

Performance of the Quasar Spectral Templates for the Dark Energy Spectroscopic Instrument

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Abstract

Millions of quasar spectra will be collected by the Dark Energy Spectroscopic Instrument (DESI), leading to a fourfold increase in the number of known quasars. High-accuracy quasar classification is essential to tighten constraints on cosmological parameters measured at the highest redshifts DESI observes (z > 2.0). We present spectral templates for identification and redshift estimation of quasars in the DESI Year 1 data release. The quasar templates are comprised of two quasar eigenspectra sets, trained on spectra from the Sloan Digital Sky Survey. The sets are specialized to reconstruct quasar spectral variation observed over separate yet overlapping redshift ranges and, together, are capable of identifying DESI quasars from 0.05 < z < 7.0. The new quasar templates show significant improvement over the previous DESI quasar templates regarding catastrophic failure rates, redshift precision and accuracy, quasar completeness, and the contamination fraction in the final quasar sample.

Unified Astronomy Thesaurus concepts: Quasars (1319); Cosmology (343); Observational cosmology (1146); Redshift surveys (1378)



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1. Introduction

The Dark Energy Spectroscopic Instrument (DESI; DESI Collaboration et al. 2016a, 2016b) will collect tens of millions of spectra from four extragalactic target classes: the bright galaxy sample (BGS; Hahn et al. 2023), luminous red galaxies (LRGs; Zhou et al. 2023), emission line galaxies

(ELGs; Raichoor et al. 2023), and quasars, also known as quasi-stellar objects (QSOs; Chaussidon et al. 2023). Roughly three million QSO spectra are expected over the five-year survey duration, increasing the number of spectroscopically confirmed QSOs by a factor of four (Lyke et al. 2020).

Owing to their high intrinsic luminosity, QSOs are vital to understanding the large-scale structure of the universe by providing unparalleled access to the highest redshifts observed by DESI. QSOs can be used as direct tracers of the matter distribution and their spectra carry signatures of matter in the intergalactic medium (IGM) that is otherwise undetectable. Measurements from QSOs complemented the low-redshift galaxy tracers in the Baryon Oscillation Spectroscopic Survey (BOSS) and its extension (eBOSS; Dawson et al. 2013, 2016) to strengthen constraints on key cosmological parameters relating to expansion history, growth of structure, and inflation (du Mas des Bourboux et al 2020; Neveux et al. 2020; Hou et al. 2021; Mueller et al. 2022).

High-accuracy, automatic classification of QSOs in DESI's larger spectroscopic sample is essential to make successful measurements that use QSOs as either direct tracers or backlights to the neutral hydrogen of the Ly α forest. QSO misclassification dilutes the observed clustering amplitude while spectroscopic redshift resolution can significantly impact the value of the $f\sigma_8$ parameter extracted from redshift space distortions of the autocorrelation function (e.g., Zarrouk et al. 2018). Additionally, random QSO redshift errors dampen the radial peak of the baryon acoustic oscillation (BAO) feature and introduce unphysical correlations at small transverse separations in Ly α -QSO cross-correlation measurements (Youles et al. 2022). Classification accuracy is complicated by the vast diversity of QSO spectral features. QSO emission lines exhibit varying degrees of asymmetry, broadening, and shifting dependent on an individual system's structure. Meanwhile, the continuum shape may be altered by both intrinsic and external absorption features.

DESI spectra are automatically classified after collection into three broad categories: galaxy, QSO, or star, and simultaneously the redshifts are estimated. The most probable spectral class and redshift are determined by the Redrock³ (S. Bailey et al. 2023, in preparation) spectral template-fitting algorithm. The QSO templates used for the DESI Survey Validation (SV) program (DESI Collaboration et al. 2023a) and the Early Data Release (EDR; DESI Collaboration et al. 2023b) were adopted from (e)BOSS. The templates consist of four empirical eigenspectra derived via a principal component analysis (PCA) and described in Section 4.2 of Bolton et al. (2012). These eigenspectra were determined from 568 QSO spectra from the Sloan Digital Sky Survey (SDSS; York et al. 2000). However, small number statistics limit the range of spectral variation that can adequately be described. For example, the luminosity-dependent blueshifting of high-ionization lines (e.g., Shen et al. 2016) is not well incorporated into these templates. This feature contributes to a redshiftdependent bias in QSO redshift estimates (e.g., Amiri et al. 2023). Further, QSO spectra exhibiting more peculiar spectral features, such as broad absorption lines (BALs; e.g., Hall et al. 2002; Gibson et al. 2009; Hall et al. 2012; Yi et al. 2019) or reddened continua (e.g., Glikman et al. 2013; Calistro Rivera et al. 2021; Fawcett et al. 2022), are often poorly modeled by the templates, leading to misclassification in some cases.

Visual inspection (VI) of early DESI data revealed high QSO sample purity and reliable redshift estimates with Redrock as the sole spectral classifier; however, approximately 11%-15% of true QSOs were misclassified as galaxies or stars (Alexander et al. 2023). Two highly successful "afterburner" algorithms were implemented to retrieve the missed OSOs: QuasarNET (QN; Busca & Balland 2018; Farr et al. 2020) and a broad Mg II emission line detection algorithm. QN is a convolutional neural network trained to identify QSO emission lines in spectra. Spectra missed by Redrock but identified as OSO by QN with a probability over a specified threshold are reclassified as QSO. The Redrock QSO templates are then refit to these spectra with a prior informed by the coarse QN redshift estimate to estimate final redshifts. The Mg II afterburner checks for significant Mg II emission, indicative of QSO activity, in spectra classified as "galaxy." A QSO classification is assumed if detected, but the redshift estimate is unchanged. Together with Redrock, the afterburners brought the completeness up to approximately 94%. A full description of the afterburners, their performance, and the criteria for a spectrum to be labeled as QSO are presented by Alexander et al. (2023) and Chaussidon et al. (2023).

This work presents new QSO templates developed for DESI and their performance. We expand upon the method presented by (Brodzeller & Dawson 2022; hereafter BD22) to create new QSO templates with a specific focus on spectral diversity, redshift evolution, and redshift-dependent bias. Our method uses a clustering technique (Section 3.1) to compress a large sample of QSO spectra into subsets that, together, span the range of the spectral variation. We use the compressed sample to remove contaminants such as misclassified spectra and to standardize the rest-frame (RF) wavelength solution of the individual spectra. We then use the filtered and reredshifted spectroscopic sample to compute eigenspectra that act as the QSO spectral templates for DESI.

The most notable difference between the previous DESI QSO templates and the new DESI QSO templates is the use of two OSO template sets trained to different redshift ranges rather than one set covering the full redshift range. We developed low-redshift and high-redshift QSO template sets to allow for a more complete description of spectral variation and redshift evolution over 0.05 < z < 7, particularly in the extremes of this range. The low-redshift templates classify QSO spectra over 0.05 < z < 1.6 and are equipped to describe the host galaxy contributions that are often more significant with lower-redshift QSOs. The high-redshift templates classify QSO spectra over 1.4 < z < 7 and are trained to reconstruct the variation observed in the highest-luminosity systems. The two template sets overlap in redshift coverage, as described in Section 3.3. These templates are integrated into the Redrock software repository³⁵ and will be used to produce the QSO classifications for the DESI Year 1 Data Release.

In Section 2, we discuss the spectroscopic samples used to train the new QSO templates and to test their performance. We outline the template development method in Section 3, highlighting changes to the method presented by BD22. In Section 4, we present the performance of the new QSO

³³ https://github.com/desihub/redrock/

³⁴ The galaxy, previous QSO, and stellar spectral templates used in Redrock are available at https://github.com/desihub/redrock-templates/releases/tag/ 0.7.2.

³⁵ https://github.com/desihub/redrock-templates/releases/tag/0.8

templates on DESI spectra. We evaluate the results for Redrock alone versus Redrock together with the QSO afterburners. Finally, we measure the redshift accuracy of the new QSO templates through cross-correlations of QSOs with other tracers in DESI. We conclude in Section 5 by summarizing this work and describing the potential for future studies. Throughout our work we assume flat Λ cold dark matter (Λ CDM) cosmology described by Planck Collaboration et al. (2016).

2. Data

We use the wealth of QSO spectra from the Sixteenth Data Release (DR16; Ahumada et al. 2020) of the fourth generation of the SDSS (Blanton et al. 2017) to develop QSO spectral templates. The classification performance of the new QSO templates in Redrock alone and in the Redrock with QSO afterburners pipeline is tested on subsets of DESI spectra collected between 2020 December and 2021 July. We compare the results to those from the previous DESI QSO templates on the same samples. In this section, we review the SDSS training sample and DESI validation samples.

2.1. Training Sample

We select spectra from SDSS DR16 using attributes from the DR16 QSO catalog (Lyke et al. 2020). The spectra were collected with the Sloan telescope (Gunn et al. 2006) using the (e)BOSS spectrographs (Smee et al. 2013). QSO targets in this analysis were selected as described in Ross et al. (2012) and Myers et al. (2015).

We use QSO spectra with a Z_PCA redshift of $0.05 \le z \le 5.0$ and ZWARN_PCA = 0 to develop the new QSO templates. The method for estimating Z_PCA is explained in Section 4.4 of Lyke et al. (2020). Pixels in SDSS spectra are binned on a logarithmic wavelength array with constant spacing. The average signal-tonoise ratio (S/N) per pixel of each spectrum is determined over all pixels with a RF wavelength of $\lambda_{RF} > 1216$ Å, after excluding pixels flagged as having poor sky subtraction. We also exclude pixels at wavelengths shorter than 1216 Å from the S/N measurement, as Ly α absorption features dominate the spectrum at these wavelengths. Spectra with an average S/N per pixel > 5 are included in the training sample. The final selection provides 207,956 unique spectra.

