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**EUROPEAN SPACE AGENCY
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AMENDMENT RECORD

This document shall be amended by releasing a new edition of the document in its entirety. The Amendment Record Sheet below records the history and issue status of this document.

AMENDMENT RECORD SHEET

ISSUE	DATE	REASON FOR CHANGE
Phase-I		
1	01 Apr 2011	First issue
2	11 Nov 2011	Amended following comments from ESA (Craig Donlon)
3	15 Mar 2013	Amended by S. Good following comments from project team
Phase-II		
1	11 Apr 2014	Correction of issues identified in Phase-I of the project and update to show Phase-II products (Simon Good)
1P	5 May 2017	Updated to reflect most recent Phase-II plans and URD updates
2	9 May 2017	Issued to ESA for review

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1. INTRODUCTION

1.1 Purpose and Scope

1.1.1 Purpose

This document provides descriptions and specifications of version 2.1 products that shall be produced by the sea surface temperature (SST) climate change initiative project (SST CCI) Phase-II, which is part of the European Space Agency (ESA) Climate Change Initiative (CCI). The specifications were originally developed from user requirements defined in the SST CCI User Requirements Documents [RD.171, RD.385, RD.393] and have subsequently been revised following experience gained within the project and from users making use of the data. SST CCI Phase II plans are to produce version 2.1 SST products as follows:

- Gridded, 0.05° resolution, swath-based, SSTs from Along Track Scanning Radiometer (ATSR) and Advanced Very High Resolution Radiometer (AVHRR) satellite data ("L3U", see Section 2 for definition).
- 1 and 4-25 km resolution swath-based SSTs from ATSR and AVHRR satellite data respectively ("L2", see Section 2 for definition).
- Analyses (gap-filled products) combining the ATSR and AVHRR data streams (gridded at 0.05° resolution, daily, "L4", see Section 2 for definition).

SST anomalies are also provided within the L2 and L3U files for retrievals from the infrared sensors as additional information. Separate products containing information on SST anomalies for the L4 are also provided and specified here. These anomalies are defined as deviations from a reference climatology calculated over the period 1981-2010.

The specifications contained in this Product Specification Document (PSD) provide a complete description of the products, including the definition of file level metadata. Specifications are defined for L2, L3U and L4 data files. These are all based on (and extend) the Group for High Resolution SST (GHRSSST) Data Specification version 2.0 (GDS2.0; document revision 2.007) [AD.1], are specified to be maximally compatible with the climate and forecasting (CF) conventions [RD.177] and include the metadata specified by the CCI Data Standards Working Group (DSWG; [RD.215]).

Additionally, prototype products including information from microwave instruments for the period 2002 to 2016 have been developed and are also described in this document:

- 10km and 35km x 61km resolution swath-based SSTs from Advanced Microwave Scanning Radiometer - Earth Observing System (AMSR-E) and Advanced Microwave Scanning Radiometer-2 (AMSR-2)
- Analyses of all of the above data streams combined (ATSR, AVHRR, AMSR-E and AMSR-2, gridded at 0.05° resolution, daily).

1.1.2 Scope

This document covers the following aspects of requirement SST-TR-12 from the CCI Phase-I statement of work, annex G [RD.165] / SST-TR-25 from the CCI Phase-II statement of work, annex G [RD.369]:

- File metadata format and structure (Sections 2 and 4).
- Discovery metadata contained in the files and their structure (Sections 2 and 4)
- Long-term document revision control procedures (Section 1.2).
- Any other requirements relevant to SST ECV product specification (for example file format and naming convention; Table 2.0 and Section 3.2).

This document does not include in its scope the analysis of the error budget for translating input data to ECV products [RD.164]. This is reported in a separate document [RD.174].

Information is included to allow the reader to trace the product specifications defined in this document back to the user requirements, by referring to the user requirements document, [RD.393].

1.2 Document revision control

Document revision control is necessary to manage any changes to the product specifications and to retain a permanent record of when and where updates were made. The following principles will be followed in order to ensure that this occurs:

- Every release of the product specification document should be archived in a central project archive. The files should be protected from accidental change or deletion and backed up to a separate location.
- For every new release the version number should be incremented. The document naming convention established for the SST CCI should be used to ensure a unique file name for every version of the document.
- A summary of changes to the document and the person responsible for making the changes should be recorded in the relevant place at the beginning of the document.

Each new release must be approved by the project science leader or a person nominated by the project science leader.

1.3 Applicable Documents

The following is a list of documents that must be read in conjunction with this document. Where referenced in the text, these are identified as AD.n, where 'n' is the number in the list below:

- AD.1 GHRSSST Science Team, cited 2017: The Recommended GHRSSST Data Specification (GDS) Revision 2.0 Technical Specifications. [Available online at <https://www.ghrsst.org/wp-content/uploads/2016/10/GDS20r5.pdf>.]

1.4 Referenced Documents

The following is a list of documents with a bearing on the content of this report. Where referenced in the text, these are identified as RD.n, where 'n' is the number in the list below:

- RD.164 ESA Climate Change Initiative phase 1 – scientific user consultation and detailed specification – statement of work, Issue 1.4, Revision 1, 09/11/2009,

- Reference EOP-SEP/SOW/0031-09/SP;
http://earth.eo.esa.int/workshops/esa_cci/ao6207SoW.pdf
- RD.165 Annex G to RD.164, Sea Surface Temperature ECV (SST_cci)
- RD.166 Taylor, K.E. and C. Doutriaux (2010), CMIP5 Model Output Requirements: File Contents and Format, Data Structure and Metadata; http://cmip-pcmdi.llnl.gov/cmip5/docs/CMIP5_output_metadata_requirements.pdf
- RD.167 Rew, R., G. Davis, S. Emmerson, H. Davies, E. Hartnett and D. Heimbigner (2010), The NetCDF Users Guide; <http://www.unidata.ucar.edu/software/netcdf/docs/netcdf.pdf>
- RD.168 Climate Modelling User Group (2010), Requirement Baseline Document; http://dialspace.dial.pipex.com/prod/dialspace/town/estate/gtp89/cmug/D1.2_U RD_v1.3.pdf
- RD.169 ESA Climate Change Initiative – CCI project guidelines, Issue 1, Revision 0, 05/11/2010, Reference EOP-DTEX-EOPS-SW-10-0002
- RD.170 NetCDF Attribute Convention on Dataset Discovery (ACDD): <http://www.unidata.ucar.edu/software/netcdf-java/formats/DataDiscoveryAttConvention.html>
- RD.171 CCI Phase 1 (SST) (2010), User Requirements Document, Reference SST_CCI-URD-UKMO-001; http://www.esa-sst-cci.org/sites/default/files/documents/admin/public/SST_cci%20URD%20UKMO-001%20Issue%202.pdf
- RD.172 CCI Phase 1 (SST), Data Access Requirements Document (in preparation)
- RD.173 CCI Phase 1 (SST), Product Validation Plan (in preparation)
- RD.174 CCI Phase 1 (SST), Error Characterisation (in preparation)
- RD.176 Olsen, L.M., G. Major, K. Shein, J. Scialdone, R. Vogel, S. Leicester, H. Weir, S. Ritz, T. Stevens, M. Meaux, C. Solomon, R. Bilodeau, M. Holland, T. Northcutt and R. A. Restrepo (2007), NASA/Global Change Master Directory (GCMD) Earth Science Keywords Version 6.0.0.0.0; <http://gcmd.nasa.gov/Resources/valids/>
- RD.177 NetCDF Climate and Forecast (CF) Metadata Convention; <http://cf-pcmdi.llnl.gov/>
- RD.178 The UDUNITS-2 package; <http://www.unidata.ucar.edu/software/udunits/udunits-2/udunits2.html>
- RD.189 CCI Phase 1 (SST): Technical note on product metrics derived from the user requirements document

- RD.215 Bennett, V. (2010), Format and Metadata Guidelines for CCI Data Products (draft).
- RD.219 Donlon, C.J. et al. (2009), The GODAE High Resolution Sea Surface Temperature Pilot Project, *Oceanography*, 22(3), 34-45.
- RD.369 ESA Climate Change Initiative Phase 2 Statement of Work, prepared by ESA Climate Office, Ref. CCI-PRGM-EOPS-SW-12-0012, Issue 1, Revision 2, June 7th, 2013
- RD.385 SST_CCI User Requirements Document (URD), SST_CCI-URD-UKMO-201.
- RD.393 SST CCI User Requirements Document (2017) SST_CCI-URD-UKMO-201, <http://www.esa-sst-cci.org/PUG/documents>
- RD.400 Carrea, L., Embury, O. and Merchant, C. J. (2015) *Datasets related to in-land water for limnology and remote sensing applications: distance-to-land, distance-to-water, water-body identifier and lake-centre co-ordinates*. *Geoscience Data Journal*, 2 (2). pp. 83-97. ISSN 2049-6060 doi: 10.1002/gdj3.32

1.5 Definitions of Terms

The following terms have been used in this report with the meanings shown.

Term	Definition
AATSR	Advanced ATSR.
ACDD	Attribute Convention for Dataset Discovery.
AMSR-E	Advanced Microwave Sounding Radiometer – Earth Observing System
AMSR2	Advanced Microwave Sounding Radiometer 2
ATSR	Along Track Scanning Radiometer; the ATSR series of instruments comprises ATSR-1, ATSR-2 and AATSR.
AVHRR	Advanced Very High Resolution Radiometer.
CDL	Network Common Data form Language.
CF	Climate and Forecasting [conventions for metadata].
CMIP	Climate Model Intercomparison Project.
DSWG	CCI Data Standards Working Group
ECMWF	European Centre for Medium-range Weather Forecasts.
ECV	Essential Climate Variable.
ERA-Interim	ECMWF reanalysis ‘interim’ product.

ERS	European Remote Sensing satellite series (ERS-1, ERS-2).
GAC	Global Area Coverage.
GCMD	Global Change Master Directory.
GDS	GHRSSST Data Specification.
GMPE	GHRSSST Multi-Product Ensemble
GHRSSST	Group for High Resolution SST.
HDF4 and 5	Hierarchical Data Format version 4 and 5
IDL	Interactive Data Language.
ISO	International Organisation for Standardisation
L1B	Level 1 B data; the data collected by the satellite sensor with processing (for example calibration) applied.
L2P	Level 2 pre-processed data; geophysical variables at the full resolution of the instrument, in a satellite projection with associated geographical information
L3U	Level 3 uncollated data; gridded version of L2P data.
L3C	Level 3 collated data; L2P data from a single instrument that have been combined and mapped onto a space-time grid.
L3S	Level 3 super-collated data; L2P data from multiple instruments that have been combined and mapped onto a space-time grid.
L4	Level 4 data; a dataset formed by analysing lower level data to create a gridded product with no data gaps. The use of an infilling procedure to remove data gaps distinguishes L4 data from lower level data.
MATLAB	Matrix Laboratory
NetCDF	Network Common Data Format.
NWP	Numerical Weather Prediction.
Obs4MIPs	Observations for Model Intercomparison Projects.
OSI SAF	Ocean and Sea Ice Satellite Applications Facility.
OSTIA	Operational Sea surface Temperature and sea Ice Analysis.
RDAC	Regional Data Assembly Centre.
SSES	Single Sensor Error Statistics.
SST	Sea Surface Temperature.
SST CCI	SST climate change initiative [project].
SLSTR	Sea and Land Surface Temperature Radiometer.

TBC	To be confirmed.
URL	Uniform Resource Locator.
UUID	Universally Unique Identifier.
WGS	World Geodetic System.
XML	Extensible Mark-up Language.

2. PRODUCT OVERVIEW

An overview of the v2.1 products to be produced by the SST CCI Phase-II project is shown in Table 1. The table also records which satellite sensors will be used to create the products and the format of the input data. The final column indicates the level of data to be produced from each sensor and the resolution/grid spacing of the data in the files.

Table 1. Summary of SST CCI products, the source and level of data to be produced. L2 and L3 products contain data from a single sensor; L4 products will include data from multiple sensors.

Category of product and description	Satellite sensors & data to be used	Level of data to be produced for each sensor (resolution/grid spacing)
ATSR and full resolution Metop-A AVHRR SSTs for 1991-2016 retrieved from data obtained from the ATSR series of sensors (comprising ATSR-1, ATSR-2, AATSR and in future SLSTR) and also full resolution Metop-A AVHRR.	ATSR series (ATSR-1, ATSR-2, AATSR, SLSTR) (Envisat format) Full resolution Metop-A AVHRR (EUMETSAT format)	L2P (1km), L3U (0.05°)
AVHRR SSTs for 1981-2016 retrieved from data obtained from the AVHRR series of sensors.	AVHRR series global area coverage (NOAA GAC) data	L2P (4-25 km), L3U (0.05°)
AMSR-E Prototype SSTs for June 2002-October 2011 retrieved from data obtained from the AMSR-E instrument.	AMSR-E (from REMSS)	L2P (10km)
AMSR2 Prototype SSTs for July 2012-December 2016 retrieved from data obtained from the AMSR2 instrument.	AMSR2 (from JAXA)	L2P (35km x 61km)
Analysis Gap-free daily analyses of the ATSR and AVHRR products for 1981-2016. Prototype gap-free daily analyses of the AATSR, AVHRR, AMSR-E and AMSR2 products for 2002-2016.	The ATSR and AVHRR products described above. The ATSR AVHRR, and prototype AMSR-E and AMSR2 products described above.	L4 (0.05°)

The table indicates that the project will produce data at levels L2P, L3U and L4. These are all defined below. User requirements indicate that all will be useful to users (SST_CCI-REQ-1, [RD.393]). As the project will receive some data at data level L1B, this is also defined below.

- L1B Level 1 B data; the data collected by the satellite sensor with processing (for example calibration) applied.
- L2P Level 2 pre-processed data; geophysical variables at the full resolution of the instrument, in a satellite projection with associated geographical information.
- L3U Level 3 uncollated data; gridded version of L2P data.
- L4 Level 4 data; a dataset formed by analysing lower level data to create a gridded product with no data gaps. The use of an infilling procedure to remove data gaps distinguishes L4 data from lower level data.

