Validation Report: Sentinel-6 NTC Level 3 gridded products (GRM-123–129, GRM-195)

Version 1.3

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1.0	9/11 2021	HGL	Version prepared for the ORR16 review.
1.1	24/11 2021	HGL	Updated version after ORR16 review in response to: RID 020: Updated last three sentences of Section 2.5. RID 021: Added two sentences to Section 3.1.1. RID 023: Section 2.1: "… processors v3.4 and v3.5." Section 2.5: Reference to Figure 4, not to Figure 3.
1.2	15/6 2022	HGL	Updated version submitted for OR14 in response to SG Action SG27-Act-03: Executive Summary: added a statement about the additional validation of GRM-195. Section 1.1: updated applicable documents. Section 1.4: updated definitions. Section 1.5: added reference to Annex A. Section 4: mentions the additional validation of GRM-195. Section 6.1: updated formulations of limitations. New Annex A: additional validation of GRM-195.
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ROM SAF

The Radio Occultation Meteorology Satellite Application Facility (ROM SAF) is a decentralised processing centre under EUMETSAT which is responsible for operational processing of GRAS radio occultation (RO) data from the Metop and Metop-SG satellites and radio occultation data from other missions. The ROM SAF delivers bending angle, refractivity, temperature, pressure, humidity, and other geophysical variables in near real-time for NWP users, as well as reprocessed Climate Data Records (CDRs) and Interim Climate Data Records (ICDRs) for users requiring a higher degree of homogeneity of the RO data sets. The CDRs and ICDRs are further processed into globally gridded monthly-mean data for use in climate monitoring and climate science applications.

The ROM SAF also maintains the Radio Occultation Processing Package (ROPP) which contains software modules that aid users wishing to process, quality-control and assimilate radio occultation data from any radio occultation mission into NWP and other models.

The ROM SAF Leading Entity is the Danish Meteorological Institute (DMI), with Cooperating Entities: i) European Centre for Medium-Range Weather Forecasts (ECMWF) in Reading, United Kingdom, ii) Institut D'Estudis Espacials de Catalunya (IEEC) in Barcelona, Spain, iii) Met Office in Exeter, United Kingdom, and iv) Wegener Center, University of Graz, in Graz, Austria. To get access to our products or to read more about the ROM SAF please go to: http://www.romsaf.org

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Executive Summary

The ROM SAF Non Time Critical (NTC) Level 3 data products are based on measurements by the Sentinel-6 Radio Occultation (RO) mission. The Level 3 data consist of monthly means on a global latitude-altitude grid (5 degrees in latitude by 200 meters in altitude), averaged from a large number of near-vertical profiles of relevant geophysical variables, including bending angle, refractivity, dry temperature, temperature, and humidity. The profile data (Level 2), used as input to the ROM SAF Level 3 processing, have been generated by the ROM SAF from bending angle data (Level 1B) provided by the EUMETSAT Secretariat.

For the purpose of validating the NTC Level 3 data, we generated 4 months of data (June to September 2021) with the ROM SAF processing system. The validation is based on a) comparing the NTC Level 3 gridded monthly mean data with the corresponding data from ECMWF operational forecasts, and b) comparing the Sentinel-6 NTC Level 3 data with the corresponding Metop Offline data. In addition to this, we check the compliance with the product requirements using the methods described in the Product Requirements Document (PRD). Finally, we define an updated set of service specifications to be used in the operational monitoring of the NTC Level 3 data.

As a response to ROM SAF Steering Group Action SG27-Act-03, the compliance of the product requirements for the Level 3 tropopause height product (GRM-195) was further checked during a longer time period, June 2021 to March 2022 (Annex A).

We conclude that the ROM SAF NTC Level 3 monthly mean data are of high quality, that they meet the expectations we have on ROM SAF data products, and that they comply with the product requirements as stated in the Product Requirements Document. The issues that were detected during the validation, and that requires further investigations, are not of a character that prevent the data products from being released.

1. Introduction

1.1 Purpose of the document

This document describes the validation of the ROM SAF Sentinel-6 NTC Level 3 data. The Level 3 data consist of gridded monthly means generated by the ROM SAF processing system using Level 1B and Level 2 profile data as input, together with ancillary information from ECMWF reanalysis data. The product requirements baseline is defined in the ROM SAF Product Requirements Document (PRD) [AD.3], and the methods and algorithms used in the generation of the Level 3 data products are described in the Algorithms Theoretical Baseline Document (ATBD) [RD.6].

An extensive range of plots with a direct bearing on the validation of the climate data can be found on the ROM SAF web site (http://www.romsaf.org). Those plots should be studied in conjunction with the present report.

1.1.1 List of data products being validated in this report

The ROM SAF data products being validated in this report are listed in Table 1. They consist of Sentinel-6 NTC Level 3 data products that are generated on a regular basis for non-time-critical applications based on algorithms that may have evolved from the last reprocessing to reflect the latest scientific developments.

Table 1. List of the ***NTC data products*** covered by this Validation Report. The Level 1B input data to the ROM SAF NTC processing is obtained from the EUMETSAT Secretariat.

Product ID	Product name	Product acronym	Satellite input	Prod. version
GRM-123	NTC bending angle grid	OBGS6	Sentinel-6	1.0
GRM-124	NTC refractivity grid	ORGS6	“	“
GRM-125	NTC temperature grid	OTGS6	“	“
GRM-126	NTC specific humidity grid	OHGS6	“	“
GRM-127	NTC dry geopotential height grid	OZGS6	“	“
GRM-128	NTC dry temperature grid	ODGS6	“	“
GRM-129	NTC dry pressure grid	OYGS6	“	“
GRM-195	NTC tropopause height grid	OCGS6	“	“

1.2 Applicable and reference documents

1.2.1 Applicable documents

The following list contains documents with a direct bearing on the contents of this document:

[AD.1] CDOP 4 Proposal: Proposal for the Fourth Continuous Development and Operations Phase (CDOP 4), Ref: SAF/ROM/DMI/MGT/CDOP4/001, Version 1.1, 5 April 2021, as approved by the EUMETSAT Council in document reference EUM/C/97/21/DOC/15

[AD.2] CDOP 4 Cooperation Agreement between EUMETSAT and DMI on the CDOP 4 of the ROM SAF (EUM/C/97/21/DOC/21), signed on 31 August and 15 September 2021

[AD.3] ROM SAF CDOP 4 Product Requirements Document, Ref: SAF/ROM/DMI/MGT/PRD/004

1.2.2 Reference documents

The following documents provide supplementary or background information, and could be helpful in conjunction with this document:

[RD.1] ROM SAF ATBD: Level 1B bending angles, SAF/ROM/DMI/ALG/BA/001.

[RD.2] ROM SAF ATBD: Level 2A refractivity profiles, SAF/ROM/DMI/ALG/REF/001.

[RD.3] ROM SAF ATBD: Level 2A dry temperature profiles, SAF/ROM/DMI/ALG/TDRY/001.

[RD.4] ROM SAF ATBD: Level 2B and 2C 1D-Var products, SAF/ROM/DMI/ALG/1DVAR/002.

[RD.5] ROM SAF ATBD: Level 2C tropopause height, SAF/ROM/DMI/ALG/TPH/001.

[RD.6] ROM SAF ATBD: Level 3 gridded data, SAF/ROM/DMI/ALG/GRD/001.

[RD.7] ROM SAF Validation Report: Reprocessed Level 3 gridded data, SAF/ROM/DMI/REP/GRD/001.

[RD.8] ROM SAF Validation Report: Offline Level 3 gridded data, SAF/ROMDMI/REP/GRD/002.

[RD.9] The ROPP Pre-processor Module User Guide, SAF/ROM/METO/UG/ROPP/004.

[RD.10] The ROPP 1D-Var Module User Guide, SAF/ROM/METO/UG/ROPP/007.

[RD.11] Simmons, A., et al., Global stratospheric temperature bias and other stratospheric aspects of ERA5 and ERA5.1, *ECMW Technical Memoranda*, 859, 2020.

[RD.12] Foelsche, U., et al., Refractivity and temperature climate records from multiple radio occultation satellites consistent with 0.05%, *Atmos. Meas. Tech.*, 4, 2007-2018, 2011.

[RD.13] Steiner, A. K., Lackner, B. C., Ladstädter, F., Scherllin-Pirscher, B., Foelsche, U., and Kirchengast, G., GPS radio occultation for climate monitoring and change detection, *Radio Sci.*, 46, RSOD24, 2011.

[RD.14] Gleisner, H., Latitudinal binning and area-weighted averaging of irregularly distributed radio occultation data, GRAS SAF Report 10, 2010.

[RD.15] Ho, S.-P., et al., Estimating the uncertainty of using GPS radio occultation data for climate monitoring: Inter-comparison of CHAMP refractivity climate records 2002-2006 from different data centers, *J. Geophys. Res.*, 114, D23107, 2009.

[RD.16] Steiner, A. K., et al., Quantification of structural uncertainty in climate data records from GPS radio occultation, *Atmos. Chem. Phys.*, 13, 1469-1484, 2013.

[RD.17] Gleisner, H., K.B. Lauritsen, J.K. Nielsen, and S. Syndergaard, Evaluation of the 15-year ROM SAF monthly mean GPS radio occultation climate data record, *Atmos. Meas. Tech*, 13, 3081-3098, doi:10.5194/amt-13-3081-2020.

