3.3 Option 3 -- Data Review Options

Data review functions include options to provide an inventory of records that have been logged into the database, view data stored in a sample record, and provide chemical validations of sample analyses. Option 3 of the main menu invokes the following Data Review Options submenu:



Data Review Options Menu

3.3.1 Option 1 -- Select Sites and/or Samples

This option is used to create three types of files; (1) lists of sites that meet user-specified site selection criteria, (2) lists of sites that have water-quality data that meet user-specified site selection and sample selection criteria, and (3) lists of record numbers for water-quality data that meet user-specified sample selection criteria. These files may be used as input to other options in the NWIS QWDATA system. The record number list file is required for <u>generating output to files -- section 3.4 -- Data Output</u>.

Sample selection is a two-step process. First, site numbers are specified using one of the first three options on the **Select Sites and/or Samples** submenu. By using option 4, site selection is skipped--in effect, all sites in the database are selected.

qwsiterec -- locate record numbers for use by QWDATA application programs QWDATA database(s): 01
You may locate records for specific sites.
If you wish to locate records for specific sites the options are:

You have a file containing site numbers
You will enter site numbers at terminal
-- You will enter sites based upon selection criteria

If you don't care which sites the option is:

Locate QWDATA records without regard to site

Site specification menu within the Select Sites and/or Samples option

In the second step, sample records are selected for the designated list of sites based on user specified criteria.

3.3.1.1 Site Selection

Station numbers may be provided to the software in three ways: (1) specified in a file provided by the user, (2) from interactive entry, or (3) selected based on user specified criteria. The user also may choose not to specify station numbers (4).

(1) If the station numbers are to be read from an input file, the user will be queried for the file pathname. Station numbers must be listed using the fixed-column format shown in *Appendix G*. An output file from a previous site selection process is also an acceptable format for input. (*Appendix C*)

(2) If the station numbers will be entered interactively, the user will be queried for agency code and station number. A null entry ends interactive station number entry.

(3) If station numbers are to be selected from user-provided criteria, a list of available criteria for site selection is displayed as shown below:

qwsiterec -- Locate sites

Enter an X to choose an item for limiting retrieval, Enter a # to remove an item.

(1) AGENCY CODE: _ (2) STATE CODE: _ (3) COUNTY CODE: _
(4) HYDROLOGIC UNIT: _ (5) DRAINAGE BASIN: _ (6) POLYGON: _
(7) RANGE OF STATION NUMBERS: _ (8) TYPE OF STATION: _

Options: ? ^D # / /x /+x /-x /@ /c /q -- Enter ?/ for help

Menu for choosing the site selection criteria within the Select Sites and/or Samples option

The available selection criteria, which may be used in combination, and the specifications for each are shown below:

	Site Selection Criteria	Specifications	Source
(1)	Agency code	up to 10 agency codes	GWSI documentation
(2)	State code	up to 10 State codes	FIPS code dictionary – See Sect. 3.6.5
(3)	County code	up to 40 county codes	FIPS code dictionary – See Sect. 3.6.5
(4)	Hydrologic unit code	up to 10 hydrologic unit codes	GWSI documentation
(5)	Drainage basin code	up to 10 drainage basin codes	GWSI documentation
(6)	Polygon	up to 50 vertices	user specified
(7)	Range of station numbers	only 1 range	user specified
(8)	Type of station	up to 10 station types	<u>Appendix A</u>

Enter a non-blank character (other than "*I*") to choose a field for limiting retrieval, or enter a "**#**" to remove a field. The options for screen navigation may be invoked during selection of retrieval criteria.

If a State code is selected for site retrieval, an additional query is included to ask for a country code:

To select by state need to specify country. Enter 2-character country code (<CR>=US):

For information on country codes, please refer to <u>GWSI documentation – Chapter 2,</u> <u>Section 1.11.</u>

(4) If records are to be retrieved by polygons, the user is queried for a file containing the vertices in fixed format. Up to 50 vertices may be specified. The vertices should be stored in the format shown below:

Column	Format	Description
1-7	dddmmss	Latitude and (right-justified in column 7)
9-16	dddmmss	Longitude (right-justified in column 16)

File format for entering polygon vertices

Vertices also may be entered or selected interactively. The user is first asked if vertices are to be stored into a file. If **YES**, the user is queried for a file name. Next, the user may

choose to retrieve latitude-longitude values from the FIPSFILE -- the 2-digit State code and the 3-digit county code are requested. A county code of 000 will retrieve the State record values. Optionally, the user may choose to enter latitude-longitude pairs interactively from the terminal.

