

Hydrogen reionisation ends by $z = 5.3$: Lyman- α optical depth measured by the XQR-30 sample

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ABSTRACT

The presence of excess scatter in the Ly- α forest at $z \sim 5.5$, together with the existence of sporadic extended opaque Gunn-Peterson troughs, has started to provide robust evidence for a late end of hydrogen reionisation. However, low data quality and systematic uncertainties complicate the use of Ly- α transmission as a precision probe of reionisation’s end stages. In this paper, we assemble a sample of 67 quasar sightlines at $z > 5.5$ with high signal-to-noise ratios of > 10 per ≤ 15 km s⁻¹ spectral pixel, relying largely on the new XQR-30 quasar sample. XQR-30 is a large program on VLT/X-Shooter which obtained deep (SNR > 20 per pixel) spectra of 30 quasars at $z > 5.7$. We carefully account for systematics in continuum reconstruction, instrumentation, and contamination by damped Ly- α systems. We present improved measurements of the mean Ly- α transmission over $4.9 < z < 6.1$. Using all known systematics in a forward modelling analysis, we find excellent agreement between the observed Ly- α transmission distributions and the homogeneous-UVB simulations Sherwood and Nyx up to $z \leq 5.2$ ($< 1\sigma$), and mild tension ($\sim 2.5\sigma$) at $z = 5.3$. Homogeneous UVB models are ruled out by excess Ly- α transmission scatter at $z \geq 5.4$ with high confidence ($> 3.5\sigma$). Our results indicate that reionisation-related fluctuations, whether in the UVB, residual neutral hydrogen fraction, and/or IGM temperature, persist in the intergalactic medium until $z = 5.3$ ($t = 1.1$ Gyr after the Big Bang). This is further evidence for a late end to reionisation.

Key words: dark ages, reionisation, first stars – quasars: absorption lines – intergalactic medium – large-scale structure of Universe

1 INTRODUCTION

The epoch of reionisation, during which the bulk of intergalactic hydrogen became ionised, is of great interest for both astrophysicists and cosmologists. The timing and morphology of the transition relate to the properties of the first galaxies and other potential reionising sources, holding crucial information on the large-scale properties of the intergalactic medium (IGM) as well as galaxy formation and evolution at early cosmic times (see e.g. [Dayal & Ferrara 2018](#)). Next-generation 21cm experiments aim to directly detect the signature of neutral gas in the first stages of reionisation at $z \gtrsim 10$ within the coming decade ([DeBoer et al. 2017](#); [Trott & Pober 2019](#)). Meanwhile, the end stages of reionisation at $z \lesssim 7$ are already being probed through quasar absorption in the Lyman- α (Ly- α) and Lyman- β (Ly- β) hydrogen transitions (e.g. [Fan et al. 2002](#); [Mesinger & Haiman 2004](#); [Mortlock et al. 2011](#); [Bosman & Becker 2015](#); [Greig et al. 2017](#); [Davies et al. 2018b](#); [Eilers et al. 2019](#); [Wang et al. 2020](#)).

Over 200 quasars are now known at $z > 5.7$, corresponding to the first billion years after the Big Bang ([Bosman 2020](#)). The first observational constraints on the end of reionisation originated from detections of Gunn-Peterson (GP; [Gunn & Peterson 1965](#)) troughs at $z > 6$: total absorption of quasar continuum emission by neutral hydrogen in the IGM ([Fan et al. 2000, 2006](#)). Saturation of Ly- α absorption occurs in the presence of IGM gas with a hydrogen neutral fraction $\gtrsim 0.01\%$, with dependence on the density and temperature of the gas. The interpretation of GP troughs for reionisation is complex. Measurements of Ly- α transmission towards quasars have revealed that saturation occurs sporadically down to $z \sim 5.6$, and also on very large contiguous scales $\gtrsim 100$ cMpc/h ([Becker et al. 2015](#)). Observed differences in Ly- α optical depth between sight-lines at fixed redshift far exceed expectations from cosmic density fluctuations alone ([Becker et al. 2015](#); [Bosman et al. 2018](#); [Eilers et al. 2018](#); [Yang et al. 2020](#)), implying a more protracted or ‘patchy’ end of reionisation than was unforeseen by standard models (but see [Lidz et al. 2006](#); [Mesinger 2010](#)).

Determining the nature of these $z < 6$ optical depth fluctuations is currently a major goal of reionisation theory. The existence of late-persisting GP troughs and the observed optical depth scatter at $z \sim 5.8$ can be matched by a late end of reionisation in which some voids with hydrogen neutral fractions $> 10\%$ persist down to $z \sim 5.6$ ([Kulkarni et al. 2019](#); [Keating et al. 2020](#); [Nasir & D’Aloisio 2020](#)). Roughly half of the cosmic volume would then be occupied by neutral gas at $z \sim 7$, with important consequences such as e.g. facilitating the observation of the 21cm signal ([Raste et al. 2021](#); [Šoltinský et al. 2021](#)). In addition, scatter in the Ly- α optical depth at $z \sim 5.8$ can also arise from a short and fluctuating photon mean free path, which alters the propagation of ionising photons through the IGM ([Davies & Furlanetto 2016](#); [D’Aloisio et al. 2018](#)). Recent observations have suggested a shorter-than-expected ionising mean free path at $z \sim 6$ ([Becker et al. 2021](#)). While not explicitly requiring a late end to reionisation, a short mean free path at $z \sim 6$ poses tight requirements on the ionising power of early galaxies ([Davies et al. 2021](#); [Cain et al. 2021](#)). Further models have explored the importance of additional sources of scatter, such as relic IGM temperature fluctuations ([D’Aloisio et al. 2015](#); [Keating et al. 2018](#)) or a potential significant role of quasars ([Chardin et al. 2017](#); [Meiksin 2020](#)). Meanwhile, observations of Ly- α transmission at $z \lesssim 5$ are fully consistent with IGM models including only the effects of density fluctuations in a homogeneous (i.e. permeated) ultra-violet background (UVB) ([Rollinde et al. 2013](#); [Becker et al. 2013, 2015](#)). The transition between these two regimes across

$5.0 \leq z \leq 5.8$ therefore holds crucial clues to the changes in IGM properties as reionisation finishes.

Furthermore, the first measurements of the Ly- α optical depth distribution at $z \sim 5.8$ with large quasar samples have led to the first results from semi-numerical models of reionisation’s patchy end stages. The Bayesian inference enabled by these semi-numerical models allowed us to statistically constrain the end of reionisation to $z < 5.6$ ([Choudhury et al. 2021](#); [Qin et al. 2021](#)), as well as disfavor a strong evolution of the ionising escape fraction in reionising galaxies ([Qin et al. 2021](#)).

The advent of expensive and specifically tuned simulations, as well as sensitive inference models of reionisation, necessitate that measurements of Ly- α optical depth have a firm grasp on possible observational biases. To capture cosmic variance, studies require very large samples of quasars – but until now, this has come at the expense of data homogeneity and potential instrumental and reduction biases which are not known accurately ([Bosman et al. 2018](#)). There has been some tension between results from different groups ([Bosman et al. 2018](#); [Eilers et al. 2018](#); [Yang et al. 2020](#)) which can be largely attributed to differing choices of methods for reconstructing the underlying quasar emission ([Bosman et al. 2021](#), thereafter [B21](#)). Out of necessity (insufficient data) and low relative importance compared to sample size, a rigorous quantitative examination of those biases and uncertainties has been neglected until now. Indeed, the existence of excess scatter in Ly- α optical depth at $z \sim 5.7$ is established very robustly even with the most pessimistic assumptions on measurement errors ([Becker et al. 2015](#)). The rigour and precision required for quantitative inference and comparison to new models, however, requires a higher level of attention to observational biases and uncertainties. The XQR-30 sample ([D’Odorico et al. in prep](#)) consisting of 30 new high-SNR spectra of $z \gtrsim 5.8$ quasars, enables such a careful analysis for the first time without sacrificing sample size.

In this paper, we use the XQR-30 sample together with archival spectra of equal quality to significantly refine measurements of Ly- α optical depth at $5.0 \leq z \leq 6.0$. The observational data is described in Section 2. Restricting the analysis to high-quality data enables the suitable treatment of a slew of systematics and rigorous error estimation, which we describe in Section 3. We present the new distributions in Section 4. Finally, we compare our measurements with expectations from a homogeneously-ionised Universe in Section 5. The comparison to models both tests whether our analysis has accounted for all significant systematics at $z \sim 5$, where no reionisation-related fluctuations are expected in Ly- α transmission, and quantifies the point of transition beyond which these fluctuations are detected. We summarise our results in Section 6.

Throughout the paper we assume a [Planck Collaboration et al. \(2020\)](#) cosmology with $H_0 = 67.74$, $\Omega_m = 0.3089$. Wavelengths always refer to the rest-frame unless explicitly stated. Comoving and proper distances are always labelled explicitly (e.g. cMpc).

2 DATA

2.1 XQR-30

We primarily use data from the XQR-30 program (1103.A-0817(A)), which is ongoingly building a legacy sample of high-resolution spectra of 30 quasars at $z \gtrsim 5.8$ with the X-Shooter instrument ([Vernet et al. 2011](#)) on the Very Large Telescope. An example spectrum from the program is shown in Figure 1. The XQR-30 quasars were selected to have the highest apparent luminosities at

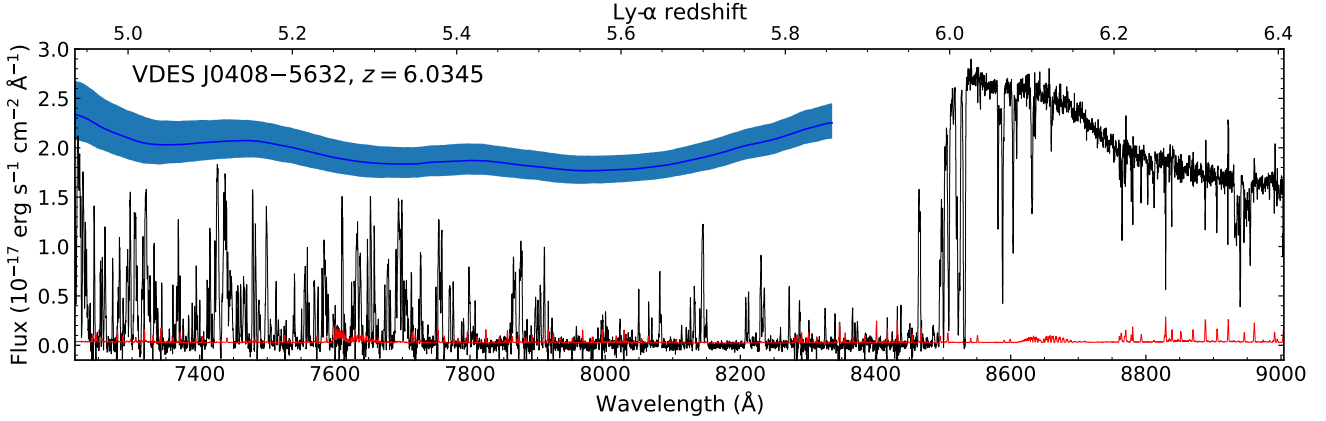


Figure 1. X-Shooter spectrum of the Ly- α transmission region in the XQR-30 quasar VDES J0408-5632 at $z = 6.0345$. The flux uncertainty is shown in red and the PCA-reconstructed continuum and its uncertainties are shown in blue. The PCA reconstruction is plotted over the wavelength range $1126\text{\AA} < \lambda < 1185\text{\AA}$ which we use in the mean flux measurement. The pixel scale is 10 km s^{-1} and the SNR of the Ly- α region (uncertainty divided by reconstruction) is $\text{SNR} = 86$. The exposure time was 13.5 hours.

Quasar ID	z_{qso}	SNR pix^{-1}	Refs.
PSO J323+12	6.5872	35.9	(1,27)
PSO J231-20	6.5869	42.3	(1,27)
VDES J0224-4711	6.5223	24.4	(3,39)
PSO J1212+0505	6.4386	55.8	(1,4)
DELS J1535+1943	6.3932	22.6	(5,-)
ATLAS J2211-3206	6.3394	37.5	(6/7,4)
PSO J060+24	6.192	49.7	(8,-)
PSO J065-26	6.1871	77.9	(8,27)
PSO J359-06	6.1722	68.8	(9,40)
PSO J217-07	6.1663	33.3	(8,8)
PSO J217-16	6.1498	73.0	(8,4)
PSO J239-07	6.1102	56.3	(8,40)
SDSS J0842+1218	6.0754	83.2	(11/12,27)
ATLAS J158-14	6.0685	60.3	(6,40)
VDES J0408-5632	6.0345	86.6	(3,3)
ATLAS J029-36	6.021	57.1	(14,13)
SDSS J2310+1855	6.0031	113.4	(15,16)
PSO J007+04	6.0015	54.4	(12/17,27)
PSO J029-29	5.984	65.6	(8,8)
PSO J108+08	5.9485	104.8	(8,8)
PSO J183-12	5.917	61.8	(17,-)
PSO J025-11	5.844	50.6	(8,-)
PSO J242-12	5.837	22.9	(8,-)
PSO J065+01	5.833	25.1	(2,-)
PSO J308-27	5.7985	53.2	(8,2)

Table 1. XQR-30 quasars with X-Shooter spectra included in this work. References correspond to (Discovery, Redshift determination). The full list of references is given in the caption of Table 3.

