_{\gamma\gamma} < 160 \text{ GeV}$ . The following sections outline the specific strategies adopted for each channel.

#### 5.1 The 1L channel

In the 1L channel, two signal-enriched regions (SR),  $6b$  and  $5b_{\text{Hi}}$ , and two background-enriched CRs with negligible signal contamination,  $5b_{\text{Lo}}$  and  $4b_{\text{Hi}}$ , are defined based on the number of  $b$ -tagged jets satisfying different WP criteria. These regions are summarised in table 2. The SRs capture  $\sim 1.1\%$  of all the produced inclusive  $t\bar{t}HH$  signal events.

The dominant background in the 1L channel arises from  $t\bar{t}$  events with additional heavy-flavour (HF) jets, originating from  $b$ - or  $c$ -quarks produced primarily via gluon emissions from higher-order QCD processes. Previous ATLAS and CMS analyses [98–101] have shown that MC simulations systematically underestimate the production rate of these events. To correct for this discrepancy, the normalisations of the  $t\bar{t}$ +jets background components are adjusted using CRs, with corrections derived according to the flavour composition of the additional jets. Their kinematic distributions are modelled using MC simulation. The  $t\bar{t}$ +jets events are categorised according to the generator-level flavour of the extra jets, identified

| Region           | Type | $N_b^{85\%}$ | $N_b^{77\%}$ | Fit variable                        |
|------------------|------|--------------|--------------|-------------------------------------|
| $4b_{\text{Hi}}$ | CR   | 4            | 4            | $\sum_{\text{jet}} w_{\text{PCBT}}$ |
| $5b_{\text{Lo}}$ | CR   | 5            | $\leq 4$     | $\sum_{\text{jet}} w_{\text{PCBT}}$ |
| $5b_{\text{Hi}}$ | SR   | 5            | 5            | Transformer output                  |
| $6b$             | SR   | $\geq 6$     | —            | Transformer output                  |

**Table 2.** Definition of regions in the 1L channel, along with the variables used in the fit. The quantities  $N_b^{85\%}$  and  $N_b^{77\%}$  represent the number of  $b$ -tagged jets identified using the 85% and 77% efficiency working points, respectively.

via a hadron–jet matching algorithm described in ref. [78]. Five categories are defined:  $t\bar{t} + \geq 1c/l(\text{light})$ ,  $t\bar{t} + 1b$ ,  $t\bar{t} + 2b$ ,  $t\bar{t} + 3b$ , and  $t\bar{t} + \geq 4b$ .

The normalisation factors (NF) for each  $t\bar{t}$ +jets category are determined simultaneously with the signal strength (see section 8) using a profile likelihood fit that incorporates both the signal and CRs defined in table 2, along with the corresponding fitting variables in each region. Pre-fit normalisations are taken directly from the generator cross-section predictions. Each category is treated as an independent process and assigned its own modelling uncertainties. The post-fit normalisations of the dominant components,  $t\bar{t} + 1b$  and  $t\bar{t} + 2b$ , are extracted through unconstrained parameters in the fit, allowing them to adjust freely to the observed data. Due to the limited constraining power of the data, the  $t\bar{t} + \geq 1c/l$ ,  $t\bar{t} + 3b$ , and  $t\bar{t} + \geq 4b$  components are normalised to their MC predictions, with associated systematic uncertainties discussed in section 7. Other minor background contributions ( $V/VV/VVV$ ,  $t\bar{t}V$ ,  $t\bar{t}H$ , multi-top and  $V(V, VV)$ +jets) are also estimated by using MC simulation.

## 5.2 The SSML channel

In the SSML channel, the SRs are defined as follows. Events in the SS2L category are required to have at least six jets, while those in the 3L category must contain at least five jets. In both cases, at least two jets must be  $b$ -tagged using the 85% WP, i.e.  $N_b^{85\%} \geq 2$ . Additionally, the scalar sum of the transverse momentum of jets and leptons,  $H_{\text{T}}^{\text{all}}$ , must exceed 400 GeV. In this channel, the SRs capture approximately 0.75% of all produced  $t\bar{t}HH$  signal events.

Background contributions in the SSML channel are classified into two main types: physics backgrounds and instrumental backgrounds. Physics backgrounds originate from processes that produce final states similar to those targeted by the SSML selection, including  $VV$ ,  $VVV$ ,  $t\bar{t}V$ ,  $t\bar{t}H$ ,  $t\bar{t}VV$ , and multi-top. In these processes, leptons arise from the prompt decays of heavy bosons ( $W$ ,  $Z$ , and  $H$ ). Among these background sources,  $t\bar{t}V$ ,  $t\bar{t}H$ , and multi-top constitute the dominant contributions limiting the search sensitivity.

All physics backgrounds, except for  $t\bar{t}W$ , are estimated by using MC simulations. For  $t\bar{t}W$ , its kinematic properties are modelled using MC, while a dedicated CR is employed to constrain its normalisation using data. This is achieved through a template fit to the jet multiplicity distribution ( $N_j$ ) in the  $t\bar{t}W$  CR. This approach accounts for a potentially enhanced  $t\bar{t}W$  production cross-section relative to the SM prediction, motivated by recent measurements [79, 102]. The selection criteria for this CR are given in table 3. The

requirements for this and other CRs described below are designed to enhance contributions from the targeted background sources while remaining orthogonal to the SR.

Instrumental backgrounds originate from leptons with misidentified charge (QmisID) and non-prompt leptons from photon conversions, heavy-flavour quark decays, and jets misidentified as leptons (Fake/non-prompt). The main process contributing to these backgrounds is  $t\bar{t}$  production. These backgrounds are challenging to simulate accurately and are therefore evaluated using a combination of MC and data-driven techniques, following the methodology described in ref. [97].

QmisID primarily affects the SS2L  $ee$  and  $e\mu$  channels, as electron identification is particularly susceptible to charge misidentification due to bremsstrahlung radiation followed by photon conversion. In Run 2 data, a boosted decision tree (BDT) based electron charge identification (ECID) tool is employed to significantly reduce the QmisID contribution [83]. The ECID tool combines tracking information with the magnitude and spatial pattern of bremsstrahlung radiation to reject electrons whose charges are likely mismeasured. However, this tool is not yet available for the Run 3 data sample, resulting in an increased QmisID background.

The charge misidentification rate is derived from  $Z \rightarrow e^+e^-$  events in data, selected with  $|m_{ee} - m_Z| < 10 \text{ GeV}$  and no charge requirement. The rate is determined from the fraction of same-sign electron pairs and parameterised as a function of the electron  $p_T$  and  $\eta$ . It is then applied to the  $ee$  and  $e\mu$  data events passing the SS2L selection, excluding the charge requirement, to estimate the QmisID background contribution. In Run 2, the rate ranges from 0.004% for electrons with  $p_T < 60 \text{ GeV}$  in the central region to 4% for those with  $p_T > 130 \text{ GeV}$  in the forward region. In Run 3, the rate increases by a factor of 2–5 depending on the electron  $p_T$  and  $|\eta|$ .

Backgrounds from photon conversions,  $\gamma^{(*)} \rightarrow e^+e^-$ , occurring either at the primary vertex or within the detector material, can lead to only one of the electrons being reconstructed. A conversion electron is identified through its small invariant mass with a nearby reconstructed track. It is classified as an internal conversion (Int. Conv.),  $\gamma^* \rightarrow e^+e^-$ , if the associated track points to the primary vertex, or as a material conversion (Mat. Conv.),  $\gamma \rightarrow e^+e^-$ , if the track instead points to a conversion vertex in the detector material. Leptons from heavy-flavour ( $b$ - and  $c$ -quark) decays generally fail to satisfy the identification criteria designed for prompt leptons from vector boson decays. However, a small fraction satisfy the selection and contribute to the non-prompt lepton background.

Similar to the  $t\bar{t}W$  background, CRs are used to improve the estimates of these fake/non-prompt lepton background contributions. MC predictions are scaled by NFs derived from a template fit to data in all the CRs, defined in table 3. Each CR targets a specific background source: ‘Int. Conv.’ for virtual photon conversions at the primary vertex, ‘Mat. Conv.’ for real photon conversions in the detector material, ‘HF  $e$ ’ for electrons from heavy flavour decays, and ‘HF  $\mu$ ’ for muons from heavy flavour decays. The selection criteria leverage the characteristic features of these background processes to enhance their contributions while ensuring orthogonality among all CRs and the SR. The distributions of event variables used in the fits are listed in the table.