If records are to be qualified by Station Type Code and GW or SW or LK station types are selected, any one or more of the additional selection options shown below may be selected.

Selection criterion	Specification	Reference source
For SW (stream), LK (lake), DV (diversion), LA (land application) or OF (outfall) sites:		
Base discharge (range)	only 1 range	user supplied
Drainage area (range)	only 1 range	user supplied
For GW (ground-water), or SP (spring) or AG (aggregate ground water) sites:		
Primary geologic unit	up to 20 geologic unit codes	Section 3.6.4
Use of site	up to 10 use-of-site codes	<u>Appendix A</u>
Use of water	up to 10 use-of-water codes	<u>Appendix A</u>
Well depth (range)	only 1 range	user supplied
Ground-water project ID	up to 10 project ID's	user supplied

Selection criteria for surface-water and ground-water station types used for site selection

To be selected, a site record must satisfy all the selected criteria. [Note: These selection criteria are optional fields in the Site File record. If the selected field has not been populated in a site record, that site will fail the selection criterion.]

The speed of the Site File retrieval will vary depending upon the degree of qualification by the selected criteria that are supplied by the user. The user is given a warning and an opportunity to abort the Site File search if the criteria are too general. If no site selection criteria are specified, the default condition is invoked and the selection criterion used is *Agency code = USGS*.

Beginning search for sites in database 01 ... (No selection made -- will search for ALL station types Searching on STATION TYPE only

This may take a long time as the entire site file must be read

Do you wish to continue (Y/N,<CR>=Y)?

Warning message when searching the entire site file

After the Site File has been queried for sites that satisfy the user selection criteria, the user is asked if selected sites should be sorted. A response of **YES**, invokes a prompt to select sorting options. All of the desired sort codes must be entered on one line with no spaces. The first field will be the primary sort; the next will be the secondary sort, and so forth. In the example below, sites are sorted according to agency code, site type, and station number.

qwsiterec total number si	tes located: 1050	
Do you wish to sort the loca	ted sites (Y/N)? Y	
You may sort on any combi	nation of the following fields:	
A Agency code	G Hydrologic unit	
B Station number	H Drainage basin	
C Station name	I Station type	
D Latitude-longitude	J Use of water	
E State	K Geologic unit	
F County	L Ground-water project	
The first field will be the primary sort the next will be the secondary sort 1, Please enter the sort codes on one line with no embedded spaces		
Enter sort code(s):		

User is given the option to sort retrieved sites

When the sort is complete or if the sort option is skipped, the user is prompted to enter a file name to hold the retrieved site numbers. The site numbers and associated location and other site information are saved in a file using a fixed-column format shown in Appendix C.

(4) If the user chooses not to specify site numbers in the **Select Sites and/or Samples** submenu, the program moves to the option to select water-quality records.

3.3.1.2 Selecting Water-Quality Records

After sites are selected, water-quality records may be selected for the specified sites or the user may return to the "Data Review" menu. To select water-quality records, a screen is displayed to specify selection criteria. If no water-quality record selection criteria are specified, by entering a *<cr>* in the *DATE* field, the program uses a default date range from 1776 to present -- in effect, selecting all records in the database.

