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Supporting information for article:

Crystal structures of *Lymphocytic choriomeningitis virus* endonuclease domain complexed with diketo acid ligands

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Figure S1 Alignment of 245 sequences of *Arenaviridae* L ENDO domain prepared with ESript.

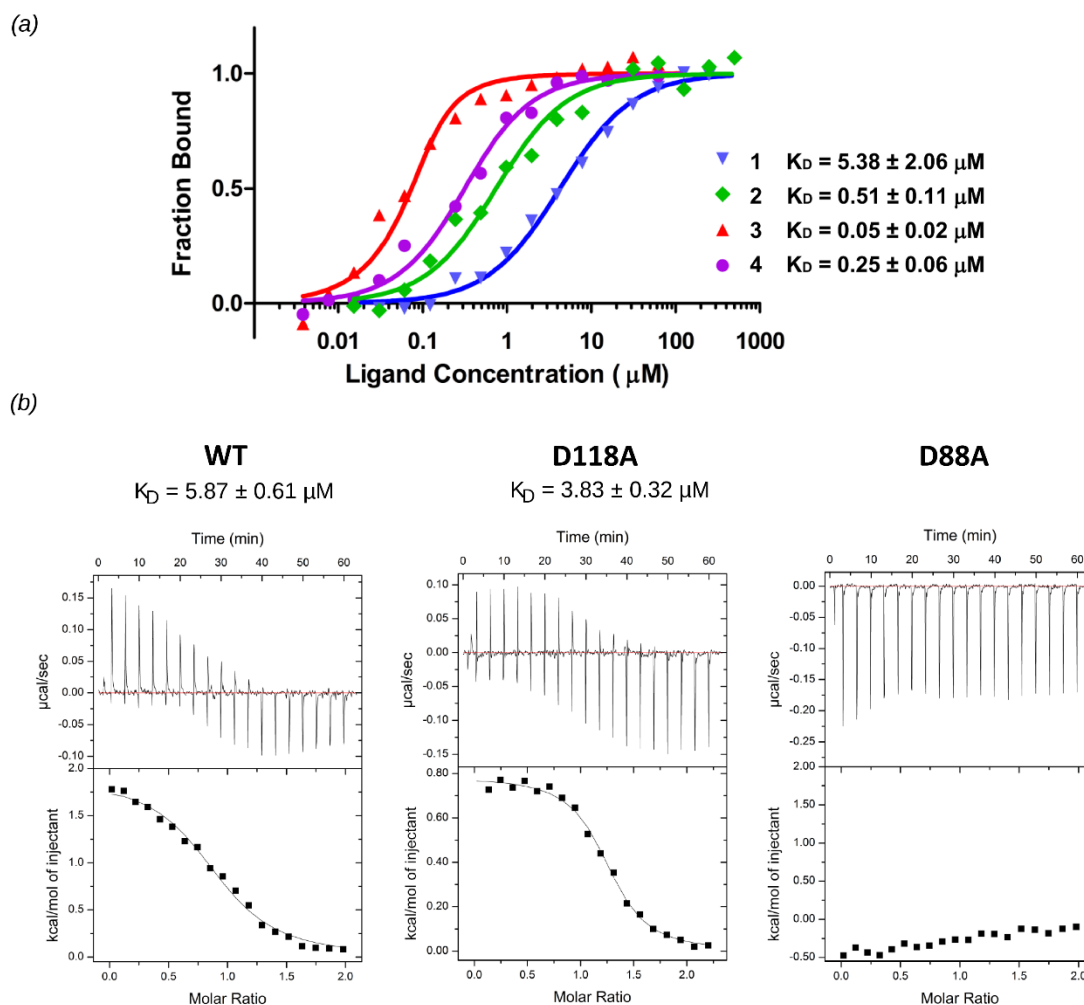


Figure S2 (a) Representative binding curves for ENDO-WT to DPBA (**1**), L-742,001 (**2**), **3** and **4**, determined by microscale thermophoresis (MST). Fraction Bound represents the baseline corrected normalized fluorescence for each compound with normalization to 1 for amplitude. (b) Representative ITC titrations for ENDO proteins with DPBA (**1**) at 25 °C as a function of the molar ratio of ligand to protein. The upper panel shows the ITC raw data and the lower panel presents the integrated heats of each injection. Binding isotherms were fitted to the raw data using one-site binding model to determine the K_D .

