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Author

James, Cassandra, Bainbridge, Zoe, Lewis, Stephen, Clech-Goods, Celine, Mann, Reinier, Huggins, Raethea, Orr, David, Welk, Kylee, Liu, Shuci, Agnew, Gordon, Bartley, Rebecca, Bramley, Robert, Buckle, Alicia, Cogle, Lex, Cross, Matthew, et al.

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Compilation of riverine water quality data from the Great Barrier Reef catchment area, northeastern Australia

Cassandra James[1]✉, Zoe Bainbridge[1], Stephen Lewis[1], Celine Clech-Goods[2], Reinier Mann[2], Raethea Huggins[2], David Orr[2], Kylee Welk[2], Shuci Liu[3], Gordon Agnew[4], Rebecca Bartley[5], Robert Bramley[6], Alicia Buckle[7], Lex Cogle[8], Matthew Cross[9], Aaron Davis[1], Michelle Devlin[10], Bradley D. Eyre[11], John Faithful[12], Miles Furnas[13], Paul Godfrey[14], Renee Gruber[13], Aaron Hawdon[15], Christina Howley[16], Heather Hunter[14,17], Mark Kennard[18], Emma Laxton[19], Stephen Mackay[14], David McJannet[5], Michael Nash[20], Dominique O'Brien[1], Fred Oudyn[21], Richard Pearson[1], Ken Rohde[22], Michelle Tink[23] & Andrew Moss[24]

This manuscript describes the collation of available water quality data from the freshwater reaches of surface streams within the Great Barrier Reef catchment area, northeastern Australia. This compilation represents one of the most comprehensive online datasets for historical tropical and subtropical freshwater quality around the world. We document the criteria for selection of the data and associated publications as well as the processes of data cleaning used to produce a qualitative assessment of the datasets. The final compilation includes 41 individual datasets that collectively report 466 sites and contain over 26,000 discrete water quality sample records totaling more than 350,000 unique water quality results. Finally, we outline the nuances of the data that end users need to take into account when combining them for spatial and temporal analyses. The dataset ensures that these valuable water quality data collected over the past four decades are preserved for the next generations of researchers, practitioners, management agencies and policy makers.

[1]Catchment to Reef Research Group, TropWATER, James Cook University, Townsville, Australia. [2]Water Quality and Investigations (Science Division), Department of the Environment, Tourism, Science and Innovation, Brisbane, Australia. [3]Water and Catchments (Science Division), Department of the Environment, Tourism, Science and Innovation, Brisbane, Australia. [4]Waterways and Catchment Management Team, Sunshine Coast Council, Nambour, Australia. [5]CSIRO Environment, Brisbane, Australia. [6]CSIRO Agriculture and Food, Adelaide, Australia. [7]Terrain Natural Resource Management, Innisfail, Australia. [8]Formerly Department of Natural Resources and Management, Mareeba, Australia. [9]Inorganic Chemistry, Queensland Health Forensic and Scientific Services, Brisbane, Australia. [10]Centre for Environment, Fisheries and Aquaculture Science, Lowestoft, Suffolk, NR33, UK. [11]Centre for Coastal Biogeochemistry, Faculty of Science and Engineering, Southern Cross University, Lismore, Australia. [12]Formerly JCU TropWATER; now WSP Australia P/L, Townsville, Australia. [13]Australian Institute of Marine Science, Townsville, Australia. [14]Formerly Australian Rivers Institute, Griffith University, Brisbane, Australia. [15]CSIRO Environment, Townsville, Australia. [16]Howley Environmental Consulting, Cooktown, Australia. [17]Formerly Department of Environment and Resource Management, Brisbane, Australia. [18]Australian Rivers Institute, Griffith University, Brisbane, Australia. [19]J.H. & E.S. Laxton - Environmental Consultants, Sydney, Australia. [20]Formerly Terrain NRM; Aquasea Enterprises, Ingham, Australia. [21]Chemistry Centre, Department of the Environment, Tourism, Science and Innovation, Brisbane, Australia. [22]Water & Catchments – Science Division, Department of the Environment, Tourism, Science and Innovation, Mackay, Australia. [23]TropWATER Laboratory, James Cook University, Townsville, Australia. [24]Aquatic Ecosystem Health (Science Division), Department of the Environment, Tourism, Science and Innovation, Brisbane, Australia. ✉e-mail: Cassandra.James@jcu.edu.au

Background & Summary

The Great Barrier Reef catchment area (GBRCA) covers a 423,000 km^2 region of northeastern Australia and hosts a diverse range of aquatic ecosystems across seven distinct biogeographical regions (Fig. 1[1]). Most of the 35 river basins that comprise the GBRCA have been extensively modified since the arrival of Europeans (c. 1850), including the introduction of grazing animals (cattle and initially sheep), cropping, mining and urban developments[2]. These land-use changes have profoundly influenced the water quality of the receiving streams that discharge to the Great Barrier Reef (GBR) lagoon and have been extensively documented by several monitoring programs conducted over the past 40 years[1,3–14]. However, the raw data collected by many of these monitoring programs were not included within published reports and most exist within fragmented and unmaintained online resources, as appendices of hard copy grey-literature reports (i.e., unavailable online) or on individual computer hard drives. Clearly, there is an urgent need to collate the available water quality data for the GBRCA so that they are readily accessible to all potential users. This compilation, its digital storage and dissemination, provides a valuable bank of water quality data accessible to water quality practitioners and management agencies. For example, the data will be available to inform regional Water Quality Improvement Plans and regional Report Cards, and available to local, state and federal government and Natural Resource Management (NRM) agencies, and the next generation of water quality practitioners and modellers. To our knowledge, this compilation represents one of the largest and most comprehensive compilations of historical freshwater quality from tropical and subtropical regions of the world. Such a collation would reveal the spatial and temporal extents of the existing monitoring, allow spatial and temporal trends to be analysed from a larger data resource, inform future monitoring activities and knowledge gaps, and pay tribute to and preserve the legacy of the pioneering practitioners.

The water quality datasets from the GBRCA that were identified for inclusion represent monitoring programs conducted by practitioners dispersed across numerous research organisations (e.g., the Australian Institute of Marine Science [AIMS], Commonwealth Scientific and Industrial Research Organisation [CSIRO], and various universities), government departments, natural resource management (NRM) groups, local councils, and private contractors over a non-continuous 40-year period to 2023. The datasets reflect the different research questions and scientific issues that the practitioners were addressing, including development of site-specific water quality guidelines/objectives and water quality improvement plans (including land use and sub-catchment water quality monitoring), baseline condition assessment and wetland processes, water quality compliance, catchment sediment and nutrient budgets, and exports of various water quality parameters to the GBR lagoon. The datasets capture considerable financial investment from numerous state and federal government funded programs over several decades back to the late 1990's. This diversity is manifested in the different methods for water quality sample collection, reporting, and the different laboratory analyses employed. Such differences present challenges to how the data are compiled and curated. In particular, the different extraction methods for total and particulate nitrogen and phosphorus can produce widely varying results[15–20] and need to be carefully addressed to avoid spurious interpretations of the data. Hence, a robust and systematic Quality Assurance/Quality Control (QA/QC) framework needs to be developed and implemented to document the overall confidence of each dataset, to acknowledge limitations, and to highlight the key metadata so that all methods are replicable should future investigations be required. Our intent was to maintain the veracity and security of the data for the future in its rawest state possible, while eliminating major errors and artifacts of any data processing.