Each entry in Table 1 is expanded in Table 2 and Table 3. These tables provide full details of each product. This includes aspects such as the file names, the file sizes, the target for stability etc.

The headings to the columns in Table 2 and Table 3 define unique names for each product. These shall be appended in brackets with the name of an individual sensor if it is necessary to distinguish between sensors in a series. For example the individual components of the ATSR product shall be referred to as ATSR (ATSR-1), ATSR (ATSR-2) and ATSR (AATSR).

Table 2. Detailed description of the SST CCI infrared-only products. The column headings define unique names for each product. Where it is necessary to distinguish between data from individual sensors in products that contain a series of sensors the name of the sensor shall be appended to the product name in brackets. For example the ATSR-1 part of the ATSR product shall be referred to as ATSR (ATSR-1). File size estimates are based on the following grid sizes: AVHRR L2P – 625 x 7000, L3 and L4 data - 7,200 x 3,600 and one time step per file. User requirements for each aspect of the products are included and are referenced as codes beginning with SST_CCI-REQ-; full details of these requirements are in [RD.393].

Product	ATSR	AVHRR	Analysis
Satellite sensors used	ATSR series (ATSR-1, ATSR-2, AATSR, SLSTR in future)	AVHRR series GAC data, Metop-A full resolution	ATSR series and AVHRR series
Satellite sensor type	Infrared	Infrared	Infrared
Satellite platform	ERS-1, ERS-2, Envisat, Sentinel-3 in future	NOAA platforms, Metop-A	ERS-1, ERS-2, Envisat, Sentinel-3 in future, NOAA platforms, Metop-A
Satellite orbit	Polar	Polar	Polar
Input data source	ESA	NOAA & EUMETSAT	SST CCI (ATSR and AVHRR products)

Product	ATSR	AVHRR	Analysis
Input data format	Envisat format	AVHRR GAC and Metop-A full resolution.	NetCDF compliant with this document
Input data level	L1B	L1B	L3U and L2P
Input data frequency	One file per orbit per sensor (typically 14 orbits per day, one sensor operating)	One file per orbit per sensor (typically 14 orbits per day, more than one sensor operating)	Typically 28 orbits per day, one file per orbit
Input data grid	1 km spaced irregular grid	1km spaced irregular grid (full resolution Metop-A AVHRR only), 4-25 km spaced irregular grid (otherwise)	0.05° grid and swath
Input data spatial coverage	Global	Global	Global
Processing to be applied by the project	SST retrieval; cloud and ice screening; depth and time adjustment to SSTs; uncertainty estimates; anomaly calculation	SST retrieval; cloud and ice screening; depth and time adjustment to SSTs; uncertainty estimates; anomaly calculation	Analysis; analysis uncertainty; anomaly calculation
User requirement for SST processing	SST_CCI-REQ-7: Provide SST anomalies relative to a long-term reference climatology SST_CCI-REQ-27: Provide comprehensively characterised uncertainties in the products, together with indicators of confidence in uncertainty		
Output data level	L2P and L3U	L2P and L3U	L4
Output data level user requirement	SST_CCI-REQ-1: provide products at levels 2, 3 (uncollated and daily collated) and 4.		
Output data frequency	One file per orbit per sensor (typically 14 orbits per day, one sensor operating)	One file per orbit per sensor (typically 14 orbits per day, more than one sensor operating)	One file per day
Output data frequency user requirement	SST_CCI-REQ-16: provide at least daily resolution.		

Product	ATSR	AVHRR	Analysis
Output grid	1 km spaced irregular grid and 0.05° grid	1 km spaced irregular grid (full resolution Metop-A AVHRR only), 4-25 km spaced irregular grid and 0.05° grid	0.05° grid
Output grid user requirement	SST_CCI-REQ-10: Provide level 3 and 4 data on a regular latitude/longitude grid. SST_CCI-REQ-14: Provide data at least at 0.1° latitude by 0.1° longitude resolution. .		
File size estimate (assuming no compression)	1160 (L2)/1140 (L3) MB	256 (L2)/1140 (L3) MB	164 MB
File size user requirement	SST_CCI-REQ-40: Consider users with the least developed computing infrastructures when designing product files and provision mechanisms.		
Output file format	CF compliant NetCDF		
Output file format user requirement	SST_CCI-REQ-42: Provide data in CF-compliant NetCDF format		
Spatial coverage	Global		
Spatial coverage user requirement	SST_CCI-REQ-9: Provide global coverage.		
Product start month	08/1991	08/1981	08/1981
Product end month	04/2012	12/2016	12/2016
Product length	approx. 21 years	35 years	35 years
Product length user requirement	SST_CCI-REQ-12: Provide products of 30 or more years in length. SST_CCI-REQ-13 also requires products of > 100 years in length, but that is out of scope of this work.		
Depth of SST	Skin and 20 cm	Skin and 20 cm	20 cm
SST depth user requirement	SST_CCI-REQ-4: Provide SSTskin. SST_CCI-REQ-5 and SST_CCI-REQ-6: provide SST20cm at observation time and as a daily average.		

Product	ATSR	AVHRR	Analysis
SST time of day	Platform dependent time (skin SST) and adjusted to a time representative of the daily average	Platform dependent time (skin SST) and adjusted to a time representative of the daily average	Representative of daily average
SST time of day user requirement	SST_CCI-REQ-5 and SST_CCI-REQ-6: Provide SST20cm at observation time and as a daily average.		
Target bias	Bias <0.1°C when evaluated over length scales of ~1000 km		
Acceptable level of bias user requirement	SST_CCI-REQ-19: Provide SST with no more than a maximum of 0.1°C bias. SST_CCI-REQ-21: Provide SST with at least 0.1°C precision.		
Target stability	0.1°C/decade		
Stability user requirement	SST_CCI-REQ-23: Provide SST with a maximum drift of 0.05°C/decade.		
Ancillary data to be included	Surface wind speed from the ERA-Interim reanalysis		Sea ice concentration and uncertainties; taken from OSI SAF data
Ancillary data user requirement	SST_CCI-REQ-39: Provide information on wind speed		SST_CCI-REQ-37: Provide information on location of sea ice and its concentration
File names – read from top to bottom to obtain the file name for each product Definitions of the fields contained in chevrons (<>) are in Section 3.2.	<Indicative Date><Indicative Time>-ESACCI-		
	L2P or L3U	L2P or L3U	L4
	_GHRSSST-		
	SSTskin-[ATSR1, ATSR2 or AATSR]	SSTskin-AVHRR<X>_G	SSTdepth-OSTIA-GLOB
	-v2.0-fv<FileVersion>.nc		

Table 3. Detailed description of the prototype SST CCI products including data from passive microwave sensors. The column headings define unique names for each product. User requirements for each aspect of the products are included and are referenced as codes beginning with SST_CCI-REQ-; full details of these requirements are in [RD.393].

Product	AMSR-E	AMSR2	Analysis
Satellite sensors used	AMSR-E	AMSR2	AATSR and AVHRR series, AMSR-E and AMSR2
Satellite sensor type	Microwave	Microwave	Infrared and microwave
Satellite sensor user requirement	SST_CCI-REQ-3; Provide some products which are a combination of infrared and microwave satellite data.		
Satellite platform	EOS Aqua	GCOM-W1	Envisat, NOAA platforms, Metop-A, EOS Aqua and GCOM-W1
Satellite orbit	Polar	Polar	Polar
Input data source	REMSS via NSIDC	JAXA	SST CCI (AATSR, AVHRR series, AMSR-E and AMSR2 products)
Input data format	HDF-4	HDF-5	NetCDF compliant with this document
Input data level	L2A	L1R	L3U (ATSR and AVHRR) and L2P (AMSR-E and AMSR2)
Input data frequency	Ascending and descending half-orbit files	Ascending and descending half-orbit files	Typically 28 orbits per day, one file per orbit
Input data grid	10km spaced irregular grid	L1R data resampled to 6GHz resolution of: 35km x 61km	0.05° grid (ATSR and AVHRR) and 10 km and 35km x 61km irregular grid (sub-sampled to native resolution of the instrument if appropriate, AMSR-E and AMSR2)
Input data spatial coverage	Global	Global	Global

Product	AMSR-E	AMSR2	Analysis
Processing to be applied by the project	SST retrieval; cloud and ice screening; uncertainty estimates	SST retrieval; cloud and ice screening; uncertainty estimates	Analysis; uncertainty estimates
User requirement for SST processing	SST_CCI-REQ-27: Provide comprehensively characterised uncertainties in the products, together with indicators of confidence in uncertainty		
Output data level	L2P	L2P	L4
Output data level user requirement	SST_CCI-REQ-1: provide products at levels 2, 3 (uncollated and daily collated) and 4.		
Output data frequency	Ascending and descending half-orbit files	Ascending and descending half-orbit files	One file per day
Output data frequency user requirement	SST_CCI-REQ-16: provide at least daily resolution.		
Output grid	10 km spaced irregular grid	35km x 61km spaced irregular grid	0.05° grid
Output grid user requirement	SST_CCI-REQ-10: Provide level 3 and 4 data on a regular latitude/longitude grid. SST_CCI-REQ-14: Provide data at least at 0.1° latitude by 0.1° longitude resolution.		
Output file format	CF compliant NetCDF		
Output file format user requirement	SST_CCI-REQ-42: Provide data in CF-compliant NetCDF format.		
Spatial coverage	Global		
Spatial coverage user requirement	SST_CCI-REQ-9: Provide global coverage.		
Product start date	01/06/2002	02/07/2012	01/06/2002
Product end date	04/10/2011	31/12/2016	31/12/2016
Product length	9 years, 4 months	4 years, 6 months	14 years, 7 months
Product length user requirement	SST_CCI-REQ-12: Provide products of 30 or more years in length. SST_CCI-REQ-13 also requires products of > 100 years in length, but that is out of scope of this work.		
SST depth	Subskin and 20 cm	Subskin and 20 cm	20 cm

Product	AMSR-E	AMSR2	Analysis
SST depth user requirement	SST_CCI-REQ-4: Provide SSTskin. SST_CCI-REQ-5 and SST_CCI-REQ-6: provide SST20cm at observation time and as a daily average.		
SST time of day	Platform dependent time (subskin SST, 1.30 am and pm local time) and adjusted to a time representative of the daily average	Platform dependent time (subskin SST, 1.30 am and pm local time) and adjusted to a time representative of the daily average	Representative of daily average
SST time of day user requirement	SST_CCI-REQ-5 and SST_CCI-REQ-6: Provide SST20cm at observation time and as a daily average.		
Target bias	Bias < 0.1°C when evaluated over length scales of ≤ 1000 km		
Acceptable level of bias user requirement	SST_CCI-REQ-19: Provide SST with no more than a maximum of 0.1°C bias. SST_CCI-REQ-21: Provide SST with at least 0.1°C precision.		
Target stability	0.1°C/decade		
Stability user requirement	SST_CCI-REQ-23: Provide SST with a maximum drift of 0.05°C/decade.		
Ancillary data to be included	Surface wind speed from the ERA-Interim reanalysis		Sea ice concentration and uncertainties; taken from OSI SAF data
Ancillary data user requirement	SST_CCI-REQ-39: Provide information on wind speed		SST_CCI-REQ-37: Provide information on location of sea ice and its concentration
File names – read from top to bottom to obtain the file name for each product Definitions of the fields contained in chevrons (<>) are in Section 3.2.	<Indicative Date><Indicative Time>-ESACCI-		
	L2P	L2P	L4
	_GHRSSST-		
	SSTsubskin-AMSRE	SSTsubskin-AMSR2	SSTdepth-OSTIA-GLOB
	-v2.0-fv<FileVersion>.nc		

3. FILE FORMAT AND METADATA

3.1 Rationale

The format of the data files shall be Network Common Data Format (NetCDF) and shall follow Climate and Forecasting (CF) conventions as far as possible. This is the format preferred by the majority of potential users of the products (user requirement SST_CCI-REQ-42, [RD.393]). The use of NetCDF also allows the use of a variety of different tools/languages to manipulate and view the data, for example the tools under development as part of the ESA CCI ToolBox and those available within languages such as the Interactive Data Language (IDL), the Matrix Laboratory (MATLAB) and Python.

CF compliant NetCDF files are already very well established in the SST user community owing to the success of the GHRSSST project ([RD.219]; <https://www.ghrsst.org/>). GHRSSST provides SST data products in a CF compliant NetCDF data format, the latest version being the GDS2.0 [AD.1]. The GDS2.0 already includes much of the data and metadata that users require and that SST CCI wish to include in the files, but also has the flexibility of allowing additional data fields to be added as required. The earlier user requirements gathered by the SST CCI project showed some limited support for the GDS2.0 for the NetCDF files (SST_CCI-UR-QUF-89, [RD.171]). Adopting the GDS2.0 specification provides benefits to users as some will already have experience with the files and may have existing software and tools to work with the data. It also ensures easy incorporation of the SST CCI products into the GHRSSST framework. ESA have mandated use of GDS2.0 for this project.

It is also desirable for the SST CCI data to be available in a form that is familiar to climate modellers to allow ease of comparison of observational data with climate model data [RD.168]. Format specifications exist to allow this ('Obs4MIPS format'; see <http://obs4mips.llnl.gov/>), However, this has some differences to the way that the storage of data in NetCDF format is implemented by GHRSSST. These differences mean that it is not possible to produce one set of data files that is consistent with both specifications. The SST CCI project shall produce files that are consistent with the GDS2.0 specification as described in this document. Files in the Obs4MIPS format will also be produced, but are not described here.