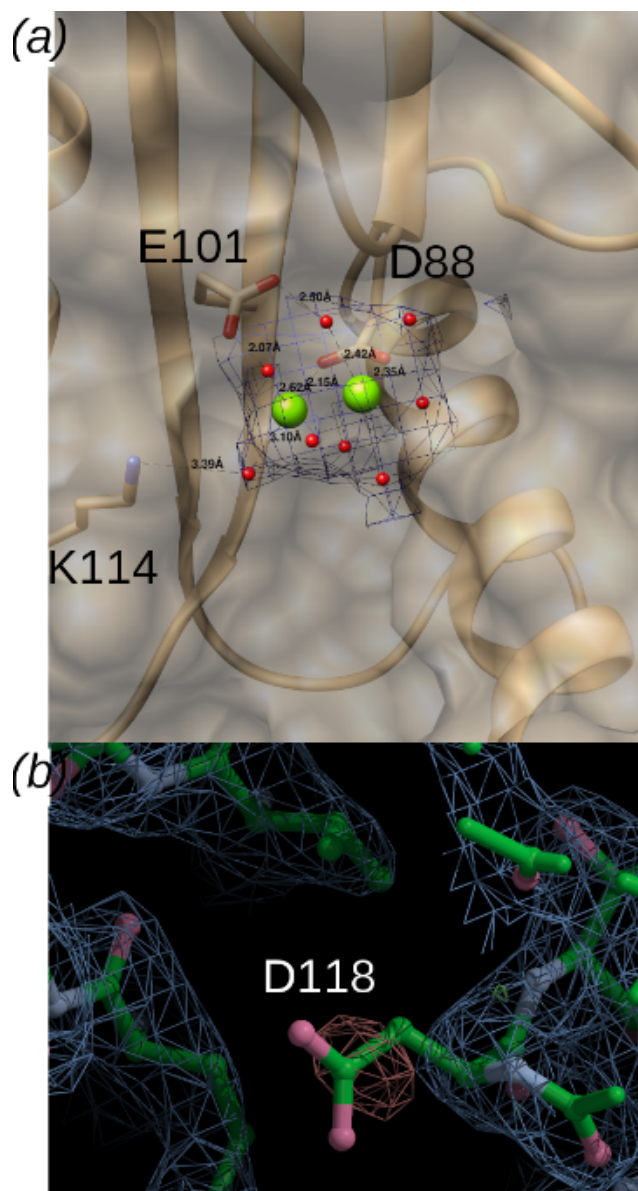


Figure S3 (a) Zoom of the catalytic site of the holo-enzyme structure of the LCMV endonuclease with the 2 catalytic Mg^{2+} coordinated by D88 and a network of water molecules. (b) $2Fo-Fc$ Map of the D118A mutant. Overall structure of the endonuclease LCMV is not affected by this mutation.