$z > 5.7$. Observations were carried out using the $0.9''$ and $0.6''$ slits in the visible and near-infrared arms of X-Shooter, respectively. We use 25 quasars from the XQR-30 sample which do not show strong broad absorption lines (BALs) precluding the modelling of the intrinsic continuum. We however retain the BAL quasars ATLAS J2211-3206, PSO J239-07 and PSO J239-07, whose BAL features are well-resolved and confined to highly-ionised absorption (Bischetti et al., in prep). All XQR-30 spectra have signal-to-noise ratios (SNRs) larger than 20 per 10 km s^{-1} pixel measured over $1165\text{\AA} < \lambda < 1170\text{\AA}$ (Table 1). We use the reconstructed continua described in Section 3.2 to calculate the SNR over the range most

Quasar ID	z_{qso}	SNR pix^{-1}	Refs.
PSO J036+03	6.5405	61.4	(18,27)
PSO J011+09	6.4695	14.5	(1,40)
PSO J159-02	6.386	22.9	(8,-)
SDSS J0100+2802	6.3269	560.5	(20,27)
ATLAS J025-33	6.318	127.3	(14,13)
SDSS J1030+0524	6.309	69.6	(21,22)
VDES J0330-4025	6.239	17.0	(3,10)
PSO J308-21	6.2355	24.4	(8,27)
VIK J2318-3029	6.1456	16.5	(7,27)
ULAS J1319+0950	6.1347	81.7	(23,27)
CFHQS J1509-1749	6.1225	43.0	(24,4)
CFHQS J2100-1715	6.0807	12.4	(25,27)
ULAS J1207+0630	6.0366	29.2	(12,4)
SDSS J1306+0356	6.033	65.3	(21,27)
PSO J340-18	5.999	29.9	(17,13)
ULAS J0148+0600	5.998	152.0	(12,13)
SDSS J0818+1722	5.997	132.1	(19,13)
VIK J0046-2837	5.9926	15.0	(28,29)
PSO J056-16	5.9676	32.0	(8,40)
SDSS J1335+3533	5.9012	10.3	(19,26)
PSO J004+17	5.8166	15.9	(8,40)
SDSS J0836+0054	5.804	73.8	(21,-)
SDSS J0927+2001	5.7722	53.8	(19,26)
PSO J215-16	5.7321	30.2	(31,31)
J1335-0328	5.693	35.0	(32,13)
J0108+0711	5.577	20.0	(32,13)
J2207-0416	5.529	16.9	(9,13)

Table 2. Quasars with literature and archival X-Shooter spectra included in this work. References correspond to (Discovery, Redshift determination). The full list of references is given in the caption of Table 3.

relevant to our study. The X-Shooter instrument has a resolution of $\sim 34\text{ km s}^{-1}$ in the visible ($5500\text{\AA} < \lambda < 10200\text{\AA}$) and $\sim 37\text{ km s}^{-1}$ in the infrared ($10200\text{\AA} < \lambda < 24800\text{\AA}$), although better-than-average seeing during observations means the effective resolution is slightly higher. Observations are first flat-fielded and sky-subtracted following the method of Kelson (2003), then the spectra extracted optimally (Horne 1986) separately for the visible and infrared arms of the instrument. Our reductions routines are described in more detail in Becker et al. (2009); further details, including comparisons

with the publicly-available *esorex* (Freudling et al. 2013) and *Pypelt* (Prochaska et al. 2020) pipelines for X-Shooter, will be presented in D’Odorico et al. (in prep). The optical and infrared arms are then stitched together over the $10110\text{\AA} < \lambda_{\text{obs}} < 10130\text{\AA}$ spectral window, by rescaling the infrared spectrum to match the observed mean flux in the optical arm after two rounds of sigma-clipping and discarding of all pixels with $\text{SNR} < 2$. The spectrum is then interpolated over the overlap window. This somewhat aggressive procedure is adopted to minimize the risk of creating an artificial ‘step’ in the spectrum between the arms, to which the continuum-fitting method may be non-linearly sensitive (c.f. §3.2).

2.2 Other X-Shooter spectra

We supplement the XQR-30 quasars with 27 archival X-Shooter spectra of equal $\text{SNR} > 10$ per 10 km s^{-1} pixel from the literature (Table 2), including three quasars at $5.5 < z < 5.7$ to better sample the Ly- α transmission at $z \leq 5.3$. The spectra were reduced in an identical manner to the XQR-30 quasars, except 6 of them which had already been reduced with *Pypelt*. *Pypelt* is an open-source Python package designed to automate the reduction of spectroscopic data for (currently) 28 different spectrographs (Prochaska et al. 2019). Similarly to our custom reduction pipeline, *Pypelt* performs joint extraction of objects and a model of sky emission in each observed frame. We conducted a comparative analysis on a sub-sample of quasars reduced via both methods, which showed only a negligible ($< 0.5\%$) effect on the large-scale Ly- α transmission.

2.3 ESI spectra

Finally, we also complement our sample with 15 archival spectra of $z \gtrsim 5.7$ quasars taken by the ESI instrument (Sheinis et al. 2002) on the Keck Telescope (Table 3). The spectral resolution of ESI is lower than that of X-Shooter, at $\sim 60 \text{ km s}^{-1}$, and ESI’s wavelength coverage only includes the optical up to $\lambda < 10500\text{\AA}$. While we strive to reduce systematics arising from instrument and data reduction by minimising the number of different instruments, we include ESI spectra with $\text{SNR} > 10$ per 15 km s^{-1} pixel since they constitute the largest collection of deep, publicly available observations of $z > 5.7$ quasar spectroscopy with a single spectrograph besides X-Shooter. The ESI spectra were reduced using the same methods and algorithms as our X-Shooter pipeline, applying optimal spectral extraction after flat-fielding and sky subtraction. All but three of the ESI spectra we employ were also included in the ‘GOLD’ sample of Bosman et al. (2018), where their reduction is further described. The three new spectra were reduced in an identical manner, but were not included in Bosman et al. (2018) due to the availability of deeper MMTRCS (Schmidt et al. 1989) or HIRES spectroscopy (Vogt et al. 1994). Here we prefer the slightly shallower ESI spectra in order to preserve instrumental consistency and reduce possible instrumentation systematics. In a preliminary study (B21), we analysed the impact of ESI’s lesser resolution and wavelength coverage on systematics arising from quasar continuum reconstruction in the context of Ly- α transmission. We found that while continuum uncertainties were increased by $\sim 50\%$ compared to using spectra with X-Shooter’s wavelength coverage, no systematic biases arose. Six of our X-Shooter spectra were also observed to $\text{SNR} > 10$ depth by ESI, enabling an empirical test of potential biases linked to instrumentation which we present in §3.3.

Quasar ID	z_{qso}	SNR pix^{-1}	Refs.
SDSS J1148+5251	6.4189	118.8	(33,34)
CFHQS J0050+3445	6.251	28.6	(25,35)
SDSS J1623+3112	6.254	16.4	(36,35)
SDSS J1250+3130	6.138	41.2	(19,35)
SDSS J2315-0023	6.124	14.6	(37,13)
SDSS J1602+4228	6.083	24.1	(36,35)
SDSS J1630+4012	6.066	10.3	(33,35)
SDSS J0353+0104	6.057	15.4	(37,35)
SDSS J2054-0005	6.0389	22.6	(37,27)
SDSS J1137+3549	6.009	23.2	(19,35)
SDSS J1411+1217	5.904	42.1	(36,30)
SDSS J0005-0006	5.847	18.4	(36,13)
SDSS J0840+5624	5.8441	34.9	(19,26)
SDSS J0002+2550	5.818	119.0	(36,35)
SDSS J1044-0125	5.7846	64.9	(38,27)

Table 3. Quasars with archival ESI spectra included in this work. References relate to (Discovery, Redshift determination). (–) This paper; (1) Mazzucchelli et al. (2017); (2) D’Odorico et al. in prep; (3) Reed et al. (2017); (4) Decarli et al. (2018); (5) Wang et al. (2019); (6) Chehade et al. (2018); (7) Farina et al. (2019); (8) Bañados et al. (2016); (9) Wang et al. (2016); (10) Eilers et al. (2020); (11) De Rosa et al. (2011); (12) Jiang et al. (2015); (13) Becker et al. (2019); (14) Carnall et al. (2015); (15) Jiang et al. (2016); (16) Wang et al. (2013); (17) Bañados et al. (2014); (18) Venemans et al. (2015); (19) Fan et al. (2006); (20) Wu et al. (2015); (21) Fan et al. (2001); (22) Jiang et al. (2007); (23) Mortlock et al. (2009); (24) Willott et al. (2007); (25) Willott et al. (2010); (26) Wang et al. (2010); (27) Venemans et al. (2020); (28) Venemans et al. (2018); (29) Schindler et al. (2020); (30) Kurk et al. (2007); (31) Morganson et al. (2012); (32) Yang et al. (2017); (33) Fan et al. (2003); (34) Willott et al. (2015); (35) Shen et al. (2019); (36) Fan et al. (2004); (37) Jiang et al. (2008); (38) Fan et al. (2000); (39) Wang et al. (2021); (40) Eilers et al. (2021). For quasars without discovery papers, we reference the first paper which showcased or used a spectrum featuring broad emission lines.

3 METHODS

The effective Ly- α optical depth τ_{eff} is defined using the mean transmitted flux fraction in the Ly- α forest,

$$\tau_{\text{eff}} = -\log \left\langle \frac{F(\lambda)}{F_{\text{cont}}(\lambda)} \right\rangle, \quad (1)$$

where F is the observed flux, F_{cont} is the reconstructed intrinsic quasar continuum and $\langle \rangle$ is the mean over a fixed interval, traditionally taken to be 50 cMpc/h (see §3.1). The usable range of observed wavelengths is limited by the quasar’s effect on its environment on one hand and overlap with Ly- β absorption on the other. To exclude the effect of the background quasars (the so-called ‘proximity zone’, Cen & Haiman 2000; Carilli et al. 2010; Eilers et al. 2017) we restrict ourselves to $\lambda < 1185\text{\AA}$, beyond which no effect on Ly- α transmission is seen even in the deepest spectral stacks ($< 0.5\%$ Ly- α flux increase: Bosman et al. 2018). No quasars are known to have proximity zones extending beyond $1185\text{\AA}$: the longest $z > 5$ proximity zone, in quasar SDSS J0100+2802, only extends to $\gtrsim 1189\text{\AA}$. In fact, we note that our proximity zone cut may be overly conservative, since no effect is seen in deep stacks even at $\lambda < 1195\text{\AA}$ at $z > 6.1$ and the more conservative cut reduces the probed volume at $z > 6.0$ by $\sim 30\%$ for our sample.

To exclude contamination by the overlapping Ly- β forest at low wavelengths, the redshift of the background quasar must be known precisely to determine its location with respect to the foreground IGM. When possible, we adopt the systemic redshifts of the quasar host galaxies, determined through the identification of

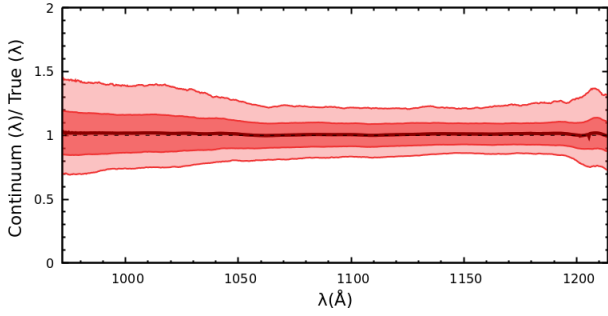


Figure 2. Residuals in the PCA reconstruction of the $\lambda < 1220\text{\AA}$ blue-side continua of 4597 eBOSS quasars at $2.7 < z < 3.5$, which were not used for training the PCA. No significant wavelength-dependent biases are seen. The average uncertainty over the $1026 < \lambda < 1185\text{\AA}$ range, used in this paper, is $-7.9/+7.8\%$.

sub-mm emission lines (these redshifts can roughly be identified in Tables 1, 2 and 3 by having five significant digits). Redshifts may also be obtained from our rest-UV spectra directly using the quasar broad emission lines, but these features are often blue-shifted from the quasar host galaxies and from each other (Meyer et al. 2019; Schindler et al. 2020; Onoue et al. 2020) with a large scatter $\sim 750 \text{ km s}^{-1}$. An alternative method, which we use here, is to adopt the redshift of the first Ly- α absorber in front of the quasar (Worseck et al. 2014). This method for locating the onset of the IGM has been shown to have relatively little offsets and scatter with respect to sub-mm emission lines, $\Delta v = 180 \pm 180 \text{ km s}^{-1}$ (Becker et al. 2021). We employ it here for cases where fits to the Mg II broad emission line are complicated by absorption, as indicated in Tables 1, 2 and 3.

To err on the side of caution, we round up the Ly- β wavelength of $1025.7\text{\AA}$ and only use wavelengths $\lambda > 1026\text{\AA}$. While the presence of the O VI broad emission line renders the continuum prediction slightly more uncertain over the $1026\text{\AA} < \lambda \lesssim 1050\text{\AA}$ wavelength range, this is carefully quantified and propagated to all our measurements and model comparisons (see Figure 2 and §3.2). We note that even if we use on occasion wavelengths contaminated by Ly- β absorption due to chance redshift errors, the corresponding Ly- β -absorbing gas would be located inside the quasar’s proximity zone, and the Ly- β absorption should therefore be relatively small (although difficult to quantify in a model-independent manner).

The data reduction procedure in principle automatically rejects outlier pixels (e.g. cosmic rays) when a large number of exposures are stacked. Nevertheless, we exclude a few ($\lesssim 0.05\%$ of total) anomalous pixels which are flagged if their SNR at the unabsorbed continuum level is < 2 per pixel (since an average $\text{SNR} \geq 10$ is enforced for all our observations) or if pixels have negative flux at $> 3\sigma$ significance. Such sigma-clipping can by definition only induce a bias $\ll 0.1\%$, while it cleans up features which are clearly reduction glitches.

3.1 Redshift or length intervals?

The traditional way of quantifying Ly- α optical depth fluctuations, motivated by efficiency when dealing with small sample sizes and by ease of comparison to theoretical models, has been to divide Ly- α transmission spectra in intervals of constant length (Becker et al. 2015; Bosman et al. 2018; Eilers et al. 2019; Yang et al.

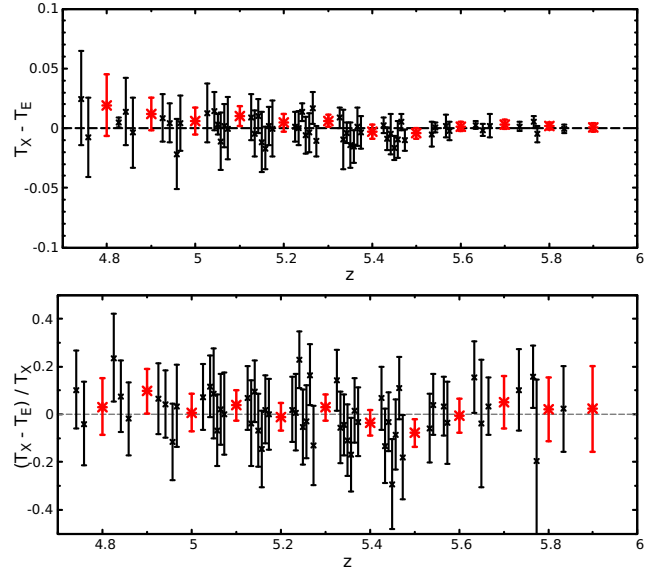


Figure 3. Differences in Ly- α transmission measured with ESI (T_E) and X-Shooter (T_X) spectra of the same six quasars. *Top:* Absolute difference in transmitted flux. The error bars account for observational uncertainties as well as continuum reconstruction uncertainties and biases. Individual measurements are shown in black with the averages in red. *Bottom:* Same as top panel, but showing the fractional differences. The diagnostics show no evidence for instrument biases beyond the ones already accounted for in the measurement uncertainties. In both plots, some random scatter along the x-axis (redshift) has been added to improve legibility.