The format of NetCDF used for GDS2.0 data files is preferentially 'NetCDF-4 classic' and therefore this shall be used for SST CCI files. The term 'NetCDF-4 classic' combines two aspects of the files: the underlying file format and the data model. These are explained briefly below:

Three different underlying formats could be used:

- 'classic': this is compatible with all versions of the NetCDF library;
- '64-bit offset': this allows larger datasets to be written but is not compatible with versions of the NetCDF library prior to 3.6.0;
- NetCDF-4; this uses Hierarchical Data Format version 5 (HDF5) as its base format and gives access to desirable features such as internal per variable compression; it is compatible with the NetCDF library from version 4.

Although the NetCDF-4/HDF5 format is not compatible with older versions of the library, the additional features such as its compression abilities gives clear advantages over the other options.

There are two NetCDF data models: 'classic' and 'enhanced' [RD.167]. The classic data model has a number of limitations compared to enhanced, for example the enhanced data model includes a greater number of allowed storage types. Either can be written using the NetCDF-4/HDF5 underlying format. The advantage of using the classic model is that it maintains compatibility with legacy software.

In summary:

- The SST CCI files shall be internally compressed NetCDF-4/HDF5 format and shall use the NetCDF classic data model.
- The file specifications shall follow CF conventions as far as possible.
- The files will be based on and be consistent with the GHRSSST GDS2.0 [AD.1] as far as possible.

3.2 Filename convention

SST CCI shall follow the file naming convention specified in [AD.1], i.e.:

<Indicative Date><Indicative Time>-<RDAC>-<Processing Level>_GHRSSST-<SST Type>-<Product String>-<Additional Segregator>-v<GDS Version>-fv<FileVersion>.<File Type>

The components to this list are summarised in [AD.1] Table 7-1 with further explanatory information in the text of that document. That table is reproduced here in Table 4 with an additional column (headed SST CCI definition) that details the implementation of the filenaming convention that shall be used by the SST CCI project. All the information required to define the SST CCI files is contained within this document. However, note that references in the Description column of the table are to sections in the [AD.1] document and these shall be referred to if further explanation is desired. In places, clarifications to the [AD.1] version of the text have been made and these are indicated in italics.

Table 4. Components of the filenames; based on [AD.1] section 7.1 – refer there for more details. The final column details the implementation for the SST CCI project. In the Description column the references refer to sections of [AD.1]. All references in the SST CCI column are to parts of this document.

Name	Definition	Description	SST CCI definition
<Indicative Date>	YYYYMMDD	The identifying date for this data set. See Section 7.2 in [AD.1]. The section states that: YYYY is the four-digit year, MM is the two-digit month from 01 to 12, and DD is the two-digit day of month from 01 to 31 and The date used should best represent the observation date for the dataset.	As stated in Description column.
<Indicative Time>	HHMMSS	The identifying time for this data set. The time used is dependent on the <Processing Level> of the data set: L2P: start time of granule L3U: start time of granule L4 and GMPE: nominal time of analysis All times should be given in UTC. See Section 7.3 in [AD.1]. The section states that: HH is the two-digit hour from 00 to 23, MM is the two-digit minute from 00 to 59, and SS is the two-digit second from 00 to 59 and All times should be given in UTC and should be chosen to best represent the observation time for this dataset. Note: RDACs should ensure the applications they use to determine UTC properly account for leap seconds.	As stated in Description column.
<RDAC>	The RDAC where the file was created.	The Regional Data Assembly Centre (RDAC) code.	For the SST CCI products, this is: ESACCI
<Processing Level>	The data processing level code (L2P, L3U, or L4)	The data processing level code, defined in Section 7.5 in [AD.1].	See Table 1 in this document.
<SST type>	The type of SST data included in the file.	Conforms to the GHRSSST definitions for SST, defined in Section 7.6 in [AD.1].	This should be set to be the primary SST stored in the file. See Table 5.

Name	Definition	Description	SST CCI definition
<Product String>	A character string identifying the SST product set. The string is used uniquely within an RDAC but may be shared across RDACs.	The unique "name" within an RDAC of the product line. See Section 7.7 <i>in [AD.1]</i> for the product string lists, one each for L2P, L3, L4, and GMPE products. See Section 7.7 <i>in [AD.1]</i> .	See Table 6 in this document.
<Additional Segregator>	Optional text to distinguish between files with the same <Product String>. Dashes are not allowed within this element.	This text is used since the other filename components are sometimes insufficient to uniquely identify a file. For example, in L2P or L3U (un-collated) products this is often the original file name or processing algorithm. Note, underscores should be used, not dashes. For L4 files, this element should begin with the appropriate regional code as defined in Section 7.8. This component is optional but must be used in those cases where non-unique filenames would otherwise result.	For L2 and L3 products this is not used. For L4 products it is GLOB (GLOB is required to indicate spatial coverage)
<GDS Version>	nn.n	Version number of the GDS used to process the file. For example, GDS 2.0 = "02.0".	To be set to "02.0".
<File Version>	xx.x	Version number for the file, for example, "02.0".	As stated in Description column.
<File Type>	NetCDF data file suffix (nc) or ISO metadata file suffix (xml).	Indicates this is a NetCDF file containing data or its corresponding ISO-19115 metadata record in XML.	Will be nc for SST CCI files.

Table 5. Values and definitions of <SST type>. Based on [AD.1] section 7.6 – refer there for more details.

SST type	Description
SSTskin	SST sensed by infrared instruments (at depth of approximately 10 µm).
SSTsubskin	SST sensed by microwave instruments (at depth of approximately 1 mm).
SSTdepth	Temperature at a specific depth. The depth shall be included in the file metadata.
SSTfnd	Temperature from which the diurnal thermocline develops each day.

Table 6: Product strings for data to be processed; based on [AD.1] Tables 7-5 to 7-7 – refer there for more details. Codes for future SLSTR products should be confirmed with the GHRSSST project before use.

Sensor/analysis	Platform (if applicable)	Product String	Comment
ATSR	ERS-1	ATSR1	
ATSR	ERS-2	ATSR2	
AATSR	Envisat	AATSR	
AVHRR_GAC	NOAA-<X> or MetOpA	AVHRR<X>_G	<X> is <i>either</i> : if the satellite hosting the AVHRR is a NOAA platform, <X> is the satellite number, <i>or</i> , if the AVHRR is on Metop-A, <X> is 'MTA'.
AMSR-E	EOS Aqua	AMSRE	
AMSR2	GCOM-W1	AMSR2	
OSTIA		OSTIA	L4 analysis using the OSTIA system
SLSTR	SENTINEL_3A	S3A_SLSTR	TBC

3.3 Global attributes

Attributes are metadata that are stored in a NetCDF file. Global attributes contain information that applies to the whole contents of the NetCDF file.

All GHRSSST format data files share the same set of global attributes. These are listed in [AD.1] Table 8-1. The CCI DSWG also specify a set of global attributes that should be included in the SST CCI data files ([RD.215]), some of which are not in the GHRSSST specification. In addition an attribute called “creator_processing_institution” has been included to indicate the institution that created products as part of the SST CCI project.

Table 7 contains a list of the global attributes. Much of this is reproduced from Table 8-1 in [AD.1]. However, annotations to the table have been made in places in order to clarify the text; these are indicated by italics. The additional attributes specified by the CCI DSWG are also included. These are the entries that include ‘CCI DSWG’ in the Source column of the table. The “creator_processing_institute” attribute has SST CCI within the Source column. Other points to note are:

- The definition of the shading of the rows in the table is given in Table 8.
- All references in the Description column refer to the contents of [AD.1]. Although all the information required to create the SST CCI files is contained here, these can be used to obtain more information about GDS2.0 files.
- The final column, headed ‘SST CCI definition’ contains information about the implementation of the attributes for the SST CCI files. All references in this column are to parts of this document.

As revealed by the column headed 'Source', the definition of the attributes was based on CF conventions, the Unidata Attribute Convention for Dataset Discovery (ACDD) [RD.170], the requirements of the GHRSSST project [AD.1] and the specifications provided by the CCI DSWG.

Table 7. Global attributes that are included in all GHRSSST format data files and additional attributes specified by the CCI DSWG. Much of the contents of this table is reproduced from [AD.1] and further information can be found there. Annotations and changes to the original text are made in places and these are written in italics. The meaning of the colours is given in Table 8. Note that attributes described as having the format 'string' shall actually be stored in the NetCDF file as an array of characters. References in the Description column are to parts of [AD.1]; references in the SST CCI definition column are to parts of this document.

Global Attribute Name	Format	Description	Source	SST CCI definition
Conventions	string	A text string identifying the netCDF conventions followed. This attribute should be set to the version of CF used and should also include the ACDD. For example: "CF-1.4, Unidata Observation Dataset v1.0".	CF	CF-1.5, Unidata Observation Dataset v1.0
title	string	A descriptive title for the GHRSSST data set	CF, ACDD	See examples in Section 4.
summary	string	A paragraph describing the dataset.	ACDD	See examples in Section 4.
references	string	Published or web-based references that describe the data or methods used to produce it.	CF	Include any relevant publications or webpages.
institution	string	GHRSSST RDAC code where the data were produced. See Table 7-2 in [AD.1] for available codes.	CF, ACDD	The RDAC code for the SST CCI products is ESACCI
history	string	History of all applications that have modified the original data to create this file.	CF, ACDD	

Global Attribute Name	Format	Description	Source	SST CCI definition
comment	String	Miscellaneous information about the data or methods used to produce it.	CF, ACDD	Used to indicate the centre where the data were produced. Set to: These data were produced at <institution> as part of the ESA SST CCI project.
license	String	Describe any restrictions to data access, use, and distribution. GHR SST data sets should be freely and openly available to comply with the R/GTS framework, with no restrictions. However, if a user should submit a simple registration via a web form, for example, the URL could be given here. Default to "GHR SST protocol describes data use as free and open."	ACDD	Creative Commons Licence by attribution (http://creativecommons.org/licenses/by/4.0/)
id	String	The unique GHR SST character string for this product. All GHR SST SST products have one, and they are listed in Table 7-10 in [AD.1].	ACDD	See Section 3.5 for the list of strings to be used by the SST CCI project.
naming_authority	String	Fixed as "org.ghrsst" following ACDD convention.	ACDD	org.ghrsst
product_version	String	The product version of this data file, which may be different than the file version used in the file naming convention (Section 7 in [AD.1]).	GDS	See Section 3.2 of this document
uuid	String	A Universally Unique Identifier (UUID). Numerous, simple tools can be used to create a UUID, which is inserted as the value of this attribute. See http://en.wikipedia.org/wiki/Universally_Unique_Identifier for more information and tools.	GDS	[RD.169] suggests the use of http://www.oss.org/pkg/lib/uuid/ , and this will be followed.

Global Attribute Name	Format	Description	Source	SST CCI definition
tracking_id	string	Identical to uuid (i.e. this shall contain the same value as uuid).	CCI DSWG	As stated in Description column. This is an alternative name for the UUID as used in the CMIP5 specification [RD.166].
gds_version_id	string	GDS version used to create this data file. For example, "2.0".	GDS	The GDS version used for the SST CCI product specification was 2.0.
netcdf_version_id	string	Version of netCDF libraries used to create this file. For example, "4.1.1"	GDS	As stated in Description column. Optionally can also include the date for example "4.2.1.1 of Oct 19 2012 14:25:16"
date_created	string	The date and time the data file was created in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	ACDD	As stated in Description column.
file_quality_level	integer	A code value: 0 = unknown quality 1 = extremely suspect (frequent problems, e.g. with known satellite problems) 2 = suspect (occasional problems, e.g. after launch) 3 = excellent (no known problems)	GDS	As stated in Description column.

Global Attribute Name	Format	Description	Source	SST CCI definition
spatial_resolution	String	A string describing the approximate resolution of the product. For example, "1.1km at nadir"	GDS	Value depends on the product. See Table 1 or Table 2 or Table 3.
start_time	String	Date and time of the first measurement in the data file in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	GDS	As stated in Description column.
time_coverage_start	String	Identical to start_time. Included for increased ACDD compliance.	ACDD	As stated in Description column.
stop_time	String	Date and time of the last measurement in the data file in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	GDS	As stated in Description column.
time_coverage_end	String	Identical to stop_time. Included for increased ACDD compliance.	ACDD	As stated in Description column.
time_coverage_duration	String	Duration of time coverage in ISO 8601 compliant format; the difference between time_coverage_end and time_coverage_start.	CCI DSWG, ACDD	In the form PdDThHmMsS or other ISO 8601 compliant format where d is the number of days, h is the number of hours, m is the number of minutes, s is the number of seconds, omitting dD etc. if the number is zero.
time_coverage_resolution	String	Time resolution of the data in the file in ISO 8601 compliant format.	CCI DSWG, ACDD	Orbit repeat period (for single orbit files) or frequency of data files.

Global Attribute Name	Format	Description	Source	SST CCI definition
northernmost_latitude	float	Decimal degrees north, range -90 to +90. This is equivalent to ACDD geospatial_lat_max.	GDS	As stated in Description column.
geospatial_lat_max	float	Identical to northernmost_latitude.	CCI DSWG, ACDD	As stated in Description column.
southernmost_latitude	float	Decimal degrees north, range -90 to +90. This is equivalent to ACDD geospatial_lat_min.	GDS	As stated in Description column.
geospatial_lat_min	float	Identical to southernmost_latitude.	CCI DSWG, ACDD	As stated in Description column.
easternmost_longitude	float	Decimal degrees east, range -180 to +180. This is equivalent to ACDD geospatial_lon_max.	GDS	As stated in Description column.
geospatial_lon_max	float	Identical to easternmost_longitude.	CCI DSWG, ACDD	As stated in Description column.
westernmost_longitude	float	Decimal degrees east, range -180 to +180. This is equivalent to ACDD geospatial_lon_min.	GDS	As stated in Description column.
geospatial_lon_min	float	Identical to westernmost_longitude.	CCI DSWG, ACDD	As stated in Description column.
geospatial_vertical_min	float	Minimum of the vertical extent of the data; positive values indicate distances above the surface.	CCI DSWG, ACDD	To be set to the representative depth of the deepest SST in the file.
geospatial_vertical_max	float	Maximum of the vertical extent of the data; positive values indicate distances above the surface.	CCI DSWG, ACDD	To be set to the representative depth of the shallowest SST in the file.