Locate QWDATA records
Enter an X to choose an item for limiting retrieval, Enter a # to remove an item.
(1) DATE: (2) ANALYSIS-LEVEL CODES: _ (3) PROJECT ID: _ (4) GEOLOGIC UNIT: _ (5) PROCESSING STATUS: _ (6) PARAMETER VALUES AND CODES: _
Options: ? ^D # / /x /+x /-x /@ /c /q Enter ?/ for help

Selection options for locating water-quality records

Water-quality records may be selected using any combination of six selection criteria, which are shown below:

	Selection criterion	Specification	Reference source
(1)	Date (range)	1 date range	user supplied
(2)	Analysis-level codes		
	Medium code	up to 10 medium codes	<u>Appendix A</u>
	Analysis source code	up to 10 analysis source codes	<u>Appendix A</u>
	Hydrologic condition code	up to 6 hydrologic condition codes	<u>Appendix A</u>
	Sample type code	up to 6 sample type codes	<u>Appendix A</u>
	Hydrologic event code	up to 10 hydrologic event codes	<u>Appendix A</u>
(3)	Project ID	up to 10 project ID's	user supplied
(4)	Geologic unit	up to 10 geologic unit codes	Function 6.4
(5)	Processing status	up to 6 processing status codes	<u>Appendix A</u>
(6)	Parameter codes and values		
	Parameter codes	up to 50 parameter codes	Function 6.2
	Parameter values	up to 50 parameter value minimums and/or maximums	user supplied
	Remark codes	up to 5 remark codes	<u>Appendix A</u>
	Quality-assurance codes	up to 5 quality-assurance codes	<u>Appendix A</u>
	Method codes	up to 5 method codes	<u>Appendix A</u>
	Prep set number	one prep set number	user supplied
	Analysis set number	one analysis set number	user supplied
	Value qualifier code	up to 5 value qualifier codes	<u>Appendix A</u>

Record selection criteria, specifications, and reference source

A user can get all stored records for a site if **DATE** is used for the selection of records and a <CR> is entered for both the begin date and end date. In any release after NWIS 4.2, the storage of times in the Universal Time Coordinate (UTC) System may result in small number of samples not being included in retrievals limited by date. The retrieval

program will use the time variable set for the Unix environment on the local computer system. To avoid missing samples in a date range, you could include an extra day on either end of the desired date range. Some examples of this behavior include:

A) Example: Sample in Arizona database from Navajo reservation (the Navajo reservation observes daylight saving time, but the rest of the state does not)

 Unix time variable is US/Arizona
 Sample begin date/time logged in as: 10-01-02 @ 0030 MDT
 Sample begin date/time stored in UTC as: 10-01-02 @ 0630 UTC
 Retrieval of all records in a water year as entered on the screen: Begin date: 10-01-02 End date: 09-30-03
 Retrieval date range converted to: Begin date: 10-01-02 @ 07:00:00 UTC End date: 10-01-03 @ 06:59:59 UTC

Due to the conversion to UTC for retrieval this sample is *not* included in the retrieval even though it was collected in the date range selected.

B) Example: Sample from Indiana in a county near Chicago, Illinois

- 1) Unix time variable is US/East-Indiana
- 2) Sample begin date/time logged in as: 09-30-02 @ 2345 CST
- 3) Sample begin date/time stored in UTC as: 10-01-02 @ 0545 UTC
- 4) Retrieval of all records in a water year as entered on the screen: Begin date: 10-01-02 End date: 09-30-03
- 5) Retrieval date range converted to: Begin date: 10-01-02 @ 05:00:00 UTC End date: 10-01-03 @ 04:59:59 UTC

Due to the conversion to UTC for retrieval this sample is included in the retrieval even though it was not collected in the date range selected.

C) Example: Sample from the east coast of the United States

- 1) Unix time variable is US/Eastern
- 2) Sample begin date/time logged in as: 09-30-02 @ 2300 EST
- 3) Sample begin date/time stored in UTC as: 10-01-02 @ 0400 UTC
- 4) Retrieval of all records in a water year as entered on the screen: Begin date: 10-01-02 End date: 09-30-03
- 5) Retrieval date range converted to: Begin date: 10-01-02 @ 04:00:00 UTC End date: 10-01-03 @ 03:59:59 UTC

Due to the conversion to UTC for retrieval this sample is included in the retrieval even though it was not collected in the date range selected.

