



Multiscale Complex Genomics



**Project Acronym:** MuG

**Project title:** Multi-Scale Complex Genomics (MuG)

**Call:** H2020-EINFRA-2015-1

**Topic:** EINFRA-9-2015

**Project Number:** 676556

**Project Coordinator:** Institute for Research in Biomedicine (IRB Barcelona)

**Project start date:** 1/11/2015

**Duration:** 36 months

## Deliverable 2.5: Project Outputs

**Lead beneficiary:** Institute for Research in Biomedicine (IRB Barcelona)

**Dissemination level:** PUBLIC

Due date: 31/10/2018

Actual submission date: 06/11/2018

Copyright© 2015-2018 The partners of the MuG Consortium



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676556.

## Document history

Version	Contributor(s)	Partner	Date	Comments
0.1	Anna Montras	IRB Barcelona	22/08/2018	First draft
0.2	Mark McDowall	EMBL-EBI	11/10/2018	Additions in sections 6.2 and 7
0.3	Anna Montras	IRB Barcelona	16/10/2018	Second draft
1.0			05/11/2018	Approved by Supervisory Board



## Table of contents

<b>1</b>	<b>INTRODUCTION .....</b>	<b>5</b>
<b>2</b>	<b>EC REPORTING DOCUMENTS .....</b>	<b>5</b>
2.1	DELIVERABLES.....	5
2.2	MILESTONES.....	5
<b>3</b>	<b>SCIENTIFIC OUTCOME .....</b>	<b>5</b>
3.1	PEER-REVIEWED SCIENTIFIC PUBLICATIONS.....	5
3.2	DATA SETS .....	12
3.2.1	<i>Senescence</i> .....	12
3.2.2	<i>Whole Yeast Data</i> .....	12
3.2.3	<i>Transcription factor binding and DNA bending</i> .....	12
<b>4</b>	<b>TECHNICAL DOCUMENTATION .....</b>	<b>12</b>
4.1	INFRASTRUCTURE.....	12
4.2	CODE.....	12
4.2.1	<i>Source code</i> .....	12
4.2.2	<i>MuG coding standards</i> .....	12
4.3	DATA.....	13
4.4	EXTERNAL TOOL INTEGRATION .....	13
4.5	VRE HELP .....	13
4.6	TOOLS HELP .....	14
4.6.1	<i>External analysis tools integrated in the MuG VRE</i> .....	14
4.6.2	<i>Other Tools</i> .....	14
4.7	TUTORIALS.....	14
<b>5</b>	<b>TRAINING MATERIALS .....</b>	<b>14</b>
5.1	WEBINARS .....	14
5.2	WORKSHOP DOCUMENTATION .....	15
<b>6</b>	<b>LEGAL AND IP .....</b>	<b>15</b>
6.1	VRE TERMS OF USE .....	15
6.2	LICENSING INFO .....	15
<b>7</b>	<b>OTHER DISSEMINATION AND COMMUNICATION TOOLS .....</b>	<b>16</b>
<b>8</b>	<b>OPEN ACCESS REPOSITORIES .....</b>	<b>17</b>



## Executive summary

The ultimate objective of MuG is to support the emerging community working in the 3D/4D genomics field in embracing the use of HPC and the adoption of standards by facilitating the way they interact with such elements. It is key in order to enable a wide uptake by the community of the MuG developments that all project outputs are properly characterized and all related documentation is easily accessible to the community of users. It has been a priority of WP2 to coordinate efforts with developers (WP3, 4, 5, 6) and lead users (pilot projects) in order to ensure that (i) the community is made aware of project results and (ii) project results are properly documented, archived and accessible. D2.5 contains a thorough list of the project outputs and provides links to relevant repositories and publications, data, technical documentation and software stored thereby.



## 1 INTRODUCTION

The main achievement of the MuG project lies in the development of the MuG VRE, a user-friendly platform that makes available to the 3D/4D genomics community tools to integrate navigation and visualization from sequence data to chromatin dynamics data. Beyond the developed software tools and pipelines, which constitute the fundamental outputs generated by the project, a number of side outputs has been generated that must as well be properly characterized and archived in order to ensure the proper uptake of the MuG VRE services by external users (e.g. scientific publications, data sets, training materials, technical documentation, tutorials, etc.) and their long-term sustainability.