The Queensland Department of the Environment, Tourism, Science and Innovation's (DETSI) Great Barrier Reef Catchment Loads Monitoring Program (GBRCLMP) has conducted monitoring of total suspended solids (TSS), total, particulate and dissolved species of nitrogen and phosphorus, and various pesticide residues across several major tributaries of the GBRCA since the 2006–07 financial year[21–23]. The GBRCLMP follows a rigorous QA/QC process across sample collection, processing, analysis, and reporting protocols and has recently set up a Microsoft Azure Data Platform and the associated public website Tahbil - Water Quality Data Portal (Water Quality & Investigations, DETSI) to collate, store and disseminate their raw and calculated water quality data. Statistical analyses of this data resource have already provided valuable insights on the spatial and temporal drivers of water quality across the GBRCA[24–26]. Undoubtedly, further insights on spatial and temporal water quality trends can be gained through the collation and curation of the earlier water quality datasets in combination with the GBRCLMP dataset.

This paper describes the processes employed to produce the historical water quality data compilation for the GBRCA and how datasets and their associated metadata were identified and curated. The identification process involved literature searches and the knowledge of the extensive authorship base, many of whom are the original custodians of the individual datasets. Due to resource constraints, the water quality data have been restricted to surface freshwater monitoring of total suspended solids, total and dissolved speciation of carbon, nitrogen and phosphorus, ionic composition (cations, anions), pesticide residues and trace metals. We also included associated field and laboratory measured physical and chemical properties where they accompanied the above water quality datasets. Some case-by-case exceptions were made to ensure the 'complete dataset' was preserved (i.e., datasets which contained some estuarine sites). The identified datasets were then subjected to a rigorous 'cleaning process' to highlight laboratory detection limits and methods as well as to convert data to standardised reporting units. Finally, a metadata compilation has been produced to thoroughly document all sample site details, collection methods and laboratory procedures for each of the datasets.

Our historical water quality data compilation for the GBRCA encompasses 41 individual datasets that collectively report over 466 individual sites and contain over 26,000 records with each record being a discrete water quality sample collected at a particular location and date/time. The coverage of sites show a clear spatial bias concentrated along the coastal section from Cairns to Mackay (Fig. 1). There are fewer monitored sites in the Cape York, Burnett Mary and Fitzroy NRM regions. The spatial bias of sampling sites on the coastal plain reflect largely where the intensive agricultural, urban and industrial land uses are found, as well as the most

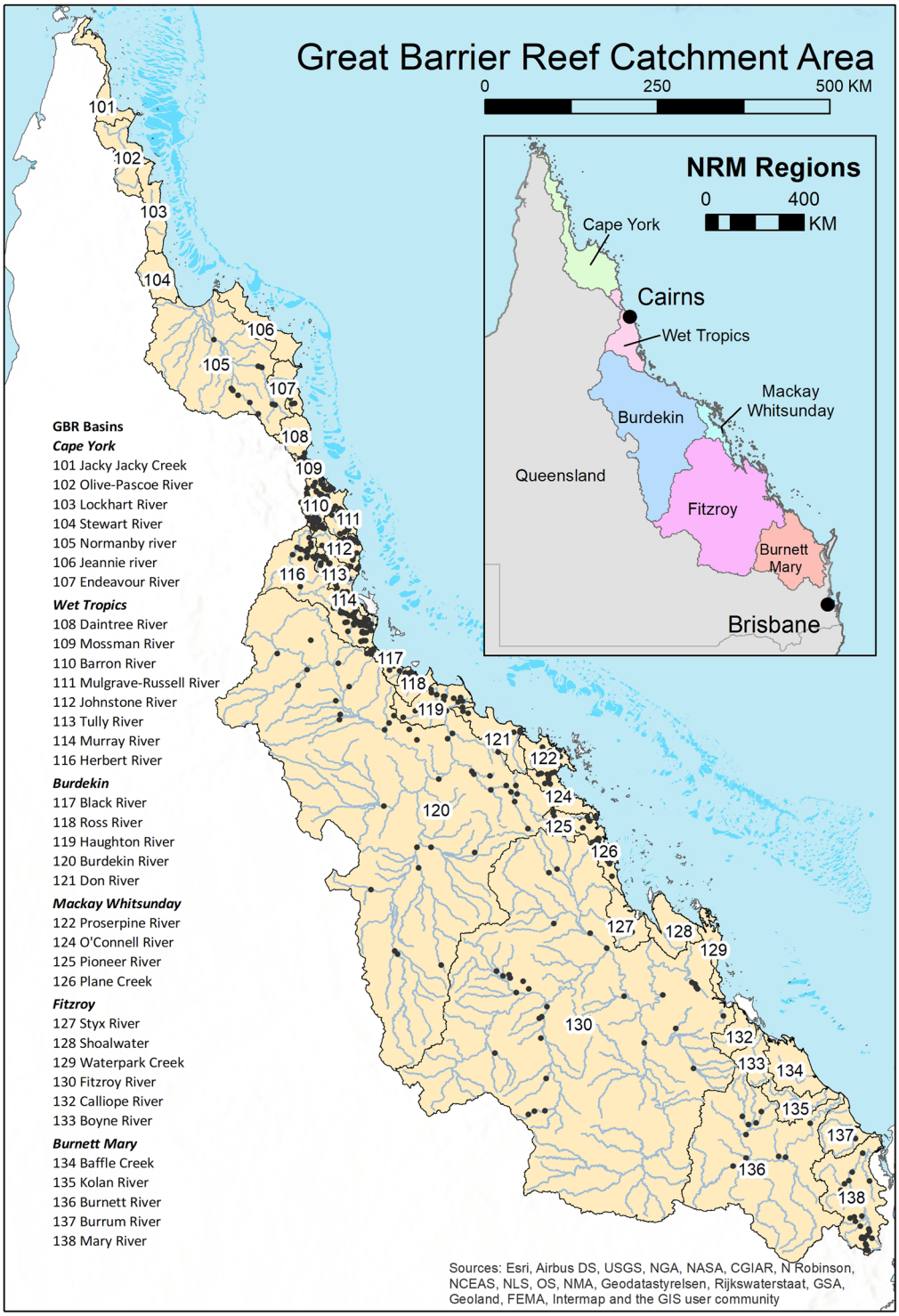

Fig. 1 Great Barrier Reef Catchment Area (GBRCA), river basins, Natural Resource Management (NRM) regions, and monitoring site locations captured in this compilation.