2020). In this approach, the average transmission beyond a quasar’s proximity zone is calculated over consecutive bins of fixed length (usually $\Delta L = 50 \text{ cMpc/h}$), and such measurements are assigned to a redshift interval depending on the mid-point of each length bin. We reproduce this approach for the purposes of comparison with the literature, but in our fiducial results we modify it for the purposes of comparison with theoretical models for two main reasons. First, the fixed length definition makes it possible for the same quasar sightline to contribute to the optical depth distribution in a single redshift bin more than once. This is a source of unwanted covariance, since IGM optical depth is known to be correlated on scales up to 100 cMpc/h (Becker et al. 2015). Second, the definition implies that up to half of pixels contributing to an optical depth measurement at a given redshift may be located outside of the redshift bin’s bounds. The result is artificial scatter in measured optical depth, especially since Ly- α optical depth evolves very quickly at $z > 5$ (B21; see also Worseck et al. 2016). To circumvent these issues, we instead measure the optical depth in bins of constant redshift intervals directly. We divide the spectra in bins of $\Delta z = 0.1$ centered at $z = 5.0, 5.1, \dots, 6.0$ and retain measurements if $> 50\%$ of the corresponding wavelength range is usable. In practice, $\sim 30\%$ of sightlines are truncated by more than 10% ; we propagate the resulting uncertainties throughout the analysis.

For the purposes of future comparisons of the data with models, sometimes binning in equal length intervals, with fixed endpoints in redshift, might be preferable. We show the resulting distributions for $\Delta L = 50 \text{ cMpc/h}$ in Appendix A. Full measurements for $\Delta L = 30, 50, 100 \text{ cMpc/h}$ and $\Delta z = 0.05, 0.1$ are also available as online material.

3.2 Continuum reconstruction

We employ Principal Component Analysis (PCA) to reconstruct $F_{\text{cont}}(\lambda)$ based on the observed quasar continuum at $\lambda > 1280\text{\AA}$. Quasar continuum PCA models use a training set of low- z quasar spectra to find optimal linear decompositions of the ‘known’ red side ($\lambda > 1280\text{\AA}$) and the ‘unknown’ blue side of the spectrum ($\lambda < 1220\text{\AA}$), then determines an optimal mapping between the linear coefficients of the two sides’ decompositions (Francis et al. 1992; Yip et al. 2004; Suzuki et al. 2005; McDonald et al. 2005; Pâris et al. 2011; Āurovčřková et al. 2020). In B21, we conducted a rigorous comparison of the precision and accuracy of six reconstruction techniques used in the literature by using a large sample of ‘blind’ tests with spectra where the true continuum was known. We found that two PCA methods outperformed both the more traditionally-employed power-law extrapolation (e.g. Bosman et al. 2018) and ‘stacking of neighbours’ methods, both in prediction accuracy and in lack of wavelength-dependent reconstruction residuals. Here, we use a further improved version of the most accurate PCA method identified in (B21), the log-PCA approach of Davies et al. (2018c) (see also Davies et al. 2018b).

Our PCA consists of 15 red-side components and 10 blue-side components. Training was performed on 4597 quasars at $2.7 < z < 3.5$ with $\text{SNR} > 7$ from the SDSS-III Baryon Oscillation Spectroscopic Survey (BOSS, Dawson et al. 2013) and the SDSS-IV Extended BOSS (eBOSS, Dawson et al. 2016). Intrinsic continua were obtained automatically using a modified version of the method of Dall’Aglio et al. (2008), originally based on the procedures outlined in Young et al. (1979) and Carswell et al. (1982). The automatically-fitted continua are re-normalised to ensure they match the observed mean Ly- α transmission at $z \sim 3$ measured from high-resolution spectra (Faucher-Giguère et al. 2008; Becker et al. 2013), as they would otherwise be biased by the lack of spectral resolution of the SDSS spectrograph (see discussion in Dall’Aglio et al. 2009).

Testing is performed by using an independent set of 4597 quasars from eBOSS. The asymmetric 1σ and 2σ bounds are measured by finding the central 68th and 95th percentile intervals of the prediction error in the testing sample at each wavelength. Figure 2 shows the wavelength-dependent 1σ and 2σ continuum reconstruction uncertainties, $\text{Continuum}(\lambda)/\text{True}(\lambda)$. No features are visible at any rest-frame wavelength in the residuals, indicating that blue-side emission lines can be reconstructed without bias. The standard deviation is $\text{PCA}/\text{True} - 1 = 0.8^{+7.8}_{-7.9}\%$, i.e. the method predicts the underlying continuum within 8%: a large improvement compared to power-law extrapolation methods ($> 13\%$) and a slight improvement over the best PCA in B21 (9%). For the ESI spectra covering a shorter red-side wavelength range, we use the ‘optical-only’ PCA developed in B21 with $\text{PCA}/\text{True} - 1 = 1.0^{+11.2}_{-11.3}\%$. The lower accuracy is unsurprising since fewer features are available to the PCA modelling. However, no significant wavelength-dependent biases are present.

In the rest of the paper, we always correct for the residual wavelength-dependent mean bias ($< 1\%$) to our reconstructions of $F_{\text{cont}}(\lambda)$ and forward-model the full wavelength-dependent uncertainties into all measurements and model comparisons. We refer the reader to B21 for further details of the PCA training and testing procedures. Figures showing all PCA fits and blue-side predictions are shown in Zhu et al. (submitted) and the PCA fits for XQR-30 spectra will be made public with the first XQR-30 data release (D’Odorico et al. in prep).

z	$\langle F_{\text{Ly-}\alpha} \rangle$	-1σ	$+1\sigma$	N_{los}
4.8	0.194	-0.015	+0.018	15
4.9	0.171	-0.014	+0.014	17
5.0	0.1581	-0.0089	+0.0082	37
5.1	0.1428	-0.0054	+0.0068	48
5.2	0.1222	-0.0054	+0.0046	55
5.3	0.1031	-0.0050	+0.0056	58
5.4	0.0801	-0.0048	+0.0061	64
5.5	0.0591	-0.0035	+0.0039	64
5.6	0.0447	-0.0036	+0.0033	59
5.7	0.0256	-0.0029	+0.0031	51
5.8	0.0172	-0.0028	+0.0022	45
5.9	0.0114	-0.0030	+0.0029	28
6.0	0.0089	-0.0029	+0.0033	19
6.1	0.0088	-0.0074	+0.0082	10
6.2	0.0047	-0.0044	+0.0045	8

Table 4. Mean Ly- α flux transmission at $4.75 < z < 6.25$, measured in $\Delta z = 0.1$ intervals centred on the redshift given in the first column. Uncertainties correspond to the 16th and 84th percentiles from bootstrap resampling. The measurement uncertainties on their own are a factor 5 – 10 smaller than the bootstrap uncertainties quoted here. N_{los} sightlines contribute to each measurement.

3.3 Instrumental effects

To empirically check whether our data reduction and continuum reconstruction methods have accounted for all differences between ESI and X-Shooter spectra, we compare optical depth measurements for six quasars which have deep spectra with both X-Shooter and ESI. Figure 3 shows the difference between the Ly- α transmission observed with X-Shooter, $T_X = F_{\text{X-Shooter}}/F_{\text{cont, X-Shooter}}$ and with ESI, $T_E = F_{\text{ESI}}/F_{\text{cont, ESI}}$. The continua were reconstructed using the two PCAs discussed in §3.2. The top and bottom panels show the absolute and fractional difference between T_X and T_E , respectively. No statistically significant bias is detected at any redshift. Across all observations, the average fractional bias between the instruments is 1.3% with an observed scatter of 2.3%. Since the effect is very sub-dominant compared to continuum uncertainties ($\sim 11\%$ for ESI spectra) and we did not detect a statistically significant bias, we disregard instrumental differences between ESI and X-Shooter spectra beyond what is already included in the reduction pipelines.

3.4 DLA exclusion

Damped Ly- α absorbers (DLAs), named after their prominent Ly- α damping wings, are intervening systems along quasar sightlines with hydrogen column densities $N_{\text{HI}} \geq 10^{20.3} \text{ cm}^{-2}$ (Wolfe et al. 2005; Rafelski et al. 2012). DLAs near quasars at $z \gtrsim 6$ can completely absorb Ly- α transmission over intervals $\Delta v = 2000 \text{ km s}^{-1}$, with significant suppression of the transmission over $\Delta v \gtrsim 5000 \text{ km s}^{-1}$ (D’Odorico et al. 2018; Bañados et al. 2019; Davies 2020). Since reionisation models typically do not include the effect of DLAs, we strive to remove them from our nominal measurements.

The detection of $z \gtrsim 5$ DLAs relies on the identification of associated low-ionisation metal absorption lines, since their Ly- α absorption may not contrast against the highly-opaque IGM. DLA metallicities at $z \gtrsim 5$ are very diverse, and some can be highly sub-solar (Bañados et al. 2019), such that even relatively weak metal absorption might indicate a DLA. The identification of intervening metal absorbers in the XQR-30 sample will be described in detail in Davies et al. (in prep). For the other quasars, we used where relevant the published lists of intervening metal systems of Cooper et al. (2019), D’Odorico et al. (2018),

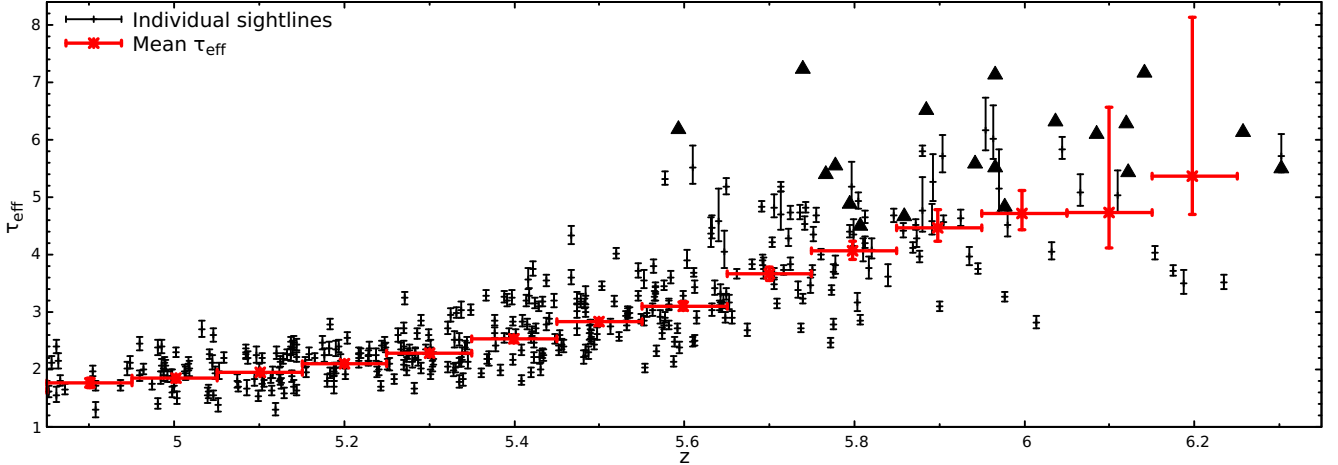


Figure 4. Mean Ly- α flux measured along 67 quasar sightlines at $4.9 < z < 6.2$, measured in 50 cMpc/h bins. Non-detections are shown with upwards pointing triangles. The mean fluxes measured in intervals of $\Delta z = 0.1$ are shown with red points. Uncertainties correspond to the 16th and 84th percentile contours of a bootstrap resampling in each redshift interval. Non-detections are shown at the 2σ limit. The observed scatter between sightlines increases drastically above $z \gtrsim 5.4$.

Meyer et al. (2019) and Becker et al. (2019). We supplemented the literature where necessary by conducting our own metal search, following closely the standard procedure described in Bosman et al. (2017). Pairs of absorption lines corresponding to the same ion or frequently co-occurring ions (C IV, Mg II, Fe II, O I+C II) are searched for automatically before being confirmed manually. Due to the high SNR of the X-Shooter spectra, we expect to be $> 90\%$ complete to absorption corresponding to $\log N_{\text{Mg II}}/\text{cm}^{-2} \gtrsim 13$. The metal identification in the ESI spectra similarly relies on literature studies which employed infrared spectra of the objects.

We adopt the following criteria: we mask the central $\Delta v = 3000 \text{ km s}^{-1}$ for systems with metal column densities $\log N_{\text{C II}}/\text{cm}^{-2} > 13$, $\log N_{\text{O I}}/\text{cm}^{-2} > 13$, or $\log N_{\text{Si II}}/\text{cm}^{-2} > 12.5$, measured through the $\lambda = 1334.53\text{\AA}$, $1302.16\text{\AA}$, and $1526\text{\AA}$ transitions, respectively. When none of these ions are accessible, we also exclude the central $\Delta v = 3000 \text{ km s}^{-1}$ for systems with $\log N_{\text{Mg II}}/\text{cm}^{-2} > 13$ based on the high rates of co-occurrence of the Mg II 2796.35, 2803.53 $\text{\AA}$ doublet (Cooper et al. 2019). We exclude a larger window of $\Delta v = 5000 \text{ km s}^{-1}$ around intervening systems with $\log N_{\text{O I}}, \text{C II}, \text{Si II}, \text{Mg II} > 14 \text{ cm}^{-2}$ due to the likely presence of extended damping wings.

We do not exclude systems based on the presence of highly-ionised ions alone (e.g. C IV, Si IV) since the corresponding gas is likely highly ionised (Cooper et al. 2019). Finally, we exclude $\Delta v = 5000 \text{ km s}^{-1}$ around the suspected location of strong O VI associated absorption (from systems detected from strong associated C IV absorption), which overlaps with the Ly- α forest in quasars J1411+1217 and J1623+3112.

4 RESULTS

Figure 4 shows the mean Ly- α transmission measured in intervals of 50 cMpc/h. The average transmission evolves smoothly over $5 < z < 6$, but an increase in scatter between measurements at equal redshift becomes clear at $z \gtrsim 5.4$. By $z = 5.6$, the sampling of the distribution is visibly limited. The number of fully opaque Gunn-Peterson troughs with non-detections (2σ) at $\tau > 6$ increases sharply, with the first occurrence found at $z \sim 5.6$.

4.1 Mean transmission across $4.8 < z < 6.2$

We calculate the mean transmission in bins of $\Delta z = 0.1$ and give the results in Table 4. We do not weight the measurement: all pixels corresponding to Ly- α transmission inside a given redshift interval contribute equally (after the masking of bad regions as described above). The uncertainties are calculated via bootstrap re-sampling in each redshift bin. We quote the 16% and 84% percentiles of the bootstrap results. The observational uncertainties, taking into account only uncertainties in individual measurements, are a factor 5 – 10 smaller than the bootstrap uncertainties at all redshifts. The uncertainties are therefore dominated by the intrinsic width of the Ly- α transmission distribution. The mean Ly- α transmission over the range $4.8 < z < 5.7$ is empirically well-described by a linear decline of the form:

$$F_{\text{Ly-}\alpha}(1+z) = a \times (1+z) + b. \quad (2)$$

We fit this functional form to our observations using least-squares regression, and obtain best-fitting parameters $a = -0.191$, $b = 1.307$. Both parameters are constrained to better than 0.1%. We show the resulting curve in Figure 5. An empirical parametric description of effective Ly- α optical depth evolution with redshift, used for instance by Becker et al. (2013), is a power-law function with a constant offset of the form:

$$\tau_{\text{eff}}(1+z) = \tau_0 \left(\frac{1+z}{1+z_0} \right)^\beta + C. \quad (3)$$

Setting $z_0 = 4.8$, we run a least-squares regression and find best-fit parameters $\tau_0 = 0.30 \pm 0.08$, $\beta = 13.7 \pm 1.5$ and $C = 1.35 \pm 0.12$. We fit this form to the mean optical depth over $4.8 < z < 5.9$ and show the resulting best-fit model in Figure 6. We sample the covariance matrix of the three parameters and calculate the upper and lower envelopes encompassing 68% of the variance about the best fit, which are shown by the orange shaded region. The evolution of τ_{eff} with redshift is much steeper at $z > 4.8$ than over $2 < z < 5$, where Becker et al. (2013) found a best-fit $\beta = 2.90$.