1.3 Acronyms and abbreviations

ATBD	Algorithm Theoretical Baseline Document
CDOP	Continuous Development and Operations Phase (EUMETSAT)
CDR	Climate Data Record
COSMIC	Constellation Observing System for Meteorology, Ionosphere and Climate
DMI	Danish Meteorological Institute; ROM SAF Leading Entity
ECMWF	European Centre for Medium-range Weather Forecasts
EPS	EUMETSAT Polar Satellite System
EUMETSAT	EUropean organisation for the exploitation of METeorological SATellites
GNSS	Global Navigation Satellite System
GPAC	GNSS Processing and Archiving Center
GPS	Global Positioning System (US)
GRAS	GNSS Receiver for Atmospheric Sounding (EPS/Metop)
GRIB	GRIdded Binary (WMO)
ICDR	Interim Climate Data Record
IEEC	Institut d'Estudis Espacials de Catalunya
L1	GPS carrier frequency, 1575.42 MHz
L2	GPS carrier frequency, 1227.6 MHz
LC	L Corrected (through linear combination of L1 and L2)
LEO	Low Earth Orbit
Met Office	United Kingdom Meteorological Office
Metop	Meteorological Operational Polar satellite (EUMETSAT)
MSL	Mean Sea Level
netCDF	Network Common Data Format

NRT	Near Real Time
NTC	Non Time Critical
NWP	Numerical Weather Prediction
PRD	Product Requirements Document (ROM SAF)
RO	Radio Occultation
ROM SAF	Radio Occultation Meteorology SAF (former GRAS SAF)
ROPP	Radio Occultation Processing Package (ROM SAF)
SAF	Satellite Application Facility (EUMETSAT)
UG-WEGC	University of Graz, Wegener Center
WMO	World Meteorological Organization

1.4 Definitions

RO data products from current and upcoming EUMETSAT satellites and other missions are grouped in data levels (Level 0, 1, 2, or 3) and product types (NRT, Offline, NTC, CDR, or ICDR). The data levels and product types are defined below.[1] The lists of variables should not be considered as the complete contents of a given data level, and not all variables may be contained in a given data level in a given file.

Data levels:

Level 0: Raw sounding, tracking and ancillary data, and other GNSS data before clock correction and reconstruction;

Level 1A: Reconstructed full resolution excess phases, total phases, pseudo ranges, SNRs, orbit information, I, Q values, NCO (carrier) phases, navigation bits, scintillation parameters, and quality information;

Level 1B: Bending angles and impact parameters, tangent point location, total electron content, and quality information;

Level 2: Refractivity, geopotential height, "dry" temperature profiles (Level 2A), pressure, temperature, specific humidity profiles (Level 2B), surface pressure, tropopause height, planetary boundary layer height (Level 2C), ECMWF model level coefficients (Level 2D), electron densities, and quality information;

Level 3: Gridded or resampled data, that are processed from Level 1 or 2 data, and that are provided as, e.g., daily, monthly, or seasonal means on a spatiotemporal grid, including metadata, uncertainties and quality information.

Product types:

NRT: Data product delivered less than: (i) 3 hours after measurement (ROM SAF Level 2 products for EPS); (ii) 150 min after measurement (ROM SAF Level 2 products for EPS-SG Global Mission); (iii) 125 min after measurement (ROM SAF Level 2 products for EPS-SG Regional Mission);

1 Note that the level definitions differ partly from the WMO definitions: *http://www.wmo.int/pages/prog/sat/dataandproducts_en.php*

Offline, NTC: Data product delivered from about 5 days to up to 6 months after measurement, depending on the applicable requirements. The evolution of this type of product is driven by new scientific developments and subsequent product upgrades;

CDR: Climate Data Record generated from a dedicated reprocessing activity using a fixed set of processing software.[2] The data record covers an extended time period of several years (with a fixed end point) and constitutes a homogeneous data record appropriate for climate usage. The CDR may be referred to as Fundamental (e.g. for Level 1B bending angles) or as Thematic (if related to a specific application area);[3]

ICDR: Interim Climate Data Record which regularly extends in time a CDR using a system having optimum consistency with and lower latency than the system used to generate the CDR.[4]

General terms:

System: GPAC (ROM SAF GNSS Processing and Archiving Center)

Web site: ROM SAF web site: http://www.romsaf.org

Product Archive: PARF (ROM SAF Product Archive and Retrieval Facility)

1.5 Overview of this document

This document is organized as follows:

Chapter 1: Contains the introduction.

Chapter 2: Contains an overview of the Level 1B and Level 2 profile data used as input to the Level 3 processing. It also contains an overview of the Level 3 gridded data, the Level 3 processing, and a list of the quality screening tests.

Chapter 3: Contains the main validation results.

Chapter 4: Contains a check of the compliance with the Product Requirements.

Chapter 5: Contains suggested Service Specifications for the NTC Level 3 products.

Chapter 6: Contains the main conclusions of the validation.

Annex A: Contains additional validation of the Tropopause Height Grid (GRM-195).

[2] *(i) GCOS 2016 Implementation Plan; (ii) http://climatemonitoring.info/home/terminology/*
[3] *http://climatemonitoring.info/home/terminology*
[4] *http://climatemonitoring.info/home/terminology/ (the ICDR definition was endorsed at the 9th session of the joint CEOS/CGMS Working Group Climate Meeting on 29 March 2018)*

2. Background

2.1 Input data to ROM SAF NTC processing

The ROM SAF NTC data products are based on data from the Sentinel-6 mission, which currently consists of the Sentinel-6A satellite. The data are processed by the ROM SAF from Level 1B data obtained from the EUMETSAT Secretariat. These input data are generated with EUMETSAT's Common Processing Facility (CPF) OPE environment, processor RO-NTC v3.4 and v3.5.

2.2 Level 1B and Level 2 profile data

The starting point for the ROM SAF Level 3 processing is a large number of near-vertical profiles, one for each occultation: bending angle, $\alpha(a)$, refractivity, $N(H)$, dry pressure, $p_{\mathrm{dry}}(H)$, dry temperature, $T_{\mathrm{dry}}(H)$, dry geopotential height, $Z(H_{p\mathrm{dry}})$, temperature, $T(H)$, specific humidity, $q(H)$, and tropopause height, H_{TP}. Here, H is the mean-sea level (MSL) altitude, a is the impact parameter, H_p is the pressure height (a logarithmic measure of pressure), and $H_{p\mathrm{dry}}$ is the dry-pressure height [RD.6]. The retrievals of the geophysical profile data are described in the associated ATBDs [RD.1-4], while the retrieval of tropopause height has its own ATBD [RD.5].

The bending angle, refractivity, and dry profiles are provided on relatively dense vertical grids reaching up to well above the region where the RO measurements provide useful information on the neutral atmosphere. The temperature and humidity profiles are given on a standard set of vertical levels ranging from the surface up to around 80 km, near the top of the atmospheric model used as *a priori* in the retrieval. Each occultation has an associated reference location and time, which is used in binning the data.

The NTC Level 1B data are obtained from EUMETSAT (See Section 2.1) while the Level 2 profiles are retrieved with the GPAC-3.0 system, which includes the ROPP-10.0 software package (an internal release with adaptions made by DMI).

2.3 Level 3 gridded data

The ROM SAF Level 3 data incorporates gridded monthly means and associated quantities (standard deviations, data numbers, sampling error estimates, etc.) of:

- Bending angle, $\alpha(a)$
- Refractivity, $N(H)$
- Dry pressure, $p_{\mathrm{dry}}(H)$
- Dry temperature, $T_{\mathrm{dry}}(H)$
- Dry geopotential height, $Z_{\mathrm{dry}} = Z(H_{p\mathrm{dry}})$
- 1D-Var temperature, $T(H)$
- 1D-Var specific humidity, $q(H)$
- Tropopause height, H_{TP}

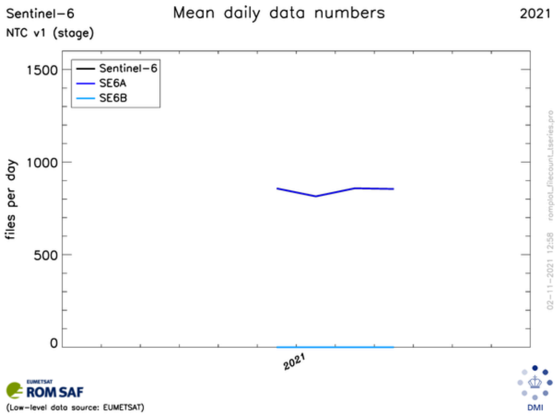

Figure 1. *Number of occultations available for NTC data generation from the single Sentinel-6A satellite during the 4-month validation period June to September 2021.*

As described in Section 2.2, H is the MSL altitude, a is the impact parameter, and $H_{p\text{dry}}$ is the dry-pressure height [RD.6]. The monthly means, and the associated variables, are defined on zonal grids, 200 meters in height by 5 degrees in latitude [RD.6].

The data numbers available from the Sentinel-6 mission are shown in Figure 1. On average, we obtain 800-900 occultations per day from the single Sentinel-6A satellite currently in orbit.

All RO missions have a relatively uniform distribution of data numbers in longitude, whereas the latitude distribution tends to be non-uniform to some extent [RD.14]. Figure 2 shows the longitudinal (left-hand panel) and latitudinal (right-hand panel) distributions of data numbers per unit area for Sentinel-6. The non-uniform latitudinal distribution is mainly a consequence of the RO satellite orbit, with impacts from the GNSS satellite orbits in combination with the limb-sounding observing geometry of the RO instrument.