We reduce the impact of nonintrinsic foreground features in the spectra by applying various corrections. The corrections applied are identical to those in BD22 except with changes to filtering outlier pixels. We first correct for galactic extinction using the dust map of Schlegel et al. (1998) and extinction law of Fitzpatrick (1999). We then mask pixels flagged for poor sky subtraction and those that deviate negatively by more than 2σ from the ratio of the measured flux to the flux smoothed by a 30 pixel median filter (corresponding to approximately 2000 km s⁻¹). The latter mask aims to remove contamination from foreground IGM absorption but may unintentionally mask some intrinsic absorption features, such as narrow BALs. Lastly, each spectrum is shifted to its RF solution.

2.2. Validation Samples

DESI is installed on the Mayall Telescope at Kitt Peak National Observatory. The focal plane holds 5000 optical fibers, steered by robotic positioners to the locations of survey targets (Myers et al. 2023; Silber et al. 2023). The focal plane is split into 10 wedges, called petals, each holding 500 fibers that

 Table 1

 VI Spectral Class of Objects in the DESI Truth Table (All Targets) and the QSO Main Subset

| Spectral | Number of Spectra | | | |
|----------|-------------------|----------|--|--|
| Class | All Targets | QSO Main | | |
| QSO | 1643 | 1368 | | |
| Galaxy | 14,991 | 915 | | |
| Star | 763 | 349 | | |

direct light to a multiobject fiber spectrograph. A single pointing of the 10 petals is collectively referred to as a tile. A complete description of DESI instrumentation is provided in Abareshi et al. (2022).

Spectra collected by DESI are processed in a fully automatic pipeline (Guy et al. 2023) and then classified by Redrock and the QSO afterburners. The spectra are binned on a wavelength array with constant linear spacing between pixels.

We use five samples of DESI spectra for validating the new QSO templates, detailed in the following paragraphs: the DESI Truth Table, QSO Main, Survey Validation (SV) Repeat Exposures, the One-Percent Survey, and the Guadalupe Internal Data Assembly (hereafter Guadalupe). All spectra were classified with Redrock version 0.15.4 and the QSO afterburners using the previous QSO templates. The SV and One-Percent spectra and corresponding catalogs with these classifications will be publicly available in the EDR. The Guadalupe data used in this work will be released as part of DESI Year 1 and will use classifications from the QSO templates presented in this paper.

DESI Truth Table. The first validation sample is selected from the SV program and consists of spectra from eight tiles: 80605, 80606, 80607, 80608, 80609, 80610, 80613, and 80742. These tiles were exposed multiple times to achieve a higher cumulative effective exposure depth than the nominal main survey. Coadding all the spectra obtained for a target enabled reliable VI of early survey data to assess pipeline performance and preliminary target selection methods (Allende Prieto et al. 2020; Raichoor et al. 2020; Ruiz-Macias et al. 2020; Yèche et al. 2020; Zhou et al. 2020). As a result, there exist VI labels for many of these spectra that include a spectral class, redshift, and confidence in the visual assessment. Confidence is provided on a scale of 0-4, with 0 indicating no signal and 4 indicating two or more secure spectral features are identifiable. A VI confidence of equal to or greater than 2.5, meaning at least one inspector indicated a probable classification with at least one clear spectral feature or several weak features, is treated as truth (see Alexander et al. 2023; Lan et al. 2023, for details).

We use the truth labels to determine the classification accuracy and sample completeness with the new QSO templates for the resulting QSO and galaxy samples (Section 4.1). In total, we test performance on 17,397 cumulative spectra with confident VI labels. The breakdown of spectral classes assigned from VI in the DESI Truth Table is given Table 1.

QSO Main. The QSO target selection for SV includes objects fainter than the main survey (Chaussidon et al. 2023). We study performance on main survey QSO targets by restricting the DESI Truth Table to target type "QSO" and r < 23. This subsample contains 2632 cumulative spectra, of which a nonnegligible fraction is non-QSOs according to VI. The VI spectral-class distribution within QSO Main is included in Table 1.

SV Repeat Exposures. The individual exposures of targets in the DESI Truth Table tiles and six additional deep tiles (80620, 80678, 80690, 80695, 80699, and 80711) were randomly sampled to create several spectra of each target equivalent to exposures at the main survey depth. We use the spectra of QSO targets in this sample to quantify the redshift precision by comparing the redshift estimates for different spectra of the same target (Section 4.2.1).

One-Percent Survey and Guadalupe. The One-Percent Survey, occasionally referred to as SV3 (Chaussidon et al. 2023), was collected primarily between 2021 April 5 and 2021 May 13, using exposure times 20% longer than the fiducial. Guadalupe is the first two months of main survey data collected by DESI between 2021 May 14 and July 9. We use these last two samples for measuring the bias on QSO redshifts and for additional testing of QSO redshift precision (Section 4.2.2). We also use Guadalupe to check the spectra of targets that change classification with the change of QSO templates (Section 4.1.3), evaluating the overall accuracy of the changes and determining any new potential failure modes.

3. QSO Template Development

This section provides a brief overview of the clustering technique and the compression of the resulting clusters into a PCA training set of composite spectra. We primarily focus on the changes from BD22, referring the reader there for complete details. We then discuss the process for reredshifting the training sample which is also used to prune noisy, misclassified, or problematic spectra from the training sample. Finally, we present the final PCA eigenspectra sets that comprise the QSO templates for classification in DESI. The overall process for template development is outlined in Figure 1.

3.1. Overview of the Clustering Procedure and Results

We use the clustering technique of BD22 to compress the training sample of QSO spectra into groups that exhibit low internal diversity. The clustering method is based on SetCoverPy,³⁶ an archetype technique developed by Zhu (2016). The only free parameter in the clustering method is the reduced χ^2 threshold (Equation (1) in BD22), below which two spectra are considered similar and therefore belong to the same cluster. This parameter is tuned to maximize the similarity of spectra in the same cluster without creating excessive outliers (i.e., spectra not within the χ^2_{red} threshold to any other spectrum). We refer to Section 3 of BD22 for a full description of the clustering technique and outlier identification. We only provide a brief overview, focusing on details specific to this work.

We use the χ^2_{red} distance metric from BD22 to measure the similarity between all pairs of spectra within a clustering bin (bins are described in the following paragraphs). The χ^2_{red} metric includes a two-parameter term $(c\lambda^{\Delta\alpha})$ that is applied to the higher S/N spectrum of each pair to account for the difference in broadband continua between the spectra. The values of *c* and $\Delta\alpha$ are determined for each pair so that the χ^2_{red} is minimized. QSO continua are well described by a single power law between the Ly α and H β emission lines (e.g., Brotherton et al. 2001; Vanden Berk et al. 2001), permitting this term to be reasonably applied to QSO pairs at z > 1. The

³⁶ https://github.com/guangtunbenzhu/SetCoverPy

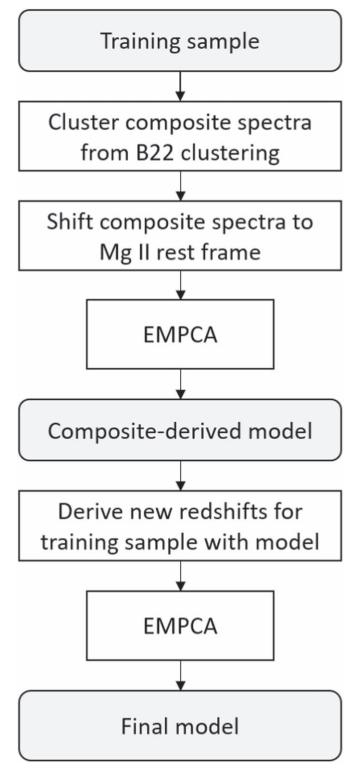


Figure 1. Flowchart of the template development process.

term's validity breaks at lower redshifts as wavelengths longer than that of the H β line enter the spectral coverage. We therefore split the training sample into two overlapping subsamples for clustering:³⁷ 1.0 < z < 2.6 and z < 1.3. For the z < 1.3 subsample, c = 1 and $\Delta \alpha = 0$ in all χ^2_{red}

 $[\]frac{37}{37}$ Note that this division of the training sample is not the same that is used to develop the final QSO templates in this work, see Section 3.3.