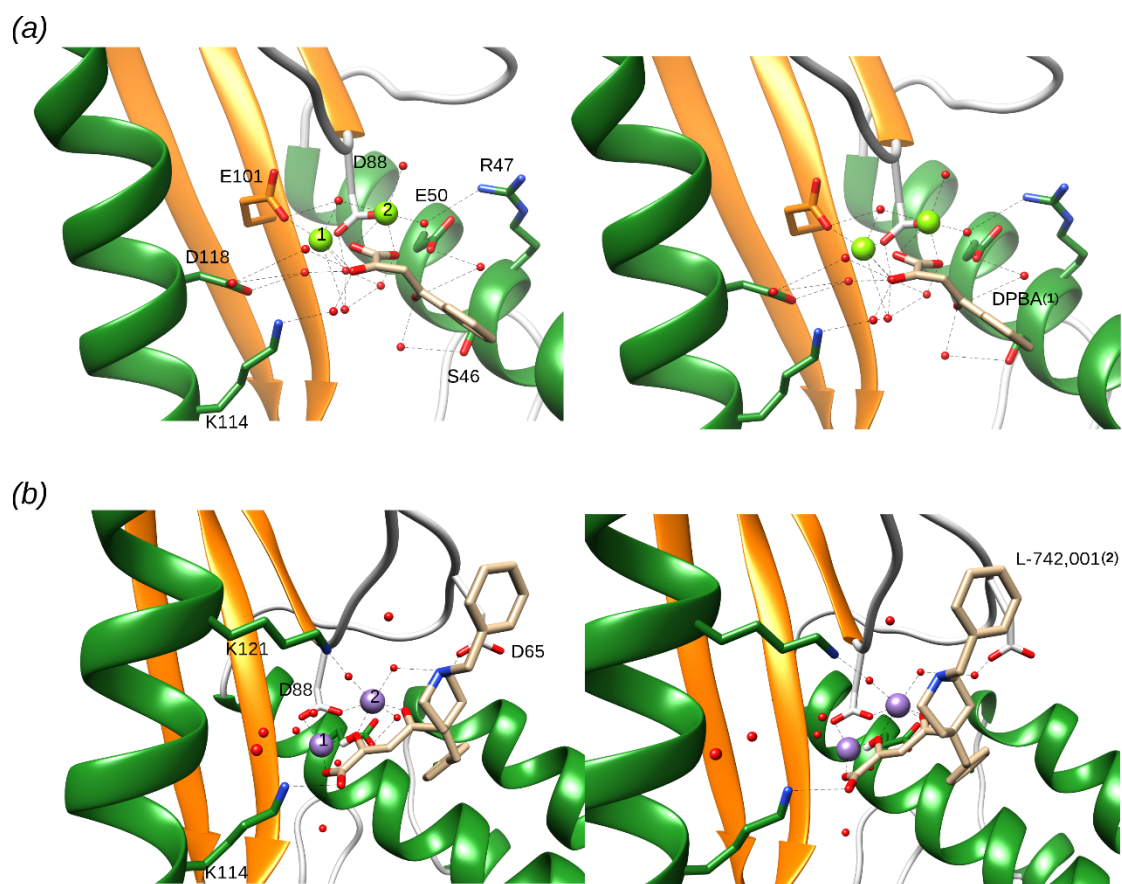


Figure S4 Zoom of the catalytic site showing the intense water ions molecule catalytic residues coordination in stereo view. Crystal structures of ENDO protein in complex with (a) DPBA (**1**) and (b) L-742,001 (**2**). Structures are represented as ribbon with helices in green and strands in gold while the compound is represented in sticks. Mg²⁺ and Mn²⁺ ions are represented as light green and purple spheres respectively.

