

Mars Science Laboratory (MSL)
Chemistry and Mineralogy (CheMin)
Reduced Data Archive
Software Interface Specification

Version 1.1

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TABLE OF CONTENTS

TABLES	iv
DOCUMENT CHANGE LOG	v
TBD ITEMS	vi
ACRONYMS AND ABBREVIATIONS.....	vii
GLOSSARY	viii
1 Introduction.....	1
1.1 Purpose and Scope.....	1
1.2 Content Overview.....	1
1.3 Applicable Documents and Constraints	2
1.4 Relationships with Other Interfaces	2
2 Archive Volume Contents	2
2.1 Root Directory Contents.....	3
2.2 Data Directory Contents and Naming	3
2.3 Index Directory Contents.....	4
2.4 Document Directory Contents.....	5
2.5 Catalog Directory Contents	5
2.6 Label Directory Contents.....	6
2.7 Software Directory Contents	Error! Bookmark not defined.
2.8 Calib Directory Contents	6
2.9 Geometry Directory Contents.....	Error! Bookmark not defined.
2.10 Browse Directory Contents	Error! Bookmark not defined.
2.11 Extras Directory Contents	6
3 Archive Volume Format.....	7
3.1 File Formats	7
3.1.1 Document File Format	7
3.1.2 Tabular File Format	7
3.1.3 PDS Label Format.....	7
3.1.4 Software File Format	8
3.1.5 Catalog File Format	8
3.1.6 Science Data File Formats	8
4 Archive Volume Generation.....	9
4.1 Data Transfer and Validation Methods	9
4.2 Data Product Sizes and Delivery Rates.....	9
4.3 Interface Media Characteristics	9
4.4 Backup	10

4.5 Revisions..... 10

4.6 Labeling and Identification..... 10

5 Support Staff and Cognizant Persons..... 10

TABLES

Table 1. MSL CheMin Derived Data Products.....	1
Table 2. Processing Levels for Science Data Sets	1
Table 3. CheMin RDR Product Type Identifiers	3
Table 4. Index Table Contents	4
Table 5. CheMin Delivery Sizes and Rates	9

DOCUMENT CHANGE LOG

Change	Date	Affected Portions
V1.1 Updated for Release 1	3/14/13	TBD table, 3.1.3, page heading

TBD ITEMS

Section	Description

ACRONYMS AND ABBREVIATIONS

ASCII	American Standard Code for Information Interchange
CD-ROM	Compact Disk - Read-Only Memory
CD-WO	Write-Once Compact Disk
ISO	International Standards Organization
JPL	Jet Propulsion Laboratory
NSSDC	National Space Science Data Center
PDS	Planetary Data System
PSG	Project Science Group
RCE	Rover Compute Element
SDVT	Science Data Validation Team
SIS	Software Interface Specification
TBD	To Be Determined

GLOSSARY

Archive – An archive consists of one or more data sets along with all the documentation and ancillary information needed to understand and use the data. An archive is a logical construct independent of the medium on which it is stored.

Archive Volume, Archive Volume Set – A volume is a unit of media on which data products are stored; for example, one CD-ROM or DVD-ROM. An *archive volume* is a volume containing all or part of an archive; that is, data products plus documentation and ancillary files. When an archive spans multiple volumes, they are called an *archive volume set*. Usually the documentation and some ancillary files are repeated on each volume of the set, so that a single volume can be used alone.

Catalog Information – Descriptive information about a data set (e.g. mission description, spacecraft description, instrument description), expressed in Object Description Language (ODL) which is suitable for loading into a PDS catalog.

Data Product – A labeled grouping of data resulting from a scientific observation, usually stored in one file. A product label identifies, describes, and defines the structure of the data. An example of a data product is a planetary image, a spectrum table, or a time series table.

Data Set – An accumulation of data products. A data set together with supporting documentation and ancillary files is an archive.

Rover Compute Element – The MSL onboard computer. This consists of primary (A) and backup (B) computer elements. CheMin data are downlinked from the RCE.

Standard Data Product – A data product generated in a predefined way using well-understood procedures, processed in "pipeline" fashion. Data products that are generated in a nonstandard way are sometimes called *special data products*.