| Region      | Channel                 | $N_j$                | $N_b^{85\%}$ | Other selection                                                                                                                                                                              | Fit variable          |
|-------------|-------------------------|----------------------|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|
| SR          | SS2L<br>3L              | $\geq 6$<br>$\geq 5$ | $\geq 2$     | $H_T^{\text{all}} > 400 \text{ GeV}$                                                                                                                                                         | Transformer<br>output |
| $t\bar{t}W$ | SS2L $e\mu, \mu\mu$     | $\geq 4$             | $\geq 2$     | $p_T^{\ell_2} > 25 \text{ GeV},  \eta(e)  < 1.5$<br>If $N_b^{85\%} = 2$ : $H_T^{\text{all}} < 400 \text{ GeV}$ or $N_j < 6$<br>If $N_b^{85\%} \geq 3$ : $H_T^{\text{all}} < 400 \text{ GeV}$ | $N_j$                 |
| Int. Conv.  | SS2L $ee, e\mu$         | $4 \leq N_j < 6$     | $\geq 1$     | Only one $e$ from $\gamma^* \rightarrow ee$<br>No $e$ from $\gamma \rightarrow ee$                                                                                                           | $N_{\text{events}}$   |
| Mat. Conv.  | SS2L $ee, e\mu$         | $4 \leq N_j < 6$     | $\geq 1$     | Only one $e$ from $\gamma \rightarrow ee$<br>No $e$ from $\gamma^* \rightarrow ee$                                                                                                           | $N_{\text{events}}$   |
| HF $\mu$    | 3L $e\mu\mu, \mu\mu\mu$ | $\geq 1$             | $= 1$        | $E_T^{\text{miss}} > 35 \text{ GeV}$<br>$100 < H_T^{\text{all}} < 275 \text{ GeV}$<br>Total lepton charge $= \pm 1$                                                                          | $p_T^{\ell_3}$        |
| HF $e$      | 3L $eee, ee\mu$         | $\geq 1$             | $= 1$        | $E_T^{\text{miss}} > 35 \text{ GeV}$<br>$100 < H_T^{\text{all}} < 275 \text{ GeV}$<br>Total lepton charge $= \pm 1$                                                                          | $p_T^{\ell_3}$        |

**Table 3.** Definitions of signal and control regions in the SSML channel. In the 3L sub-channel, leptons are labelled as  $\ell_1, \ell_2$ , and  $\ell_3$  in decreasing order of  $p_T$ .  $N_j$ , and  $N_b^{85\%}$  denote the numbers of jets and  $b$ -tagged jets identified using the 85% working point.

For the Run 3 data, photon conversion CRs (Int. Conv. and Mat. Conv.) are not used due to the larger QmisID background contribution stemming from the absence of the ECID tool. Instead, the NFs obtained from the Run 2 data are used to estimate the conversion background contributions in Run 3 data.

Fake/non-prompt lepton background contributions from light hadron decays or misidentified jets are expected to be minimal and are estimated by using simulation without additional corrections.

### 5.3 The $b\bar{b}\gamma\gamma$ channel

Three SRs are defined for the  $b\bar{b}\gamma\gamma$  channel using BDTs, as described in section 6. The background model in this channel comprises a dominant non-resonant (continuum) component, along with several resonant contributions from Higgs boson production in the diphoton invariant-mass spectrum.

The continuum background primarily originates from  $\gamma\gamma$ +jets events, with smaller contributions from  $\gamma$ +jet or dijet events where one or two jets are misidentified as photons. Due to the tight event selection, this background is dominated by processes with associated heavy-flavour production. Therefore, two dedicated samples,  $\gamma\gamma b\bar{b}$  and  $t\bar{t}\gamma\gamma$  are used to model the continuum background composition and kinematics. MC simulation is used solely for optimising the event selection and for training multivariate classifiers.

The continuum background is modelled with an exponential function chosen using the spurious-signal procedure [103], which evaluates a broad range of candidate parameterisations. The exponential form is retained because it satisfies statistical criteria ensuring that it does

not artificially absorb or generate a signal. The exponential shape parameter is determined from data via an unbinned maximum-likelihood fit to the diphoton invariant mass distribution,  $m_{\gamma\gamma}$ , performed in the sidebands of all the  $b\bar{b}\gamma\gamma$  SRs described in section 6. The fit uses independent normalisations for each region while enforcing a common exponential shape correlated across them. Allowing the shape parameter to vary independently in each SR changes the overall sensitivity by less than 1%, and the resulting parameter values are consistent across regions within statistical uncertainties.

Resonant backgrounds from single Higgs boson production and non- $t\bar{t}HH$  Higgs boson pair production processes are modelled using simulated samples and are normalised to their corresponding theoretical cross-sections. Their shapes are described by double-sided Crystal Ball (DSCB) functions [104] derived from simulation.

The complete background model is thus constructed as the sum of the analytic continuum and resonant MC templates. A combined likelihood fit simultaneously determines the normalisations and the correlated continuum shape across the signal and sideband regions, while the resonant contributions remain constrained to their theoretical predictions.

## 6 Multivariate discriminants

Multivariate analysis techniques are employed to exploit the kinematic differences between signal and background events that satisfy the SR selection in the 1L and SSML channels. A transformer architecture is used, incorporating the scaled dot-product attention mechanism described in ref. [81].

MC samples are used to train the transformer models, which are designed to distinguish among various event classes, including both signals and backgrounds. The training process aims to minimise a loss function that quantifies the fraction of misclassified events within the training data samples.

Signal and background samples used to develop the transformer models are partitioned into three statistically independent subsamples: one for training (training set), one for hyperparameter optimisation (validation set), and one for performance evaluation (test set). This strategy facilitates the study and mitigation of over-training effects. The test set is also used to predict the expected signal and background distributions of the transformer output scores for the final statistical analyses. A  $k$ -fold method, with  $k = 3$  for 1L and  $k = 4$  for SSML, is performed by rotating the three sets in order to evaluate independently all data samples and maximise the number of MC events used in the final statistical analyses. The training is performed separately for the Run 2 and Run 3 data samples.

The input features to the transformer consist of kinematic variables, complemented by  $b$ -tagging. These include the momentum vectors  $(p_T, \eta, \phi)$  of leptons, jets and  $E_T^{\text{miss}}$ , along with the jet  $w_{\text{PCBT}}$  and the charge information for leptons.

For the 1L channel, a binary transformer classifier is trained to distinguish the  $t\bar{t}HH$  signal from all background processes. In contrast, the SSML channel employs a three-class training scheme to separately identify the  $t\bar{t}HH$  signal, the multi-top background, and all other backgrounds. The multi-top contribution is treated separately due to its comparatively large cross-section uncertainty. The transformer provides class-likelihood scores that are between zero and one for each event:  $p_{t\bar{t}HH}$  and  $p_{\text{bkgd}}$  in 1L and  $p_{t\bar{t}HH}$ ,  $p_{\text{multi-top}}$ , and  $p_{\text{others}}$

in SSML. These scores are used to construct discriminants,  $D_{1L}$  for 1L and  $D_{SSML}$  for SSML, for the final signal-background separation:

$$D_{1L} = p_{t\bar{t}HH}, \quad D_{SSML} = \ln \left( \frac{p_{t\bar{t}HH}}{0.2 \cdot p_{\text{multi-top}} + 0.8 \cdot p_{\text{others}}} \right).$$

The weights assigned to the multi-top and other background components in the SSML discriminant are optimised to maximise sensitivity to the  $t\bar{t}HH$  signal. These weights closely reflect the relative contributions of the corresponding background processes in the highest  $D_{SSML}$  regime.

The  $b\bar{b}\gamma\gamma$  channel employs a set of BDTs to define SRs of varying purities, rather than serving as the final discriminant. Signal-to-background discrimination is achieved through a multi-BDT strategy, implemented using the XGBOOST algorithm [105] and the OPTUNA framework [106] for hyperparameter optimisation.

Four independent BDTs, shown in figure 2, are trained on the combined Run 2 and Run 3 data samples to distinguish the  $t\bar{t}HH$  signal from the four major backgrounds:  $\gamma\gamma b\bar{b}$ ,  $t\bar{t}\gamma\gamma$ ,  $t\bar{t}H$ , and other Higgs processes. Key input features include the reconstructed di-Higgs boson invariant mass and the kinematics of photons and  $b$ -tagged jets. Training is validated with independent test samples, and overtraining is assessed by comparing training and test BDT-score distributions. Three mutually exclusive SRs (SR1, SR2, and SR3), ordered from the lowest to highest sensitivity, are defined for events with  $N_b^{90\%} \geq 3$  using three thresholds ( $c_i^1 < c_i^2 < c_i^3$ ) on each of the four BDTs ( $i = 1, 2, 3, 4$ ). SR3 contains events satisfying all highest thresholds ( $c_i^3$ ), SR2 consists of events satisfying the intermediate thresholds ( $c_i^2$ ) but fail to satisfy the SR3 requirement. Finally SR1 includes events satisfying the baseline thresholds ( $c_i^1$ ), excluding those already assigned to SR2 or SR3. The threshold values,  $c_i^k$ , are optimised to maximise the expected signal significance within the diphoton mass window  $120 < m_{\gamma\gamma} < 130$  GeV, while ensuring at least three sideband events in each SR. In the  $b\bar{b}\gamma\gamma$  channel, the SRs retain approximately 0.05% of all  $t\bar{t}HH$  signal.

## 7 Systematic uncertainties

Systematic uncertainties in the  $t\bar{t}HH$  search are categorised into three main groups: experimental uncertainties, which affect reconstructed objects such as leptons, photons, and jets; theoretical uncertainties, related to the modelling of signal and background processes; and data-driven uncertainties, associated with background estimates derived from data. These uncertainties impact both the shape of kinematic distributions and the normalisation of signal and background contributions. While the specific objects and processes may vary across channels, the methodologies for evaluating experimental and theoretical uncertainties are similar. In contrast, the estimation of uncertainties for data-driven background contributions is channel-specific. In the 1L and SSML channels, systematic variations are propagated through the transformer-output templates used in the binned fit. For the  $b\bar{b}\gamma\gamma$  channel, the uncertainties are incorporated via the  $m_{\gamma\gamma}$  model (signal DSCB parameters and background-shape parameters) entering the unbinned fit in each category.

