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References and set-up descriptions for the MC16 campaign

The ATLAS Collaboration

This document is intended as a template for referencing ATLAS Monte Carlo set-ups for Standard Model processes produced in the MC16 campaign. It includes descriptions of the generator configurations and the appropriate references.

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1 Introduction

This document is a collection of short descriptions of the baseline Standard Model processes produced as part of the ATLAS MC16 production campaign. Often a short and a long description is provided, depending on whether a sample is used as a background or a signal sample in an analysis, respectively.

It is assumed that paper editors will make a final pass through the wording, e.g. to avoid acronyms being introduced multiple times. The descriptions contain the appropriate citations which are included by default in the `atlaslatex` package as well. These citations often reflect decades of theory work and would have typically been agreed upon with the generator developers, who rely on them to secure funding for future generator development. PMG therefore strongly encourages *keeping all recommended citations* for any given snippet.

Please note that the generator versions can generally change from sample to sample. A change in the third digit typically indicates some sort of technical bug fix that does not affect the physics modelling otherwise. In order to save CPU time, samples are often regenerated only when they are affected by a (sufficiently severe) bug and so even within a set of final states of any given process, the generator version may differ.

You may have to add the `process` or `hepprocess` option to the `atlasphysics` package for some generators. In addition, some useful macros for processes are defined in the style file `MC_snippets-defs.sty`.

2 Pile-up overlay

Description: The effect of multiple interactions in the same and neighbouring bunch crossings (pile-up) was modelled by overlaying the simulated hard-scattering event with inelastic proton–proton (pp) events generated with Pythia 8.186 [1] using the NNPDF2.3lo set of parton distribution functions (PDF) [2] and the A3 set of tuned parameters [3].

Optional description: The Monte Carlo (MC) events were weighted to reproduce the distribution of the average number of interactions per bunch crossing ($\langle\mu\rangle$) observed in the data. The $\langle\mu\rangle$ value in data was rescaled by a factor of 1.03 ± 0.04 to improve agreement between data and simulation in the visible inelastic proton–proton (pp) cross-section [4].

3 Single-boson processes

In the following paragraphs, the set-up of the current ATLAS single-boson baseline samples is described. Details of the full process configuration are given in the PUB note [5]. In the case of Sherpa samples, a minimal description of built-in systematic uncertainties is also given.

3.1 Sherpa (MEPS@NLO)

3.1.1 QCD V+jets

Samples

The descriptions below correspond to the samples in Table 3.1.

Table 3.1: V+jets samples with Sherpa.

DSID range	Description
364100–364113	$Z \to \mu\mu$
364198–364203	$Z \to \mu\mu$ (10 GeV $< m_{\ell\ell} <$ 40 GeV)
364359, 364362, 364281	$Z \to \mu\mu$ (very low mass)
364114–364127	$Z \to ee$
364204–364209	$Z \to ee$ (10 GeV $< m_{\ell\ell} <$ 40 GeV)
364358, 364361, 364282	$Z \to ee$ (very low mass)
364128–364141	$Z \to \tau\tau$
364210–364215	$Z \to \tau\tau$ (10 GeV $< m_{\ell\ell} <$ 40 GeV)
364282, 364360, 364363	$Z \to \tau\tau$
364142–364155	$Z \to \nu\nu$
364156–364169	$W \to \mu\nu$
364170–364183	$W \to e\nu$
364184–364197	$W \to \tau\nu$
364216–364229	$Z \to \ell\ell, W \to \ell\nu$ (high p_{T})

Short description: The production of V+jets was simulated with the Sherpa 2.2.1 [6] generator using next-to-leading-order (NLO) matrix elements (ME) for up to two partons, and leading-order (LO) matrix elements for up to four partons calculated with the Comix [7] and OpenLoops [8–10] libraries. They were matched with the Sherpa parton shower [11] using the MEPS@NLO prescription [12–15] using the set of tuned parameters developed by the Sherpa authors. The NNPDF3.0nnlo set of PDFs [16] was used and the samples were normalised to a next-to-next-to-leading-order (NNLO) prediction [17].

Long description: The production of V+jets was simulated with the SHERPA 2.2.1 [6] generator. In this set-up, NLO-accurate matrix elements for up to two partons, and LO-accurate matrix elements for up to four partons were calculated with the Comix [7] and OPENLOOPS [8–10] libraries. The default SHERPA parton shower [11] based on Catani–Seymour dipole factorisation and the cluster hadronisation model [18] were used. They employed the dedicated set of tuned parameters developed by the SHERPA authors and the NNPDF3.0NNLO PDF set [16].

The NLO matrix elements for a given jet multiplicity were matched to the parton shower (PS) using a colour-exact variant of the MC@NLO algorithm [12]. Different jet multiplicities were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which was extended to NLO accuracy using the MEPS@NLO prescription [13]. The merging threshold was set to 20 GeV.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ± 0.001.

The V+jets samples were normalised to a next-to-next-to-leading-order (NNLO) prediction [17].

3.1.2 Electroweak Vjj (VBF)

The descriptions below correspond to the samples in Table 3.2. Samples include the VBF and V-strahlung diagrams, but they do not include semileptonic VV diagrams and do not overlap with QCD V+jets samples.

Table 3.2: Electroweak Vjj samples with SHERPA.

DSID range	Description
700358–700364	EWK Vjj (baseline)
308092–308096	EWK Vjj (legacy)

Description (baseline setups): Electroweak production of $\ell\ell jj$, $\ell\nu jj$ and $\nu\nu jj$ final states was simulated with SHERPA 2.2.11 [6] using leading-order (LO) matrix elements with up to one additional parton emission. The matrix elements were merged with the SHERPA parton shower [11] following the MEPS@LO prescription [14] and using the set of tuned parameters developed by the SHERPA authors. The NNPDF3.0NNLO set of PDFs [16] was employed. The samples were produced using the VBF approximation, which avoids overlap with semileptonic diboson topologies by requiring a t-channel colour-singlet exchange. The starting conditions of the CS shower are set according to the large-N_c amplitudes supplied by Comix [22] to achieve the correct VBF-appropriate radiation pattern.

Description (legacy setups): Electroweak production of $\ell\ell jj$, $\ell\nu jj$ and $\nu\nu jj$ final states was simulated with SHERPA 2.2.1 [6] using leading-order (LO) matrix elements with up to two additional parton emissions. The matrix elements were merged with the SHERPA parton shower [11] following the MEPS@LO prescription [14] and using the set of tuned parameters developed by the SHERPA authors. The NNPDF3.0NNLO set of PDFs [16] was employed. The samples were produced using the VBF approximation, which avoids overlap with semileptonic diboson topologies by requiring a t-channel colour-singlet exchange.

3.2 MadGraph (CKKW-L)

Samples

The descriptions below correspond to the samples in Table 3.3. The set-ups of N_{parton}- and H_{T}-sliced samples differ slightly between the two slicing schemes with regard to the matrix element PDF, the jet-clustering radius parameter and the scale used in the evaluation of α_{s} to determine the weight of each splitting. The short description merges the two set-ups and requires the paper editors to select the appropriate PDF set (or gracefully describe both); the long description is left unmerged.

Table 3.3: V+jets samples with MADGRAPH5+PYTHIA 8 using CKKW-L merging.

DSID range	Description
363123–363146	H_{T}-sliced $Z \to \mu\mu$
363147–363170	H_{T}-sliced $Z \to ee$
361510–361514	N_{parton}-sliced $Z \to \tau\tau$
361515–361519	N_{parton}-sliced $Z \to \nu\nu$
363624–363647	H_{T}-sliced $W \to \mu\nu$
363600–363623	H_{T}-sliced $W \to e\nu$
363648–363671	H_{T}-sliced $W \to \tau\nu$

Short description for H_{T}-sliced and N_{parton}-sliced V+jets: QCD V+jets production was simulated with MADGRAPH5_aMC@NLO 2.2.2 [23], using LO-accurate matrix elements (ME) with up to four final-state partons. The ME calculation employed the NNPDF3.0NLO set of PDFs [16] (H_{T}-sliced) / NNPDF2.3LO set of PDFs [2] (N_{parton}-sliced). Events were interfaced to PYTHIA 8.186 [1] for the modelling of the parton shower, hadronisation, and underlying event. The overlap between matrix element and parton shower emissions was removed using the CKKW-L merging procedure [24, 25]. The A14 tune [26] of PYTHIA 8 was used with the NNPDF2.3LO PDF set [2]. The decays of bottom and charm hadrons were performed by EVTGEN 1.2.0 [27]. The V+jets samples were normalised to a next-to-next-to-leading-order (NNLO) prediction [17].

H_{T}-sliced long description: QCD V+jets production was simulated with LO-accurate matrix elements (ME) for up to four partons with MADGRAPH5_aMC@NLO 2.2.2 [23]. The ME calculation was interfaced with PYTHIA 8.186 [1] for the modelling of the parton shower, hadronisation, and underlying event. To remove overlap between the matrix element and the parton shower the CKKW-L merging procedure [24, 25] was applied with a merging scale of 30 GeV and a jet-clustering radius parameter of 0.2. In order to better model the region of large jet p_{T}, the strong coupling constant α_{s} was evaluated at the scale of each splitting to determine the weight. The matrix element calculation was performed with the NNPDF3.0NLO PDF set [16] with $\alpha_{\mathrm{s}} = 0.118$. The calculation was done in the five-flavour number scheme with massless b- and c-quarks. Quark masses were reinstated in the Pythia 8 parton shower. The renormalisation and factorisation scales were set to the MadGraph default values, based on a clustering of the event. The A14 tune [26] of Pythia 8 was used with the NNPDF2.3LO PDF set [2] with $\alpha_{\mathrm{s}} = 0.13$. The decays of bottom and charm hadrons were performed by EvtGen 1.2.0 [27].

$N_{\mathbf{parton}}$-sliced long description: QCD V+jets production was simulated with LO-accurate matrix elements (ME) for up to four partons with MadGraph5_aMC@NLO 2.2.2 [23]. The ME calculation was interfaced with Pythia 8.186 [1] for the modelling of the parton shower and underlying event. To remove overlap between the matrix element and the parton shower the CKKW-L merging procedure [24, 25] was applied with a merging scale of 30 GeV and a jet-clustering radius parameter of 0.4. In order to better model the region of large jet p_{T}, the strong coupling constant α_{s} was evaluated at the scale of each splitting to determine the weight. The matrix element calculation was performed with the NNPDF2.3LO PDF set [2] with $\alpha_{\mathrm{s}} = 0.13$. The calculation was done in the five-flavour number scheme with massless b- and c-quarks. Quark masses were reinstated in the Pythia 8 parton shower. The renormalisation and factorisation scales were set to the MadGraph default values, based on a clustering of the event. The A14 tune [26] of Pythia 8 was used with the NNPDF2.3LO PDF set [2] with $\alpha_{\mathrm{s}} = 0.13$. The decays of bottom and charm hadrons were performed by EvtGen 1.2.0 [27].

3.3 Inclusive Powheg V

3.3.1 QCD V+jets

The descriptions below correspond to the samples in Table 3.4.

Table 3.4: Inclusive V samples with Powheg.

DSID range	Description
361100–361108	$W^+, W^-, Z/\gamma^*$ with e, μ, τ decays
301000–301178, 344722	high-mass slices: W^+, W^-, Z with e, μ, τ decays
361664–361669	Z/γ^* low-mass slices (m = 6–10–60 GeV)
426335–426336	Z/γ^* high-$p_{\mathrm{T},\ell\ell} > 150$ GeV slices

Description: The Powheg Box v1 MC generator [28–31] was used for the simulation at NLO accuracy of the hard-scattering processes of W and Z boson production and decay in the electron, muon, and τ-lepton channels. It was interfaced to Pythia 8.186 [1] for the modelling of the parton shower, hadronisation, and underlying event, with parameters set according to the AZNLO tune [32]. The CT10NLO PDF set [33] was used for the hard-scattering processes, whereas the CTEQ6L1 PDF set [34] was used for the parton shower. The effect of QED final-state radiation was simulated with Photos++ 3.52 [35, 36]. The EvtGen 1.2.0 program [27] was used to decay bottom and charm hadrons.

3.3.2 Electroweak Vjj (VBF)

The descriptions below correspond to the samples in Table 3.5. Samples include the VBF and V-strahlung diagrams, but they do not include semileptonic VV diagrams and do not overlap with the QCD V+jets samples.

Table 3.5: Electroweak Vjj samples with POWHEG.

DSID range	Description
600931–600939	EWK Vjj

Description: Electroweak production of $\ell\ell jj$ and $\ell\nu jj$ final states was simulated with POWHEG BOX v2 [28–30, 37] using the NNPDF3.0NLO [16] parton distribution functions (PDF) and is accurate to next-to-leading order (NLO) in perturbative QCD. The sample was produced with the VBF approximation, which requires a t-channel colour-singlet exchange to remove overlap with diboson topologies [38, 39]. The parton-level events were passed to PYTHIA 8.245 to add parton-showering hadronisation and underlying-event activity, using the A14 [26] set of tuned parameters. The correct VBF-appropriate radiation pattern was achieved by using the dipole-recoil option. The EVTGEN 1.7.0 program [27] was used for the properties of the bottom and charm hadron decays.

4 Multiboson processes

In the following paragraphs, the set-ups of the current ATLAS multiboson baseline samples are described. Details of the full process configuration are given in the PUB note [40].

4.1 Inclusive Powheg

The descriptions below correspond to the samples in Table 4.1.

Table 4.1: Inclusive VV samples with Powheg.