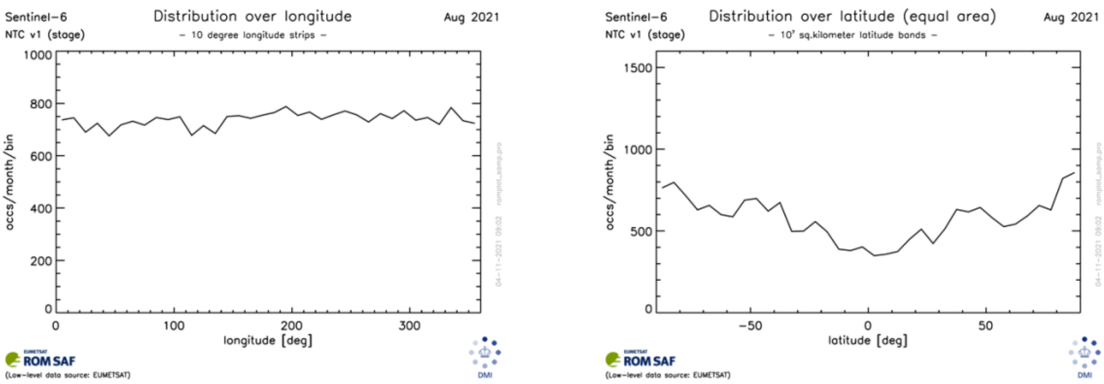

Figure 2. *Distribution of occultations over longitude (left panel) and latitude (right panel) for the Sentinel-6 mission. On a monthly time scale the distributions over longitude are relatively uniform while the latitude distribution is less uniform, with larger data numbers (per unit area) towards the poles.*

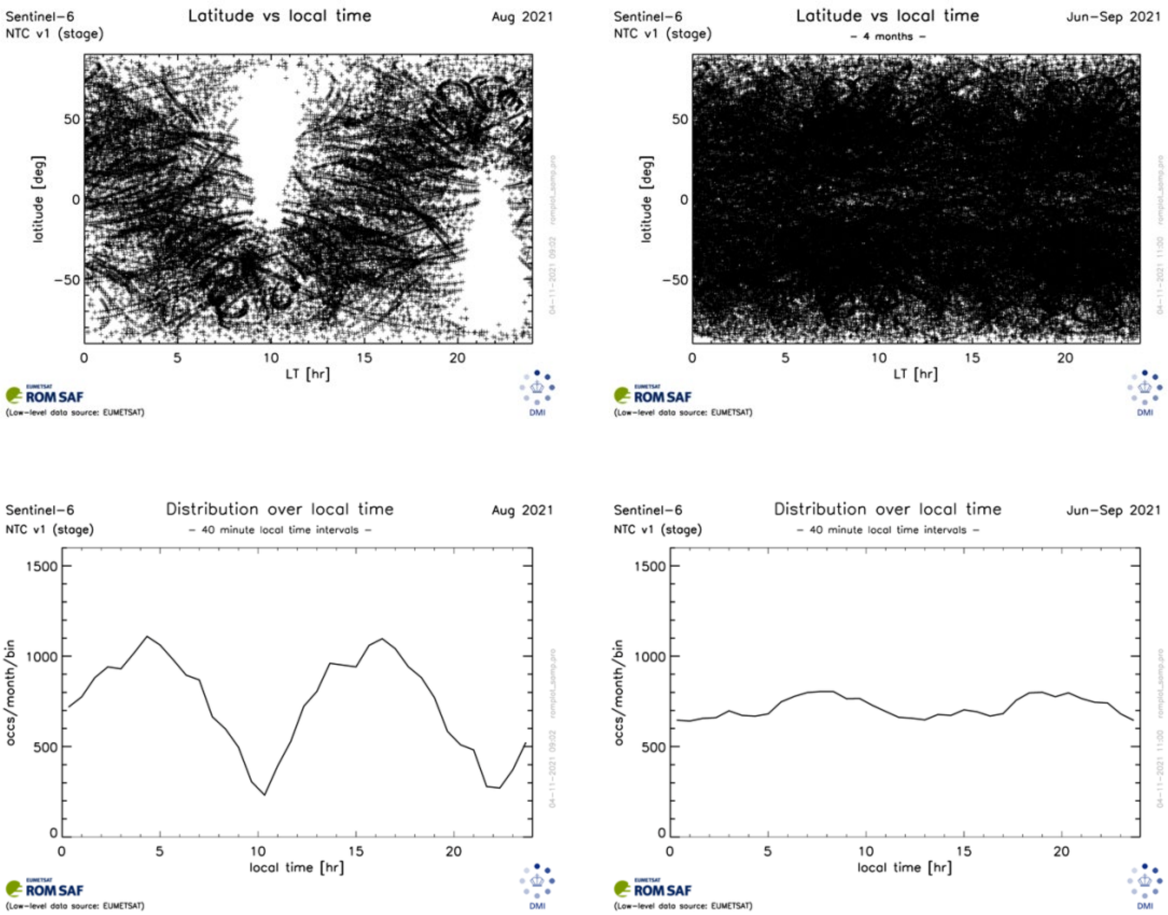

Figure 3. *The upper panels show the scatter of occultations in latitude and local time for a single month (upper left) and for a 4-month time period (upper right) for the Sentinel-6 mission. The lower panels show the corresponding distributions over local time for a single month (lower left) and for a 4-month period (lower right).*

Unlike Metop, the Sentinel-6 satellite is not Sun-synchronous. The nodal precession of the Sentinel-6 orbit is such that over a 4-month period, the equatorial crossings drift through 24 hours of local time. As a consequence, the individual monthly means are generated from non-uniform local time distributions of data that slowly change with time (Figure 3, lower left panel). However, all local times, i.e. the complete diurnal cycle, is sampled over half the nodal-precession cycle, approximately 2 months.

2.4 ROM SAF Level 3 processing

The Level 3 gridded data are generated from the Level 1B and Level 2 profile data through rather straight-forward *binning and averaging* [RD.6]. A set of equal-angle latitudinal bins are defined and all valid observations that fall within a latitude bin and calendar month undergo a weighted averaging to form a zonal mean for that latitude and month. The purpose of the weighting is to more closely approximate an area-weighted average.

The sampling errors are estimated by sub-sampling an atmospheric model (ECMWF operational forecasts in the present validation, ERA5 reanalysis forecasts in the operational setting) at the observed times and locations. Based on these estimates, we do a sampling-error correction, or adjustment, by subtracting the estimated sampling errors from the observed means [RD.12,13,16]. The errors remaining after the sampling-error correction are referred to as residual sampling errors.

The uncertainty of the monthly mean is estimated as a combination of the per-profile measurement uncertainties and the uncertainties due to the residual errors remaining after the sampling-error correction [RD.6]. In principle, there is also a structural uncertainty due to algorithmic choices and underlying processing assumptions, but these are not explicitly quantified by the ROM SAF Level 3 algorithms. However, the ROM SAF has participated in activities with the explicit purpose to quantify structural uncertainties by comparing independent processing of the same input data. Results from these studies have been published in the scientific literature [RD.15,16].

In summary, the RO Level 3 gridded data products are generated by the following steps:

1) quality control and flagging of profiles that are identified as non-nominal (‘bad’)
2) vertical interpolation of profiles onto a regular Level 3 height grid
3) weighted averaging into monthly latitude bins
4) estimation of sampling errors in the monthly means
5) estimation of uncertainties (measurement and sampling) in the monthly means
6) estimation of *a priori* information in the monthly means
7) formatting of the Level 3 gridded data and meta-data into netCDF files

The generation of zonally gridded monthly mean data is followed by further averaging into seasonal and annual means, and into regional, hemispheric, and global means.

The Level 3 NTC gridded data, which are validated in the present document, were retrieved with the ROMCLIM-1.3 software.

2.5 Quality control of profiles

The purpose of the quality control is to identify profiles that are likely to provide an invalid representation of the atmosphere. Before processing the atmospheric profiles into gridded monthly-mean data, all profiles are checked against a set of criteria indicating non-nominal conditions (listed in Table 2). Some of these criteria are seldom met – they are only a basic sanity check to ensure that corrupt data do not affect the climate data (*QC-0*). Other tests are designed to identify occultations with degraded bending angles (*QC-2*), that could be regarded as outliers (*QC-3*), or that have problems with the 1D-Var processing (*QC-4*).

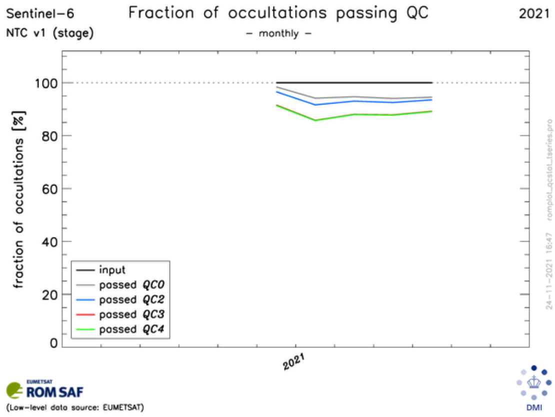

Figure 4. *Fraction of occultations available for the Level 3 gridded data generation, after the consecutive QC steps during the 5-month period June to October 2021. QC-0 is a fundamental sanity check of bending-angle and refractivity profiles, QC-2 is a check based on the SO quality scores, QC-3 consists of systematic removal of outliers through comparison with ERA5, and QC-4 is a check on the 1D-Var solution.*

The first step (*QC-0*) in the quality screening procedure is a basic check to ensure that the bending angle and refractivity profiles have the required quality. Bending angles are checked through the QC provided by the EUMETSAT Secretariat, with the requirement that they must be nominal. Refractivities must reach above an altitude of 60 km and below 20 km, all values must fall within the range 0 to 500 N-units, and the altitude series must vary monotonously.

In the next step (*QC-2*), the bending angle quality is checked through the two *SO scaling factors* which quantify the degree of fit to a background bending angle profile. This QC step also includes a requirement that the background bending-angle data should only play a minor role below 40 km altitude, which is indicated by the *LC weighting factor*.

The next QC step (*QC-3*) removes data identified as outliers. This is done by comparing the observed bending angles, refractivities, and dry temperatures to ECMWF reanalysis data within specified height intervals.