Our measurements are in fair agreement with past literature, as shown in Figure 5. The quasars used in this work have considerable overlap ($\sim 30 - 50\%$) with the ones employed by Becker et al. (2015); Eilers et al. (2018); Bosman et al. (2018) and Yang

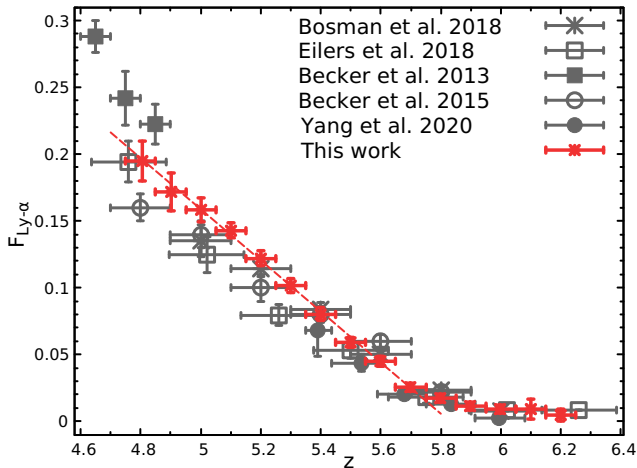


Figure 5. Average Ly- α transmission evolution with redshift. Uncertainties are obtained via bootstrap resampling in this work as well as in the literature comparison samples of [Becker et al. \(2013, 2015\)](#); [Bosman et al. \(2018\)](#); [Eilers et al. \(2018\)](#), and should therefore encompass cosmic variance as long as the underlying optical depth distributions are well-sampled. Differences at $z \gtrsim 5.5$ are due to under-sampling of cosmic variance, as well as systematic biases in older work. At $z > 5.4$, cosmic variance is 5–10 times larger than measurement uncertainties. The red dashed line shows the optimal linear fit to the data over $4.8 < z < 5.7$ (Equation 2, see text).

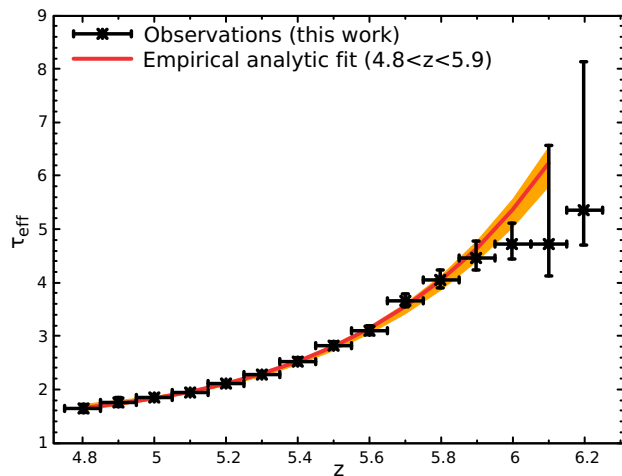


Figure 6. Evolution of τ_{eff} with redshift measured in our sample across $4.8 < z < 6.2$ in steps of $\Delta z = 0.1$ (black). The red line shows the best-fit power-law model and its 68% uncertainty envelope (Equation 3, see text). Observational uncertainties are obtained via bootstrap resampling.

[et al. \(2020\)](#), such that differences are unlikely to be due to cosmic variance alone. Systematic differences in continuum reconstruction methods are a known cause of bias: as shown in B21, the tension between the measurements of [Bosman et al. \(2018\)](#) and [Eilers et al. \(2018\)](#) can be explained almost entirely by the different continuum reconstruction methods employed (power-law extrapolation and a PCA based on [Pâris et al. 2011](#), respectively). Both methods were found to introduce non-trivial wavelength-dependent biases which depend sensitively on the redshifts of the background quasars; such corrections unfortunately cannot be applied post-hoc. [Becker et al. \(2015\)](#), [Bosman et al. \(2018\)](#) and [Yang et al. \(2020\)](#) all employed

power-law reconstructions, and therefore carry similar biases; this may explain why our results are offset from all three studies in the same direction at $z < 5.4$ (where power-law-induced uncertainties and biases are the largest). We also note that [Eilers et al. \(2018\)](#), [Bosman et al. \(2018\)](#) and [Becker et al. \(2015\)](#) had substantial overlap in quasar sightlines, and should therefore be affected by cosmic variance in a coherent way compared to our sample. [Yang et al. \(2020\)](#) calculated mean optical depths by using a weighted spectral stack, without providing measurements of scatter between sightlines. In order to provide a better comparison with this study, we re-calculate the optical depth values from [Yang et al. \(2020\)](#)’s sample by using their published list of measured optical depths in each quasar sightline, and we estimate the cosmic variance uncertainties via bootstrap resampling.

We find a very smooth, linear evolution of the mean Ly- α transmitted flux across $4.8 < z < 5.7$, with no sudden steepening, in contrast with several past studies. Matching the results of [Becker et al. \(2013\)](#) at $z < 4.8$ still seems to require a faster steepening at $z \sim 4.7$ (Fig. 5). However, both their measurements and ours are at the (opposite) edges of their redshifts of validity at $z \sim 4.8$. In our study, measurements at $z < 5$ rely on $N < 20$ objects, and are the most sensitive to errors in background quasar redshift via contamination by Ly- β absorption. Conversely, the measurements of [Becker et al. \(2013\)](#) at $z > 4.5$ use the Ly- α forest at the shortest separations from the background quasars, where the continuum is under-predicted by power-law extrapolations due to the large width of the broad Ly- α emission line (B21); the measurements of [Becker et al. \(2013\)](#) are also based on spectra with much lower SNR than our sample. Properly sampling the overlapping region would therefore require a sample of deep quasar spectra of intermediate redshifts, i.e. $5 < z_{\text{qso}} < 5.5$.

4.2 Optical depth distributions at $5.0 < z < 6.1$

We show the distributions of Ly- α optical depth at $5.0 < z < 6.1$ for comparison with previous studies in Figure 7. We first use the traditional method of measuring the optical depth in constant 50 cMpc/h intervals whose centres are then binned by redshift, since this definition was employed by all past studies. We will highlight the biases created by this definition later in Figure 8.

Non-detections of transmission over a given interval (defined at the 2σ level) give rise to lower limits on optical depth. Limits can either be represented as corresponding to flux equal to twice the measurement uncertainty (i.e. just below the detection threshold, e.g. [Becker et al. 2015](#)) or as corresponding to infinite optical depth. Following [Bosman et al. \(2018\)](#), we display the cumulative distribution functions (CDFs) showing both bounds. The lower CDF assumes that all non-detections are infinitely opaque, while the upper CDF assumes all non-detections correspond to flux just below the detection limit.

Owing to the much higher SNR of our sample, the number of non-detections over 50 cMpc/h is highly reduced at $5.5 < z < 5.9$ compared to [Bosman et al. \(2018\)](#), which used a sample of size comparable to ours ($N_{\text{qso}} = 64$ compared to our $N_{\text{qso}} = 67$) but with widely varying SNR. Our study only employs spectra which are able to probe optical depths up to (at least) $\tau = 4.5$ in $\Delta z = 0.1$ bins. At $5.5 < z < 5.7$, the only non-detection is in quasar PSO J025-11 (1/67 sightlines) while $\sim 10\%$ of sightlines were undetected in [Bosman et al. \(2018\)](#). The quasar J0148+0600 (the longest trough from [Becker et al. 2015](#)) was formerly the most opaque at this redshift, but a slight update to the quasar’s redshift shifts the exact start and end of the measurement bin in our study such that trans-

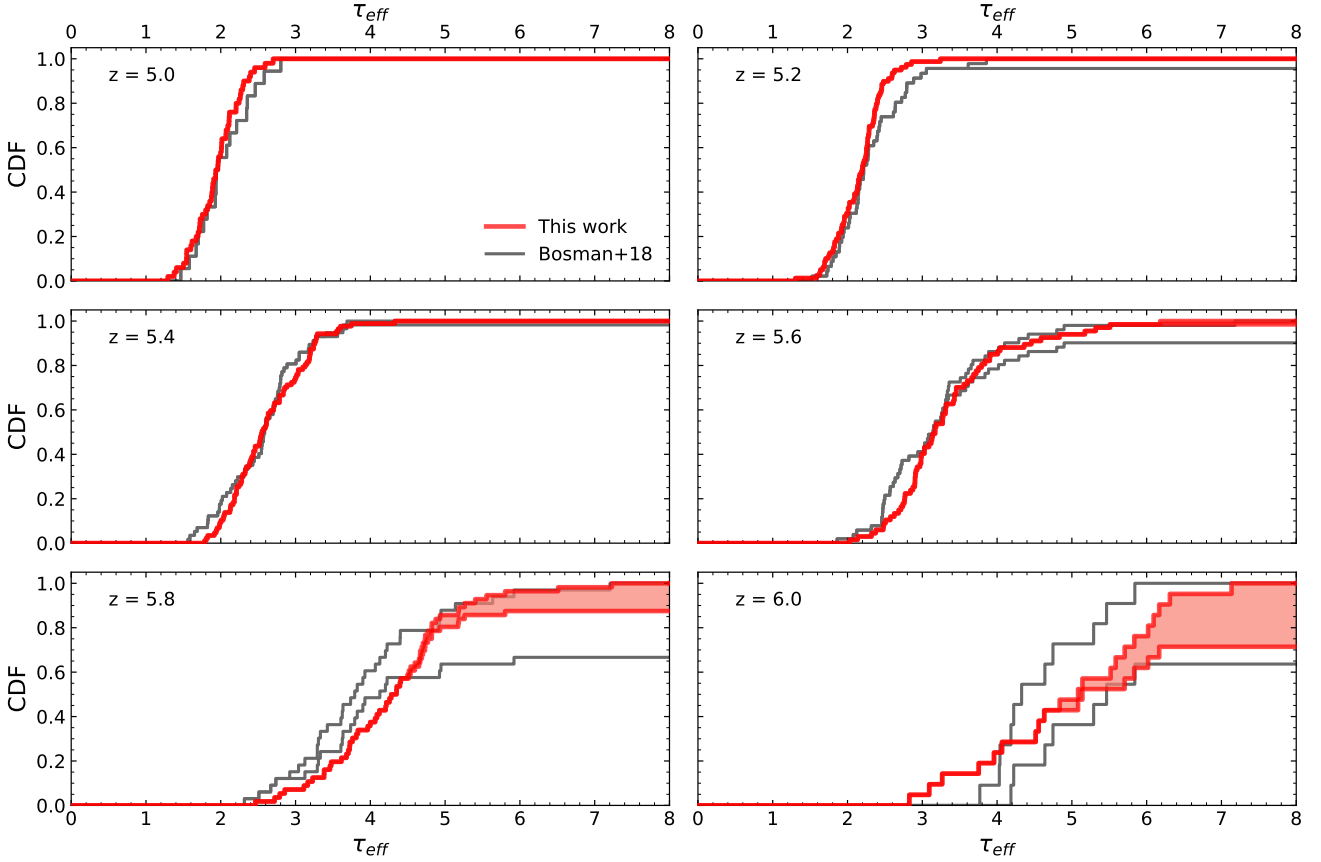


Figure 7. CDFs of Ly- α optical depth (red) computed in 50 cMpc/h intervals, compared to results from Bosman et al. (2018) (black). The lower and upper CDFs correspond to assumptions that non-detections are infinitely opaque, or just below the detection threshold, respectively. While the sample sizes are comparable ($N = 67$ and $N = 64$, respectively), the highly improved data quality and new correction of systematic biases linked to instrumentation and continuum reconstruction result in overall smoother distributions and fewer non-detections. The most transparent sightlines at $z = 6.0$ are shown in Figure 10

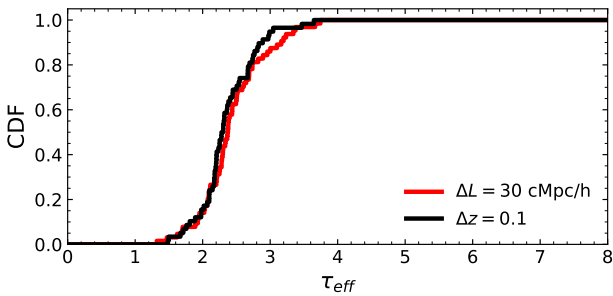


Figure 8. Comparison of the optical depth distribution measured over the same interval, $5.25 < z < 5.35$, using bins of constant length with boundaries that vary (red) or constant Δz boundaries (black). The length of 30 cMpc/h corresponds to the redshift interval $\Delta z = 0.1$; the only difference between the distributions is the definition of binning and not the lengths over which the optical depth is intrinsically computed. The excess of highly opaque sightlines in the red curve originates from length bins whose centres lie near the top end of the range ($z \sim 5.35$), artificially increasing the scatter by including contributions from pixels outside the nominal redshift range. To avoid this bias, we adopt binning in constant redshift for the purposes of inference.

mission is detected ($\tau = 5.33$) in a bin centred at $z = 5.577$. This issue highlights one of the problems with the classical definition of

optical depth binning: results depend non-trivially on the assumed redshifts of the background quasars (while our binning explicitly does not). At $5.7 < z < 5.9$, the number of non-detections is reduced from $\sim 35\%$ (in Bosman et al. 2018) to 12.5% (7/56 sightlines have $\tau > 4.5$). In contrast, our increased sensitivity does not reduce the number of sightlines with non-detections at $5.9 < z < 6.1$, where $\sim 30\%$ of sightlines (6/21) remain fully absorbed. A large fraction of $z \gtrsim 5.9$ sightlines are therefore more opaque than $\tau = 4.5$, a limit which is unlikely to be exceeded for large samples of quasars with current instrumentation. Significant advances in sensitivity, which may be required to detect residual transmission in the bulk of quasars at $z > 6$, could be brought by the next-generation Extremely Large Telescope (Gilmozzi & Spyromilio 2007) or the Thirty Meter Telescope (Sanders 2013).

