



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:21 AM UTC

PDB ID : 7F0D / pdb_00007f0d
EMDB ID : EMD-31398
Title : Cryo-EM structure of Mycobacterium tuberculosis 50S ribosome subunit bound with clarithromycin
Authors : Zhang, W.; Sun, Y.; Gao, N.; Li, Z.
Deposited on : 2021-06-03
Resolution : 3.30 Å(reported)
Based on initial model : 5V7Q

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

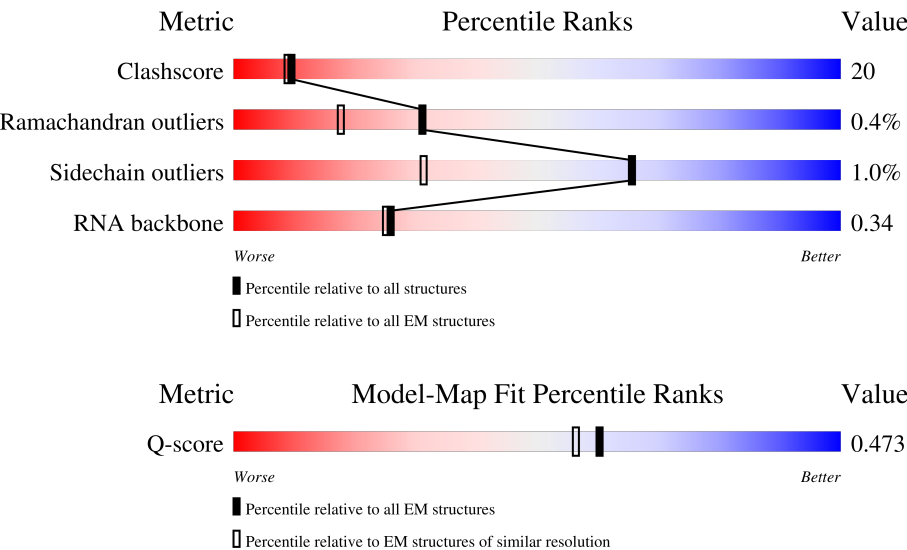
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	47	

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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	37	
6	6	80	
7	A	3138	
8	B	115	
9	C	280	
10	D	217	
11	E	223	
12	F	187	
13	G	179	
14	H	152	
15	J	147	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	

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Mol	Chain	Length	Quality of chain
29	X	64	16% 52% 45%
30	Y	77	14% 39% 45% 16%
31	Z	65	12% 38% 52% 9%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 94362 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	53	Total	C	N	O	0	0
			421	262	93	66		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	-	expression tag	UNP A0A3E0V5U0

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	45	Total	C	N	O	S	0	0
			345	214	60	66	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	1	0
			66978	29855	12345	21659	3119		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	170	Total	C	N	O	S	0	0
			1335	834	254	242	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	-	expression tag	UNP A0A045HTP7

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	142	Total	C	N	O	S	0	0
			1060	656	215	187	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	VAL	-	expression tag	UNP A0A654TTE7

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	98	Total	C	N	O		0	0
			742	472	136	134			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP P9WHC3

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	98	Total	C	N	O	0	0
			759	480	141	138		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	90	Total	C	N	O	S	0
			699	430	138	129	2	0

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	V	177	Total	C	N	O		0
			1319	822	243	254		0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	74	Total	C	N	O	0	0
			546	336	111	99		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	X	63	Total	C	N	O	S	0
			476	289	101	81	5	0

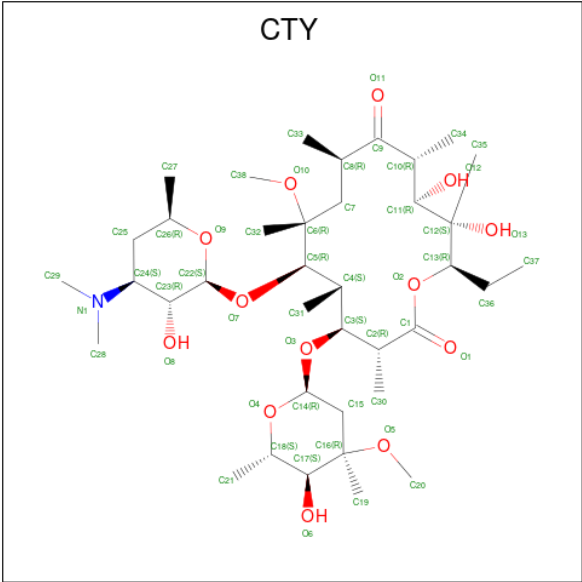
- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	65	Total	C	N	O	S	0
			541	331	106	103	1	0

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	59	Total	C	N	O	0	0
			476	293	101	82		

- Molecule 32 is CLARITHROMYCIN (CCD ID: CTY) (formula: $C_{38}H_{69}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	N	O	0
			52	38	1	13	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	3	Total	O	0
			3	3	

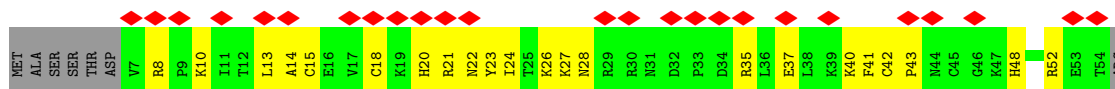
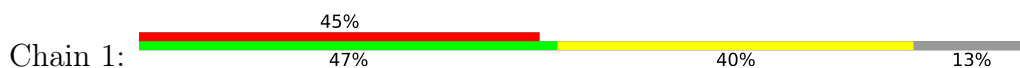
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