D) Example: Sample from the east coast of the United States

1) Unix time variable is US/Eastern

- 2) Sample begin date/time logged in as: 09-30-03 @ 2330 EST
- 3) Sample begin date/time stored in UTC as: 10-01-03 @ 0430 UTC
- 4) Retrieval of all records in a water year as entered on the screen: Begin date: 10-01-02

End date: 09-30-03

5) Retrieval date range converted to:

Begin date: 10-01-02 @ 04:00:00 UTC End date: 10-01-03 @ 03:59:59 UTC

Due to the conversion to UTC for retrieval this sample is *not* included in the retrieval even though it was collected in the date range selected.

Selection of criteria based on (2) analysis-level codes or (6) parameter codes and values each invoke another menu described below.

If the user specifies a selection based on **analysis-level codes**, the following menu is invoked. The user may select one or more of the selection criteria.

Locate QWDATA records

Enter an X to choose an item for limiting retrieval, Enter a # to remove an item.

(1) MEDIUM CODE: _ (2) ANALYSIS SOURCE: _ (3) HYDROLOGIC CONDITION: _
(4) SAMPLE TYPE: _ (5) HYDROLOGIC EVENT: _

Options: ? ^D # / /x /+x /-x /@ /c /q -- Enter ?/ for help

Options for selecting water quality records based on analysis-level codes

If the user specifies a selection based on *parameter codes and values* the following series of menus are invoked. On the first menu, the user has the option of restricting parameter selection by selecting *NOT*. This option is used to select records for which parameter(s) identified in the next step do not exist. For example, if the *NOT* option is selected and parameter code 00010 is selected, only records without parameter code 00010 (water temperature) are retrieved.

Next, the user is asked to specify the first parameter code for selection. The user may also specify minimum and maximum values for that parameter code as well as other result level codes listed in the screen below. Null values can be retrieved by inserting a '.' in the MIN field.

Paramatar coda/valua tests			
i arameter coue, value tests			
NOT: (X qualifies records if specified	ed parameters d	lo not exist))
Enter up to 50 testsquit? (Y/N): N	-	,	
(1) PARM: 00010 MIN: 15	MAX: 30	RMK:	
QA: METH:	_ PREP SET N	NUMBER:	
ANL SET NUMBER:	VAL QUAI	L CODE:	
(2) A/O: O PARM: 00300 MIN: 4	MAX:	RM	K :
OA: METH:	PREP SET N	NUMBER:	
ANL SET NUMBER:	- VAL OUAI	CODE:	
(3) A/O: PARM: MIN:	MAX:		RMK:
OA: METH:	PREP SET	NUMBER:	
ANL SET NUMBER:	- VAL OUAI	CODE:	
Options: ? ^D # / /x /+x /-x /@ /c /q Enter ?/ for help			

Screen for selecting water-quality records based on parameter codes

More than one parameter code may be selected. Selection by parameter codes and values is the only selection that does not require that the specified criteria must be satisfied to qualify a water-quality record for selection. If more than one parameter code is specified, for **each parameter after the first**, the user is asked whether the relation to the previous parameter is **AND** or **OR**. The **AND** or **OR** options in combination with the **NOT** option results in specific actions based on the rules of *boolean logic (Getting started, 2.2.6)*. Examples are shown in the table below.

First specification	Second specification (P1=parameter code 1, etc.)	Action selects records that
NOT	P1, AND P2	do not contain values for both P1 and P2
NOT	P1, <i>OR</i> P2	do not contain values for either P1 or P2
	P1, AND P2	contain values for both P1 and P2
	P1, <i>OR</i> P2	contain values for either P1 or P2
	P1, OR P2, AND P3	contain values for either P1 or both P2 and P3
NOT	P1, OR P2, AND P3	do not contain values for either P1 or both P2 and P3

Actions of NOT, AND, and OR specifications for record selection based on result level codes

After the specifications are complete, the user is asked to select if records flagged as local use (code z) or proprietary (code 9) should be included in the retrieval. If 1 is entered, records with a processing status of "z" are included in the retrieval; if 2 is entered, records with an analysis status = "9" are included; if 12 is entered, both local use and proprietary records are included; a carriage return $\langle cr \rangle$ results in the default condition in which local use and proprietary records are excluded from the retrieval. Additional information about setting the processing status code is available in <u>section 3.7.5</u>; general information about analysis status codes and processing status codes is available in <u>section 2.4.10</u> and <u>2.4.15</u> respectively.