DSID range	Description
361600–361605	inclusive $WW(2\ell 2\nu)$, $WZ(3\ell\nu)$, $ZZ(4\ell)$, $ZZ(4\nu)$, $ZZ(2\ell 2\nu)$ (all lepton flavours)
361606–361611	inclusive $WW/WZ/ZZ$ semileptonic decays ($\ell\ell qq$, $\ell\nu qq$, $\nu\nu qq$, all lepton flavours)

Description: The Powheg Box v2 [28–30] generator was used to simulate the WW, WZ and ZZ [41] production processes at NLO accuracy in QCD. The effect of singly resonant amplitudes and interference effects due to Z/γ^* and same-flavour lepton combinations in the final state were included, where appropriate. Interference effects between WW and ZZ for same-flavour charged leptons and neutrinos were ignored. Events were interfaced to Pythia 8.210 [42] for the modelling of the parton shower, hadronisation, and underlying event, with parameters set according to the AZNLO tune [32]. The CT10 PDF set [33] was used for the hard-scattering processes, whereas the CTEQ6L1 PDF set [34] was used for the parton shower. The EvtGen 1.2.0 program [27] was used to decay bottom and charm hadrons.

The factorisation and renormalisation scales were set to the invariant mass of the boson pair. An invariant mass of $m_{\ell\ell} > 4$ GeV was required at matrix-element level for any pair of same-flavour charged leptons.

4.2 Sherpa

4.2.1 Fully leptonic, semileptonic and loop-induced VV

The descriptions below correspond to the samples in Table 4.2. They describe the almost identical set-ups of fully leptonic (including loop-induced VV production) and semileptonic VV decays. For loop-induced processes $gg \to VV$, the description below assumes that the 'nominal' samples with Higgs contributions are used. If you are using specialised set-ups that exclude the Higgs component, the description should be modified appropriately. (Get in touch with the PMG Weak Boson Processes subgroup if you are unsure.)

Table 4.2: VV samples with SHERPA: fully leptonic, semileptonic, loop-induced fully leptonic, loop-induced semileptonic. SFOS stands for 'same flavour opposite-charge sign'.

DSID range	Description
364250–364255, 363494 364288–364290	$4\ell, 3\ell\nu, 2\ell2\nu, 4\nu$ with $m_{\ell\ell}(\text{SFOS}) > 4\,\text{GeV}$, $p_{\text{T}}^{\ell}(1,2) > 5\,\text{GeV}$ fully leptonic low $m_{\ell\ell}$ and p_{T}^{ℓ} complement
345705–345727	loop-induced leptonic
363355-363360, 363489	semileptonic, on-shell diboson production with factorised decays
364302-364305	loop-induced semileptonic, using factorised on-shell decays)

Description: Samples of diboson final states (VV) were simulated with the SHERPA 2.2.1 or 2.2.2 [6] generator depending on the process, including off-shell effects and Higgs boson contributions, where appropriate. Fully leptonic final states and semileptonic final states, where one boson decays leptonically and the other hadronically, were generated using matrix elements at NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional parton emissions. Samples for the loop-induced processes $gg \to VV$ were generated using LO-accurate matrix elements for up to one additional parton emission for both the cases of fully leptonic and semileptonic final states. The matrix element calculations were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@NLO prescription [12–15]. The virtual QCD corrections were provided by the OPENLOOPS library [8–10]. The NNPDF3.0NNLO set of PDFs was used [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which is extended to NLO accuracy using the MEPS@NLO prescription [13]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OPENLOOPS library [8–10]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ± 0.001.

4.2.2 Electroweak $VVjj$

The descriptions below correspond to the samples in Table 4.3.

Table 4.3: Electroweak $VVjj$ samples with SHERPA.

DSID range	Description
364283–364284	$\ell\ell\ell jj$, $\ell\ell\ell\nu jj$
364285	$\ell\ell\nu\nu jj$ opposite-sign
364287	$\ell\ell\nu\nu jj$ same-sign
366086–366089	$\ell\ell\ell jj$, $\ell\ell\ell\nu jj$, $\ell\ell\nu\nu jj$, with the triboson contributions removed

Description: Electroweak production of a diboson in association with two jets ($VVjj$) was simulated with the SHERPA 2.2.2 [6] generator. The LO-accurate matrix elements were matched to a parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@LO prescription [12–15]. Samples were generated using the NNPDF3.0NNLO PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ± 0.001.

4.2.3 $V\gamma$ (NLO, biased)

The descriptions below correspond to the samples in Table 4.4.

Table 4.4: NLO $V\gamma$ samples with SHERPA.

DSID range	Description
700011–700017	biased in $\log_{10}(\max[p_T(V), p_T(\gamma)])$

Description: The production of $V\gamma$ final states was simulated with the SHERPA 2.2.8 [6] generator. Matrix elements at NLO QCD accuracy for up to one additional parton and LO accuracy for up to three additional parton emissions were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@NLO prescription [12–15]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OPENLOOPS 2 library [8–10, 43]. Samples were generated using the NNPDF3.0NNLO PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which was extended to NLO accuracy using the MEPS@NLO prescription [13]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OpenLoops 2 library [8–10, 43]. Multijet merging at NLO accuracy in the electroweak coupling was based on the NLO $\mathrm{EW}_{\mathrm{virt}}$ approach [44, 45]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14nnlo [20] and MMHT2014nnlo [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ± 0.001.

4.2.4 $V\gamma$ (NLO, sliced)

The descriptions below correspond to the samples in Table 4.5.

Table 4.5: NLO $V\gamma$ samples with Sherpa.

DSID range	Description
364500–364535	sliced in p_{T}^{γ}
345887–345900	sliced in $m_{\ell\ell}$

Description: The production of $V\gamma$ final states was simulated with the Sherpa 2.2.2 [6] generator. Matrix elements at NLO QCD accuracy for up to one additional parton and LO accuracy for up to three additional parton emissions were matched and merged with the Sherpa parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@NLO prescription [12–15]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OpenLoops library [8–10]. Samples were generated using the NNPDF3.0nnlo PDFset [16], along with the dedicated set of tuned parton-shower parameters developed by the Sherpa authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which was extended to NLO accuracy using the MEPS@NLO prescription [13]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OpenLoops library [8–10]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ±0.001.

4.2.5 $V\gamma$ (LO)

The descriptions below correspond to the samples in Table 4.6.

Table 4.6: LO $V\gamma$ samples with SHERPA.

DSID range	Description
366140–366154	SHERPA 2.2.4, $Z(\rightarrow ee/\mu\mu/\tau\tau)\gamma$, sliced in p_T^γ

Description: The production of $V\gamma$ final states was simulated with the SHERPA 2.2.4 [6] generator. Matrix elements at LO accuracy in QCD for up to three additional parton emissions were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@LO prescription [12–15]. Samples were generated using the NNPDF3.0NNLO PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ±0.001.

4.2.6 Tribosons (NLO)

The descriptions below correspond to the samples in Table 4.7.

Table 4.7: NLO VVV samples (factorised decays) with SHERPA.

DSID range	Description
363507–363509	$3\ell 1\nu 2j$, $4\ell 2j$
364242–364249	fully leptonic decays
364336–364339	$WWW \rightarrow 2\ell 2\nu jj$

Description: The production of triboson (VVV) events was simulated with the SHERPA 2.2.2 [6] generator using factorised gauge-boson decays. Matrix elements, accurate to NLO for the inclusive process and to LO for up to two additional parton emissions, were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@NLO prescription [12–15]. The virtual QCD corrections for matrix elements at NLO accuracy were provided by the OPENLOOPS library [8–10]. Samples were generated using the NNPDF3.0NNLO PEF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which is extended to NLO accuracy using the MEPS@NLO prescription [13]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ±0.001.

4.2.7 Tribosons (LO)

The descriptions below correspond to the samples in Table 4.8.

Table 4.8: LO VVV samples with SHERPA.

DSID range	Description
407311–407315	on- and off-shell contributions to 6-lepton production

Description: The production of triboson (VVV) events was simulated with the SHERPA 2.2.1 [6] generator. Matrix elements accurate to LO in QCD for up to one additional parton emission were matched and merged with the SHERPA parton shower based on Catani–Seymour dipole factorisation [7, 11] using the MEPS@LO prescription [12–15]. Samples were generated using the NNPDF3.0NNLO PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Additional description: The ME+PS matching [12] was employed for different jet multiplicities which were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15]. The calculation was performed in the G_μ scheme, ensuring an optimal description of pure electroweak interactions at the electroweak scale.

Uncertainties from missing higher orders were evaluated [19] using seven variations of the QCD factorisation and renormalisation scales in the matrix elements by factors of 0.5 and 2, avoiding variations in opposite directions.

Uncertainties in the nominal PDF set were evaluated using 100 replica variations. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets. The effect of the uncertainty in the strong coupling constant α_s was assessed by variations of ±0.001.

5 Higgs boson processes

In this chapter, the set-up of the current ATLAS samples for Higgs boson production in gluon–gluon fusion, vector-boson fusion and Higgs-strahlung processes is described.

5.1 H via gluon–gluon fusion

Powheg+Pythia 8 samples

The descriptions below correspond to the samples in Table 5.1.

Table 5.1: Powheg Higgs gluon–gluon fusion samples with Powheg+Pythia 8 for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
343981	$H \rightarrow \gamma\gamma$	
345316	$H \rightarrow Z\gamma$	
345060	$H \rightarrow ZZ^* \rightarrow 4\ell$	$\ell = e, \mu, \tau$
345324	$H \rightarrow WW^* \rightarrow 2\ell 2\nu$	$p_{\mathrm{T},\ell 1} > 15$ GeV and $p_{\mathrm{T},\ell 2} > 5$ GeV
308284	$H \rightarrow ZZ^* \rightarrow 4\nu$	$E_{\mathrm{T}}^{\mathrm{miss}} > 75$ GeV
345342	$H \rightarrow b\bar{b}$	
345097	$H \rightarrow \mu\mu$	
345120	$H \rightarrow \tau\tau \rightarrow \ell^+\ell^-$	$p_{\mathrm{T},\ell 1} > 13$ GeV and $p_{\mathrm{T},\ell 2} > 7$ GeV
345121	$H \rightarrow \tau\tau \rightarrow h^+\ell^-$	$p_{\mathrm{T},\ell} > 15$ GeV and $p_{\mathrm{T},h} > 20$ GeV
345122	$H \rightarrow \tau\tau \rightarrow \ell^+h^-$	$p_{\mathrm{T},\ell} > 15$ GeV and $p_{\mathrm{T},h} > 20$ GeV
345123	$H \rightarrow \tau\tau \rightarrow h^+h^-$	$p_{\mathrm{T},h1} > 30$ GeV and $p_{\mathrm{T},h2} > 20$ GeV
345124	$H \rightarrow \tau\tau \rightarrow \mu\tau$	
345125	$H \rightarrow \tau\tau \rightarrow e\tau$	

Short description: Higgs boson production via gluon–gluon fusion was simulated at next-to-next-to-leading-order (NNLO) accuracy in QCD using Powheg Box v2 [28–30, 46, 47]. The simulation achieved NNLO accuracy for arbitrary inclusive $gg \rightarrow H$ observables by reweighting the Higgs boson rapidity spectrum in Hj-MiNLO [48–50] to that of HNNLO [51]. The PDF4LHC15nnlo PDF set [52] and the AZNLO tune [32] of Pythia 8 [42] were used.

The gluon–gluon fusion prediction from the Monte Carlo samples was normalised to the next-to-next-to-next-to-leading-order cross-section in QCD plus electroweak corrections at next-to-leading order (NLO) [53–63]. The decays of bottom and charm hadrons were performed by EvtGen [27]. The normalisation of all

Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

Long description: Higgs boson production via gluon–gluon fusion was simulated at next-to-next-to-leading-order (NNLO) accuracy in QCD using POWHEG BOX v2 [28–30, 46, 47]. The simulation achieved NNLO accuracy for arbitrary inclusive $gg \rightarrow H$ observables by reweighting the Higgs boson rapidity spectrum in HJ-MINLO [48–50] to that of HNNLO [51]. The transverse momentum spectrum of the Higgs boson obtained with this sample was found to be compatible with the fixed-order HNNLO calculation and the HRES 2.3 calculation [70, 71] performing resummation at next-to-next-to-leading-logarithm accuracy matched to a NNLO fixed-order calculation (NNLL+NNLO). Top- and bottom-quark mass effects were included up to next-to-leading order (NLO).

The renormalisation and factorisation scales were set to half of the Higgs boson mass and the PDF4LHC15NNLO PDF set [52] was used. The matrix elements were matched to the parton shower of PYTHIA 8 [42] which uses the AZNLO tune [32]. The decays of bottom and charm hadrons were performed by EVTGEN [27].

The QCD scale uncertainties were obtained using nine-point scale variations of the NLO renormalisation and factorisation scales and applying the NNLO reweighting to those variations, including up and down variations of $\mu_{\mathrm{r}} = \mu_{\mathrm{f}}$ around the central value for the NNLO part, yielding a total of 27 scale variations. PDF and α_{s} uncertainties were estimated using the PDF4LHC15NLO set of eigenvectors. The envelope of the resulting 27 scale variations was taken to estimate the QCD scale uncertainty. Uncertainties were also provided for switching off bottom- and top-quark mass effects.

The prediction from the Monte Carlo samples was normalised to the next-to-next-to-next-to-leading-order cross-section in QCD in the infinite top-quark mass limit [53, 56–58, 72] and including exact corrections for all finite quark-mass effects at NLO in QCD as well as NLO electroweak effects [55, 63]. Additionally, corrections to the inverse of the top-quark mass were taken into account at NNLO [59–62]. The normalisation of all Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

5.2 *H* via vector-boson fusion

POWHEG+PYTHIA 8 samples

The descriptions below correspond to the samples in Table 5.2.