All three channels remain statistically limited, especially the  $b\bar{b}\gamma\gamma$  channel. The dominant systematic uncertainties stem from the modelling of  $t\bar{t}$  production with at least three  $b$ -jets

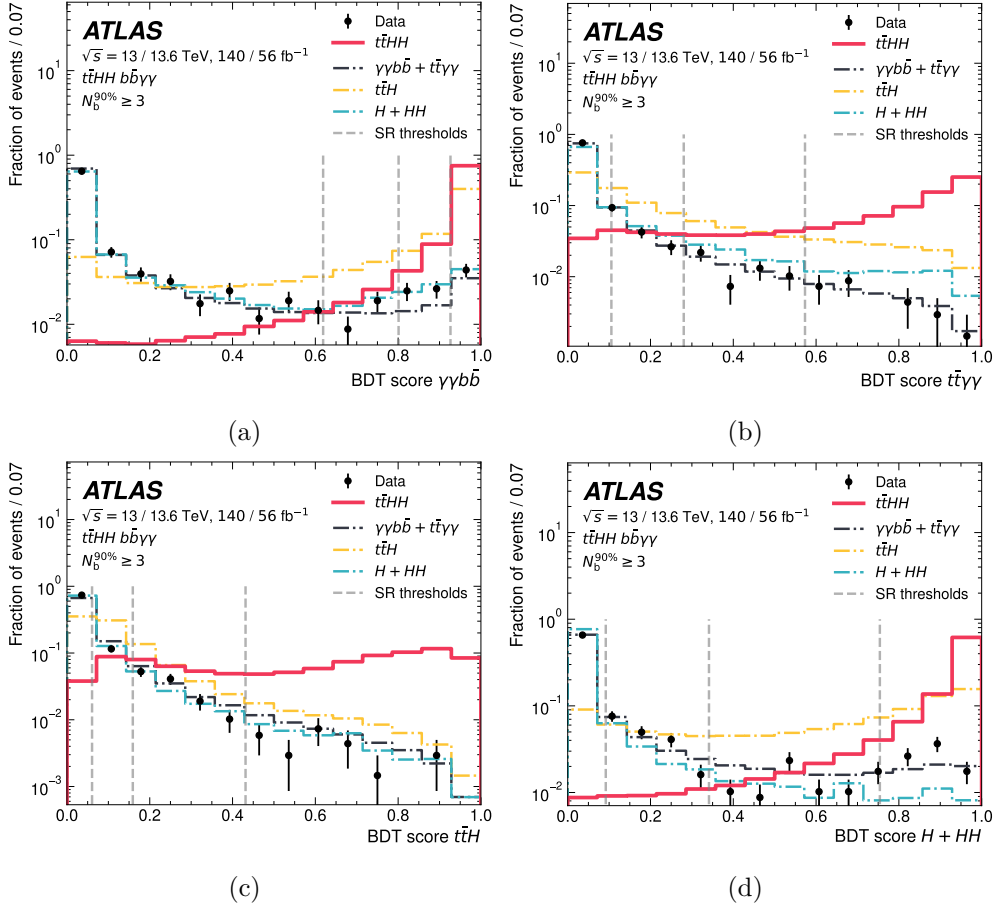


**Figure 2.** BDT score distributions obtained from the combined Run 2 and Run 3 data samples, used to discriminate the  $t\bar{t}HH$  signal from the main background processes: (a)  $\gamma\gamma b\bar{b}$ , (b)  $t\bar{t}\gamma\gamma$ , (c)  $t\bar{t}H$ , and (d) single Higgs boson and di-Higgs boson production. All histograms are normalised to unity. Vertical dashed lines indicate the BDT score thresholds used to define the signal regions, whose boundaries are determined simultaneously across the four BDT scores.

in the 1L channel, the theoretical uncertainty on the four-top production cross section in the SSML channel, and the modelling of  $t\bar{t}H$  production with extra heavy-flavour jets in the  $b\bar{b}\gamma\gamma$  channel.

The subsections below first describe systematic uncertainties common to all channels, followed by those specific to each channel and their corresponding impacts.

## 7.1 Experimental uncertainties

Jet-related uncertainties arise from several sources, including the jet energy scale (JES), jet energy resolution (JER), flavour tagging, and JVT used for pile-up rejection. JES and JER uncertainties are evaluated using control samples where jets recoil against well-calibrated reference objects — such as photons,  $Z$  bosons, or other calibrated jets [91]. Flavour tagging uncertainties originate from uncertainties in tagging efficiencies and misidentification rates. These are assessed using  $t\bar{t}$  events for  $b$ - and  $c$ -jets, and  $Z$ +jets events for light-quark and gluon jets [107–109]. Additional uncertainties are considered for the JVT efficiency [93].

Furthermore, a separate uncertainty is applied in simulation to account for differences in detector response between  $b$ -jets, light-quark jets and gluon jets.

Uncertainties in the reconstruction, identification, isolation and trigger efficiencies of electrons, photons, and muons are also considered, along with uncertainties in their energy scale and resolution [83, 88]. The latter uncertainties for jets and leptons are propagated to the calculation of  $E_T^{\text{miss}}$ , which also incorporates contributions from the modelling of the underlying event and the reconstruction efficiency of tracks used to compute the soft term [110].

The uncertainty in the integrated luminosity is 0.83% [31] for the Run 2 data sample, and 2.0% [32, 33] for the Run 3 data sample. These values are derived using the LUCID-2 detector [111], supplemented by measurements from the inner detector and calorimeters. An additional uncertainty is considered for corrections applied to the pile-up profile in simulated samples.

## 7.2 Theoretical uncertainties

Uncertainties in the modelling of signal and background processes arise from several sources: the PDFs,  $\alpha_s$ , missing higher-order QCD corrections in the partonic MEs, and initial- and final-state radiation (ISR and FSR). PDF uncertainties are evaluated following the PDF4LHC recommendations [72], while  $\alpha_s$  uncertainties are estimated by varying its value within the current measurement range. Uncertainties due to missing high-order corrections are assessed by varying the renormalisation and factorisation scales relative to their central values. Generator-related uncertainties are determined by comparing nominal predictions with those obtained using alternative generators or parton shower models, as specified in table 1. ISR and FSR uncertainties are evaluated by varying the renormalisation scales in the parton shower, as well as the renormalisation and factorisation scales in the MEs.

## 7.3 1L specific uncertainties

Modelling uncertainties for  $t\bar{t}$ +jets are evaluated by comparing the nominal POWHEG+PYTHIA 8 (5FS) sample with four alternative samples: POWHEG+PYTHIA 8 configurations with `pThard=1` and with  $h_{\text{damp}} = 3m_t$ , a POWHEG+HERWIG 7 sample, and a POWHEGBOXRES +HERWIG7 (4FS) sample. Each alternative generator and each  $t\bar{t}$ +jets component ( $t\bar{t} + c/l$ ,  $t\bar{t} + 1b$ ,  $t\bar{t} + 2b$ ,  $t\bar{t} + 3b$ , and  $t\bar{t} + \geq 4b$ ) is treated independently. The normalisations of the  $t\bar{t} + 1b$  and  $t\bar{t} + 2b$  components are constrained in data through two independent free NFs. For these two, the alternative samples are normalised to the nominal phase space, so that the uncertainties account for shape and acceptance effects, separated from overall normalisation variations. For the  $t\bar{t} + 3b$ ,  $t\bar{t} + \geq 4b$ , and the subdominant  $t\bar{t} + c/l$  components, additional normalisation uncertainties of 40%, 50%, and 6%, respectively, are assigned. These values are derived, for each component, from the sum in quadrature of the relative differences between the nominal prediction and all alternative samples. In this case, the alternative samples are not normalised to the nominal phase space. The resulting uncertainty includes their intrinsic normalisation differences and therefore includes normalisation, shape, and acceptance effects.

## 7.4 SSML specific uncertainties

For the SSML channel, a conservative uncertainty is assigned to the  $t\bar{t}t\bar{t}$  production. The ATLAS Collaboration has previously measured the  $t\bar{t}t\bar{t}$  cross-section to be about two standard deviations above the SM prediction [97]. To account for both the 15% theoretical uncertainty [69] and the discrepancy with the ATLAS measurement, normalisation uncertainties of  $^{+70\%}_{-15\%}$  are applied, similar to the approach taken in ref. [77]. These uncertainties are also applied to the minor  $t\bar{t}t\bar{t}$  background in the 1L channel.

Uncertainties in the fake/non-prompt lepton and QmisID background contributions are evaluated following the methodology outlined in ref. [97]. For the fake/non-prompt lepton background, only shape uncertainties in the distributions used in the template fit are considered, as their normalisations are free parameters in the fit. These uncertainties are estimated by comparing data with the background predictions in regions kinematically similar to the control regions. For the heavy-flavour non-prompt background, a loose lepton selection is employed, while for the conversion background, comparisons are made using  $\mu\mu\gamma^{(*)}$  events in the 3L sub-channel.

Additional systematic uncertainties associated with the ECID are also included. As discussed in section 5.2, the photon-conversion backgrounds for Run 3 are estimated by using the NFs derived from Run 2 data. Extra systematic uncertainties are applied to account for differences in event yields between the Run 3 and the Run 2 extrapolations without the ECID tool.

## 7.5 $b\bar{b}\gamma\gamma$ specific uncertainties

The dominant uncertainty in the continuum  $\gamma\gamma$ +jets background arises from the choice of analytic function for its modelling. This background modelling uncertainty is evaluated using the *spurious signal* method that quantifies the fitted signal yield obtained when a signal-plus-background fit is applied to background-only templates [103]. In all categories, the resulting bias is treated as a systematic uncertainty in the signal yield.