If an occultation does not pass one or several of the above tests, the bending angle, refractivity, and dry variables are marked as non-nominal. Otherwise, they are regarded as nominal, and the refractivity profiles are passed on to the 1D-Var processing. This is followed by another QC step (*QC-4*) which checks the quality of the 1D-Var solution. The impacts of a sequential application of the QC tests are shown in Figure 4. For Sentinel-6, around 10-12% of the occultations with an associated EUMETSAT netCDF-4 file are rejected, which is similar to the rejection rate for Metop Offline data.

Table 2. *Summary of the ROM SAF quality control of the Level 1 and 2 data used as input to the Level 3 processing. QC-1 is currently not used operationally.*

QC-0: basic sanity check
Identification of occultations with too small vertical extension, too few useful data points, the presence of invalid data points, or height variables that form a non-monotonous series.
- $\alpha(H_a)$ must be nominal as provided by the EUMETSAT Secretariat - H_a values must form a monotonous series - $N(H)$ must reach below 20 km and above 60 km - $N(H)$ values must fall within valid range: [0,500] N-units - H must form a monotonous series
QC-1: (not used)
QC-2: bending angle quality
Checking of a) the quality of the bending angles, as quantified by the noise on the L2 impact parameter series, b) the fit of the raw LC bending angle to a background bending angle profile, and c) that the background bending-angle data only play a minor role below 40 km altitude.
- SO scaling factor 1 must fall in the interval [0.92,1.08] - SO scaling factor 2 must fall in the interval [0.60,1.40] - LC weighting factor must be larger than 0.90 below 40 km altitude
QC-3: identification of outliers
Identification of outliers by comparing with ECMWF reanalysis data mapped to refractivity, bending angle, and dry temperature.
- N must deviate from reanalysis by less than 10% between 5-35 km - N must deviate from reanalysis by less than 20% below 5 km - T_{DRY} must deviate from reanalysis by less than 20 K between 30-40 km
QC-4: quality of 1D-Var solution
Identification of occultations that have problems converging at an acceptable 1D-Var solution.
- the 1D-var algorithm must converge within 25 iterations - the penalty function $2J/N_{obs}$ must be smaller than 5.0 at convergence

3. Gridded data comparisons

The purpose of the validation is to demonstrate that the ROM SAF NTC Level 3 monthly-mean data products have the expected quality and characteristics, and that the Level 3 data products meet the formal requirements as stated in the ROM SAF Product Requirements Document (PRD) [*AD.3*]. The latter is done by demonstrating that the gridded monthly mean data are consistent with the reference data (here, ECMWF operational forecasts), using the methods and accuracy specifications described in the PRD.

The Level 3 data set to be validated contains eight geophysical variables distributed over latitude and height. The data used in the validation only covers a limited time period of 4 months, which obviously is not enough to cover the whole seasonal cycle. Some selection of data and properties to be investigated is also required. In the present validation report we have chosen to discuss the following:

- Comparison of Sentinel-6 NTC gridded monthly-mean data with the corresponding ECMWF operational forecast data (Section 3.1)
- Comparison of Sentinel-6 NTC gridded monthly-mean data with the corresponding Metop Offline data (Section 3.2)

3.1 Comparison with ECMWF operational forecast data

In this section, the ROM SAF NTC Level 3 monthly-mean data are compared to the corresponding means generated from co-located ECMWF operational short-term forecasts.

There are a few issues to consider when comparing observed RO data with Numerical Weather Prediction (NWP) data. First, RO data are commonly assimilated by the ECMWF NWP system [RD.11], although that does not seem to be the case for Sentinel-6 data at the time of writing this report. Second, the ECMWF short-term forecasts have been used as *a priori* data in the ROM SAF 1D-Var retrieval of temperature and humidity profiles [RD.4]. These two factors complicate the choice of reference for the comparison. We have chosen to use ECMWF *short-term forecast data* as reference. By using forecast data, we avoid comparison of two data sets containing the same observational data, which would be the consequence of using ECMWF analysis data as reference. However, the ECMWF operational forecasts have a significant influence on the comparison of geophysical variables obtained by 1D-Var retrieval – temperature and humidity – particularly at altitudes and/or latitudes where the background information dominates the 1D-Var solution.

Throughout the RO-NWP comparison it should be acknowledged that ECMWF data is not the truth. In some cases, we are able to spot problems with the NWP data from differences with respect to the observational RO data. The RO–NWP comparisons can also be used to check the consistency of data from different RO missions or different RO satellites, and they are further used to demonstrate the formal compliance with the ROM SAF PRD requirements (Section 4).

In Section 3.1.1 we show RO–NWP time-averaged differences on a latitude-height cross-section for all eight variables up to 50 km (the humidity only up to 12 km). In Section 3.1.2 we show RO–NWP difference time-height plots for four geophysical variables (bending angle, refractivity, dry temperature, and humidity) in five latitude bands as well as for globally averaged data.

3.1.1 Sentinel-6–NWP differences on latitude-height cross section

In Figure 5 we show the spatial pattern of differences between RO data and ECMWF operational forecasts obtained by time averaging over the 4-month time series, from June to September 2021. We do this averaging for all 8 geophysical variables included in the NTC Level 3 data product.

Note that since we only assess a 4-month time period, it is possible that some of the biases are seasonally varying and that averaging over complete seasonal cycles would reduce them.

The dominant feature in the refractivity plot is a positive bias extending between 35 and 50 km and covering nearly all latitudes except for the very highest altitudes and latitudes. The corresponding bias features are clearly evident also in the dry variables (pressure, temperature, geopotential height). Above 40 km, at low- and mid-latitudes, dry temperature is biased 2 K relative to the ECMWF operational forecasts. In the lower troposphere we find negative biases in both bending angle and refractivity, largest at low and mid-latitudes and gradually smaller toward higher latitudes.

The 1D-Var temperatures show a characteristic banded bias pattern that we also saw in previous validations of Reprocessed and Offline data. Note that a) the temperature plot is essentially a 1D-Var *solution minus background* plot, and b) the bias pattern has very much smaller amplitude than the other panels shown in Figure 5. The humidity biases are dominated by negative biases at mid-latitudes and weak, positive biases at low latitudes. The extents to which these biases represent seasonal effects are unclear.

The tropopause heights based on dry temperatures lapse rate exhibit a characteristic pattern with relatively large, negative biases at mid-latitudes, while the tropopause heights based on the bending angle profiles are more uniform with latitude. The tropopause heights based on refractivity fall somewhere between these two cases. The negative biases may be caused by a systematic bias towards identification of the lower tropopause in regions with multiple tropopauses. It should also be pointed out that the large negative biases at high southern latitudes may be a seasonal phenomenon caused by the thermal tropopause not being well-defined. Such a tendency to large negative biases (relative to ERA5) at high southern latitudes around southern hemisphere mid-winter is seen in Metop Offline data.

Sentinel-6 – NWP

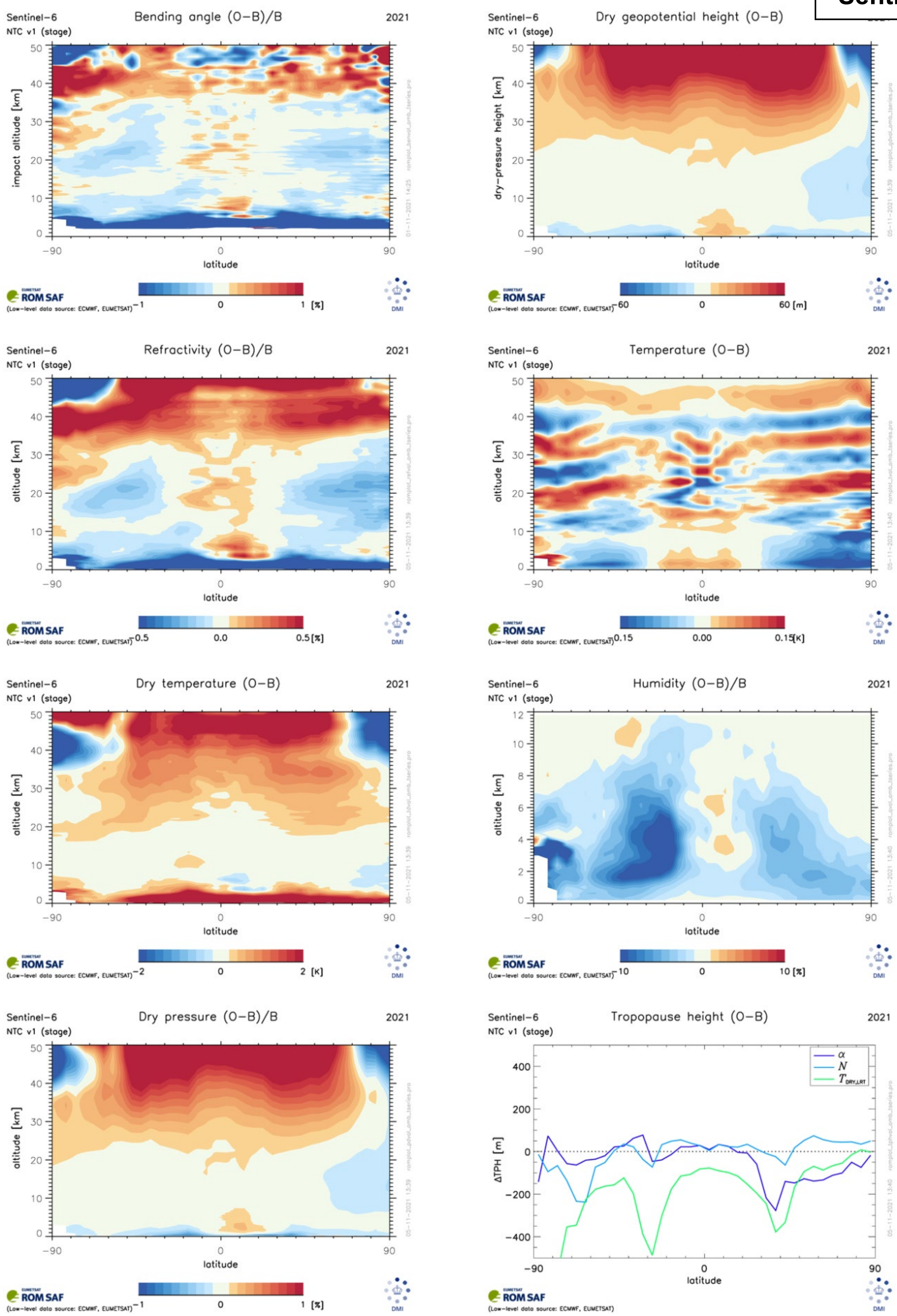

***Figure 5.** Sentinel-6–NWP differences on a latitude-height cross-section. The time averages are computed for the 4-month period June to September 2021.*

3.1.2 Sentinel-6–NWP difference time-height plots

In Figs. 6a-d we show spatial averages of RO-NWP differences in five latitude bands as well as globally. The data are presented as time-height plots extending up to 50 km (except for humidity which is only provided up to 12 km) and covering the time period from June to September 2021. Data are shown for bending angle, refractivity, dry temperature, and humidity.