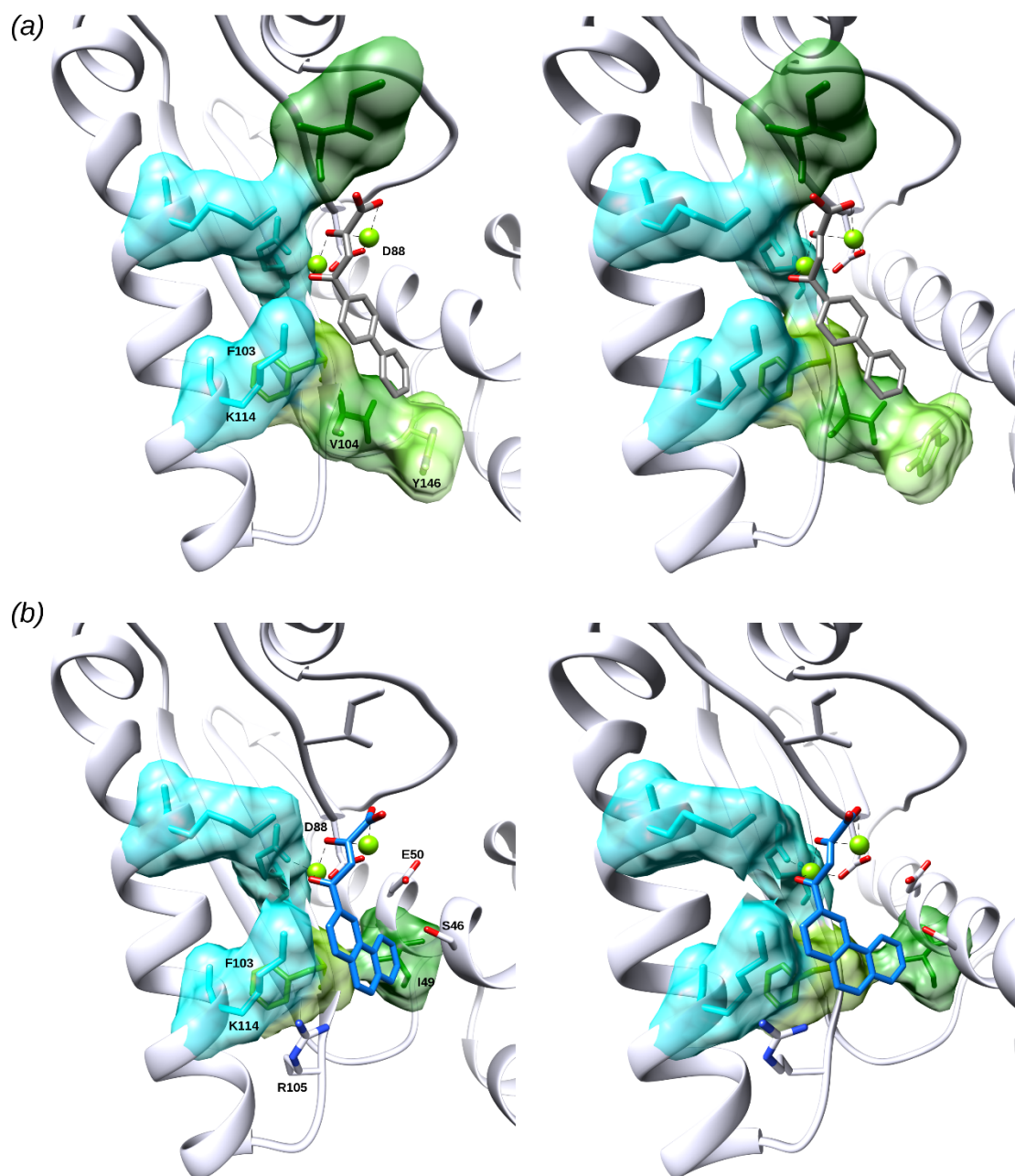


Figure S5 Zoom of best pose of molecules **3** (a) and **4** (b) in stereo view. Residues and their surface involved in binding are coloured according to hydrophobicity from cyan (the least) to green (the most). Structures are represented as ribbon while the compound is represented in sticks. Mg²⁺ ions are represented as light green spheres.

Table S1 Arenaviridae Endonuclease domain L NCBI reference number.