For resonant processes, a conservative 100% uncertainty is assigned to single and di-Higgs boson processes to account for modelling limitations in heavy-flavour-jet-associated production. An exception is made for  $t\bar{t}H$  production with additional heavy-flavour jets, for which a 50% normalisation uncertainty is assigned, derived from the measurement in refs. [98, 99].

## 8 Statistical analysis and results

To assess the compatibility of the observed data with background expectations and to search for the presence of a  $t\bar{t}HH$  signal, simultaneous maximum-likelihood fits are performed across the SRs and CRs. In the 1L and SSML channels, binned likelihood fits to data are performed using the transformer discriminant in the SRs and the fit variables listed in tables 2 and 3 for the CRs. For the  $b\bar{b}\gamma\gamma$  channel, an unbinned maximum-likelihood fit is performed to the diphoton invariant mass  $m_{\gamma\gamma}$  in each of the three BDT-defined SRs.

The parameter-of-interest (POI) in the fit is the signal strength,  $\mu_{t\bar{t}HH}$ , defined as the ratio of the observed  $t\bar{t}HH$  signal cross-section to the SM expectation. The fit also includes

normalisation parameters, which constrain background contributions using data from CRs in the 1L and SSML channels, and background parameters for the  $b\bar{b}\gamma\gamma$  channel. Systematic uncertainties are incorporated via nuisance parameters (NPs).

Likelihood functions are constructed separately for each SR and CR. In the 1L and SSML channels, the likelihood is built from binned Poisson probabilities of the corresponding fitting variable. In the  $b\bar{b}\gamma\gamma$  channel, the likelihood is unbinned and defined as the product of per-event probability densities evaluated at the observed  $m_{\gamma\gamma}$ . Gaussian or log-normal constraints are applied to the NPs in both cases. These individual likelihoods are then aggregated across all regions to form the final likelihood function, which is subsequently maximised in the fit.

For the 1L and SSML channels, the final likelihood function is:

$$\mathcal{L}(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta}) = \prod_r \left[ \prod_i^{N_{\text{bins}}^r} \text{Pois}(n_i^r | \nu_i^r(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta})) \right] \cdot G(\vec{\theta}),$$

where  $\prod_r$  denotes the product of all regions,  $\text{Pois}(n_i^r | \nu_i^r(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta}))$  represents the Poisson probability in bin  $i$  from region  $r$ , with  $n_i^r$  and  $\nu_i^r(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta})$  representing the observed and expected event counts, respectively. The variables  $\vec{\kappa}$  and  $\vec{\theta}$  correspond to NFs and NPs. The expected count in each bin is given by

$$\nu_i^r(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta}) = \mu_{t\bar{t}HH} S_i^r(\vec{\theta}) + B_i^r(\vec{\kappa}, \vec{\theta}), \quad (8.1)$$

where  $S_i^r$  is the expected signal yield from the SM, and  $B_i^r$  is the estimated background contribution, in bin  $i$  from region  $r$ . The function  $G(\vec{\theta})$  encodes the prior constraints on the NPs.

For  $b\bar{b}\gamma\gamma$ , the final likelihood function has the form:

$$\mathcal{L}(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta}) = \prod_r \left[ \text{Pois}(n_r | \nu_r(\mu_{t\bar{t}HH}, \vec{\kappa}, \vec{\theta})) \times \prod_i^{n_r} f_r(m_{\gamma\gamma}^i, \vec{\kappa}, \vec{\theta}) \right] \cdot G(\vec{\theta}).$$

Here  $n_r$  and  $\nu_r$  are the observed and expected event counts in region  $r$ , respectively. The function  $f_r(m_{\gamma\gamma}^i, \vec{\kappa}, \vec{\theta})$  represents the probability density for the diphoton mass of event  $i$  in the region  $r$ , summing over both signal and background contributions, analogous to eq. (8.1):

$$f_r(m_{\gamma\gamma}^i, \vec{\kappa}, \vec{\theta}) = \mu_{t\bar{t}HH} S_r(m_{\gamma\gamma}^i) + B_r(m_{\gamma\gamma}^i, \vec{\kappa}, \vec{\theta}) \quad (8.2)$$

where  $S_r$  and  $B_r$  denote the probability densities for the SM signal and background contributions in region  $r$ , respectively. The vector  $\vec{\kappa}$  parameterises the background model and  $G(\vec{\theta})$  represents the NP constraints as described above.

For the 1L and SSML channels, the Run 2 and Run 3 data samples are first fitted independently and then combined. In contrast, the  $b\bar{b}\gamma\gamma$  channel employs a single fit to the two data samples, motivated by the limited numbers of events and the similarity of their kinematic distributions. Experimental systematic uncertainties are assumed to be correlated across channels within the same run period, but uncorrelated between run periods except for most of the jet-related uncertainties, which are treated as correlated. Theoretical uncertainties in the process cross-sections are considered correlated across both run periods and all channels, while other modelling uncertainties are uncorrelated across run periods to

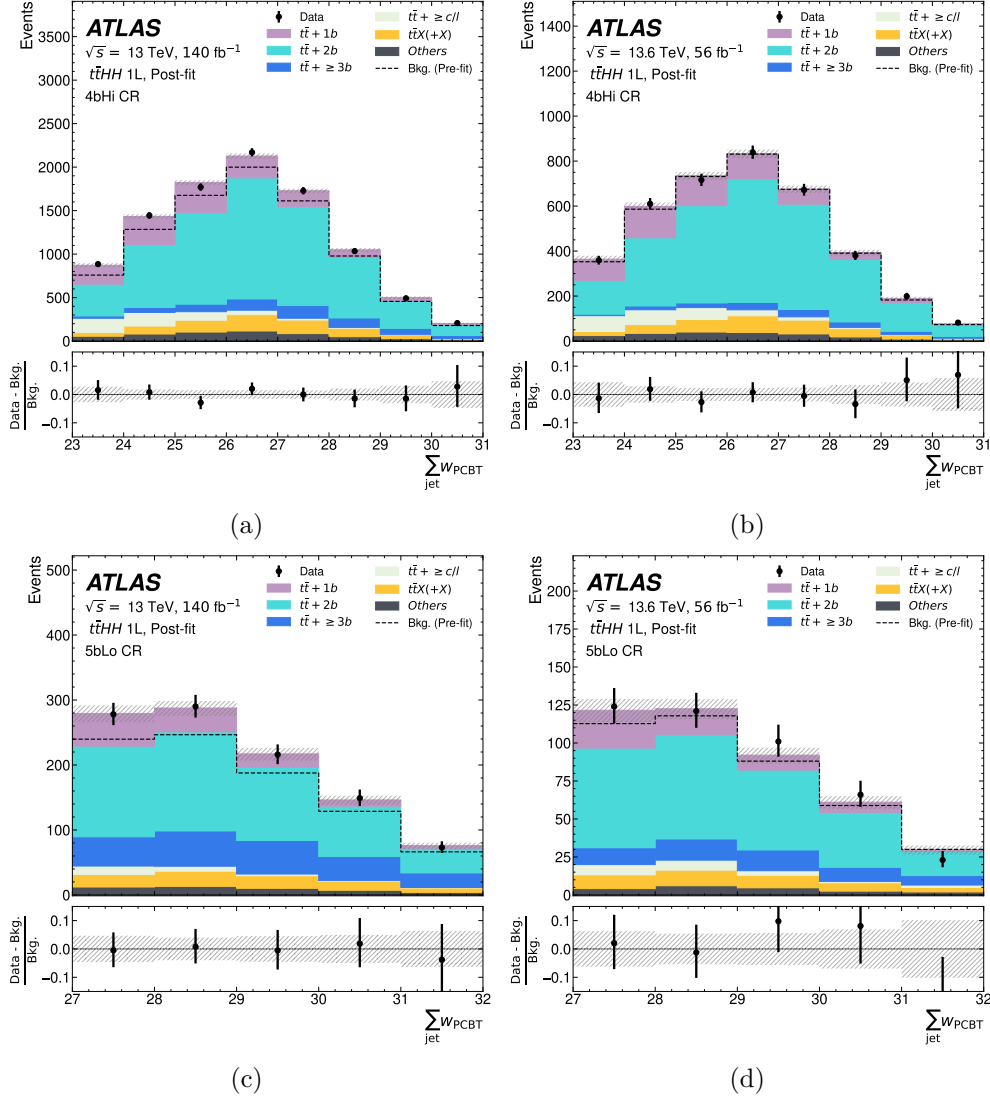


**Figure 3.** Distributions of the sum of jet pseudo-continuous  $b$ -tagging scores in the  $4b_{\text{Hi}}$  and  $5b_{\text{Lo}}$  control regions of the 1L channel for the (a, c) Run 2 and (b, d) Run 3 data samples, comparing the data with the post-fit stacked background predictions. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit background predictions are overlaid as dashed histograms.

account for differences in the MC generator configurations used in the two runs. The NFs for the  $t\bar{t} + 1b$ ,  $t\bar{t} + 2b$ , and  $t\bar{t}W$  processes, introduced to account for differences between data and theoretical predictions, are treated as correlated between the run periods, while all other NFs, related to instrumental backgrounds in the SSML channel, are kept uncorrelated.

The fits are performed under the signal-plus-background hypothesis. Good agreement is observed between the data and background expectations across all fit variables, for all channels and data-taking periods. Figures 3 and 4 show the post-fit background composition in the 1L and SSML CRs, respectively, for the combined Run 2 and Run 3 data samples.