downstream ('end of pipe') locations on rivers discharging into the GBR lagoon. Each record usually contains multiple parameter measurements. Due to the array of project intents and budgets, there is a high degree of variability in the water quality parameters collected for a particular location and datetime stamp. Overall, oxidised nitrogen (NO_X) was the most common water quality parameter measured across the monitoring sites (20,559 records), followed by ammonium (19,945), filterable reactive phosphorus (FRP) (19,746 records), and total suspended solids (TSS) or total solids (18,355 records) (Fig. 2). These parameters have been the foundation of most end-of-catchment load and land-use-specific monitoring programs since the late 1980s and generally

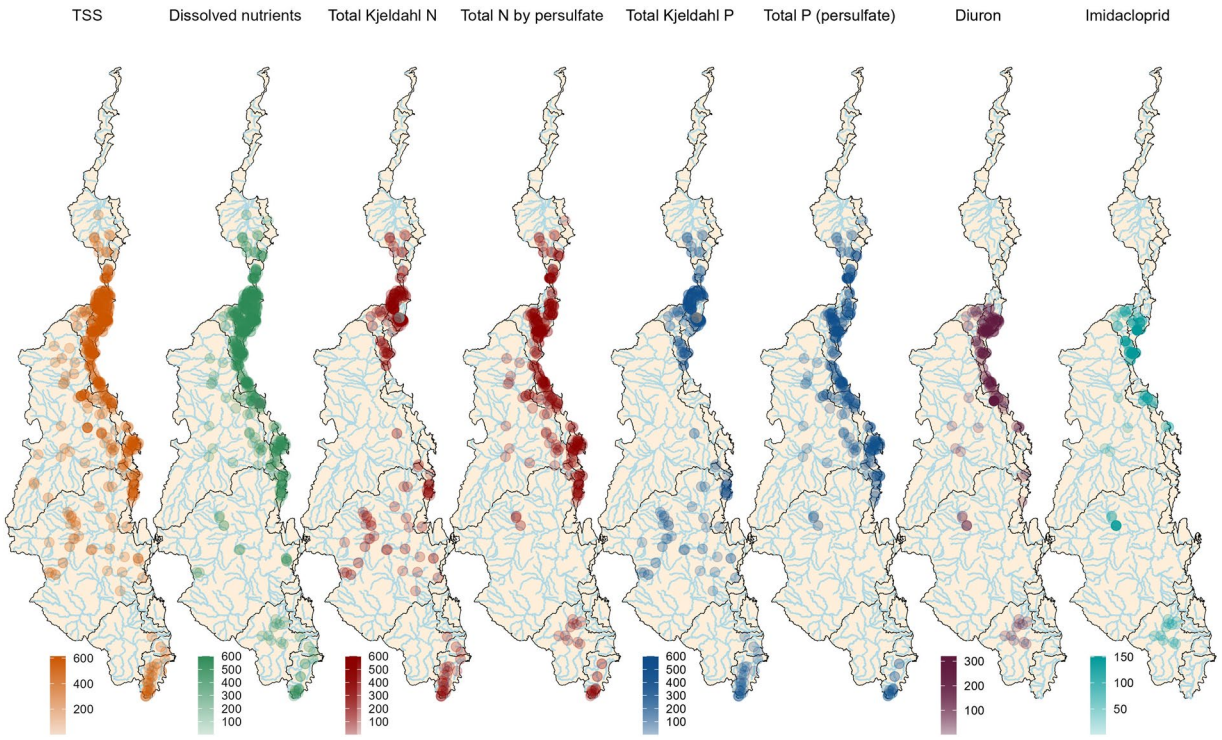

Fig. 2 Distribution and counts of selected parameters across the GBR catchments aggregated over time. Dissolved nutrients include nitrogen oxides, ammonium and filterable reactive phosphorus as counts for these were extremely similar across the catchments.

demonstrate the same spatial bias as the site distributions, although some differences in spatial coverage between the parameters are evident (Fig. 2).

Methods

Data acquisition. Potential datasets were identified through a review of available literature including the historical review of Mitchell *et al.*[3] and subsequent reviews by Brodie and Mitchell[27,28] and Bartley *et al.*[29]. Much of the water quality data for the region resides in grey literature such as project reports. Word of mouth was also an important avenue through which potential data were identified. Once potential datasets were identified, requests were sent to the data proponents by email for permission to access the data and any associated documentation including original laboratory reports, and to provide each data custodian with a data usage agreement. Most datasets were provided in electronic form, but a small number were only available in hard copy and had to be transcribed. Unfortunately, some datasets were excluded at this early stage due to loss of the raw data from computer hard drives, data confidentiality concerns, or the unreachability of the lead practitioners. Datasets with limited sampling (i.e., <5 samples in total per site) were also excluded from this compilation, as were datasets collected at the finer farm (or block) scale due to the focus on waterways. Overall, this process yielded 41 water quality datasets from the GBRCA suitable for compiling (Table 1).

Data criteria. *Location and date time.* All contributing datasets were initially assessed to ensure that essential metadata for the sites (location, date and time) were available. We mapped the location provided for each site and referenced this against maps provided in the corresponding publications. The site descriptions in most instances provided a relatively accurate location. For example, many sites were described by their proximity to a road bridge and hence could be located with reasonable confidence. In some earlier datasets, the location information provided was not of sufficient accuracy to locate the site on the stream network. Where possible we verified the locations with the individual data providers. If the site could not be located with a degree of confidence it was removed from the dataset (this related to two datasets).

All site latitudes and longitudes are presented in Geocentric Datum of Australia 2020 (GDA2020). In many cases, data were provided with coordinates but without information on the reference datum. In these instances, we mapped the locations based on the most likely datum used and verified them against the site descriptions and maps. The majority of the data were provided with a date when sampling occurred, and our preference was for data with a date and time of sampling. However, a few datasets provided only a month and year of sampling but were deemed to be important early datasets. In these instances, we used the middle of the month date (15th) to estimate a sampling date. This has been flagged in the metadata associated with these datasets. When a sampling time was not provided the timestamp defaults to the sample being collected at midnight.