Short description: Higgs boson production via vector-boson fusion was simulated with POWHEG BOX v2 [28–30, 73] and interfaced with PYTHIA 8 [42] for parton shower and non-perturbative effects, with parameters set according to the AZNLO tune [32]. The POWHEG BOX prediction is accurate to next-to-leading order (NLO) and uses the PDF4LHC15NLO PDF set [52]. It was normalised to an approximate-NNLO QCD cross-section with NLO electroweak corrections [74–76]. The decays of bottom and charm hadrons were performed by EVTGEN [27]. The normalisation of all Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

Table 5.2: POWHEG+PYTHIA 8 Higgs vector-boson fusion samples for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
346317	$H \to \text{all}$	
346214	$H \to \gamma\gamma$	
345833	$H \to Z\gamma$	$Z \to \ell^+\ell^-$
345834	$H \to \gamma\gamma^*$	$\gamma^* \to \ell^+\ell^-$
346228	$H \to ZZ^* \to 4\ell$	$\ell = e, \mu$
450576	$H \to ZZ^* \to 2\ell 2b$	
345948	$H \to WW^* \to 2\ell 2\nu$	$p_{\text{T},\ell 1} > 15\,\text{GeV}$ and $p_{\text{T},\ell 2} > 5\,\text{GeV}$
346600	$H \to ZZ^* \to 4\nu$	$E_{\text{T}}^{\text{miss}} > 75\,\text{GeV}$
345949	$H \to b\bar{b}$	
346190	$H \to \tau\tau \to \ell^+\ell^-$	$p_{\text{T},\ell 1} > 13\,\text{GeV}$ and $p_{\text{T},\ell 2} > 7\,\text{GeV}$
346191	$H \to \tau\tau \to h^+\ell^-$	$p_{\text{T},\ell} > 15\,\text{GeV}$ and $p_{\text{T},h} > 20\,\text{GeV}$
346192	$H \to \tau\tau \to \ell^+h^-$	$p_{\text{T},\ell} > 15\,\text{GeV}$ and $p_{\text{T},h} > 20\,\text{GeV}$
346193	$H \to \tau\tau \to h^+h^-$	$p_{\text{T},h1} > 30\,\text{GeV}$ and $p_{\text{T},h2} > 20\,\text{GeV}$
346194	$H \to \tau\tau \to e\tau$	
346195	$H \to \tau\tau \to \mu\tau$	

Long description: Higgs boson production via vector-boson fusion was simulated with POWHEG BOX v2 [28–30, 73]. A factorised approximation, where cross-talk between the fermion lines is neglected, was used. The implementation is based on the respective NLO QCD calculations for genuine W/Z vector-boson fusion topologies (VBF approximation). Quark–antiquark annihilation and interference contributions between t- and u-channel contributions were disregarded.

The renormalisation and factorisation scales were set to the W boson mass and the PDF4LHC15NLO PDF set [52] was used. The matrix elements were matched to the parton shower of PYTHIA 8 [42] which uses the AZNLO tune [32]. A dipole-recoil strategy was used for the parton shower.The decays of bottom and charm hadrons were performed by EVTGEN [27].

The QCD scales μ_{r} and μ_{f} were varied independently by factors of 0.5 and 2.0, both in the matrix element and in the parton shower.

The prediction from the POWHEG BOX sample was normalised to the next-to-next-to-leading-order cross-section in QCD using the VBF approximation [74–76]. Relative next-to-leading-order electroweak corrections were also taken into account for the t- and u-channel contribution considered in the VBF approximation. The normalisation of all Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

5.3 *VH*

This section describes the generation details of nominal samples for Higgs-strahlung production.

POWHEG+PYTHIA 8 samples

The descriptions below correspond to the samples in Tables 5.3 to 5.6.

Table 5.3: POWHEG+PYTHIA 8 samples of Higgs boson production in association with a Z boson for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
345038	$H \to ZZ^* \to 4\ell$	$Z \to$ all
345319	$H \to \gamma\gamma$	$Z \to$ all
345322	$H \to Z\gamma$	$Z \to$ all
345103	$H \to \mu\mu$	$Z \to$ all
345217	$H \to \tau\tau$	$Z \to$ all
345218	$H \to e\tau$	$Z \to$ all
345219	$H \to \mu\tau$	$Z \to$ all
345445	$H \to WW^* \to 2\ell 2\nu$	$Z \to$ all
345876	$H\, toee$	$Z \to$ all
345965	$H \to \gamma\gamma^*$	$\gamma^* \to \ell^+\ell^-$; $Z \to$ all
346310	$H \to$ all	$Z \to$ all
346607	$H \to ZZ^* \to 4\nu$	$Z \to \ell^+\ell^-$
345055	$H \to b\bar{b}$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \ell^+\ell^-$
345111	$H \to c\bar{c}$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \ell^+\ell^-$
345337	$H \to WW^* \to 2\ell 2\nu$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \ell^+\ell^-$
346326	$H \to \tau\tau$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \ell^+\ell^-$
346693	$H \to ZZ^* \to 4\nu$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \ell^+\ell^-$
345056	$H \to b\bar{b}$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \nu\bar{\nu}$
345112	$H \to c\bar{c}$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \nu\bar{\nu}$
345445	$H \to WW^* \to 2\ell 2\nu$	$p_{\mathrm{T},Z}$ enhancement; $Z \to \nu\bar{\nu}$

Short description: Higgs boson production in association with a vector boson was simulated using POWHEG BOX v2 [28–30, 73] and interfaced with PYTHIA 8 [42] for parton shower and non-perturbative effects. The POWHEG BOX prediction is accurate to next-to-leading order for VH boson plus one-jet production. The loop-induced $gg \to ZH$ process was generated separately at leading order. The PDF4LHC15NLO PDF set [52] and the AZNLO tune [32] of PYTHIA 8 [42] were used. The decays of bottom and charm hadrons were performed by EVTGEN [27]. The Monte Carlo prediction was normalised to cross-sections calculated at NNLO in QCD with NLO electroweak corrections for $q\bar{q}/qg \to VH$ and at NLO and next-to-leading-logarithm accuracy in QCD for $gg \to ZH$ [77–83]. The normalisation of all Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

Long description: Higgs boson production in association with a vector boson was simulated using POWHEG BOX v2 [28–30, 73]. The computation was carried out using the MINLO [84] prescription, which achieves NLO accuracy for the VH and VH boson plus one-jet production inclusive distributions and dictates the choice of renormalisation and factorisation scales. Virtual amplitudes were constructed through

Table 5.4: POWHEG+PYTHIA 8 samples of Higgs boson production in association with a W^+ boson for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
345039	$H \to ZZ^* \to 4\ell$	$W^+ \to$ all
345318	$H \to \gamma\gamma$	$W^+ \to$ all
345104	$H \to \mu\mu$	$W^+ \to$ all
345212	$H \to \tau\tau$	$W^+ \to$ all
345214	$H \to e\tau$	$W^+ \to$ all
345216	$H \to \mu\tau$	$W^+ \to$ all
345321	$H \to Z\gamma$	$W^+ \to$ all
345325	$H \to WW^* \to 2\ell 2\nu$	$W^+ \to q\bar{q}$
345877	$H \to e^+e^-$	$W^+ \to$ all
345964	$H \to \gamma\gamma^*$	$\gamma^* \to \ell^+\ell^-$; $W^+ \to$ all
346311	$H \to$ all	$W^+ \to$ all
346605	$H \to ZZ^* \to 4\nu$	$W^+ \to$ all
346699	$H \to 4\ell$	interfaced to PROPHECY4F
346705	$H \to 4\ell$	interfaced to Hto4l
345054	$H \to b\bar{b}$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$
345110	$H \to c\bar{c}$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$
345327	$H \to WW^* \to 2\ell 2\nu$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$
346561	$H \to WW^* \to q\bar{q}\ell\nu$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$
346325	$H \to \tau\tau$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$
346729	$H \to ZZ^* \to 4\nu$	$p_{\mathrm{T},W}$ enhancement; $W^+ \to \ell^+\nu$

the interface to the GOSAM package [85]. The loop-induced $gg \to ZH$ process was generated separately at leading order with POWHEG BOX. In all cases, the PDF4LHC15NLO PDF set [52] was used.

The matrix elements were matched to the parton shower of PYTHIA 8 [42] which uses the AZNLO tune [32]. The decays of bottom and charm hadrons were performed by EVTGEN [27]. The QCD scales μ_r and μ_f were varied independently by factors of 0.5 and 2.0 to account for their uncertainties.

The predictions from POWHEG BOX were normalised to the best available theoretical prediction. The $q\bar{q}/qg \to VH$ cross-sections were calculated at NNLO in QCD with NLO electroweak corrections and the $gg \to ZH$ cross-sections were calculated at NLO and next-to-leading-logarithm accuracy [77–83]. The normalisation of the $q\bar{q} \to ZH$ samples was extracted from the subtraction of the latter from the former. Differential NLO EW corrections were available from the HAWK program [81] to be applied to $q\bar{q}$-initiated VH production as a function of the vector boson's transverse momentum. The normalisation of all Higgs boson samples accounts for the decay branching ratio calculated with HDECAY [64–66] and PROPHECY4F [67–69].

Table 5.5: POWHEG+PYTHIA 8 samples of Higgs boson production in association with a W^- boson for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
345040	$H \to ZZ^* \to 4\ell$	$W^- \to$ all
345317	$H \to \gamma\gamma$	$W^- \to$ all
345105	$H \to \mu\mu$	$W^- \to$ all
345211	$H \to \tau\tau$	$W^- \to$ all
345213	$H \to e\tau$	$W^- \to$ all
345215	$H \to \mu\tau$	$W^- \to$ all
345320	$H \to Z\gamma$	$W^- \to$ all
345333	$H \to WW^* \to 2\ell 2\nu$	$W^- \to q\bar{q}$
345878	$H \to e^+e^-$	$W^- \to$ all
345963	$H \to \gamma\gamma^*$	$\gamma^* \to \ell^+\ell^-$; $W^- \to$ all
346312	$H \to$ all	$W^- \to$ all
346606	$H \to ZZ^* \to 4\nu$	$W^- \to$ all
346700	$H \to 4\ell$	interfaced to PROPHECY4F
346706	$H \to 4\ell$	interfaced to Hto4l
345053	$H \to b\bar{b}$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$
345109	$H \to c\bar{c}$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$
345326	$H \to WW^* \to 2\ell 2\nu$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$
346560	$H \to WW^* \to q\bar{q}\ell\nu$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$
346324	$H \to \tau\tau$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$
346730	$H \to ZZ^* \to 4\nu$	$p_{\mathrm{T},W}$ enhancement; $W^- \to \ell^-\bar{\nu}$

Table 5.6: POWHEG+PYTHIA 8 samples of loop-induced Higgs boson production in association with a Z boson for different Higgs boson decay channels.

DSID	Decay channel	Additional comment
345061	$H \to \gamma\gamma$	$Z \to$ all
345066	$H \to ZZ^* \to 4\ell$	$Z \to$ all
345098	$H \to \mu\mu$	$Z \to$ all
345596	$H \to ZZ^* \to 4\nu$	$Z \to$ all
346524	$H \to WW^* \to 2\ell 2\nu$	$Z \to$ all
346697	$H \to ZZ^* \to 4\nu$	interfaced to PROPHECY4F
346703	$H \to ZZ^* \to 4\nu$	interfaced to Hto4l
345057	$H \to b\bar{b}$	$Z \to \ell^+\ell^-$
345113	$H \to c\bar{c}$	$Z \to \ell^+\ell^-$
345446	$H \to WW^* \to 2\ell 2\nu$	$Z \to \ell^+\ell^-$
346329	$H \to \tau\tau$	$Z \to \ell^+\ell^-$
346694	$H \to ZZ^* \to 4\nu$	$Z \to \ell^+\ell^-$
345058	$H \to b\bar{b}$	$Z \to \nu\bar{\nu}$
345114	$H \to c\bar{c}$	$Z \to \nu\bar{\nu}$

6 Top-quark processes

This chapter describes the samples used for top-quark processes. The $t\bar{t}$ samples are described in Section 6.1. Single-top samples are described in Section 6.2 for tW associated production, in Section 6.3 for t-channel production, and in Section 6.3.4 for s-channel production. Finally, $t\bar{t}$+HF samples are described in Section 6.4.

6.1 $t\bar{t}$ production

This section describes the MC samples used for the modelling of $t\bar{t}$ production. Section 6.1.1 describes the Powheg+Pythia 8 samples, Section 6.1.2 describes the Powheg+Herwig 7 samples, Section 6.1.4 describes the MadGraph5_aMC@NLO+Pythia 8 samples, and finally Section 6.1.6 describes the Sherpa samples.

The reference cross-section values are extracted from Ref. [86]. Studies of MC simulation performance including comparisons with unfolded data are collected in the PUB notes [87–89].

6.1.1 Powheg+Pythia 8

Samples The descriptions below correspond to the samples in Tables 6.1 to 6.3.

Table 6.1: Nominal $t\bar{t}$ samples produced with Powheg+Pythia 8. The h_{damp} value is set to $1.5\,m_{\mathrm{top}}$.

DSID range	Description
410470	$t\bar{t}$ non-all-hadronic
410471	$t\bar{t}$ dileptonic
410472	$t\bar{t}$ all-hadronic

Table 6.2: $t\bar{t}$ samples produced with Powheg+Pythia 8 used to estimate initial-state radiation systematic uncertainties. The h_{damp} value is set to $3.0\,m_{\mathrm{top}}$.