In agreement with the EU open access policies, all documents, software and data generated by the project have been deposited in open access repositories, making them traceable and findable beyond the end of the MuG 3-year grant period independently from the maintenance of the MuG website.

The present deliverable compiles a thorough list of project outputs and provides links to their locations in the MuG project website and in external open access repositories.

## 2 EC REPORTING DOCUMENTS

All reports generated in MuG are tagged as public and are thus accessible to the community. Documentation is available for download from the MuG website, and as the reports become approved, they are incorporated into the MuG community created in Zenodo (see section 8 below).

### 2.1 Deliverables

<http://www.multiscalegenomics.eu/MuG/deliverables/>

### 2.2 Milestones

<http://www.multiscalegenomics.eu/MuG/about-mug/milestones/>

## 3 SCIENTIFIC OUTCOME

### 3.1 Peer-reviewed scientific publications

According to EC rules on open access, publication in either green or gold open access has been adopted by all partners. Regardless of the open access route chosen by partners, a copy of all publications has been deposited in open access repositories to ensure its long-term accessibility. A full list of publications, organized by year, is kept in the MuG website: <http://www.multiscalegenomics.eu/MuG/category/publications/>

A full table with papers and links to the public repository where each paper is deposited is provided in the table below for easy reference.

In total, consortium members have published **31** MuG-related scientific papers in high-impact journals, including 5 reviews, which have accumulated **326 citations** thus far. It is worthy of note that 3 MuG co-PIs have co-authored a position paper on 4D nucleome data and model standards with leading worldwide researchers in the field.



	Year		Title	Authors	Reference	DOI	Public repository
1	2016	ARTICLE	<a href="#">BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data</a>	Hospital A, Andrio P, Cugnasco C, Codo L, Becerra Y, Dans P, Battistini F, Torres J, Goñi R, <b>Orozco M, Gelpí J.</b>	Nucleic Acids Res 44 (D1) D272-278	<a href="http://dx.doi.org/10.1093/nar/gkv1301">http://dx.doi.org/10.1093/nar/gkv1301</a>	<a href="http://upcommons.upc.edu/handle/2117/84242">http://upcommons.upc.edu/handle/2117/84242</a>
2	2016	REVIEW	<a href="#">Multiscale simulation of DNA</a>	Dans P, Walther J, Gómez H, <b>Orozco M.</b>	Curr Opin Struct Biol 37, 29–45.	<a href="https://doi.org/10.1016/j.jsb.2015.11.011">https://doi.org/10.1016/j.jsb.2015.11.011</a>	<a href="http://deposit.ub.edu/dspace/handle/2445/103226">http://deposit.ub.edu/dspace/handle/2445/103226</a>
3	2016	ARTICLE	<a href="#">Long-timescale dynamics of the Drew-Dickerson dodecamer</a>	Dans P, Danilāne L, Ivani I, Dršata T, Lankaš F, Hospital A, Walther J, Pujagut R, Battistini F, Gelpí J, Lavery R, <b>Orozco M.</b>	Nucleic Acids Res 44 (9): 4052-4066	<a href="http://dx.doi.org/10.1093/nar/gkw264">http://dx.doi.org/10.1093/nar/gkw264</a>	<a href="https://upcommons.upc.edu/handle/2117/86576?locale-attribute=en">https://upcommons.upc.edu/handle/2117/86576?locale-attribute=en</a>
4	2016	ARTICLE	<a href="#">Small details matter: the 2'Hydroxyl as a conformational switch in RNA</a>	Darre L, Ivani I, Dans PD, Gómez H, Hospital A and <b>Orozco M</b>	J. Am. Chem. Soc. 138 (50), 16355–16363	<a href="http://dx.doi.org/10.1021/jacs.6b09471">http://dx.doi.org/10.1021/jacs.6b09471</a>	<a href="http://deposit.ub.edu/dspace/handle/2445/105631">http://deposit.ub.edu/dspace/handle/2445/105631</a>
5	2016	ARTICLE	<a href="#">Coordinate redeployment of PRC1 proteins suppresses tumor formation during Drosophila development</a>	Vincent Loubiere, Anna Delest, Aubin Thomas, Boyan Bonev, Bernd Schuettengruber, Satish Sati, Anne-Marie Martinez & <b>Giacomo Cavalli.</b>	Nature Genetics 48, 1436–1442	<a href="https://doi.org/10.1038/ng.3671">https://doi.org/10.1038/ng.3671</a>	<a href="https://hal.archives-ouvertes.fr/hal-01393390">https://hal.archives-ouvertes.fr/hal-01393390</a>
6	2016	REVIEW	<a href="#">Organization and function of the 3D genome</a>	Boyan Bonev & <b>Giacomo Cavalli.</b>	Nature Reviews Genetics 17, 661–678	<a href="https://doi.org/10.1038/nrg.2016.112">https://doi.org/10.1038/nrg.2016.112</a>	<a href="https://hal.archives-ouvertes.fr/hal-01386805">https://hal.archives-ouvertes.fr/hal-01386805</a>