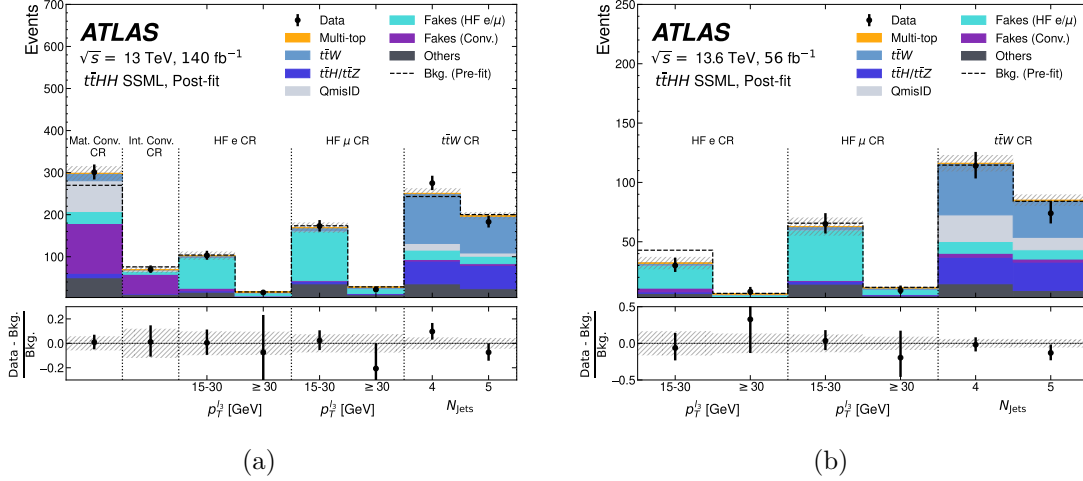


**Figure 4.** Distributions of the fit variables of the SSML control regions, using the same binning as in the fit, for the (a) Run 2 and (b) Run 3 data samples, comparing the data with the post-fit stacked background predictions. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit background predictions are overlaid as dashed histograms.

In the 1L channel, the post-fit NFs for the  $t\bar{t} + 1b$  and  $t\bar{t} + 2b$  processes are  $1.2 \pm 0.4$  and  $0.91 \pm 0.11$ , respectively, while in the SSML channel the  $t\bar{t}W$  NF is  $1.04 \pm 0.20$ . These NFs are consistent within uncertainties between Run 2 and Run 3.

The corresponding post-fit discriminant distributions are shown in figure 5 for the 1L channel and in figure 6 for the SSML channel, presented separately for the Run 2 and Run 3 data samples. Figure 7 shows the post-fit diphoton invariant mass distribution for the  $b\bar{b}\gamma\gamma$  channel, combining the Run 2 and Run 3 data samples. The measured signal-strength values are all compatible with the SM prediction of unity,  $\mu_{t\bar{t}HH}^{1L} = -5^{+15}_{-15}$  from 1L,  $\mu_{t\bar{t}HH}^{SSML} = 5^{+17}_{-21}$  from SSML, and  $\mu_{t\bar{t}HH}^{b\bar{b}\gamma\gamma} = -13^{+35}_{-6}$  from  $b\bar{b}\gamma\gamma$ . The asymmetry in the measured signal-strength uncertainty in the  $b\bar{b}\gamma\gamma$  channel arises from the physical constraint that the total expected event yield must remain non-negative. Combining three channels yields a best-fit signal-strength value of  $\mu_{t\bar{t}HH} = -3^{+11}_{-12}$ . Distributions of representative kinematic variables in the Run 2 signal regions are shown in figure 8 for 1L and figure 9 for SSML, demonstrating good agreement between the observed data and the post-fit background predictions. Comparable agreement is observed in Run 3.

Upper limits on the signal strength at the 95% CL are derived using the modified frequentist method [112], commonly referred to as the CL<sub>s</sub> method, and employing the  $\tilde{q}_\mu$  test statistic in the asymptotic approximation [113]. The observed (expected) 95% CL upper limits on the signal strength are 26 (29), 40 (38), and 75 (79) for the 1L, SSML, and  $b\bar{b}\gamma\gamma$  channels, respectively. In all cases, the expected limits are computed under the background-only hypothesis ( $\mu_{t\bar{t}HH} = 0$ ). Combining the three channels results in an observed upper limit of 20 at 95% CL, compared with an expected limit of 21. Figure 10 shows the observed and expected limits for the individual 1L, SSML, and  $b\bar{b}\gamma\gamma$  channels, as well as their combination.

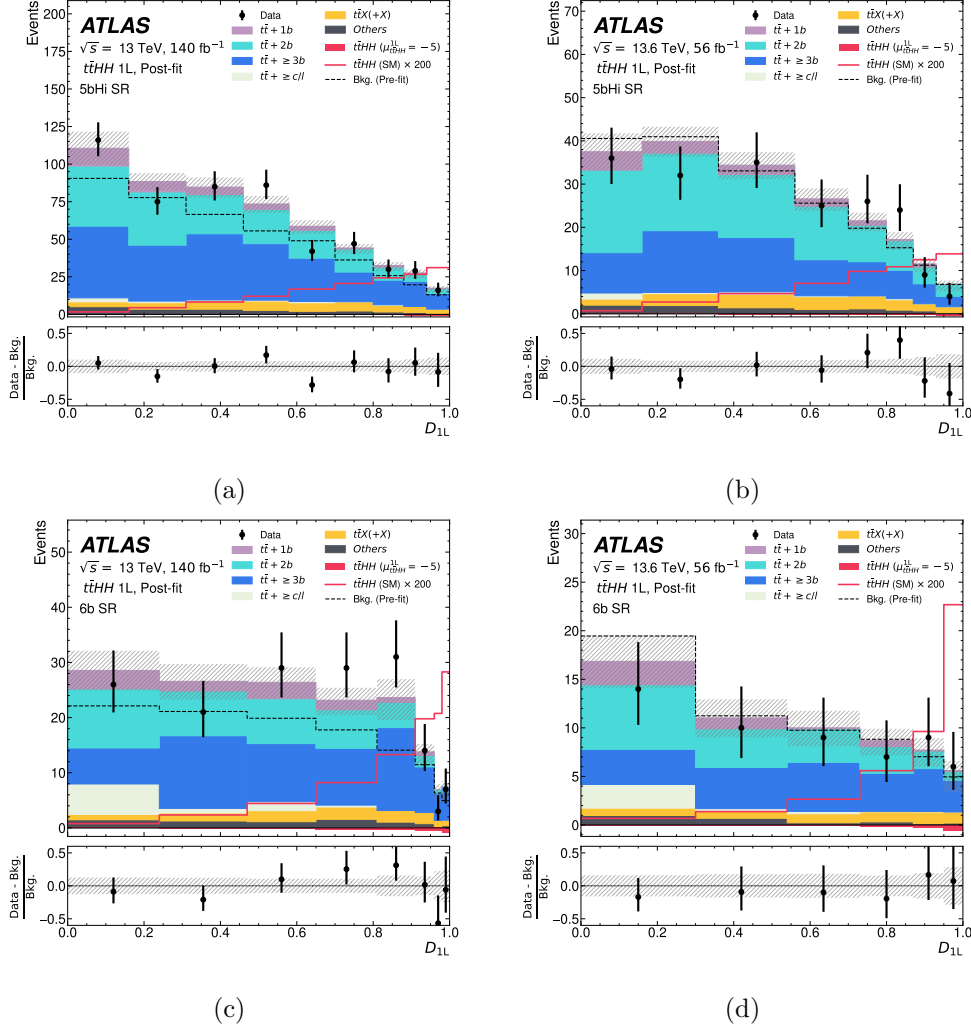


**Figure 5.** Distributions of the  $D_{1L}$  discriminant in the  $5b_{Hi}$  and  $6b$  signal regions of the 1L channel for the (a, c) Run 2 and (b, d) Run 3 data samples, comparing the data with the post-fit stacked background predictions. The observed  $t\bar{t}HH$  signal in this channel, corresponding to a measured signal strength of  $\mu_{t\bar{t}HH}^{1L} = -5^{+15}_{-15}$ , is overlaid as a negative contribution. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit background predictions are overlaid as dashed lines, and the SM  $t\bar{t}HH$  signal distribution — scaled up by a factor of 200 — are shown as solid lines.

For the 1L and SSML channels, the results from the Run 2 and Run 3 data samples are compatible within uncertainties, with the Run 2 data sample providing more stringent limits due to its larger integrated luminosity.