The user is notified that the database search has begun. After water-quality records are retrieved (and if the number of records retrieved is greater than zero), the number of records and number of sites are displayed to the screen:

qwsiterec -- locating QWDATA records

Beginning search for QWDATA records in database 01 end of search. 12227 records (212 sites) located in database 01

Do you wish to save a list of sites that have QW data (Y/N)? Y

Enter pathname of file to hold list of sites with QW data for database /n --

User is notified of the number of water-quality records retrieved and the number of sites for those records. The user is given the option to save a list of sites for which water-quality records were selected.

The user is asked if the list of sites with water quality data should be saved. If the response is **YES**, the user is prompted to enter the path name for the file. Next, the user is asked if the water-quality record numbers should be sorted. The retrieved record numbers may be sorted on any combination of the following fields:



User is notified of the number of water-quality records retrieved and given the option to sort the record numbers

All of the desired sort codes must be entered on one line with no spaces. The first field will be the primary sort; the next will be the secondary sort, and so forth. When the sort is complete or if the sort option is skipped, the user is prompted to enter a file name to hold the retrieved list of record numbers. An example of output of record numbers from this program are shown in <u>Appendix C</u>.

3.3.2 Option 2 -- Produce Inventory of Samples

This option is used to produce a table of information for records that have been logged into the database for samples collected within a specific water year. This program has historically been identified as the `loglist' program. The table may be limited to a user-supplied list of station numbers (up to 50) and/or range of dates within the specified water year. An example of the output from this program is included in <u>Appendix C</u>. This tabular output is written to a file and may be spooled to a printer at the user's request.

Some of the information included in this output indicates the storage of results for some types of analyses. Column entries in the types of analyses can be marked as R, which means that when the sample was logged in, the indicated type of analyses was included in the sample header information; C, which means that when the sample was logged in, the indicated type of analyses was included in the sample header information and at least one of the parameter codes in the type of analysis group has a result stored for the record; or 'blank', which means that nothing was done during login. In the table below are the types of analyses and the parameter codes that are included in each group:

Type of Analyses	Parameter Codes
CH, Chemical	00915, 00925, 00930, 00940, 00945,
	00955, 90095
NU, Nutrients	00608, 00610, 00625, 00630, 00631,
	00665, 00666
ME, Metals	01025, 01027, 01030, 01034, 01040,
	01042, 01045, 01046, 01049, 01051,
	01056, 01065, 01067, 01090, 01092
BI, Biological	00573, 60050, 70943, 70944, 70945,
	70946, 70949, 70950, 70960, 70964,
	70968, 71100, 81354, 82555, 95100,
	95200
PE, Pesticides	39370, 39516, 00550, 06801
RA, Radiological	80050, 80060, 80030, 80040
SE, Sediment	80154, 70344, 70346
BE, Bed material	80160, 80162, 80169, 80171

Note: This feature should be used with caution, because it does not indicate when all results for requested analyses have been stored in the database. The results in the types of analyses columns are based on a very limited set of parameters.

The user is first queried for the name of a file to hold the output. The file name may include the pathname if the user does not wish to save the file in the current directory. If the specified file already exists, it may be either appended or overwritten, according to the user response. The water year is entered next. Within the selected water year, the table may be restricted to specific station numbers and a range of dates. Station numbers may be entered interactively or from a *fixed-column format file*. Station numbers also are accepted in the format used to output stations under *menu option 3.3.1*. Sites may also be input without an agency code.



Screen queries for producing an inventory of samples in the water-quality database

When the selected records have been retrieved, they are ordered by record number. The user is given the option to sort the records by up to seven sort fields (station number, project code, processing status code (*Appendix A*, date of last update, record number, sample start date, and lab ID). Sort selections are entered one at a time. The first sort option entered is the secondary sort; the primary sort is on the record number, the second sort option entered is the tertiary sort, and so forth.