In bending angle (Fig. 6a), the dominating feature is a positive bias extending between 35 and 45 km. In refractivity (Fig. 6b) and dry temperature (Fig. 6c) we also find positive biases above 35-40 km, except for the polar upper stratosphere where the biases are mostly negative. In the refractivity low-latitude panel (Fig. 6b, lowest panel) there is a pattern that may be part of a 2-month oscillation. This is consistent with findings in the Level 2 validation and may be related to the 4-month nodal precession cycle of the Sentinel-6 satellite orbit.

In 1D-Var humidity (Fig. 6d), negative biases are clearly dominating, with peaks at mid-latitudes around 4 km, and also a peak at high southern latitudes in association with the Antarctic plateau.

In previous validations, we found pronounced seasonal cycles in the bias structures and we can expect that to be the case also for the NTC data. However, because of the short validation time series – only 4 months – we cannot presently say very much about it.

Sentinel-6 – NWP
Bending angle

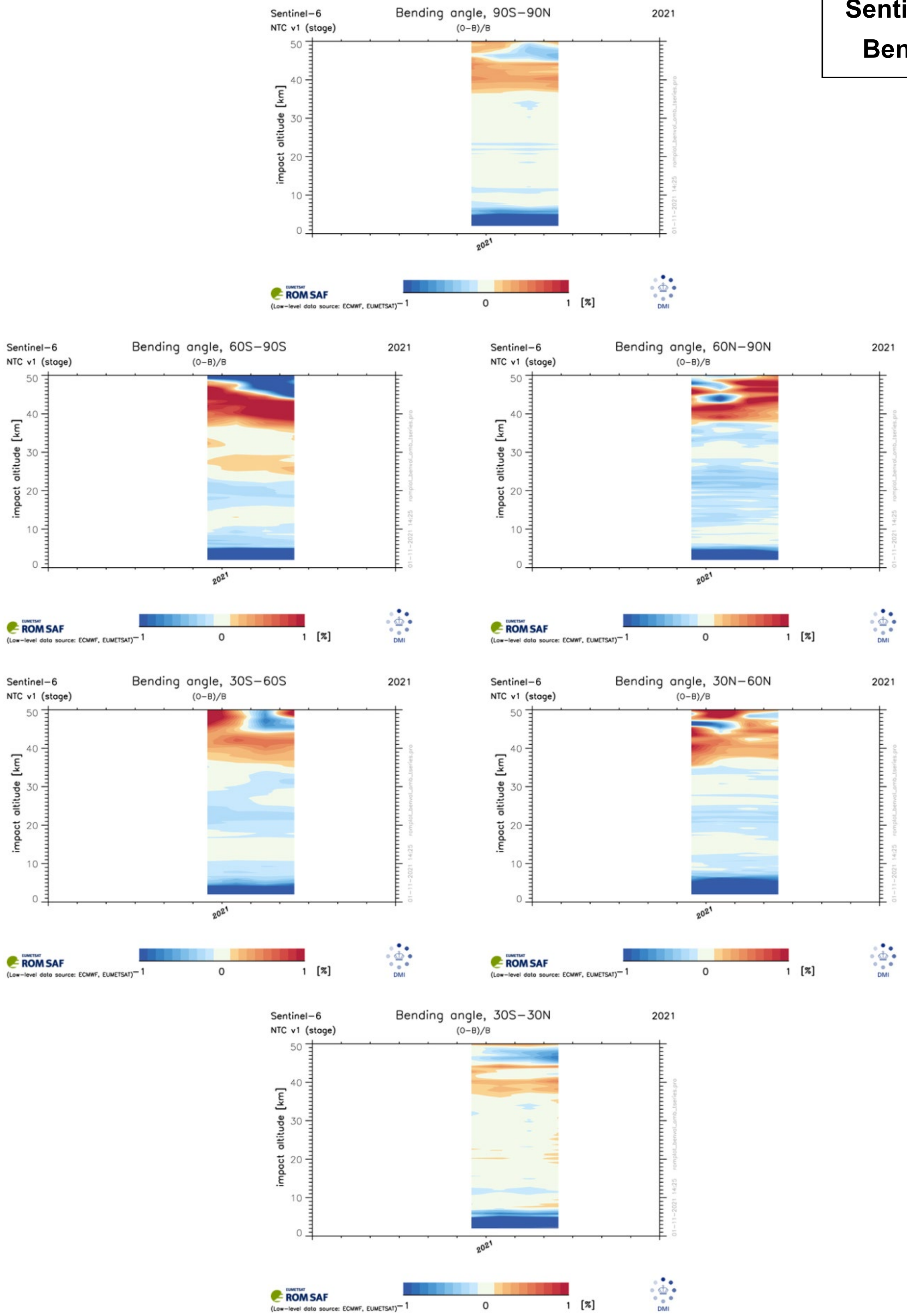

Figure 6a. *Sentinel-6–NWP bending angle differences for the 4-month period June to September 2021. The Level 3 monthly-mean Sentinel-6 NTC data have been aggregated into five latitude bands plus global data.*

Sentinel-6 – NWP Refractivity

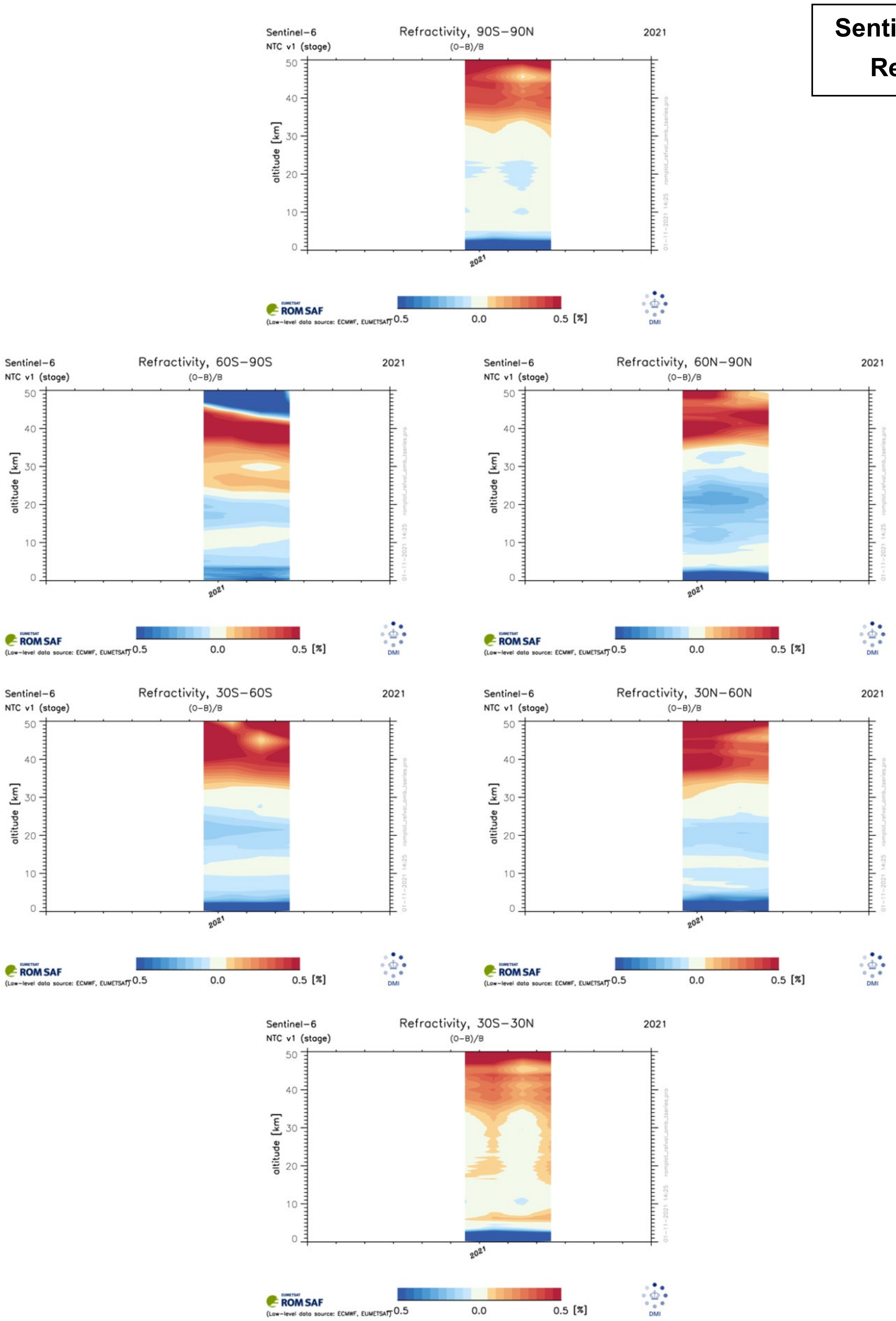

Figure 6b. *Sentinel-6–NWP refractivity differences for the 4-month period June to September 2021. The Level 3 monthly-mean Sentinel-6 NTC data have been aggregated into five latitude bands plus global data.*