DSID range	Description
410480	$t\bar{t}$ single lepton
410481	$t\bar{t}$ all-hadronic
410482	$t\bar{t}$ dileptonic

Table 6.3: $t\bar{t}$ samples produced with Powheg+Pythia 8 with alternative h_{damp} values which can be used to estimate the uncertainty due to the Powheg+Pythia 8 matching scheme.

DSID (1.3 m_{top})	DSID (1.8 m_{top})	DSID (2.0 m_{top})	Description
411350	411353	411356	$t\bar{t}$ single lepton
411351	411354	411357	$t\bar{t}$ all-hadronic
411352	411355	411358	$t\bar{t}$ dileptonic

Short description: The production of $t\bar{t}$ events was modelled using the Powheg Box v2 [28–30, 37] generator at NLO with the NNPDF3.0nlo [16] PDF set and the h_{damp} parameter[1] set to 1.5 m_{top} [89]. The events were interfaced to Pythia 8.230 [42] to model the parton shower, hadronisation, and underlying event, with parameters set according to the A14 tune [26] and using the NNPDF2.3lo set of PDFs [2]. The decays of bottom and charm hadrons were performed by EvtGen 1.6.0 [27].

The uncertainty due to initial-state radiation (ISR) was estimated by simultaneously varying the h_{damp} parameter and the μ_{r} and μ_{f} scales, and choosing the Var3c up/down variants of the A14 tune as described in Ref. [88]. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up or down by a factor two.

Long description: The production of $t\bar{t}$ events was modelled using the Powheg Box v2 [28–30, 37] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_{s}, and the NNPDF3.0nlo [16] parton distribution function (PDF). The h_{damp} parameter, which controls the matching in Powheg and effectively regulates the high-p_{T} radiation against which the $t\bar{t}$ system recoils, was set to 1.5 m_{top} [89]. The functional form of the renormalisation and factorisation scales was set to the default scale $\sqrt{m_{\text{top}}^2 + p_{\text{T}}^2}$. The events were interfaced with Pythia 8.230 [42] for the parton shower and hadronisation, using the A14 set of tuned parameters [26] and the NNPDF2.3lo set of PDFs [2]. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

The $t\bar{t}$ sample was normalised to the cross-section prediction at next-to-next-to-leading order (NNLO) in QCD including the resummation of next-to-next-to-leading logarithmic (NNLL) soft-gluon terms calculated using Top++ 2.0 [90–96]. For proton–proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross-section corresponds to $\sigma(t\bar{t})_{\text{NNLO+NNLL}} = 832 \pm 51$ fb using a top-quark mass of $m_{\text{top}} = 172.5$ GeV. The uncertainties in the cross-section due to the PDF and α_{s} were calculated using the PDF4LHC15 prescription [52] with the MSTW2008nnlo [97, 98], CT10nnlo [33, 99] and NNPDF2.3lo [2] PDF sets in the five-flavour scheme, and were added in quadrature to the effect of the scale uncertainty.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}$ sample with two additional samples [88]. To simulate higher parton radiation, the factorisation and renormalisation scales were reduced by a factor of 0.5 while simultaneously increasing the h_{damp} value to 3.0 m_{top} and using the Var3c up variation from the A14 tune. For lower parton radiation, μ_{r} and μ_{f} were increased by a factor of two while keeping the h_{damp} value set to 1.5 m_{top} and using the Var3c down variation in the parton shower. The Var3c A14 tune variation [26] largely corresponds to the variation of α_{s} for ISR in the A14 tune. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up and down by a factor of two.

[1] The h_{damp} parameter is a resummation damping factor and one of the parameters that controls the matching of Powheg matrix elements to the parton shower and thus effectively regulates the high-p_{T} radiation against which the $t\bar{t}$ system recoils.

The NNPDF3.0LO replicas were used to evaluate the PDF uncertainties for the nominal PDF. In addition, the central value of this PDF was compared with the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets.

6.1.2 POWHEG+HERWIG 7.04

Samples The descriptions below correspond to the samples in Table 6.4.

Table 6.4: $t\bar{t}$ samples produced with POWHEG+HERWIG 7.

DSID range	Description
410557	$t\bar{t}$ single lepton
410558	$t\bar{t}$ dileptonic
410559	$t\bar{t}$ all-hadronic

Short description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal $t\bar{t}$ sample with another event sample produced with the POWHEG BOX v2 [28–30, 37] generator using the NNPDF3.0NLO [16] parton distribution function (PDF). Events in the latter sample were interfaced with HERWIG 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21]. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal $t\bar{t}$ sample with an event sample also produced with the POWHEG BOX v2 [28–30, 37] generator but interfaced with HERWIG 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21]. POWHEG BOX provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s, and used the NNPDF3.0NLO [16] parton distribution function (PDF) and an h_{damp} parameter value of 1.5 m_{top} [89]. The functional form of the renormalisation and factorisation scales was set to the default scale $\sqrt{m_{\mathrm{top}}^2 + p_{\mathrm{T}}^2}$. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

6.1.3 POWHEG+HERWIG 7.13

Samples The descriptions below correspond to the samples in Table 6.5.

Table 6.5: $t\bar{t}$ samples produced with POWHEG+HERWIG 7.13.

DSID range	Description
411233	$t\bar{t}$ single lepton
411234	$t\bar{t}$ dileptonic
411316	$t\bar{t}$ all-hadronic

Short description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal $t\bar{t}$ sample with another event sample produced with the POWHEG BOX v2 [28–30, 37] generator using the NNPDF3.0NLO [16] parton distribution function (PDF). Events in the latter sample were interfaced with HERWIG 7.13 [100, 101], using the HERWIG 7.1 default set of tuned parameters [101, 102] and the MMHT2014LO PDF set [21]. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal $t\bar{t}$ sample with an event sample also produced with the POWHEG BOX v2 [28–30, 37] generator but interfaced with HERWIG 7.13 [100, 101], using the HERWIG 7.1 default set of tuned parameters [101, 102] and the MMHT2014LO PDF set [21]. POWHEG BOX provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s, and used the NNPDF3.0NLO [16] parton distribution function (PDF) and an h_{damp} parameter value of 1.5 m_{top} [89]. The functional form of the renormalisation and factorisation scales was set to the default scale $\sqrt{m_{\text{top}}^2 + p_{\text{T}}^2}$. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

6.1.4 MADGRAPH5_aMC@NLO+PYTHIA 8

Samples The descriptions below correspond to the samples in Table 6.6.

Table 6.6: $t\bar{t}$ samples produced with MADGRAPH5_aMC@NLO+PYTHIA 8.

DSID range	Description
410464	$t\bar{t}$ single lepton
410465	$t\bar{t}$ dileptonic
410466	$t\bar{t}$ all-hadronic

Short description: To assess the uncertainty in the matching of NLO matrix elements to the parton shower, the POWHEG sample was compared with a sample of events generated with MADGRAPH5_aMC@NLO 2.6.0 [23] interfaced with PYTHIA 8.230 [42]. The MADGRAPH5_aMC@NLO calculation used the NNPDF3.0NLO set of PDFs [16] and PYTHIA 8 used the A14 set of tuned parameters [26] and the NNPDF2.3LO set of PDFs [2]. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

Long description: To assess the uncertainty due to the choice of matching scheme, the POWHEG sample was compared with a sample generated by MADGRAPH5_aMC@NLO+PYTHIA 8. For the calculation of the hard-scattering, MADGRAPH5_aMC@NLO 2.6.0 [23] with the NNPDF3.0NLO [16] PDF set was used. The events were interfaced with PYTHIA 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3LO set of PDFs [2]. Top quarks were decayed at LO using MADSPIN [103, 104] to preserve spin correlations. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27]. The parton-shower starting scale had the functional form $\mu_q = H_T/2$ [88], where H_T is defined as the scalar sum of the p_T of all outgoing partons. The renormalisation and factorisation scale choice was the same as for the POWHEG BOX set-up.

6.1.5 MadGraph5_aMC@NLO+Herwig 7.13

Samples The descriptions below correspond to the samples in Table 6.7.

Table 6.7: $t\bar{t}$ samples produced with MadGraph5_aMC@NLO+Herwig 7.13.

DSID range	Description
412116	$t\bar{t}$ single lepton
412117	$t\bar{t}$ dileptonic
412175	$t\bar{t}$ all-hadronic

Short description: To assess the uncertainty in the matching of NLO matrix elements to the parton shower, a sample produced with the Powheg Box v2 generator was compared with a sample generated with MadGraph5_aMC@NLO 2.6.0 [23], both using the NNPDF3.0nlo [16] parton distribution function (PDF) and interfaced with Herwig 7.13 [100, 101], using the Herwig 7.1 default set of tuned parameters [101] and the MMHT2014lo PDF set [21]. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

Long description: To assess the uncertainty in the matching of NLO matrix elements to the parton shower, a Powheg sample was compared with a sample generated by MadGraph5_aMC@NLO [23]. The first sample was produced with the same hard-scatter set-up as the nominal sample using the Powheg Box v2 [28–30, 37] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s, with the NNPDF3.0nlo [16] parton distribution function (PDF) and the h_{damp} parameter set to 1.5 m_{top} [89]. The functional form of the renormalisation and factorisation scales was set to the default scale $\sqrt{m_{\text{top}}^2 + p_{\text{T}}^2}$. The second sample used MadGraph5_aMC@NLO 2.6.0 with the NNPDF3.0nlo [16] PDF set for the calculation of the hard-scattering. Top quarks were decayed at LO using MadSpin [103, 104] to preserve spin correlations. The parton-shower starting scale had the functional form $\mu_q = H_T/2$ [88], where H_T is defined as the scalar sum of the p_T of all outgoing partons. The events from both generators were interfaced with Herwig 7.13 [100, 101], using the Herwig 7.1 default set of tuned parameters [101] and the MMHT2014lo PDF set [21]. The renormalisation and factorisation scale choice in the MadGraph5_aMC@NLO set-up was the same as for the Powheg Box set-up. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27] in both set-ups.

6.1.6 Sherpa 2.2.1

Samples The descriptions below correspond to the samples in Table 6.8.

Short description: Additional samples of $t\bar{t}$ events were produced with the Sherpa 2.2.1 [6] generator using NLO-accurate matrix elements for up to one additional parton, and LO-accurate matrix elements for up to four additional partons calculated with the Comix [7] and OpenLoops [8–10] libraries. They were

Table 6.8: $t\bar{t}$ samples produced with SHERPA 2.2.1.

DSID range	Description
410249	$t\bar{t}$ all-hadronic
410250	$t\bar{t}$ single lepton
410251	$t\bar{t}$ single lepton
410252	$t\bar{t}$ dileptonic

matched with the SHERPA parton shower [11] using the MEPS@NLO prescription [12–15] and the set of tuned parameters developed by the SHERPA authors to match the NNPDF3.0NNLO set of PDFs [16].

Additional information: The central scale had the functional form $\mu^2 = m_{\text{top}}^2 + 0.5 \times (p_{\text{T},t}^2 p + p_{\text{T},\bar{t}}^2)$. The CKKW matching scale of the additional emissions was set to 30 GeV.

6.2 Single-top tW associated production

This section describes the MC samples used for the modelling of single-top tW associated production. Section 6.2.1 describes the POWHEG+PYTHIA 8 samples – both for the diagram removal (DR) set-ups, which are used for the nominal prediction as well as uncertainties due to additional radiation and PDFs, and for the diagram subtraction (DS) set-ups, which are used for the uncertainty due to the treatment of the overlap with $t\bar{t}$ production. Section 6.2.2 describes the POWHEG+HERWIG 7 samples used for the uncertainty due to parton showering and hadronisation modelling, and Section 6.2.3 describes the MADGRAPH5_AMC@NLO+PYTHIA 8 samples used for the uncertainty due to the choice of matching scheme.

The reference cross-section values are extracted from Ref. [105].

6.2.1 POWHEG+PYTHIA 8

Samples Table 6.9 gives the DSIDs of the tW POWHEG+PYTHIA 8 samples, for both the DR and DS schemes. Single-top and single-anti-top (tW^- and $\bar{t}W^+$) events were generated in different samples. The dileptonic samples overlap with the inclusive ones.

Short description: The associated production of top quarks with W bosons (tW) was modelled by the POWHEG BOX v2 [28–30, 106] generator at NLO in QCD using the five-flavour scheme and the NNPDF3.0NLO set of PDFs [16]. The diagram removal scheme [107] was used to remove interference and overlap with $t\bar{t}$ production. The related uncertainty was estimated by comparison with an alternative sample generated using the diagram subtraction scheme [89, 107].[2] The events were interfaced to PYTHIA 8.230 [42] using the A14 tune [26] and the NNPDF2.3LO set of PDFs [2].

The uncertainty due to initial-state radiation (ISR) was estimated by simultaneously varying the h_{damp} parameter and the μ_{r} and μ_{f} scales, and choosing the Var3c up/down variants of the A14 tune as described

[2] Analyses which do not use this approach should obviously not use this sentence in their description.

Table 6.9: Single-top tW associated production samples produced with Powheg+Pythia 8.

DSID	Description
410646	tW^- (DR) inclusive
410647	$\bar{t}W^+$ (DR) inclusive
410648	tW^- (DR) dileptonic
410649	$\bar{t}W^+$ (DR) dileptonic
410654	tW^- (DS) inclusive
410655	$\bar{t}W^+$ (DS) inclusive
410656	tW^- (DS) dileptonic
410657	$\bar{t}W^+$ (DS) dileptonic

in Ref. [88]. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up or down by a factor two.