 Table 2

 The Number of QSOs in Each Redshift Bin, the Median S/N of Spectra in the Bin, and RF Wavelength Range Used for Clustering

| | QSOs | | | | | | High S/N | | | Low S/N | |
|-----------------------|--------|--------------------|--|------|----------------------------|----------|----------|----------------------------|----------|----------|--|
| Redshift | | QSOs Median S/N | $\begin{array}{ccc} \lambda_{\min} & \lambda_{\max} & \lambda_{\max} & \lambda_{\max} & (A) & (A) \end{array}$ | | Initial $\chi^2_{\rm red}$ | Clusters | Outliers | Initial $\chi^2_{\rm red}$ | Clusters | Outliers | |
| 0.0 < z < 0.35 | 3289 | | 3611 | 7687 | 2.477 | 138 | 259 | | | | |
| 0.35 < z < 0.7 | 15,847 | 7.89 | 2674 | 6104 | 1.320 | 451 | 305 | 1.053 | 464 | 228 | |
| 0.7 < z < 0.85 | 11,541 | 7.45 | 2124 | 5617 | 1.241 | 362 | 140 | 1.067 | 390 | 82 | |
| 0.85 < z < 1.0 | 12,125 | 7.47 | 1952 | 5189 | 1.100 | 411 | 102 | 0.989 | 392 | 55 | |
| 1.0 < <i>z</i> < 1.15 | 12,218 | 7.49 | 1805 | 4818 | 1.034 | 335 | 43 | 0.950 | 296 | 29 | |
| 1.15 < z < 1.3 | 13,048 | 7.42 | 1679 | 4519 | 1.016 | 337 | 58 | 0.950 | 330 | 51 | |
| 1.0 < z < 1.2 | 16,463 | 7.47 | 1805 | 4724 | 1.083 | 472 | 66 | 0.950 | 496 | 61 | |
| 1.2 < z < 1.4 | 18,117 | 7.43 | 1641 | 4332 | 1.080 | 445 | 83 | 0.952 | 489 | 57 | |
| 1.4 < z < 1.6 | 17,992 | 7.34 | 1505 | 3999 | 1.149 | 480 | 167 | 1.017 | 527 | 83 | |
| 1.6 < z < 1.8 | 16,918 | 7.36 | 1389 | 3714 | 1.266 | 432 | 300 | 1.083 | 473 | 109 | |
| 1.8 < z < 2.0 | 17,310 | 7.76 | 1289 | 3460 | 1.376 | 398 | 510 | 1.123 | 438 | 154 | |
| 2.0 < z < 2.2 | 17,145 | 7.71 | 1203 | 3249 | 1.609 | 369 | 569 | 1.255 | 399 | 242 | |
| 2.2 < z < 2.4 | 20,155 | 7.60 | 1128 | 3058 | 1.899 | 435 | 670 | 1.441 | 531 | 296 | |
| 2.4 < z < 2.6 | 14,796 | 7.60 | 1062 | 2889 | 2.077 | 330 | 602 | 1.516 | 423 | 344 | |
| 2.6 < z < 5.0 | 26,258 | | | | | | 616 | | | 464 | |

Note. The median S/N is used to split the redshift bin into two evenly sized subbins in which clustering is performed independently. The final number of clusters and outliers are reported after the outlier retrieval stage. The lowest-redshift bin is not split on S/N owing to small numbers and the results are for the full bin. A different clustering method is used for the highest-redshift bin, described in the text.

calculations. Spectra with redshifts above z = 2.6 are excluded from initial clustering and incorporated into clusters at a subsequent stage, as described later in this section.

The training subsamples are binned on discrete intervals of $\Delta z \approx 0.15-0.35$ to account for redshift evolution of spectral features, described in Table 2. Within each redshift bin, the spectra are cropped to the overlapping wavelength range defined by the shortest wavelength of the lowest-redshift spectrum and the longest wavelength of the highest-redshift spectrum in the bin. Additionally, pixels with an RF wavelength shorter than 1216 Å are masked to avoid the spurious signal from the Ly α forest. The spectra are then normalized according to the median flux density measured over the common RF wavelength range. The pixel diversity mask (Section 3.2.1 in BD22) is applied at this stage. This mask focuses spectral comparisons on the top 32% of pixels exhibiting the most flux variation within a given redshift bin to maximize the information content in the resulting clusters.

Each redshift bin is further binned on its median S/N, excluding the lowest-redshift bin owing to low numbers. Our motivation for subbinning on S/N is twofold. First, the noise levels vary greatly across the sample and splitting on S/N allows us to tune the threshold distance for clustering to achieve a meaningful measure of similarity between spectra, given their noise levels. Second, many spectral features are known to evolve with luminosity (e.g., Shields 2007; Jensen et al. 2016). We can treat S/N as a loose proxy for luminosity since the QSOs are at the same approximate redshift and SDSS exposure times are relatively consistent.

Clustering is performed independently in the high-S/N and low-S/N bins of each redshift bin. We enforce $\chi^2_{red} \ge 0.95$ when determining the initial clustering threshold distances. The same outlier retrieval method in BD22 is applied to the resulting clusters to maximize diversity coverage. The initial threshold χ^2_{red} and final clustering results are summarized in Table 2.

The clustering technique produces 11,043 nonexclusive clusters of similar spectra and 6388 unique outliers. The cluster sizes range from two spectra to several hundred spectra. The smaller clusters often contain more peculiar QSOs such as BALOSOs, dust-reddened OSOs, systems with extremely shifted lines, or QSOs with unusually high equivalent widths, while larger clusters contain more typical QSO spectra displaying blue continua. Though the degree of overlap between clusters varies greatly, larger clusters tend to share more spectra with other larger clusters than smaller clusters do in general. To first order, the collection of the clusters represents the range of spectral diversity observed across the full training sample. Many spectra identified as outliers in clustering exhibit calibration or classification errors, peculiar features such as BALs or atypical emission line strengths or ratios, or have incorrect redshifts from Z PCA, as determined from VI. The natural segregation of these spectra facilitate contaminant rejection before training the final spectral model (See Section 3.2).

The χ^2_{red} used to cluster QSO spectra excludes pixels in the Ly α forest. Above z = 2.6, the Ly α forest is present in an increasingly significant portion of the spectrum. For this reason, QSOs at 2.6 < z < 5.0 have been excluded from the first stage of clustering. We retrieve these high-redshift spectra by adding them to the existing clusters of the 2.4 < z < 2.6 bin in a similar fashion to the outliers.

We first divide the z > 2.6 spectra on the median S/N of the 2.4 < z < 2.6 redshift bin. The χ^2_{red} is calculated between pairs of the z > 2.6 spectra and cluster representative spectra in the S/N bin corresponding to the high-redshift spectrum's S/N. The distance metric is determined in the overlapping wavelength range of the pair, restricting the comparison to 1216 Å $< \lambda_{RF} < 2884$ Å. A high-redshift spectrum is then added to all clusters for which the χ^2_{red} to the representative spectrum is less than 150% of the initial distance threshold of that bin.

An error-weighted mean composite spectrum is then computed from all clusters as follows. The processed spectra (Section 2.1) belonging to clusters from the z < 1.3 subsample are normalized over 3620-4510 Å in the RF. The processed spectra belonging to clusters from the 1.0 < z < 5.0 subsample, excluding z > 2.4, are normalized over 1815-2880 Å. A different RF range of 1275-1725 Å is required to normalize the spectra in clusters at z > 2.4 owing to the extended wavelength coverage of the clusters.

All individual spectra are adjusted to the continuum slope of the representative spectrum using the $c\lambda^{\Delta\alpha}$ correction when taking the error-weighted mean of a cluster in the 1.0 < z < 5.0subsample. The cluster composite spectra from the z < 1.3subsample are simple error-weighted means. Thirty pixels on each extreme of a composite spectrum are removed to reduce edge noise. Lastly, we mask missing flux values and outlier pixels in each composite spectrum. Outlier pixels are identified identically as in the training sample, except if the threshold to be masked is 3σ positive or negative.

3.2. Correcting Redshifts in the Training Sample

We reported a redshift-dependent bias on \mathbb{Z}_PCA in BD22. We showed the bias could be stabilized by eigenspectra trained in the RF of the Mg II emission line (see BD22 Figure 9). The use of Mg II as a stable redshift estimator is similarly reported by Hewett & Wild (2010). We therefore shift all composite spectra so that the Mg II line is at the expected RF wavelength using an improved version of the redshift correction method in BD22 (see Section 3.3 of BD22). This correction is enabled by the high S/N of the composite spectra, which facilitates a direct fit to the line location.

We approximate the underlying flux that is not associated with Mg II emission by fitting a power law over 2600-2725 Å and 2875–2950 Å. After subtracting the power-law fit, a double Gaussian is fit to 2730–2870 Å. We impose a lower bound on the dispersion of 250 km s^{-1} for both components of the Gaussian and require the two peak positions to be identical. The continuum and line profile are fit twice with pixels that deviate by more than 3σ from the first fit masked in the second. The iterative fitting reduces the influence of associated absorption features on estimating the line location. The wavelength solution of the spectrum is then shifted so the line center is at the RF wavelength of 2798.75 Å (consistent with Vanden Berk et al. 2001). This method for fitting the continuum and line profile neglects Fe II emission (e.g., Wills et al. 1980, 1985; Vestergaard & Wilkes 2001), which can impact the measured line widths. Since we are only concerned with determining the line center, we do not include an iron template and rely on the continuum estimate to absorb iron contributions. Systematic offsets on our Mg II location estimate will contribute to redshift errors in the final QSO templates for DESI. We explore the magnitude of systematic redshift offsets in Section 4.2.2.

Cluster composite spectra of the 10,905 clusters from z > 0.35 redshift–S/N subbins (Table 2) are corrected with this method. The procedure fails to fit the Mg II emission line in 134 cases. VI of these spectra reveals clear contamination from stellar spectra or redshift errors in most cases. We reject these composite spectra and their contributing spectra from the further analyses.

The Mg II emission line falls off the blue end of (e)BOSS spectra at $z \leq 0.35$. It therefore cannot be used to correct for

potential redshift offsets in the composite spectra of z < 0.35clusters. We use a different approach to place these composite spectra in the same frame as the others. We apply a weighted expectation maximization principal component analysis (EMPCA;³⁸ Bailey 2012) to the mean-subtracted reredshifted cluster composite spectra of the z < 1.3 subsample. EMPCA was designed to determine eigenvectors of data sets with noise or gaps, using measurement uncertainties to weight the input data. The composite spectra are median normalized over their common wavelength coverage and weighted by their propagated inverse variance. We then fit the mean spectrum plus the first five eigenspectra from EMPCA to the composite spectra of the z < 0.35 clusters. We fit only 3100–7000 Å by the current RF solution to ensure coverage by the eigenspectra. Each spectrum is fit at intervals of 69 km s⁻¹, the resolution of (e) BOSS spectra, over ± 2070 km s⁻¹ and then shifted to the new redshift solution.