18	2017	ARTICLE	<a href="#">The spatial position of budding yeast chromosomes affects gene expression</a>	Di Giovanni F, Di Stefano M, Bàu D, Carey LB, <b>Marti-Renom MA</b> and Mendoza M	BioRxiv (preprint)	2017	<a href="https://doi.org/10.1101/237263">https://doi.org/10.1101/237263</a>	<a href="https://www.biorxiv.org/content/early/2017/12/20/237263">https://www.biorxiv.org/content/early/2017/12/20/237263</a>
19	2017	ARTICLE	<a href="#">Single-cell absolute contact probability detection reveals chromosomes are organized by multiple low-frequency yet specific interactions</a>	Cattoni DI, Cardozo Gizzi AM, Georgieva M, DiStefano M, Valeri A, Chamousset D, Houbron Ch, Déjardin S, Fiche JB, González I, Chang JM, Sexton T, <b>Marti-Renom MA</b> , Bantignies F, Cavalli G and Nollmann M	Nature Communications 8, 1753		<a href="#">doi: 10.1038/s41467-017-01962-x</a>	<a href="https://www.biorxiv.org/content/early/2017/10/24/159814">https://www.biorxiv.org/content/early/2017/10/24/159814</a>
20	2017	ARTICLE	<a href="#">DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p</a>	Chakraborty A, Lyonnais S, Battistini F, Hospital A, Medicì G, Prohens R, Orozco M, Vilardell J and Solà M	Nucleic Acids Res. 45(2), 951–967.		<a href="https://doi.org/10.1093/nar/gkw1147">10.1093/nar/gkw1147</a>	<a href="http://europemc.org/articles/PMC5314765">http://europemc.org/articles/PMC5314765</a>
21	2017	ARTICLE	<a href="#">Expanding the repertoire of DNA shape features for genome-scale studies of transcription factor binding</a>	Jinsen Li, Jared M. Sagendorf, Tsu-Pei Chiu, <b>Marco Pasi</b> , Alberto Perez, Remo Rohs	Nucleic Acids Res. 45(2), 12877–12887		<a href="https://doi.org/10.1093/nar/gkx1145">10.1093/nar/gkx1145</a>	<a href="http://europemc.org/articles/PMC5728407">http://europemc.org/articles/PMC5728407</a>
22	2017	PROCEEDINGS PAPER	<a href="#">Transparent Execution of Task-Based Parallel Applications in Docker with COMP Superscalar</a>	Victor Anton, Cristian Ramon-Cortes, Jorge Ejarque, <b>Rosa M. Badia</b>	2017 Euromicro International Conference on Parallel, Distributed and Network-based Processing (PDP)	25th		<a href="http://hdl.handle.net/2117/104660">http://hdl.handle.net/2117/104660</a>





				<b>M</b> , Pombo A and Torres-Padilla ME			
29	2018	ARTICLE	<a href="#"><u>Polycomb-Dependent Chromatin Looping Contributes to Gene Silencing during Drosophila Development</u></a>	Ogiyama Y, Schuettengruber B, Papadopoulos GL, Chang JM and Cavalli G	Molecular Cell 71 (1), 73-88.E5	<a href="https://doi.org/10.1016/j.molcel.2018.05.032">https://doi.org/10.1016/j.molcel.2018.05.032</a>	<a href="http://europepmc.org/abstract/med/30008320">http://europepmc.org/abstract/med/30008320</a>
30	2018	ARTICLE	<a href="#"><u>Loss of PRC1 induces higher-order opening of Hox loci independently of transcription during Drosophilaembryogenesis</u></a>	Cheutin T and Cavalli G	Nature communications 9, 3898	<a href="https://doi.org/10.1038/s41467-018-05945-4">https://doi.org/10.1038/s41467-018-05945-4</a>	<a href="https://europepmc.org/articles/PMC6156336">https://europepmc.org/articles/PMC6156336</a>
31	2018	ARTICLE	<a href="#"><u>SKEMPI 2.0: An updated benchmark of changes in protein-protein binding energy, kinetics and thermodynamics upon mutation.</u></a>	Jankauskaité, J., Jiménez-García, B., Dapkūnas, J., Fernández-Recio, J., Moal, I.H.	Bioinformatics (in press)	<a href="https://doi.org/10.1093/bioinformatics/bty635">https://doi.org/10.1093/bioinformatics/bty635</a>	Will be deposited in UPCommons when published. <a href="https://upcommons.upc.edu/handle/2117/23714?locale-attribute=ca">https://upcommons.upc.edu/handle/2117/23714?locale-attribute=ca</a>