Table 4 summarises the breakdown of contributions to the observed and expected uncertainties,  $\Delta\mu_{t\bar{t}HH}$ , in the signal strength of the combined 1L, SSML, and  $b\bar{b}\gamma\gamma$  analysis from different groups of uncertainty sources. These breakdowns are derived by performing conditional profile-likelihood fits in which all NPs associated with a given uncertainty group are fixed to their best-fit values, while all remaining parameters are profiled. The uncer-

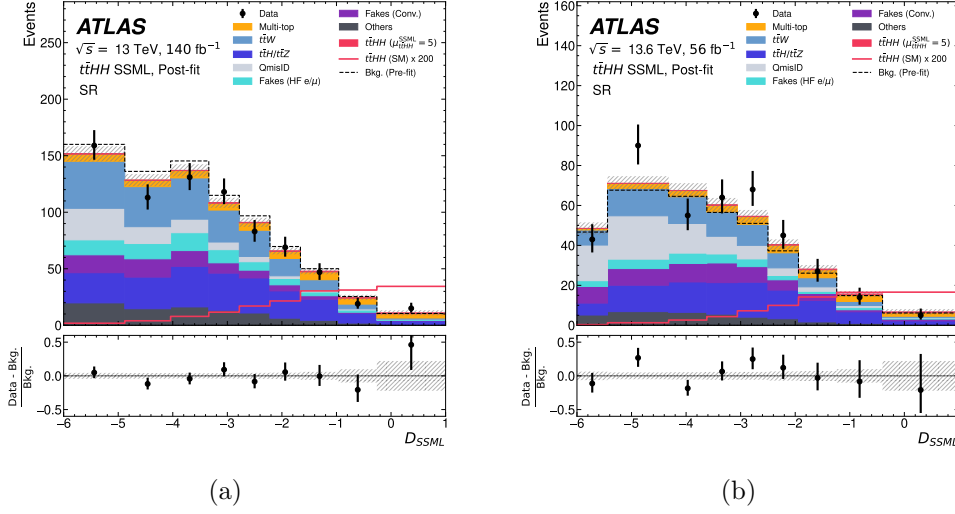


**Figure 6.** Distributions of the  $D_{\text{SSML}}$  discriminant in the SSML signal regions for the (a) Run 2 and (b) Run 3 data samples, comparing the data with the post-fit stacked signal-plus-background predictions. The observed  $t\bar{t}HH$  signal in this channel, corresponding to a measured signal strength of  $\mu_{t\bar{t}HH}^{\text{SSML}} = 5_{-21}^{+17}$ , is displayed stacked on top of the backgrounds. The first and last bins include contributions from underflow and overflow, respectively. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit background predictions are overlaid as dashed lines, and the SM  $t\bar{t}HH$  signal distribution — scaled up by a factor of 200 — are shown as solid lines.

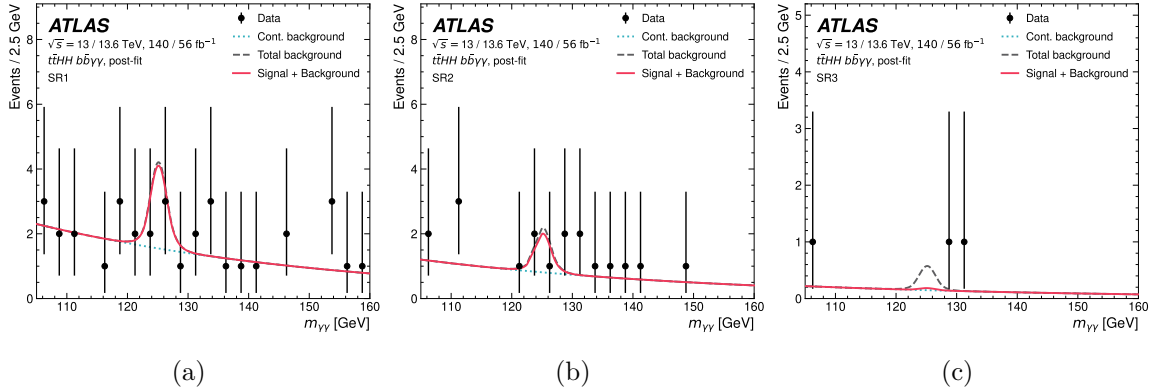


**Figure 7.** Comparison of the  $m_{\gamma\gamma}$  distributions between the observed data and the signal-plus-background fitted estimate (solid) for the  $b\bar{b}\gamma\gamma$  channel in the three signal regions: (a) SR1, (b) SR2 and (c) SR3, where SR1 is the least sensitive and SR3 the most sensitive. The continuous background (dotted) and the total background (dashed) are also shown. The observed  $t\bar{t}HH$  signal strength in this channel is  $\mu_{t\bar{t}HH}^{b\bar{b}\gamma\gamma} = -13_{-6}^{+35}$ .

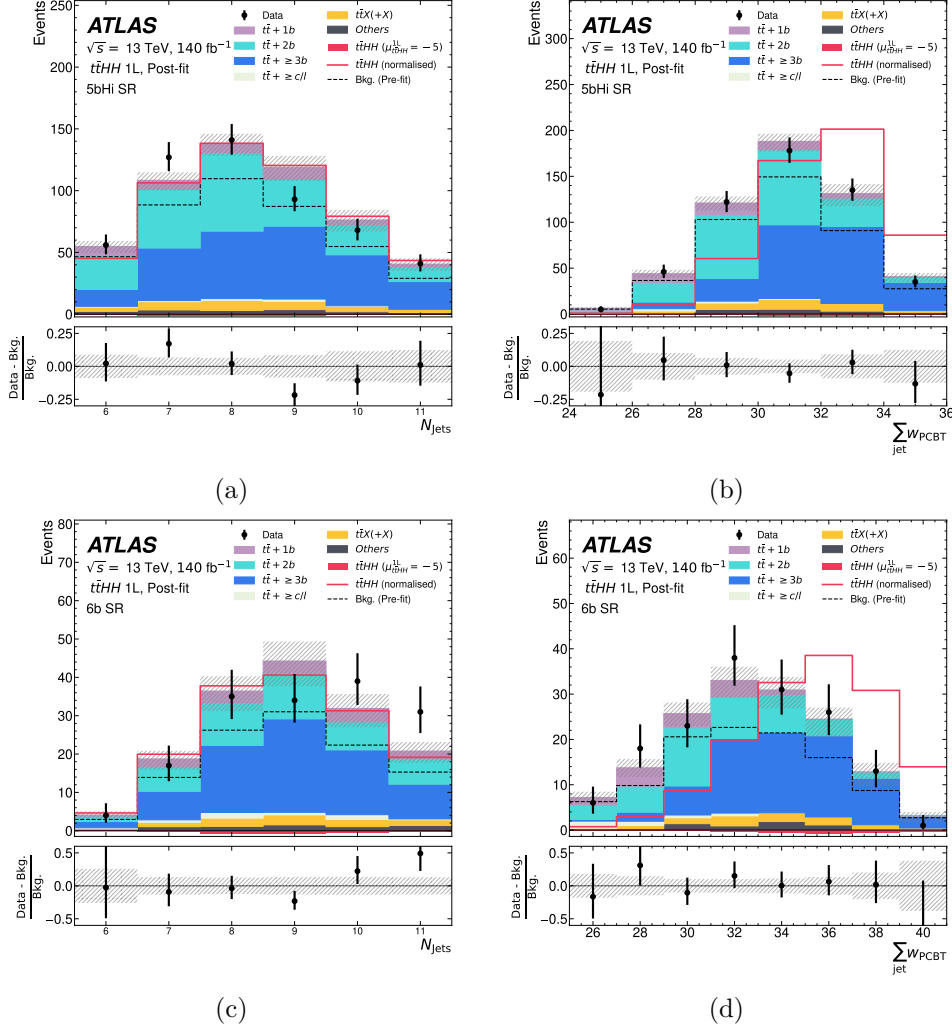


**Figure 8.** Distributions of the (a, c) jet multiplicity and (b, d) sum of pseudo-continuous  $b$ -tagging scores in the (a, b)  $5b_{\text{Hi}}$  and (c, d)  $6b$  signal regions of the 1L channel for the Run 2 data sample, comparing the data with the post-fit stacked background predictions. The fitted  $t\bar{t}HH$  signal in this channel,  $\mu_{t\bar{t}HH}^{1L} = -5^{+15}_{-15}$ , is overlaid as a negative contribution. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit backgrounds are overlaid as dashed lines, and the SM  $t\bar{t}HH$  signal distributions — normalised to the total background yield — are shown as solid lines.

tainty attributed to each group is then defined as the difference in quadrature between the total post-fit uncertainty and the uncertainty from the corresponding conditional fit. The expected breakdowns are evaluated assuming  $\mu_{t\bar{t}HH} = 1$ , and correlations among different groups are neglected. The systematic uncertainties are categorised into signal modelling, background modelling, number of MC events and detector systematic uncertainties, with the background-modelling contribution further decomposed by background source. The uncertainties from the floating NFs, which are limited by the available number of data events, are included in the data statistical uncertainty category. Data statistical and systematic