As shown in Figure 2, larger redshift corrections are required with increasing redshift and the corrections tend more red (Z_PCA is underestimated relative to the Mg II RF). The trend is possibly driven by the blueshifting of high-ionization lines, such as C IV and Ly α , with respect to Mg II, a less biased line. The greater flux density of these lines relative to Mg II tends to dominate the fit during redshift estimation. Further, the Ly α forest is present in spectra at z > 1.92, a clear inflection point in this figure.

After redshift corrections, we subtract the error-weighted mean of cluster composite spectra of the z < 1.3 subsample from all composite spectra within that subsample. We then derive eigenspectra from the residuals using EMPCA. We weight the flux values by the propagated inverse variance. This results in a model consisting of a mean vector and the first five eigenspectra from EMPCA that covers approximately 1800–9600 Å in the RF. We repeat these steps with the cluster composite spectra from the 1.0 < z < 5.0 subsample, creating a second spectral model with different RF wavelength coverage of approximately 600-5200 Å. The high-redshift model is padded with an exponential decay out to $\lambda_{\rm RF} = 590$ Å to provide redshift coverage up to z = 5.05.

New to BD22, these eigenspectra do not comprise our final QSO templates. There are two main issues with using the composite-derived templates for classification in DESI. First, all the spectra within a cluster have individual redshift errors. Although small, the varying redshift offsets within a cluster lead to blurring and peak dampening of the emission lines in the composite spectrum. These features may negatively affect modeling. Second, the clusters overlap in membership with one spectrum potentially belonging to tens of clusters. The cluster overlap is desirable to avoid harsh boundaries on smooth population gradients, but, if we use eigenspectra from the cluster composites as the QSO templates, we introduce an artificial up-weighting of more common spectral features.

We instead use Redrock with the high- and low-redshift QSO models derived from the composite spectra to fit the calibrated spectra of the training sample and derive new redshifts. We mask pixels in the Z_PCA RF at $\lambda_{RF} < 1216$ Å while fitting. Additionally, if the spectrum has a nonzero BAL_PROB attribute indicating BALs are present (Guo & Martini 2019), we mask pixels in the following Z_PCA RF ranges: 1479–1549 Å, 1326–1397 Å, and 1216–1240 Å. These

³⁸ https://github.com/sbailey/empca/

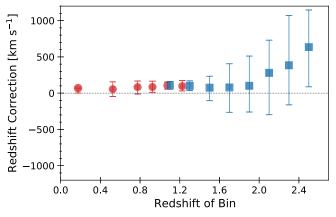


Figure 2. Red circles (blue squares) indicate the median redshift correction applied to cluster composite spectra of each low (high) redshift bin, including the z < 0.35 bin. Error bars indicate the 16th and 84th percentiles of each distribution.

ranges correspond to the typical wavelengths of C IV, Si IV, and N V BALs. Lastly, we also remove pixels at $\lambda_{obs} > 9700$ Å owing to a lack of coverage from the low-redshift templates as they approach $z \approx 0.05$. This reredshifting step aims to reduce the redshift bias seen in Figure 2 while addressing the issues outlined in the previous paragraph.

In the overlap redshift range of the models, we observe strong agreement in the redshift estimates from the two eigenspectra sets. For these spectra, we use the redshift from the model that provided the lowest χ^2_{red} fit. We reject spectra from the final training sample that have a nonzero ZWARN attribute or $|\Delta z| > 0.05$ between the new redshift and Z_PCA. This cut effectively removes all the outlier spectra that exhibit calibration errors, incorrect classifications, or little signal and leaves most true QSO systems in the final sample except those displaying extreme peculiarities. We refine the redshifts of spectra with a new redshift of z > 1.92 by updating the Ly α forest mask and refitting over $\pm 5000 \text{ km s}^{-1}$ from the initial redshift estimate. On average, the initial redshift estimate with these templates is redder than Z_PCA and the refined redshifts are almost always redder than the initial redshift. Our final model is trained using these new redshifts.

3.3. The Eigenspectra

We suggested in BD22 that using multiple QSO template sets, each trained to reconstruct the variation observed over limited redshift intervals, should improve spectral modeling over the full QSO population (supported by Yip et al. 2004). Toward this goal, we create two QSO eigenspectra sets that together serve as the QSO templates for spectral classification in DESI. The new DESI QSO templates consist of a lowredshift eigenspectra set and a high-redshift eigenspectra set. The sets are trained on subsamples of the individual spectra of the reredshifted, pruned training sample introduced in the previous subsection. The templates are derived with EMPCA, weighting flux values by their inverse variance.

We tested several redshift boundaries when defining the training subsamples for the high- and low-redshift QSO eigenspectra. The maximum redshift for the low-redshift training sample varied between z = 1.4 to z = 1.9 while the minimum redshift for the high-redshift training sample varied between z = 1.0 to z = 1.5. The two training samples always

overlapped in redshift by $\Delta z = 0.4$ to allow a smooth transition from one set to the next when classifying DESI spectra with Redrock.

All high-redshift templates are padded with a fast exponential decay beyond $\lambda \approx 600$ Å to extend the redshift coverage to z = 7.0. Though the QSO number density is low beyond $z \approx 4.5$ as seen by DESI, the padding ensures coverage for classifying the highest-redshift observations. The choice of exponential decay is so that the flux at these wavelengths is close to zero, as expected beyond the Lyman break, while avoiding zeros and discontinuities. A single template set that was trained on all redshifts, analogous to the previous DESI QSO templates, was also created for comparison.

In all cases, the templates consisted of the mean spectrum of its training sample plus the first N eigenspectra from EMPCA on the residual spectra. N was varied for each template option to determine how many eigenspectra were necessary to achieve high-accuracy QSO classification on the DESI Truth Table without introducing problems in the galaxy sample from overflexibility. We evaluated the accuracy, completeness, and catastrophic failure rates of classifications with Redrock on the DESI Truth Table (similar to Section 4.1) as well as the quality of the fits to determine the optimal choice for classification in DESI. The full redshift range template set underperformed relative to all high- and low-redshift template combinations evaluated in this work for all N tested.

We find that a mean plus three eigenspectra model in which the low-redshift set, trained on z < 1.7 spectra, classifies QSOs over 0.05 < z < 1.6 and the high-redshift set, trained on z > 1.3spectra, classifies QSOs over 1.4 < z < 7.0 performs the best. This choice of redshift boundaries outperformed other models by $\sim 5\%$ -10% in terms of completeness. Including higher-order eigenspectra marginally improves completeness but at the expense of reduced galaxy sample completeness and quasar sample purity below z = 1.5. The redshift range for classification differs from training due to the differences in wavelength coverage between SDSS and DESI and template binning in Redrock. We report only the results from the best-performing templates in Section 4, omitting the performance of the alternative options for brevity.

The new QSO template sets are shown in Figure 3 along with previous DESI QSO templates for comparison. Spectrophotometric calibration is degraded at the shortest observerframe wavelengths in SDSS spectra (see Margala et al. 2016). As such, both the previous and high-redshift QSO templates suffer from reduced modeling power at the shortest wavelengths, namely beyond the Lyman limit, where SDSS QSO numbers are sparse. On the red side of the Lyman limit, the most notable difference from the previous to the current templates is an overall reduction of random noise attributed to the increased training sample size.

Figure 3 also highlights the improvement of using template sets specialized for specific redshift intervals. The high-redshift set is overall similar to the previous templates, but there is a marked difference at low redshift. Particularly, the spectra lack the unphysical break in continuum present in the previous templates near 4000 Å. This is likely a result of the greater flux density and high variance at shorter wavelengths dominating the previous templates and leading to unphysical continua at longer wavelengths to maintain orthogonality.

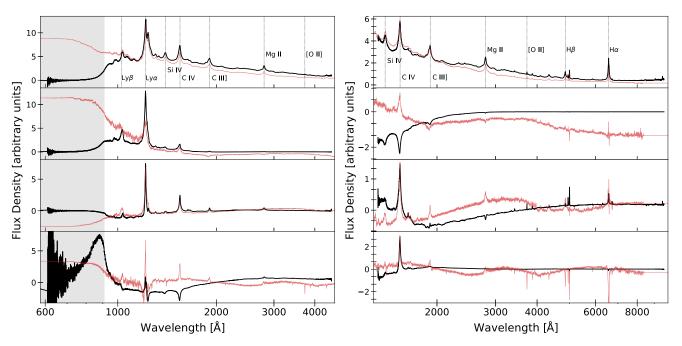


Figure 3. The high-redshift templates are shown on the left in black and cover 1.4 < z < 7.0. The low-redshift templates are shown on the right in black and cover 0.05 < z < 1.6. The previous DESI QSO templates are overlaid in red in both figures. The previous templates are trimmed to the wavelength coverage of the new templates and scaled for clarity in comparison. Prominent QSO emission lines are annotated on the mean spectra. The gray shading indicates the wavelength region that is poorly constrained in both eigenspectra sets owing to low QSO numbers and degraded spectrophotometric calibration at the shortest wavelengths of SDSS spectra.

4. Performance on DESI Spectra

We test the performance of the new QSO templates in Redrock on the DESI spectral samples introduced in Section 2.2. The results are presented alongside the performance of the previous QSO templates to quantify improvements to QSO classification in DESI. DESI also uses the two QSO afterburner algorithms, QN and a broad Mg II line finder (described in Section 1), post-Redrock to improve QSO sample completeness. These algorithms are dependent on Redrock output, so we rerun the QSO afterburners on the spectral samples to assess how the new templates impact their performance. Additionally, we evaluate the resulting galaxy samples, as a primary concern with improving the QSO templates is degrading the galaxy sample quality (e.g., Guy et al. 2023).