Supplementary Table1 : Liste of L protein sequences used in bioinformatic analysis.	
N°	NCBI GI Number
1	gi 221272070 sp Q6XQI9.2 L_ALLVP/1-203 RecName: Full=RNA-directed RNA polymerase L
2	gi 156103994 gb ABU39911.1 /1-203 L polymerase [Pichinde mammarenavirus]
3	gi 16226196 gb AAL16099.1 AF427517_1/1-203 L polymerase [Pichinde mammarenavirus]
4	gi 48696026 ref YP_025093.1 /1-203 L protein [Pital mammarenavirus]
5	gi 186909558 gb ACC94304.1 /1-206L protein [Tamiami mammarenavirus]
6	gi 189026273 ref YP_001936024.1 /1-203L protein [Flexal mammarenavirus]
7	gi 221272054 sp B2MW51.1 L_PARVP/1-203 RecName: Full=RNA-directed RNA polymerase L
8	gi 62766434 gb AA939344.1 /1-203 RNA-dependent RNA polymerase [Bear Canyon mammarenavirus]
9	gi 33868628 gb AAQ55263.1 /1-209L protein [Sabia mammarenavirus]
10	gi 164519642 gb AAP44542.2 /1-209 L protein [Sabia mammarenavirus]
11	gi 164607197 ref YP_001649214.1 /1-204 L protein [Oliveros mammarenavirus]
12	gi 62766431 gb AA939342.1 /1-205 RNA-dependent RNA polymerase [Amapari mammarenavirus]
13	gi 48095770 gb AAT40454.1 /1-205 L protein [Machupo mammarenavirus]
14	gi 221272059 sp B2C4J3.1 L_CHAVB/1-205 RecName: Full=RNA-directed RNA polymerase L
15	gi 81941884 sp Q6IUF8.1 L_MACHU/1-205 RecName: Full=RNA-directed RNA polymerase L
16	gi 48095764 gb AAT40450.1 /1-205 L protein [Machupo mammarenavirus]
17	gi 34365537 ref NP_899215.1 /1-205 L protein [Machupo mammarenavirus]
18	gi 221272060 sp B2MW49.1 L_LATVB/1-204 RecName: Full=RNA-directed RNA polymerase L
19	gi 927338583 gb ALE15102.1 /1-205 RNA-directed RNA polymerase L [Guanarito mammarenavirus]
20	gi 927338568 gb ALE15093.1 /1-205 RNA-directed RNA polymerase L [Guanarito mammarenavirus]
21	gi 927338578 gb ALE15099.1 /1-205 RNA-directed RNA polymerase L [Guanarito mammarenavirus]
22	gi 927338573 gb ALE15096.1 /1-205 RNA-directed RNA polymerase L [Guanarito mammarenavirus]
23	gi 927338558 gb ALE15087.1 /1-205 RNA-directed RNA polymerase L [Guanarito mammarenavirus]
24	gi 607235393 gb AHW46357.1 /1-205 RNA-dependent RNA polymerase [Tacaribe mammarenavirus]
25	gi 335149 gb AAA47901.1 /1-205 L protein [Tacaribe mammarenavirus]
26	gi 164519657 gb AAP44555.2 /1-205 L protein [Cupixi mammarenavirus]
27	gi 695315673 gb AIT17761.1 /1-204 polymerase [Lassa mammarenavirus]
28	gi 927338588 gb ALE15105.1 /1-205 RNA-directed RNA polymerase L [Junin mammarenavirus]
29	gi 695315073 gb AIT17551.1 /1-204 polymerase [Lassa mammarenavirus]
30	gi 316308864 gb ADU56613.1 /1-204 polymerase [Lassa mammarenavirus]
31	gi 695315039 gb AIT17543.1 /1-204 polymerase [Lassa mammarenavirus]
32	gi 695315003 gb AIT17537.1 /1-204 polymerase [Lassa mammarenavirus]
33	gi 695314650 gb AIT17457.1 /1-204 polymerase [Lassa mammarenavirus]
34	gi 927338593 gb ALE15108.1 /1-205 RNA-directed RNA polymerase L [Junin mammarenavirus]
35	gi 695315187 gb AIT17579.1 /1-204 polymerase [Lassa mammarenavirus]
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37	gi 695315172 gb AIT17575.1 /1-204 polymerase [Lassa mammarenavirus]
38	gi 695314803 gb AIT17497.1 /1-204 polymerase [Lassa mammarenavirus]
39	gi 695315332 gb AIT17661.1 /1-204 polymerase [Lassa mammarenavirus]
40	gi 695314618 gb AIT17449.1 /1-204 polymerase [Lassa mammarenavirus]
41	gi 695315240 gb AIT17603.1 /1-204 polymerase [Lassa mammarenavirus]
42	gi 695315834 gb AIT17797.1 /1-204 polymerase [Lassa mammarenavirus]
43	gi 695315768 gb AIT17781.1 /1-204 polymerase [Lassa mammarenavirus]
44	gi 695315508 gb AIT17721.1 /1-204 polymerase [Lassa mammarenavirus]
45	gi 695315285 gb AIT17633.1 /1-204 polymerase [Lassa mammarenavirus]
46	gi 695315392 gb AIT17689.1 /1-204 polymerase [Lassa mammarenavirus]
47	gi 695315530 gb AIT17727.1 /1-204 polymerase [Lassa mammarenavirus]
48	gi 695315432 gb AIT17703.1 /1-204 polymerase [Lassa mammarenavirus]
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51	gi 927338598 gb ALE15111.1 /1-205 RNA-directed RNA polymerase L [Junin mammarenavirus]
52	gi 226374504 gb ACO52427.1 /1-205L protein [Junin mammarenavirus]
53	gi 695315246 gb AIT17607.1 /1-204 polymerase [Lassa mammarenavirus]
54	gi 695315354 gb AIT17673.1 /1-204 polymerase [Lassa mammarenavirus]
55	gi 695315622 gb AIT17751.1 /1-204 polymerase [Lassa mammarenavirus]
56	gi 695315749 gb AIT17777.1 /1-204 polymerase [Lassa mammarenavirus]
57	gi 695316024 gb AIT17835.1 /1-204 polymerase [Lassa mammarenavirus]
58	gi 695315316 gb AIT17653.1 /1-204 polymerase [Lassa mammarenavirus]
59	gi 695315798 gb AIT17789.1 /1-204 polymerase [Lassa mammarenavirus]
60	gi 316308876 gb ADU56621.1 /1-204 polymerase [Lassa mammarenavirus]
61	gi 695314511 gb AIT17433.1 /1-204 polymerase [Lassa mammarenavirus]
62	gi 695315375 gb AIT17681.1 /1-204 polymerase [Lassa mammarenavirus]
63	gi 695314632 gb AIT17453.1 /1-204 polymerase [Lassa mammarenavirus]
64	gi 695314771 gb AIT17489.1 /1-204 polymerase [Lassa mammarenavirus]
65	gi 695315155 gb AIT17571.1 /1-204 polymerase [Lassa mammarenavirus]
66	gi 695314974 gb AIT17531.1 /1-204 polymerase [Lassa mammarenavirus]
67	gi 328679015 gb AEB32435.1 /1-205 L protein [Junin mammarenavirus]
68	gi 52222820 gb AAU34183.1 /1-205 L protein [Junin mammarenavirus]
69	gi 695313836 gb AIT17283.1 /1-204 polymerase [Lassa mammarenavirus]
70	gi 399125347 gb AFP21519.1 /1-204 large RNA-dependent RNA polymerase [Lujo mammarenavirus]
71	gi 695313220 gb AIT17137.1 /1-204 polymerase [Lassa mammarenavirus]