Project code	Project name, date range and parameter groupings	Data custodian
E_AIMSGBR	GBR river water quality; 1986–00	The Australian Institute of Marine Science (AIMS)[1,3,4,39,47]
E_EPAGBR	EPA GBR river water quality; 1992–22	Queensland Government[6]
E_LAXTGBR	Laxton GBR river water quality; 1998–03	Laxton - Environmental Consultants P/L[48]
E_SCUGBR	GBR DIC study; 2014–17	Southern Cross University[49]
E_HECNR	Normanby catchment water quality; 2006–18	Howley Environmental Consulting[14,50,51]
E_HECAR	Annan-Jeannie catchments water quality; 2002–12	Howley Environmental Consulting[52]
E_SCUEST	Annan-Daintree estuarine water quality study; 1995	Southern Cross University[53]
E_DSWQIP	Douglas Shire WQIP; 2003–04	Commonwealth Scientific and Industrial Research Organisation (CSIRO)[54]
E_NHTBR	NHT Barron River water quality; 1992–99	Queensland Government[55]
E_GBRMPA	Barron Russell-Mulgrave water quality; 1997–00	Great Barrier Reef Marine Park Authority (GBRMPA)[56]
E_ECOTOUR	Wet Tropics Ecotourism study; 1995	TropWATER, James Cook University (JCU)[57,58]
E_PROJ25	Project 25 Russell-Mulgrave water quality; 2016–20	TropWATER, JCU[13,59]
E_NHTJR	NHT Johnstone River water quality; 1991–98	Queensland Government[7,60,61]
E_WTMIP	Wet Tropics Major Integrated Project (WTMIP); 2018–23	Terrain Natural Resource Management on behalf of the WTMIP consortium[62]
E_TWQIP	Tully WQIP; 2005–07	TropWATER, JCU[8,63]
E_HYDRO	Tully-Millstream Hydroelectric Scheme; 1990	TropWATER, JCU[64,65]
E_MTSRF7	MTSRF Tully-Murray floodplain wetlands; 2008–09	TropWATER, JCU; Australian Rivers Institute (ARI), Griffith University[66]
E_DPIFOR	Whitfield Creek DPI Forestry; 2003–04	TropWATER, JCU[67]
E_KYAMBUL	Kyambul Lagoon water quality; 2007–09	CSIRO[68]
E_CSIROHR	Lower Herbert River water quality; 1992–95	CSIRO[5,69]
E_HWQMP	Herbert Water Quality Monitoring Program; 2011–17	TropWATER, JCU; Herbert Cane Productivity Services Ltd.; Terrain NRM[70–72]
E_BRWQIP	Black Ross WQIP; 2007–08	TropWATER, JCU[73,74]
E_TCCWEIR	TCC Selected weir water quality data; 2013–22	Townsville City Council (TCC; 2023).
E_CSIROWW	Wheel Weany event water quality; 2000–17	CSIRO[75,76]
E_NHTBKN	Townsville Burdekin water quality; 2001–02	TropWATER, JCU[77]
E_BCWQ	Burdekin Community water quality; 2003–11	TropWATER, JCU[9,78–84]
E_MYUNA	Bowen River water quality at Myuna; 2003–08	CSIRO; TropWATER, JCU; North Queensland Dry Tropics (NQDT)[10,79–81]
E_LDCBBB	LDC Bowen community water quality; 2018–22	TropWATER, JCU; NQ Dry Tropics[10]
E_LWRRBAR	LWRR Barratta Wetlands study; 1991–93	TropWATER, JCU[85]
E_RRRDBAR	RRRD Barratta intensive study; Jan 2013	University of Queensland; TropWATER, JCU[86,87]
E_LBWQIP	Lower Burdekin WQIP; 2004–11	TropWATER, JCU[45,79–82,88,89]
E_WRICMA	WRICMA Coast and Clean Seas Whitsunday; 2000–02	TropWATER, JCU[90]
E_MWHW03	Mackay Whitsunday Healthy Waterways; 2002–03	Queensland Government[91,92]
E_MWHW08	Mackay Whitsunday Healthy Waterways; 2004–08	Queensland Government[93–95]
E_LAXTSAR	Sarina, Broadsound shires water quality; 1989–93	Laxton - Environmental Consultants P/L[96]
E_NAPFR	NAP Fitzroy River water quality; 1994–98; 2002–08	Queensland Government[11,97]
E_FBAFR	Fitzroy Priority Neighbourhood Catchments; 2006–10	Fitzroy Basin Association Inc.[98,99]
E_P2RGOR	Gordonstone Creek paddock to reef study; 2000–21	Fitzroy Basin Association Inc.[100–102]
E_BCCANBR	North Burnett water quality post TC Oswald; 2014–17	Burnett Catchment Care Association[103]
E_SCCMR	Mary Catchment nutrient water quality; 2019–20	Sunshine Coast Council (2023)
E_GRUMR	Griffith Mary Catchment water quality; 1994–97	ARI, Griffith University[104,105]

Table 1. Project, date range, basins covered, key parameter groups, data custodian, original report reference(s).

Sampling methods. We have included data collected by traditional discrete manual grab sampling, autosamplers and rising stage samplers. In the cases where data were collected using rising stage samplers, we direct the user to the original publication as listed on relevant metadata statements. We excluded data collected by continuous probes or passive samplers relating to three datasets. Grab samples were often collected to validate the continuous sampling probes and, where available, these grab samples have been included in this dataset.

Spatial scope. An initial criterion for inclusion of a dataset involved the use of digitalised watercourses (i.e., Inland waters: Watercourse layer) available on Queensland Globe[30] within the GBRCA to define the main surface flow pathways and riverine locations. However, in heavily modified areas (both urban and agricultural sectors), waterways have been substantially modified and, in some instances, re-routed from their original paths. These waterways (often referred to as "drains" in these settings) now represent key flow pathways within a catchment. Hence, drains were included where they were considered to represent a major surface flow pathway.

We excluded some sites in the interests of landholder privacy. We did not include locations where the data could be attributed to a single, or small group of upstream landholders. Whilst this was not a clear-cut criterion, there were only a few locations where this occurred, and data exclusion was determined on a case-by-case basis in consultation with the data provider.

The spatial scope of the data compilation was also limited in terms of the downstream extent of sampling sites. We largely excluded sites deemed estuarine or strongly tidally influenced. However, this was not a definitive criterion. Due to the hydrological variability of many rivers in this region, sampling locations some distance inland can at times receive brackish waters particularly if a high spring tide occurs during periods of low river discharge. In some instances, barrages and dams will prevent upstream brackish water intrusion. We assessed the tidal influences through the water chemistry (e.g., salinity, conductivity, and ionic composition). We only included freshwater sites that predominantly run fresh (i.e., electrical conductivity $<1{,}000\ \mu S$). Exceptions were made for larger datasets, where a small number of sites were tidally influenced for some or all samples; these sites were included to retain the 'complete project dataset'. Such data have been identified and recorded on project metadata statements.

We excluded water quality samples taken from within large lacustrine and palustrine systems such as dams and lakes because of the need to capture spatial water quality variations and the relevant in-stream biological drivers (e.g., instream and riparian vegetation). However, we included data from inputs and outputs to these water bodies where available. In drier regions of the GBRCA, many waterways cease flowing and form a series of disconnected waterholes during the dry season. We included samples from these in-channel environments (waterholes and interconnected wetlands) as these are riverine systems with flowing water for at least some periods of the year.

Temporal scope. We collated data from the late 1980s through to 2023. The timeframe of water quality datasets ranges from a single wet season (or even flow event) to more than 10 years of continuous data. Comparison of data across such a wide range of time is hampered by the changes in analytical methods and available sampling equipment. We did not eliminate any early data but rather included the necessary information on the analytical methods and detection limits where we were able to source them so that the data utility can be assessed by the user.