Global Attribute Name	Format	Description	Source	SST CCI definition
source	String	Comma separated list of all source data present in this file. List SST sources first, followed by Auxiliary sources. If the source is a GHRSSST product, use the GHRSSST unique string listed in Table 7-10. For other sources, following the best practice described in Section 7.9 in [AD.1].	CF	See Section 3.5 in this document for the source codes relevant to the SST CCI products.
platform	String	Satellite(s) used to create this data file. Select from the entries found in the Satellite Platform column of Table 7-5 in [AD.1] and provide as a comma separated list if there is more than one.	GDS	See Table 6 in this document for the platforms relevant to the SST CCI products.
sensor	String	Sensor(s) used to create this data file. Select from the entries found in the Satellite Sensor column of Table 7-5 in [AD.1] and provide as a comma separated list if there is more than one.	GDS	See Table 6 in this document for the platforms relevant to the SST CCI products.
Metadata_Conventions	String	Unidata Dataset Discovery v1.0	ACDD	As stated in Description column.
metadata_link	String	Link to collection metadata record at archive	ACDD	http://www.esa-cci.org
keywords	String	Typically GCMD Science Keyword: "Oceans > Ocean Temperature > Sea Surface Temperature"	ACDD	As stated in Description column.
keywords_vocabulary	String	"NASA Global Change Master Directory (GCMD) Science Keywords" as defined in [RD.176].	ACDD	As stated in Description column.
standard_name_vocabulary	String	"NetCDF Climate and Forecast (CF) Metadata Convention"	ACDD	As stated in Description column.
geospatial_lat_units	String	Units of the latitudinal resolution. Typically "degrees_north"	ACDD	degrees_north

Global Attribute Name	Format	Description	Source	SST CCI definition
geospatial_lat_resolution	float	Latitude Resolution in units matching geospatial_lat_units.	ACDD	
geospatial_lon_units	string	Units of the longitudinal resolution. Typically "degrees_east"	ACDD	degrees_east
geospatial_lon_resolution	float	Longitude Resolution in units matching geospatial_lon_resolution.	ACDD	
acknowledgment	string	Information about funding source and how to cite the use of these data.	ACDD	Funded by ESA.
creator_name	string	Provide a name and email address for the most relevant point of contact at the producing RDAC, as well as a URL relevant to this data set.	ACDD	SST_cci
creator_email	string		ACDD	science.leader@esa-sst-cci.org
creator_url	string		ACDD	http://www.esa-sst-cci.org
creator_processing_institution	string	Contains additional information about the institution that created the product within the CCI project.	SST_cci	These data were produced at <institution> as part of the ESA SST CCI project.
project	string	"Group for High Resolution Sea Surface Temperature"	ACDD	Climate Change Initiative – European Space Agency
publisher_name	string	<i>The name of the data publisher; for GHRSSST data this is The GHRSSST Project Office</i>	ACDD	ESACCI
publisher_url	string	<i>The web address of the data published; for GRHSST data this is http://www.ghrsst.org</i>	ACDD	http://www.esa-sst-cci.org
publisher_email	string	<i>The email address of the data publisher; for GHRSSST data this is ghrsst-po@nceo.ac.uk</i>	ACDD	science.leader@esa-sst-cci.org

Global Attribute Name	Format	Description	Source	SST CCI definition
processing_level	String	GHRSSST definitions are the options: L2P, L3U, L4 and GMPE	ACDD	Value depends on the product. See Table 1 or Table 2 or Table 3.
cdm_data_type	String	"swath" or "grid"	ACDD, GDS	"swath" if L2P file, otherwise "grid"
product_specification_version	String	The file name (excluding extension) of the product specification document to which the file relates.	SST_cci	For example SST_CCI-PSD-UKMO-201-Issue-2-signed

Table 8. Key to colours used in Table 7 and Table 9. Based on Table 4-2 in [AD.1].

Colour	Meaning
Blue	Mandatory item.
Violet	An item that is mandatory for only certain situations.

3.4 Variable attributes

In the context of a NetCDF file a variable refers to an array of data stored within the file. Each variable can have attributes associated with it. [AD.1] defines attributes that should be provided with variables. As for the global attributes, the table of variable attributes from [AD.1] (Table 8-2) is reproduced here (Table 9). Annotations to the original text are indicated by italics. References within the table in the Description column refer to the contents of [AD.1] or to other external references. The SST CCI implementation of the variables is given in the column headed 'SST CCI definition'. All references in this column are to parts of this document. There are some differences to the attributes to be used that depends on the nature of the data being stored; these are identified using violet shading (see Table 8).

Table 9. List of variable attributes. The contents of the first four columns of this table are reproduced from [AD.1] and further information can be found there. References in those columns refer to parts of [AD.1]. Annotations and changes to the [AD.1] text are identified by italics. The final column contains the SST CCI implementation of the attributes. All references in that column refer to parts of this document. The meaning of the colours is given in Table 8. Note that attributes described as having the format ‘string’ shall actually be stored in the NetCDF file as an array of characters.

Variable attribute name	Format	Description	Source	SST CCI definition
_FillValue	Must be same as the variable type	A value used to indicate array elements containing no valid data. This value must be of the same type as the storage (packed) type; should be set as the minimum value for this type. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report fill as 128. Some cases will be reported as unsigned bytes 0 to 255.	CF	As stated in Description column.
units	string	Text description of the units, preferably S.I., and must be compatible with the Unidata UDUNITS-2 package [RD.178]. For a given variable (e.g. wind speed), these must be the same for each dataset.	CF, ACDD	See specifications in Section 4.
scale_factor	Must be expressed in the unpacked data type	To be multiplied by the variable to recover the original value. Defined by the producing RDAC. Valid values within valid_min and valid_max should be transformed by scale_factor and add_offset, otherwise skipped to avoid floating point errors.	CF	See specifications in Section 4. The type of this attribute defines the type of the unpacked data.
add_offset	Must be expressed in the unpacked data type	To be added to the variable after multiplying by the scale factor to recover the original value. If only one of scale_factor or add_offset is needed, then both should be included anyway to avoid ambiguity, with scale_factor defaulting to 1.0 and add_offset defaulting to 0.0. Defined by the producing RDAC.	CF	See specifications in Section 4. The type of this attribute defines the type of the unpacked data.
long_name	string	A free-text descriptive variable name.	CF, ACDD	See specifications in Section 4.

Variable attribute name	Format	Description	Source	SST CCI definition
valid_min	Expressed in same data type as variable	Minimum valid value for this variable once they are packed (in storage type). The fill value should be outside this valid range. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report valid min as 129. Some cases as unsigned bytes 0 to 255. Values outside of valid_min and valid_max will be treated as missing values.	CF	See specifications in Section 4.
valid_max	Expressed in same data type as variable	Maximum valid value for this variable once they are packed (in storage type). The fill value should be outside this valid range. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report valid min as 127.	CF	See specifications in Section 4.
standard_name	String	Where defined, a standard and unique description of a physical quantity. For the complete list of standard name strings, see [RD.177]. Do not include this attribute if no standard_name exists.	CF, ACDD	See specifications in Section 4.
comment	String	Miscellaneous information about the data or the methods used to produce it.	CF	As stated in Description column.
source	String	<p>For L2P and L3 files: For a data variable with a single source, use the GHRSSST unique string listed in Table 7-10 in [AD.1] if the source is a GHRSSST SST product. For other sources, following the best practice described in Section 7.9 in [AD.1] to create the character string.</p> <p>If the data variable contains multiple sources, set this string to be the relevant “sources of” variable name. For example, if multiple wind speed sources are used, set source = sources_of_wind_speed.</p> <p>For L4: follow the source convention used for the global attribute of the same name, but provide in the comma-separated list only the sources relevant to this variable.</p>	CF	<p>String containing the source of data, or comma separated list if there are multiple sources.</p> <p>Section 3.5 details the sources of data to be used by the SST CCI products and the names for these that shall be used to fill this attribute.</p>

Variable attribute name	Format	Description	Source	SST CCI definition
references	string	Published or web-based references that describe the data or methods used to produce it. Note that while at least one reference is required in the global attributes (See Table 8-1 in [RD.87], references to this specific data variable may also be given.	CF	As stated in Description column. Note that the equivalent in this document to the table that is referred to is Table 7.
axis	string	For use with coordinate variables only. The attribute 'axis' may be attached to a coordinate variable and given one of the values "X", "Y", "Z", or "T", which stand for a longitude, latitude, vertical, or time axis respectively. See: http://cf-pcmdi.llnl.gov/documents/cf-conventions/1.4/cf-conventions.html .	CF	See specifications in Section 4.
positive	string	For use with a vertical coordinate variables only. May have the value "up" or "down". For example, if an oceanographic netCDF file encodes the depth of the surface as 0 and the depth of 1000 meters as 1000 then the axis would set positive to "down". If a depth of 1000 meters was encoded as -1000, then positive would be set to "up". See the section on vertical-coordinate in <i>the CF conventions document</i> [RD.177].	CF	This is not used in SST CCI files.
coordinates	string	Identifies auxiliary coordinate variables, label variables, and alternative coordinate variables. See the section on coordinate-system in <i>the CF conventions document</i> [RD.177].	CF	As stated in Description column.

Variable attribute name	Format	Description	Source	SST CCI definition
grid_mapping	String	Use this for data variables that are on a projected grid. The attribute takes a string value that is the name of another variable in the file that provides the description of the mapping via a collection of attached attributes. That named variable is called a grid mapping variable and is of arbitrary type since it contains no data. Its purpose is to act as a container for the attributes that define the mapping. See the section on mappings-and-projections in <i>the CF conventions document</i> [RD.177].	CF	This is not used in SST CCI files.
flag_meanings	String	Space-separated list of text descriptions. Words within a phrase should be connected with underscores. Used only for flag and “sources_of_xxx” variables.	CF	See specifications in Section 4.
flag_values	Array of the data type of variable (Note that this is listed incorrectly as ‘string’ in [AD.1])	Comma-separated array of valid, mutually exclusive variable values (required when the bit field contains enumerated values). Used only for flag and “sources_of_xxx” variables.	CF	See specifications in Section 4.
flag_masks	Array of the data type of variable (Note that this is listed incorrectly as ‘string’ in [AD.1])	Array of valid variable masks (required when the bit field contains independent Boolean conditions). Used only for flag and “sources_of_xxx” variables.	CF	See specifications in Section 4.

3.5 Unique product identifiers

Some of the attributes described in Table 7 and Table 9 contain identifiers for the data that have been used to create the file. Section 7.9 of [AD.1] describes these strings. For completeness a brief summary can be found below. In Table 10 all the source data to be used by the project are listed together with the unique text strings that shall be used by to refer to these in the SST CCI files. The entries to the table are based on the information in [AD.1] and [RD.172].

The format of the text is:

<Product String>-<RDAC>-<Processing Level>-<Additional Segregator>-v<Product Version>

The definition of these elements can be found in Table 4, with the exception of the following points:

- <Product Version> - this specifies the version of the dataset and should have the form x.y, where x is the major and y the minor version number.
- <Additional Segregator> - for wind speed data, <Additional Segregator> should be set to WSP, and to ICE for sea ice fraction.
- If there is no predefined GHRSSST RDAC for a data source an appropriate acronym can be substituted instead.

[AD.1] includes a number of predefined text strings. Some existing text strings predate the format described above and hence do not conform.

Table 10. Table of source data and unique product identifiers. The unique text string for future SLSTR products should be checked against the GHRSSST specification before use.

Source data	Unique text string	Comment
ATSR1 Level 1	ATSR1-ESA-L1-v3.0	
ATSR2 Level 1	ATSR2-ESA-L1-v3.0	
AATSR Level 1	AATSR-ESA-L1-v3.0	
AVHRR GAC Level 1	AVHRR<X>_G-ESACCI- L1C-v<Y>	<X> is the satellite number; <Y> is the format version number in form x.y where x is the major format version (1, 2, 3, 4 or 5) and y is used to denote format changes where the major format number is unchanged (possible values are 0, 1 and 2).
AVHRR MetOp Level 1	AVHRRMTA-EUMETSAT- L1-v1	
SLSTR Level 1	S3A_SLSTR-ESA-L1-v<x.y>	TBC
NWP wind speed	ERA_INTERIM-ECMWF- WSP-v1.0	
Sea Ice CCI/OSI SAF sea ice fractions	TBD	This is an adaptation of the source field used in current OSTIA files

Source data	Unique text string	Comment
Land mask	Derived from the Landcover CCI water bodies map	Generated within the Land Cover ESA CCI project (http://maps.elie.ucl.ac.be/CCI/viewer/index.php). It is 1/360 deg resolution and it was derived from multi-temporal metrics based on time series of the backscattered intensity recorded by the ASAR instrument between 2005 and 2010. The main source of ASAR imagery is the Wide Swath Mode (WSM) at 150 m spatial resolution. The post-processing of this dataset for use in the project is described in Carrea (2015) [RD.400].
Lake mask	ARCLake_lakemask	
Data files created by SST CCI	<Product String>-ESACCI- <Processing Level>- v<Version Number>	See text for definition of these fields.

4. PRODUCT SPECIFICATION

This section contains detailed specifications for the files to be produced by the SST CCI project. The structure of the files is fully specified, including the geophysical variables, the metadata and aspects of the data such as the grid.

4.1 Format of the product description tables

Tables are used to describe the detailed structure of the data files in the following subsections. An example of the layout of the tables is shown in Table 11. The points to note are:

- Colours are used to show the start and end of sections of the file structure.
- The column headed 'T' contains the storage type of the variables and attributes; the abbreviations used are explained in Table 12.
- The column headed 'D' contains the dimensionality of the variables. Dimensions are ordered as in the network Common Data form Language (CDL) definition i.e. with the fastest changing dimension last.
- The 'Bytes' column indicates the storage requirement for each item.