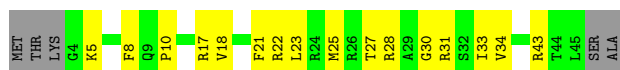
- Molecule 1: 50S ribosomal protein L32



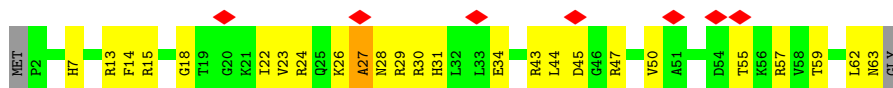
- Molecule 2: 50S ribosomal protein L33



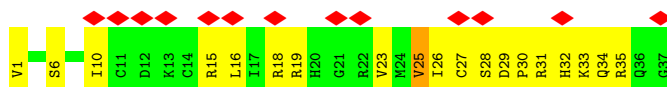
- Molecule 3: 50S ribosomal protein L34



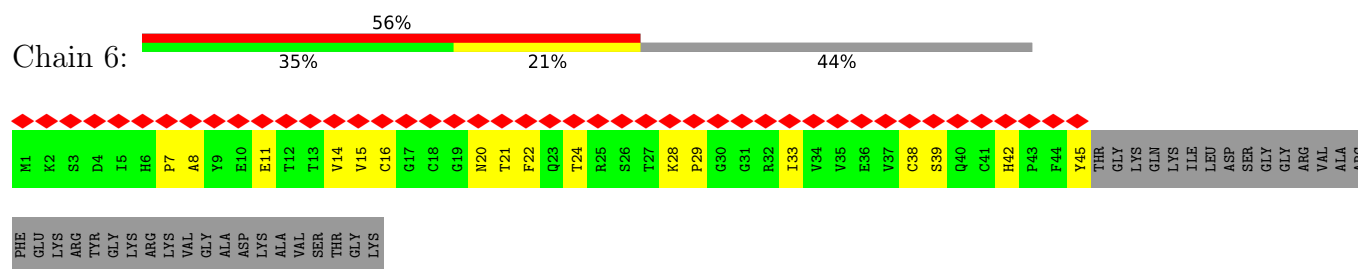
- Molecule 4: 50S ribosomal protein L35



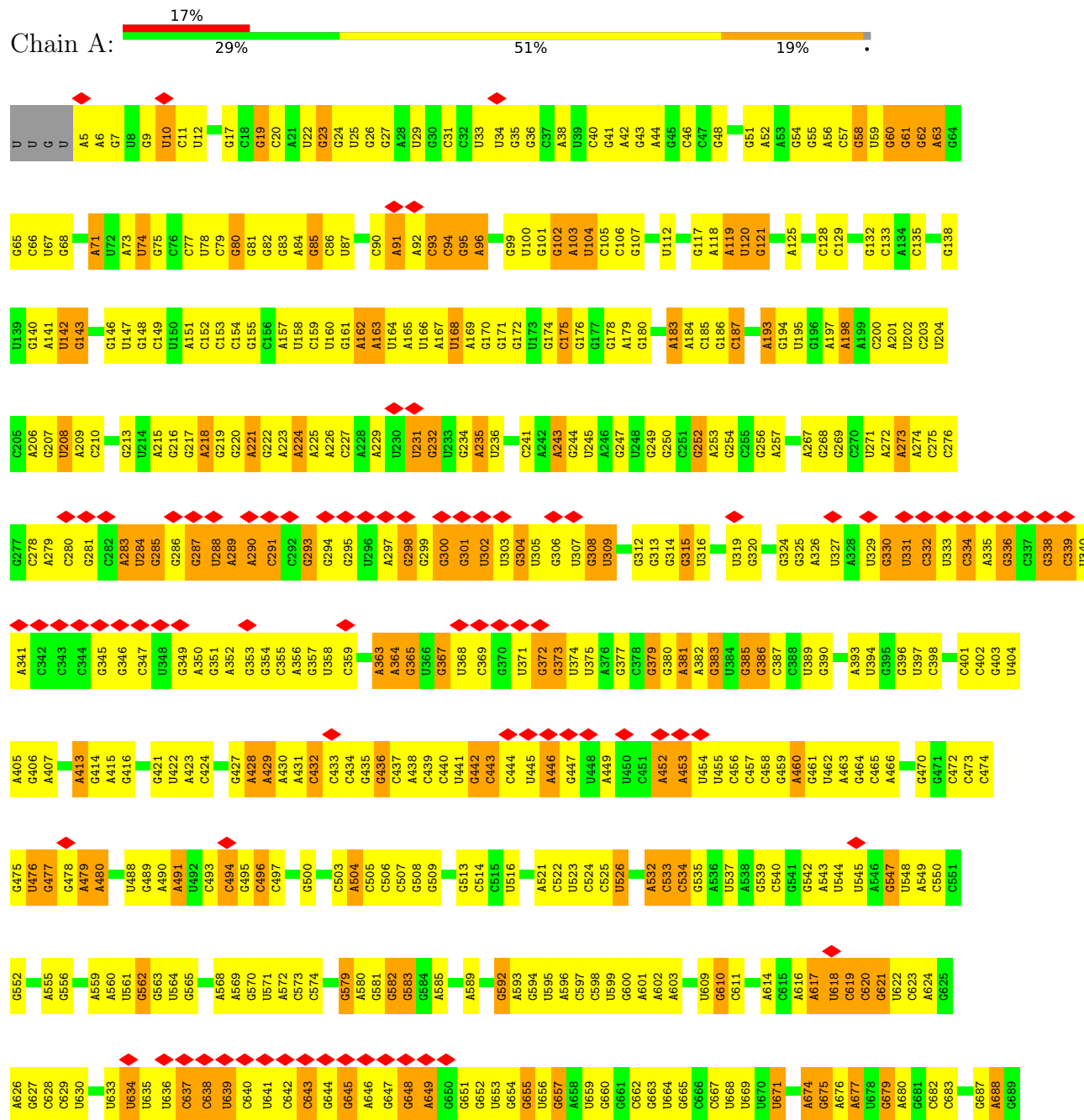
- Molecule 5: 50S ribosomal protein L36

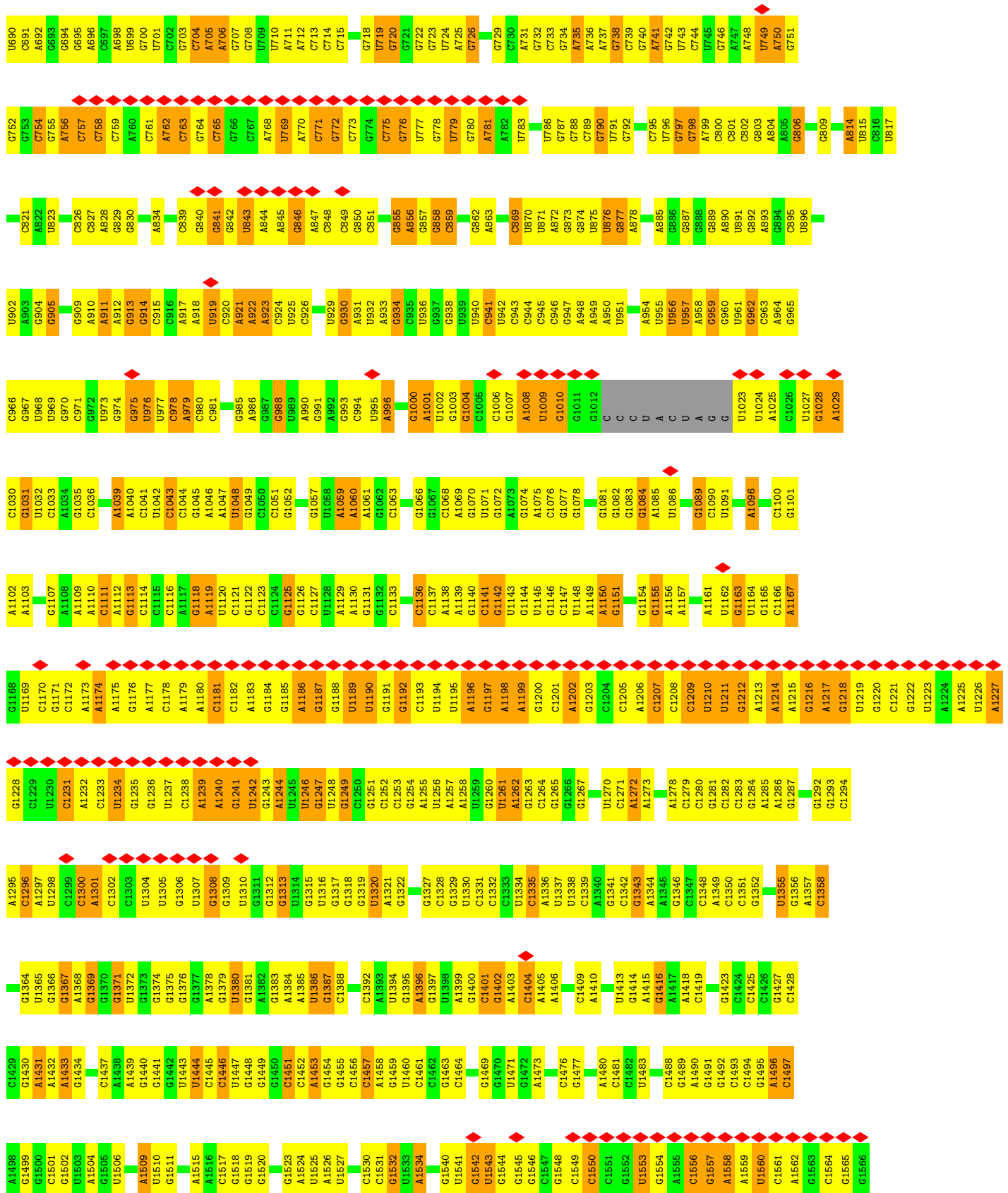


- Molecule 6: 50S ribosomal protein L31

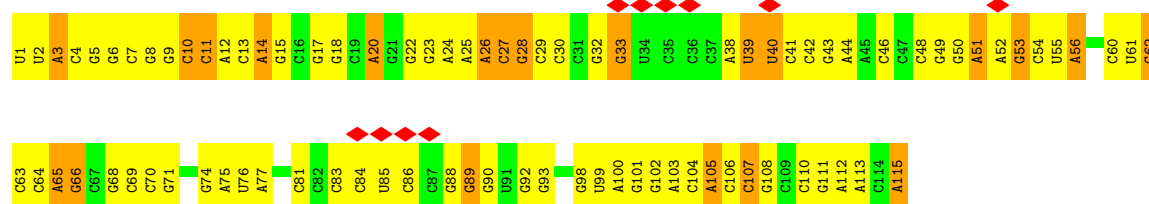


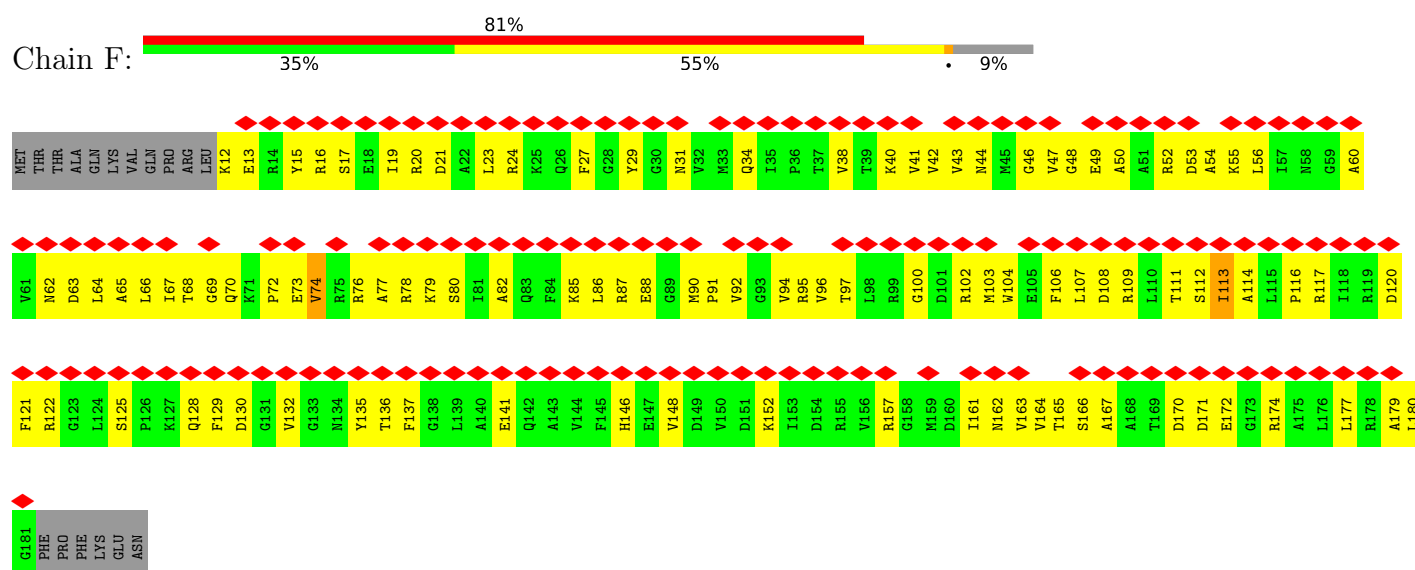
- Molecule 7: 23S rRNA



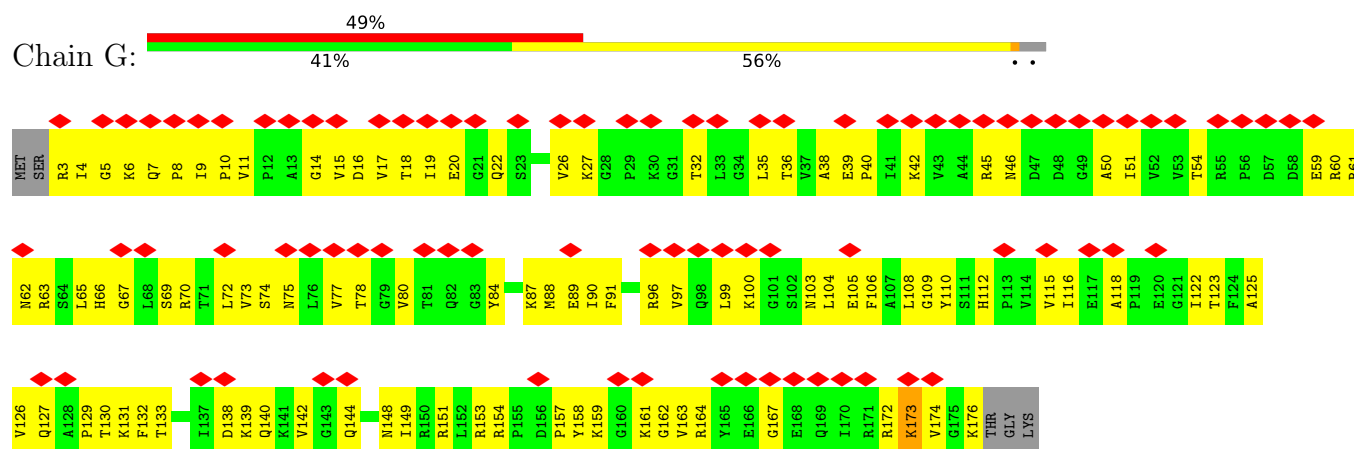


A2373	C2374	C2375	U2376	C2378	A2379	C2380	C2381	C2382	C2383	C2384	U2386	U2387	C2388	G2389	C2390	C2391	C2392	C2393	C2394	A2395	C2396	U2397	C2398	C2399	U2400	U2401	C2402	U2403	U2404	G2405	U2406	A2407	A2408	U2409	A2410	C2411	C2412	A2413	C2414	U2415	C2416	U2417	G2418	A2419	U2420	C2421	G2422	U2423	A2424	U2425	U2426	G2427	G2428	G2429	C2430	A2431	U2432		
C2309	C2310	C2311	U2312	C2313	A2314	A2317	C2318	A2319	A2320	C2321	U2322	U2323	G2324	U2328	U2329	G2330	G2333	U2334	U2335	C2336	G2337	C2338	U2339	A2340	C2341	C2342	G2343	U2344	U2345	U2346	G2347	U2348	G2349	U2350	A2351	C2352	G2353	A2354	U2355	A2356	G2357	C2358	U2359	G2360	G2361	C2362	A2363	G2364	A2365	C2366	U2367	G2368	U2369	G2370	A2371	A2372			
U2240	C2244	G2247	G2248	C2249	G2250	A2251	A2252	A2253	U2254	U2255	A2258	C2259	U2260	U2261	A2262	G2263	G2265	A2268	A2269	C2270	A2271	U2272	C2273	G2274	U2275	C2276	G2277	C2278	U2279	A2280	C2281	G2284	C2285	G2286	G2287	C2288	A2289	G2290	A2291	C2292	G2293	G2294	A2297	A2298	G2299	A2300	C2301	C2302	C2303	G2307	A2308								
A2166	G2167	U2168	U2169	G2170	G2171	C2172	G2173	A2174	A2175	U2176	U2177	U2178	C2179	U2180	U2181	U2182	G2183	U2184	C2185	G2186	U2189	A2190	A2191	G2192	U2193	U2194	C2200	U2201	G2202	A2203	A2204	C2205	A2208	U2209	G2210	G2211	C2212	G2213	U2214	A2215	A2216	C2217	G2218	A2219	C2220	A2226	A2227	G2228	U2229	G2230	U2233	C2234	A2239						