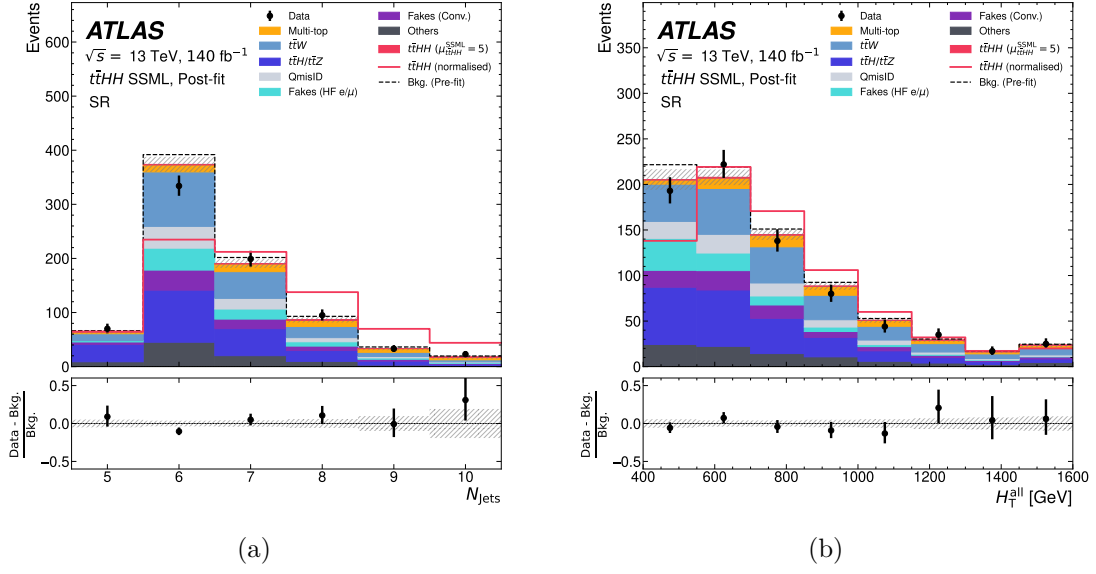


**Figure 9.** Distributions of the (a) jet multiplicity and (b)  $H_T^{\text{all}}$  in the SSML signal region for the Run 2 data sample, comparing the data with the post-fit stacked signal-plus-background predictions. The fitted  $t\bar{t}HH$  signal in this channel,  $\mu_{t\bar{t}HH}^{\text{SSML}} = 5_{-21}^{+17}$ , is shown stacked on top of the backgrounds. The first and last bins include contributions from underflow and overflow, respectively. The lower panels display the relative differences between the data and the background predictions. The hatched bands indicate the combined statistical and systematic uncertainties in the background predictions. For reference, the pre-fit backgrounds are overlaid as dashed lines, and the SM  $t\bar{t}HH$  signal distributions — normalised to the total background yield — are shown as solid lines.

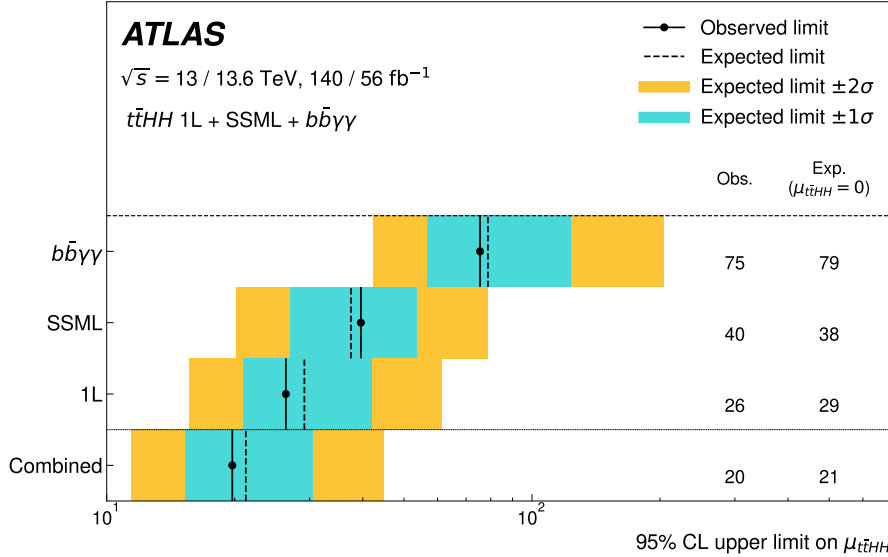


**Figure 10.** Observed and expected 95% CL upper limits on the signal strength from the individual 1L, SSML, and  $b\bar{b}\gamma\gamma$  channels, and from their combination. The expected limits are derived under the background-only hypothesis, i.e. assuming  $\mu_{t\bar{t}HH} = 0$ .

| Uncertainty Source   | Observed       | Expected       |
|----------------------|----------------|----------------|
| Signal modelling     | (+0.9, −1.8)   | (+1.3, −1.0)   |
| Background modelling | (+6.8, −8.2)   | (+5.7, −6.2)   |
| $t\bar{t}$ + jets    | (+5.3, −6.5)   | (+4.7, −5.0)   |
| $t\bar{t}t\bar{t}$   | (+4.6, −6.4)   | (+2.9, −4.0)   |
| $t\bar{t}H$          | (+2.1, −1.6)   | (+2.0, −1.9)   |
| others               | (+0.9, −0.7)   | (+0.9, −0.8)   |
| MC statistical       | (+2.8, −3.7)   | (+2.5, −2.7)   |
| Detector systematic  | (+2.2, −3.4)   | (+1.9, −1.5)   |
| Total systematic     | (+8.3, −9.4)   | (+7.3, −7.4)   |
| Data statistical     | (+7.2, −6.8)   | (+7.2, −6.7)   |
| Total                | (+11.0, −11.6) | (+10.3, −10.0) |

**Table 4.** Breakdowns of the contributions to the observed and expected uncertainties,  $\Delta\mu_{t\bar{t}HH}$ , in the signal strength of the combined 1L, SSML, and  $b\bar{b}\gamma\gamma$  analysis for different groups of uncertainty sources, neglecting correlations among groups.

uncertainties contribute comparably to the total uncertainty, while background modelling dominates the systematic uncertainty.

## 9 Higgs effective field theory interpretation

Beyond-the-SM (BSM) self-interactions of the Higgs boson, or its non-standard interactions with other gauge fields and fermions, could lead to modifications to the  $t\bar{t}HH$  event rate as well as affect the kinematic properties of the signal events. The results obtained with the two most sensitive channels of this analysis, i.e. the 1L and SSML channels, are thus interpreted in the context of the HEFT formalism, with a focus on anomalous interactions between Higgs boson pairs and top quark pairs.

Similarly to the SM effective field theory (SMEFT) [114, 115], HEFT assumes the SM field content. However, unlike in SMEFT, where the Higgs boson is part of an SU(2) doublet alongside unphysical Goldstone bosons, in HEFT the Higgs boson is a gauge singlet. This allows the Higgs boson dynamics to be decoupled from the symmetry-breaking pattern [116]. Consequently, HEFT enables more general deviations in Higgs boson couplings, which must be independently constrained through precision measurements, and features a more intricate power counting compared to SMEFT [117–119]. The HEFT approach employed in this study is implemented in a model specifically developed for this purpose and is interfaced through MADGRAPH [51] using the FeynRules UFO model format [120, 121].

State-of-the-art constraints on  $c_{t\bar{t}HH}$  have been derived from the ggF  $HH$  channel by both the ATLAS [8] and CMS [9] collaborations, ( $-0.19 < c_{t\bar{t}HH} < 0.7$  and  $-0.28 < c_{t\bar{t}HH} < 0.59$ , respectively), which remains the most sensitive channel to date for  $c_{t\bar{t}HH}$ . However, assuming a weakly interacting ultraviolet completion [122], ggF is parameterised by two additional Higgs–gluon couplings,  $c_{ggH}$  and  $c_{ggHH}$ , in comparison with  $t\bar{t}HH$  where these enter at higher

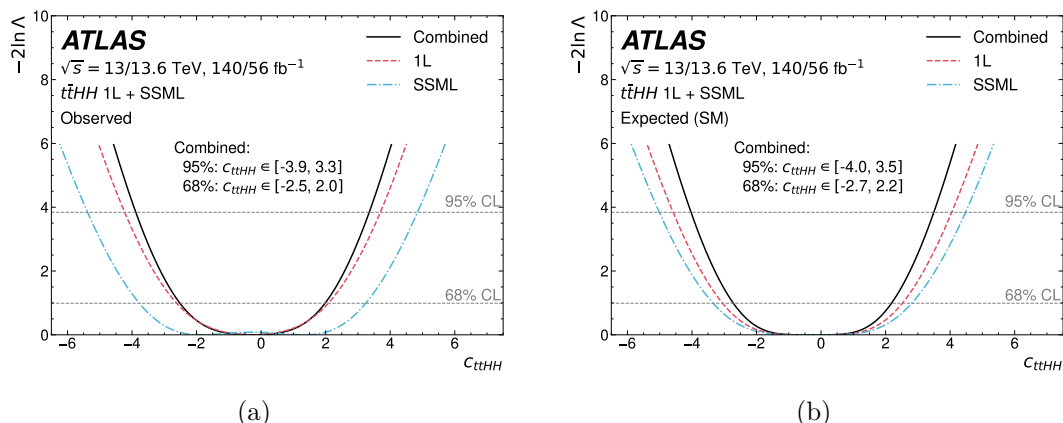


**Figure 11.** (a) Observed and (b) expected values of the profile likelihood as a function of  $c_{t\bar{t}HH}$  for the 1L channel (dashed curve), the SSML channel (dot-dashed curve), and their combination (solid curve).

loop order. As a result, obtaining robust bounds from ggF is more challenging unless further assumptions are imposed. The quoted limits are obtained by setting all other couplings of the Higgs boson to their SM values. Relaxing this assumption requires a multidimensional fit, weakening the obtained constraints. The work presented here aims to provide a complementary constraint on  $c_{t\bar{t}HH}$  independent of the ggF  $HH$  channel. The underlying assumption of the analysis, that only  $c_{t\bar{t}HH}$  differs from its SM value, is consistent with those used to derive the values for the ggF  $HH$  channel. In this context, only cross-section effects are considered, while acceptance and kinematic shape variations are not explicitly parameterised. Acceptance effects are evaluated for values of  $c_{t\bar{t}HH}$  close to the exclusion limits and are covered by an additional 30% uncertainty in the signal yield included in the measurement. An estimate of the kinematic-shape effects is found to impact the 95% CL interval on  $c_{t\bar{t}HH}$  by at most 10%, which is not included in the quoted limits.