To determine the lowest redshift at which the optical depth distribution is in agreement with fluctuations from density alone, we use redshift bins with $\Delta z = 0.1$. We choose this binning size in order to resolve the fast evolution in the mean optical depth (Figure 5). In Section 3.1 we highlighted some potential biases inherent to the classical definition of binning optical depth measurements of constant length. In Figure 8 we demonstrate these biases, which become more pronounced as the redshift intervals are shortened. The optical depth distribution at $z = 5.3$ is artificially broadened by the inclusion of transmission outside the nominal redshift range, as shown in the red curve. This effect is non-negligible when the

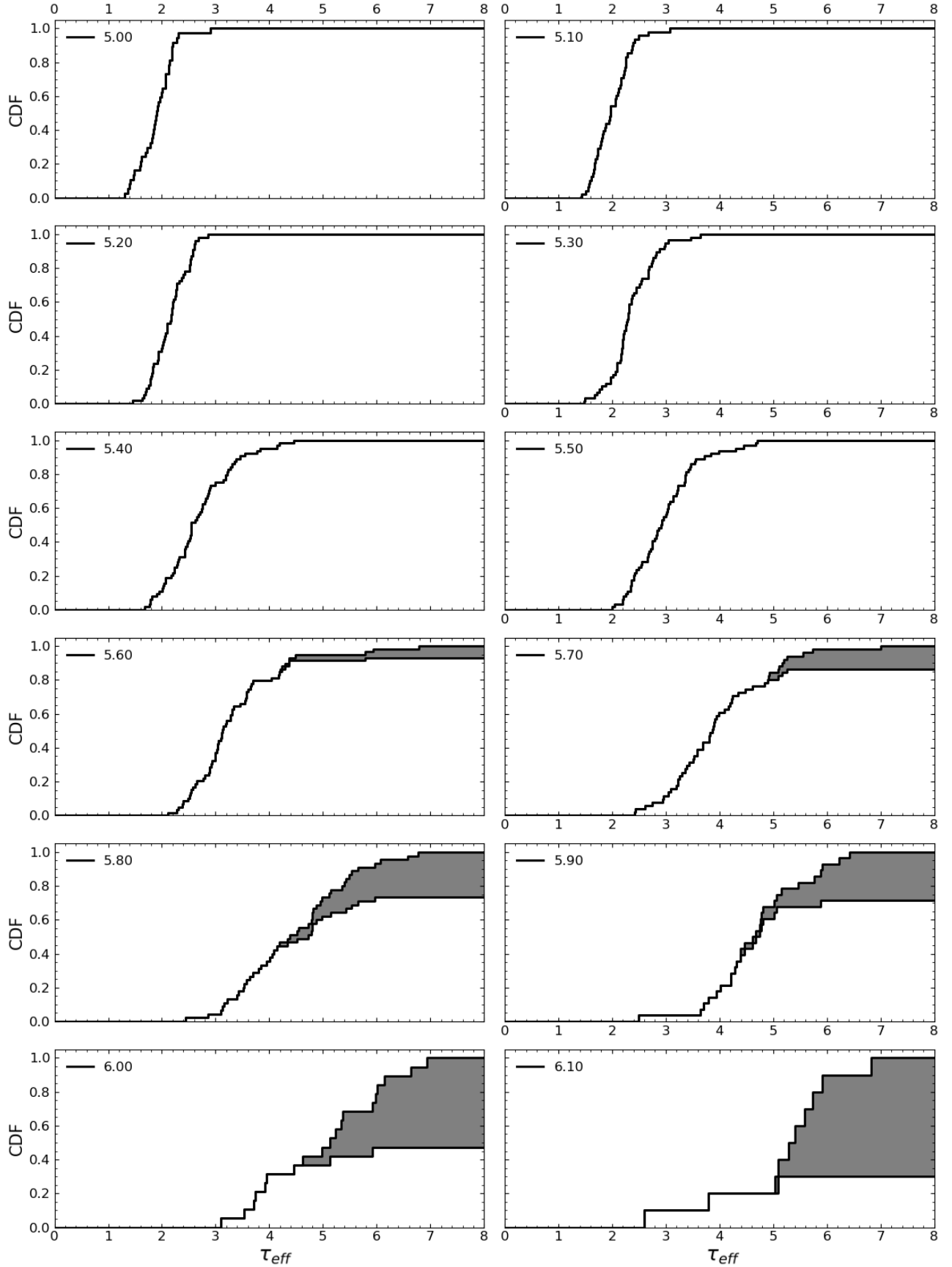


Figure 9. CDFs of Ly- α optical depth in bins of constant $\Delta z = 0.1$. The distributions begin to appear ‘elongated’ around $z \sim 5.4$. The fraction of non-detections (as seen by the difference between the curves at the right edges of the CDFs) increases sharply above $z = 5.7$, but some transparent sightlines remain even at $z = 6.1$. The most transparent sightlines at $z = 5.9$ and $z = 6.1$ are shown in Figure 10.

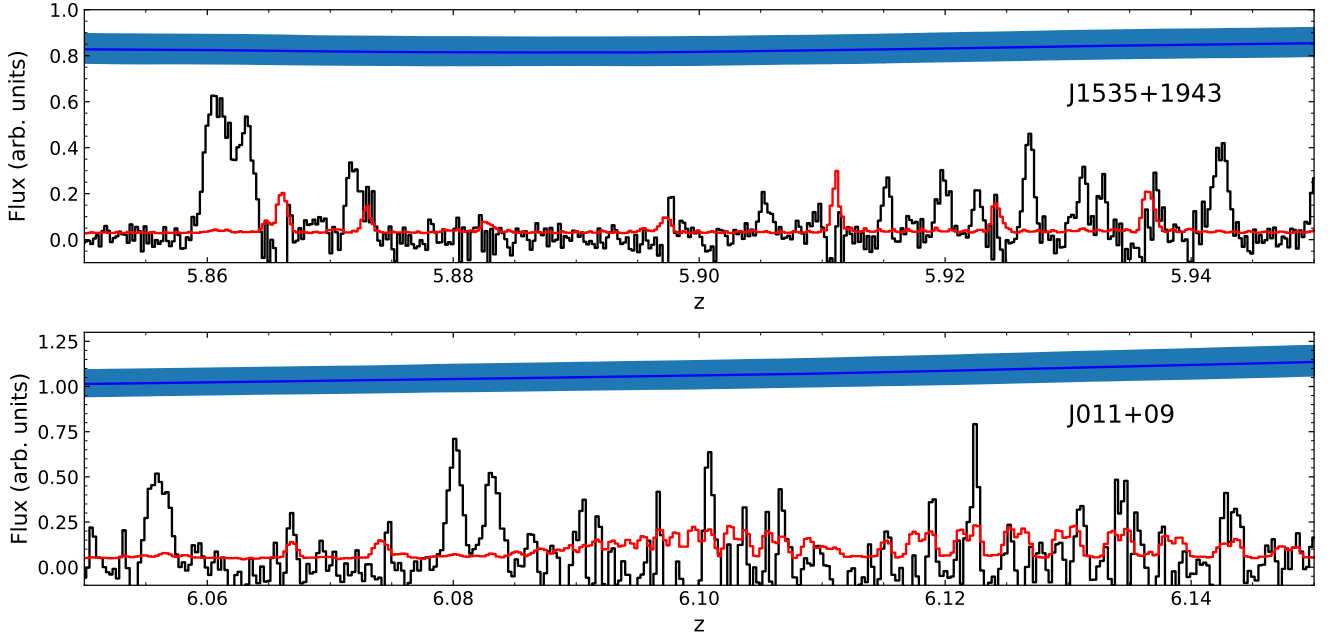


Figure 10. Black: Transmitted Ly- α flux in the most transmissive sightlines at $z = 5.9$ (J1535+1943, top) and at $z = 6.1$ (J1535+1943, middle; PSO J011+09, bottom). Red: observational uncertainties. Blue: PCA continuum reconstruction and its $\pm 1\sigma$ uncertainties. The $6.10 < z < 6.14$ range is affected by increased uncertainties due to sky emission corrections, but excluding this region slightly raises the mean transmitted flux over the $6.05 < z < 6.15$ interval.

binning length becomes comparable to the redshift interval, when the evolution in the mean is rapid (as shown in Figure 5), or when using sightlines near the end of their usable wavelength ranges (i.e. the lowest redshift bins). We adopt binning in constant redshift intervals for the purposes of inference in order to avoid this bias, and show the resulting CDFs in $\Delta z = 0.1$ in Figure 9. The new definition also avoids any covariance of sightlines in distributions at fixed redshift. The distributions will still be covariant between redshifts, since opaque sightlines show coherence over scale $\Delta z > 0.1$.

4.3 $z \geq 5.9$ transmissive sightlines

In Figure 10 we show the most transmissive sightlines at $z = 5.9$ and $z = 6.1$ which stand out from the distributions in Figure 9. The XQR-30 quasar J1535+1943 is the most transmissive at $z = 5.9$ with $\tau_{\text{eff}} = 2.50$, showing Ly- α transmission over the entire $5.85 < z < 5.95$ interval (top panel). The same quasar is the second most transmissive at $z = 6.1$, with 2 strong transmission spikes at $z \sim 6.07$ resulting in $\tau_{\text{eff}} = 3.79$; this suggests elevated transmission over scales $\gtrsim 100$ cMpc/h. At $z = 6.1$, the X-Shooter archival quasar PSO J011+09 is the most transmissive by far, with 3 very strong transmission spikes resulting in $\tau_{\text{eff}} = 2.59$ (bottom panel). The transmission is affected by increased uncertainties due to corrections for telluric absorption; however, excluding the regions affected by these increased uncertainties actually further lowers the measured optical depths.

These transparent sightlines stand out at $> 10\sigma$ from the mean transmission at $z = 5.9$ and $z = 6.1$, respectively (see Figure 9). The discovery of such rare transmissive sightlines is only possible by employing large samples of quasars to sample cosmic variance: at $z = 5.9$, only 1/51 sightlines has an optical depth $\tau_{\text{eff}} < 3$. Characterising the extrema of the optical depth distribution at fixed redshift

	Sherwood	Nyx
$z = 5.0$	0.5475	1.0825
$z = 5.1$	0.555	1.1475
$z = 5.2$	0.5525	1.2
$z = 5.3$	0.5575	1.085
$z = 5.4$	0.6075	1.24
$z = 5.5$	0.62	1.4275
$z = 5.6$	0.755	1.775
$z = 5.7$	0.78	1.975
$z = 5.8$	0.7775	2.015

Table 5. Rescaling factors which maximise the likelihood of the observed optical depth distributions for Sherwood and Nyx at each redshift. Values are determined at the nearest multiple of 0.0025.

is crucial in order to design models of UVB fluctuations which reproduce the full variety of environments at the end of reionisation. The quasar J1535+1943 was not included in any previous measurements of optical depth; its addition to our sample raises the average transmitted flux by $\sim 10\%$. While this change is comfortably included within our quoted bootstrap uncertainties, it may account for some of the systematic disagreements between our study and past work which did not include this quasar (Figure 5).

In addition, Ly- α transmission spikes can be used to measure the thermal state of the IGM (e.g. Gaikwad et al. 2020) and to pose constraints on reionisation history through their statistical distribution (Barnett et al. 2017; Chardin et al. 2018). The identification of strong transmission spikes at $z > 5.8$ therefore opens up complementary analyses, which will be explored in a separate paper (XQR-30 in prep).

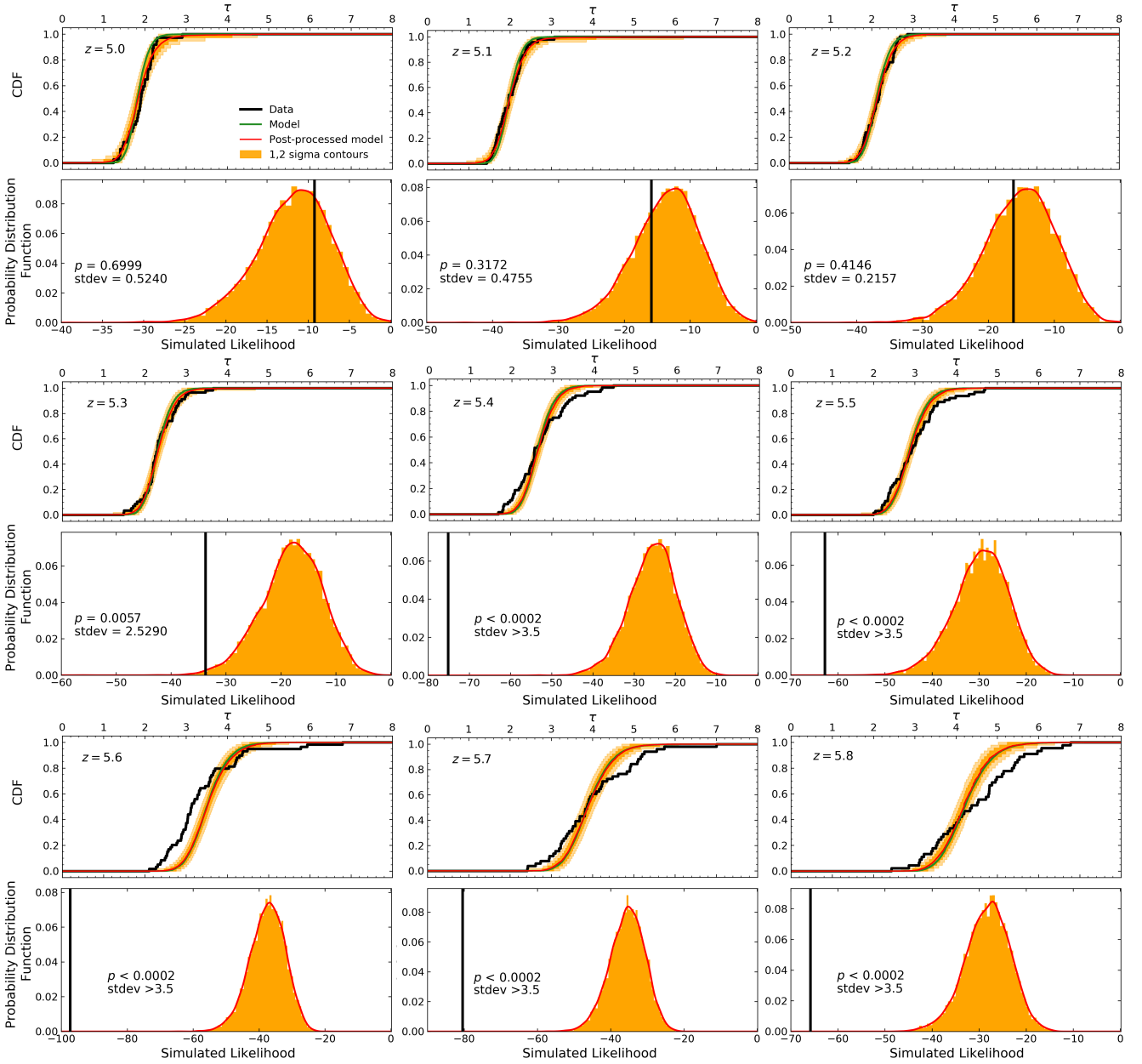


Figure 11. Top panels: observed Ly- α optical depth distribution (black), compared to the Sherwood simulations without any post-processing (green) and with post-processing (red, orange). The light and dark orange contours show 1σ and 2σ envelopes from bootstrap resampling the post-processed models. Bottom panels: probability distribution of log-likelihoods for fully forward-modelled datasets (orange). The distributions are used to build KDEs (red) which are evaluated at the location of the likelihood of the observed dataset (thick vertical black lines). The Sherwood model is a great fit to observations at $z \leq 5.2$, but excluded at $> 3.5\sigma$ at $z \geq 5.4$.