Long description: Single-top tW associated production was modelled using the Powheg Box v2 [28–30, 106] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0nlo [16] parton distribution function (PDF) set. The functional form of the renormalisation and factorisation scales was set to the default scale, which is equal to the top-quark mass ($m_{\text{top}} = 172.5$ GeV). The diagram removal scheme [107] was employed to handle the interference with $t\bar{t}$ production [89]. The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

The inclusive cross-section was corrected to the theory prediction calculated at NLO in QCD with NNLL soft-gluon corrections [108, 109]. For proton–proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross-section corresponds to $\sigma(tW)_{\text{NLO+NNLL}} = 71.7 \pm 3.8$ pb, using a top-quark mass of $m_{\text{top}} = 172.5$ GeV. The uncertainty in the cross-section due to the PDF was calculated using the MSTW2008nnlo 90% CL [97, 98] PDF set, and was added in quadrature to the effect of the scale uncertainty.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}$ sample with two additional samples [88]. To simulate higher parton radiation, the factorisation and renormalisation scales were reduced by a factor of 0.5 while simultaneously increasing the h_{damp} value to $3.0\,m_{\text{top}}$ and using the Var3c up variation from the A14 tune. For lower parton radiation, μ_r and μ_f were increased by a factor of two while keeping the h_{damp} value set to $1.5\,m_{\text{top}}$ and using the Var3c down variation in the parton shower. The Var3c A14 tune variation [26] largely corresponds to the variation of α_s for ISR in the A14 tune. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up and down by a factor of two.

The nominal Powheg+Pythia 8 sample was compared with an alternative sample generated using the diagram subtraction scheme [89, 107] to estimate the uncertainty arising from the interference with $t\bar{t}$ production.

To evaluate the PDF uncertainties for the nominal PDF, the 100 variations for NNPDF3.0nlo were taken into account. In addition, the central value of this PDF was compared with the central values of the CT14nnlo [20] and MMHT2014nnlo [21] PDF sets.

6.2.2 Powheg+Herwig 7

Samples Table 6.10 gives the DSIDs of the tW Powheg+Herwig 7 DR samples. Single-top and single-anti-top (tW^- and $\bar{t}W^+$) events were generated in different samples. The dileptonic samples overlap with the inclusive ones.

Table 6.10: Single-top tW associated production samples produced with Powheg+Herwig 7.

DSID	Description
411036	tW^- (DR) inclusive
411037	$\bar{t}W^+$ (DR) inclusive
411038	tW^- (DR) dileptonic
411039	$\bar{t}W^+$ (DR) dileptonic

Short description: The uncertainty due to the parton shower and hadronisation model was evaluated by comparing the nominal sample of events with a sample where events generated with the Powheg Box v2 [28–30, 106] generator were interfaced to Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014lo PDF set [21].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal tW sample with another sample produced with the Powheg Box v2 [28–30, 106] generator but interfaced with Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014lo PDF set [21]. Powheg Box provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0nlo [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to the default scale, which is equal to the top-quark mass. The diagram removal scheme [107] was employed to handle the interference with $t\bar{t}$ production [89]. The decays of bottom and charm hadrons are simulated using the EvtGen 1.6.0 program [27].

6.2.3 MadGraph5_aMC@NLO+Pythia 8

Samples Table 6.11 gives the DSIDs of the tW MadGraph5_aMC@NLO+Pythia 8 samples. The dileptonic sample overlaps with the inclusive one.

Table 6.11: Single-top tW associated production samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID	Description
412002	tW inclusive
412003	tW dileptonic

Short description: To assess the uncertainty in the matching of NLO matrix elements to the parton shower, the nominal tW sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator at NLO in QCD using the five-flavour scheme and the NNPDF2.3nlo [16] PDF set. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo PDF.

Long description: To assess the uncertainty due to the choice of matching scheme, the nominal tW sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme, using the NNPDF2.3nlo [16] PDF set. The functional form of the renormalisation and factorisation scale was set to the default scale, which is equal to the top-quark mass. The parton-shower starting scale had the functional form $\mu_q = H_T/2$ [88], where H_T is defined as the scalar sum of the p_T of all outgoing partons. The diagram removal scheme [107] was employed to handle the interference with $t\bar{t}$ production [89]. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo PDF. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

6.3 Single-top t-channel production

This section describes the MC samples used for the modelling of single-top t-channel production. Section 6.3.1 describes the Powheg+Pythia 8 samples used for the nominal prediction and for the uncertainty from additional radiation and due to PDFs. Section 6.3.2 describes the Powheg+Herwig 7 samples used for the uncertainty due to the choice of parton shower and hadronisation model, and Section 6.3.3 describes the MadGraph5_aMC@NLO+Pythia 8 samples used for the uncertainty due to the choice of matching scheme.

The reference cross-section values are extracted from Ref. [105].

6.3.1 Powheg+Pythia 8

Samples Table 6.12 gives the DSIDs of the t-channel Powheg+Pythia 8 samples. Single-top and single-anti-top events were generated in distinct samples.

Table 6.12: Single-top t-channel event samples produced with Powheg+Pythia 8.

DSID	Description
410658	t-channel t leptonic
410659	t-channel $\bar{t}$ leptonic

Short description: Single-top t-channel production was modelled using the POWHEG BOX v2 [28–30, 110] generator at NLO in QCD using the four-flavour scheme and the corresponding NNPDF3.0NLO set of PDFs [16]. The events were interfaced with PYTHIA 8.230 [42] using the A14 tune [26] and the NNPDF2.3LO set of PDFs [2].

The uncertainty due to initial-state radiation (ISR) was estimated by simultaneously varying the h_{damp} parameter and the μ_{r} and μ_{f} scales, and choosing the Var3c up/down variants of the A14 tune as described in Ref. [88]. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up or down by a factor two.

Long description: Single-top t-channel production was modelled using the POWHEG BOX v2 [28–30, 110] generator, which provided matrix elements at next-to-leading-order (NLO) accuracy in the strong coupling constant α_{s} in the four-flavour scheme with the corresponding NNPDF3.0NLO [16] parton distribution function (PDF) set. The functional form of the renormalisation and factorisation scales was set to $\sqrt{m_b^2 + p_{\text{T},b}^2}$ following the recommendation of Ref. [110]. Top quarks were decayed at LO using MADSPIN [103, 104] to preserve all spin correlations. The events were interfaced with PYTHIA 8.230 [42] using the A14 tune [26] and the NNPDF2.3LO PDF set. The decays of bottom and charm hadrons were simulated using the EVTGEN 1.6.0 program [27].

The inclusive cross-section was corrected to the theory prediction calculated at NLO in QCD with HATHOR 2.1 [111, 112]. For proton–proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross-section corresponds to $\sigma(t, t\text{-chan})_{\text{NLO}} = 136.02^{+5.40}_{-4.57}$ pb ($\sigma(\bar{t}, t\text{-chan})_{\text{NLO}} = 80.95^{+4.06}_{-3.61}$ pb) for single-top (single-anti-top) production, using a top-quark mass of $m_{\text{top}} = 172.5$ GeV. The uncertainties in the cross-section due to the PDF and α_{s} were calculated using the PDF4LHC prescription [52] with the MSTW2008NLO 68% CL [97, 98], CT10NLO [33] and NNPDF2.3NLO [2] PDF sets, and were added in quadrature to the effect of the scale uncertainty.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}$ sample with two additional samples [88]. To simulate higher parton radiation, the factorisation and renormalisation scales were reduced by a factor of 0.5 while simultaneously increasing the h_{damp} value to $3.0\,m_{\text{top}}$ and using the Var3c up variation from the A14 tune. For lower parton radiation, μ_{r} and μ_{f} were increased by a factor of two while keeping the h_{damp} value set to $1.5\,m_{\text{top}}$ and using the Var3c down variation in the parton shower. The Var3c A14 tune variation [26] largely corresponds to the variation of α_{s} for ISR in the A14 tune. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up and down by a factor of two.

To evaluate the PDF uncertainties for the nominal PDF, the 100 variations for NNPDF3.0NLO were taken into account. In addition, the central value of this PDF was compared with the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets.

6.3.2 POWHEG+HERWIG 7

Samples Table 6.13 gives the DSIDs of the t-channel POWHEG+HERWIG 7 samples. Single-top and single-anti-top events were generated in distinct samples.

Table 6.13: Single-top t-channel event samples produced with Powheg+Herwig 7.

DSID	Description
411032	t-channel $\bar{t}$ leptonic
411033	t-channel t leptonic

Short description: The uncertainty due to the parton shower and hadronisation model was evaluated by comparing the nominal sample of events with a sample where the events generated with the Powheg Box v2 [28–30, 110] generator were interfaced to Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014lo PDF set [21].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal sample with another sample produced with the Powheg Box v2 [28–30, 110] generator but interfaced with Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014lo PDF set [21]. Powheg Box provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the four-flavour scheme with the corresponding NNPDF3.0nlo [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to $\sqrt{m_b^2 + p_{\mathrm{T},b}^2}$ following the recommendation of Ref. [110]. Top quarks were decayed at LO using MadSpin [103, 104] to preserve all spin correlations. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

6.3.3 MadGraph5_aMC@NLO+Pythia 8

Samples Table 6.14 gives the DSIDs of the t-channel MadGraph5_aMC@NLO+Pythia 8 samples.

Table 6.14: Single-top t-channel event samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID	Description
412004	t-channel leptonic

Short description: To assess the uncertainty in the matching of NLO matrix elements to the parton shower, the nominal sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator at NLO in QCD using the five-flavour scheme and the NNPDF2.3nlo [16] PDF set. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo PDF set.

Long description: To assess the uncertainty due to the choice of matching scheme, the nominal sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the four-flavour scheme, using the corresponding NNPDF3.0nlo [16] PDF set. The functional form of the renormalisation and factorisation scales was set to $\sqrt{m_b^2 + p_{\mathrm{T},b}^2}$ following the recommendation of Ref. [110].

The parton-shower starting scale had the functional form $\mu_q = H_T/2$ [88], where H_T is defined as the scalar sum of the p_T of all outgoing partons. Top quarks were decayed at LO using MadSpin [103, 104] to preserve all spin correlations. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

6.3.4 Single-top s-channel production

This section describes the MC samples used for the modelling of single-top s-channel production. Section 6.3.5 describes the Powheg+Pythia 8 samples used for the nominal prediction and for the uncertainty from additional radiation and due to PDFs. Section 6.3.6 describes the Powheg+Herwig 7 samples used for the uncertainty due to the parton shower and hadronisation model, and Section 6.3.7 describes the MadGraph5_aMC@NLO+Pythia 8 samples used for the uncertainty due to the choice of matching scheme.

The reference cross-section values are extracted from Ref. [105].

6.3.5 Powheg+Pythia 8

Samples Table 6.15 gives the DSIDs of the s-channel Powheg+Pythia 8 samples. Single-top and single-anti-top events were generated in distinct samples.

Table 6.15: Single-top s-channel event samples produced with Powheg+Pythia 8.

DSID	Description
410644	s-channel t leptonic
410645	s-channel $\bar{t}$ leptonic

Short description: Single-top s-channel production was modelled using the Powheg Box v2 [28–30, 113] generator at NLO in QCD in the five-flavour scheme with the NNPDF3.0nlo [16] parton distribution function (PDF) set. The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo PDF set.

The uncertainty due to initial-state radiation (ISR) was estimated by simultaneously varying the h_{damp} parameter and the μ_r and μ_f scales, and choosing the Var3c up/down variants of the A14 tune as described in Ref. [88]. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up or down by a factor two.

Long description: Single-top s-channel production was modelled using the Powheg Box v2 [28–30, 113] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0nlo [16] parton distribution function (PDF) set. The functional form of the renormalisation and factorisation scales was set to the default scale, which was equal to the top-quark mass. The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3LO PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

The inclusive cross-section was corrected to the theory prediction calculated at NLO in QCD with Hathor 2.1 [111, 112]. For proton–proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross-section corresponds to $\sigma(t, s\text{-chan})_{\text{NLO}} = 6.35^{+0.23}_{-0.20}$ pb ($\sigma(\bar{t}, s\text{-chan})_{\text{NLO}} = 3.97^{+0.19}_{-0.17}$ pb) for single-top (single-anti-top) production, using a top-quark mass of $m_{\text{top}} = 172.5$ GeV. The uncertainties in the cross-section due to the PDF and α_{s} were calculated using the PDF4LHC prescription [52] with the MSTW2008NLO 68% CL [97, 98], CT10NLO [33] and NNPDF2.3NLO [2] PDF sets, and were added in quadrature to the effect of the scale uncertainty.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}$ sample with two additional samples [88]. To simulate higher parton radiation, the factorisation and renormalisation scales were reduced by a factor of 0.5 while simultaneously increasing the h_{damp} value to $3.0\,m_{\text{top}}$ and using the Var3c up variation from the A14 tune. For lower parton radiation, μ_{r} and μ_{f} were increased by a factor of two while keeping the h_{damp} value set to $1.5\,m_{\text{top}}$ and using the Var3c down variation in the parton shower. The Var3c A14 tune variation [26] largely corresponds to the variation of α_{s} for ISR in the A14 tune. The impact of final-state radiation (FSR) was evaluated by varying the renormalisation scale for emissions from the parton shower up and down by a factor of two.

To evaluate the PDF uncertainties for the nominal PDF, the 100 variations for NNPDF3.0NLO were taken into account. In addition, the central value of this PDF was compared with the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets.