Parameter scope. We included parameters in the dataset that describe the physical and chemical conditions (with specification on whether the data were field collected or laboratory derived where appropriate), including: nutrient concentrations (nitrogen, phosphorus and carbon), sediments, ionic composition (cations, anions), metal concentrations, and pesticide concentrations (Table 2). We included properties such as true colour, water temperature, pH, turbidity, electrical conductivity, dissolved oxygen, water hardness, alkalinity and chlorophyll *a* concentrations where they were collected in association with the other water quality data listed above. Where possible, we included only directly-measured parameters and not those derived or calculated from other measurements. For example, we did not include dissolved inorganic nitrogen (DIN) *per se* but rather the individual constituent nutrient concentrations [nitrite (NO_2^-), nitrate (NO_3^-), and ammonia (NH_3/NH_4^+)] where measured. Similarly, we have not included particulate nitrogen and particulate phosphorus for the majority of the datasets where they have been calculated. For a small number of datasets, particulate nutrients were measured directly (e.g., AIMS GBR river water quality, GBRMPA Barron Russell-Mulgrave water quality and CSIRO Lower Herbert water quality) and therefore were included. This decision was made to encourage the user to consider how they handle error propagation and metrics that may be ambiguous in their determination (e.g., DIN calculations may sometimes exclude nitrite as it is often considered a very minor component in freshwaters). In a few cases only the calculated data were available (i.e., not the constituent nutrient fractions), and in those instances, we have retained the derived data and these have been noted in the associated metadata statements. A small number of standard calculated metrics provided in laboratory analysis such as water hardness and dissolved inorganic carbon were also included where available. The methods of laboratory analysis were also compiled. This is of particular importance for parameters that may be analysed using different methods, which has implications for the estimated parameter concentrations.

Once most of the derived parameters were removed, we created a final list of the parameters reported across all the collated datasets and considered their inclusion based on their relevance to the freshwater riverine systems of the GBRCA. We considered datasets that included at a minimum: total suspended solids, nutrients, metals, and/or pesticide parameters but excluded datasets that reported only a limited suite of field and/or physical properties.

Defining a water quality monitoring site. Many of the collated water quality datasets represent relatively short sampling campaigns (~1 to 3 years) but could create a broader picture of spatial and temporal water quality trends when combined with data collected at the same site as part of another project/program. In some instances, a "site" had been sampled by several different parties over the past 40 or so years with minor variability in the sampling location. In general, slight shifts in sampling location do not influence water quality results[31]; however, more substantial changes to "site" water chemistry can be expected where a tributary joins the stream network between the two sampled points. For this reason, the physical distance between two locations was not a sufficient criterion to evaluate unique site identity. Rather, to consolidate data from different sampling programs (and in some cases where site locations shifted within the same program), it was necessary to assess to what extent any differences in the location between successive sampling events would affect the water quality results. The criteria to associate water quality data with a common site were based on:

Analyte group	Details
Field properties	pH, electrical conductivity, dissolved oxygen, water temperature, turbidity
Physical properties (laboratory measured)	True colour, electrical conductivity, pH, turbidity, chlorophyll *a*, phaeophytin *a*
Cations, Anions, Alkalinity & Hardness	Water hardness, cation and anion composition, alkalinity
Sediments	Total suspended solids (TSS), total solids, suspended sediment concentration (SSC). Nominal pore size ranges from 0.4 – 1.5 µm.
Nutrients	Total nitrogen (TN), total phosphorus (TP), total Kjeldahl nitrogen (TKP), total Kjeldahl phosphorus (TKP), total dissolved nitrogen (TDN), total dissolved phosphorus (TDP), dissolved Kjeldahl nitrogen (DKN), dissolved Kjeldahl phosphorus (DKP), oxidised nitrogen (NO_x: nitrate and nitrite), ammonia/ammonium, filterable reactive phosphorus (FRP), urea, particulate nitrogen and particulate phosphorus, dissolved organic carbon (DOC), total organic carbon (TOC), dissolved inorganic carbon (DIC)
Metals and metalloids	Total metals, dissolved metals
Pesticides	Herbicides, insecticides, fungicides

Table 2. The parameters incorporated into the collated dataset. Note that each dataset usually included only a subset of the parameters listed. Further details regarding laboratory methods and key references are given in the metadata statements. Dissolved here refers to the filtrate passing through a standard 0.45 µm filter. It should be noted that the filtrate may possess fine particulate material (colloids) that pass through a 0.45 µm filter and associated adsorbed nutrients and metals.

- No tributaries or drains that could affect downstream water quality located between the two sampling locations;
- No discharges from point sources (e.g., sugar cane mills);
- No major changes in land use that could result in water quality alterations over short spatial extents;
- The absence of major infrastructure within a stream (e.g., bridges or roads);
- The distance between locations did not exceed 1 km.

We created a single GIS layer of all the sampling sites to visualise their locations and identify sample locations that were near to each other and might be consolidated by applying the above criteria. Those locations which met the criteria for consolidation were ascribed a common site name. A full list of the sites and their locations are housed within the repository as a separate document.

Following this process, we created a list of unique sites and where possible matched them to existing or current Queensland Government site codes (i.e. termed unique DETSI site reference). In some cases, this involved adjusting the site's location by a small distance to match the existing government monitoring site provided the criteria for merging the sites were met. The remaining sites that were independent of existing Queensland Government sites were assigned their own unique DETSI site code. The resulting list of sampling locations was then further streamlined with the review of the available water quality data from each site (or consolidated sites). We excluded sites where fewer than five samples were collected but provided no minimum time span as we recognised the importance of short but intensive sampling campaigns to the overall understanding of water quality variability (e.g. the delivery of nutrient and sediment loads during short-lived flood events).

Chemical form. Water chemistry data can be reported by the laboratory as either an elemental or compound form. It was critically important that these forms were clearly identified when the datasets were compiled. In many instances, laboratory naming conventions such as "nitrate-N" clearly indicated that the elemental form was provided. However, some datasets only reported, for example, "nitrate", and we could not be confident of the actual measurement reported. In these cases, we approached the original laboratory to clarify the reported chemical form and compared the results with the original laboratory output files where available.

Detection limits. Inconsistencies were noted across the datasets in the reporting of values below the analytical detection limits (censored data). For example, values below detection for some of the earlier datasets were originally assigned a zero value. In other cases, the censored data were treated by replacing the values with half the detection limit. Where information on laboratory detection limits was provided either within the data itself or in accompanying publications, we reinstated the value at the detection limit and provided the operator (e.g., "<") in a contiguous column. Where detection information was not provided, we obtained the detection limits via contact with the original laboratories. We note that detection limits can vary substantially in a single laboratory as methods and instrumentation evolve, the required analytical resolution (e.g., trace versus standard) and, due to particular water quality issues (e.g., saline water may require dilution to prevent interference in the analysis). Where we could not establish a reasonable detection limit, we assigned a value based on contemporary detection limits.