1 Introduction

1.1 Purpose and Scope

This Software Interface Specification is intended to be used by those who wish to understand the format and content of the Mars Science Laboratory (MSL) Chemistry and Mineralogy (CheMin) Reduced Data Record (RDR) Archive. Typically, these individuals would be software engineers, data analysts, or planetary scientists. The specifications in this document apply to all CheMin RDR standard product archive volumes that are generated by the MSL Project.

1.2 Content Overview

The MSL CheMin RDR archive consists of the following derived products, which are described in the CheMin RDR Software Interface Specification, applicable document 1. All CheMin derived products are generated by the CheMin Science Team. Level 1B data products will be delivered to PDS with data set identification as MSL-M-CHEMIN-4-RDR-V1.0. Tables with Level 2 mineral identifications and abundances will be delivered separately, with data set identification as MSL-M-CHEMIN-5-RDR-V1.0. The separate delivery of Level 2 mineral identification and abundance data allows analysis and revision of these data independently of the processed 1D source data.

Table 1. MSL CheMin Derived Data Products

NASA Level	CODMAC Level	Description
1B	4	Co K α XRD data summed along 2-theta radii, adjusted for arc length and presented as 2-theta versus intensity tables.
1B	4	Co K β XRD data summed along 2-theta radii, adjusted for arc length and presented as 2-theta versus intensity tables.
1B	4	Single-pixel EDS histogram of energy versus intensity (counts).
1B	4	Split-pixel EDS histogram of energy versus intensity (counts).
1B	4	Total EDS histogram of energy versus intensity (counts).
1B	4	XRD data from stacked raw frames, summed along 2-theta radii, adjusted for arc length and presented as 2-theta versus intensity tables.
1B	4	XRD data from modified raw frames, summed along 2-theta radii, adjusted for arc length and presented as 2-theta versus intensity tables.
2	5	Mineral identification, abundance, and estimated errors.

NASA and CODMAC data processing levels are described in Table 2.

Table 2. Processing Levels for Science Data Sets

NASA	CODMAC	Description
Packet data	Raw – Level 1	Telemetry data stream as received at the ground station, with science and engineering data embedded.
Level-0	Edited – Level 2	Instrument science data (e.g., raw voltages, counts) at full resolution, time ordered, with duplicates and transmission errors removed.
Level 1-A	Calibrated - Level 3	Level 0 data that have been located in space and may have been transformed (e.g., calibrated, rearranged) in a

NASA	CODMAC	Description
		reversible manner and packaged with needed ancillary and auxiliary data (e.g., radiances with the calibration equations applied).
Level 1-B	Resampled - Level 4	Irreversibly transformed (e.g., resampled, remapped, calibrated) values of the instrument measurements (e.g., radiances, magnetic field strength).
Level 2	Derived - Level 5	Geophysical parameters, generally derived from Level 1 data, and located in space and time commensurate with instrument location, pointing, and sampling.
Level 3	Derived - Level 5	Geophysical parameters mapped onto uniform space-time grids.

This Software Interface Specification (SIS) describes the format, content, and generation of the CheMin RDR Archive. Section 2, Archive Volume Contents, describes the structure of the archive volumes and the contents of each file. Section 3, Archive Volume Format, describes the file formats used on the archive volumes. Section 4, Archive Volume Generation, describes the procedure for assembling the archive and transferring it to the Planetary Data System (PDS). Finally, Section 5, Support Staff and Cognizant Persons, lists the individuals responsible for generating and receiving the archive volumes.

1.3 Applicable Documents and Constraints

This Archive Volume SIS is intended to be consistent with the following documents:

1. Mars Exploration Program Data Management Plan, R. E. Arvidson, S. Slavney and J. Ward, Rev. 4, June 15, 2011.
2. Mars Science Laboratory Archive Generation, Validation, and Transfer Plan, J. Crisp and P. Theisinger, JPL D-35281, MSL-214-1333, May 28, 2010.
3. MSL CheMin Reduced Data Record (RDR) Software Interface Specification (SIS), D. Vaniman, JPL D-69260, MSL 576-3503, Version 1.0, April 4, 2011.
4. Planetary Data System Archive Preparation Guide, Version 1.4, JPL D-31224, April 1, 2010.
5. Planetary Data System Standards Reference, February 27, 2009, Version 3.8, JPL D-7669, Part 2.
6. MSL CheMin Science Team and PDS Geosciences Node Interface Control Document (ICD), Version 2.0, May 14, 2007.