6.3.6 Powheg+Herwig 7

Samples Table 6.16 gives the DSIDs of the s-channel Powheg+Herwig 7 samples. Single-top and single-anti-top events were generated in distinct samples.

Table 6.16: Single-top s-channel event samples produced with Powheg+Herwig 7.

DSID	Description
411034	s-channel t leptonic
411035	s-channel $\bar{t}$ leptonic

Short description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal sample with another sample produced with the Powheg Box v2 [28–30, 113] generator at NLO in the strong coupling constant α_{s} in the five-flavour scheme using the NNPDF3.0NLO [16] parton distribution function (PDF). Events in the latter sample were interfaced with Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal sample with another sample produced with the Powheg Box v2 [28–30, 113] generator but interfaced with Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21]. Powheg Box provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0NLO [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to the default scale, which is equal to the top-quark mass. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

6.3.7 MadGraph5_aMC@NLO+Pythia 8

Samples Table 6.17 gives the DSIDs of the s-channel MadGraph5_aMC@NLO+Pythia 8 samples.

Table 6.17: Single-top s-channel event samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID	Description
412005	s-channel leptonic

Short description: To assess the uncertainty due to the choice of matching scheme, the nominal sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator at NLO in the strong coupling constant α_s in the five-flavour scheme, using the NNPDF3.0NLO [16] PDF set. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3LO PDF set.

Long description: To assess the uncertainty due to the choice of matching scheme, the nominal sample was compared with a sample generated with the MadGraph5_aMC@NLO 2.6.2 [23] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0NLO [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to the default scale, which is equal to the top-quark mass. The parton-shower starting scale had the functional form $\mu_q = H_T/2$ [88], where H_T is defined as the scalar sum of the p_T of all outgoing partons. Top quarks were decayed at LO using MadSpin [103, 104] to preserve all spin correlations. The events were interfaced with Pythia 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3LO PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

6.4 $t\bar{t}$+HF

In the following subsections, the set-ups of the current baseline samples for the production of $t\bar{t}$ quark pairs in association with b-quarks ($t\bar{t}$+HF) are described. NLO predictions with massive b-quarks in the matrix element and matched to parton shower programs are available within the Sherpa+OpenLoops, MadGraph5_aMC@NLO and, more recently, Powheg Box frameworks.

6.4.1 Sherpa

The descriptions below refer to the Sherpa 2.2.1 samples. Details of the set-up are given in Ref. [114] and reported below.

Samples The descriptions below correspond to the samples in Table 6.18.

Table 6.18: Nominal $t\bar{t}$ +HF samples produced with SHERPA. Variation samples are not explicitly listed.

DSID range	Description
410323–4	$t\bar{t}$ single lepton
410325	$t\bar{t}$ dilepton
410369	$t\bar{t}$ all-hadronic

Description: Samples for $t\bar{t}$+HF processes were produced with the SHERPA 2.2.1 [6] generator, using the MEPS@NLO prescription [13] and interfaced with OPENLOOPS [8–10] to provide the virtual corrections for matrix elements at NLO accuracy. The four-flavour scheme is used with the b-quark mass set to 4.75 GeV. The renormalisation scale μ_r has the functional form $\sqrt[4]{m_T(t) \cdot m_T(\bar{t}) \cdot m_T(b) \cdot m_T(\bar{b})}$. The factorisation scale μ_f was set to $H_T/2$, where H_T is the transverse-mass sum of the partons in the matrix element, and this value was also the resummation scale μ_q of the parton shower. The CT10NLO PDF set was used in conjunction with a dedicated PS tune developed by the SHERPA authors.

6.4.2 MADGRAPH5_aMC@NLO+PYTHIA 8

In the following, set-ups are described for PYTHIA only. Details of the set-up are given in Ref. [114] and reported below.

Samples The descriptions below correspond to the samples in Table 6.19.

Table 6.19: Nominal $t\bar{t}$ +HF samples produced with MADGRAPH5_aMC@NLO+PYTHIA 8.

DSID range	Description
410265	$t\bar{t}$ non-all-hadronic
410266	$t\bar{t}$ dileptonic
410267	$t\bar{t}$ all-hadronic

Description: Samples for $t\bar{t}$+HF processes were produced with the MADGRAPH5_aMC@NLO generator with the NNPDF3.0NLO [16] PDF set. It was interfaced with PYTHIA 8.230 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3LO PDF. The four-flavour scheme was used with the b-quark mass set to 4.75 GeV. The renormalisation scale μ_r has the functional form $\sqrt[4]{m_T(t) \cdot m_T(\bar{t}) \cdot m_T(b) \cdot m_T(\bar{b})}$. The factorisation scale μ_f was set to $H_T/2$, where H_T is the transverse-mass sum of the partons in the matrix element. The resummation scale μ_q has the form $\mu_q = f_Q\sqrt{\hat{s}}$, where the prefactor f_Q is an external parameter randomly distributed in the range $[f_Q^{min}, f_Q^{max}] = [0.1, 0.25]$.

6.4.3 POWHEG BOX RES +PYTHIA 8

In the following, set-ups are described for PYTHIA 8 only.

Samples The descriptions below correspond to the samples in Table 6.20.

Table 6.20: Nominal $t\bar{t}$ +HF samples produced with Powheg Box Res +Pythia 8.

DSID range	Description
411179–80	$t\bar{t}$ non-all-hadronic
411178	$t\bar{t}$ dileptonic
411275	$t\bar{t}$ all-hadronic

Description: Samples for $t\bar{t}$+HF processes were produced with the Powheg Box Res [115] generator and OpenLoops [8–10], using a pre-release of the implementation of this process in Powheg Box Res provided by the authors [116], with the NNPDF3.0nlo [16] PDF set. It was interfaced with Pythia 8.240 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo PDF set. The four-flavour scheme was used with the b-quark mass set to 4.95 GeV. The factorisation scale was set to $0.5 \times \Sigma_{i=t,\bar{t},b,\bar{b},j} m_{\mathrm{T},i}$, the renormalisation scale was set to $\sqrt[4]{m_{\mathrm{T}}(t) \cdot m_{\mathrm{T}}(\bar{t}) \cdot m_{\mathrm{T}}(b) \cdot m_{\mathrm{T}}(\bar{b})}$, and the h_{damp} parameter was set to $0.5 \times \Sigma_{i=t,\bar{t},b,\bar{b}} m_{\mathrm{T},i}$.

7 Rare top-quark processes

This chapter describes the samples used for rare top-quark processes. Section 7.1 describes the $t\bar{t}H$ samples. Section 7.2 describes the $t\bar{t}V$ ($V = W/Z$) samples. Section 7.3 describes the $t\bar{t}\gamma$ samples. Section 7.4 describes the tH samples. Section 7.6 describes the tZq samples. Section 7.7 describes the tWZ samples. Finally, Section 7.8 describes the $t\bar{t}t\bar{t}$ samples.

7.1 $t\bar{t}H$

7.1.1 Powheg+Pythia 8

Nominal $t\bar{t}H$ samples are produced with Powheg+Pythia 8. The h_{damp} value is set to 352.5 GeV $= 3/4 \cdot (m_H + 2m_{\text{top}})$.

Samples Table 7.1 gives the nominal $t\bar{t}H$ samples.

Table 7.1: Nominal $t\bar{t}H$ samples produced with Powheg+Pythia 8.

DSID range	Description
346343	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ all-hadronic
346344	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ semileptonic
346345	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ dileptonic
346525	$t\bar{t}H$, $H \to \gamma\gamma$, $t\bar{t} \to$ all

Short description: The production of $t\bar{t}H$ events was modelled using the Powheg Box v2 [28–30, 37, 117] generator at NLO with the NNPDF3.0nlo [16] PDF set. The events were interfaced to Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were performed by EvtGen 1.6.0 [27].

Long description: The production of $t\bar{t}H$ events was modelled using the Powheg Box v2 [28–30, 37, 117] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s in the five-flavour scheme with the NNPDF3.0nlo [16] PDF set. The functional form of the renormalisation and factorisation scales was set to $\sqrt[3]{m_T(t) \cdot m_T(\bar{t}) \cdot m_T(H)}$. The events were interfaced to Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were performed by EvtGen 1.6.0 [27].

The cross-section was calculated at NLO QCD and NLO EW accuracy using MadGraph5_aMC@NLO as reported in Ref. [53]. The predicted value at $\sqrt{s} = 13$ TeV is 507^{+35}_{-50} fb, where the uncertainties were estimated from variations of α_s and the renormalisation and factorisation scales.

The uncertainty in the initial-state radiation (ISR) was estimated using the Var3c up/down variations of the A14 tune. Uncertainties due to missing higher-order corrections were evaluated through simultaneous variations of the renormalisation and factorisation scales by factors of 2.0 and 0.5. Uncertainties in the PDFs were evaluated using the 100 variations of the NNPDF3.0NLO set.

7.1.2 Powheg+Herwig 7

Samples Table 7.2 presents alternative $t\bar{t}H$ samples.

Table 7.2: Alternative $t\bar{t}H$ Powheg+Herwig 7 samples produced to evaluate systematic uncertainties due to different MC models for parton showering and hadronisation.

DSID range	Description
346346	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ all-hadronic
346347	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ semileptonic
346348	$t\bar{t}H$, $H \to$ all, $t\bar{t} \to$ dileptonic
346526	$t\bar{t}H$, $H \to \gamma\gamma$, $t\bar{t} \to$ all

Short description: The impact of using a different parton shower and hadronisation model was evaluated by showering the nominal hard-scatter events with Herwig 7.04 [100, 101] using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21].

Long description: The impact of using a different parton shower and hadronisation model was evaluated by comparing the nominal sample with another sample produced with the Powheg Box v2 [28–30, 37] generator but interfaced with Herwig 7.04 [100, 101], using the H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21]. Powheg Box provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s with the NNPDF3.0NLO [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to $\sqrt[3]{m_T(t) \cdot m_T(\bar{t}) \cdot m_T(H)}$. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

7.2 $t\bar{t}V$ production

This section describes the MC samples used for the modelling of $t\bar{t}V$ ($V = W/Z$) production. Section 7.2.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples, and Section 7.2.2 describes the Sherpa samples. (NOTE: this section is not frozen as the Sherpa samples are likely to be updated and become the nominal samples in the near future.)

7.2.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Tables 7.3 and 7.4.

Table 7.3: Nominal $t\bar{t}V$ samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
410155	$t\bar{t}W$
410156	$t\bar{t}Z(\to \nu\nu)$
410157	$t\bar{t}Z(\to qq)$
410218	$t\bar{t}e^+e^-$, $m_{\ell\ell} > 5$ GeV
410219	$t\bar{t}\mu^+\mu^-$, $m_{\ell\ell} > 5$ GeV
410220	$t\bar{t}\tau^+\tau^-$, $m_{\ell\ell} > 5$ GeV
410276	$t\bar{t}e^+e^-$, $m_{\ell\ell} \in [1, 5]$ GeV
410277	$t\bar{t}\mu^+\mu^-$, $m_{\ell\ell} \in [1, 5]$ GeV
410278	$t\bar{t}\tau^+\tau^-$, $m_{\ell\ell} \in [1, 5]$ GeV

Table 7.4: $t\bar{t}V$ samples produced with MadGraph5_aMC@NLO+Pythia 8 used to estimate initial-state radiation systematic uncertainties.

DSID range	Description
410376	$t\bar{t}W$ A14Var3c up
410377	$t\bar{t}W$ A14Var3c down
410378	$t\bar{t}Z(\to \nu\nu)$ A14Var3c up
410379	$t\bar{t}Z(\to \nu\nu)$ A14Var3c down
410380	$t\bar{t}Z(\to qq)$ A14Var3c up
410381	$t\bar{t}Z(\to qq)$ A14Var3c down
410370	$t\bar{t}e^+e^-$ A14Var3c up
410371	$t\bar{t}e^+e^-$ A14Var3c down
410372	$t\bar{t}\mu^+\mu^-$ A14Var3c up
410373	$t\bar{t}\mu^+\mu^-$ A14Var3c down
410374	$t\bar{t}\tau^+\tau^-$ A14Var3c up
410375	$t\bar{t}\tau^+\tau^-$ A14Var3c down

Short description: The production of $t\bar{t}V$ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced to Pythia 8.210 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.2.0 program [27].

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal event sample with two samples where the Var3c up/down variations of the A14 tune were employed.

Long description: The production of $t\bar{t}V$ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s with the NNPDF3.0NLO [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to the default of $0.5 \times \sum_i \sqrt{m_i^2 + p_{T,i}^2}$, where the sum runs over all the particles generated from the matrix element calculation. Top quarks were decayed at LO using MadSpin [103, 104] to preserve spin correlations. The events were interfaced with Pythia 8.210 [42] for the parton shower and hadronisation, using the A14 set of tuned parameters [26] and the NNPDF2.3LO [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.2.0 program [27].

The cross-sections were calculated at NLO QCD and NLO EW accuracy using MadGraph5_aMC@NLO as reported in Ref. [53]. In the case of $t\bar{t}\ell\ell$ the cross-section was scaled by an off-shell correction estimated at one-loop level in α_s. (*Optionally:*) The predicted values at $\sqrt{s} = 13$ TeV are $0.88^{+0.09}_{-0.11}$ pb and $0.60^{+0.08}_{-0.07}$ pb for $t\bar{t}Z$ and $t\bar{t}W$, respectively, where the uncertainties were estimated from variations of α_s and the renormalisation and factorisation scales.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}V$ sample with two additional samples, which have the same settings as the nominal one, but employed the Var3c up or down variation of the A14 tune, which corresponds to the variation of α_s for initial-state radiation (ISR) in the A14 tune.