4.1. Classification Accuracy and Completeness

The VI labels in the DESI Truth Table and QSO Main samples include a spectral class and redshift, allowing us to estimate the contamination fraction, incompleteness, and catastrophic failure rates in the QSO samples from Redrock with the new QSO templates. We also review the Redrock galaxy sample from the DESI Truth Table for potential impacts from updating the QSO templates.

A contaminant in a sample is defined as a spectrum for which the VI and Redrock spectral classes disagree or the Redrock redshift is bad. A good Redrock redshift for a QSO spectrum requires that

$$|\Delta v| = \frac{|z_{VI} - z_{\text{Redrock}}|}{1 + z_{VI}} \times c < 3000 \text{ km s}^{-1}.$$
 (1)

We use a stricter definition of a good redshift for the galaxy sample, requiring $|\Delta v| < 1000$ km s⁻¹. The catastrophic failure

rate is a subset of the contamination fraction, isolating only bad Redrock redshifts regardless of spectral-class correctness. The incompleteness of each sample is the number of spectra with VI spectral class of QSO (galaxy) that is not included in the Redrock QSO (galaxy) sample.

The contamination fraction, catastrophic failure rate, and incompleteness for the Redrock QSO and galaxy samples from the DESI Truth Table and the Redrock QSO sample from QSO Main are reported in Table 3. The same metrics for the previous QSO templates are also included in the table. Overall, both QSO samples show clear improvement with the change of templates while the galaxy sample exhibits minimal change. Assuming a binomial distribution, the new QSO templates lower the incompleteness of the QSO Main sample by $32\% \pm 3\%$ and reduce the catastrophic failure rate by $50\% \pm 11\%$. A similar gain in completeness is achieved for the broader QSO sample as well, with a reduction in catastrophic failures of $32\% \pm 8\%$

Figure 4 shows the contamination fraction and incompleteness with redshift for the three samples. With the new templates, Redrock achieves a more complete QSO sample on the DESI Truth Table and QSO Main at all redshifts z > 0.5. This is reflected by the reduced contamination in the galaxy sample, indicating some QSOs previously misclassified as galaxies are now being placed in the correct sample. At all redshifts, the new QSO templates reduce the contamination in the QSO sample from QSO Main while achieving a lower or comparable contamination fraction in the QSO sample from the DESI Truth Table.

There are 132 objects in the DESI Truth Table that are classified as QSO by Redrock with the new QSO templates and were not classified as QSO with the previous templates. Figure 5 shows a representative selection of these spectra, illustrating the types of QSO recovered. Many of the new

 Table 3

 The Performance Metrics of Redrock Alone and Redrock with the QSO Afterburners on Spectra from the DESI Truth Table and QSO Main

| | | Previous | QSO Templates | | New QSO Templates | | | |
|----------|--------|---------------|--------------------------|----------------|-------------------|---------------|--------------------------|----------------|
| Sample | Size | Contamination | Catastrophic Failures | Incompleteness | Size | Contamination | Catastrophic Failures | Incompleteness |
| QSO | 1422 | 62 (4.4%) | 37 (2.6%) | 283 (17%) | 1497 | 58 (3.9%) | 25 (1.7%) | 204 (12%) |
| QSO Main | 1200 | 25 (2.1%) | 20 (1.7%) | 193 (14%) | 1253 | 16 (1.3%) | 10 (0.8%) | 131 (9.6%) |
| Galaxy | 15,310 | 491 (3.2%) | 268 (1.8%) | 172 (1.1%) | 15,237 | 431 (2.8%) | 258 (1.7%) | 185 (1.2%) |
| | | | | with QSO | afterburners | | | |
| QSO | 1781 | 216 (12%) | 77 (4.3%) | 78 (4.7%) | 1779 | 202 (11%) | 58 (3.3%) | 66 (4.0%) |
| QSO Main | 1387 | 64 (4.6%) | 31 (2.2%) | 45 (3.3%) | 1384 | 48 (3.5%) | 16 (1.2%) | 32 (2.3%) |
| Galaxy | 14,951 | 271 (1.8%) | 193 (1.3%) | 311 (2.1%) | 14,955 | 289 (1.9%) | 210 (1.4%) | 325 (2.2%) |

Note. The QSO Main is a subset of the DESI Truth Table mimicking main survey QSO performance by limiting to QSO targets with r < 23. The left section of the table lists the performance metrics when using the previous QSO templates and the right section is with the new QSO templates.

Redrock QSOs display dust-reddened continua or strong absorption features that likely contributed to misclassification under the previous templates. A known issue with the previous templates is missing narrow or weak Mg II emission, necessitating the Mg II QSO afterburner (Alexander et al. 2023; Chaussidon et al. 2023). The new templates recover many of these as Redrock QSOs, though the afterburner is still necessary to reach the desired QSO completeness.

Figure 5 also highlights a failure mode of Redrock generally. A small number of high-redshift Ly α emitter (LAE) galaxies are inadvertently targeted as QSO or galaxy. These systems are not classifiable as galaxy at the correct redshift with Redrock owing to the range of the galaxy templates (0 < z < 1.7). As a result, many of these objects appear in the QSO sample, with the Ly α line flux fit by the QSO template Ly α . The redshifts of true LAEs classified as QSO are only approximate since Ly α emission is broad in a QSO spectrum. Future work in DESI may explore an intentional LAE target class with a devoted template set for classification and redshift fitting.

4.1.1. Classification Accuracy and Completeness from Redrock with QSO Afterburners

The results reported so far are from Redrock alone. The QSO afterburners are necessary to achieve the required classification performance for cosmological analyses. In this subsection, we evaluate the impact that the new QSO templates have on classification for the full Redrock plus QSO afterburners pipeline.

The contamination fraction, catastrophic failure rate, and incompleteness of the QSO and galaxy samples from Redrock with QSO afterburners on the DESI Truth Table are reported in the bottom half of Table 3. As with the top half of the table, results are shown for both the previous and new QSO templates. Also included in the table are the metrics for the QSO samples from QSO Main.

The inclusion of the QSO afterburners results in an 8% (12.3%) gain in completeness for the QSO sample from the DESI Truth table and a 7.3% (10.7%) gain in completeness for the QSO sample from QSO Main with the new (previous) templates. The contamination fraction of the QSO sample from the DESI Truth Table, however, increases by about 7%–8% with both template sets compared to Redrock alone. These QSO samples include all spectra classified as QSO regardless of target type. The majority of the contamination (\sim 75% with previous and \sim 84% with new) is from spectra with a VI

spectral class of "galaxy" for which there is strong agreement between the VI redshift and QSO template redshift. This type of contamination is inconsequential as the redshifting is successful. The remaining contamination results from incorrect redshift estimates compared to the VI redshift.

Considering only the Redrock plus QSO afterburners performance, the new QSO templates improve both QSO samples across all metrics while the galaxy sample is minimally affected. The QSO sample from QSO Main is the most reflective of main survey QSOs and therefore the Year 1 QSO sample owing to the target type and magnitude restriction. For this sample, the catastrophic failure rate is improved by $48\% \pm 9\%$, the incompleteness by $29\% \pm 7\%$, and contamination by $25\% \pm 5\%$ using the new templates.

Overall, the new QSO templates produce QSO samples with higher completeness, less contamination, and a reduced rate of catastrophic failures compared to the previous QSO templates. The improvement to the QSO classification performance is achieved with minimal impact on the galaxy sample.

4.1.2. Average Spectral Properties of Redrock QSOs

The median composite of spectra in the DESI Truth Table classified as QSO by Redrock with the new QSO templates is shown in the top panel of Figure 6. Also shown is the median composite of QSO spectra that were missed by Redrock but recovered by the QSO afterburners. This figure does not fully convey the diversity of Redrock and missed QSOs but illustrates the average spectral properties seen in a typical Redrock QSO spectrum while providing insight into the type of spectral features that the new QSO templates struggle to reconstruct.

The bottom panel of Figure 6 shows similarly constructed composite spectra for the previous QSO templates, originally presented by Alexander et al. (2023). The missed QSO composite is constructed from a larger sample than with the new QSO templates, as their study focused on afterburner performance.

The typical spectrum classified as QSO by Redrock with the new QSO templates differs most from the typical missed QSO spectrum at $\lambda_{RF} < 3700$ Å where their underlying continua diverge. The QSOs missed by the new QSO templates tend to display more reddened continua in this range, similar to those missed by the previous QSO templates. For both template sets, a typical missed QSO may also display stronger host galaxy features such as the Balmer series and Ca H + K stellar

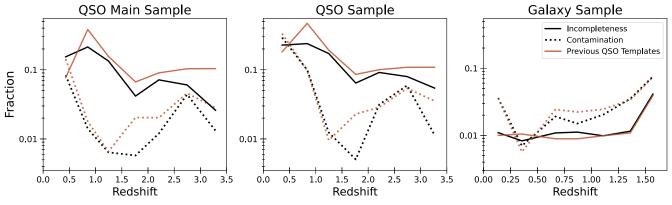


Figure 4. The contamination fraction (dashed) and incompleteness (solid) of the QSO Main sample, and of the QSO and galaxy samples from the DESI Truth Table with redshift from Redrock with the new QSO templates. The same metrics for the previous QSO templates are shown in red.

absorption lines observed over 3700–4000 Å as well as increased [O II] and [O III] flux. While the afterburners recover many of the QSO spectra that Redrock missed, a few percent of QSOs are still missed entirely (Table 4). Often, these QSOs have low S/N, very red continua, or strong absorption features.

A notable difference in the missed QSO spectra from changing the QSO templates appears in the equivalent width of broad lines such as C IV, C III], and Mg II. The equivalent widths of these lines in the typical missed QSO are smaller with the new QSO templates than with the previous QSO templates. This change indicates the new templates can describe more of the line profile parameter space, typically missing only the most narrow of broad line systems.