G2031	U2032	G2033	C2034	G2035	A2036	A2037	G2041	C2042	A2043	A2046	G2047	G2048	A2049	U2050	G2051	U2052	G2057	C2060	U2061	G2062	A2063	C2064	C2071	G2072	G2073	G2074	U2075	G2076	C2077	U2078	G2079	G2080	A2081	A2082	G2083	G2084	U2085	U2086	A2087	A2088	G2091	G2092	A2093	C2094	G2095	C2096	G2097	U2098	U2099	A2100	A2101	C2102	C2103						
C2104	G2105	C2106	A2107	A2108	G2109	G2110	G2111	U2112	G2113	A2114	A2115	G2116	C2117	G2118	G2119	A2120	G2121	A2122	A2123	U2124	U2125	U2126	A2127	G2128	C2129	C2130	C2131	C2132	C2133	A2134	A2138	A2139	C2140	G2141	G2142	C2143	G2144	G2145	U2146	C2147	G2148	U2149	A2150	A2151	C2152	U2153	A2154	U2155	A2156	A2157	C2158	C2159	A2160	U2161	C2162	C2163	U2164	A2165	
C1962	U1963	U1964	G1965	C1966	G1967	U1968	U1969	G1970	U1971	G1972	A1973	G1974	C1975	G1976	G1977	A1978	A1979	U1980	U1981	C1982	G1983	G1984	G1987	C1988	A1989	G1990	A1991	A1992	A1993	A1996	G1997	U1998	A2003	G2004	A2007	C2008	U2009	G2010	U2013	A2016	U2017	A2018	A2019	A2020	A2021	C2022	A2023	C2024	A2025	G2026	U2028								
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G1821	C1822	A1823	C1824	A1825	C1826	A1827	C1828	A1829	G1830	A1831	G1832	C1833	G1836	U1837	A1838	C1842	A1843	A1844	A1845	C1846	C1847	G1848	A1849	C1850	A1851	C1852	A1853	G1854	G1855	C1860	A1861	G1862	G1863	U1864	A1865	G1866	A1867	C1868	C1869	C1873	C1874	A1875	A1876	G1877	G1878	C1879	G1880	U1881	A1882	C1883	G1884	A1885	G1886	A1887	U1888				
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U1567	A1568	C1569	U1570	A1571	A1572	C1573	C1574	A1575	C1576	C1577	C1578	A1579	A1580	A1581	A1582	C1583	C1584	G1585	G1586	A1587	U1588	C1589	G1590	A1591	U1592	C1593	A1594	C1595	C1596	C1597	C1598	C1599	C1600	U1601	U1602	C1603	G1604	G1605	G1606	G1607	G1608	U1609	G1610	U1611	G1612	G1613	A1614	G1615	U1616	U1617	C1618	U1619	G1620	G1621	G1622	C1623	C1624	U1625	C1626