Uncertainties due to missing higher-order corrections were evaluated by simultaneously varying the renormalisation and factorisation scales by factors of 2.0 and 0.5. Uncertainties in the PDFs were evaluated using the 100 replicas of the NNPDF3.0NLO set.

7.2.2 Sherpa

Samples The descriptions below correspond to the samples in Table 7.5.

Table 7.5: $t\bar{t}V$ samples produced with Sherpa.

DSID range	Description
410142	$t\bar{t}\ell\ell$
410143	$t\bar{t}Z(\rightarrow qq)$, $t\bar{t}Z(\rightarrow \nu\nu)$
410144	$t\bar{t}W$

Description: Additional $t\bar{t}V$ samples were produced with the Sherpa 2.2.0 [6] generator at LO accuracy, using the MEPS@LO set-up [14, 15] with up to one additional parton for the $t\bar{t}\ell\ell$ sample and two additional partons for the others. A dynamic renormalisation scale was used and is defined similarly to that of the nominal $t\bar{t}V$ samples. The CKKW matching scale of the additional emissions was set to 30 GeV. The default Sherpa 2.2.0 parton shower was used along with the NNPDF3.0NNLO [16] PDF set.

7.3 $t\bar{t}\gamma$ production

This section describes the MC samples used for the modelling of $t\bar{t}\gamma$ production. Section 7.3.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples, and Section 7.3.2 describes the MadGraph5_aMC@NLO+Herwig 7 samples.

7.3.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Tables 7.6 and 7.7.

Table 7.6: Nominal $t\bar{t}\gamma$ samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
410389	$t\bar{t}\gamma$, non-all-hadronic
410394	$t\bar{t}\gamma$, all-hadronic

Table 7.7: $t\bar{t}\gamma$ samples produced with MadGraph5_aMC@NLO+Pythia 8 used to estimate initial-state radiation systematic uncertainties.

DSID range	Description	
410404	$t\bar{t}\gamma$	non-all-hadronic, A14Var3c up
410405	$t\bar{t}\gamma$	non-all-hadronic, A14Var3c down
410410	$t\bar{t}\gamma$	all-hadronic, A14Var3c up
410411	$t\bar{t}\gamma$	all-hadronic, A14Var3c down

Short description: The production of $t\bar{t}\gamma$ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at LO with the NNPDF2.3lo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.212 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}\gamma$ sample with two additional samples, where the Var3c up/down variations of the A14 tune were employed.

Long description: The $t\bar{t}\gamma$ sample was simulated as a $2\rightarrow7$ process at LO including the decay of the top quarks by MadGraph5_aMC@NLO 2.3.3 [23] with the NNPDF2.3lo [16] parton distribution function (PDF), interfaced with Pythia 8.212 [42], using the A14 set of tuned parameters [26] and the NNPDF2.3lo [16] PDF set. The photon could be radiated from an initial charged parton, an intermediate top quark, or any of the charged final-state particles. The top-quark mass, top-quark decay width, W-boson decay width, and fine structure constant were set to 172.5 GeV, 1.320 GeV, 2.085 GeV, and 1/137, respectively. The five-flavour scheme was used, where all the quark masses are set to zero, except for the top quark. The renormalisation and the factorisation scales were set to $0.5 \times \sum_i \sqrt{m_i^2 + p_{\mathrm{T},i}^2}$, where the sum runs over all the particles generated from the matrix element calculation. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

The cross-section was calculated at NLO in QCD as reported in Ref. [118], resulting in a K-factor of 1.24 which was applied to the samples, with a relative uncertainty of 14% from variations of renormalisation and factorisation scales as well as the choice of PDF set.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal $t\bar{t}V$ sample with two additional samples, which had the same settings as the nominal one, but employed the Var3c up or down variation of the A14 tune, which corresponds to the variation of α_s for initial-state radiation (ISR) in the A14 tune.

To evaluate the effect of renormalisation and factorisation scale uncertainties, the two scales were varied simultaneously by factors 2.0 and 0.5. To evaluate the PDF uncertainties for the nominal PDF, the 100 replicas for NNPDF2.3LO were taken into account.

7.3.2 MadGraph5_aMC@NLO+Herwig 7

Samples The descriptions below correspond to the samples in Table 7.8.

Table 7.8: $t\bar{t}\gamma$ samples produced with MadGraph5_aMC@NLO+Herwig 7.

DSID range	Description
410395	$t\bar{t}\gamma$ non-all-hadronic
410396	$t\bar{t}\gamma$ all-hadronic

Short description: Additional $t\bar{t}\gamma$ samples were produced with the parton shower of the nominal samples replaced by Herwig 7.04 [100, 101] to evaluate the impact of using using a different parton shower and hadronisation model. The H7UE set of tuned parameters [101] and the MMHT2014LO PDF set [21] were used.

7.4 *tHq*

This section describes the MC samples used for the modelling of tH production. Section 7.4.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples,

7.4.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Table 7.9.

Table 7.9: Nominal tH samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
346188	tHq $H \to \gamma\gamma$ four flavour
346229	tHq $H \to b\bar{b}$ four flavour
346230	tHq $H \to \tau\tau/H \to ZZ/H \to W^+W^-$ four flavour
346414	tHq $H \to \ell\ell\ell\ell$, four flavour
346676	tHq $H \to$ inclusive, four flavour, UFO model
346677	tHq $H \to \gamma\gamma$, four flavour, UFO model
346799	tHq $H \to \tau\tau/H \to ZZ/H \to W^+W^-$ + Nleptons=2 filter, four flavour, UFO model

Table 7.10: Nominal tHW samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID	Description
346486	tHW $H \to \gamma\gamma$
346511	tHW $H \to \ell\ell\ell\ell$
346678	tHW $H \to$ inclusive, UFO model
346759	tHW $H \to \gamma\gamma$, UFO model

Exceptions: If and only if you are using the UFO model sample: the correct version is MadGraph5_aMC@NLO 2.6.2.

Short description: The production of tHq events was modelled using the MadGraph5_aMC@NLO 2.6.0 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

Long description: The tHq samples were simulated using the MadGraph5_aMC@NLO 2.6.0 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The top quark was decayed at LO using MadSpin [103, 104] to preserve spin correlations, whereas the Higgs boson was decayed by Pythia in the parton shower. The samples were generated in the four-flavour scheme. The functional form of the renormalisation and factorisation scales was set to the default scale $0.5\times\sum_i \sqrt{m_i^2 + p_{\mathrm{T},i}^2}$, where the sum runs over all the particles generated from the matrix element calculation. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

7.5 *tHW*

This section describes the MC samples used for the modelling of tHW production. Section 7.5.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples.

7.5.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Table 7.10.

Short description: The tHW production is modelled using the MadGraph5_aMC@NLO 2.6.2 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The overlap with the $t\bar{t}H$ production is removed using the diagram removal scheme [107, 119]. The events are interfaced with Pythia 8.235 [42] using the A14 parameter set [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons are simulated using the EvtGen 1.6.0 program [27].

Long description: The tHW samples were simulated using the MadGraph5_aMC@NLO 2.6.2 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.235 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The top quark was decayed at LO using MadSpin [103, 104] to preserve spin correlations, whereas the Higgs boson was decayed by Pythia in the parton shower. The samples were generated in the five-flavour scheme. The functional form of the renormalisation and factorisation scales was set to the default scale $0.5\times\sum_i \sqrt{m_i^2 + p_{\mathrm{T},i}^2}$, where the sum runs over all the particles generated from the matrix element calculation. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

7.6 tZq

This section describes the MC samples used for the modelling of tZq production. Section 7.6.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples,

7.6.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Tables 7.11 and 7.12.

Table 7.11: Nominal tZq samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
412063	tZq

Table 7.12: tZq samples produced with MadGraph5_aMC@NLO+Pythia 8 used to estimate initial-state radiation systematic uncertainties.

DSID range	Description
412065	tZq, A14Var3c up
410064	tZq, A14Var3c down

Short description: The production of tZq events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal tZq sample with two additional samples, which had the same settings as the nominal one, but employed the Var3c up and down variations of the A14 tune.

Long description: The tZq sample was simulated using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. Off-resonance events away from the Z mass peak were included. The top quark was decayed at LO using

MadSpin [103, 104] to preserve spin correlations. The four-flavour scheme was used, where all the quark masses are set to zero, except for the top and bottom quarks. Following the discussion in Ref. [110], the functional form of the renormalisation and factorisation scales was set to $4\sqrt{m_b^2 + p_{\mathrm{T},b}^2}$, where the b-quark was the one produced by a gluon splitting in the event. The decays of bottom and charm hadrons were simulated using the EvtGen program [27].

The tZq total cross-section, calculated at next-to-leading order (NLO) using MadGraph5_aMC@NLO 2.3.3 with the NNPDF3.0nlo PDF set, is 800 fb, with an uncertainty of $^{+6.1}_{-7.4}$%. The uncertainty was computed by varying the renormalisation and factorisation scales by a factor of two and by a factor of 0.5.

The uncertainty due to initial-state radiation (ISR) was estimated by comparing the nominal tZq sample with two additional samples, which have the same settings as the nominal one, but employed the Var3c up or down variation of the A14 tune, which corresponds to the variation of α_{s} for ISR in the A14 tune.

To evaluate the effect of renormalisation and factorisation scale uncertainties, the two scales were varied simultaneously by factors 2.0 and 0.5. To evaluate the PDF uncertainties for the nominal PDF, the 100 variations for NNPDF2.3lo were taken into account.

7.7 tWZ

This section describes the MC samples used for the modelling of tWZ production. Section 7.7.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples,

7.7.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Table 7.13.

Table 7.13: Nominal tWZ samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
410408	tWZ DR1
410409	tWZ DR2

Short description: The production of tWZ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.212 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.2.0 program [27].

Long description: The production of tWZ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.0nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.212 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The top quark and the Z boson were decayed at LO using MadSpin [103, 104] to preserve spin correlations. While the top quark was allowed to decay inclusively, the Z boson decay was restricted to a pair of charged leptons.

The five-flavour scheme was used, where all the quark masses are set to zero, except the top quark. The renormalisation and factorisation scales were set to the top-quark mass. The diagram removal scheme described in Ref. [107] was employed to handle the interference between tWZ and $t\bar{t}Z$, and was applied to the tWZ sample. A sample with the alternative scheme described in Ref. [119] was produced to assess the associated systematic uncertainty. The decays of bottom and charm hadrons were simulated using the EvtGen 1.2.0 program [27].

7.8 $t\bar{t}t\bar{t}$ production

This section describes the MC samples used for the modelling of $t\bar{t}t\bar{t}$ production. Section 7.8.1 describes the MadGraph5_aMC@NLO+Pythia 8 samples, and Section 7.8.2 describes the MadGraph5_aMC@NLO+Herwig 7 samples.

7.8.1 MadGraph5_aMC@NLO+Pythia 8

Samples The descriptions below correspond to the samples in Table 7.14.

Table 7.14: Nominal $t\bar{t}t\bar{t}$ samples produced with MadGraph5_aMC@NLO+Pythia 8.

DSID range	Description
412043	$t\bar{t}t\bar{t}$

Short description: The production of $t\bar{t}t\bar{t}$ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator at NLO with the NNPDF3.1nlo [16] parton distribution function (PDF). The events were interfaced with Pythia 8.230 [42] using the A14 tune [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

Long description: The production of $t\bar{t}t\bar{t}$ events was modelled using the MadGraph5_aMC@NLO 2.3.3 [23] generator, which provided matrix elements at next-to-leading order (NLO) in the strong coupling constant α_s with the NNPDF3.1nlo [16] parton distribution function (PDF). The functional form of the renormalisation and factorisation scales was set to $0.25 \times \sum_i \sqrt{m_i^2 + p_{\text{T},i}^2}$, where the sum runs over all the particles generated from the matrix element calculation, following the Ref. [120]. Top quarks were decayed at LO using MadSpin [103, 104] to preserve all spin correlations. The events were interfaced with Pythia 8.230 [42] for the parton shower and hadronisation, using the A14 set of tuned parameters [26] and the NNPDF2.3lo [16] PDF set. The decays of bottom and charm hadrons were simulated using the EvtGen 1.6.0 program [27].

7.8.2 MadGraph5_aMC@NLO+Herwig 7

Samples The descriptions below correspond to the samples in Table 7.15.

Table 7.15: $t\bar{t}t\bar{t}$ samples produced with MadGraph5_aMC@NLO+Herwig 7.

DSID range	Description
412044	$t\bar{t}t\bar{t}$

Description: Additional $t\bar{t}t\bar{t}$ samples were produced with the parton shower of the nominal samples replaced by Herwig 7.04 [100, 101] to evaluate the impact of using a different parton shower and hadronisation model. The H7UE set of tuned parameters [101] and the MMHT2014lo PDF set [21] were used.

8 Jet processes

This section describes the MC samples used for the modelling of multijet production. Section 8.1 describes the PYTHIA 8 samples, Section 8.2 describes the HERWIG 7 samples, Section 8.3 describes the POWHEG+PYTHIA 8 samples, and finally Section 8.4 describes the SHERPA samples.

8.1 PYTHIA 8

The descriptions below correspond to the samples in Table 8.1.

Table 8.1: Nominal multijet samples produced with PYTHIA.

DSID range	Description
364700–364712	PYTHIA with shower weights

Description: Multijet production was generated using PYTHIA 8.230 [42] with leading-order matrix elements for dijet production which were matched to the parton shower.