5 COMPARISON WITH HOMOGENEOUS-UVB MODELS

The existence of completely opaque troughs with $\tau > 5$ at $z \sim 5.8$ rules out models of reionisation with a homogeneous UVB and IGM temperature-density relation (Becker et al. 2015; Bosman et al. 2018). Even in the absence of large opaque troughs, the observed scatter in Ly- α optical depth at fixed redshift suggests excess fluctuations at even later times (Fig. 4). Determining the redshift evolution of these fluctuations can quantify the transition redshift beyond

which the IGM no longer retains reionisation-related structure from the point of view of Ly- α absorption.

We compare our results to predictions from two different homogeneous-UVB simulations, Sherwood (Bolton et al. 2017) and Nyx (Almgren et al. 2013). In both models, scatter between sight-lines results solely from fluctuations in the density field within a constant, fully-permeated UVB. Compared to Nyx, the Sherwood simulation is run with smaller boxes but provides finer redshift sampling ever $\Delta z = 0.1$ in redshift, while in Nyx the optical depth distribution must be extrapolated from 3 snapshots at $z = 5.0$, $z = 5.5$ and $z = 6.0$. The two simulation suites also employ differ-

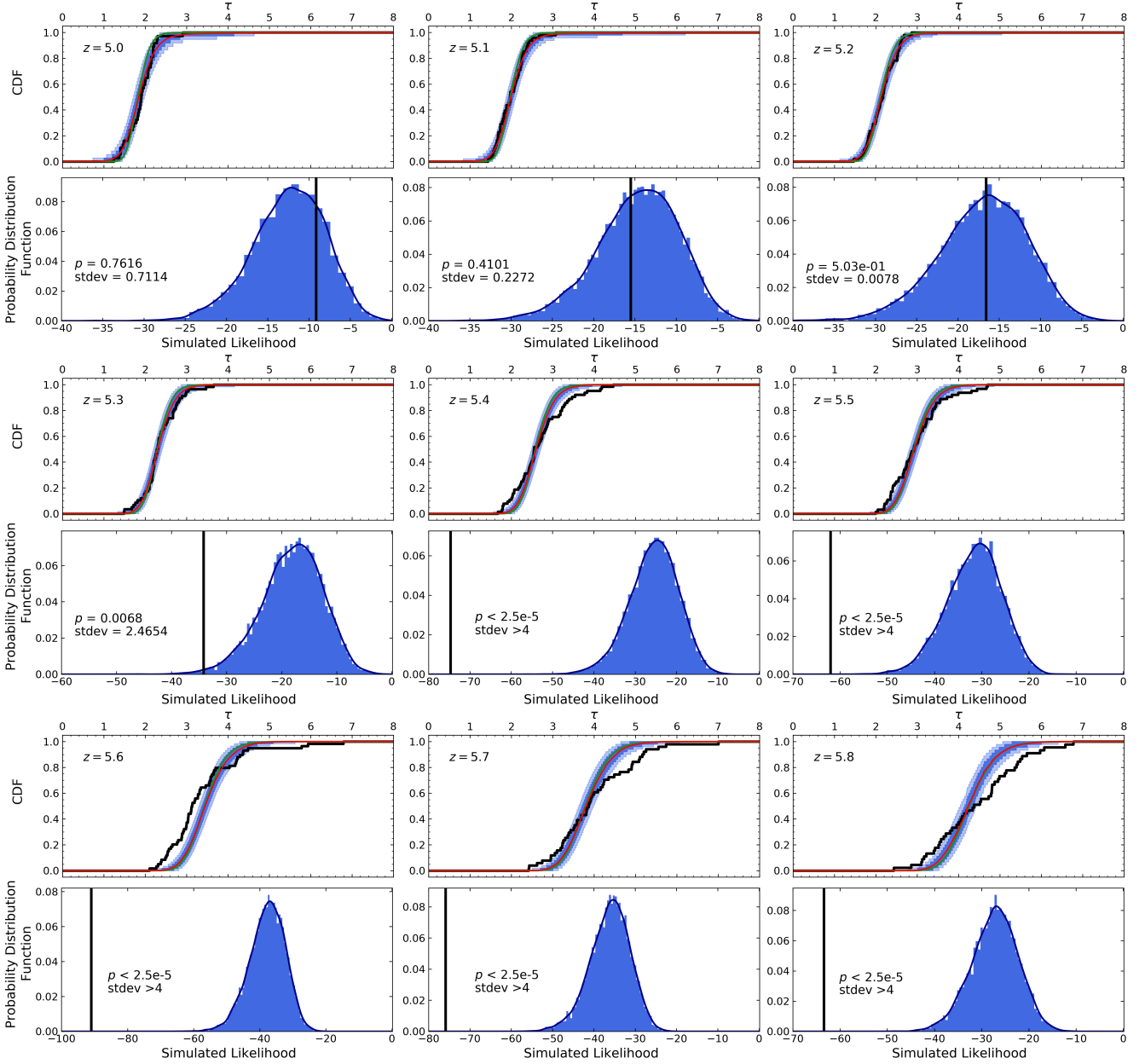


Figure 12. Same as Figure 11 but for the Nyx simulation (blue). The Nyx model is a great fit to observations at $z \leq 5.2$, is in mild tension with data at $z = 5.3$ (1.5σ) and excluded at $< 3.5\sigma$ at $z \geq 5.4$.

ent models of the UVB with different base rescalings of the ionising intensity. Neither simulation resolves the gas densities corresponding to DLAs nor Lyman-limit systems. We give more details of the simulation suites below.

The Sherwood simulation suite was designed to reproduce Ly- α transmission post-reionisation, at $2 < z < 5$, where it is in remarkable agreement with observations (Bolton et al. 2017). Sherwood employs the hydrodynamics code P-GADGET 3 (Springel 2005) and a uniform Haardt & Madau (2012) UVB. The gas particle masses are $M_{\text{gas}} = 9.97 \cdot 10^4 M_{\odot}$ and the box includes 2×2048^3 particles. We use the simulated boxes which are 40 cMpc/h on the side; we prefer those boxes over the lower-resolution 80 cMpc/h runs of Sherwood since they resolve the Ly- α transmission and thus

provide a closer comparison to the Nyx simulation. Snapshots were taken every $\Delta z = 0.1$ from $z = 5.0$ to $z = 6.0$. We draw 5000 lines of sight through the simulation box with lengths corresponding to $\Delta z = 0.1$ at each redshift.

Nyx is an Eulerian grid cosmological hydrodynamical simulation code which is optimized for simulations of the Ly α forest (Lukić et al. 2015). We use the Nyx simulation described in Davies et al. (2018a), 100 cMpc/h on a side with 4096^3 dark matter particles and 4096^3 baryon grid cells, sufficient box size and resolution for converged Ly α forest statistics at $z \lesssim 6$ (Oñorbe et al. 2017). Snapshots at $z = 5.0, 5.5$, and 6.0 were used to simulate the Ly α forest at $z = 5.0$ – 5.2 , 5.3 – 5.7 , and 5.8 , respectively. At redshifts not equal to the snapshot redshift, we re-scaled the physical gas densi-

ties by $(1+z)^3$ to account for cosmological expansion, effectively ignoring the impact of structure formation over these intervals of cosmic time. We draw 40000 lines of sight through each snapshot starting from random positions within the volume towards a random direction along the grid axes. While the simulation was originally run with the [Haardt & Madau \(2012\)](#) UVB for heating and cooling rates, here we initially construct Ly α forest skewers assuming a fixed photoionisation rate $\Gamma_{\text{HI}} = 10^{-12.1} \text{ s}^{-1}$ comparable to observational estimates at $z \sim 5$ ([Becker & Bolton 2013](#)).

We post-process sightlines drawn from simulations in the following way. First, we shorten sightlines to the length corresponding to $\Delta z = 0.1$ and project them onto a wavelength array with constant velocity sampling. We then randomly assign each simulated sightline to a real observation in the same redshift interval, and interpolate the simulated flux onto the observed wavelength array (including any masking of bad regions). We add random noise sampled from the corresponding observed error array by drawing from a gaussian with width of the 1σ uncertainty at each pixel. Finally, we multiply the sightline by a wavelength-dependent continuum error drawn from a normal distribution with scale of the observed 1σ bound of the continuum uncertainty. This assumes that the continuum uncertainty is fully covariant, while formally we would need to draw from the full PCA posterior (see e.g. [Davies et al. 2018b](#)). However, since we care not about the details of wavelength-dependence, our approach is both more computationally efficient and conservative. Shifting the continuum reconstruction at all wavelengths by the same standard deviation introduces a more coherent shift than selecting a random draw with the same PCA likelihood. This procedure will tend to introduce ‘‘pessimistic’’ continuum-reconstruction scatter into the post-processed simulations, in the sense that it slightly lowers the evidence for fluctuations (which is conservative for our purposes). Note that we do not need to convolve our simulated sightlines to match the observed instrumental resolutions, since the convolution operation explicitly conserves the total flux.

5.1 Maximum likelihood analysis

In order to calculate the likelihood of our observations given a model, optical depths at each simulated pixel must first be rescaled in bulk. The optical depth rescaling is expressed as a multiplicative factor on optical depth, $\tau_{\text{rescaled}} = A\tau_{\text{sim}}$ where the rescaling factor A is different at each redshift¹. Rescaling corresponds to adjusting the ionising background intensity in the simulations, i.e. it reflects a deviation from [Haardt & Madau \(2012\)](#) in the average ionising emissivity which can be a factor of a few. Optical depth rescaling factors are usually chosen to match the observed mean fluxes at each redshift, $\langle e^{A\tau_{\text{sim}}} \rangle = \langle F \rangle_{\text{obs}}$, but this may lead to bias when large sightline scatter is present. A few highly transmissive sightlines will lead to a very low average τ , which might make it difficult to match opaque sightlines. However, the highly transmissive sightlines also carry uncertainties. Therefore, a rescaling to a slightly lower average flux than observed leads to a better agreement between models and observations, because both opaque and transmissive sightlines can be produced by random noise. Motivated by this observation, we choose the rescaling factor to *maximise the likelihood of the observations* instead of matching the mean flux explicitly. We note our rescaling factors still give rise to mean simulated fluxes consis-

¹ Note that this rescaling is applied at each simulated pixel before computing the mean optical depth

tent with observed mean fluxes at $< 1\sigma$ at all redshifts where the simulations are a good fit to the data (see below).

We determine the likelihood of the observations by combining the likelihoods of each individual measurement τ_n made in sightline S_n :

$$\mathcal{L}_{\text{data}} = \prod_{n=1..N} p(\tau_n | S_n)$$

where N is the total number of sightlines contributing to the distribution at a given redshift. The probability $p(\tau_n | S_n)$ is obtained by post-processing all simulated sightlines with the observational properties of sightline S_n : wavelength sampling and masking, random flux uncertainties, and a random continuum uncertainty. The resulting distribution of predicted τ given S_n is then used to build a kernel density estimator (KDE). To obtain a smooth KDE from the Sherwood simulation with a relatively small number of sightlines, we over-sample each sightline 6 times². The KDE is then evaluated at the observed value τ_n to produce $p(\tau_n | S_n)$. The process is repeated for each observation S_n to obtain $\mathcal{L}_{\text{data}}$ via Equation (2).

For the purposes of comparison with models, we always assume that flux non-detections correspond to intrinsic flux just below the detection threshold (i.e. the upper CDF bounds in Figure 9). We pick the rescaling factor to maximise $\mathcal{L}_{\text{data}}$ by sampling A in steps of 0.0025. Table 5 lists the optimal rescaling factors at each redshift. We thus ensure that simulations are given the ‘best possible chance’ at reproducing the optical depth scatter in the observations.

We now calculate the probability of drawing a full dataset with $\mathcal{L}_{\text{data}}$ from the simulations. We generate 10000 fully forward-modelled datasets by post-processing N randomly-selected model sightlines, each assigned to the uncertainties of an observed sightline S_n . All simulated datasets therefore have the same size as the observations. The likelihood is calculated for each simulated dataset in the same manner as the data³, giving rise to a distribution of $\{\mathcal{L}_{\text{sim}}\}$. We build a KDE on the distribution of simulated likelihoods and evaluate it at $\mathcal{L}_{\text{data}}$ to finally obtain the probability of the entire set of observations given the simulation model. These probabilities p formally coincide with the p-values, and we also convert them to standard deviations via $\text{stdev} = \sqrt{2}\text{erf}^{-1}(2p)$ where erf^{-1} is the inverse error function.

5.2 Results

Figures 11 and 12 show the results of the likelihood analysis for the Sherwood and Nyx simulations, respectively. The data likelihood falls within $\pm 1\sigma$ expectations at $5.0 \leq z \leq 5.2$ for both Sherwood and Nyx. Forward-modelling introduces some optical depth scatter due to uncertainties, most visible at $z = 5.0$. The extra scatter is expected, and provides a better fit to observations: e.g. at $z = 5.1$ and $z = 5.2$ in Sherwood, the post-processed elongated distribution (red line) provides a better fit to the data than the model without post-processing (green line). The excellent agreement with models at $z \leq 5.2$ implies that the intrinsic physics within the simulations combined with our known observational uncertainties account for all the variance observed in the data. A homogeneous UVB acting

² meaning the observational uncertainties are chosen at random 6 times for each sightline to produce 6 predicted values of τ

³ However, we do not apply the optimal choice of rescaling factor to each simulated dataset as for the data, since this would be computationally unfeasible. A test of the impact reveals that the wings of the likelihood distribution may shift to higher values by up to $\Delta\mathcal{L} \sim 2$, which is insufficient to quantitatively affect our results.

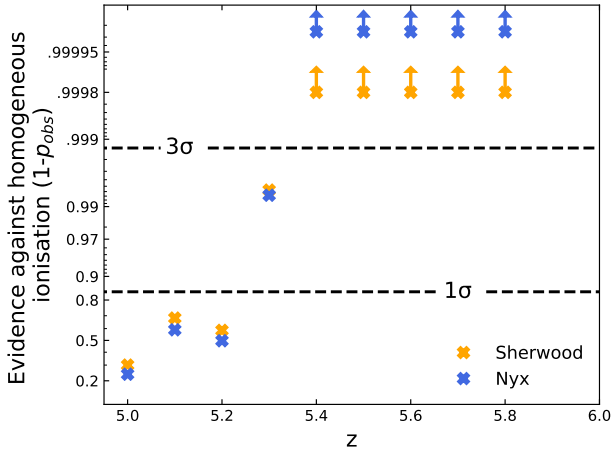


Figure 13. Summary of the likelihood analysis comparing the observed distributions of optical depth to the homogeneous-UVB Sherwood (orange) and Nyx (blue) simulations. By including forward-modelling of all known uncertainties, both models provide an excellent fit to the data at $z \leq 5.2$ but are in strong tension at $z \geq 5.4$.

on density fluctuations is therefore a sufficient description of Ly- α transmission up to $z = 5.2$.