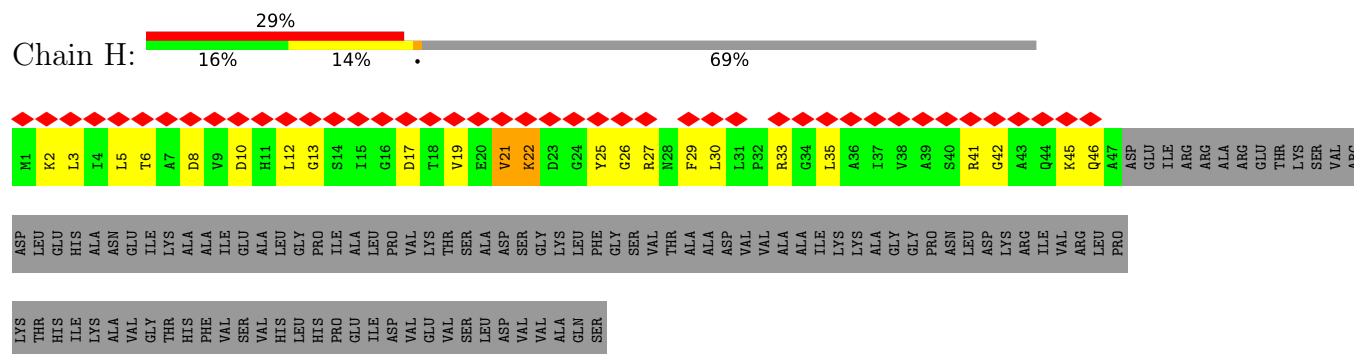




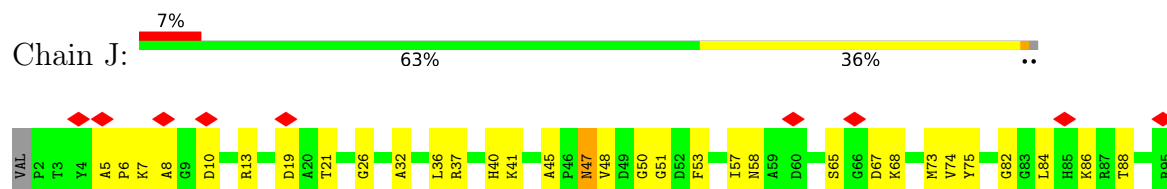
- Molecule 13: 50S ribosomal protein L6



- Molecule 14: 50S ribosomal protein L9

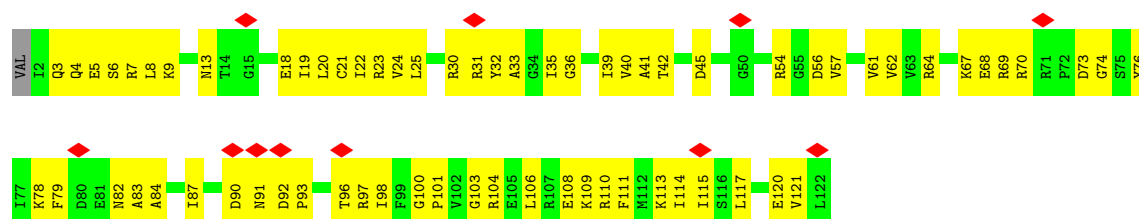
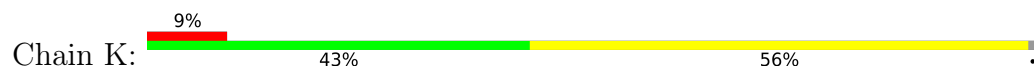


- Molecule 15: 50S ribosomal protein L13

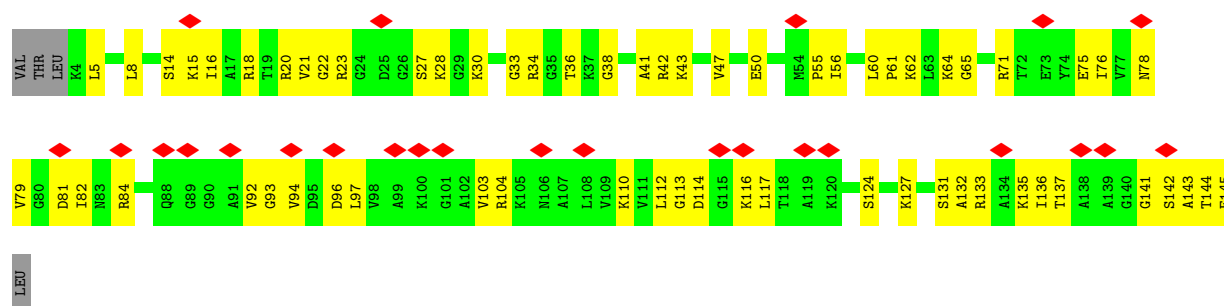




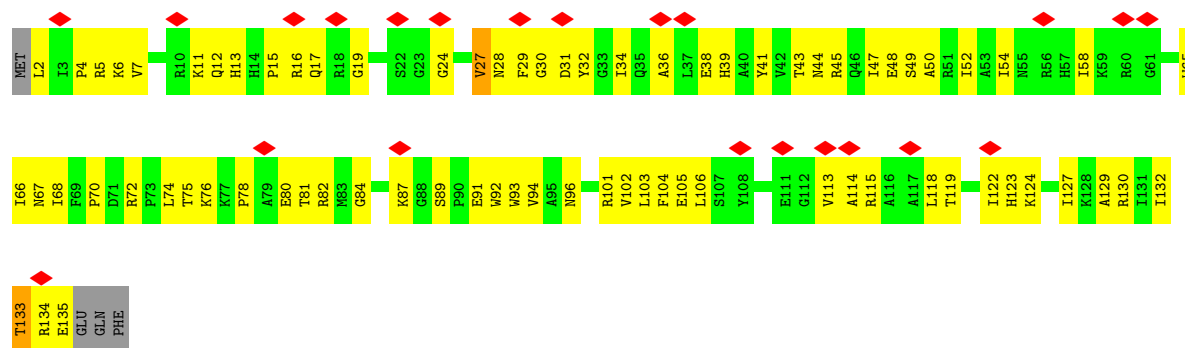
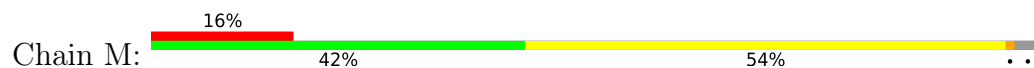
• Molecule 16: 50S ribosomal protein L14