1.4 Relationships with Other Interfaces

This Archive Volume SIS could be affected by changes to the design of the CheMin RDR standard data products (Applicable Document 3).

2 Archive Volume Contents

This section describes the contents of the MSL CheMin RDR Archive volumes, including the file names, file contents, file types, and organization responsible for providing the files.

2.1 Root Directory Contents

Files in the Root Directory include an overview of the archive, a description of the volume for the PDS Catalog, and a list of errata or comments about the archive. The following files are contained in the Root Directory.

File Name	File Contents	File Provided By
AAREADME.TXT	Volume content and format information	Geosciences Node
ERRATA.TXT	A cumulative listing of comments and updates concerning all archive volumes published to date. More than just errata, this file should be updated with release notes for each data release, including an explanation of any revisions or omissions.	CheMin Team
VOLDESC.CAT	A description of the contents of this volume in a PDS format readable by both humans and computers	Geosciences Node

2.2 Data Directory Contents and Naming

Files in the Data Directory are grouped into subdirectories by sol (Mars day) number, with directory names in the form SOLnnnn (example: SOL0001). Files in the Data Directory consist of data products and the PDS labels that describe them. Both data products and labels are provided by the CheMin Team.

The file naming scheme is fully explained in the CheMin RDR SIS, Applicable Document 3. In brief, the scheme is as follows:

<instr><config><sclk><prod><sol><site><drive><seqid><producer><ver>.<ext>

where

instr = CM for CheMin

config = A_ for primary Rover Compute Element (RCE) , B_ for backup RCE, or __ (two underscores) for a special case where partial downlinks may have been obtained from both the primary and the backup RCE and compiled into a single RDR

sclk = 9-character Spacecraft Clock Start Count

prod = 3-character product type identifier, one of the following for CheMin RDRs:

Table 3. CheMin RDR Product Type Identifiers

CheMin RDR Product Type	Identifier
Diffraction Single, K-alpha or K-beta	RD1
Diffraction Split, K-alpha or K-beta	RDS
Diffraction All, Raw	RDA
Diffraction All, Raw	RTR
Energy All	REA
Energy Single	RE1
Energy Split	RES
Mineral Identification and Abundance	MIN

sol = 4-digit sol number

site = 3-character site location number

drive = 4-character drive location (position within site)

seqid = 4-character Category subfield and 5-digit sequence ID

producer = "P" for CheMin Principal Investigator; other characters A through L to be assigned to CheMin Co-Investigators

ver = 1-character version identifier

ext = TAB for ASCII text table data, DAT for binary table data, LBL for ASCII text PDS label

2.3 Index Directory Contents

Files in the Index Directory are provided to help the user locate products in the archive. The following files are contained in the Index Directory.

File Name	File Contents	File Provided By
INDXINFO.TXT	A description of the contents of this directory	Geosciences Node
INDEX.TAB	A table listing all data products on this volume	CheMin Team
INDEX.LBL	A PDS detached label that describes INDEX.TAB	CheMin Team

The index table contains one row for each product on an archive volume. Table 4 lists the columns of the index table.

Table 4. Index Table Contents

Column Name	Description	Source
VOLUME_ID	PDS archive volume on which a data product is stored	Specified at time of index table creation
PATH_NAME	Directory path to data product, relative to volume root	Determined by location of PDS label file
FILE_NAME	Name of <i>label</i> file for data product	PDS label file name
PRODUCT_ID	Unique identifier for data product	PDS label
PRODUCT_TYPE	Type of RDR product, from Table 3.	PDS label
PRODUCT_VERSION_ID	Version number of data product	PDS label
PRODUCT_CREATION_TIME	Date and time of data product creation	PDS label
RELEASE_ID	ID of scheduled data release to PDS in which this product was included	PDS label
START_TIME	UTC date and time of start of observation	PDS label
SPACECRAFT_CLOCK_START_COUNT	Spacecraft clock count at start of observation	PDS label

2.4 Document Directory Contents

The Document Directory contains documentation to help the user understand and use the archive data. The following files are contained in the Document Directory.