Conversely, the Ly- α transmission scatter observed at $z \geq 5.4$ is in excess of model predictions at $> 3.5\sigma$ in both models. Since we sampled 5000 sightlines from the Sherwood simulation, we are limited in determining the nature of outliers to the $\lesssim 1/5000 \approx 3.5\sigma$ level. The 40000 sightlines from the Nyx simulation enable us to push the analysis to $\lesssim 1/40000 \approx 4\sigma$ outliers. We find that the post-processed Sherwood simulations fail to match the observations at the saturation level (3.5σ) at all redshifts $z \geq 5.4$. Nyx similarly fails to match observations at the corresponding 4σ level at $z \geq 5.4$. In both models, the rescaling factor which maximises the likelihood of observations results in mean simulation fluxes in close agreement with observed values (within 1σ of the values in Table 4) at $z \leq 5.3$; but the mean fluxes are in disagreement at $z \geq 5.4$ where the ‘most likely’ mean fluxes are closer to the median (Figs 11, 12). As expected, matching the median transmission increases the likelihood of an extended distribution since both extremely opaque and extremely transmissive sightlines then have reasonable probabilities.

Both the Nyx and Sherwood simulations transition from providing good fits to the data to being in strong tension with observations at $z = 5.3$, where they are in mild tension with the data (excluded at 2.4σ and 2.5σ , respectively). We conclude that extra Ly- α optical depth scatter is present in the observations, and its magnitude is in excess of differences between simulations due to box size and different choices of UVB models. However, the tension is mild and we cannot completely rule out either homogeneous UVB model. Examining the difference between Nyx and Sherwood in more detail, we find that Nyx provides a statistically better fit to the data at all redshifts in the absolute (i.e. the likelihood of the observed dataset is higher in Nyx). We attribute this to Nyx’s larger box size, which makes the model more apt to capture density fluctuations on large scales. However, both models are in agreement with the data at $z < 5.3$, in strong tension at $z > 5.3$, and in mild tension at $z = 5.3$.

Redshift $z = 5.4$ is the lowest redshift at which the observed distribution of optical depths is in strong tension with both mod-

els ($> 3.5/4\sigma$). To evaluate the robustness of the result, we test whether the tension is driven primarily by the most opaque sightlines at $z = 5.4$ or by the extended shape of the entire distribution. We arbitrarily remove the most opaque 3 sightlines, which have observed $\tau > 4$ – corresponding to 5% of the sample. While none of them show signs of foreground absorption by DLAs in the form of intervening metal absorbers, some DLAs at $z > 5$ may be particularly metal-poor. Even though we find no evidence for such metal-poor DLAs in the other redshift bins, unlucky alignment cannot be completely excluded. We roughly estimate that such DLAs would need metallicities of $[X/H] \lesssim -2.5$ to avoid detection in our spectra; this will be calculated in more detail in Davies et al. (in prep).

However, we find that even after arbitrarily removing the most opaque 3 sightlines from the distribution, the observations are still in strong tension with the $z = 5.4$ Sherwood simulation at 3.43σ ($p = 0.0305\%$ with $A = 0.58$). A similar result is obtained with Nyx, where omitting the most opaque sightlines still results in tension at 3.68σ . We show the corresponding likelihood distributions in Appendix B. We therefore conclude that the whole extended shape of the distribution, and not just a few sightlines, are driving the disagreement between homogeneous UVB models and observations at $z = 5.4$.

5.3 Discussion

Figure 13 summarises the results of the likelihood analysis. Both homogeneous-UVB simulations, Sherwood and Nyx, provide an excellent fit to observations at $z \leq 5.2$. Post-processing the simulations slightly broadens the predicted distribution of optical depths in this regime, bringing predictions in agreement with the data. There is no evidence that any extra sources of fluctuations are necessary at $z \leq 5.2$, such as, for example, a spatially varying thermal state of the IGM. In particular, the Sherwood simulation successfully matches Ly- α optical depth over $2 \leq z \leq 5.2$ without any such modifications (Bolton et al. 2017). The tension observed at $z \geq 5.4$ is therefore highly significant, and marks the breakdown of one or more simplifying assumptions in the post-reionisation high- z IGM.

The presence of large opaque troughs $\gtrsim 100$ cMpc/h in length in the Ly- α forest down to $z \sim 5.6$ already independently rules out homogeneous ionisation at that redshift (Becker et al. 2015; Bosman et al. 2018). Opaque troughs persisting at late times have been theorised to arise from patches of significantly neutral gas ($x_{\text{HI}} > 10\%$, Kulkarni et al. 2019; Keating et al. 2020; Nasir & D’Aloisio 2020; see also Lidz et al. 2006; Mesinger 2010). At the same time, recent measurements have reported a very short mean free path of ionising photons at $z = 6$, of ~ 0.75 pMpc (Becker et al. 2021). Evidence therefore points to a late end of reionisation, with remnant fluctuations in the UVB and/or IGM temperature persisting for 70–80 Myr after the demise of the last highly neutral ‘patches’ at $z \approx 5.6$ (see also Davies et al. 2021; Cain et al. 2021). From the point of view of Ly- α transmission homogeneity, hydrogen reionisation is not over before $z = 5.3$.

5.3.1 Hydrogen neutral fraction

We calculate the volume-averaged x_{HI} directly from the 40000 Nyx skewers at each redshift assuming ionisation equilibrium, shown in Figure 14. Our nominal measurements correspond to re-scalings of the UVB which maximize the likelihood of the τ_{eff} distribution (Table 6). We also measure upper and lower bounds corresponding to

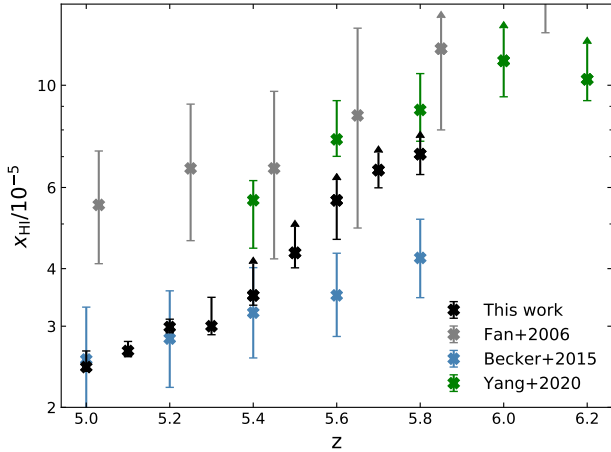


Figure 14. Evolution of the volume-averaged neutral fraction x_{HI} with redshift. We only provide lower limits in the regime where the Nyx simulation, which we use in the calculation of x_{HI} , is excluded by the observations. The model is a fairly poor fit to the data at $z = 5.3$ (2.5σ tension), which may be causing an offset. Our measurements employ samples factors 5 – 10 larger than past measurements. Tension with the Fan et al. (2006) values (blue) may be the result of a number of observational, systematic, or modelling differences.

re-scalings that reproduce, respectively, the lower and upper bounds of the mean transmitted flux. At $z = 5.3$, we find a significant difference between the x_{HI} values obtained from rescaling the $z = 5.0$ snapshot of Nyx as opposed to the $z = 5.5$ snapshot; we attribute this difference to evolution in the cosmic structure which neither snapshot captures perfectly. We list the most pessimistic bounds on x_{HI} among both snapshot re-scalings. For redshifts $z \geq 5.4$, the strong tension between our data and the maximum-likelihood Nyx τ_{eff} distribution implies that reionisation may not yet be complete (see also Kulkarni et al. 2019; Nasir & D’Aloisio 2020; Qin et al. 2021; Choudhury et al. 2021). The x_{HI} estimate from the mean flux is not sensitive to the fraction of fully-neutral regions, so we show our measurements at $z \geq 5.4$ as lower limits.

The calculation of x_{HI} has traditionally assumed an optically-thin IGM without self-shielding by dense fluctuations Fan et al. (2006); Becker et al. (2015); Yang et al. (2020). To estimate the impact of this assumption on our measurements, we post-process a set of skewers with the prescription of Rahmati et al. (2013) and show the results in Table 6. The inclusion of self-shielding results in an increase of x_{HI} by $\sim 25\%$. Unlike previous works where the effect was comparatively negligible, uncertainties related to the treatment of self-shielding dominate over our statistical uncertainties. Since the Nyx simulations do not resolve dense gas, we cannot provide a physically realistic inclusion of self-shielding at the $< 5\%$ level required to match the statistical uncertainties. We show the best-fit values without self-shielding in Figure 14 in order to compare to past work which universally assumed an optically-thin IGM.

We are consistent with the inferred x_{HI} values of Yang et al. (2020), who employed a homogeneous UVB model up to $z = 5.8$. Our values of the neutral fraction at $5.0 \leq z \leq 5.4$ are a factor ~ 2 lower than reported by Fan et al. (2006). This tension ($\sim 2\sigma$) may be due to a number of factors, such as a much smaller sample size than our study, continuum reconstruction systematics, lower SNR, or the very significant differences in the IGM model. We are in good agreement with Becker et al. (2015) up to $z = 5.4$. The mea-

z	$x_{\text{HI}}/10^{-5}$ (no s-s)	$x_{\text{HI}}/10^{-5}$ (with s-s)
5.0	$2.446 - 0.051 + 0.205$	$3.020 - 0.058 + 0.230$
5.1	$2.651 - 0.075 + 0.129$	$3.336 - 0.164 + 0.064$
5.2	$2.988 - 0.085 + 0.119$	$3.636 - 0.095 + 0.131$
5.3	$3.000 - 0.125 + 0.466$	$3.598 - 0.145 + 0.566$
5.4	$(3.498) > 3.332$	–
5.5	$(4.328) > 4.016$	–
5.6	$(5.627) > 4.630$	–
5.7	$(6.544) > 5.990$	–
5.8	$(7.087) > 6.401$	–

Table 6. Values of the hydrogen neutral fraction and $\pm 1\sigma$ bounds computed by comparison with the homogeneous-UVB Nyx simulations. We show the values both with and without self-shielding included (s-s). The numbers in brackets have the highest likelihood according our model, but note that above $z \geq 5.4$, homogeneous-UVB simulations are a poor match to data and only enable lower limits on x_{HI} .

surements of Becker et al. (2015) correspond to the neutral fraction specifically *inside of ionised regions*, which explains the divergence with our lower limits at higher redshifts. The uncertainties of our low- z x_{HI} measurements are very small, reflecting the exquisite precision of the measurement of the mean flux (Fig. 5). We warn that homogeneous UVB models are a fairly poor fit to observations at $z = 5.3$ (2.5σ tension), such that systematic errors in x_{HI} may be present in that redshift bin. The use of a -1σ lower bound on x_{HI} as a lower limit may therefore be an equally justified choice.

The conversion of mean flux measurements to values of the IGM neutral fraction x_{HI} is only valid under the assumption of completely homogeneous ionisation. This is because, fundamentally, the translation is model-dependent and relies on simulations assuming homogeneous ionisation. Models which reproduce the mean flux with late reionisation, such as that of Kulkarni et al. (2019), predictably result in significantly higher x_{HI} than simulations with homogeneous ionisation even when they match the *same observed mean flux* (Yang et al. 2020).

5.3.2 Non-homogeneous UVB models

We compare our new measurements of Ly- α optical depth distributions with the late-reionisation model of Keating et al. (2020) (first described in Kulkarni et al. 2019). Their model uses high-resolution cosmological radiative transfer simulations in boxes of 160 cMpc/h on the side. Similarly to the Sherwood suite, the late-reionisation simulation is run with the P-GADGET 3 code and uses the same cosmological initial conditions. The radiative transfer is conducted in post-processing with the ATON code (Aubert & Teyssier 2008, 2010). The simulation employed 2×2048^3 gas and dark matter particles. Lightcones of 50 cMpc/h are extracted from the simulation on-the-fly, resulting in sightlines with H I fraction and temperature that evolve along the line of sight with redshift. The centre of each such sightline is matched to the mid-point redshift of a measurement from the Bosman et al. (2018) sample, such that all sightlines are at slightly different redshifts. Five hundred such simulated datasets are generated for each redshift. Figure 15 shows the resulting 1σ (70%) bounds of the corresponding CDFs.

In order to compare these simulations to our observations, we re-bin the spectra in intervals of 50 cMpc/h centred on the mid-point redshift of each snapshots. The resulting bins cover redshifts of $5.3245 < z < 5.4754$ for the $z = 5.4$ snapshot, $5.5210 < z < 5.6710$ for the $z = 5.6$ snapshot, etc. In addition to the like-to-like sightline matching detailed above, the predicted

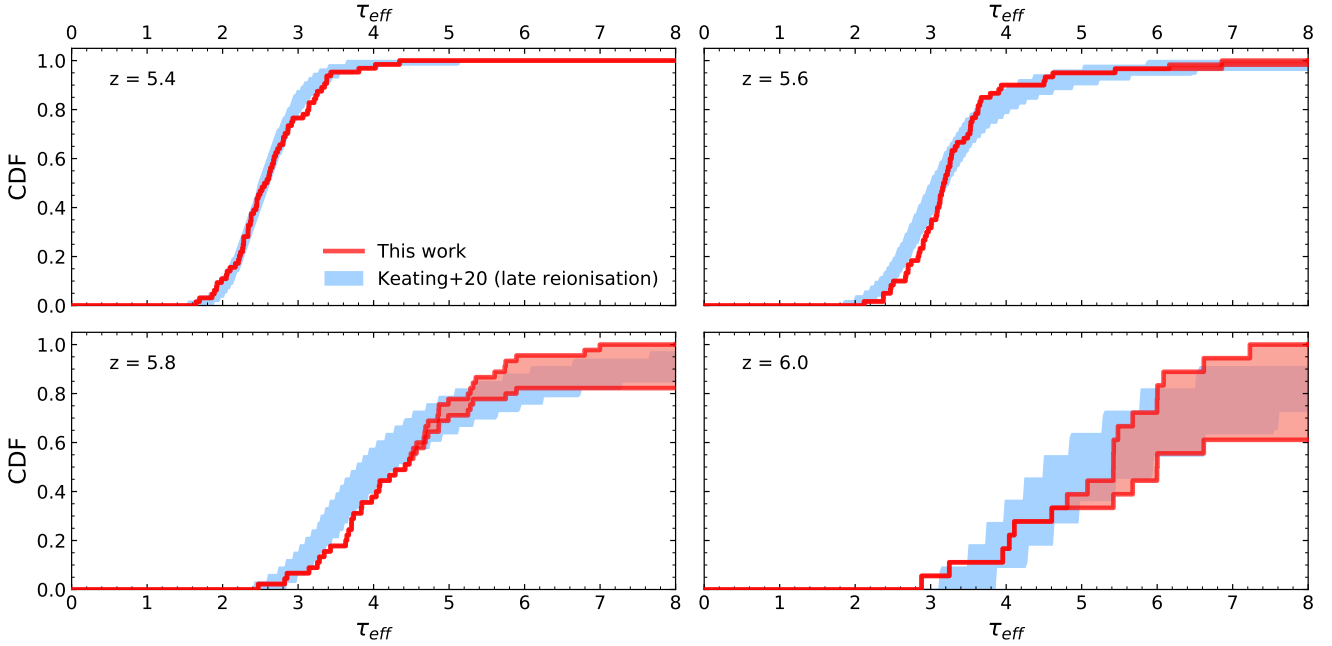


Figure 15. Comparison of the optical depth distributions measured in this work (red) to a model of late reionisation (Keating et al. 2020, blue). The contours of the blue distribution correspond to the central 1σ (70%) bounds of the simulated distributions. Late reionisation provides an excellent qualitative description of the Ly- α optical depth scatter above ≈ 5.4 . The late reionisation model was not calibrated to reproduce our updated measurements to mean Ly- α transmitted flux, precluding a direct quantitative comparison.