• Molecule 17: 50S ribosomal protein L15

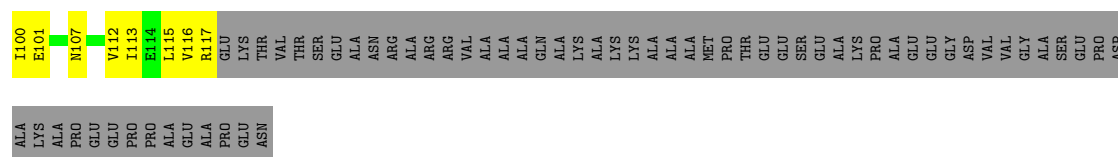


• Molecule 18: 50S ribosomal protein L16

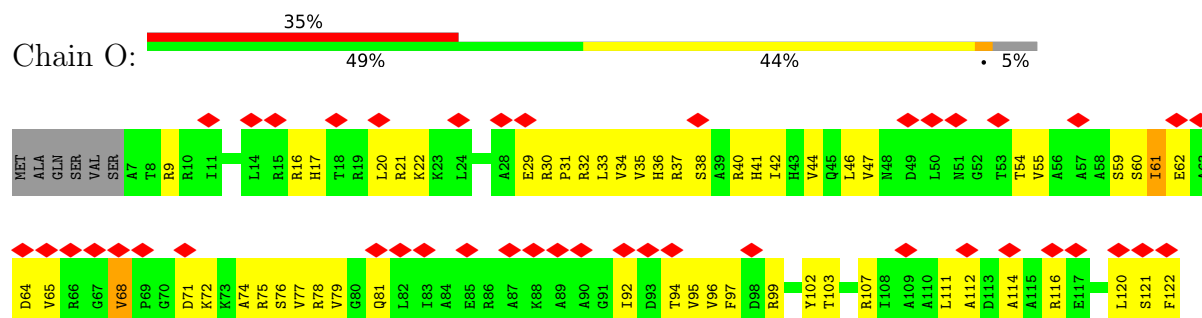


• Molecule 19: 50S ribosomal protein L17





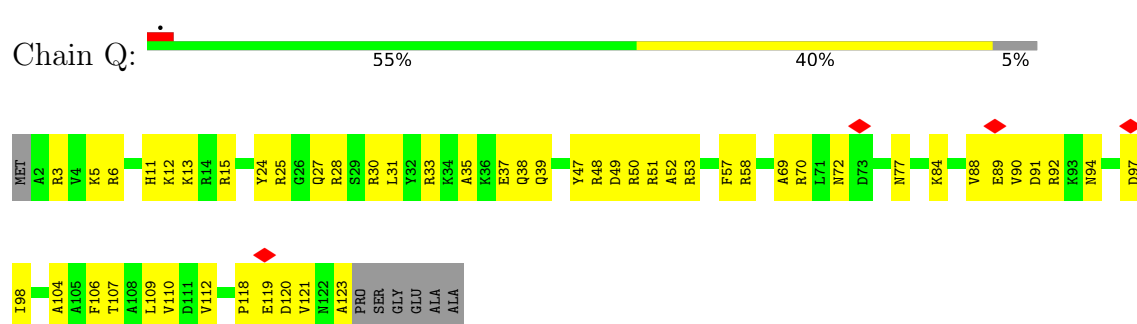
• Molecule 20: 50S ribosomal protein L18



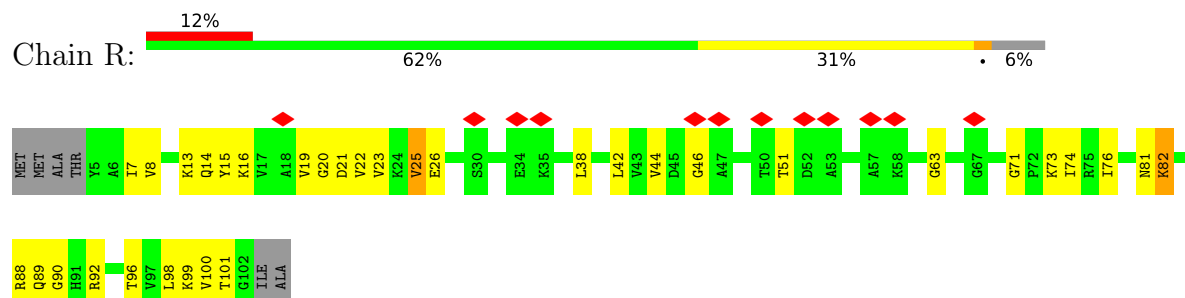
• Molecule 21: 50S ribosomal protein L19



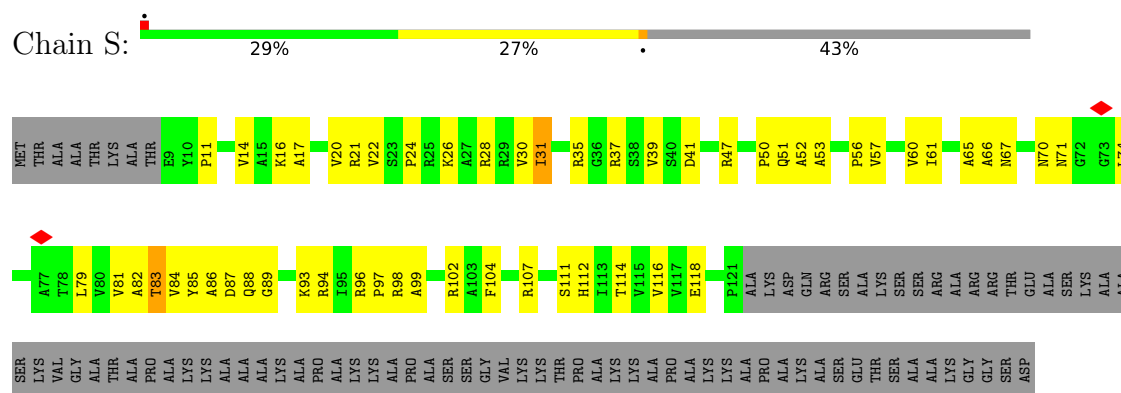
• Molecule 22: 50S ribosomal protein L20



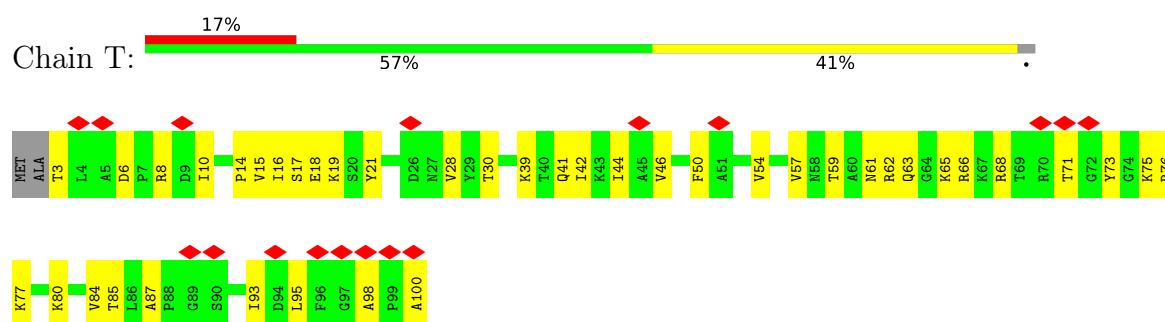
• Molecule 23: 50S ribosomal protein L21



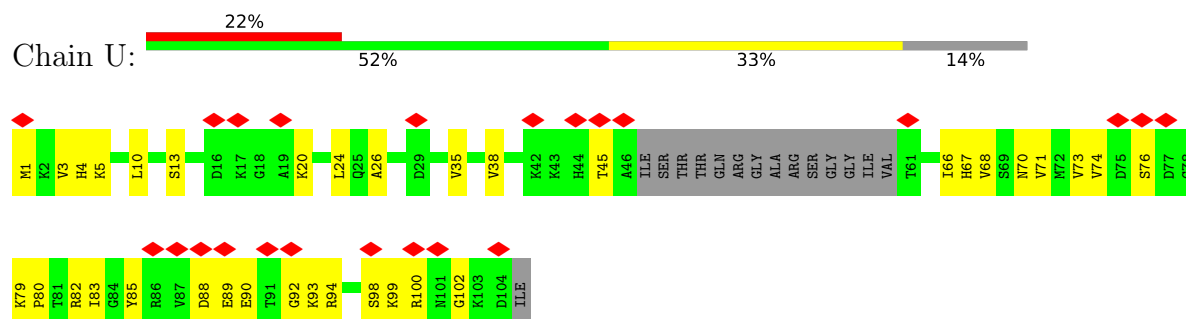
- Molecule 24: 50S ribosomal protein L22



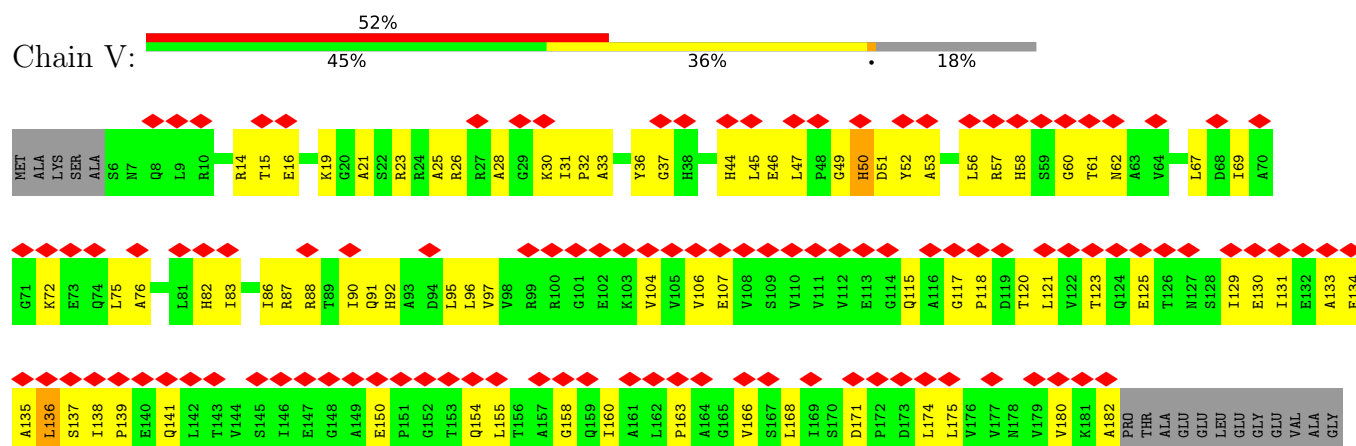
- Molecule 25: 50S ribosomal protein L23