Table 11. Example of a table showing file structure. Colours are used to denote the beginning and end of sections of the structure.

Element name	Description	Range/value	Unit	T	D	Bytes
Dataset	Begin of dataset					
Dimensions	Begin of dimensions					
dimension1						
dimension2						
dimensionN						
Dimensions	End of dimensions					
Variables	Begin of variables					
Variable	Begin of variable					
variable_name						
Attributes	Begin of attributes					
attribute1						
attribute2						
attributeN						
Attributes	End of attributes					
Variable	End of variable					
More variable definitions as required						
Variables	End of variables					
Attributes	Begin of global					

Element name	Description	Range/value	Unit	T	D	Bytes
	attributes					
Global attributes that have values that are consistent between data levels are defined in Table 14.						
global_attribute1						
global_attribute2						
global_attributeN						
Attributes	End of global attributes					
Dataset	End of dataset					

4.2 Storage type definitions

Storage types and abbreviations used to refer to them are listed in Table 12. Storage types are limited to those available in the classic NetCDF format. For information the names given to these types in [AD.1] are also listed.

Note that although the abbreviation 'st' is used to indicate text strings, in the NetCDF classic data model there is actually no 'string' storage type [RD.167]. This type of data is instead stored as an array of characters.

Table 12. Abbreviations used for storage types.

Type	Description	Name used in [AD.1]	Comment
Sc	8-bit signed integer	Byte	The NetCDF data type names match those used in [AD.1] for these types.
Ss	16-bit signed integer	Short	
Sl	32-bit signed integer	int (or long)	
Fl	32-bit floating point	float	
Db	64-bit floating point	double	
St	Character array	string	To be stored in the NetCDF file as an array of characters (8-bit unsigned integers)

4.3 L2P data

4.3.1 Description

L2P data files contain swath based SST data. In the context of the SST CCI project, they will be produced from ATSR, AVHRR Global Area Coverage (GAC), AMSR-E and AMSR-2 data.

Each file shall contain a single orbit of data (some orbits may be incomplete). The swath geometry of the input level 1 data is preserved in the L2P output in each case. The "pixel" in the case of GAC is a subsampling of full resolution. For the across track scans of

AVHRR, the pixel resolution varies across the swath. For the conical scanning instruments (ATSRs and microwave instruments) the pixel resolution is more constant (although coarser in the forward view of ATSRs than the nadir view).

L2P files shall include confidence information. Single sensor error statistics (SSES) (bias and standard deviation) are included only for compatibility with GHRSSST data standards and are set to zero.

Multiple different types of retrieval are possible using different views and channels. The L2P files shall contain the best available retrievals.

4.3.2 Summary of contents

The files produced by SST CCI will follow the specification of the 'L2Pcore' files defined in [AD.1] where possible. The primary SST provided is the skin (or subskin, in the case of the prototype passive microwave products) SST obtained at the satellite observation time.

In GHRSSST L2Pcore files, "single sensor error statistics" (SSES) fields are provided that do not fit the SST CCI approach, and are superseded by the uncertainty fields described below.

19 variables are included in the L2P "experimental" fields (although the data provided are not considered experimental scientifically in this case). There are four groups of variables: (i) those relating to SST at the observation time; (ii) those relating to SST adjusted to depth and to the daily mean; (iii) those relevant to users wishing to derive an alternative retrieval type; and (iv) those relating to aspects of the effectiveness of the retrievals.

Group (i):

- type of retrieval used for the primary SST (sea_surface_temperature_retrieval_type);
- uncertainty in primary skin SST from random effects, independent between measured values (uncertainty_random);
- uncertainty in primary skin SST from locally systematic effects, correlated on local spatio-temporal scales (uncertainty_correlated);
- uncertainty in primary skin SST from systematic effects, correlated on large scales (uncertainty_systematic);
- uncertainty in primary skin SST from all effects (sea_surface_temperature_total_uncertainty);
- Adjustment for depth which when added to skin SST gives an estimate of SST-20cm at time of observation (depth_adjustment);
- uncertainty in depth adjustment, which is locally correlated (uncertainty_correlated_depth_adjustment);

Group (ii):

- estimate of daily mean SST at 20 cm (sea_surface_temperature_depth);

- UTC time to which the mean daily SST estimate applies – will be noon for a particular day (daymean_time)
- uncertainty in adjustment to daily mean SST (uncertainty_correlated_time_and_depth_adjustment);
- total uncertainty for estimate of daily mean SST at 20 cm (sea_surface_temperature_depth_total_uncertainty); and
- SST anomaly: the difference between the SST at depth and a reference climatology of SST at depth (sea_surface_temperature_depth_anomaly).

Group (iii):

- type of retrieval used for the alternative SST (alt_sst_retrieval_type);
- adjustment to add to primary SST to obtain alternative SST, which will be zero when there is no alternative (adjustment_alt)
- uncertainty in alternative skin SST from random effects, independent between measured values (uncertainty_random_alt)
- uncertainty in alternative skin SST from locally systematic effects, correlated on local spatio-temporal scales (uncertainty_correlated_alt)
- uncertainty in alternative skin SST from systematic effects, correlated on large scales (uncertainty_systematic_alt)

Group (iv):

- sensitivity of skin SST retrieval to actual changes in SST (sst_sensitivity); and
- adjustment based on comparison to *in situ* data applied to the primary SST retrieval in the absence of a satellite reference sensor (empirical_adjustment).

Information about how to combine the uncertainties is provided in the comment attributes within the files and correlation length and time scales are provided for the synoptically (locally) correlated components. CF standard name modifiers do not exist for individual uncertainty components and so no standard names are defined for them.

A summary of the data fields is given in Table 13.

Table 13. Variables to be included within the L2P data files; some of the name and description information in this table is reproduced from Section 9.1 of [AD.1]. The shading (see Table 8) and the OCC column indicate the number of occurrences of each variable. These are either mandatory (1, blue shading) or optional (0, violet shading).

Name	Description	OCC
lat	Coordinate variable; central latitude of each spatial point of the data arrays	1
lon	Coordinate variable; central longitude of each spatial point of the data arrays	1

Name	Description	OC C
time	Coordinate variable; time of each temporal point of the data arrays; the start time of the granule	1
sea_surface_temperature	Best available skin/subskin SST retrievals (unadjusted for time and depth); fill values to be provided where there is land, cloud or total sea ice cover	1
sst_dtime	Time differences of SST retrievals from the base time in the time coordinate variable	1
sses_bias	SST single sensor error statistic measurement bias estimate (to contain zeroes)	1
sses_standard_deviation	SST single sensor error statistic measurement standard deviation estimate (to contain zeroes)	1
l2p_flags	Flags specific to each L2P dataset that help users interpret data	1
quality_level	A quality level for each measurement	1
wind_speed	An estimate of surface wind speed (from the ERA-Interim reanalysis)	1
sea_surface_temperature_retrieval_type	Type of retrieval used for the primary SST: 1. single view, two channel 2. single view, three channel 3. dual view, two channel 4. dual view, three channel 5. single view, 11 and 3.7 two channel	1
uncertainty_random	uncertainty in skin SST from random effects, independent between measured values	1
uncertainty_correlated	uncertainty in skin SST from locally systematic effects, correlated on local spatio-temporal scales	1
uncertainty_systematic	uncertainty in skin SST from systematic effects, correlated on large scales	1
sea_surface_temperature_total_uncertainty	uncertainty in skin SST from all effects	1
depth_adjustment	modelled vertical temperature difference between skin and 20 cm at time of skin observation	1
uncertainty_correlated_depth_adjustment	uncertainty in estimate of skin to 20 cm temperature difference at time of skin observation ¹	1

¹ Assume a locally systematic effect on same scale as synoptic effects of the atmosphere

Name	Description	OC C
sea_surface_temperature_depth	Estimate of daily mean SST at 20 cm	1
daymean_time	UTC time to which the mean daily SST estimate applies	1
uncertainty_correlated_time_and_depth_adjustment	uncertainty in adjustment to daily mean SST	1
sea_surface_temperature_depth_total_uncertainty	total uncertainty for estimate of daily mean SST at 20 cm	1
sea_surface_temperature_depth_anomaly	SST anomaly: the difference between the SST at depth and a reference climatology of SST at depth	1
alt_sst_retrieval_type	alternative type of retrieval for sea_surface_temperature 1. single view, two channel 2. single view, three channel 3. dual view, two channel 4. dual view, three channel 5. single view, 11 and 3.7 two channel	1
adjustment_alt	adjustment to add to best available skin SST to obtain the alternative retrieval ²	1
uncertainty_random_alt	uncertainty in skin SST from random effects, independent between measured values, for retrieval type alt	1
uncertainty_correlated_alt	uncertainty in skin SST from locally systematic effects, correlated on local spatio-temporal scales, for retrieval type alt	1
uncertainty_systematic_alt	uncertainty in skin SST from systematic effects, correlated on large scales, for retrieval type alt	1
sst_sensitivity	sensitivity of skin/subskin SST retrieval to actual changes in SST	1
empirical_adjustment	adjustment, based on comparison to in situ data, applied to the primary SST retrieval in the absence of a contemporary satellite reference sensor	1

The contents of these files meet the following user requirements:

- The inclusion of wind speed meets user requirement SST_CCI-REQ-39: Provide information on wind speed [RD.393].

² For ATSRs, primary hierarchy is D3 > D2 , and adjustment gives D2 (most consistent through time series) when D3 is provided as best. For AVHRRs, hierarchy is N3 > N2, and adjustment provides N2 when N3 is best. Reason for providing an alternative: can then use N2 or D2 consistently for whole record if consistency (rather than minimum point uncertainty) is user's top priority.

- The SST plus adjustment for depth meets SST_CCI-REQ-6: Provide SST20cm at the observation time [RD.393].
- The SST plus adjustments for depth and time meets requirement SST_CCI-REQ-5: provide daily average SST20cm [RD.393]. Note that provision of skin SST meets requirement SST_CCI-REQ-4: Provide SSTskin.
- Provision of SST anomalies meets SST_CCI-REQ-7 [RD.393].
- The separate uncertainty components and correlation scales provide information to the user about the correlation structure of the uncertainties (requirements: SST_CCI-REQ-27: Provide comprehensively characterised uncertainties in the products and SST_CCI-REQ-29: Provide information about the spatial and temporal correlation structure of errors [RD.393]).
- The files also include a simple quality flag (SST_CCI-REQ-35: Provide simple-to-use quality information for each SST value [RD.393]).

4.3.3 Detailed contents

The detailed contents of the L2P products are defined in Table 14 and Table 15. The former is used to specify the global attributes that have common values in files for all data levels. Together the tables specify the structure of the NetCDF files.

Table 14. Global attributes common to all data files. Contents were taken from [AD.1] Table 8-1 and adapted for the SST_cci data files.

Element name	Description	Range/ value	Unit	T	D	Bytes
Attributes	Beginning of global attributes					
Conventions	The version of the netCDF conventions followed.	CF-1.5, Unidata Observation Dataset v1.0		st		
title	Insert satellite sensor name and data level into the string to create a descriptive name for the data.	ESA SST CCI <Product String> <Data Level> product		st		
summary	Insert satellite sensor name, data level and algorithm name/brief description.	<Product String> <Data Level> product from the ESA SST CCI project, produced using <algorithm name>.		st		
references	Published or web-based references.			st		
institution	RDAC code.	ESACCI		st		

Element name	Description	Range/ value	Unit	T	D	Bytes
history	To contain a history of applications that have been used to process the data. For example this can be used to record the version of the retrieval algorithm applied to the data, the identity of intermediate files used in the processing etc.			st		
license	The GHRSSST standard data license.	GHRSSST protocol describes data use as free and open		st		
id	Unique text string for this product. See Section 3.5.			st		
naming_authority	Defined in [RD.87] as org.ghrsst.	org.ghrsst		st		
product_version	Product version (see Section 3.5).			st		
uuid	Universally Unique Identifier. For example see http://www.ossfp.org/pkg/lib/uuid/ [RD.169]			st		
tracking_id	Identical to uuid (i.e. this shall contain the same value as uuid)			st		
gds_version_id	Version of [GDS] that files are based on.	2.0		st		
netcdf_version_id	NetCDF library.	Format examples: 4.1.1 or 4.2.1.1 of Oct 19 2012 14:25:16		st		
date_created	File creation	Format: yyyymmddThh mmssZ		st		

Element name	Description	Range/ value	Unit	T	D	Bytes
file_quality_level	Select from: 0 = unknown quality 1 = extremely suspect (frequent problems, e.g. with known satellite problems) 2 = suspect (occasional problems, e.g. after launch) 3 = excellent (no known problems)	[0, 3]		sl		4
spatial_resolution	A string describing the approximate resolution of the product. For example, "1.1km at nadir". See Table 1 for values to use.	[1 km at nadir, 0.05°]		st		
start_time	Date and time of the first measurement in the data file.	Format: yyyyymmddThhmmssZ		st		
time_coverage_start	Identical to start_time.	Format: yyyyymmddThhmmssZ		st		
stop_time	Date and time of the last measurement in the data file in the form.	Format: yyyyymmddThhmmssZ		st		
time_coverage_end	Identical to stop_time.	Format: yyyyymmddThhmmssZ		st		
time_coverage_duration	Difference between time_coverage_end and time_coverage_start in the form PdDThHmMsS, replacing the lower case letters with the appropriate numbers.	Format: PdDThHmMsS (see description column for more details) or other ISO 8601 compliant format		st		