Ly- α optical depth distributions from Keating et al. (2020) were also calibrated to the mean Ly- α transmitted flux measurements of Bosman et al. (2018). The late reionisation model cannot be trivially re-scaled to our updated mean flux values, because the radiative transfer simulations rescale the emissivity of reionising sources to match the mean flux and predict Ly- α optical depth fluctuations self-consistently. As such, the model requires time-consuming runs of the simulation to calibrate. We therefore leave a quantitative comparison of the late reionisation model with our observations to future work. Figure 15 shows the excellent qualitative agreement between our new observations and the Keating et al. (2020) model without rescaling to match the new measurements of mean transmitted flux, nor sightline matching. At $z = 6.0$, the late reionisation model predicted a significantly larger fraction of sightlines $\tau_{\text{eff}} < 4$ than observed in previous work (compare with Figure 7). At $z = 5.8$, the model also predicted a larger number of highly opaque sightlines, closer to our present measurements than to previous measurements. The agreement with our updated results is therefore excellent despite the lack of specific re-calibration. This is encouraging evidence for a patchy, late end to hydrogen reionisation.

6 CONCLUSIONS

We have measured the mean Ly- α optical depth at $4.8 < z < 6.2$ by assembling a sample of 67 high-SNR quasar sightlines, leveraging the new XQR-30 sample of X-Shooter spectra of $z \gtrsim 5.8$ quasars. Our sample represents a ~ 3 -fold increase in the number of high-quality spectra of Ly- α transmission at the end stages of reionisation. We only employ observations taken with 2 spectrographs, enabling us to rigorously quantify systematics in instrumentation and continuum reconstruction for all our observations. The depth

of observations, $\text{SNR} > 10$ per spectral pixel, also enables a more careful removal of possible DLA contaminants than previous studies.

Our measurement of the evolution of the mean Ly- α evolution with redshift is in rough agreement with previous work (Figure 5). Differences are more likely to originate in previously-uncorrected systematics than in cosmic variance, given our large sample size and overlap with previous studies. We detect no sudden acceleration in the mean flux evolution over $4.8 < z < 5.5$.

We present an extremely transparent sightline with $\tau < 3$ at $z = 5.9$, and 2 rare sightlines with $\tau < 4$ at $z = 6.1$. These rare sightlines correspond to patches of the IGM with factors 5–15 times more transmitted flux than the median. The existence of transparent patches may help constrain future models of reionisation, which must be able to generate both sightlines with $\tau \sim 2.5$ and $\tau > 6$ at the same redshift ($z = 5.9$).

Next, we determine the lowest redshift at which excess optical depth scatter in Ly- α emerges, signalling a departure from a uniformly ionised IGM. Using an improved grasp on systematics, we forward-model two simulation models employing homogeneous UVBs, the Sherwood and Nyx simulations. We conduct a maximum-likelihood analysis to obtain the probability of the full observed dataset at each step of $\Delta z = 0.1$. All observational systematics (wavelength masking, observational uncertainties, continuum uncertainties, etc) are included in post-processing of the simulations. These uncertainties result in increased Ly- α optical depth scatter which improves the agreement between models and observations.

We find excellent agreement between the forward-modelled simulations and observations at $5.0 \leq z \leq 5.2$, where the observed data has a high probability of being observed by chance ($< 1\sigma$). A homogeneous UVB is in mild tension with observations at $z =$

5.3 (2.5σ) and strongly excluded at $z \geq 5.4$ ($> 4\sigma$). To check whether the disagreement at $z = 5.4$ is driven by a few opaque sightlines which may contain DLAs, we arbitrarily remove the 3 least transmissive sightlines which have $\tau > 4$. Homogeneous UVB models remain excluded at $z = 5.3$ at $> 3.5\sigma$ confidence, meaning that the intrinsically large width of the observed distribution, and not just a few sightlines, is driving the tension. Despite differences in the box size, snapshot density, and UVB models between the two suites, our results are consistent between the Sherwood and Nyx simulations.

Since the Sherwood model has been highly successful in modelling the Ly- α forest over a wide range of redshifts ($2 < z < 5.2$), a sudden failure by $z = 5.4$ represents a breakdown of one or more simplifying assumptions. Whether fluctuations in the UVB are present at very late times and/or whether the thermal state of the IGM retains the imprint of recent ionisation, it is clear that reionisation-related fluctuations persist in the IGM until at least $z = 5.3$.

Finally, we convert our measurements of the mean Ly- α flux to volume-averaged neutral fraction x_{HI} . We stress that this conversion is model-dependent; here we use the Nyx simulation suite. Since Nyx (and homogeneous-UVB models in general) provides a very poor fit to data at $z \geq 5.4$, only lower limits on x_{HI} can be quoted. Our results at $5.0 \leq z \leq 5.3$ are in mild tension with those of Fan et al. (2006) ($\sim 2\sigma$), but the vast improvements in data quality, quantity and understanding of systematics and IGM modelling over the last 15 years makes it difficult to pinpoint the source of the disagreement.

The XQR-30 sample has qualitatively changed the landscape of the late stages of reionisation. Analysis of Ly- α transmission at $z > 5$ has become a precision probe of the post-reionisation era, with exciting prospects both on the analysis and theoretical fronts. Through excellent complementarity with upcoming 21cm probes, IGM transmission studies make it possible to uncover the entire history of reionisation from start to end.

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APPENDIX A: ALTERNATIVE DATA BINNING

In this paper, we bin the data in fixed redshift intervals of equal size $\Delta z = 0.1$. Fixed redshift bins to equal comoving length may sometimes be more convenient for model comparison. In Figure A1 we show a such a sub-division of the data between $4.9 \lesssim z \lesssim 6.2$ in 8 bins with fixed $\Delta L = 50$ cMpc/h. The mid-points and edges of each bin are given in each panel as well as in Table A1. The average optical depths measured in this manner, as well as the qualitative evolution of the optical depth distribution, are fully consistent with those obtained in the paper’s main body. The number of non-detections is slightly lessened due to averaging of the optical depth over a larger interval. Distributions of optical depths on different scales are expected to be sensitive to different optical effects. We make these distributions available as supplemental online material, as well as the distributions with intervals of $\Delta z = 0.05, 0.1, 0.2$ and $\Delta L = 30, 50, 70$ cMpc/h. Note that intervals $\Delta z \gtrsim 0.1$ are subject to variations of the mean flux $> 1\sigma$ between their edges (Fig. 5).

z	$z_{\min}$	$z_{\max}$	$\langle F_{\text{Ly-}\alpha} \rangle$	-1σ	$+1\sigma$	N_{los}
5.000	4.932	5.069	0.1545	-0.0085	$+0.0080$	37
5.140	5.069	5.210	0.1329	-0.0056	$+0.0054$	52
5.284	5.210	5.357	0.1073	-0.0043	$+0.0046$	58
5.433	5.357	5.509	0.0741	-0.0039	$+0.0047$	65
5.588	5.509	5.667	0.0458	-0.0032	$+0.0031$	61
5.748	5.667	5.830	0.0192	-0.0025	$+0.0022$	48
5.915	5.830	5.999	0.0126	-0.0031	$+0.0028$	28
6.087	5.999	6.175	0.0091	-0.0051	$+0.0051$	12

Table A1. Mean Ly- α flux transmission at $4.9 \lesssim z \lesssim 6.2$, measured in $\Delta L = 50$ cMpc/h bins with fixed redshift bounds $z_{\min}$ and $z_{\max}$. Uncertainties correspond to the 16th and 84th percentiles from bootstrap resampling. The measurement uncertainties on their own are a factor 5 – 10 smaller than the bootstrap uncertainties quoted here. N_{los} sightlines contribute to each measurement.

APPENDIX B: $Z = 5.4$ DISTRIBUTION WITHOUT MOST OPAQUE SIGHTLINES

To determine whether the tension at $z = 5.4$ is due to outlier sightlines (potential DLAs), we arbitrarily remove the top 3 most opaque sightlines and re-run the likelihood analysis. The results are shown in Figure B1. While the tension is reduced compared to including the opaque sightlines, the tension remains above 3σ for both the Sherwood and Nyx simulations. The test therefore indicates that the entire shape of the Ly- α optical depth distribution at $z = 5.4$, and not just a few outliers, drive the tension with homogeneous UVB models.

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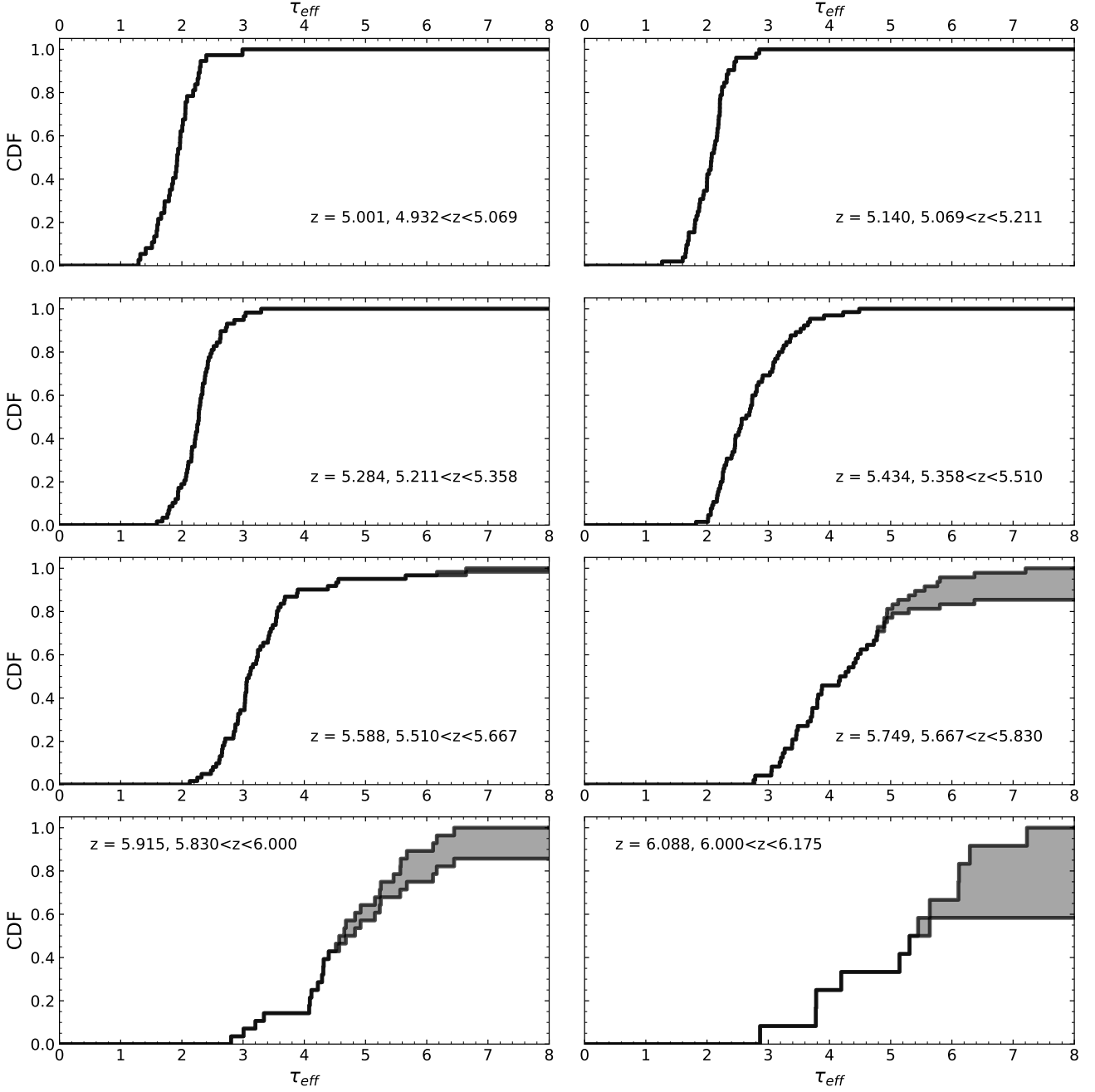


Figure A1. Same as Figure 9, but with fixed redshift intervals of constant length $\Delta L = 50$ cMpc/h as indicated in each panel. The qualitative evolution is unchanged: the first opaque troughs emerge at $z \sim 5.6$.

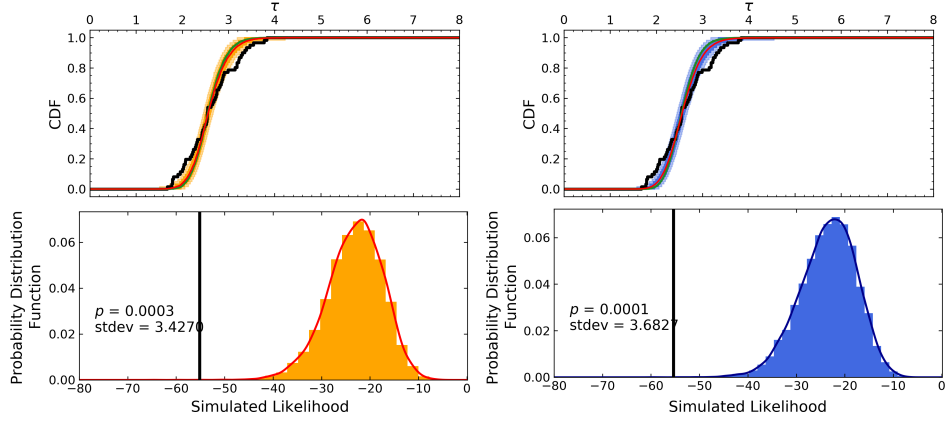


Figure B1. Same as Figure 11 but distributions at $z = 5.4$ arbitrarily excluding the most opaque 3 sightlines with $\tau > 4$. Left: results for Sherwood. Right: results for Nyx. In both simulations, a tension at $> 3\sigma$ remains even after removing the most opaque sightlines.