Sentinel-6 – NWP
Dry temperature

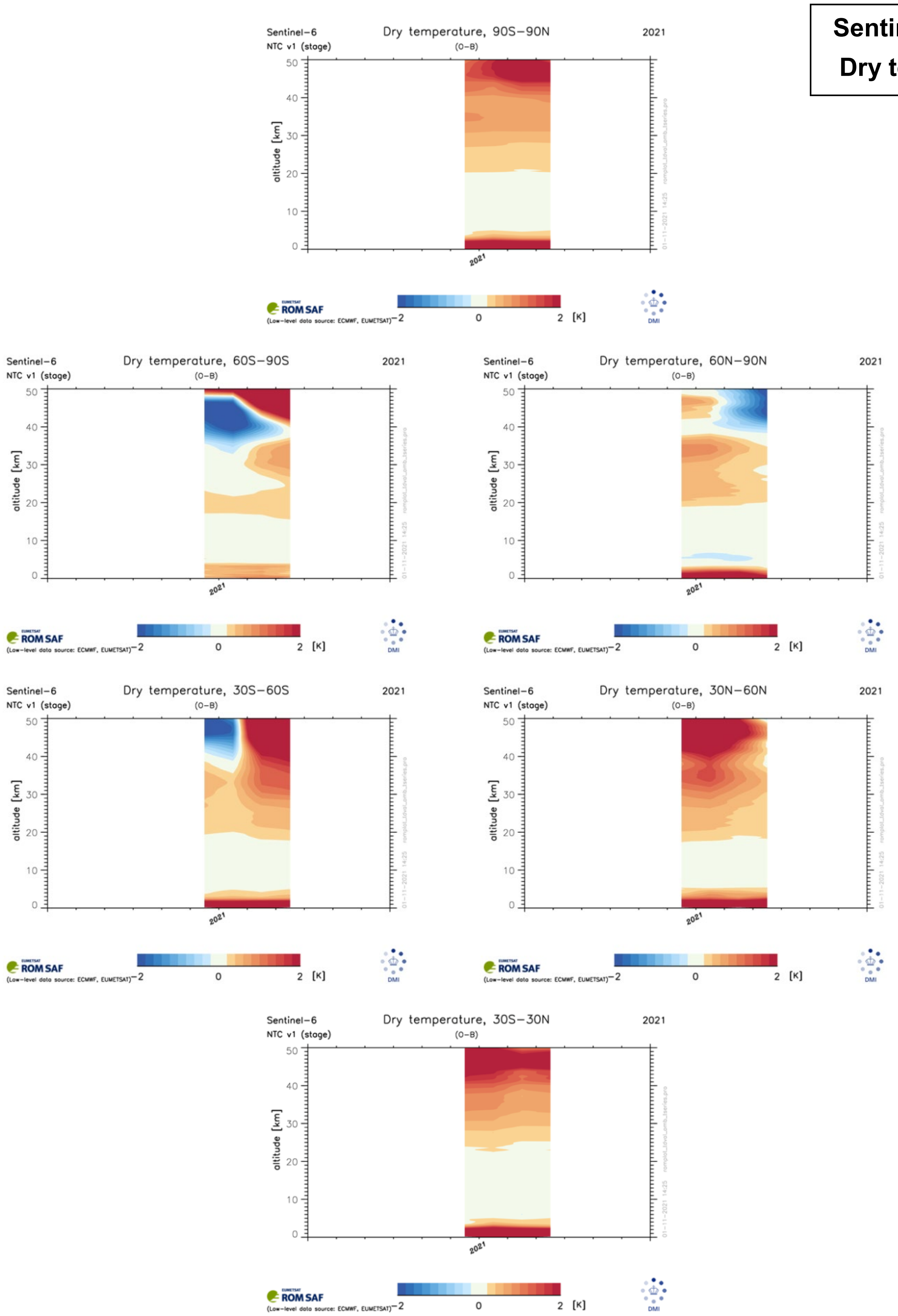

Figure 6c. *Sentinel-6–NWP dry temperature differences for the 4-month period June to September 2021. The Level 3 monthly-mean Sentinel-6 NTC data have been aggregated into five latitude bands plus global data.*

Sentinel-6 – NWP Humidity

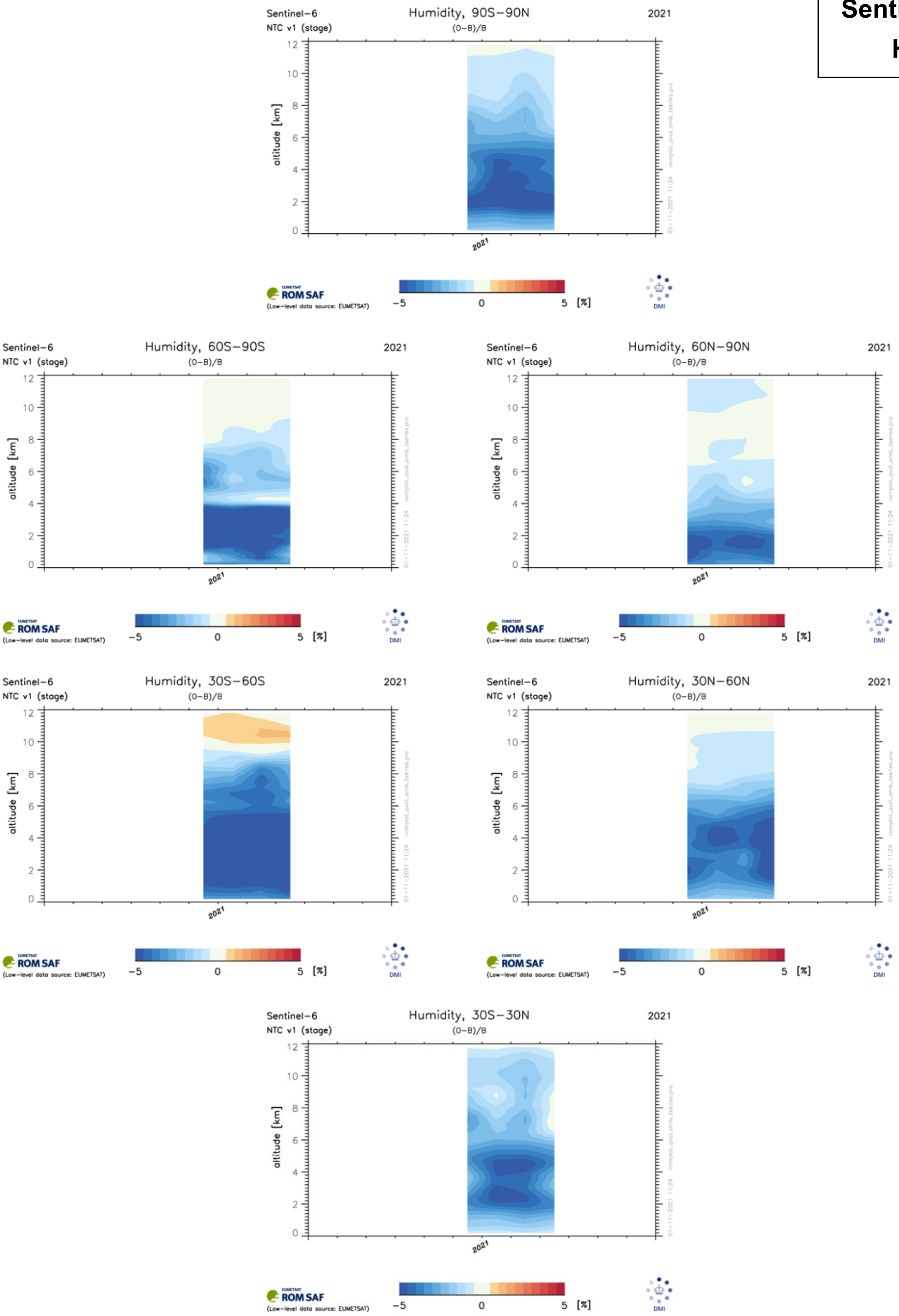

Figure 6d. *Sentinel-6–NWP humidity differences for the 4-month period June to September 2021. The Level 3 monthly-mean Sentinel-6 NTC data have been aggregated into five latitude bands plus global data. The humidity profiles are retrieved by 1D-Var processing.*

3.2 Comparison with Metop Offline data

In this section, the Sentinel-6 NTC gridded monthly-mean data are compared to the corresponding Metop Offline data.

There is an expectation that data from different RO instruments, and different RO missions, should have sufficiently small systematic differences to allow data to be merged into longer time series [RD.17]. In the altitude range from the lower troposphere up to 30 km – for bending angle up to 40 km – we expect the cross-mission biases to be small.

Such cross-mission biases could be investigated from the relatively rare cases when two RO instruments happen to measure roughly the same volume of the atmosphere. Here we instead take the approach that by using an atmospheric model (here, ECMWF operational forecasts) we can remove the influence of sampling effects, and thus directly compare monthly averages computed from two different missions. The same approach is used in *sampling-error correction* of gridded monthly mean data. An underlying assumption is that the relevant modes of atmospheric variability are correctly described by the model. Should, for example, the diurnal cycle be incorrectly described, a residual sampling error would remain when comparing two missions that sample the diurnal cycle differently, like Sentinel-6 and Metop.