Element name	Description	Range/ value	Unit	T	D	Bytes
time_coverage_resolution	Temporal resolution of data in the file i.e. the orbit repeat period or the frequency of L3/L4 data.	Format: PdDThHmMs S (see description of time_coverage_duration for more details)		st		
source	Comma separated list of all source data present in this file. List SST sources first, followed by auxiliary sources. See Section 3.5 for source data names.			st		
Platform	Satellite(s) used to create this data file. Select from the entries found in Table 6			st		
Sensor	Satellite(s) used to create this data file. Select from the entries found in Table 6			st		
Metadata_Conventions		Unidata Dataset Discovery v1.0		st		
metadata_link	Link to collection metadata record at archive.	http://www.esa-cci.org		st		
Keywords	Standard words that describe the data, taken from the source specified in keywords_vocabulary.	Oceans > Ocean Temperature > Sea Surface Temperature		st		
keywords_vocabulary	Defines the source of the text in the keywords attribute; [RD.176].	NASA Global Change Master Directory (GCMD) Science Keywords		st		

Element name	Description	Range/ value	Unit	T	D	Bytes
standard_name_vocabulary	Defines the source of the standard names for the variables; [RD.177].	NetCDF Climate and Forecast (CF) Metadata Convention		st		
geospatial_lat_units	Units of the latitudinal resolution.	degrees_north		st		
geospatial_lat_resolution	Latitude resolution in units matching geospatial_lat_units. See values in Table 1.	[0.009, 0.05]		fl		4
geospatial_lon_units	Units of the longitudinal resolution.	degrees_east		st		
geospatial_lon_resolution	Longitude resolution in units matching geospatial_lon_units. See values in Table 1.	[0.009, 0.05]		fl		4
geospatial_vertical_min	Depth of the deepest SST in the file (negative value as the direction is downwards) – see Table 5	-10 ⁻⁶ or -0.001 or -0.2		fl		4
geospatial_vertical_max	Depth of the shallowest SST in the file (negative value as the direction is downwards) – see Table 5	-10 ⁻⁶ or -0.001 or -0.2		fl		4
acknowledgment	Information about funding source and how to cite the use of these data.	Funded by ESA		st		
creator_name	Description of data creators.	ESA SST CCI		st		
creator_email		science.leader@esa-sst-cci.org		st		
creator_url		http://www.esa-sst-cci.org/		st		

Element name	Description	Range/ value	Unit	T	D	Bytes
creator_processing_institution	Contains additional information about the institution that created the product within the CCI project. Insert institution name (for example 'the University of Reading' or 'the Met Office') to indicate where the data were produced.	These data were produced at <institution> as part of the ESA SST CCI project.		st		
project	The name of the project.	Climate Change Initiative – European Space Agency		st		
publisher_name	Information about the data publisher.	ESACCI		st		
publisher_url		http://www.esa-sst-cci.org		st		
publisher_email		science.leader@esa-SST-cci.org		st		
product_specification_version	Version of this document used to define the file.	The filename of the PSD (without extension)		st		
attributes	End of global attributes					

Table 15. Detailed specification of the SST CCI L2P files.

Element name	Description	Range/value	Unit	T	D	Bytes
Dataset	Begin of dataset					
dimensions	Begin of dimensions					
ni	Across track dimension.			sl	1	4
nj	Along track dimension.			sl	1	4
time	Time dimension; must be 1 for L2P data.	1		sl	1	4

Element name	Description	Range/value	Unit	T	D	Bytes
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
lat	Latitude coordinates.	[-90, 90]		fl	nj, ni	nj × ni × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_north		st		
long_name	A free-text descriptive variable name.	Latitude coordinates		st		
standard_name	Unique descriptive name for data.	Latitude		st		
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lon	Longitude coordinates.	[-180, 180]		fl	nj, ni	nj × ni × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude coordinates		st		
standard_name	Unique descriptive name for data.	Longitude		st		

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
time	Time coordinate ; the start time of the granule	[0, 2 ³¹]		sl	time	time x 4
attributes	Begin of attributes					
units	Text description of the units.	seconds since 1981-01-01 00:00:00		st		
long_name	A free-text descriptive variable name.	reference time of sst file		st		
standard_name	Unique descriptive name for data.	Time		st		
calendar	Defines the calendar used to define the times.	gregorian		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
sea_surface_temperature	Best available sea surface temperature retrievals; to contain fill values if land, cloud or full sea ice cover.	[271.15, 323.15] (after scaling)	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name. First option is for infrared data, second for passive microwave data; see also Table 5.	sea surface skin temperature or sea surface subskin temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-200		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
standard_name	Unique descriptive name for data. Choose appropriate value from Table 5.	sea_surface_skin_temperature or sea_surface_subskin_temperature		st		
comment	Miscellaneous information about the data or the methods used to produce it. Includes method of calculating total uncertainty.	Temperature of the skin of the ocean; total uncertainty = $\sqrt{\text{uncertainty_systematic}^2 + \text{uncertainty_correlated}^2 + \text{uncertainty_random}^2}$		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
depth	Effective depth of the sea_surface_temperature variable. Choose appropriate value from Table 5.	10 micrometres or 1 millimetre		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sst_dtime	Time differences of SST retrievals from the reference time.	[-32767, 32767]	secs	ss	time, nj, ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
units	Text description of the units.	Seconds		st		
scale_factor	To be multiplied by the variable to recover the original value.	1.0		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	time difference from reference time		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-32767		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	32767		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	time plus sst_dtime gives seconds after 1981-01-01 00:00:00		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sses_bias	Single sensor error statistic bias error.	Zero for all SST values	K	sc	time, nj, ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1

Element name	Description	Range/value	Unit	T	D	Bytes
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	SSES bias estimate		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		sc		1
comment	Miscellaneous information about the data or the methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sses_standard_deviation	Single sensor error statistic standard deviation.	Zero for all SST values	K	sc	time, nj, ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	Kelvin		st		

Element name	Description	Range/value	Unit	T	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	1.27		fl		4
long_name	A free-text descriptive variable name.	SSES standard deviation		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		sc		1
comment	Miscellaneous information about the data or the methods used to produce it.	Uncertainty information is contained in the variables uncertainty_systematic, uncertainty_correlated, and uncertainty_random.		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
l2p_flags	Specifies type of input data and provide flags and information to the user. See Table 16.	[0, 255] (this may change if extra flags are defined)		ss	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					

Element name	Description	Range/value	Unit	T	D	Bytes
_FillValue	A value used to indicate array elements containing no valid data.	-32768		sc		1
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	255		sc		1
long_name	A free-text descriptive variable name.	L2P flags		st		
comment	Miscellaneous information about the data or the methods used to produce them.	These flags are important to properly use the data		st		
coordinates	Identifies coordinate variables.	lon lat		st		
flag_meanings	Meaning attached to each flag value.	microwave land ice lake river spare views channels aerosol		st		
flag_masks	Bit masks corresponding to the flags described in flag_meanings.	1, 2, 4, 8, 16, 32, 64, 128, 256		ss		2
attributes	End of attributes					
variable	Begin of variable					
quality_level	Indicator of the quality of each SST.	[0, 5]		sc	time x nj x ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5		sc		1
long_name	A free-text descriptive variable name.	quality level of SST pixel		st		
comment	Miscellaneous information about the data or the methods used to produce it.	These are the overall quality indicators and are those used for all GHRSSST SSTs		st		
coordinates	Identifies coordinate variables.	lon lat		st		
flag_meanings	Meaning attached to each flag value.	no_data bad_data worst_quality low_quality acceptable_q uality best_quality		st		
flag_values	Values that correspond to the flags described in flag_meanings. The b after the numbers is to indicate that they are single byte numbers.	0b, 1b, 2b, 3b, 4b, 5b		sc		1
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
wind_speed	Surface wind speed at 10 m height. Resolution should be no less than 1 m s ⁻¹ and has been defined here to be 0.1 m s ⁻¹ . The range of wind speeds that can be represented is 0 – 25.4 m s ⁻¹ ; values higher than this should be set to the maximum.	[0, 25.4] (after scaling)	ms ⁻¹	sc	time, nj, ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	m s-1		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.1		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	12.7		fl		4
long_name	A free-text descriptive variable name.	10m wind speed		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		sc		1
standard_name	Unique descriptive name for data.	wind_speed		st		

Element name	Description	Range/value	Unit	T	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it.	Wind speeds sourced from ECMWF ERA Interim reanalysis; wind speeds greater than 25.4 m/s are set to 25.4.		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
height	Height that the wind values correspond to.	10 m		st		
time_offset	Difference in hours between the SST reference time and the time of the wind speed value.			fl		4
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature_retrieval_type	Type of retrieval used for the primary SST.	[1,5]		sc	time x nj x ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
long_name	A free-text descriptive variable name.	Type of retrieval used for the primary SST		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	1		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	1. single view, two channel 2. single view, three channel 3. dual view, two channel 4. dual view, three channel 5. single view, 11 and 3.7 two channel		st		
coordinates	Identifies coordinate variables.	lon lat		st		
retrieval_type_meanings	Meaning attached to each value.	single view, two channel single view, three channel dual view, two channel dual view, three channel single view, 11 and 3.7 two channel		st		
retrieval_type_values	Values that correspond to the values described in retrieval_type_meanings. The b after the numbers is to indicate that they are single byte numbers.	1b, 2b, 3b, 4b, 5b		sc		1
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
uncertainty_random	Component of uncertainty that is uncorrelated between SST retrievals separated by any spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
Units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be uncorrelated between SSTs		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
Comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is uncorrelated between SSTs; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncertainty_correlated	Component of uncertainty that is highly correlated between SST retrievals separated by sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
long_name	A free-text descriptive variable name.	Uncertainty from errors like to be correlated over synoptic scales		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is correlated over synoptic scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
uncertainty_systematic	Component of uncertainty that is highly correlated between SST retrievals separated by larger than sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
Attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be correlated over large scales		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is correlated over large scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
Attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature _total_uncertainty	Combination of all uncertainty components.	Total uncertainty from combining uncertainties as described in the comment attribute to the sea_surface_temperature variable	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.00		fl		4
long_name	A free-text descriptive variable name.	Total uncertainty in sea_surface_temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Total uncertainty in each sea_surface_temperature data point		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
depth_adjustment	Adjustment to give SST at 20 cm depth at observation time.	[-10.,10.] (after scaling)	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Adjustment to sea surface temperature at 0.2 m		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-1000		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	1000		ss		2
standard_name	Unique descriptive name for data.			st		
comment	Miscellaneous information about the data or the methods used to produce it.	Add to sea_surface_temperature, if SST at 20cm at observation time is required		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
Coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
uncertainty_correlated_depth_adjustment	Uncertainty in adjustment for depth, correlated between SST estimates separated by sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Depth adjustment uncertainty		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Adjustment uncertainty; can be combined with other uncertainty estimates to form a total uncertainty		st		

Element name	Description	Range/value	Unit	T	D	Bytes
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
Attributes	End of attributes					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature _depth	SSTs adjusted to time representative of the daily average and 20 cm.	[271.15, 323.15] (after scaling)	K	ss	time, nj, ni	time × nj × ni × 2
Attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name.	sea surface temperature at 0.2 m		st		

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-200		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
standard_name	Unique descriptive name for data.	sea_water_temperature		st		
comment	Miscellaneous information about the data or the methods used to produce it. Includes method of calculating total uncertainty.	Temperature of the ocean at 20 cm depth; total uncertainty = $\sqrt{\text{uncertainty_systematic}^2 + \text{uncertainty_correlated}^2 + \text{uncertainty_random}^2 + \text{uncertainty_correlated_time_and_depth_adjustment}^2}$		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
depth	Effective depth of the SST data.	0.2 metre		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
daymean_time	UTC time to which the mean daily SST estimate applies	[0, 2 ³¹]		sl	time	time x 4
Attributes	Begin of attributes					

Element name	Description	Range/value	Unit	T	D	Bytes
units	Text description of the units.	seconds since 1981-01-01 00:00:00		st		
long_name	A free-text descriptive variable name.	UTC time to which the mean daily SST estimate applies		st		
calendar	Defines the calendar used to define the times.	Gregorian		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncertainty_correlated_time_and_depth_adjustment	Uncertainty in adjustment for time and depth, correlated between SST estimates separated by sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
Units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
long_name	A free-text descriptive variable name.	Time and depth adjustment uncertainty		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Adjustment uncertainty; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature_depth_total_uncertainty	Combination of all uncertainty components.	Total uncertainty from combining uncertainties as described	K	ss	time, nj, ni	time x nj x ni x 2

Element name	Description	Range/value	Unit	T	D	Bytes
		in the comment attribute to the sea_surface_temperature_depth variable				
Attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.00		fl		4
long_name	A free-text descriptive variable name.	Total uncertainty in sea_surface_temperature_depth		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Total uncertainty in each sea_surface_temperature_depth data point		st		
coordinates	Identifies coordinate variables.	lon lat		st		

Element name	Description	Range/value	Unit	T	D	Bytes
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature _depth_anomaly	SSTs adjusted to daily average and 20 cm, expressed as a deviation for the long-term average for that day.	[-40., 40.] (after scaling)	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	sea surface temperature anomaly at 0.2 m		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-4000		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	4000		ss		2
standard_name	Unique descriptive name for data.	sea_water_temperature_anomaly		st		

Element name	Description	Range/value	Unit	T	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it. Includes method of calculating total uncertainty. Neglects uncertainty in reference climatology.	Temperature of the ocean at 20 cm depth; total uncertainty = $\sqrt{\text{uncertainty_systematic}^2 + \text{uncertainty_correlated}^2 + \text{uncertainty_random}^2 + \text{uncertainty_time_and_depth_adjustment}^2}$		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
depth	Effective depth of the SST data.	0.2 metre		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
alt_sst_retrieval_type	Type of retrieval used for the alternative SST retrieval	[1,5]		sc	time x nj x ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
long_name	A free-text descriptive variable name.	Type of retrieval used for the alternative SST retrieval		st		

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable once they are packed (in storage type).	1		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	For ATSRs, adjustment gives D2 (most consistent through time series) when D3 is provided as best. For AVHRRs, adjustment provides N2 when N3 is best. Reason for providing an alternative: can then use N2 or D2 consistently for whole record if consistency (rather than minimum point uncertainty) is top priority.		st		
coordinates	Identifies coordinate variables.	lon lat		st		