## 3.2 Data sets

Data generated by the pilot projects throughout the MuG project have been deposited in public repositories according to the MuG data management policies defined in D4.2 (Data Management Plan).

### 3.2.1 *Senescence*

"Differential 4D genome rewiring in different types of cell senescence"

- Public repository link:  
<https://www.ebi.ac.uk/arrayexpress/experiments/E-MTAB-5829/>
- Status: under embargo (publication pending)

### 3.2.2 *Whole Yeast Data*

"Chromatin structure changes upon oxidative stress or UV irradiation in the yeast *Saccharomyces cerevisiae*":

- Public repository link:  
<https://www.ebi.ac.uk/arrayexpress/experiments/E-MTAB-5825>
- Status: under embargo (publication pending)

### 3.2.3 *Transcription factor binding and DNA bending*

Atomic resolution structural data generated by this pilot project have been deposited in a MuG-specific section of the BIGNASim nucleic acids simulation database.

A more detailed description of the datasets is provided in the description for [milestones MS29-MS33](#).

## 4 TECHNICAL DOCUMENTATION

### 4.1 Infrastructure

A detailed description of the infrastructure and all the elements that compose the MuG VRE is accessible from the main menu in the MuG VRE homepage: <http://www.multiscalegenomics.eu/MuGVRE/> ("What's MuG VRE")

- Clouds: <http://www.multiscalegenomics.eu/MuGVRE/clouds/>
- Components: <http://www.multiscalegenomics.eu/MuGVRE/components/>
- Tool catalog: <http://www.multiscalegenomics.eu/MuGVRE/tools-catalog/>
- Visualizers: <http://www.multiscalegenomics.eu/MuGVRE/visualizers-catalog/>

### 4.2 Code

#### 4.2.1 *Source code*

All the code been developed by MuG is stored in a GitHub repository (<https://github.com/Multiscale-Genomics>).

Links to the repository are available from the <http://www.multiscalegenomics.eu/MuGVRE/source-code/>

#### 4.2.2 *MuG coding standards*

[http://multiscale-genomics.readthedocs.io/en/latest/coding\\_standards.html#](http://multiscale-genomics.readthedocs.io/en/latest/coding_standards.html#)



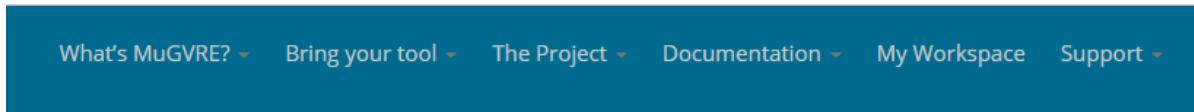
## 4.3 Data

- Supported File types: <http://www.multiscalegenomics.eu/MuGVRE/file-types/>
- Supported data types: <http://www.multiscalegenomics.eu/MuGVRE/data-types/>
- Available assemblies <http://www.multiscalegenomics.eu/MuGVRE/available-assemblies/>

## 4.4 External tool integration

The MuGVRE tool integration API has been conceived to facilitate collaborative work in further development of the VRE, allowing external tool developers to integrate their tools, subject to terms of use (<http://www.multiscalegenomics.eu/MuGVRE/terms-of-use/>).