File Name	File Contents	File Provided By
DOCINFO.TXT	A description of the contents of this directory	Geosciences Node
CHEMIN_BASICS.PDF	A PDF file that explains basic operation and data generation from the CheMin instrument	CheMin Team
CHEMIN_BASICS.HTM	CHEMIN_BASICS as hypertext	CheMin Team
CHEMIN_BASICS.LBL	A PDS label that describes both versions of CHEMIN_BASICS	CheMin Team
CHEMIN_RDR_AVVIS.PDF	The Archive Volume SIS (this document) as a PDF file	CheMin Team
CHEMIN_RDR_AVVIS.HTM	The Archive Volume SIS (this document) as hypertext	CheMin Team
CHEMIN_RDR_AVVIS.LBL	A PDS label that describes both versions of CHEMIN_RDR_AVVIS.	CheMin Team
CHEMIN_RDR_SIS.PDF	The Data Product SIS as a PDF file	CheMin Team
CHEMIN_RDR_SIS.HTM	The Data Product SIS as hypertext	CheMin Team
CHEMIN_RDR_SIS.LBL	A PDS label that describes both versions of CHEMIN_RDR_SIS.	CheMin Team
MSL_LDD.FUL, .LBL	MSL Local Data Dictionary and label	Geosciences Node
PDSDD.FUL, .LBL	PDS Data Dictionary and label	Geosciences Node

2.5 Catalog Directory Contents

The files in the Catalog Directory provide a top-level understanding of the mission, spacecraft, instruments, and data sets. The files in this directory are coordinated with the PDS data engineer, who is responsible for loading them into the PDS catalog. The following files are found in the Catalog Directory.

File Name	File Contents	File Provided By
CATINFO.TXT	A description of the contents of this directory	Geosciences Node
CHEMIN_INST.CAT	Instrument information for the PDS catalog	CheMin Team
CHEMIN_L1_RDRDS.CAT, CHEMIN_L2_RDRDS.CAT	Data set information for the PDS catalog	CheMin Team
CHEMIN_REF.CAT	References mentioned in other CHEMIN*.CAT files	CheMin Team
MSL_INSTHOST.CAT	Instrument host (i.e., spacecraft) information for the PDS catalog	MSL Project
MSL_MISSION.CAT	Mission information for the PDS catalog	MSL Project
MSL_REF.CAT	References mentioned in other MSL*.CAT files	MSL Project
PERSON.CAT	Personnel information for the PDS catalog (Team and PDS personnel responsible for generating the archive)	CheMin Team

2.6 Label Directory Contents

The Label Directory contains format files, e.g., excerpts from PDS labels that describe data format and organization. These files are referred to in the PDS labels that accompany the data products. They are "include" files that are intended to be parsed as if they were part of the PDS labels that refer to them. This is an optional directory. It is present only if the data product labels refer to format files using the ^STRUCTURE keyword. The following files are contained in the Label Directory.

File Name	File Contents	File Provided By
LABINFO.TXT	A description of the contents of this directory	Geosciences Node
CHEMIN_EDH.FMT	Format of CheMin RDR energy data products	CheMin Team
CHEMIN_MIN.FMT	Format of CheMin mineral abundance data products	CheMin Team
CHEMIN_XRD.FMT	Format of CheMin X-ray Diffraction data products	CheMin Team

2.7 Calib Directory Contents

The Calib Directory contains calibration files used to process the data products, or calibration data needed to use the data products. This directory is optional. It appears only if there are calibration data, plans, or reports included in the archive. The following files are contained in the Calib Directory.

File Name	File Contents	File Provided By
CALINFO.TXT	A description of the contents of this directory	Geosciences Node
CALREPORT.PDF	PDF documentation of results obtained from analyses of calibration standards carried on the CheMin flight instrument.	CheMin Team
CALREPORT.HTM	CALREPORT as hypertext	CheMin Team
CALREPORT.LBL	PDS label that describes both versions of CALREPORT	CheMin Team

2.8 Extras Directory Contents

The Extras Directory contains a listing of commercial or public-domain software available for processing Level 2 CheMin X-ray diffraction data. The following files are contained in the Extras Directory.

File Name	File Contents	File Provided By
EXTRINFO.TXT	A description of the contents of this directory	Geosciences Node
XRDINFO.PDF	A listing of commercial or public-domain software capable of processing CheMin XRD data	CheMin team

The purpose of this directory is to provide the reader with a list of software that can process and analyze CheMin XRD data. The software listed will be a partial listing, since there are many commercial and public-domain programs that may be used, with varying degrees of

sophistication in XRD pattern processing. The list provided will represent software commonly used by various members of the CheMin team, but the ASCII format in which CheMin XRD RDRs are provided can be handled by most software.