Element name	Description	Range/value	Unit	T	D	Bytes
retrieval_type_meanings	Meaning attached to each value.	single view, two channel single view, three channel dual view, two channel dual view, three channel single view, 11 and 3.7 two channel		st		
retrieval_type_values	Values that correspond to the values described in retrieval_type_meanings. The b after the numbers is to indicate that they are single byte numbers.	1b, 2b, 3b, 4b, 5b		sc		1
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
adjustment_alt	Adjustment to give alternative SST retrieval.	[-10.,10.] (after scaling)	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
long_name	A free-text descriptive variable name.	Adjustment to alternative sea surface temperature retrieval		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-1000		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	1000		ss		2
standard_name	Unique descriptive name for data.			st		
comment	Miscellaneous information about the data or the methods used to produce it.	Add to sea_surface_temperature, if alternative SST retrieval is required		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncertainty_random_alt	Component of uncertainty in alternative SST retrieval that is uncorrelated between SST retrievals separated by any spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					

Element name	Description	Range/value	Unit	T	D	Bytes
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
Units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty in alternative SST retrieval from errors likely to be uncorrelated between SSTs		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
Comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty in alternative SST retrieval that is uncorrelated between SSTs; can be combined with other uncertainty estimates to form a total uncertainty		st		

Element name	Description	Range/value	Unit	T	D	Bytes
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncertainty_correlated_alt	Component of uncertainty in alternative SST retrieval that is highly correlated between SST retrievals separated by sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty in alternative SST retrieval from errors like to be correlated over synoptic scales		st		

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty in alternative SST retrieval that is correlated over synoptic scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
uncertainty_systematic_attribute	Component of uncertainty in alternative SST retrieval that is highly correlated between SST retrievals separated by larger than sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	K	ss	time x nj x ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty in alternative SST retrieval from errors likely to be correlated over large scales		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		ss		2

Element name	Description	Range/value	Unit	T	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty in alternative SST retrieval that is correlated over large scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sst_sensitivity	Sensitivity of the retrieval to actual changes in sea surface temperature	0 to 1		ss	time, nj, ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
scale_factor	To be multiplied by the variable to recover the original value.	0.001		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.00		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
long_name	A free-text descriptive variable name.	Sensitivity of the retrieval to actual changes in sea surface temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	1000		ss		2
Comment	Miscellaneous information about the data or the methods used to produce it.	Sensitivity of the retrieval to actual changes in sea surface temperature		st		
Coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
empirical_adjustment	Adjustment, based on comparison to in situ data, applied to the primary SST retrieval in the absence of a contemporary satellite reference sensor	[-10.,10.] (after scaling)	K	ss	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	Kelvin		st		

Element name	Description	Range/value	Unit	T	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Adjustment, based on comparison to in situ data		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-1000		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	1000		ss		2
standard_name	Unique descriptive name for data.			st		
comment	Miscellaneous information about the data or the methods used to produce it.	If not applied, fill with zeros to indicate independence from in situ		st		
source	See Table 10.			st		
references	Published or web-based references that describe the data or methods used to produce it.			st		
Coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variables	End of variables					
attributes	Begin of global attributes					

Element name	Description	Range/value	Unit	T	D	Bytes
Global attributes as described in Table 7.						
comment	To contain any miscellaneous information about the data and methods. Delete the 'and sea_surface_temperature_depth' part of the second sentence if the sea_surface_temperature_depth variable is not included in the file.	For information about uncertainty estimates see the comment attributes to the sea_surface_temperature and sea_surface_temperature_depth variables.		st		
northernmost_latitude	Decimal degrees north, range -90 to +90. May vary from orbit to orbit.	[-90, 90]		fl		4
geospatial_lat_max	Identical to northernmost_latitude	[-90, 90]		fl		4
southernmost_latitude	Decimal degrees north, range -90 to +90. May vary from orbit to orbit.	[-90, 90]		fl		4
geospatial_lat_min	Identical to southernmost_latitude	[-90, 90]		fl		4
easternmost_longitude	Decimal degrees east, range -180 to +180. May vary from orbit to orbit.	[-180, 180]		fl		4
geospatial_lon_max	Identical to easternmost_longitude	[-180, 180]		fl		4
westernmost_longitude	Decimal degrees east, range -180 to +180. May vary from orbit to orbit.	[-180, 180]		fl		4
geospatial_lon_min	Identical to westernmost_longitude	[-180, 180]		fl		4
processing_level	Data level.	L2P		st		
cdm_data_type	"swath" or "grid"	Swath		st		

Element name	Description	Range/value	Unit	T	D	Bytes
attributes	End of global attributes					
dataset	End of dataset					

Table 16. Meaning of each bit in a l2p_flags field. Reformatted version of Table 9-19 of [AD.1] with additional entries denoted by italics. Bits 6-15 are available for use by the SST CCI project; two of these are used to describe the retrieval.

Bit	Description	Meaning if 0	Meaning if 1
0	Type of sensor	Infrared	Microwave
1	Ocean or land indicator	Over the ocean	Over land
2	Sea ice indicator	Not sea ice contaminated	Sea ice contaminated
3	Lake indicator (if known)	Not over lake	Over lake
4	River indicator (if known)	Not over river	Over river
5	Reserved for future use		
6	<i>Number of satellite views used in retrieval (or, if no retrieval possible, what it would have been if a retrieval had been performed))</i>	<i>Single (nadir only) view</i>	<i>Dual view</i>
7	<i>Number of channels used in retrieval (or, if no retrieval possible, what it would have been if a retrieval had been performed)</i>	<i>Two channels</i>	<i>Three channels</i>
8	Aerosol dynamic indicator	No significant additional stratospheric aerosol present	Significant additional stratospheric aerosol present, e.g. as a result of a volcanic eruption
9-15	<i>Available for use by SST CCI</i>		

Table 17. Quality level indicators for SST data. Reproduced from Section 9.18 of [AD.1] with shading added to indicate flags that will not be used by SST CCI. In the case of prototype PMW products, quality flags also reflect the presence of Radio Frequency Interference (RFI).

Value	Meaning
0	Missing data
1	These data are not valid and should not be used

Value	Meaning
2	Data are of the lowest quality that still could be usable
3	Low quality data
4	Acceptable quality data
5	Best quality data

4.4 L3U data

4.4.1 Description

Level 3 data files contain gridded SST data (but not analysis data, i.e. they do not include values where no retrieval could be made). In the context of all the data to be produced by SST CCI these will be uncollated (L3U) data files – these contain a single orbit of data from a single sensor (i.e. a gridded version of L2P data).

The grid used shall be a regular 0.05° latitude-longitude grid (SST_CCI-REQ-14, [RD.393]). As with L2P files, the level 3 files shall contain the best available SST data. L3C files – daily collations of data from a sensor – can also be produced following the specification described in this document.

The contents of the files are very similar to those of L2P files and hence meet the same user requirements described in Section 4.3.2.

4.4.2 Summary of contents

The files are almost identical to the L2P files. They differ in the specification of the grid and in some of the attributes. Note that the time dimension in level 3 (and 4) files is set to be unlimited. In practice only one time field is contained in each file, but this allows utilities that operate on the files to concatenate the data [AD.1].

Table 18. Fields within a L3 data file; some of the name and description information in this table is reproduced from Section 9.1 of [AD.1]. The shading (see Table 8) and the OCC column indicate the number of occurrences of each variable. These are either mandatory (1, blue shading) or optional (0..1, violet shading).

Name	Description	OCC
Lat	Vector specifying the central latitude of each spatial point in the data grid	1
lat_bnds	Latitude bounds of each grid cell; included from [RD.166].	1
Lon	Vector specifying the central longitude of each spatial point in the data grid	1
lon_bnds	Longitude bounds of each grid cell; included from [RD.166].	1
time	Vector specifying the reference time of each temporal point in the data grid; this is either the start time of the L3U granule or the mid-point of the collation window for L3C (the midpoint of the day the data represent)	1
time_bnds	Time bounds of each time point (either start and end times of the data collection for L3U or start and end of the day for L3C); included from [RD.166]	1
sea_surface_temperature	Best available sea surface	1

	temperature retrievals (unadjusted for time and depth); fill values to be provided where there is land, cloud or total sea ice cover	
sst_dtime	Time differences of SST retrievals from the reference time	1
sses_bias	SST single sensor error statistic measurement bias estimate (to contain zeroes)	1
sses_standard_deviation	SST single sensor error statistic measurement standard deviation estimate (to contain zeroes)	1
l2p_flags	Flags that help users interpret data	1
quality_level	A quality level for each SST	1
wind_speed	An estimate of surface wind speed (from the ERA-Interim reanalysis)	1
uncertainty_random	uncertainty in skin SST from random effects, independent between measured values	1
uncertainty_correlated	uncertainty in skin SST from locally systematic effects, correlated on local spatio-temporal scales	1
uncertainty_systematic	uncertainty in skin SST from systematic effects, correlated on large scales	1
sea_surface_temperature_total_uncertainty	uncertainty in skin SST from all effects	1
depth_adjustment	modelled vertical temperature difference between skin and 20 cm at time of skin observation	1
uncertainty_correlated_depth_adjustment	uncertainty in estimate of skin to 20 cm temperature difference at time of skin observation ³	1
sea_surface_temperature_depth	Estimate of daily mean SST at 20 cm	1
daymean_time	UTC time to which the mean daily SST estimate applies	1
uncertainty_correlated_time_and_depth_adjustment	uncertainty in adjustment to daily mean SST	1
sea_surface_temperature_depth_total_uncertainty	total uncertainty for estimate of daily mean SST at 20 cm	1
sea_surface_temperature_depth_anomaly	SST anomaly: the difference between the SST at depth and a reference climatology of SST at depth	1
alt_sst_retrieval_type	alternative type of retrieval for	1

³ Assume a locally systematic effect on same scale as synoptic effects of the atmosphere

	sea_surface_temperature 1. single view, two channel 2. single view, three channel 3. dual view, two channel 4. dual view, three channel 5. single view, 11 and 3.7 two channel	
adjustment_alt	adjustment to add to best available skin SST to obtain the alternative retrieval ⁴	1
uncertainty_random_alt	uncertainty in skin SST from random effects, independent between measured values, for retrieval type alt	1
uncertainty_correlated_alt	uncertainty in skin SST from locally systematic effects, correlated on local spatio-temporal scales, for retrieval type alt	1
uncertainty_systematic_alt	uncertainty in skin SST from systematic effects, correlated on large scales, for retrieval type alt	1
empirical_adjustment	adjustment, based on comparison to in situ data, applied to the primary SST retrieval in the absence of a contemporary satellite reference sensor	1

4.4.3 Detailed contents

The detailed contents of the products are defined in Table 19. The table specifies the structure of the NetCDF files. Much of this is done with reference to Table 15. However, note that in keeping with the examples in [AD.1] the spatial dimensions are given different names in level 3 files compared to L2P (lat and lon in the former, ni and nj in the latter).

Table 19. Description of L3 file contents; this follows the specification defined in [AD.1].

Element name	Description	Range/value	Unit	T	D	Bytes
dataset	Begin of dataset					
dimensions	Begin of dimensions					
lon	Zonal dimension.	7200		sl		4
lat	Meridional dimension.	3600		sl		4
time	Time dimension; in practice will be 1.	Unlimited		sl		4

⁴ For ATSRs, primary hierarchy is D3 > D2 , and adjustment gives D2 (most consistent through time series) when D3 is provided as best. For AVHRRs, hierarchy is N3 > N2, and adjustment provides N2 when N3 is best. Reason for providing an alternative: can then use N2 or D2 consistently for whole record if consistency (rather than minimum point uncertainty) is user's top priority.

Element name	Description	Range/value	Unit	T	D	Bytes
bnds	Dimension for the latitude, longitude and time bounds.	2		sl		4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
lat	Latitude coordinates	[-90, 90]		fl	lat	lat x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_north		st		
long_name	A free-text descriptive variable name.	Latitude		st		
standard_name	Unique descriptive name for data.	latitude		st		
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	Y		st		
bounds	Indicates the variable containing the latitude cell boundaries	lat_bnds		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lat_bnds	Bounds of the latitude cells	[-90, 90]		fl	bnds x lat	bnds xlat x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_north		st		
long_name	A free-text descriptive variable name.	Latitude cell boundaries		st		

Element name	Description	Range/value	Unit	T	D	Bytes
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the northern and southern boundaries of the grid cells.		st		
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lon	Longitude coordinates	[-180, 180]		fl	lon	lon x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude		st		
standard_name	Unique descriptive name for data.	longitude		st		
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	X		st		
bounds	Indicates the variable containing the longitude cell boundaries	lon_bnds		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		

Element name	Description	Range/value	Unit	T	D	Bytes
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lon_bnds	Bounds of the longitude cells	[-180, 180]		fl	bnds x lon	bnds x lon x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude cell boundaries		st		
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the eastern and western boundaries of the grid cells.		st		
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
time	Time coordinate	[0, 2 ³¹]		sl	time	time x 4
attributes	Begin of attributes					
units	Text description of the units.	seconds since 1981-01-01 00:00:00		st		
long_name	A free-text descriptive variable name.	reference time of sst file		st		
standard_name	Unique descriptive name for data.	time		st		
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	T		st		

Element name	Description	Range/value	Unit	T	D	Bytes
calendar	Defines the calendar used to define the times.	gregorian		st		
bounds	Indicates the variable containing the time cell boundaries	time_bnds		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
time_bnds	Bounds of the time cells	$[0, 2^{31}]$		sl	bnds × time	bnds × time × 4
attributes	Begin of attributes					
units	Text description of the units.	seconds since 1981-01-01 00:00:00		st		
long_name	A free-text descriptive variable name.	Time cell boundaries		st		
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the start and end times for the time period the data represent.		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
sst_dtime	As specified in Table 15 (except that the coordinates attribute is optional, the storage type is sl, fill value is -2^{31} and valid min and valid max are -43200 and 43200 respectively since 43200 is half a day in units of seconds)					
variable	End of variable					
variable	Begin of variable					
sses_bias	As specified in Table 15 (except that the coordinates attribute is optional)					