A “Bring your tool” section is visible on top of the MuG VRE home page:



From there, a drop-down menu provides external tool developers all necessary information to integrate their tool into the MuG VRE:

- Why bring your tool to the VRE? <http://www.multiscalegenomics.eu/MuGVRE/policy/>
- Instructions: <http://www.multiscalegenomics.eu/MuGVRE/instructions/>
- Tool integration: <http://www.multiscalegenomics.eu/MuGVRE/integration-of-tools/>

## 4.5 VRE help

Help is fully integrated into the MuG VRE. The user can access the help from the menu bar accessible from the VRE user interface.



The help information is divided into the following categories:

- General: <https://vre.multiscalegenomics.eu/help/general.php>
- Getting started: <https://vre.multiscalegenomics.eu/help/starting.php>



- Data upload: <https://vre.multiscalegenomics.eu/help/upload.php>
- Workspace: <https://vre.multiscalegenomics.eu/help/ws.php>
- Job launching: <https://vre.multiscalegenomics.eu/help/launch.php>

## 4.6 Tools help

Help for each tool integrated in the VRE is likewise available from the same drop-down menu:

### 4.6.1 External analysis tools integrated in the MuG VRE

Individual help for each tool integrated in the MuG VRE

<https://vre.multiscalegenomics.eu/help/tools.php>

- Chromatin dynamics
- MC-DNA
- MD Energy Refinement
- NAFlex Analyses
- Nucleosome dynamics
- 3D consensus
- Process Genomes
- TADbit

### 4.6.2 Other Tools

- MuG information network:  
<http://www.multiscalegenomics.eu/MuGVRE/modules/ConnectivityBrowser/>
- BiGNASim:  
<http://www.multiscalegenomics.eu/MuGVRE/modules/BigNASimMuG/>
- Flexibility browser: <http://www.multiscalegenomics.eu/MuGVRE/flexibility-browser/>

## 4.7 Tutorials

From the drop-down menu “support” on the MuG VRE homepage, tutorials for different integrated tools are available.

<http://www.multiscalegenomics.eu/MuGVRE/nucleosome-dynamics/>

## 5 TRAINING MATERIALS

### 5.1 Webinars

MuG has collaborated with the BioExcel CoE in delivering different webinars. Such collaboration allows MuG to take advantage of established training infrastructure by the BioExcel CoE and provides BioExcel with the specialized expertise in different topics of relevance to the 3D/4D genomics community and the wider computational biomolecular research community. Recordings of webinars delivered by MuG in collaboration with BioExcel are available through the BioExcel YouTube channel ([https://www.youtube.com/channel/UCd2hq8Q\\_ZyTU4YafEhweE5g](https://www.youtube.com/channel/UCd2hq8Q_ZyTU4YafEhweE5g))

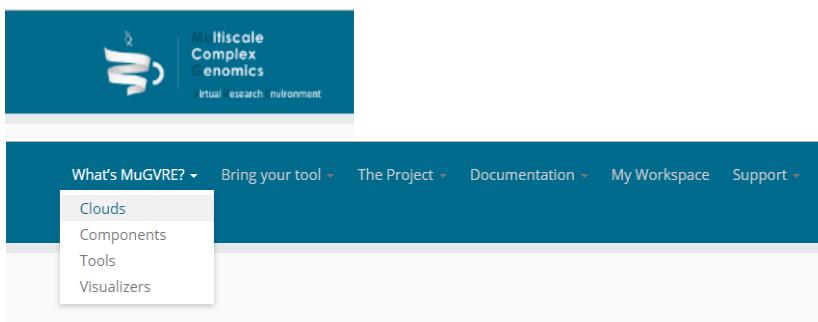
- BioExcel MDWeb (<https://www.youtube.com/watch?v=-dZpGKifp2I>)
- BioExcel NA Flex ([https://www.youtube.com/watch?v=ZTUFsFPU\\_kw&t=100s](https://www.youtube.com/watch?v=ZTUFsFPU_kw&t=100s))