Common methods for dealing with values below detection can introduce bias into analysis of the data. Because of the different data types being collated here, there is no single correct method for imputing the missing values. Indeed, a suitable substitute value for a nutrient parameter, where we can be confident that it is naturally present, will be different from a synthetic pesticide where the chemical may be truly absent from the

sample. In the latter case, the application of even a very low substitute value could result in an artificially high load if accumulated over time. For this reason, we have not provided any substitute values and leave this to the discretion of the user.

Data Records

The dataset has been deposited in the James Cook University research data repository which can be accessed here: https://doi.org/10.25903/pase-na93[32]. The data includes an MS Excel (.xlsx) file (workbook) for each contributing dataset containing 3 worksheets: a metadata statement related to the project, a site location lookup table and the water quality data related to that project. The data are arranged in wide format with each variable attributed two columns; an operator column with the suffix "OP" affixed to the variable name and, in the second column, the variable itself. Units are provided beneath the variable name. We also provide a table of sites (.xlsx) and a table of parameters with units (.xlsx) as separate documents.

The workbooks contain the following headers:

- **project_code:** Code for the project for which the data were collected (see Table 1).
- **project_name:** Name of the project for which the data were collected (see Table 1).
- **source_site_name:** The name of the site in the source dataset.
- **site_name**: Name of the site in the compiled dataset.
- **basin_name:** Name of the river drainage area as defined by the Australian Water Resources Management Committee via Geosciences Australia (1997) in which the sample was taken.
- **catchment_name:** The name of the natural drainage area in which the sample was taken.
- **river_name:** Name of the river in which the sample was taken.
- **source_site_code:** Site code in the source data (if available).
- **site_code:** A Queensland Government site code for the compiled dataset.
- **source_latitude_DD:** Source latitude coordinate for collection site location in decimal degrees (if supplied).
- **source_longitude_DD:** Source longitude coordinate for collection site location in decimal degrees (if supplied).
- **source_datum:** Source Datum (if supplied).
- **latitude_DD:** Latitude coordinate for collection site location in decimal degrees for compiled dataset.
- **longitude_DD:** Longitude coordinate for collection site location in decimal degrees for compiled dataset.
- **datum:** Datum (GDA2020) for compiled dataset.
- **n:** Number of rows in source dataset for each site.
- **sampling_date_time:** Date and time in dd/mm/yyyy hh:mm (24 hours clock). Where time is missing time is included as 00:00.
- **sample_unique_identifier:** Unique code attributed to all water quality samples (codes start with a '9').
- **sample_collection_method:** Method by which sample was collected. This is usually as a manual grab sample or by automatic sampler. Note the latter also distinguishes between discrete samples and composite samples.
- **laboratory_name:** Name of laboratory where sample was analysed.
- **analysis_method:** This field states "See metadata". Because of the array of different analytical methods and technical details the user is referred to the metadata statements.
- **depth_m:** Depth below water surface (m) of where sample was collected. May be blank but the user is referred to the metadata for further information.
- **comment:** Any comments from the original records that are relevant to the water sample (for example observations on river flow or condition).
- **variable name_OP:** An operator code (e.g. <) for non-numerical laboratory results for a given analyte.
- **variable name:** Concentration value for a given analyte.

For each project dataset we have created a metadata statement and had these checked and endorsed by the data provider where possible. These statements provide key detailed information about the project, funding, key references, technical details, laboratory analysis methods and any relevant notes about the data. These statements also document any assumptions that were made regarding the data and any identified limitations. This information will be a particularly important reference for datasets where associated publications are difficult to access. Users are expected to take into consideration this resource and the reference therein to determine the utility of data for their specific purpose. A pdf of the full set of metadata statements including a table defining the acronyms used is also included in the data package.

Many Australian river and stream systems have high hydrological variability, over days, months and years[33,34]. Where contextual information was provided through description of a flow condition, this information was incorporated as a comment for each record. We note that sites matched to an existing Queensland Government site code often have flow data freely available from the Queensland Government Water Monitoring Information Portal[35]. In addition, daily modelled flow data for the individual sites may also be available through the eWater Source model[36].

These data are also publicly accessible on the Queensland Government Tahbil – Water Quality Data Portal alongside the GBRCLMP water quality monitoring data. They can be selected by including third-party data in the search criteria, and can be filtered by analyte, location and date and downloaded in long data format as a csv file. The Tahbil – Water Quality Data Portal is an invaluable online resource that will continue to grow and update. Some earlier datasets are at the same sampling locations (i.e. sites) that were later absorbed into the GBRCLMP or finer spatial scale (land-use focused) sites that collectively strengthen the spatial and temporal

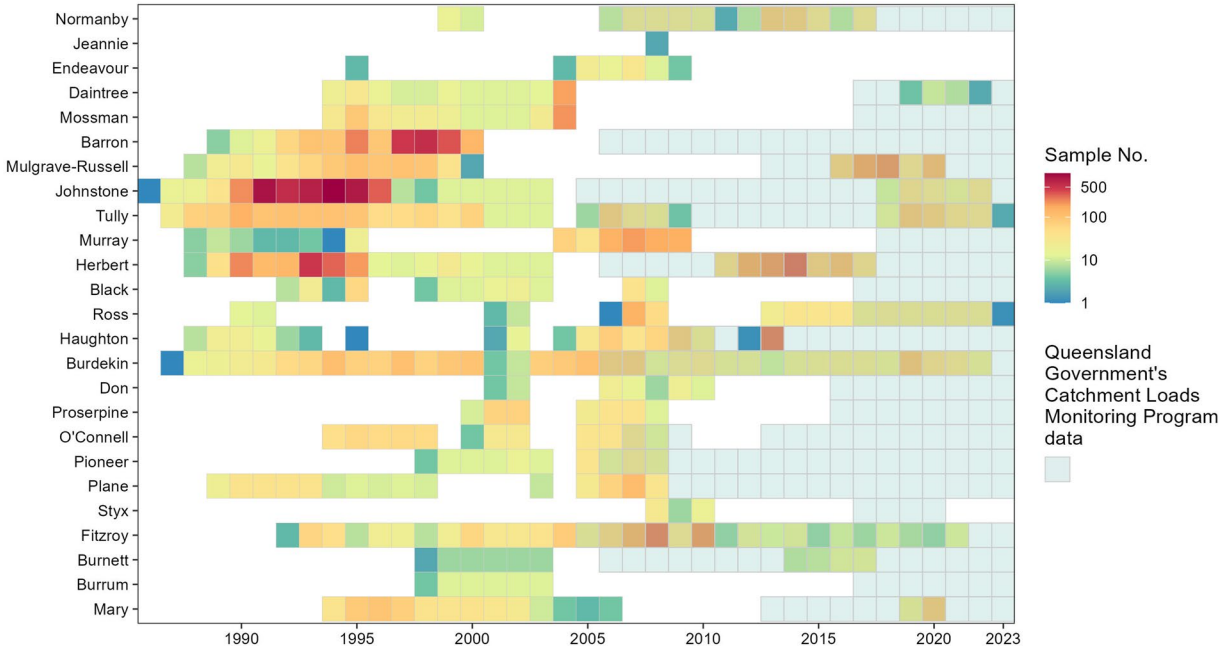

Fig. 3 Numbers of nutrient water quality samples included in this data compilation per year per river basin. Additional sample collection undertaken by the Queensland Government's Catchment Loads Monitoring Program within each of these basins has also been provided for historical completeness.

aspects of the water quality dataset resource. For example, catchments such as the Burdekin have been effectively monitored continuously for more than 30 years and some Wet Tropics catchments (Tully, Johnstone and Herbert) have water quality data collectively spanning several decades (Fig. 3).