Screen queries for sorting the sample inventory file

When the sort request is complete, the user is asked if data for another water year are to be retrieved. If a response of **YES** is provided, the queries described above are repeated beginning with entry of station numbers and/or date range. If the response is **NO**, the name of the file containing the output is displayed to the screen and the user is given the option to spool the output file to a printer. The user may enter a destination printer or print to the default local printer. Upon completion of the inventory table, the user is returned to the Data Review menu.

3.3.3 Option 3 -- List Samples and Results

Sample information and analytical results for requested records can be displayed to the screen or a file. Records may be identified by record number or by agency, station number, date, time, and medium code. The user is first given the option to enter record selection information interactively or to input this information using an existing file. **Note:** The minimum identifying information needed to uniquely identify a sample is agency code, station number, date, and medium code.

To retrieve a record using sample identification information, all information that has been entered for a particular sample must be specified. The fields that could be completed are agency, station number, date, medium code, time, end date, and end time. For example, if all of these fields were populated for a particular sample, then all of the fields must be used to identify and retrieve the sample. Typically, samples are uniquely identified with agency, station number, date, time, and medium code.

If the list of records is to be entered from a file, the user is prompted for the file name and input format (1 -- record number, or 2 -- agency code, station number, date, time, and medium code).

qwlist program processing in database: 01
Do you want to enter record selection info at the terminal (Y/N, <cr>=Y)? N</cr>
Enter the pathname of the input file (99 to end) test3
What is the format of this file? That is, does it contain record numbers or agency-site-date-medium?
Do you want to identify records by:
1 Decend Number
1 Kecora Number
2 Agency Code, Station Number, Date, Time
Please enter option (1/2, <cr>=1):</cr>

Entering a file to retrieve a list of sample information

If the records are to be identified by record number, the format of the file is one record number per line, with the 8-digit record number beginning in column 1 of each line as shown in <u>Appendix G</u>.

Additional information may be included beyond column 8 so that output from other options (such as the record file output from the <u>Select Sites and/or Samples</u> option shown in <u>Appendix C</u>).

Input files containing records identified by agency, station number, date, time, and medium code must follow the format shown in Appendix G:

The next query gives the user the option to print the output to the screen or to a file. The user is queried for an output file name if the file output option is selected. If the output is to a file, the file will contain the long form (132 characters wide) of the output; footnotes for remarks and qualifiers and result comments can be included. There are three options for display to the screen. An example of each display is in *Appendix C*. After selection of the display to the screen, if either of the long output formats (options 2 and 3) are selected, the user may choose to include footnotes at the bottom of the page to define remarks and qualifiers that appear with the sample information. If the short form (option 1) is chosen, footnotes to define remarks and qualifiers cannot be included. Next, the user is given the option to include result comments (field and/or lab text comments pertaining to a result). Note: The analytical results are displayed using unrounded values from the database.

Do you want output to terminal (T) or to a file (F) (<CR>=T)? T You have 3 options for display of parameters: 1 -- short form, 2-columns 2 -- long form, folded into 80 characters 3 -- long form, 132 characters Enter option desired (1-3,<CR>=1): 3 Do you want to include footnotes for remarks and qualifiers (Y/N,<CR>=Y)? Do you want to include result comments (Y/N,<CR>=N)?

Output option queries for List Samples and Results. This example specifies output to the terminal using the 132-character, long-form to include footnotes explaining remark and qualifier codes.

If the user has chosen to input record information interactively, the next screen allows the user to enter record numbers or agency code station number, date, time, and medium code.

qwlist program -- processing in database: 01

Enter record number:

(Q to quit, <CR> to select by agency-site-date-time-medium)

Interactive record input screen for producing output from the List Samples and Results option

qwlist program -- processing in database: 01

(1) Agency Code: USGS (2) Site Number: ______
 (3) Begin Date: YYYYMMDD (4) Begin Time: HHMM
 (5) End Date: YYYYMMDD (6) End Time: HHMM
 (7) Medium Code: _____

Options: ? ^D # / /x /+x /-x /@ /c /q -- Enter ?/ for help



Note: Begin time, end time, and end date are not required fields on input. However, if these fields have been populated in a sample record, they must be entered here in order to retrieve the record.