- Molecule 26: 50S ribosomal protein L24



- Molecule 27: 50S ribosomal protein L25



ALA
GLU
GLU
ALA
LYS
GLU
GLU
ALA
ALA
VAL
SER
GLU
ALA
GLY
GLU
ALA
GLU
ALA
GLY
GLY
SER
GLU

• Molecule 28: 50S ribosomal protein L27

Chain W: 7% 45% 37% .. 14%

MET
ALA
HIS
LYS
LYS
GLY
ALA
SER
SER
VAL
SER
ARG
N12
G13
R14
D15
S16
A17
A18
Q19
R20
R25
Q29
V30
V31
E35
I36
L37
Q40
R41
G42
T43
K44
F45
H46
V49
N50
V51
D57
F60
A61
K62
T63
A64
V67
E68
F69
G70
I71
K72
R73
G74
R75
K76
T77
V78
S79
I80
R81
Q82
S83
T84
T85
ALA

• Molecule 29: 50S ribosomal protein L28

Chain X: 16% 52% 45% ..

M1
A2
A3
V4
I7
C8
G11
P12
G13
K16
S17
V18
S19
H20
S21
R24
T25
S26
R27
R28
H29
D30
V36
H37
A38
V39
T40
R41
P42
G43
Q44
H45
K46
K47
R48
L49
C55
A58
G59
K60
I61
T62
R63
GLY

• Molecule 30: 50S ribosomal protein L29

Chain Y: 14% 39% 45% 16%

MET
ALA
VAL
G4
V5
S6
P7
G8
E9
E12
L13
T14
E17
L18
R21
R22
R23
E24
E27
E28
L32
R33
F34
Q35
R36
A37
T38
G39
Q40
L41
H42
H43
H44
R45
R46
L47
R48
T49
V50
R51
Q52
E53
I54
A55
R56
I57
V58
T59
R62
E63
R64
L68
ALA
THR
GLY
PRO
ASP
GLY
LYS
GLU
SER

• Molecule 31: 50S ribosomal protein L30

Chain Z: 12% 38% 52% 9%

MET
S2
Q3
L4
K5
I6
T7
Q8
V9
R10
S11
T12
I13
R16
R20
E21
S22
L23
R24
T25
L26
G27
L28
R29
R30
S34
R37
E38
D39
N40
T43
R44
G45
L46
T47
A48
V49
V50
R51
H52
L53
V54
E55
V56
E57
F58
A59
Q60
THR
GLY
GLY
LYS
THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTY, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.56	0/427	0.66	0/570
2	1	0.35	0/407	0.61	0/543
3	2	0.56	0/361	0.68	0/473
4	3	0.48	0/499	0.62	0/664
5	4	0.34	0/303	0.54	0/402
6	6	0.21	0/353	0.46	0/478
7	A	0.51	0/74998	0.50	0/117018
8	B	0.37	0/2749	0.45	0/4284
9	C	0.51	0/2129	0.66	0/2861
10	D	0.52	0/1613	0.66	0/2174
11	E	0.44	0/1575	0.59	0/2129
12	F	0.26	0/1352	0.53	0/1817
13	G	0.30	0/1351	0.60	0/1824
14	H	0.25	0/353	0.51	0/474
15	J	0.50	0/1170	0.57	0/1584
16	K	0.44	0/944	0.60	0/1268
17	L	0.46	0/1073	0.61	0/1432
18	M	0.44	0/1098	0.58	0/1481
19	N	0.52	0/925	0.55	0/1242
20	O	0.34	0/895	0.53	0/1202
21	P	0.45	0/922	0.59	0/1236
22	Q	0.61	0/992	0.65	0/1329
23	R	0.47	0/751	0.52	0/1009
24	S	0.52	0/874	0.60	0/1186
25	T	0.42	0/770	0.59	0/1038
26	U	0.37	0/705	0.58	0/941
27	V	0.31	0/1336	0.54	0/1820
28	W	0.50	0/551	0.67	0/735
29	X	0.52	0/484	0.63	0/648
30	Y	0.40	0/544	0.64	0/727
31	Z	0.50	0/480	0.67	0/645
All	All	0.49	0/102984	0.52	0/155234

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
3	2	0	1
4	3	0	1
11	E	0	2
13	G	0	1
14	H	0	1
16	K	0	1
25	T	0	1
27	V	0	2
28	W	0	3
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	16	ARG	Peptide
3	2	43	ARG	Peptide
4	3	27	ALA	Peptide
11	E	11	ILE	Peptide
11	E	137	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	421	0	461	35	0
2	1	400	0	413	27	0
3	2	358	0	390	15	0
4	3	494	0	533	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	299	0	326	18	0
6	6	345	0	332	12	0
7	A	66978	0	33731	1891	0
8	B	2458	0	1253	87	0
9	C	2088	0	2123	137	0
10	D	1590	0	1633	97	0
11	E	1552	0	1593	96	0
12	F	1335	0	1372	97	0
13	G	1330	0	1390	93	0
14	H	350	0	367	22	0
15	J	1143	0	1173	44	0
16	K	934	0	993	61	0
17	L	1060	0	1119	78	0
18	M	1072	0	1115	70	0
19	N	908	0	956	51	0
20	O	886	0	924	57	0
21	P	907	0	947	43	0
22	Q	980	0	1028	49	0
23	R	742	0	799	31	0
24	S	860	0	903	44	0
25	T	759	0	809	36	0
26	U	699	0	738	27	0
27	V	1319	0	1365	60	0
28	W	546	0	567	35	0
29	X	476	0	496	31	0
30	Y	541	0	551	29	0
31	Z	476	0	509	31	0
32	A	52	0	69	9	0
33	A	1	0	0	0	0
34	A	3	0	0	0	0
All	All	94362	0	60978	3028	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 3028 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1222:G:H21	7:A:1227:A:N6	1.30	1.29
7:A:842:G:H21	7:A:847:A:N6	1.32	1.27
7:A:842:G:N2	7:A:847:A:H62	1.35	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1222:G:N2	7:A:1227:A:H62	1.35	1.23
7:A:1185:G:N2	7:A:1232:A:H62	1.37	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	51/57 (90%)	38 (74%)	13 (26%)	0	100	100
2	1	46/55 (84%)	35 (76%)	11 (24%)	0	100	100
3	2	40/47 (85%)	32 (80%)	8 (20%)	0	100	100
4	3	60/64 (94%)	50 (83%)	10 (17%)	0	100	100
5	4	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
6	6	43/80 (54%)	31 (72%)	12 (28%)	0	100	100
9	C	270/280 (96%)	207 (77%)	63 (23%)	0	100	100
10	D	211/217 (97%)	160 (76%)	51 (24%)	0	100	100
11	E	205/223 (92%)	166 (81%)	38 (18%)	1 (0%)	24	55
12	F	168/187 (90%)	133 (79%)	35 (21%)	0	100	100
13	G	172/179 (96%)	131 (76%)	41 (24%)	0	100	100
14	H	45/152 (30%)	37 (82%)	8 (18%)	0	100	100
15	J	144/147 (98%)	125 (87%)	19 (13%)	0	100	100
16	K	119/122 (98%)	93 (78%)	26 (22%)	0	100	100
17	L	140/146 (96%)	107 (76%)	33 (24%)	0	100	100
18	M	132/138 (96%)	109 (83%)	23 (17%)	0	100	100
19	N	114/180 (63%)	103 (90%)	11 (10%)	0	100	100
20	O	114/122 (93%)	93 (82%)	21 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	P	110/113 (97%)	80 (73%)	30 (27%)	0	100	100
22	Q	120/129 (93%)	106 (88%)	12 (10%)	2 (2%)	7	30
23	R	96/104 (92%)	82 (85%)	12 (12%)	2 (2%)	5	26
24	S	111/197 (56%)	93 (84%)	18 (16%)	0	100	100
25	T	96/100 (96%)	81 (84%)	15 (16%)	0	100	100
26	U	86/105 (82%)	62 (72%)	24 (28%)	0	100	100
27	V	175/215 (81%)	124 (71%)	49 (28%)	2 (1%)	11	39
28	W	72/86 (84%)	51 (71%)	17 (24%)	4 (6%)	1	9
29	X	61/64 (95%)	43 (70%)	17 (28%)	1 (2%)	7	31
30	Y	63/77 (82%)	57 (90%)	6 (10%)	0	100	100
31	Z	57/65 (88%)	41 (72%)	16 (28%)	0	100	100
All	All	3156/3688 (86%)	2497 (79%)	647 (20%)	12 (0%)	31	60