72	gi 695313464 gb AIT17199.1 /1-204 polymerase [Lassa mammarenavirus]
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74	gi 567840457 gb AHC95551.1 /1-206 L polymerase [Lassa mammarenavirus]
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93	gi 49037379 gb AAT48998.1 /1-204 L protein [Lassa mammarenavirus]
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96	gi 695313531 gb AIT17215.1 /1-204 polymerase [Lassa mammarenavirus]
97	gi 695313149 gb AIT17125.1 /1-204 polymerase [Lassa mammarenavirus]
98	gi 695314109 gb AIT17343.1 /1-204 polymerase [Lassa mammarenavirus]
99	gi 374095908 gb AEY85215.1 /1-204 L protein [Lassa mammarenavirus]
100	gi 81919817 sp O09705.1 L_LASSJ/1-204 RecName: Full=RNA-directed RNA polymerase L
101	gi 316308870 gb ADU56617.1 /1-204 polymerase [Lassa mammarenavirus]
102	gi 695313387 gb AIT17179.1 /1-204 polymerase [Lassa mammarenavirus]
103	gi 316308917 gb ADU56645.1 /1-204 polymerase [Lassa mammarenavirus]
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105	gi 695314003 gb AIT17321.1 /1-204 polymerase [Lassa mammarenavirus]
106	gi 695314315 gb AIT17383.1 /1-204 polymerase [Lassa mammarenavirus]
107	gi 695313855 gb AIT17287.1 /1-204 polymerase [Lassa mammarenavirus]
108	gi 695313434 gb AIT17191.1 /1-204 polymerase [Lassa mammarenavirus]
109	gi 695313820 gb AIT17279.1 /1-204 polymerase [Lassa mammarenavirus]
110	gi 695315264 gb AIT17619.1 /1-204 polymerase [Lassa mammarenavirus]
111	gi 258489191 gb ACV72587.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
112	gi 115383199 gb ABI96821.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
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114	gi 695313870 gb AIT17291.1 /1-204 polymerase [Lassa mammarenavirus]
115	gi 1032562909 gb ANH09748.1 /1-204 polymerase [Lassa mammarenavirus]
116	gi 37729911 gb AAO59509.1 /1-204 polymerase [Lassa mammarenavirus]
117	gi 695313566 gb AIT17223.1 /1-204 polymerase [Lassa mammarenavirus]
118	gi 383212122 dbj BAM08950.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
119	gi 695313928 gb AIT17297.1 /1-204 polymerase [Lassa mammarenavirus]
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126	gi 115383205 gb ABI96825.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
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128	gi 383385889 gb AFH08746.1 /1-204 polymerase [Lymphocytic choriomeningitis mammarenavirus]
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130	gi 567840446 gb AHC95544.1 /1-204 L polymerase [Lassa mammarenavirus]
131	gi 258489184 gb ACV72583.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
132	gi 162945389 gb ABY20732.1 /1-204 RNA-dependent RNA polymerase [Dandenong virus]
133	gi 331369 gb AAA66591.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
134	gi 158726685 gb ABW80746.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
135	gi 385140458 gb AFI42020.1 /1-204 large RNA-dependent RNA polymerase protein [Lymphocytic choriomeningitis mammarenavirus]
136	gi 258489195 gb ACV72589.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
137	gi 749717247 ref YP_009116793.1 /1-204 polymerase [Gairo virus]
138	gi 86440169 gb ABC96004.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
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142	gi 290791119 gb ADD63340.1 /1-204 L [Merino Walk mammarenavirus]
143	gi 316997267 dbj BAJ52730.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
144	gi 1032562918 gb ANH09754.1 /1-204 polymerase [Lassa mammarenavirus]
145	gi 258489172 gb ACV72577.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
146	gi 169641155 gb ACA61300.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
147	gi 115383211 gb ABI96829.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
148	gi 37955037 gb AAO59515.1 /1-204 polymerase [Lassa mammarenavirus]
149	gi 1032562924 gb ANH09758.1 /1-204 polymerase [Lassa mammarenavirus]
150	gi 85542281 gb ABC71137.1 /1-204 L protein [Mopeia mammarenavirus]