The requested record information will be listed on the screen or to a file in the specified format until a response of "q" is entered for record number to end the program

3.3.4 Option 4 -- Sample List and/or Cation-Anion Balance

From this option, output is produced that includes: **1**) a list of parameters and their values, **2**) a cation-anion balance table, or **3**) both for specific samples.

Unless sample identification is to be entered from the terminal, the user is queried for the name of a file (full pathname allowed, up to 32 characters) that contains a list of sample identifiers. This file should contain the necessary identification information. This information may be record numbers or agency code, station number, date, time, and medium code in the format shown above. Next, the user is queried for the name of a file to hold the output.

```
qwbal program – processing in database: 01
Do you want to enter record selection numbers from the terminal (Y/N, <CR>=Y)? y
Enter name of file to hold output –
: output.file
Do you want a listing of parameters and values (Y/N, <CR>=Y)? y
Do you want a cation-anion balance table (Y/N, <CR>=Y)? y
```

Queries for producing a sample list and/or cation-anion balance

The user may select from two output options--parameter list and values and/or an anioncation balance table. If the user chooses to enter sample identifications from the terminal, there will be a request for the next record identifier after processing each record. An entry of **q** or **quit** in the record or station number field terminates processing. The user is asked if the file should be sent to the printer. If so, the user is asked for the destination printer. A **<cr>** sends output to the default printer. The file is saved with fortran page-control characters and should be printed using these page-control characters. The following Unix command usually works:

asa filename\lp -ylandscape -dprintername

An example of output from this program is shown in <u>Appendix C.</u>

Note: Analytical results are included in this output using *rounding* as identified in the *parameter code dictionary*.

3.3.5 Option 5 -- Chemical Validation Checks

Chemical logic and validation checks are performed for specified samples when this option is selected. The user must specify samples by record number. These may be entered from the terminal or a file. The user is queried for an output file name. If record numbers are entered from the terminal, the program queries the user for another record number after each sample is processed. An entry of **q** or **quit** in the record number field terminates processing. The output file name is displayed to the screen and the user is asked if the file should be sent to the printer. If so, the user is asked for the destination printer. A **<cr>** sends output to the default printer. The file is saved with fortran page-control characters. To print the file, the following Unix command usually works:

asa filename |lp -ylandscape -dprintername

Data written to the output file include:

sample identifying information:

- record number,
- station number and name,
- collection date and time,
- analysis level codes, and
- number of parameters stored for the analysis;

notations of regulatory alerts and chemical logic checks, including:

- parameters and values that exceed USEPA Drinking-water maximum contaminant levels (MCL), and
- failed chemical logic checks;
- a list of parameters and their values is produced; and
- a table showing the sum of cations and anions and the ionic balance is produced.

Alerts are based on USEPA drinking-water MCLs and are referenced to all relevant parameter codes ($\underline{Appendix E}$).

NOTE: In some cases, the alert may be for a constituent that does not exactly match the constituent to which the MCL applies. For example, the MCL for nitrate is compared to values for nitrate plus nitrite as well as to nitrate alone.

The chemical validation and logic checks are identical to the checks performed when the laboratory data are stored in the database and *WATLIST* tables are produced. These checks (*see QWDATA table - Section 2.7.1*) include comparisons of total and dissolved values of the same constituent, computed and analyzed values, and logic checks such as verifying that the concentration reported for ammonia is less than that for ammonia plus total nitrogen. When comparing computed values to stored values, both values are first rounded using the precision information stored in the *Parameter Code Dictionary*

An error message is generated only if the rounded values do not match. Invalid parameters (not in the Parameter Code Dictionary), parameters with invalid negative values, invalid fixed value codes, and results with a remark code of 'X' are deleted from the record. Sample output from this program is included in <u>Appendix C</u>.

Note: This program may require a relatively long time to execute; if many analyses are to be checked, a script file should be prepared with answers to the program queries and run in the background or as a batch job. The analytical results that appear in output from this program are rounded using the information stored in the parameter-code dictionary.