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	W	73	ARG
28	W	74	GLY
22	Q	118	PRO
23	R	82	LYS
27	V	137	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/47 (92%)	43 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	36/40 (90%)	36 (100%)	0	100	100
4	3	53/54 (98%)	52 (98%)	1 (2%)	50	68
5	4	35/35 (100%)	34 (97%)	1 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	40/66 (61%)	40 (100%)	0	100	100
9	C	212/219 (97%)	210 (99%)	2 (1%)	70	78
10	D	163/166 (98%)	160 (98%)	3 (2%)	51	70
11	E	159/172 (92%)	157 (99%)	2 (1%)	61	74
12	F	139/155 (90%)	136 (98%)	3 (2%)	45	66
13	G	143/147 (97%)	143 (100%)	0	100	100
14	H	36/121 (30%)	35 (97%)	1 (3%)	38	62
15	J	120/121 (99%)	119 (99%)	1 (1%)	73	79
16	K	100/101 (99%)	100 (100%)	0	100	100
17	L	106/110 (96%)	106 (100%)	0	100	100
18	M	110/114 (96%)	108 (98%)	2 (2%)	51	70
19	N	94/139 (68%)	94 (100%)	0	100	100
20	O	88/93 (95%)	86 (98%)	2 (2%)	44	66
21	P	98/99 (99%)	97 (99%)	1 (1%)	68	76
22	Q	95/99 (96%)	95 (100%)	0	100	100
23	R	79/83 (95%)	76 (96%)	3 (4%)	29	57
24	S	87/140 (62%)	84 (97%)	3 (3%)	32	59
25	T	82/83 (99%)	82 (100%)	0	100	100
26	U	77/88 (88%)	77 (100%)	0	100	100
27	V	142/164 (87%)	142 (100%)	0	100	100
28	W	54/62 (87%)	54 (100%)	0	100	100
29	X	52/52 (100%)	51 (98%)	1 (2%)	50	68
30	Y	58/66 (88%)	58 (100%)	0	100	100
31	Z	51/55 (93%)	51 (100%)	0	100	100
All	All	2597/2942 (88%)	2571 (99%)	26 (1%)	65	76

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	M	27	VAL
20	O	68	VAL
24	S	83	THR
20	O	61	ILE
21	P	69	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
12	F	162	ASN
27	V	82	HIS
15	J	132	HIS
27	V	58	HIS
23	R	77	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	3115/3138 (99%)	965 (30%)	15 (0%)
8	B	114/115 (99%)	33 (28%)	1 (0%)
All	All	3229/3253 (99%)	998 (30%)	16 (0%)

5 of 998 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	10	U
7	A	12	U
7	A	17	G
7	A	19	G
7	A	23	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	2994	U
7	A	2338	G
7	A	1605	G
7	A	2179	C
7	A	1567	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	CTY	A	3201	-	54,54,54	2.15	19 (35%)	83,83,83	2.08	20 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CTY	A	3201	-	-	34/75/110/110	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	3201	CTY	O9-C26	6.19	1.55	1.44
32	A	3201	CTY	O2-C1	4.74	1.45	1.34
32	A	3201	CTY	O4-C18	4.59	1.55	1.44
32	A	3201	CTY	C25-C24	-4.12	1.45	1.53
32	A	3201	CTY	C21-C18	-3.92	1.42	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	3201	CTY	O5-C16-C17	7.49	114.73	103.86
32	A	3201	CTY	C19-C16-C15	-5.64	100.79	110.64
32	A	3201	CTY	C15-C16-C17	4.83	115.91	107.64
32	A	3201	CTY	C36-C13-C12	-4.44	107.08	115.20
32	A	3201	CTY	C6-C5-C4	-4.13	107.23	113.54

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

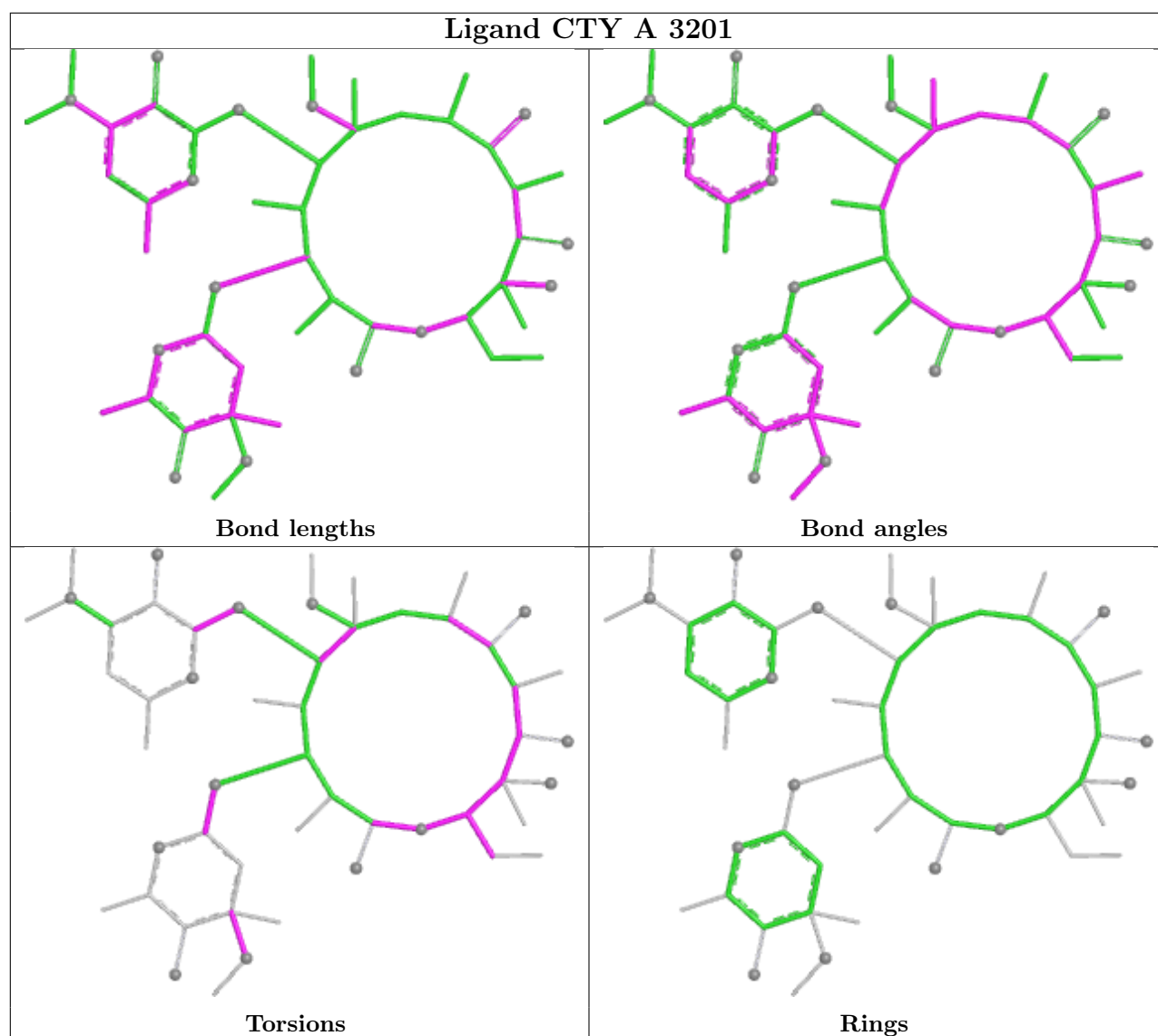
Mol	Chain	Res	Type	Atoms
32	A	3201	CTY	C9-C10-C11-C12
32	A	3201	CTY	C9-C10-C11-O12
32	A	3201	CTY	C34-C10-C11-C12
32	A	3201	CTY	C34-C10-C11-O12
32	A	3201	CTY	C10-C11-C12-C35

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	3201	CTY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

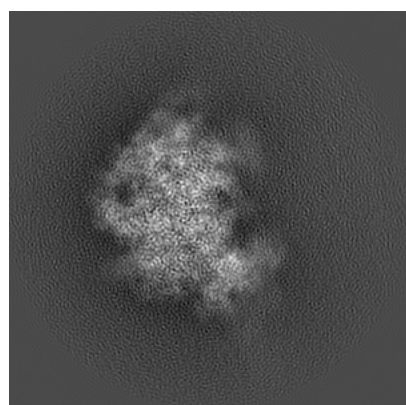
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31398. These allow visual inspection of the internal detail of the map and identification of artifacts.