151	gi 308097145 gb ADO14126.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
152	gi 356491222 ref YP_004933733.1 /1-204 L gene product [Luna mammarenavirus]
153	gi 407326379 dbj BAM45327.1 /1-204 L protein [Luna mammarenavirus]
154	gi 570339339 gb AHE76152.1 /1-204 RNA-dependent RNA polymerase [Loie River virus]
155	gi 258489202 gb ACV72593.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
156	gi 570339336 gb AHE76150.1 /1-204 RNA-dependent RNA polymerase [Loie River virus]
157	gi 404312015 dbj BAM42785.1 /1-204 RNA-dependent RNA polymerase [Luna mammarenavirus]
158	gi 349731813 dbj BAL03418.1 /1-204 RNA-dependent RNA polymerase [Luna mammarenavirus]
159	gi 1032562927 gb ANH09760.1 /1-204 polymerase [Lassa mammarenavirus]
160	gi 770340473 gb AJW68782.1 /1-204 L protein [Rat arenavirus 1]
161	gi 821351021 gb AKH39838.1 /1-204 RNA-dependent RNA polymerase [Mariental virus]
162	gi 383212119 dbj BAM08948.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
163	gi 258489198 gb ACV72591.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
164	gi 425867865 gb AFY05541.1 /1-204 polymerase RDRP [Mopeia Lassa virus reassortant 29]
165	gi 258489176 gb ACV72579.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
166	gi 399769798 dbj BAM36053.1 /1-204 L protein [Luna mammarenavirus]
167	gi 258489180 gb ACV72581.1 /1-204 L protein [Lymphocytic choriomeningitis mammarenavirus]
168	gi 570339333 gb AHE76148.1 /1-204 RNA-dependent RNA polymerase [Cardamones virus]
169	gi 255237731 ref YP_003090217.1 /1-204 polymerase [Morogoro virus]
170	gi 570339330 gb AHE76146.1 /1-204 RNA-dependent RNA polymerase [Cardamones virus]
171	gi 89903003 ref YP_516229.1 /1-204 L protein [Mobala mammarenavirus]
172	gi 123827694 sp Q27YE.1 L_IPPYV/1-204 RecName: Full=RNA-directed RNA polymerase L
173	gi 821492491 gb AKH49109.1 /1-207 L polymerase [unidentified Reptarenavirus]
174	gi 821492261 gb AKH49019.1 /1-207 L polymerase [unidentified Reptarenavirus]
175	gi 459996700 gb AGH06042.1 /1-207 L polymerase [ROUT virus]
176	gi 821492218 gb AKH48997.1 /1-207 L polymerase [unidentified Reptarenavirus]
177	gi 821492224 gb AKH49001.1 /1-207 L polymerase [unidentified Reptarenavirus]
178	gi 821492010 gb AKH48903.1 /1-207 L polymerase [unidentified Reptarenavirus]
179	gi 821492100 gb AKH48953.1 /1-207 L polymerase [unidentified Reptarenavirus]
180	gi 821492015 gb AKH48905.1 /1-207 L polymerase [unidentified Reptarenavirus]
181	gi 821492321 gb AKH49045.1 /1-204 L polymerase [unidentified Reptarenavirus]
182	gi 821492461 gb AKH49099.1 /1-207 L polymerase [unidentified Reptarenavirus]
183	gi 821492279 gb AKH49027.1 /1-207 L polymerase [unidentified Reptarenavirus]
184	gi 821492234 gb AKH49005.1 /1-207 L polymerase [unidentified Reptarenavirus]
185	gi 821492248 gb AKH49013.1 /1-207 L polymerase [unidentified Reptarenavirus]
186	gi 846119579 gb AKN10715.1 /1-207 RdRp [Aurora borealis virus]
187	gi 821492199 gb AKH48987.1 /1-207 L polymerase [unidentified Reptarenavirus]
188	gi 821492373 gb AKH49063.1 /1-207 L polymerase [unidentified Reptarenavirus]
189	gi 846119307 gb AKN10698.1 /1-207 RdRp [Suri Vanera virus]
190	gi 821492367 gb AKH49059.1 /1-207 L polymerase [unidentified Reptarenavirus]
191	gi 821492032 gb AKH48915.1 /1-207 L polymerase [unidentified Reptarenavirus]
192	gi 821492207 gb AKH48991.1 /1-207 L polymerase [unidentified Reptarenavirus]
193	gi 821492216 gb AKH48996.1 /1-207 L polymerase [unidentified Reptarenavirus]
194	gi 821492018 gb AKH48907.1 /1-207 L polymerase [unidentified Reptarenavirus]
195	gi 846119216 gb AKN10692.1 /1-207 RdRp [Aurora borealis virus]
196	gi 821492282 gb AKH49029.1 /1-207 L polymerase [unidentified Reptarenavirus]
197	gi 821492343 gb AKH49051.1 /1-207 L polymerase [unidentified Reptarenavirus]
198	gi 821492295 gb AKH49035.1 /1-207 L polymerase [unidentified Reptarenavirus]
199	gi 821492441 gb AKH49091.1 /1-207 L polymerase [unidentified Reptarenavirus]
200	gi 821492421 gb AKH49083.1 /1-207 L polymerase [unidentified Reptarenavirus]
201	gi 821492165 gb AKH48975.1 /1-201 L polymerase [unidentified Reptarenavirus]
202	gi 821492076 gb AKH48941.1 /1-207 L polymerase [unidentified Reptarenavirus]
203	gi 821492450 gb AKH49096.1 /1-207 L polymerase [unidentified Reptarenavirus]
204	gi 821492105 gb AKH48955.1 /1-207 L polymerase [unidentified Reptarenavirus]
205	gi 821492042 gb AKH48921.1 /1-207 L polymerase [unidentified Reptarenavirus]
206	gi 821492290 gb AKH49033.1 /1-207 L polymerase [unidentified Reptarenavirus]
207	gi 821492426 gb AKH49085.1 /1-207 L polymerase [unidentified Reptarenavirus]
208	gi 821491990 gb AKH48895.1 /1-207 L polymerase [unidentified Reptarenavirus]
209	gi 821492210 gb AKH48993.1 /1-207 L polymerase [unidentified Reptarenavirus]
210	gi 821492110 gb AKH48957.1 /1-206 L polymerase [unidentified Reptarenavirus]
211	gi 821492258 gb AKH49017.1 /1-206 L polymerase [unidentified Reptarenavirus]
212	gi 821492244 gb AKH49011.1 /1-207 L polymerase [unidentified Reptarenavirus]
213	gi 821492446 gb AKH49093.1 /1-207 L polymerase [unidentified Reptarenavirus]
214	gi 821492241 gb AKH49009.1 /1-207 L polymerase [unidentified Reptarenavirus]
215	gi 821491995 gb AKH48897.1 /1-207 L polymerase [unidentified Reptarenavirus]
216	gi 821492062 gb AKH48933.1 /1-206 L polymerase [unidentified Reptarenavirus]
217	gi 821492518 gb AKH49119.1 /1-207 L polymerase [unidentified Reptarenavirus]
218	gi 821492084 gb AKH48945.1 /1-207 L polymerase [unidentified Reptarenavirus]
219	gi 821492253 gb AKH49015.1 /1-207 L polymerase [unidentified Reptarenavirus]
220	gi 821492316 gb AKH49043.1 /1-207 L polymerase [unidentified Reptarenavirus]
221	gi 821492036 gb AKH48918.1 /1-207 L polymerase [unidentified Reptarenavirus]
222	gi 821492232 gb AKH49004.1 /1-207 L polymerase [unidentified Reptarenavirus]
223	gi 821492045 gb AKH48923.1 /1-207 L polymerase [unidentified Reptarenavirus]
224	gi 821492089 gb AKH48947.1 /1-207 L polymerase [unidentified Reptarenavirus]
225	gi 821492095 gb AKH48951.1 /1-207 L polymerase [unidentified Reptarenavirus]
226	gi 821492115 gb AKH48959.1 /1-207 L polymerase [unidentified Reptarenavirus]
227	gi 821492452 gb AKH49097.1 /1-207 L polymerase [unidentified Reptarenavirus]
228	gi 821492092 gb AKH48949.1 /1-207 L polymerase [unidentified Reptarenavirus]
229	gi 821492021 gb AKH48909.1 /1-207 L polymerase [unidentified Reptarenavirus]