Element name	Description	Range/value	Unit	T	D	Bytes
variable	End of variable					
variable	Begin of variable					
sses_standard_deviation	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
l2p_flags	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
quality_level	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
wind_speed	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature_retrieval_type	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
uncertainty_random	As specified in Table 15 (except that the coordinates attribute is optional)					
variable	End of variable					
variable	Begin of variable					
uncertainty_correlated	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
uncertainty_systematic	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature_total_uncertainty	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
depth_adjustment	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
uncertainty_correlated_depth_adjustment	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature_depth	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
daymean_time	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
uncertainty_correlated_time_and_depth_adjustment	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature_depth_total_uncertainty	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
sea_surface_temperature_depth_anomaly	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
alt_sst_retrieval_type	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
adjustment_alt	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
uncertainty_random_alt	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
uncertainty_correlated_alt	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
uncertainty_systematic_alt	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variable	Begin of variable					
empirical_adjustment	As specified in Table 15 (except that the coordinates attribute is optional)					
Variable	End of variable					
Variables	End of variables					
Attributes	Begin of global attributes					
Global attributes as described in Table 14.						
Comment	To contain any miscellaneous information about the data and methods. Delete the 'and sea_surface_temperature_depth' part of the second sentence if the sea_surface_temperature_depth variable is not included in the file.	For information about uncertainty estimates see the comment attributes to the sea_surface_temperature and sea_surface_temperature_depth variables.		st		
northernmost_latitude	Decimal degrees north, range -90 to +90.	90.0		fl		4
geospatial_lat_max	Identical to northernmost_latitude	90.0		fl		4
southernmost_latitude	Decimal degrees north, range -90 to +90.	-90.0		fl		4
geospatial_lat_min	Identical to southernmost_latitude	-90.0		fl		4

Element name	Description	Range/value	Unit	T	D	Bytes
easternmost_longitude	Decimal degrees east, range -180 to +180.	180.0		fl		4
geospatial_lon_max	Identical to easternmost_longitude	180.0		fl		4
westernmost_longitude	Decimal degrees east, range -180 to +180.	-180.0		fl		4
geospatial_lon_min	Identical to westernmost_longitude	-180.0		fl		4
processing_level	Data level.	L3U or L3C		st		
cdm_data_type	"swath" or "grid"	grid		st		
Attributes	End of global attributes					
Dataset	End of dataset					

4.5 L4 data

4.5.1 Description

Level 4 data – SST data that have been analysed to remove data gaps – are to be produced by the SST CCI project using the Operational Sea surface Temperature and sea Ice Analysis (OSTIA) system. The contents of these files are largely as defined in [AD.1]. A summary of the specification is included here for completeness.

4.5.2 Summary of contents

As described in [AD.1], the contents of the L4 files include SSTs, uncertainties and information about locations of land and sea ice. Separate files of SST anomaly will also be provided in v2. The files containing actual SST are summarised in Table 20 and those containing SST anomaly are summarised in Table 21.

The contents of the files meets user requirements:

- Provision of a product that does not contain data gaps, such as a L4 product, is required (SST_CCI-REQ-1 and SST_CCI-REQ-2, [RD.393]).
- SST_CCI-REQ-5 [RD.393]: the product will contain SSTs corresponding to 20 cm depth, representative of the UTC-daily average.
- Sea ice fraction and sea ice flags are provided in the L4 files (SST_CCI-REQ-37 and SST_CCI-REQ-39, [RD.393]).
- Provision of anomalies is required by SST_CCI-REQ-7. For practical reasons, these are provided in separate files for the L4 analysis.

Table 20. Variables to be included within the SST CCI L4 data files containing actual SST; some of the name and description information in this table is reproduced from Section 11.2 of [AD.1]; see [AD.1] for more details. The shading (see Table 8) and the OCC column indicate the number of occurrences of each variable. All variables listed are mandatory (1, shaded blue).

Name	Description	OCC
lat	Central latitude of each spatial point of the data arrays	1
lat_bnds	Latitude bounds of each grid cell; included from [RD.166].	1
lon	Central longitude of each spatial point of the data arrays	1
lon_bnds	Longitude bounds of each grid cell; included from [RD.166].	1
time	Time of each temporal point of the data arrays; time should be the middle of the day that the data represents	1
time_bnds	Time bounds of each time point (start and end of the day); included from [RD.166]	1
analysed_sst	Sea surface temperature data; this will either be a foundation SST (demonstration ECV) or 20 cm depth SST (long term ECV); fill values to be used where there is land; where there is total sea ice cover the analysis will contain temperatures that relax over time towards -1.8°C.	1
analysed_sst_uncertainty	Analysis uncertainty (estimate of one standard deviation of the error probability distribution)	1
sea_ice_fraction	Sea ice concentration; taken from OSI SAF data	1
sea_ice_fraction_uncertainty	Estimated error standard deviation of sea ice fraction; taken from OSI SAF data	0..1
mask	Indicates if a location is land, sea-ice or lake	1

Table 21. Variables to be included within the SST CCI L4 data files containing SST anomalies. The shading (see Table 8) and the OCC column indicate the number of occurrences of each variable. All variables listed are mandatory (1, shaded blue).

Name	Description	OCC
lat	Central latitude of each spatial point of the data arrays	1
lat_bnds	Latitude bounds of each grid cell; included from [RD.166].	1

lon	Central longitude of each spatial point of the data arrays	1
lon_bnds	Longitude bounds of each grid cell; included from [RD.166].	1
time	Time of each temporal point of the data arrays; time should be the middle of the day that the data represents	1
time_bnds	Time bounds of each time point (start and end of the day); included from [RD.166]	1
analysed_sst_anomaly	Sea surface temperature at 20cm anomaly relative to the period 1981-2010; fill values to be used where there is land.	1
analysed_sst_uncertainty	Analysed sst uncertainty (one error standard deviation), to be used as anomaly uncertainty since the underlying climatology is treated as an error-free reference	1
sea_ice_fraction	Sea ice concentration; taken from OSI SAF data	1
sea_ice_fraction_uncertainty	Estimated error standard deviation of sea ice fraction; taken from OSI SAF data	0..1
mask	Indicates if a location is land, sea-ice or lake	1

4.5.3 Detailed contents

The detailed contents of the files are specified in Table 22. To avoid duplication, we include both analysed_sst and sst_anomaly below in one table, but they will be provided in separate files.

Table 22. Detailed contents of the SST CCI L4 files.

Element name	Description	Range/value	Unit	T	D	Bytes
dataset	Begin of dataset					
dimensions	Begin of dimensions					
lon	Zonal dimension	7200		sl	1	4
lat	Meridional dimension	3600		sl	1	4
time	Time dimension; in practice will be 1.	Unlimited		sl	1	4
bnds	Dimension for the latitude, longitude and time bounds.	2		sl		4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
lat	As Table 19.					
variable	End of variable					
variable	Begin of variable					
lat_bnds	As Table 19.					
variable	End of variable					
variable	Begin of variable					
lon	As Table 19.					
variable	End of variable					
variable	Begin of variable					
lon_bnds	As Table 19.					
variable	End of variable					
variable	Begin of variable					
time	As Table 19.					
variable	End of variable					
variable	Begin of variable					
time_bnds	As Table 19.					
variable	End of variable					
variable	Begin of variable					
analysed_sst	SST values	[270.15, 318.15] (after scaling)	K	ss	time x lat x lon	time x lat x lon x 2

Element name	Description	Range/value	Unit	T	D	Bytes
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name.	analysed sea surface temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-300		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	4500		ss		2
standard_name	set to "sea_water_temperature" and include the depth attribute.	sea_water_temperature		st		
source	Set to comma separated list of the values of the global source attribute in the input files; see Section 3.5.			st		
depth	Include only if standard_name is set to sea_water_temperature. Effective depth of the SST data.	20 cm		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
Variable	End of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
variable	Begin of variable					
analysed_sst_anomaly	SST anomalies	[-40, 40] (after scaling)	K	ss	time x lat x lon	time x lat x lon x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0		fl		4
long_name	A free-text descriptive variable name.	analysed sea surface temperature anomaly		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-4000		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	4000		ss		2
standard_name	set to "sea_water_temperature" and include the depth attribute.	sea_water_temperature_anomaly		st		
source	Set to comma separated list of the values of the global source attribute in the input files; see Section 3.5.			st		
depth	Include only if standard_name is set to sea_water_temperature. Effective depth of the SST data.	20 cm		st		

Element name	Description	Range/value	Unit	T	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Start of variable					
analysed_sst_uncertainty	Uncertainty in the SSTs	[0, 327.68] (after scaling)	K	ss	time × lat × lon	time × lat × lon × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		ss		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	estimated error standard deviation of analysed_sst		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		ss		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	32767		ss		2
standard_name	Unique descriptive name for data.	sea_water_temperature_standard_error		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		

Element name	Description	Range/value	Unit	T	D	Bytes
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_ice_fraction	Sea ice concentration	[0, 1]	Fraction	sc	time x lat x lon	time x lat x lon
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	1		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	sea ice area fraction		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	100		sc		1
standard_name	Unique descriptive name for data.	sea_ice_area_fraction		st		
source	Source of the sea ice concentrations, including version number (to be confirmed).	EUMETSAT_OSI-SAF-ICE-v1.2		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
sea_ice_fraction_uncertainty	Uncertainty in sea ice concentration	[0, 1]	Fraction	sc	time x lat x lon	time x lat x lon
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	1		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	sea ice area fraction uncertainty estimate		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	100		sc		1
standard_name	Unique descriptive name for data.	sea_ice_area_fraction_standard_error		st		
source	Source of the sea ice concentrations, including version number (to be confirmed).	EUMETSAT_OSI-SAF-ICE-v1.2		st		
comment	Miscellaneous information about the data or the methods used to produce it.	Estimated error standard deviation of sea ice fraction		st		
attributes	End of attributes					
variable	End of variable					
variable	Start of variable					

Element name	Description	Range/value	Unit	T	D	Bytes
mask	Specifies if a location is land, sea-ice or lake	[1, 31]	None	sc	time x lat x lon	time x lat x lon
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
long_name	A free-text descriptive variable name.	sea/land/lake /ice field composite mask		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	1		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	31		sc		1
source	Source of the mask, including version numbers.	Based on CCI LC water body mask applied at L3 grid resolution, EUMETSAT_ OSI- SAF_icemas k, ARCLake_la kemask		st		
comment	Miscellaneous information about the data or methods used to produce them.	b0: 1=grid cell is open sea water b1: 1=grid cell is land b2: 1=grid cell is lake surface b3: 1=grid cell is sea ice b4-b7: reserved for future grid mask data		st		
flag_meanings	Meaning attached to each flag value.	water land optional_lake _surface sea_ice optional_river _surface		st		

Element name	Description	Range/value	Unit	T	D	Bytes
flag_masks	Values that correspond to the flags described in flag_meanings.	1b, 2b, 4b, 8b, 16b		sc		1
attributes	End of attributes					
variable	End of variable					
variables	End of variables					
attributes	Begin of global attributes					
As Table 14.						
comment	To contain any miscellaneous information about the data and methods.			st		
northernmost_latitude	Decimal degrees north, range -90 to +90.	90.0		fl		4
geospatial_lat_max	Identical to northernmost_latitude	90.0		fl		4
southernmost_latitude	Decimal degrees south, range -90 to +90.	-90.0		fl		4
geospatial_lat_min	Identical to southernmost_latitude	-90.0		fl		4
easternmost_longitude	Decimal degrees east, range -180 to +180.	180.0		fl		4
geospatial_lon_max	Identical to easternmost_longitude	180.0		fl		4
westernmost_longitude	Decimal degrees west, range -180 to +180.	-180.0		fl		4
geospatial_lon_min	Identical to westernmost_longitude	-180.0		fl		4
processing_level	Data level.	L4		st		
cdm_data_type	"swath" or "grid"	Grid		st		
attributes	End of global attributes					
dataset	End of dataset					

5. FILE SIZE ESTIMATES

An estimate of product size per file for each file type is provided in Table 23. The product sizes are broken down into components with different dimensionality and the number of bytes used for each component is recorded. For example the table reveals that a level 2 file stores data with dimensionality $n_i \times n_j$ and the total amount of storage required per element of the arrays with these dimensions is 8 bytes (these are the arrays containing the latitudes and longitudes of the data, which are both stored as floating point numbers and use 4 bytes per value). The total storage requirement for these data are therefore $n_i \times n_j \times 8$ bytes, The total file size can be estimated by assuming values for the dimensions and totalling the storage requirements for all the components.

The size estimates give an indication of the data processing and writing requirements. However, they exclude storage for arrays of characters, which use negligible space compared to the data arrays.

Note that these sizes are for uncompressed files. The sizes for L2 data will vary according to sensor but are representative of the largest files that might be expected. In practice the compression capability of the NetCDF-4/HDF5 format will result in much smaller files.

Table 23. File size estimates in bytes unless otherwise stated, divided into components with different dimensionality. Total size estimate assumes that $n_i = 625$, $n_j = 7,000$, $lon = 7,200$, $lat = 3,600$, $time = 1$, $bnds = 2$. Size of level 2 files will vary from sensor to sensor and level 3/4 file sizes depend on the grid that is used.

Dimensionality	Level 2	Level 3	Level 4
n_i or lon	0	4	4
n_j or lat	0	4	4
Time	4	4	4
$(n_i$ or $lon) \times bnds$	0	4	4
$(n_j$ or $lat) \times bnds$	0	4	4
$time \times bnds$	0	4	4
$(n_i$ or $lon) \times (n_j$ or $lat)$	8	0	0
$(n_i$ or $lon) \times (n_j$ or $lat) \times time$	46	46	8
Total uncompressed size estimate	236 MB	1140 MB	164 MB