4.1.3. Classification Discrepancies Between the Previous and New QSO Templates

As a last step in evaluating the catastrophic failures, completeness, and contamination, we visually inspect spectra in Guadalupe that have discrepant Redrock-only classifications between the previous and new QSO templates. Classification discrepancies occur when Redrock assigns a different spectral class (galaxy, QSO, or star) or redshift to the same spectrum depending on the QSO templates used. The threshold for a redshift to be considered discrepant is defined as

$$|\Delta v| = \frac{|z_{\text{previous}} - z_{\text{new}}|}{1 + z_{\text{previous}}} \times c > 3000 \text{ km s}^{-1}.$$
 (2)

The breakdown of classification discrepancies by target type is shown in Table 5.

VI is a time-consuming task and inspecting all spectra in Guadalupe that change classification is infeasible. Instead, we VI only a subset of spectra from Table 5 to estimate the consequences of the changed classifications. We choose 100 spectra that are discrepant in spectral class and 100 that have discrepant redshifts randomly from each target class over 40 tiles. Exclusivity is not enforced between the samples of discrepant spectra within a target type. Only 48 and 90 spectra have redshift disagreements over the selected tiles for BGS and LRG targets, respectively. This leaves a final selection of 738 spectra for VI.

Each spectrum in our VI sample was assigned to four inspectors who evaluated it using Prospect.³⁹ Prospect is a VI tool developed for evaluating DESI's pipeline performance and target selection methods in the early survey. In short, Prospect

displays an observed spectrum that can be interactively smoothed by the inspector. The top nine best template fits from Redrock can be overlaid on the spectrum for reference. Properties associated with each fit are also available in the VI tool, including the χ^2 , redshift, and spectral class (see Lan et al. 2023 for detailed descriptions of Prospect). Each inspector indicates a spectral class and redshift of the spectrum along with the confidence of their assessment on a scale of 0 to 4. A confidence of 0 indicates no signal, 1 indicates there is one strong spectral feature present with a probable identification, 2 indicates more than one spectral feature has been identified, but features may be weak, and 4 indicates two or more spectral features are securely identified. An average confidence of 2.5 is the minimum value to be considered a confident classification.

The VI results of the four inspectors inform a final classification "truth" table for the sample. Special attention is given to resolving the classifications of spectra for which the inspectors disagree. We use only confident VI classifications in our analysis, reporting the remainder as "Low Quality."

The classification under a given QSO template set is considered correct if (1) the Redrock spectral class agrees with the VI spectral class and (2) the Redrock redshift is less than 3000 km s^{-1} from the VI redshift for QSO targets or less than 1000 km s^{-1} from the VI redshift for galaxy targets. A few instances exist where both template sets satisfy these criteria on a given spectrum. For these cases, the template set that provides the redshift estimate closest to the VI redshift is labeled as correct. Discrepant classifications for which neither template set satisfies both criteria are reported under "Neither Correct." The results from VI of the discrepant spectra are summarized in Table 4, broken down by target type and type of discrepancy.

The confident VI classifications of both spectral-class- and redshift-discrepant spectra indicate an improvement with the new QSO templates for all target types. Redshift-discrepant spectra with an LRG or BGS target type, however, have a high occurrence rate of neither template set achieving the correct classification. In most cases, the failure stems from problematic reductions of the spectra, such as discontinuities in flux, that impact the template-fitting ability rather than a problem with the QSO templates themselves.

4.2. Redshift Precision and Bias

This subsection is devoted to the redshift performance of the final classifications (Redrock with QSO afterburners) with the new QSO templates. We present estimates of the redshift precision, the

³⁹ https://github.com/desihub/prospect

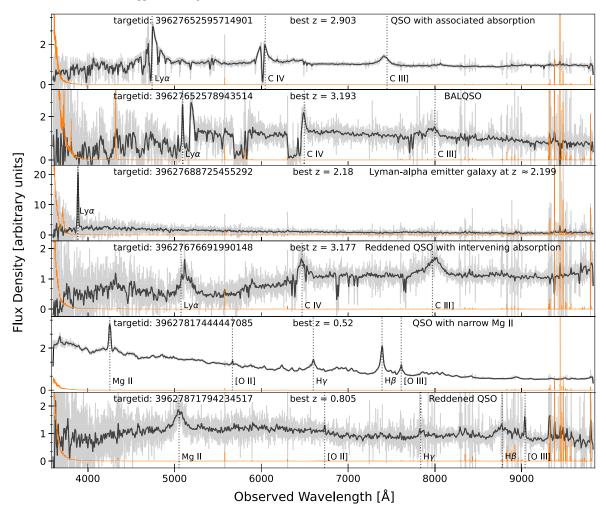


Figure 5. A subset of spectra from the DESI Truth Table that are classified as QSO by Redrock with the new QSO templates, but not classified as QSO with the previous QSO templates (pre-QSO afterburners). The observed flux is shown in gray, the error on the flux is shown in orange, and the flux after applying a Gaussian smoothing filter is shown in black. The DESI target ID, redshift estimate from the new templates (best *z*), and basic information on the type of spectrum are annotated at the top of each subplot. Prominent emission lines are indicated in the observer frame with vertical lines and labeled.

catastrophic failure rate, and average redshift bias. We also briefly discuss the redshift performance specific to BALQSOs.

4.2.1. Redshift Precision Measured by Repeat Exposures

The multiple spectra for QSO targets in the SV Repeat Exposures sample can be used to determine a lower bound on the redshift precision and estimate the catastrophic failure rate at the main survey depth. We measure the precision as the dispersion of the velocity offsets between pairs of repeat exposures. The dispersion is calculated using the median absolute standard deviation (MAD) scaled by 1.4828 $\times 2^{-\frac{1}{2}}$, following Alexander et al. (2023) and Lan et al. (2023). The catastrophic failure rate is defined as the percentage of these pairs with an absolute velocity offset, scaled by $2^{-\frac{1}{2}}$ to account for the measurement error on each redshift, over the typical failure threshold for QSOs of 3000 km s⁻¹ and a stricter threshold of 1000 km s⁻¹.

The measure of precision from repeat exposures provides only a lower-bound estimate on the true precision of QSO redshift estimates owing to the complex dynamics of QSO spectral features. Emission lines are often shifted nonuniformly from the systemic redshift, impacting the ability of a templatefitting software to extract the systemic redshift. Line dynamics that impact the redshift estimate obtained by the QSO templates will impact the redshift estimate in every exposure. The scaled MAD effectively estimates consistency or statistical precision.

The evolution of the scaled MAD with redshift is shown in Figure 7 for both the new and previous QSO templates along with their corresponding catastrophic failure rates. Redshift estimates from both QSO template sets are less precise as redshift increases until turning over at $z \approx 1.75$, also reported by Yu et al. (2023). The rise and fall of redshift precision between $1.35 \leq z \leq 2.5$ may be due to the presence of both the Mg II and C IV emission lines in the spectra. These lines have different expected velocity offsets from the systemic redshift, which could introduce additional errors.

At the main survey depth, the new templates clearly improve the precision at all redshifts. The redshift precision improves from $100^{+2.7}_{-2.4}$ km s⁻¹ to $57^{+1.5}_{-1.3}$ km s⁻¹ globally. The precision of both template sets is well below the DESI scientific and survey requirement for random errors between individual QSO redshift estimates of 750 km s⁻¹ (Abareshi et al. 2022), even at the redshift where the uncertainty peaks. The new QSO templates do not appear to impact the catastrophic failure rate at the failure threshold of 3000 km s⁻¹. DESI scientific and survey requirements dictate that the rate of catastrophic failures exceeding 1000 km s⁻¹ shall be less than 5% for tracer QSOs. Using this failure threshold on the SV Repeat Exposures sample yields a catastrophic failure rate of

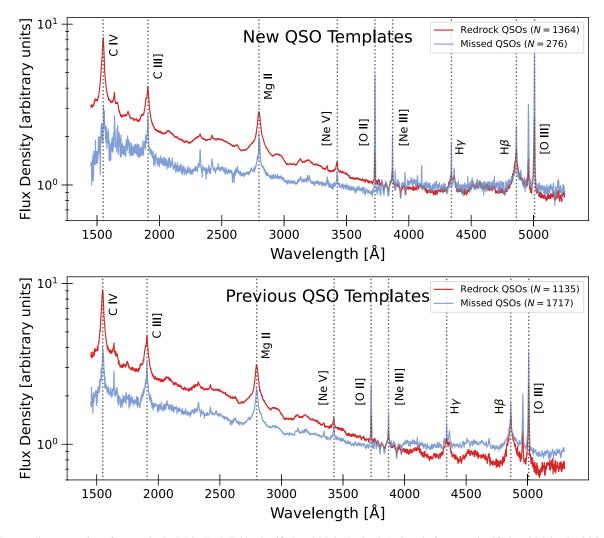


Figure 6. Top: median composites of spectra in the DESI Truth Table classified as QSO by Redrock (red) and of spectra classified as QSO by the QSO afterburners but missed by Redrock (blue). The spectra are normalized over 3800–3900 Å. Vertical lines indicate prominent QSO emission lines. Bottom: similar to above but with the previous QSO templates and an expanded sample of afterburner-identified QSOs (Figure 12 of Alexander et al. 2023).

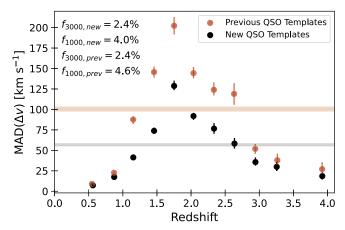


Figure 7. Redshift precision of QSO targets from the SV Repeat Exposures sample estimated by the scaled MAD of the dispersion of velocity offsets between redshift pairs. The error bars indicate the 95% confidence interval, and the shaded regions show the redshift precision measured over all redshifts. f_{1000} and f_{3000} are the catastrophic failure rate over the failure thresholds of 1000 km s⁻¹ and 3000 km s⁻¹, respectively.