230	gij821492264 gb AKH49021.1 /1-207 L polymerase [unidentified Reptarenavirus]
231	gij821492410 gb AKH49079.1 /1-207 L polymerase [unidentified Reptarenavirus]
232	gij821492274 gb AKH49025.1 /1-207 L polymerase [unidentified Reptarenavirus]
233	gij846119443 gb AKN10706.1 /1-207 RdRp [Hans Kompis virus]
234	gij821492073 gb AKH48939.1 /1-207 L polymerase [unidentified Reptarenavirus]
235	gij821492388 gb AKH49069.1 /1-207 L polymerase [unidentified Reptarenavirus]
236	gij821492000 gb AKH48899.1 /1-207 L polymerase [unidentified Reptarenavirus]
237	gij846119379 gb AKN10702.1 /1-207 RdRp [Tavallinen suomalainen mies virus]
238	gij821492039 gb AKH48919.1 /1-207 L polymerase [unidentified Reptarenavirus]
239	gij821492202 gb AKH48989.1 /1-207 L polymerase [unidentified Reptarenavirus]
240	gij821492477 gb AKH49103.1 /1-207 L polymerase [unidentified Reptarenavirus]
241	gij821492357 gb AKH49055.1 /1-207 L polymerase [unidentified Reptarenavirus]
242	gij821492301 gb AKH49037.1 /1-207 L polymerase [unidentified Reptarenavirus]
243	gij821492005 gb AKH48901.1 /1-207 L polymerase [unidentified Reptarenavirus]
244	gij821492486 gb AKH49107.1 /1-207 L polymerase [unidentified Reptarenavirus]
245	gij821492287 gb AKH49031.1 /1-207 L polymerase [unidentified Reptarenavirus]