Technical Validation

All the contributed datasets were formatted to a consistent template (including standardising to a common set of units) and, in some cases, this involved a degree of data manipulation and transposition, while some data had to be entered manually. To ensure no transcription errors were made during this process, we checked a minimum of 10% of the data items against the original supplied data. Where possible when performing these data checks, we used the rawest available datasets, including laboratory raw data sheets. Additionally, we performed a series of checks to identify any issues with the data, including checks to identify errors such as changes in units (e.g., between mg and μg), unreasonable values indicative of transcription errors, decimal place shifts, entire column shifts, and the presence of zeros within the data. We have aimed to avoid unnecessary modification of the original data apart from correcting obvious errors.

Information provided with datasets indicates that many of them have a high degree of integrity and rigour through implementation of standard sampling procedures and many have undergone 'within house' QA/QC processes, including checks of field blanks and analysis of duplicates. We have performed no further validation of the data because, primarily, it is the users' responsibility to ensure the data are suitable for the intended use. Furthermore, technical validation of historical water quality data can be very limited. For example, standard inspections such as nutrient balance checks may not be possible due to the constraints imposed by the suite of nutrients analysed; or, when a nutrient or a metal balance check is otherwise feasible, the measurement uncertainty of the method may not be available.

All water quality datasets have limitations. Our ability to recognise them and make informed decisions regarding the utility of the data are dependent on the availability of metadata and any accompanying information provided within associated publications. Based on the available metadata, we have produced quality codes for each dataset. Our assigned codes reflect the quality of metadata information available for a given dataset, rather than the data themselves. We identified four broad groups of information issues related to the metadata (Table 3).

Within the compilation, each dataset was ascribed one of three quality codes (Table 4). Datasets were attributed these primary quality codes based on the presence of information regarding issues identified in Table 3. If information on the sample location (in time and space), sampling strategy (sample collection and handling), laboratory analysis and data processing were adequately described, a dataset was assigned a 'good' quality code of 910. If one or two of the above items were not adequately described, the dataset was assigned a fair quality code (920), and if the dataset was deemed to have three or more issues it was allocated a poor code (930) (Table 4). We note that the utility of any dataset is dependent on its intended use, and therefore, even when a poor code is ascribed, the data may still have applications if their limitations are carefully considered.

Information issue	Example issue identified
Sampling location and time	Uncertainty in sample site locations, Uncertainty in sampling date
Sampling integrity	Sampling collection procedures not adequately described, Sample holding conditions not described.
Laboratory analysis	Uncertainty around the analytical methods employed and their associated detection limits.
Data processing	Uncertainty in post processing treatment of the data (e.g. unclear when data less than detection limits were substituted).

Table 3. Metadata information issues identified related to the collection and processing of water quality data.

Data quality code	Quality characterisation	Description
910	Good	Sampling location, procedures, analytical methods, and data handling processes are well documented.
920	Fair	Most components of the sampling are well documented, with one to two minor issues identified in relation to sampling location, procedures, analytical methods or data handling processes.
930	Poor	Sampling is not well documented and multiple issues were identified (three or more) in relation to sampling location, procedures, analytical methods or data handling processes.

Table 4. Quality codes and descriptions for project datasets.

Usage Notes

Cautions around utilising data combined from multiple sources. The spatial and temporal breadth of this compilation offer a valuable resource for water quality practitioners to examine spatial and temporal trends in the data and relate them to climatic and geographic variability in hydrology, land use, soil type, lithology, and vegetation in the GBRCA. However, there are necessary considerations when combining datasets before such analysis can be undertaken. For instance, water quality data can vary greatly over a hydrograph[29], so different sample collection methods (grab samples, autosamplers and rising stage samplers) will collect different stages of the flow[37]. In addition, the compiled datasets have been derived from various laboratories, using different extraction procedures, analyses and instrumentation over time. Differences in analytical methods can profoundly impact the resulting water quality measurements[29]. We note that while many of the conventional inorganic analytical methods have not changed substantially over time, how these methods are implemented has changed. Key changes include the transition to digitalised signals for laboratory analysis via automated methods such as flow injection analysis/segmented flow analysis. These changes have generally resulted in improved standards for, and adherence to, detection limits and so reporting has changed over time, which needs to be considered when combining long-term data.

There is a distinct geographical separation in the methods employed for the analysis of total nutrients. Monitoring programs in the Fitzroy, and earlier datasets from the Wet Tropics and the Mary River, used the Kjeldahl digestion method whereas the persulfate digestion method was generally preferred for samples from the Burdekin and more recent monitoring from the Wet Tropics (Fig. 2). These approaches for determining nitrogen have different chemistries and their suitability/effectiveness depends on characteristics of the water sample, including salinity, suspended solids concentration, organic loads and nitrogen concentrations[15,17,18]. In the compiled dataset, total nitrogen analysed directly by a persulfate digestion has been distinguished from total Kjeldahl nitrogen. However, for the latter, an estimate of TN can be generated by combining the TKN and NO_X with the calculated and direct approaches having high agreement in freshwater[20]. We strongly advocate caution when combining water quality results that have used these different digestion methods. It is well-established that both methods have their own nuances and do not always represent a 'complete extraction'[15–20].

Protocols for analysing total phosphorus and total dissolved phosphorus within the collated datasets include acid persulfate digestion, alkaline persulfate digestion and Kjeldahl digestion. Total phosphorus and total dissolved phosphorus analysis by the acid persulfate digestion is generally considered to be comparable to the Kjeldahl approach in freshwater. The methods convert all forms of phosphorus to orthophosphate and measured phosphorus is generally not significantly different[18]. More recently, acid persulfate digestion was reported to have better recoveries of total phosphorus compared with the alkaline persulfate method in waters with high suspended solids, typical of agricultural runoff[38]. As with total nitrogen, we caution against combining water quality results from the different digestion methods for total phosphorus unless the user can have confidence that the extractions have provided comparable results.

The UV approach to the analysis of dissolved organic nitrogen and phosphorus is unreliable for freshwaters with low and unpredictable recovery rates[16]. This was also confirmed by comparisons between dissolved total nutrients measured by two different approaches on field data in the Wet Tropics[39]. Given the freshwater focus of the compiled dataset and consultation with the data provider, samples for dissolved organic nitrogen and dissolved organic phosphorus analysed using the UV oxidation digestion method were excluded.