mg-rest-util	Common library for the RESTful interfaces. Currently only covers authorisation	<a href="https://github.com/Multiscale-Genomics/mg-rest-util">https://github.com/Multiscale-Genomics/mg-rest-util</a>	Apache 2.0
mg-rest-dm	RESTful interface to the DM API	<a href="https://github.com/Multiscale-Genomics/mg-rest-dm">https://github.com/Multiscale-Genomics/mg-rest-dm</a>	Apache 2.0
mg-rest-files	RESTful interface to the Dparts for the DM API that allow file access	<a href="https://github.com/Multiscale-Genomics/mg-rest-file">https://github.com/Multiscale-Genomics/mg-rest-file</a>	Apache 2.0
mg-rest-service	RESTful meta server for linking between the distinct RESTful servers	<a href="https://github.com/Multiscale-Genomics/mg-rest-service">https://github.com/Multiscale-Genomics/mg-rest-service</a>	Apache 2.0
mg-rest-adjacency	RESTful interface to retrieve values from calculated adjacency matrices	<a href="https://github.com/Multiscale-Genomics/mg-rest-adjacency">https://github.com/Multiscale-Genomics/mg-rest-adjacency</a>	Apache 2.0
mg-rest-3d	RESTful interface to models generated by TADbit	<a href="https://github.com/Multiscale-Genomics/mg-rest-3d">https://github.com/Multiscale-Genomics/mg-rest-3d</a>	Apache 2.0
mg-docs	Documentation for developers about creating pipelines and tools to run within the VRE. Includes descriptions about coding standards, testing, license and how this is enforced	<a href="https://github.com/Multiscale-Genomics/mg-docs">https://github.com/Multiscale-Genomics/mg-docs</a>	Apache 2.0
VRE	VRE core release 1.0. Web interface and backend	<a href="https://github.com/Multiscale-Genomics/VRE">https://github.com/Multiscale-Genomics/VRE</a>	Apache 2.0

In addition, a full inventory of external tools, components, visualizers and other external infrastructure elements integrated, used, or partially developed within the MuG framework is accessible from the main menu on the MuG website (<http://www.multiscalegenomics.eu/MuGVRE>). Licensing information for external tools will be available from the Tools' Help section within the VRE.



## 7 OTHER DISSEMINATION AND COMMUNICATION TOOLS

In addition to peer-reviewed scientific publications, other contributions to scientific gatherings have been key to make the community aware of the MuG advances. Contributions to conferences or relevant workshops have been widely announced in the MuG website, with links to download related dissemination materials when available.

Materials and information devoted to disseminating the project are available from the MuG website:

- Press releases and news items:



<http://www.multiscalegenomics.eu/MuG/category/news-events/>

- Project brochure:

[http://www.multiscalegenomics.eu/MuG/wp-content/uploads/2016/05/MuG\\_Factsheet.pdf](http://www.multiscalegenomics.eu/MuG/wp-content/uploads/2016/05/MuG_Factsheet.pdf)

- Newsletter archive:

<http://www.multiscalegenomics.eu/MuG/about-mug/newsletters/>

- MuG visual identity and acknowledgement kit:

<https://vre.multiscalegenomics.eu/help/ackn.php>

Finally, social media have been a key tool to enhance both dissemination and communication. MuG has active accounts in the following social media networks:

- YouTube channel:

[https://www.youtube.com/channel/UCzDZ3b80ecK24S\\_m2oKq6-g/videos?view\\_as=public](https://www.youtube.com/channel/UCzDZ3b80ecK24S_m2oKq6-g/videos?view_as=public)

- Twitter: [https://twitter.com/MuG\\_genomics](https://twitter.com/MuG_genomics)
- LinkedIn: <https://www.linkedin.com/groups/8572323/>

## 8 OPEN ACCESS REPOSITORIES

To ensure long-term public availability and findability of all outputs generated by the MuG project, all publications (peer-reviewed or not – including project deliverables, milestones, etc), data and technical documentation generated by the project have been deposited in public repositories.

- **Peer-reviewed publications:** all partner institutions have agreements with open access repositories in which MuG published papers have been deposited, e.g. [HAL archives-ouvertes](#) (CNRS), [UPCommons](#) (BSC), [Deposit Digital UB](#) (IRB Barcelona). The publication of pre-prints (e.g. [biorxiv.org](#)) has also been favoured by partners.
- **Data repositories:** data sets generated within the project have been deposited in open access repositories according to the policies defined in the MuG data management plan ([D4.2](#)).
- **Other publications and outputs:** All publications and materials generated by MuG are accessible for download from the MuG website. IRB Barcelona as coordinator has agreed to maintain the MuG domain beyond the end of the MuG 3-year grant period. However, in order to guarantee long-term availability of the generated publications and to facilitate its findability, all publications are also being deposited in the Zenodo MuG community: (<https://zenodo.org/communities/mug/?page=1&size=20>).
- **Software:** Software and documentation is stored in the MuG Github repository: <https://github.com/Multiscale-Genomics>