4.0% and 4.6% for the new and previous QSO templates, respectively, meeting the requirements in both cases.

4.2.2. Cross-correlation With Other Tracers

Bias and systematic uncertainty on QSO redshifts manifest in the characteristics of the small-scale peak of cross-correlation functions in the radial direction. The radial shift of the peak from zero, Δr_{\parallel} , quantifies the average bias of the QSO redshift estimates while the width of the peak, σ_{ν} , is influenced by redshift precision (Font-Ribera et al. 2013; du Mas des Bourboux et al 2017; A. Bault et al. 2023, in preparation). An absolute value of QSO redshift precision cannot be determined from this measurement, however, as several cosmological parameters and nonlinear effects contribute to σ_v in addition to redshift errors. We instead use the relative σ_v between the correlation functions produced by the different QSO template sets with a given non-QSO tracer to quantify the change in QSO redshift precision from changing templates. We assume these distortions of the small-scale peak of the cross-correlation functions arise from the QSO redshift errors and not from the redshift errors on the other tracers. The physics of

Table 4 Results from VI of Spectra in Guadalupe That Have Discrepant Redrock-only Classifications between the Previous and New QSO Templates

| Target | Discrepancy | Total | New Templates | Previous Templates | Neither | Low |
|--------|----------------|-----------|---------------|--------------------|---------|---------|
| Type | | Inspected | Correct | Correct | Correct | Quality |
| QSO | Redshift | 100 | 70 | 16 | 5 | 9 |
| | Spectral Class | 100 | 70 | 8 | 12 | 10 |
| ELG | Redshift | 100 | 48 | 9 | 20 | 23 |
| | Spectral Class | 100 | 61 | 9 | 5 | 25 |
| LRG | Redshift | 90 | 28 | 9 | 28 | 25 |
| | Spectral Class | 100 | 59 | 0 | 33 | 8 |
| BGS | Redshift | 48 | 13 | 4 | 14 | 17 |
| | Spectral Class | 100 | 72 | 1 | 24 | 3 |

Note. We select two samples from each target type: redshift discrepant and spectral-class discrepant. Spectra in a given sample may exhibit both types of discrepancies however. Low Quality indicates spectra that could not be confidently classified through VI.

Table 5 Occurrences of Classification Discrepancies between the Previous and New QSO Templates by Target Type in the Guadalupe Sample

| | | | - | - |
|----------------|---------|---------|---------|-----------|
| Target Type | QSO | ELG | LRG | BGS |
| Total Targets | 435,538 | 498,367 | 404,361 | 1,149,884 |
| Spectral Class | 21,911 | 8,623 | 7184 | 7704 |
| Redshift | 23,009 | 7037 | 1448 | 695 |
| Both | 13,326 | 4394 | 1254 | 497 |

non-QSO tracer systems is better constrained, so we treat non-QSO redshifts as effectively error free relative to the QSO redshifts.

We calculate the two-point cross-correlation function between QSOs and galaxies in the One-Percent Survey and between QSOs and Ly α absorbers in Guadalupe using the pycorr⁴⁰ software package and the picca⁴¹ software package, respectively. All correlation functions are determined over radial separations of $-40 < r_{||} < 40$ Mpc h⁻¹ and integrated from 0 to 200 Mpc h⁻¹ in the transverse direction.

We determine the cross-correlation function between QSOs and LRGs over 0.8 < z < 1.1, QSOs and ELGs over 0.8 < z < 1.6, and QSOs with redshifts of 2.0 < z < 4.0 and $Ly\alpha$ absorbers along their sight lines. The $Ly\alpha$ -QSO crosscorrelation function is fit jointly with the Ly α autocorrelation function to reduce parameter degeneracy. DESI ELG targets overlap with DESI QSO targets, so we require a "galaxy" classification for ELGs in these measurements. The ELG and $Ly\alpha$ cross-correlation measurements are split on redshift to check for any evolution in the bias and precision of the QSO redshifts.

Figure 8 shows an example of the small-scale signal we are measuring in the Ly α -QSO cross-correlation. The x-axis corresponds to $|r_{||}| \lesssim 37$ Mpc h⁻¹, converted to km s⁻¹ for interpretation as redshift errors. The amplitude of the smallscale peak is negative because $Ly\alpha$ is a negative bias tracer. The difference in peak width between the previous and new QSO templates seen in Figure 8 corresponds to the difference in QSO redshift precision. This change in precision is captured by the ratio of σ_v in Table 6. We determine the best-fit value for

⁴¹ https://github.com/igmhub/picca



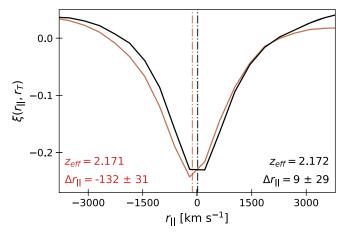


Figure 8. The Ly α -QSO cross-correlation measured with QSOs at 2.0 < z < 2.5 using the new QSO templates (black) and the previous QSO templates (red). The best-fit $\Delta r_{||}$ for each measurement is indicated with a vertical line. z_{eff} is the effective redshift of the correlation function.

the radial shift of the small-scale peak, Δr_{\parallel} , and the corresponding peak width, σ_{v} , for each correlation function. The best-fit Δr_{\parallel} values are given in Table 6 for each tracer population along with the ratio of σ_{ν} between the correlation functions produced by the different QSO templates.

Redshifts from the new QSO templates are significantly less biased in most correlations. Δr_{\parallel} is consistent with zero at 68% confidence over two of the redshift ranges evaluated, a statement that is not true at any redshift with previous QSO templates. The exception to improvement in absolute bias comes from the ELG-QSO cross-correlation. The new QSO templates produce absolute biases consistent with the previous QSO templates over 0.8 < z < 1.1, but the biases over 1.1 < z < 1.6 increase as a result of the general 70 km s⁻¹ shift seen in all galaxy-QSO cross-correlations. This shift can likely be attributed to the slight difference in RF between the previous and new template sets (Section 3.2).

A large reduction in σ_v is observed at the highest redshifts, indicating greatly improved redshift precision. The value of σ_{ν} decreases with the new OSO templates across all tracers at the other redshifts evaluated, indicating some improvement at z < 2.5 though to a lesser extent. The observed improvement in precision is consistent with the findings of Section 4.2.1.

⁴⁰ https://github.com/cosmodesi/pycorr

 Table 6

 QSO Redshift Uncertainties Measured from Cross-correlations with LRGs, ELGs, and Ly α Absorbers

| | | Previous QSO Templates | | New QSO Templates | | | |
|----------------|-----------------------|------------------------|--|-------------------|---------------------------------------|--|--|
| Redshift Range | Data Set | Zeff | $\Delta r_{ } (\mathrm{km \ s}^{-1})$ | Zeff | $\Delta r_{ }$ (km s ⁻¹) | $\sigma_{v,\text{new}}/\sigma_{v,\text{prev}}$ | |
| 0.8 < z < 1.1 | $LRG \times QSO$ | 0.954 | -75 ± 10 | 0.954 | -3 ± 10 | 0.990 ± 0.038 | |
| 0.8 < z < 1.1 | $ELG \times QSO$ | 0.961 | -40 ± 11 | 0.961 | 31 ± 8 | 0.986 ± 0.046 | |
| 1.1 < z < 1.6 | $ELG \times QSO$ | 1.353 | -17 ± 8 | 1.352 | 59 ± 8 | 0.921 ± 0.035 | |
| 2.0 < z < 2.5 | $Ly\alpha \times QSO$ | 2.171 | -132 ± 31 | 2.172 | $9{\pm}29$ | 0.948 ± 0.307 | |
| 2.5 < z < 4.0 | $Ly\alpha \times QSO$ | 2.753 | -236 ± 46 | 2.756 | -84 ± 31 | 0.501 ± 0.152 | |

Note. z_{eff} is the effective redshift of the correlation function, Δr_{\parallel} characterizes the average bias of the QSO redshifts estimates, and σ_{ν} captures the effects of several redshift uncertainties including redshift errors. A reduction of σ_{ν} demonstrates an improvement in the combination of statistical and systematic errors on the redshift estimates when using the new QSO templates.

 Table 7

 The Average Bias on and Relative Uncertainty between Redshifts From the Previous and New QSO Templates for BALQSOs (AI >0), as Measured from Cross-correlation with $Ly\alpha$ Absorbers

| Previous QSO Templates | | | | | | | |
|--|-------|---------------------------------------|--|-------|---------------------------------------|--|--|
| Data Set | Zeff | $\Delta r_{ }$ (km s ⁻¹) | $\sigma_{v,\mathrm{mask}}/\sigma_{v,\mathrm{no}\ \mathrm{mask}}$ | Zeff | $\Delta r_{ }$ (km s ⁻¹) | $\sigma_{v,\rm mas}/\sigma_{v,\rm no\ mask}$ | $\sigma_{v,\mathrm{new}}/\sigma_{v,\mathrm{prev}}$ |
| $Ly\alpha \times BALQSO$ (masking) | 2.402 | -254 ± 60 | 0.527 ± 0.213 | 2.413 | -64 ± 43 | 0.643 ± 0.288 | 0.584 ± 0.261 |
| $Ly\alpha \times BALQSO$ (no masking) | 2.403 | -177 ± 63 | | 2.414 | 56 ± 47 | | 0.478 ± 0.193 |

Note. We report $\Delta r_{||}$ for two correlation functions under each QSO template set: using the Redrock with QSO afterburner redshifts (no masking) and updated redshifts after masking BALs (masked). Additionally, the relative uncertainty (relative σ_{ν}) between the two correlation functions under a given template set is also reported, measuring the impact of masking BALs on redshift uncertainty.