This software listing does not cover processing of energy histograms (EDS data). The EDS data are interpretable from widely available lookup tables of X-ray energy. Quantification of EDS data is desired but currently not a CheMin RDR product. Study is being devoted to EDS quantification and, should this prove practical, an amendment will be made to the CheMin RDR archive.

3 Archive Volume Format

This section describes the format of CheMin RDR Archive Volumes. Data that comprise the Archive are formatted in accordance with Planetary Data System specifications [Applicable Documents 4 and 5].

3.1 File Formats

This section describes file formats for the kinds of files contained on Archive Volumes.

3.1.1 Document File Format

Document files with the .TXT suffix exist in all directories except Data. They are ASCII files which may have embedded PDS labels. Lines in a .TXT file end with a carriage return character (ASCII 13) and a line feed character (ASCII 10). This allows the files to be readable under various operating systems.

Documents in the Document directory may contain formatting and figures that cannot be rendered as ASCII text. These documents are given as PDF (Portable Document Format) files, which may be viewed with free PDF reader software. To comply with the PDS requirement that a text copy of the documentation be archived, an HTML version of each PDF file is also provided.

3.1.2 Tabular File Format

Tabular files (.TAB suffix) exist in the Index directory and the Data directory. Tabular files are ASCII files formatted for direct reading into many database management systems on various computers. All fields are separated by spaces and/or commas, and character fields are enclosed in double quotation marks ("). (Character fields are padded with spaces to keep quotation marks in the same columns of successive records.) Character fields are left justified, and numeric fields are right justified. The "start byte" and "bytes" values listed in the labels do not include the commas between fields or the quotation marks surrounding character fields. The records are of fixed length, and the last two bytes of each record contain the ASCII carriage return (ASCII 13) and line feed (ASCII 10) characters. This allows a table to be treated as a fixed length record file on computers that support this file type and as a text file with embedded line delimiters on those that don't.

3.1.3 PDS Label Format

All tabular files in the archive are described by detached PDS labels. A label has the same name as the data file it describes, but with the extension .LBL. For examples of PDS labels for each

type of CheMin data product, see the CheMin RDR Data Product SIS [Applicable Document 3]. Other types of files in the archive may have either detached or attached PDS labels. An attached label is embedded at the beginning of the file it describes.

A PDS label, whether attached or detached from its associated file, consists of lines of ASCII text in the form of keyword = value statements that provide descriptive information about the data file. The label is intended to be readable both by humans and by software. Details of the syntax and semantics of PDS labels can be found in the PDS Standards Reference (Applicable Document 5), and definitions of the keywords used in the label can be found by using the PDS Data Dictionary Lookup web service at http://pds.nasa.gov/tools/ddlookup/data_dictionary_lookup.cfm.

Lines of text in detached labels end with a carriage return character and a line feed character. This allows the files to be read under various operating systems.

3.1.4 Software File Format

No executable software files are posted within the CheMin Reduced Data Archive.

3.1.5 Catalog File Format

Catalog files (suffix .CAT) exist in the Root and Catalog directories. Like PDS labels, they are made up of keyword = value statements, but most of their content is descriptive text intended to be read by the user. They contain descriptions of the data set, instrument, spacecraft, and mission, as well as personnel contact information and references to published literature. They are called Catalog Files because they are loaded into the PDS online catalog to make the information available to users searching for data.

3.1.6 Science Data File Formats

CheMin RDR data products are ASCII text tables with detached PDS labels, as described in section 3.1.2 above.

For more information about the format and content of the data products, see the CheMin RDR Data Product SIS [Applicable Document 3].

4 Archive Volume Generation

4.1 Data Transfer and Validation Methods

CheMin RDR data products are generated by the CheMin Science Team, either at JPL or at investigator institutions. The RDR data products are prepared from calibrated and transformed CheMin EDR (raw) data products according to the CheMin RDR Data Product SIS [3]. The team uses metadata from telemetry data headers to populate the PDS labels. The CheMin Team delivers data products to the Geosciences Node of the PDS, along with the other components of the archive for which the team is responsible, according to the archive delivery schedule in the MSL Archive Plan [2] and agreement between the CheMin Team and the Geosciences Node [6]. Deliveries occur approximately every 90 sols.