A further issue is method differences in determining TSS concentrations. In most instances the gravimetric APHA standard method 2540D was used with the filter pore size recommended being 2 μm or less[40]. Where filter membrane details were available, the nominal pore size ranged from 0.4 to 1.5 μm, and this detail has been noted in the metadata statements. Although research suggests that pore size does not make a significant difference within this range[41], when TSS data are aggregated over time to derive a load, the propagation of small differences can lead to much greater variability, so care is needed in analysis of combined datasets using different membrane porosities. Furthermore, some rivers of the GBRCA can transport fine colloidal grainsize fractions and so a proportion (likely relatively small) of the concentration may be missed when larger pore size filters are

used[42]. These differences can be much larger where a greater concentration of colloidal particles are present such as waters that are stored in large reservoirs[43,44].

The analytical approaches used in individual datasets were not necessarily tailored to the specific water sample and its collection purpose, but rather may simply reflect laboratory convention or even regulatory requirements[20]. When combining data for the same parameter from different analytical methods, the user should be aware of qualifying information that may affect the efficacy of the analytical methods employed. This includes different filters used for TSS and nutrient analysis as well as the different digestion/extraction procedures for nutrient and trace metal analysis. The datasets collated here were collected for different purposes and the collector may have requested different detection limits from the testing laboratory (e.g., high level versus low level/trace). The user should be aware that this may limit the utility of the data if the detection limits are not sufficiently low, for example, to detect the natural concentrations of that parameter.

Various terminologies are used to describe dissolved inorganic phosphorus across the datasets. Some terms reference the analytical method employed e.g., molybdate-reactive phosphorus, soluble reactive phosphorus and filterable reactive phosphorus, while other terms used include orthophosphate and phosphate phosphorus. All samples analysed using the molybdate-reactive method have been assigned filterable reactive phosphorus. There are further nuances around terminology. For example, for pesticide analyses, there is a general assumption that samples were run on unfiltered water samples unless otherwise stated. It is possible (and there were limited examples within the datasets we collated) to filter and explore the distribution of herbicides associated with dissolved and particulate solids separately[45]. Additionally, the word 'total' has different connotations for different parameters. For metals and nutrients, the term implies analysis of the whole water sample (an unfiltered water sample) after digestion of the particulate/organic fractions. For pesticides, however, 'total' is used to refer to the sum of a specific pesticide concentration as well as any of its breakdown products also measured. Such nuances are not necessarily problematic but can cause confusion.

Improved metadata collection and attribution. Often datasets were missing key pieces of information that would facilitate assessment of the utility of the data. Such information may have been considered standard practice at the time and so was not explicitly recorded. Particularly noteworthy was the frequent lack of key information around sample handling. This includes information on how soon samples were retrieved after initial collection and how they were stored and transported. For example, samples collected using autosamplers cannot always be retrieved within recommended ISO holding times due to the logistics of site access under wet season conditions. Detailed information about these issues is not always provided in reporting. These aspects make a substantial difference to the accuracy and reliability of the data, particularly for more unstable water quality parameters such as ammonium, nitrate, and nitrite. Information on detection limits or practical quantifiable limits should be retained with the data wherever possible to indicate the level of confidence associated with the data. Subsequent handling of data has led in some instances to uncertainty regarding whether the measurements provided represent the actual measurement, half of the measurement, or something else.

We acknowledge that most contemporary large-scale water quality monitoring programs now store data in specially designed storage platforms where qualifying information (e.g., detection limits, quality flags, contextual information) can be held alongside the values. This is undoubtedly an improvement; however, the upkeep of such databases and their continuing costs particularly in the case of commercial products, gives cause for concern regarding their continued maintenance, capacity to update and future access.

Other water quality data sources for the GBR catchments. Although our compilation has produced an extensive resource of surface water quality data from the tributaries of the GBRCA for a range of parameters, several other outlets likely host valuable data for this region. These include water quality monitoring data from compliance-based programs associated with environmentally relevant activities (ERAs) such as mining and other industries, within environmental impact statements and from other aquatic environments such as reservoirs/lakes, groundwater, estuaries and the GBR lagoon. There has also been a wealth of paddock-scale monitoring conducted throughout the GBRCA, which, largely due to the scale of the data (i.e., individual farm), remains unobtainable due to confidentiality concerns. The increasing use of sensor technologies in the GBRCA to measure turbidity and nitrate[46] will need a central repository for data storage and preservation. Similarly, passive sampler deployments in the GBRCA for pesticide and trace metal analysis do not have a dedicated central storage platform. The compilation of the forms of data outlined above each presents its own challenges and would require specific data formatting, QA/QC analysis and associated metadata statements. The high volumes of data collected from sensor technologies present additional storage and analysis challenges. However, the extensive efforts needed to compile and curate such datasets should not deter us from undertaking these compilations, as the alternative is that they become unusable to future users and permanently lost. We have observed the loss of corporate memory in some basins where there are perceptions of a 'lack of water quality monitoring'. Our hope is that this compilation raises the profile of existing water quality monitoring programs and provides a strong base to guide further endeavors.

Code availability

No custom code was used in creating the dataset.

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Author contributions

Apart from first, and senior authors, all are listed in alphabetical order. We follow the CreDiT taxonomy[106]. Conceptualisation (C. James, Z. Bainbridge, S. Lewis, R. Mann, A. Moss), methodology (C. James, Z. Bainbridge, S. Lewis, C. Clech-Goods, R. Mann, R. Huggins, D. Orr, K. Welk, S. Liu), software (C. James, C. Clech-Goods), validation (C. James, Z. Bainbridge, S. Lewis, M. Cross, F. Oudyn, M. Tink), data provision (Z. Bainbridge, S. Lewis, G. Agnew, R. Bartley, R. Bramley, A. Buckle, L. Cogle, A. Davis, M. Devlin, B. Eyre, J. Faithful, M. Furnas, P. Godfrey, R. Gruber, A. Hawdon, C. Howley, H. Hunter, M. Kennard, E. Laxton, S. Mackay, D. McJannet, M. Nash, D. O'Brien, K. Rohde, R. Pearson, A. Moss), data curation (C. James, Z. Bainbridge, S. Lewis), writing-original draft (C. James, Z. Bainbridge, S. Lewis), writing – review and editing (C. James, Z. Bainbridge, S. Lewis, C. Clech-Goods, R. Mann, R. Huggins, D. Orr, K. Welk, S. Liu, G. Agnew, R. Bartley, R. Bramley, A. Buckle, L. Cogle, M. Cross, A. Davis, M. Devlin, B. Eyre, J. Faithful, M. Furnas, P. Godfrey, R. Gruber, A. Hawdon, C. Howley, H. Hunter, M. Kennard, E. Laxton, S. Mackay, D. McJannet, M. Nash, D. O'Brien, F. Oudyn, R. Pearson, K. Rohde, M. Tink, A. Moss), visualization (C. James, S. Liu), project administration (Z. Bainbridge), funding acquisition (Z. Bainbridge, A. Moss).

Competing interests

The authors declare no competing interests.

Additional information

Correspondence and requests for materials should be addressed to C.J.

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