Hence, we assume that the sampling errors are correctly described by the model. These errors are B_{SE6}-B_{GRID} and B_{MET}-B_{GRID}, respectively for the two satellite missions, where B_{SE6} and B_{MET} are model (”background”) means computed from data collocated with the observed RO profiles, and B_{GRID} is the model mean based on the full model grid.

Mission differences between sampling-error corrected monthly mean data can now be formulated as $(O_{\mathrm{SE6}} - B_{\mathrm{SE6}}) - (O_{\mathrm{MET}} - B_{\mathrm{MET}})$, where O_{SE6} *and* O_{MET} are the observed means for the two satellite missions.

In Section 3.2.1 we show Sentinel-6–Metop time-averaged differences on a latitude-height cross-section for bending angle, refractivity, and dry temperature, and discuss the RO mission biases detected.

3.2.1 Sentinel-6–Metop differences on latitude-height cross section

In Figure 7 we show the spatial pattern of differences between Sentinel-6 NTC monthly mean data and the corresponding Metop Offline data. The differences shown are time averages over 3 months from June to August 2021 (Metop Offline data for September were not available at the time of writing this report). In the following, we discuss the differences for bending angle, refractivity, and dry temperature.

The Sentinel-6–Metop differences in bending angle are small up to 40 km. They are predominantly below 0.1% over a broad low- and mid-latitude span. At high latitudes the differences tend to be slightly larger, but still mostly below about 0.3% up to 40 km. Above 40 km, the differences are larger with a tendency to a large-scale north-south asymmetry. This is most likely attributed to Metop data where an hemispherically asymmetric bias structure was identified in the validation of the ROM SAF Reprocessed data [RD.7] as well as in the validation of the ROM SAF Offline data [RD.8]. From the comparisons between Sentinel-6 and ECMWF operational forecasts (Section 3.1), there are no indications of a similar asymmetry in Sentinel-6 data.

The differences in refractivity are consistent with the bending angle differences, with the biases propagated downward in the processing from bending angle to refractivity. Up to 30-35 km the differences are mostly smaller than 0.1%. At higher altitudes and latitudes, the mission differences become larger, but they are still below 0.5% well above 40 km.

The dry temperature differences are consistent with the picture given above. The mission differences are further propagated downward, and the north-south asymmetry is even further pronounced. At an altitude of 25 km, the differences are mostly below 0.2 K.

In the lower troposphere we find a negative bias in bending angle and refractivity for Sentinel-6 relative to Metop, The biases are largest at low latitudes and become gradually smaller at higher latitudes, except for Antarctica where the mission differences once again is larger than in the surrounding mid-latitudes. Dry temperature is consistent with this picture.

Sentinel-6 – Metop

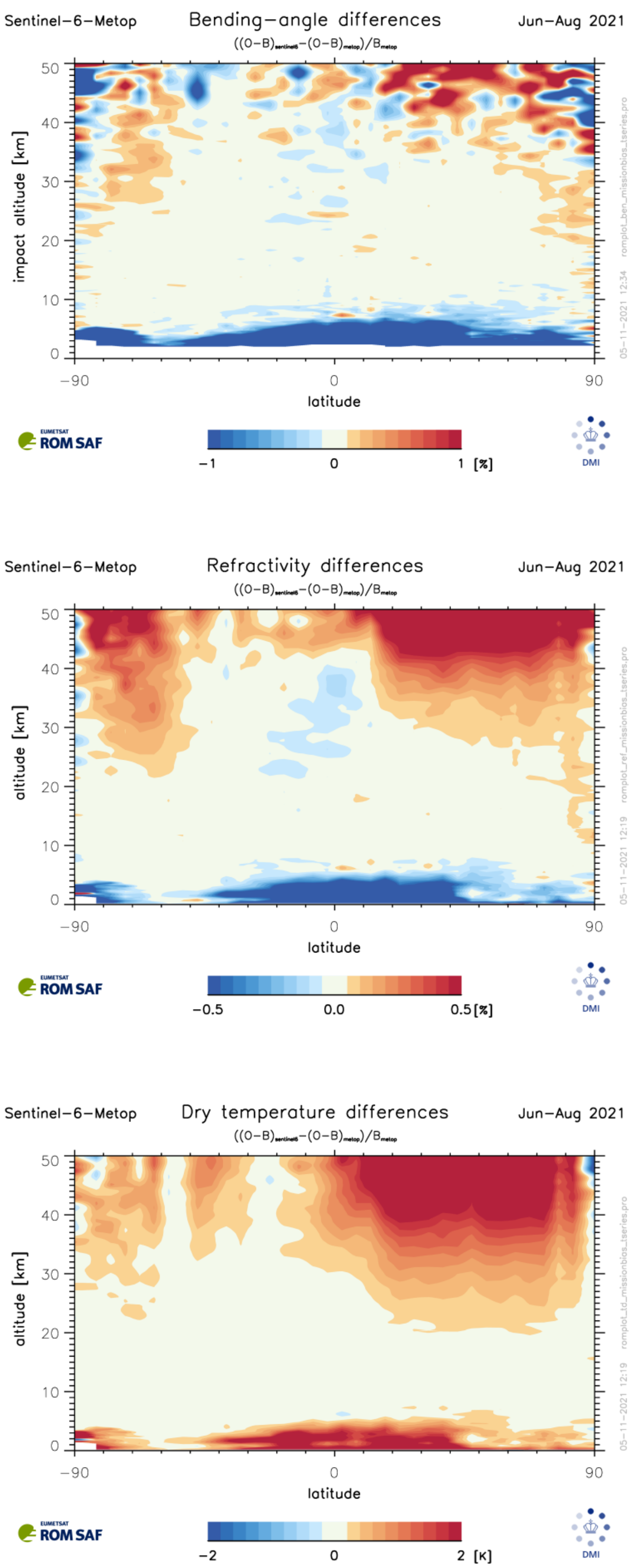

Figure 7. *Sentinel-6–Metop sampling-error corrected differences on a latitude-height cross-section. The time averages are computed for the 3-month period June to August 2021.*

4. Compliance with product requirements

The product requirements express the commitment of the ROM SAF team for the development of data products. The formal requirements for the ROM SAF data products are stated in the PRD [AD.3]. There are three sets of accuracy requirements (*threshold*, *target*, and *optimal*). The requirements are defined as functions of height (except for the tropopause height requirements). In the present report, the PRD accuracy requirements are colour coded: orange for *threshold*, yellow for *target*, and green for *optimal*. Data that do not reach the threshold are coded with *red* colour.

The compliance with the PRD accuracy requirements is determined in the following way. First, we define 3 latitude regions: tropics (30˚S–30˚N), mid-latitudes (30˚N–60˚N and 30˚S–60˚S), and polar (60˚N–90˚N and 60˚S–90˚S), and 3 altitude regions: low (0-8 km), middle (8-20 km), and high (20-50 km). That defines 9 broad latitude-height regions. Each of these 9 regions includes several hundred monthly values (though not independent, the data are more or less strongly correlated). For each observed monthly value, we compute the absolute deviation from collocated ECMWF operational forecast data, |O-B|, and determine whether the absolute deviation is smaller than the threshold, target, or optimal accuracies. We then *determine the PRD compliance, for each one of the 9 latitude-height regions, by requiring that at least 60% of the monthly mean data within that region reach the corresponding accuracy*. This quantity is also used in the definition of the Service Specifications (Section 6).

It should be noted that here is a degree of circularity arising from the fact that the ECMWF short-term forecasts have been used as *a priori* data in the ROM SAF 1D-Var processing of temperature and humidity data. At altitudes and/or latitudes where the background information dominates the 1D-Var solution, ECMWF data have a significant influence on the RO-NWP comparison of 1D-Var temperature and humidity. However, even though the differences found in the comparisons cannot be naively interpreted as an expression of errors in the ECMWF or RO data, such comparisons can nevertheless be useful to detect unexpected anomalies in the operational retrievals.

In Figure 8, we present plots of the formal compliance with the PRD requirements for all eight geophysical variables for the Sentinel-6 NTC Level 3 data. An addition check of the Tropopause Height Grid (GRM-195), covering a longer time period, is found in Annex A.

We consider all ROM SAF NTC Level 3 data products to be compliant with the PRD requirements. The lowest degree of compliance is found for the tropopause heights (where we find a single red cell in Figure 8), and to some extent the dry variables at low and mid-latitudes between 40-50 km. These are regions where some biases relative to ECMWF data are to be expected. A certain degree of seasonality in the compliance is also expected, particularly at high altitudes. The additional validation, described in Annex A, confirms the compliance of the Level 3 tropopause height product.

We conclude that the ROM SAF NTC Level 3 monthly mean data products are formally compliant with the PRD requirements.