The constraints on  $c_{t\bar{t}HH}$  are extracted from the same phase space as the rest of the analysis using the same multivariate discriminant described in section 6 and in the same analysis regions. The results are presented in figure 11. The  $c_{t\bar{t}HH}$  is constrained, at the 95% CL, in the range of  $-3.9 < c_{t\bar{t}HH} < 3.3$  for the observed results, while the expected range is  $-4.0 < c_{t\bar{t}HH} < 3.5$ . The expected profile exhibits a double-minimum structure due to the quadratic dependence of the signal cross-section on  $c_{t\bar{t}HH}$ . Given the observed results, the two minima are nearly degenerate, resulting in an almost flat region in the likelihood scan.

Benefiting from the quadratic dependence of the cross-section on  $c_{t\bar{t}HH}$ , the bounds derived in this analysis are only about one order of magnitude weaker than those obtained in the ggF  $HH$  channel in ref. [8], even though the predicted cross-section for  $t\bar{t}HH$  production is smaller by a factor of about 40.

## 10 Conclusion

The non-resonant production of Higgs boson pairs in association with top-quark pairs,  $t\bar{t}HH$ , is predicted to be a rare process in the SM. This paper describes the first search for this process using the full Run 2 data sample, corresponding to  $140 \text{ fb}^{-1}$  of  $pp$  collisions at  $\sqrt{s} = 13 \text{ TeV}$

collected between 2015 and 2018, and a Run 3 data sample of  $56 \text{ fb}^{-1}$  at  $\sqrt{s} = 13.6 \text{ TeV}$  collected between 2022 and 2023, recorded with the ATLAS detector at the LHC.

The presented  $t\bar{t}HH$  search targets the 1L, SSML, and  $b\bar{b}\gamma\gamma$  final states. The background contributions are estimated through a combination of simulation and data-driven techniques. Machine-learning-based discriminants are employed to improve separation between signal and background.

No significant excess above the background expectation is observed in any channel. A simultaneous fit across all the channels and analysis regions yields a measured signal-strength value of  $\mu_{t\bar{t}HH} = -3_{-12}^{+11}$ , consistent with the SM prediction, and results in an observed upper limit of  $\mu_{t\bar{t}HH} < 20$  at 95% CL. The results are further interpreted within the Higgs effective field theory framework, leading to a 95% CL interval on the  $t\bar{t}HH$  quartic interaction parameter of  $-3.9 < c_{t\bar{t}HH} < 3.3$ .

## Acknowledgments

We thank CERN for the very successful operation of the LHC and its injectors, as well as the support staff at CERN and at our institutions worldwide without whom ATLAS could not be operated efficiently.

The crucial computing support from all WLCG partners is acknowledged gratefully, in particular from CERN, the ATLAS Tier-1 facilities at TRIUMF/SFU (Canada), NDGF (Denmark, Norway, Sweden), CC-IN2P3 (France), KIT/GridKA (Germany), INFN-CNAF (Italy), NL-T1 (Netherlands), PIC (Spain), RAL (U.K.) and BNL (U.S.A.), the Tier-2 facilities worldwide and large non-WLCG resource providers. Major contributors of computing resources are listed in ref. [123].

We gratefully acknowledge the support of ANPCyT, Argentina; YerPhI, Armenia; ARC, Australia; BMWFW and FWF, Austria; ANAS, Azerbaijan; CNPq and FAPESP, Brazil; NSERC, NRC and CFI, Canada; CERN; ANID, Chile; CAS, MOST and NSFC, China; Minciencias, Colombia; MEYS CR, Czech Republic; DNRF and DNSRC, Denmark; IN2P3-CNRS and CEA-DRF/IRFU, France; SRNSFG, Georgia; BMFTR, HGF and MPG, Germany; GSRI, Greece; RGC and Hong Kong SAR, China; ICHEP and Academy of Sciences and Humanities, Israel; INFN, Italy; MEXT and JSPS, Japan; CNRST, Morocco; NWO, Netherlands; RCN, Norway; MNiSW, Poland; FCT, Portugal; MNE/IFA, Romania; MSTDI, Serbia; MSSR, Slovakia; ARIS and MVZI, Slovenia; DSI/NRF, South Africa; MICIU/AEI, Spain; SRC and Wallenberg Foundation, Sweden; SERI, SNSF and Cantons of Bern and Geneva, Switzerland; NSTC, Taipei; TENMAK, Türkiye; STFC/UKRI, United Kingdom; DOE and NSF, United States of America.

Individual groups and members have received support from BCKDF, CANARIE, CRC and DRAC, Canada; CERN-CZ, FORTE and PRIMUS, Czech Republic; COST, ERC, ERDF, Horizon 2020 and Marie Skłodowska-Curie Actions, European Union; Investissements d’Avenir Labex, Investissements d’Avenir Idex and ANR, France; DFG and AvH Foundation, Germany; Herakleitos, Thales and Aristeia programmes co-financed by EU-ESF and the Greek NSRF, Greece; BSF-NSF and MINERVA, Israel; NCN and NAWA, Poland; La Caixa Banking Foundation, CERCA and AGAUR programs from Generalitat de Catalunya and PROMETEO and GenT Programmes Generalitat Valenciana, Spain; Göran Gustafssons

Stiftelse, Sweden; The Royal Society and Leverhulme Trust, United Kingdom; Eric and Wendy Schmidt Fund for Strategic Innovation, United States of America.

In addition, individual members wish to acknowledge support from Chile: Agencia Nacional de Investigación y Desarrollo (ANID FONDECYT reg. 1230987, FONDECYT 1230812, FONDECYT 1240864, Fondecyt 3240661, Fondecyt Regular 1240721); China: Chinese Ministry of Science and Technology (MOST-2023YFA1605700, MOST-2023YFA1609300), National Natural Science Foundation of China (NSFC 12275265, NSFC-W2543005); Czech Republic: Czech Science Foundation (GACR – 24-11373S), Ministry of Education Youth and Sports (ERC-CZ-LL2327, FORTE CZ.02.01.01/00/22\_008/0004632), PRIMUS Research Programme (PRIMUS/21/SCI/017); EU: H2020 European Research Council (ERC – 101002463); European Union: European Research Council (BARD No. 101116429, ERC – 101219398, ERC – 948254, ERC 101089007), European Regional Development Fund (HE COFUND GA No.101081355, ERDF), Marie Skłodowska-Curie Actions (GAP-101168829); France: Agence Nationale de la Recherche (ANR-21-CE31-0013, ANR-22-EDIR-0002, ANR-24-CE31-0504-01); Germany: Deutsche Forschungsgemeinschaft (DFG – 469666862); China: Research Grants Council (GRF); Italy: Ministero dell’Università e della Ricerca (NextGenEU 153D23001490006 M4C2.1.1, NextGenEU I53D23000820006 M4C2.1.1, NextGenEU I53D23001490006 M4C2.1.1, SOE2024\_0000023); Japan: Japan Society for the Promotion of Science (JSPS KAKENHI JP25H0063, JSPS KAKENHI JP22H01227, JSPS KAKENHI JP22H04944, JSPS KAKENHI JP22KK0227, JSPS KAKENHI JP24K23939, JSPS KAKENHI JP24KK0251, JSPS KAKENHI JP25H00650, JSPS KAKENHI JP25H01291, JSPS KAKENHI JP25K01011, JSPS KAKENHI JP25K01023); Norway: Research Council of Norway (RCN-314472); Poland: Polish National Science Centre (NCN 2021/42/E/ST2/00350, NCN OPUS 2023/51/B/ST2/02507, NCN OPUS nr 2022/47/B/ST2/03059, NCN UMO-2019/34/E/ST2/00393, UMO-2022/47/O/ST2/00148, UMO-2023/49/B/ST2/04085, UMO-2023/51/B/ST2/00920, UMO-2024/53/N/ST2/00869); Spain: Agència de Gestió d’Ajuts Universitaris i de Recerca. (AGAUR – 2023 BP 00141), Ministry of Science and Innovation (RYC2019-028510-I, RYC2020-030254-I, RYC2021-031273-I, RYC2022-038164-I), Ministerio de Ciencia, Innovación y Universidades/Agencia Estatal de Investigación (EU NextGenerationEU (PRTR-C17.I1), PID2022-142604OB-C22); Sweden: Carl Trygger Foundation (Carl Trygger Foundation CTS 22:2312), Swedish Research Council (Swedish Research Council 2023-04654, VR 2021-03651, VR 2022-03845, VR 2022-04683, VR 2023-03403, VR 2024-05451, VR 2025-05940), Knut and Alice Wallenberg Foundation (KAW 2023.0366); Switzerland: Swiss National Science Foundation (SNSF – PCEFP2\_194658); United Kingdom: The Binks Trust, Royal Society (NIF-R1-231091); United States of America: U.S. Department of Energy (ECA DE-AC02-76SF00515), John Templeton Foundation (John Templeton Foundation 63206), Neubauer Family Foundation.

**Data Availability Statement.** The public release of data supporting the findings of this article will follow the CERN Open Data Policy [124]. Inquiries about plots and tables associated with this article can be addressed to atlas.publications@cern.ch.

**Code Availability Statement.** The ATLAS Collaboration’s Athena software, including the configuration of the event generators, is open source (<http://gitlab.cern.ch/atlas/athena>).

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