4.2 Data Product Sizes and Delivery Rates

Table 5 summarizes expected sizes and production rates for the CheMin RDR Standard Products.

Table 5. CheMin Delivery Sizes and Rates

CheMin RDR Product ID	CheMin RDR Product Type	Product Size	Production Rate (e.g., number of products per sol or per 90-sol delivery)	Expected Number of Products for Primary Mission (669 sols)	Expected Total Data Volume for Primary Mission
RD1	Diffraction Single, K-alpha or K-beta	816 Kb	3	22	350 Kb
RDS	Diffraction Split, K-alpha or K-beta	816 Kb	3	22	350 Kb
RDA	Diffraction All, K-alpha or K-beta	816 Kb	<1	8	130 Kb
RTR	Diffraction All, Raw	816 Kb	<1	5	80 Kb
RDF	Diffraction, Film Mode	816 Kb	<1	5	80 Kb
REA	Energy All	100 Kb	3	22	2200 Kb
RE1	Energy Single	100 Kb	3	22	2200 Kb
RES	Energy Split	100 Kb	3	22	2200 Kb
MIN	Mineral Identification and Abundance	5 Kb	3	22	100 Kb

4.3 Interface Media Characteristics

All volumes in the CheMin RDR Standard Product Archive conform to ISO 9660 standards as specified in the PDS Standards Reference [5].

4.4 Backup

The PDS Geosciences Node maintains backup copies of MSL CheMin RDR archives according to its general policy for backups, including off-site storage belonging to the Node and long-term storage at the National Space Science Data Center.

4.5 Revisions

It is expected that CheMin RDR data products may be revised during the course of the mission due to improvements in the understanding of the instrument, better calibration information, etc. When the CheMin Team delivers revised versions of CheMin RDR data products to the PDS, the team must identify the revisions at or before the time of delivery. Labels for revised products must have a later value for the `PRODUCT_CREATION_TIME` keyword and an updated value for the `PRODUCT_VERSION_ID` keyword. They may also have a different value in the `VERSION` field of the file name as described in section 2.2, Data Directory Contents and Naming. The reasons for the revisions must be documented in `ERRATA.TXT`.

Previous versions of revised products are handled according to PDS policy for "draft" data sets, as the CheMin RDR archive is considered a work in progress until the final delivery. If revisions consist of minor changes to labels or corrections of typographical errors, the previous versions are not retained. If the revisions are done to correct serious errors in previously released products such that the older products are unfit for use, then the older products are not retained. In the typical case of revisions done as part of routine updates in calibration, etc., the Geosciences Node retains previous versions, making them accessible to users, for at least six months.

4.6 Labeling and Identification

The CheMin RDR Archive has unique PDS data set identifiers that reflect either Level 1B data (labeled `MSL-M-CHEMIN-4-RDR-V1.0`) or Level 2 data (labeled `MSL-M-CHEMIN-5-RDR-V1.0`). Use of separate labels allows for expected multiple or iterative analyses of mineral abundances or for advanced pattern analysis methods, based on the methods used in generating Level 2 mineral identification and abundance data, separate from Level 1B data processing.

The volume on which the CheMin RDR Archive is stored has the PDS-assigned unique identifier `MSLCMN_1XXX`. This is the value of the keyword `VOLUME_ID` in catalog files and in the index table.

If ever the archive is divided among multiple physical volumes for data transfer or for another reason, the `XXX` in the volume ID is replaced by sequential volume numbers 001, 002, etc.

5 Support Staff and Cognizant Persons

The CheMin Principal Investigator is David Blake, NASA Ames Research Center. The CheMin Archive Representatives are CheMin Science Team members David Vaniman, Planetary Science institute, and Michael Wilson, NASA Ames Research Center. The MSL Deputy Project Scientist, who is responsible for coordinating MSL archiving, is Joy Crisp, Jet Propulsion Laboratory.

The PDS Geosciences Node Archivist for the CheMin RDR Archive is Susan Slavney, Washington University, St. Louis; she is also the MSL Mission Lead for PDS. The PDS

Geosciences Node Manager is Raymond Arvidson, Washington University. The PDS Data Engineer for MSL is Betty Sword, PDS Engineering Node, Jet Propulsion Laboratory.