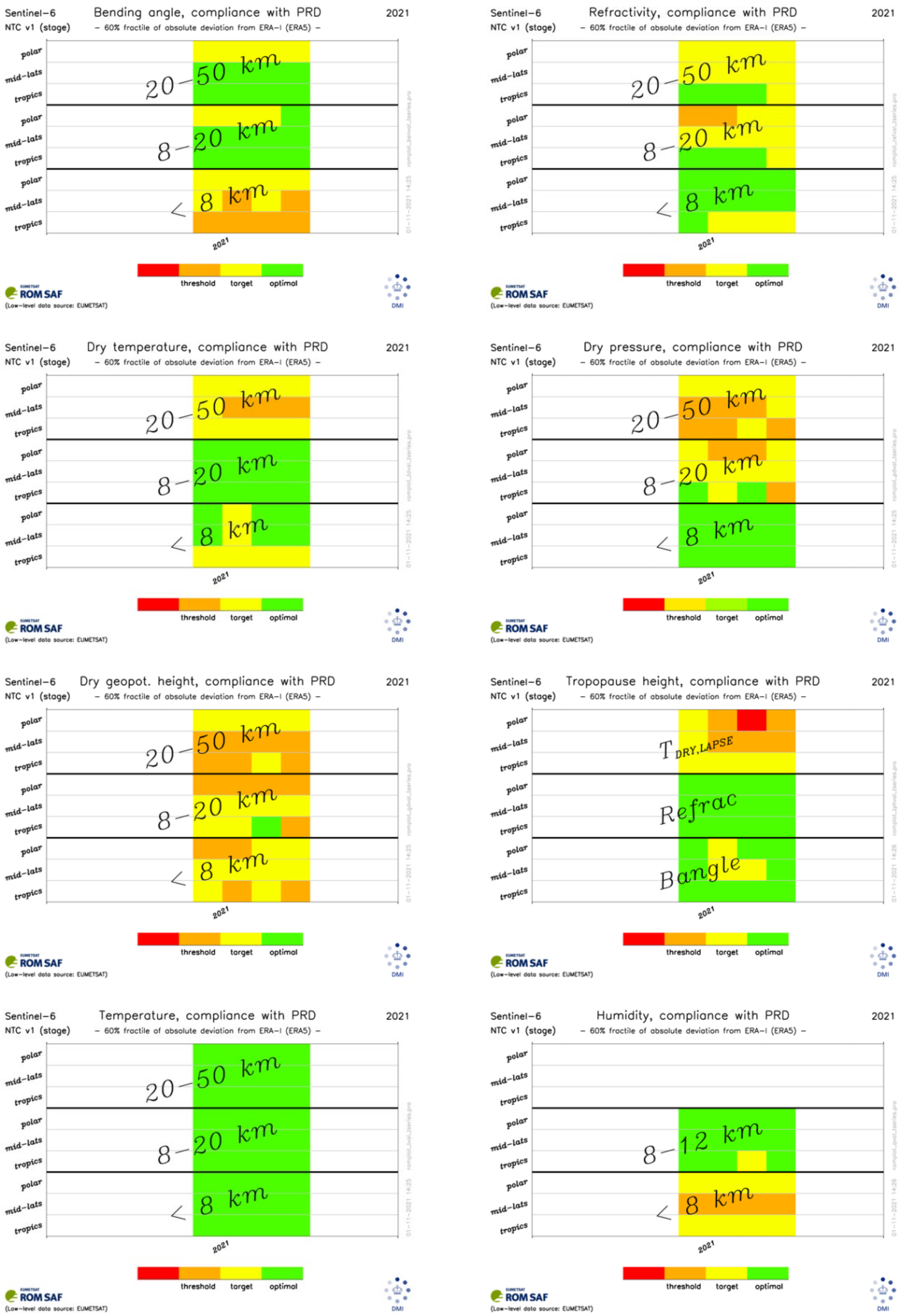

Figure 8. *Compliance with the PRD requirements of the Level 3 Sentinel-6 NTC data, based on the |O-B| distributions within 9 latitude-height regions. Red colour indicates non-compliance. There were only 4 months available for validation (June to September 2021).*

5. Service Specifications

The Service Specifications describe the commitments by the ROM SAF related to the services and products provided to the users. These commitments include a set of operational accuracy targets that should be met by the Level 3 gridded data products, and which should be regularly monitored and documented as a part of normal operations.

The accuracies proposed to be included in the service specifications for the Level 3 NTC data products are listed in Table 3. The methods used for comparing RO data with the service specifications are identical to the methods defined in the PRD. Compliance is determined by requiring that *a certain percentile of the Level 3 grid point values have absolute deviations from ECMWF operational forecast data smaller than the corresponding specifications* as stated in the Service Specifications Document. We use the 60% percentile, similar to the PRD. Hence, the service specifications for the NTC data are identical to the *target accuracies* in the PRD requirements. The outcome of the regular monitoring against the service specifications is provided on the ROM SAF web page.

Table 3. *Proposed Service Specifications for the ROM SAF NTC Level 3 data products. The accuracies are stated separately in three height layers; below 8 km, 8-25 km, and 25–50 km (for humidity only up to 12 km). Where both absolute and relative numbers are given, the requirement is given by the greater of these two.*

GRM-123–129, GRM-195 (Sentinel-6)
Bending angle
25 – 50 km: 0.3 % or 0.6 μrad[1] 8 – 25 km: 0.3 % 0 – 8 km: 3.0 – 0.3 %
Refractivity
25 – 50 km: 0.12 % or 0.006 N-units[1] 8 – 25 km: 0.12 % 0 – 8 km: 1.2 – 0.12 %
Dry temperature
25 – 50 km: 0.3 – 3.0 K 8 – 25 km: 0.3 K 0 – 8 km: 1.5 – 0.3 K
Dry pressure
25 – 50 km: 0.12 – 0.60 % 8 – 25 km: 0.12 % 0 – 8 km 0.60 – 0.12 %
Dry geopotential height
25 – 50 km: 6 – 60 m 8 – 25 km: 6 m 0 - 8 km: 6 m
Temperature
25 – 50 km: 0.3 – 3.0 K 8 – 25 km: 0.3 K 0 – 8 km: 1.0 – 0.3 K
Specific humidity
8 – 12 km: 4.0 % 0 – 8 km: 4.0 %
Tropopause Height
200.0 m
[1] Whichever is greater. [2] An accuracy interval means a linearly changing quantity between the two values over the given height interval.
Methods for validation
Nine broad latitude-height regions (tropics, mid-latitudes, high latitudes and low, middle, high altitudes) are defined. The absolute values of the differences between the monthly-mean RO data and the ECMWF operational forecast data are computed on the Level 3 grid, and each grid point value is compared to the service specification valid for that altitude. The compliance with the Service Specifications is determined, within each region and for each calendar month, by requiring that 60% of the Level 3 grid point values have absolute differences smaller than the corresponding specification.

6. Conclusions

We conclude that the ROM SAF Sentinel-6 NTC Level 3 gridded monthly mean data are of high quality, that they meet the expectations we have on ROM SAF data products, and that they comply with the product requirements as stated in the PRD [AD.3]. The issues that were detected during the validation, and that requires further investigations, are not of a character that prevent the data products from being released. These issues are described in Section 6.1 below.

6.1 Limitations

As a result of the validation activity a few issued appeared. These are:

- In certain latitude regions, the tropopause heights based on dry temperature lapse rate are consistently negatively biased relative to ECMWF forecasts as well as relative to the tropopause height based on the bending angle profile. This bias is related to the transition from the low-latitude tropopause to the mid/high latitude tropopause, a region where we frequently find multiple tropopauses.

- The dry-temperature lapse rate tropopause height is often negatively biased at high southern latitudes during southern hemisphere winter. This is part of a seasonal pattern, which may be related to the Antarctic thermal tropopause occasionally becoming less well-defined. The persistence, seasonality, and underlying cause of these biases, as well as how they are manifested in the different definitions of tropopause height, should be further investigated.

- There are relatively large negative biases in the 1D-Var humidity retrievals at high southern latitudes, apparently concentrated to the Antarctic plateau. The persistence and underlying cause of these biases should be further investigated.

ANNEX A: Additional validation of the Level 3 tropopause height product (GRM-195)

During the ORR16 review for the Sentinel-6 NTC products, it was decided that the Level 3 tropopause height product GRM-195 should have status as pre-operational until further validation could be done using a longer time period (formulated as ROM SAF Steering Group action SG27-Act-03). The result of the extended validation is shown in Figure A-1. After detecting a non-compliant value for the polar regions during August 2021 in the pre-operational period (Fig. A-1, left-hand panel), the following months are compliant for all regions, and the degree of compliance improves with time (Fig A-1, right-hand panel).

Based on this additional validation, we conclude that the Level 3 tropopause height product GRM-195 is compliant with the product requirements as stated in the PRD [AD.3].

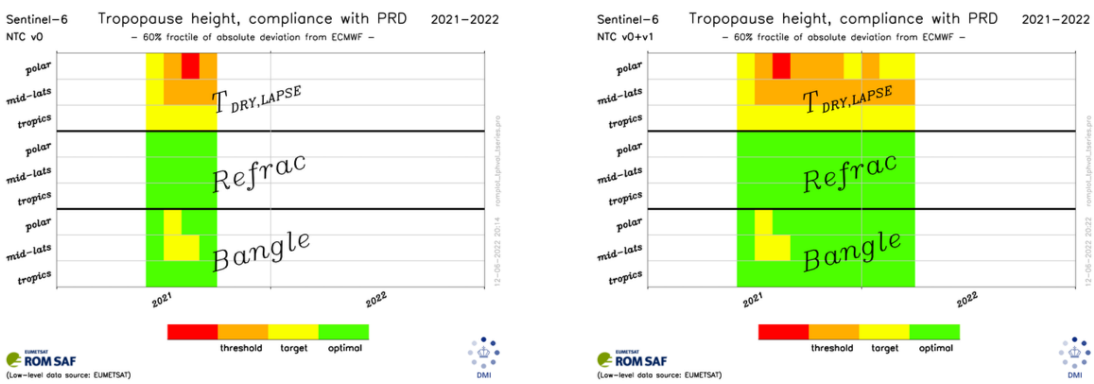

Figure A-1. *Compliance with the product requirements of the Level 3 tropopause height product GRM-195, based on the |O-B| distributions within 9 latitude-height regions. The left-hand panel shows the validation during the original time period (June – September 2021), while the right-hand panel shows the validation during the extended time period (June 2021 to March 2022). Red colour indicates non-compliance.*