The renormalisation and factorisation scales were set to the geometric mean of the squared transverse masses of the two outgoing particles in the matrix element, $p_{\mathrm{T}}^{\mathrm{hat}} = \sqrt{(p_{\mathrm{T},1}^2 + m_1^2)(p_{\mathrm{T},2}^2 + m_2^2)}$. The NNPDF2.3LO PDF set [2] was used in the ME generation, the parton shower, and the simulation of the multi-parton interactions. The A14 [26] set of tuned parameters was used. Perturbative uncertainties were estimated through event weights [121] that encompass variations of the scales at which the strong coupling constant is evaluated in the initial- and final-state shower as well as the PDF uncertainty in the shower and the non-singular part of the splitting functions.

Additional description: The modelling of fragmentation and hadronisation was based on the Lund string model [122, 123]. To populate the inclusive jet p_{T} spectrum efficiently, the sample used a biased phase-space sampling which was compensated for by a continuously decreasing weight for the event. Specifically, events at a scale $p_{\mathrm{T}}^{\mathrm{hat}}$ scale were oversampled by a factor of $(p_{\mathrm{T}}^{\mathrm{hat}}/10\,\mathrm{GeV})^4$.

8.2 HERWIG 7.1

The descriptions below correspond to the samples in Table 8.2.

Table 8.2: Multijet samples produced with HERWIG 7.

DSID range	Description
364922–364929	angular ordering in shower HERWIG 7
364902–364909	dipole shower HERWIG 7

Description: Multijet production at next-to-leading order (NLO) was generated using HERWIG 7.1.3 [102]. The renormalisation and factorisation scales were set to the p_T of the leading jet. The MMHT2014NLO [21] PDF set was used for the matrix element calculation. Two sets of samples were generated, where one makes use of the default parton shower with angular ordering, and the other uses the dipole shower as an alternative. The description of hadronisation was based on the cluster model [18] for both of these samples. Two different samples with the same matrix elements and hadronisation allow the effects of using different parton shower models to be investigated. These samples include variations from the hard scattering and shower.

8.3 POWHEG+PYTHIA 8

The descriptions below correspond to the samples in Table 8.3.

Table 8.3: Multijet samples produced with POWHEG BOX v2.

DSID range	Description
361281–361289	POWHEG+PYTHIA 8

Description: Alternative samples of multijet production at NLO accuracy were produced with POWHEG BOX v2 [28, 29] interfaced to PYTHIA 8. These were generated with the dijet process as implemented in POWHEG BOX v2 [30]. The p_T of the underlying Born configuration was taken as the renormalisation and factorisation scales and the NNPDF3.0NLO [16] parton distribution function (PDF) was used. PYTHIA with the A14 tune and the NNPDF2.3LO [2] PDF was used for the shower and multi-parton interactions. These samples included per-event weight variations for different perturbative scales in the matrix element, different parton distribution functions and their uncertainties, and the PYTHIA perturbative shower uncertainties.

8.4 SHERPA 2.2

The descriptions below correspond to the samples in Table 8.4.

Table 8.4: Multijet samples produced with SHERPA.

DSID range	Description
364677–364685	SHERPA AHADIC
364686–364694	SHERPA Lund

Description: Multijet production samples were also generated using the SHERPA 2.2.5 [6] generator. The matrix element calculation was included for the $2 \to 2$ process at leading order, and the default SHERPA parton shower [11] based on Catani–Seymour dipole factorisation was used for the showering with p_{T} ordering, using the CT14NNLO PDF set [20]. The first of these samples made use of the dedicated SHERPA AHADIC model for hadronisation [18], based on cluster fragmentation ideas. A second sample was generated with the same configuration but using the SHERPA interface to the Lund string fragmentation model of PYTHIA 6 [124] and its decay tables. These two sets of samples were used to evaluate uncertainties stemming from the hadronisation modelling.

9 Photon processes

The following paragraphs describe the set-up of the current ATLAS γ+jets and $\gamma\gamma$+jets baseline samples.

9.1 Sherpa (MEPS@NLO)

Samples

The descriptions below correspond to the samples in Table 9.1.

Table 9.1: γ+jets and $\gamma\gamma$+jets samples with Sherpa NLO.

DSID range	Description
364541–364547	single photon
364350–364354	diphoton

9.1.1 γ+jets

Short description: Prompt single-photon production was simulated with the Sherpa 2.2 [6] generator. In this set-up, NLO-accurate matrix elements for up to two partons, and LO-accurate matrix elements for up to four partons were calculated with the Comix [7] and OpenLoops [8–10] libraries. They were matched with the Sherpa parton shower [11] using the MEPS@NLO prescription [12–15] with a dynamic merging cut [125] of 20 GeV. Photons were required to be isolated according to a smooth-cone isolation criterion [126]. Samples were generated using the NNPDF3.0nnlo PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the Sherpa authors.

Long description: Prompt single-photon production was simulated with the Sherpa 2.2 [6] parton shower Monte Carlo generator. In this set-up, NLO-accurate matrix elements for up to two partons, and LO-accurate matrix elements for up to four partons were calculated with the Comix [7] and OpenLoops [8–10] libraries. The default Sherpa parton shower [11] based on Catani–Seymour dipole factorisation and the cluster hadronisation model [18] were used. They employed the dedicated set of tuned parameters developed by the Sherpa authors for this generator version and the NNPDF3.0nnlo PDF set [16].

The NLO matrix elements for a given jet multiplicity were matched to the parton shower using a colour-exact variant of the MC@NLO algorithm [12]. Different jet multiplicities were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which was extended to NLO accuracy using the MEPS@NLO prescription [13]. The merging cut was set dynamically at a scale of 20 GeV according to the prescription in Ref. [125].

The renormalisation and factorisation scales for the photon-plus-jet core process were set to the transverse energy of the photon, E_{T}^{γ}. The strong coupling constant was set to $\alpha_{\mathrm{s}}(m_Z) = 0.118$ and the QED coupling constant was evaluated in the Thomson limit. Photons from the matrix elements were required to be central, by being within the rapidity range $|y_\gamma| < 2.7$, and isolated according to a smooth-cone isolation criterion [126] with $\delta_0 = 0.1$, $\epsilon_\gamma = 0.1$ and $n = 2$.

The effects of QCD scale uncertainties were evaluated [19] using seven-point variations of the factorisation and renormalisation scales in the matrix elements. The scales were varied independently by factors of 0.5 and 2, avoiding variations in opposite directions.

PDF uncertainties for the nominal PDF set were evaluated using the 100 variation replicas, as well as ±0.001 shifts of α_{s}. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets.

9.1.2 $\gamma\gamma$+jets

Short description: Prompt diphoton production was simulated with the SHERPA 2.2 [6] generator. In this set-up, NLO-accurate matrix elements for up to one parton, and LO-accurate matrix elements for up to three partons were calculated with the Comix [7] and OPENLOOPS [8–10] libraries. They were matched with the SHERPA parton shower [11] using the MEPS@NLO prescription [12–15] with a dynamic merging cut [125] of 10 GeV. Photons were required to be isolated according to a smooth-cone isolation criterion [126]. Samples were generated using the NNPDF3.0NNLO PDF set [16], along with the dedicated set of tuned parton-shower parameters developed by the SHERPA authors.

Long description: Prompt diphoton production was simulated with the SHERPA 2.2 [6] parton shower Monte Carlo generator. In this set-up, NLO and LO-accurate matrix elements were calculated with the Comix [7] and OPENLOOPS [8–10] libraries. The default SHERPA parton shower [11] based on Catani–Seymour dipole factorisation and the cluster hadronisation model [18] were used. They employed the dedicated set of tuned parameters developed by the SHERPA authors for this generator version and the NNPDF3.0NNLO PDF set [16].

The NLO matrix elements for a given jet multiplicity were matched to the parton shower using a colour-exact variant of the MC@NLO algorithm [12]. Different jet multiplicities were then merged into an inclusive sample using an improved CKKW matching procedure [14, 15] which was extended to NLO accuracy using the MEPS@NLO prescription [13]. The merging cut was set dynamically to a scale of 20 GeV, according to the prescription in Ref. [125].

The renormalisation and factorisation scales for the diphoton core process were set to the invariant mass of the photon pair, $m_{\gamma\gamma}$. The strong coupling constant was set to $\alpha_{\mathrm{s}}(m_Z) = 0.118$ and the QED coupling constant was evaluated in the Thomson limit. Photons from the matrix elements were required to be central, by being within the rapidity range $|y_\gamma| < 2.7$, and isolated according to a smooth-cone isolation criterion [126] with $\delta_0 = 0.1$, $\epsilon_\gamma = 0.1$ and $n = 2$. Additionally, the photons were required to be separated by $\Delta R(\gamma_1, \gamma_2) > 0.2$.

The effects of QCD scale uncertainties were evaluated [19] using seven-point variations of the factorisation and renormalisation scales in the matrix elements. The scales were varied independently by factors of 0.5 and 2, avoiding variations in opposite directions.

PDF uncertainties for the nominal PDF set were evaluated using the 100 variation replicas, as well as ±0.001 shifts of α_s. Additionally, the results were cross-checked using the central values of the CT14NNLO [20] and MMHT2014NNLO [21] PDF sets.

9.2 Sherpa (MEPS@LO)

Samples

The descriptions below correspond to the samples in Table 9.2.

Table 9.2: γ+jets and $\gamma\gamma$+jets samples with Sherpa LO.

DSID range	Description
361039–361062	single photon
303727–303742	diphoton
700442	EWK γjj

9.2.1 γ+jets

Description: Prompt single-photon production was simulated using the Sherpa 2.1 [6] generator. The tree-level matrix elements, generated for up to three additional partons, were merged with the initial- and final-state parton showers using the MEPS@LO prescription [15]. The CT10NLO set of PDFs [33] was used to parameterise the proton structure in conjunction with the dedicated set of tuned parton-shower parameters developed by the Sherpa authors for this generator version. A modified version of the cluster model [18] was used for the description of the fragmentation into hadrons. Photons from the matrix elements were required to be isolated according to a smooth-cone hadronic isolation criterion [126] with $\delta_0 = 0.3$, $\epsilon_\gamma = 0.025$ and $n = 2$.

9.2.2 $\gamma\gamma$+jets

Description: Prompt diphoton production was simulated using the Sherpa 2.1 [6] generator. The tree-level matrix elements, generated for up to two additional partons, were merged with the initial- and final-state parton showers using the MEPS@LO prescription [15]. The CT10NLO set of PDFs [33] was used to parameterise the proton structure in conjunction with the dedicated set of tuned parton-shower parameters developed by the Sherpa authors for this generator version. A modified version of the cluster model [18] was used for the description of the fragmentation into hadrons. Photons from the matrix elements were required to be isolated according to a smooth-cone hadronic isolation criterion [126] with $\delta_0 = 0.3$, $\epsilon_\gamma = 0.025$ and $n = 2$. Additionally, the photons were required to be separated by $\Delta R(\gamma_1, \gamma_2) > 0.2$.

9.2.3 γjj

The descriptions below correspond to the samples in Table 9.3. The samples do not overlap with the QCD γ+jets samples.

Table 9.3: Electroweak γjj samples with SHERPA.

DSID range	Description
700442	EWK γjj

Description: Electroweak production of the γjj final state was simulated with SHERPA 2.2.11 [6] using leading-order (LO) matrix elements with up to one additional parton emission. The matrix elements were merged with the SHERPA parton shower [11] following the MEPS@LO prescription [14] and using the set of tuned parameters developed by the SHERPA authors. The NNPDF3.0NNLO set of PDFs [16] was employed. The samples were produced using the VBF approximation, which avoids overlap with semileptonic diboson topologies by requiring a t-channel colour-singlet exchange. The starting conditions of the CS shower are set according to the large-N_c amplitudes supplied by Comix [22] to achieve the correct VBF-appropriate radiation pattern. Photons from the matrix elements were required to be isolated according to a smooth-cone hadronic isolation criterion [126] with $\delta_0 = 0.1$, $\epsilon_\gamma = 0.1$ and $n = 2$.

9.3 PYTHIA (LO)

The descriptions below correspond to the samples in Table 9.4.

Table 9.4: γ+jets and $\gamma\gamma$+jets samples with PYTHIA.

DSID range	Description
423099–423112	single photon
344008, 302520–34, 364423	diphoton

9.3.1 γ+jets

Description: Prompt single-photon production was simulated using the PYTHIA 8.186 [1] generator. Events were generated using tree-level matrix elements for photon-plus-jet final states as well as LO QCD dijet events, with the inclusion of initial- and final-state parton showers. The fragmentation component was modelled by final-state QED radiation arising from calculations of all $2 \to 2$ QCD processes. The NNPDF2.3LO [2] PDF set was used in the matrix element calculation, the parton shower, and the simulation of the multi-parton interactions. The samples include a simulation of the underlying event with parameters set according to the A14 tune [26]. The Lund string model [122, 123] was used for the description of the fragmentation into hadrons.

9.3.2 $\gamma\gamma$+jets

Description: Prompt diphoton production was simulated using the PYTHIA 8.186 [1] generator. Events were generated using tree-level matrix elements for diphoton final states, with the inclusion of initial- and final-state parton showers. The fragmentation component was modelled by final-state QED radiation arising from calculations of photon-plus-jet processes in dedicated samples. The NNPDF2.3LO [2] PDF set was used in the matrix element calculation, the parton shower, and in the simulation of the multi-parton interactions. The samples include a simulation of the underlying event with parameters set according to the A14 tune [26]. The Lund string model [122, 123] was used for the description of the fragmentation into hadrons.

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