4.2.3. Redshift Success for BALQSOs

BALQSOs are notorious for degraded redshift success relative to non-BALQSOs. The presence of BALs increases the catastrophic failure rate as well as the random and systematic redshift errors of the total QSO sample. A PCA template-fitting algorithm that uses the eigenspectra of Guo & Martini (2019) was developed to classify high-ionization BALQSOs in the DESI QSO sample over 1.57 < z < 5.0. The classifier records the locations and widths of BALs associated with the C IV and Si IV emission lines. In this work, we define a BALQSO as having an intrinsic absorption index (AI; Hall et al. 2002) relative to C IV that is greater than zero.

Refined redshifts for BALQSOs in Guadalupe are provided in the DESI EDR BAL catalog presented by S. Filbert et al. (2023, in preparation). The authors refit affected spectra with the Redrock QSO templates after masking BAL features identified by the BAL classifier. The updated fit can vary up to $|\Delta z| = 0.1$ from the initial redshift estimate given by Redrock with the QSO afterburners. We repeat this reredshifting procedure for BALQSOs in Guadalupe when the new QSO templates are used in Redrock.

We compute the cross-correlation between BALQSOs (AI >0) in Guadalupe and the Ly α absorber sample from the previous subsection. As in Section 4.2.2, we determine the average bias on BALQSO redshifts and the relative redshift uncertainty between the previous and new QSO template sets. We compute the cross-correlations using both the initial redshift estimates from Redrock with QSO afterburners and the updated redshifts after masking BALs, leading to a total of four cross-correlation measurements.

The best-fit $\Delta r_{||}$ value for each correlation function is given in Table 7 along with the relative σ_{ν} between the correlation functions produced by the different template sets. The new QSO templates significantly improve the BALQSO redshift performance. The average absolute bias on both the initial and masked redshifts is reduced by over 100 km s^{-1} . Additionally, the redshift uncertainty improves by an estimated 40%–50%.

The relative σ_{ν} between the correlation functions produced by the masked and initial redshifts under each template set are also reported in Table 7. For both template sets, the masking procedure greatly improves the redshift uncertainty for BALQSOs while shifting the average bias toward more negative velocity offsets. These findings agrees with Ángela García et al. (2023) in that masking BAL features improves redshift errors and with S. Filbert et al. (2023, in preparation) that it results in lower redshifts for BALQSOs on average.

5. Summary

The new DESI QSO templates are a significant update to the automatic spectral classification procedure in DESI. The previous DESI QSO templates, inherited from (e)BOSS, were designed to classify QSO spectra across the full range of 0.05 < z < 7.0. This broad redshift coverage limits the ability to reconstruct the full range of spectral diversity adequately, contributing to poor completeness when used as the sole method for identifying QSO spectra in DESI. We have developed new QSO templates for DESI consisting of lowand high-redshift sets trained to classify QSOs over 0.05 < z < 1.6 and 1.4 < z < 7.0, respectively. We have shown that these QSO templates produce more complete QSO samples while providing higher-accuracy redshift estimates.

The new QSO templates were trained on approximately 200,000 (e)BOSS QSO spectra over 0.0 < z < 5.0. Clusters of similar spectra were identified using the clustering technique of BD22 and combined into high-S/N composite spectra. The enhanced S/N enabled direct fitting of the Mg II emission line,

a relatively stable emission feature with low bias relative to the systemic redshift. The wavelength solutions of all composite spectra were corrected so that the Mg II line was at its proper RF wavelength. Eigenspectra of the redshift-corrected composite spectra were used to rederive redshifts for the individual spectra of the training sample, placing all spectra in a consistent RF. Poor fits from the eigenspectra indicated problematic and misclassified spectra in the training sample, facilitating their removal. The high- and low-redshift QSO template sets that comprise the final QSO templates for DESI were derived from PCA on subsets of the updated training sample in redshift space. The redshift boundaries of the high- and low-redshift template sets were determined through maximizing the completeness and redshift success of Redrock on the DESI Truth Table.

We compared the classifications from Redrock with the new QSO templates and with the previous QSO templates on the DESI Truth Table and the QSO Main sample. Both samples include spectra that are exposed beyond the main survey depth, facilitating classification via VI. The QSO Main sample is a subset of the DESI Truth Table limited to QSO targets that are representative of DESI main survey QSO targets (r < 23). For this sample, the catastrophic failure rate is reduced by approximately half with the new templates while the QSO incompleteness problem with Redrock is mitigated.

DESI's two QSO afterburner algorithms work in conjunction with Redrock to achieve the required QSO completeness for scientific analyses. The new QSO templates provide less contaminated and more complete QSO samples from the Redrock plus QSO afterburners classification scheme than the previous QSO templates. The improvements to QSO classification are achieved with minimal consequences observed in the galaxy sample.

The most significant impact of the new QSO templates is observed in the redshift precision and accuracy. The velocity dispersion of repeat exposure redshifts in the SV Repeat Exposures sample indicates that the statistical redshift precision of QSOs at the main survey depth is improved by 40%-50% globally with no apparent change in the catastrophic failure rate at the 3000 km s⁻¹ threshold. The improvement in precision is largest over 1.0 < z < 2.75. The small-scale cross-correlations of QSOs with other DESI tracers reveal a reduction in the absolute bias of the QSO redshifts in most measurements, though a redshift dependency in the bias persists (Table 6). We also measure a significant reduction in the absolute bias of the redshift estimates for BALQSOs while improving their redshift uncertainties by an estimated 40%-50% (Table 7). In future template versions, further improvement in redshift performance may be achieved with more complete modeling of the Mg II emission line in the training sample spectra.

Future work will explore potential solutions to reduce or remove the redshift-dependent bias of the QSO redshifts at the highest redshifts. One possible method to reduce the bias and mitigate its redshift dependency is through correcting for the optical depth of the Ly α forest while determining the redshift. This would require a new set of high-redshift templates trained with a model of the Ly α forest optical depth evolution folded in. These upgraded high-redshift templates could be constructed with DESI QSOs to capture better the spectral diversity specific to DESI QSO targets. Incorporating the Ly α forest optical depth evolution into a template set would also allow predictions of the average continuum for unbiased estimates of the Ly α absorption field. Such continuum predictions would allow modeling of the density field on all scales for cosmological studies, including determining clustering amplitudes through cross- correlations with the cosmic microwave background. A more aggressive approach to reducing bias is masking pixels in the Ly α forest during redshift determination. This option is at the sacrifice of information of the forest, though the typical S/N of forest pixels is much less than that in the rest of the spectrum.

5.1. DESI Science Requirements

The scientific and survey requirements for DESI as a Stage IV dark energy survey are detailed in Table 3 of Abareshi et al. (2022). Below, we map the performance of the new QSO templates to the relevant scientific and survey requirements for redshift success of tracer (z < 2.1) and Ly α (z > 2.1) QSOs.

L2.4.2, L2.5.2: the random redshift error shall be less than $\sigma_v = 0.0025(1 + z)$, or equivalently 750 km s⁻¹ rms.

The MAD of velocity offsets between redshift pairs in the SV Repeat Exposures sample measures the statistical precision, or the random redshift error, of redshift estimates for QSO targets in DESI. As shown in Figure 7, the statistical redshift precision of the new QSO templates is less than 150 km s⁻¹ over 0.0 < z < 4.0 and drops below 50 km s⁻¹ for z < 1.25 and z > 2.75.

L2.4.3: systematic inaccuracy in the mean redshift of tracer QSOs shall be less than $\Delta z = 0.0004(1 + z)$ or equivalently, 120 km s⁻¹.

The average inaccuracy, or bias, of QSO redshifts is measured as $\Delta r_{||}$ in the fit to cross-correlation functions with other DESI tracers (Section 4.2.2). We only measure the bias of tracer QSO redshifts over 0.8 < z < 1.6, defined by the overlap in redshift distributions with the other non-QSO tracers targeted by DESI. The maximum average inaccuracy in this range is 59 ± 10 km s⁻¹. Additionally, the average inaccuracy of Ly α QSO and BALQSO redshifts over 2.0 < z < 4.0 is less than 120 km s⁻¹ with the new templates, though no minimum redshift accuracy is specified for high redshifts.

L2.4.4: catastrophic failures exceeding 1000 km s⁻¹ shall be less than 5% for tracer QSOs.

The typical tracer QSO in DESI will receive an exposure equivalent to the main survey depth. Therefore, the projected catastrophic failure rate is adequately estimated by limiting the SV Repeat Exposures sample to z < 2.1. This yields a catastrophic failure rate of 3.9% for tracer QSOs at the 1000 km s⁻¹ threshold.

L2.5.3: catastrophic failures shall be less than 2% for Ly α QSOs.

Similar to above, a catastrophic failure rate for Ly α QSOs is estimated by limiting the SV Repeat Exposures sample to z > 2.1. The rate of catastrophic failures exceeding 1000 km s⁻¹ is 4.1% with the new QSO templates, compared to 5.6% with the previous QSO templates. The new QSO templates achieve a catastrophic failure rate of 1.7% if the failure threshold is relaxed to 3000 km s⁻¹, compared to 1.9% with the previous templates. Ly α QSOs, unlike tracer QSOs, will be observed at least four times to enhance the S/N of their spectra. As such, the catastrophic failure rates determined here may be an overestimate.

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Data Availability

All data shown in figures are available at doi:10.5281/ zenodo.7872747

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