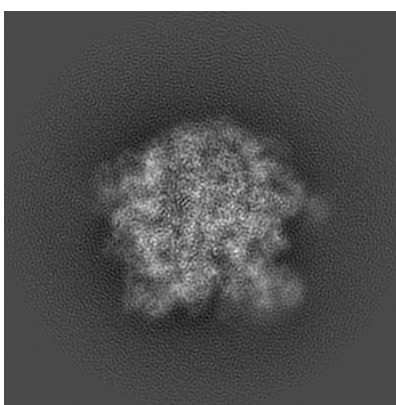
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

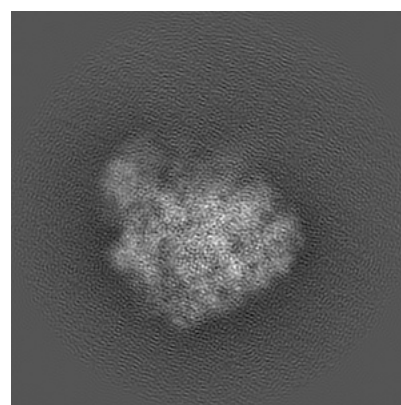
6.1.1 Primary map



X



Y

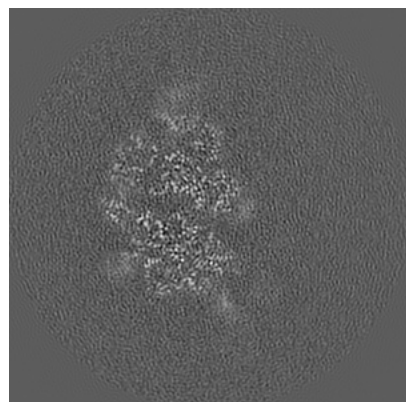


Z

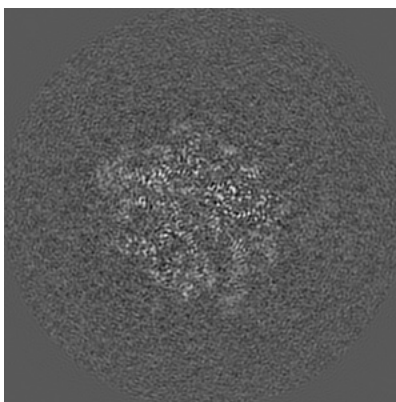
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

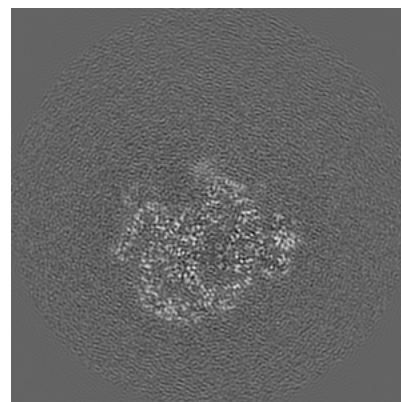
6.2.1 Primary map



X Index: 180



Y Index: 180

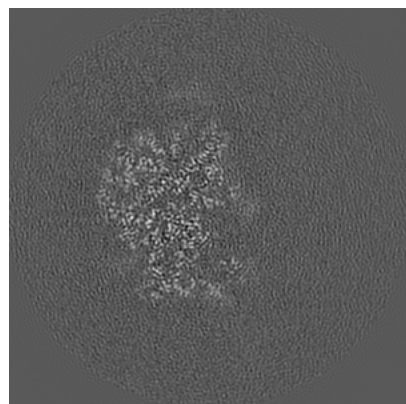


Z Index: 180

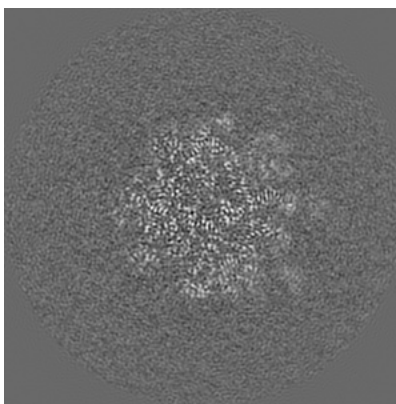
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

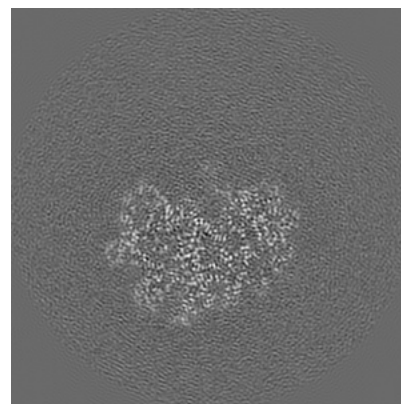
6.3.1 Primary map



X Index: 172



Y Index: 156

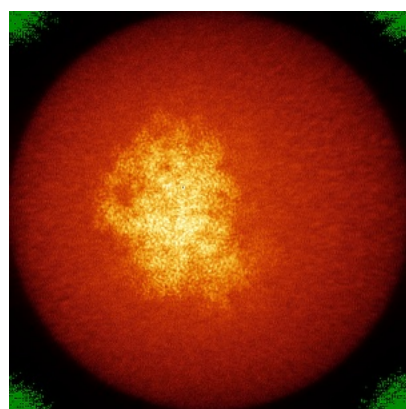


Z Index: 169

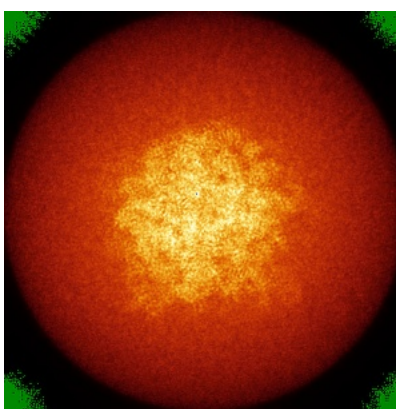
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

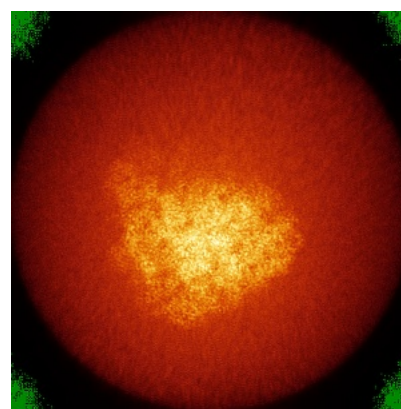
6.4.1 Primary map



X



Y

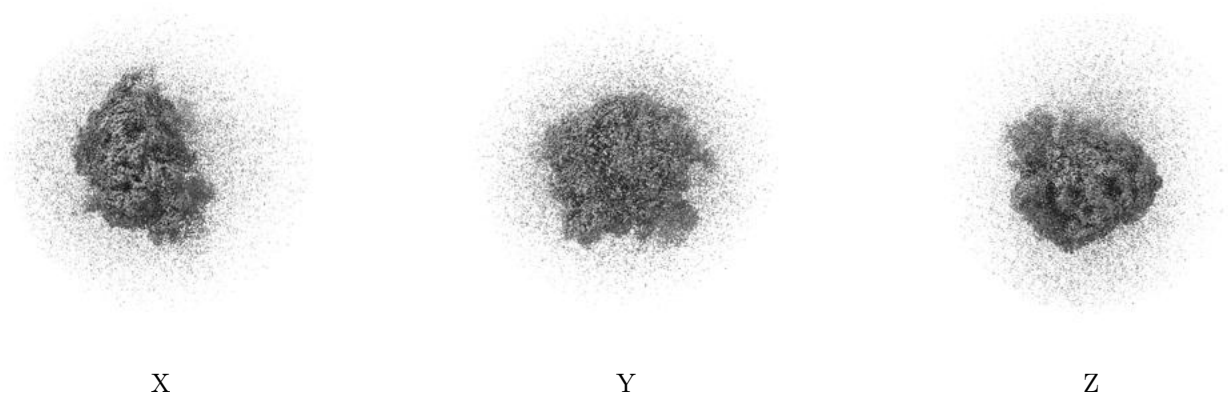


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

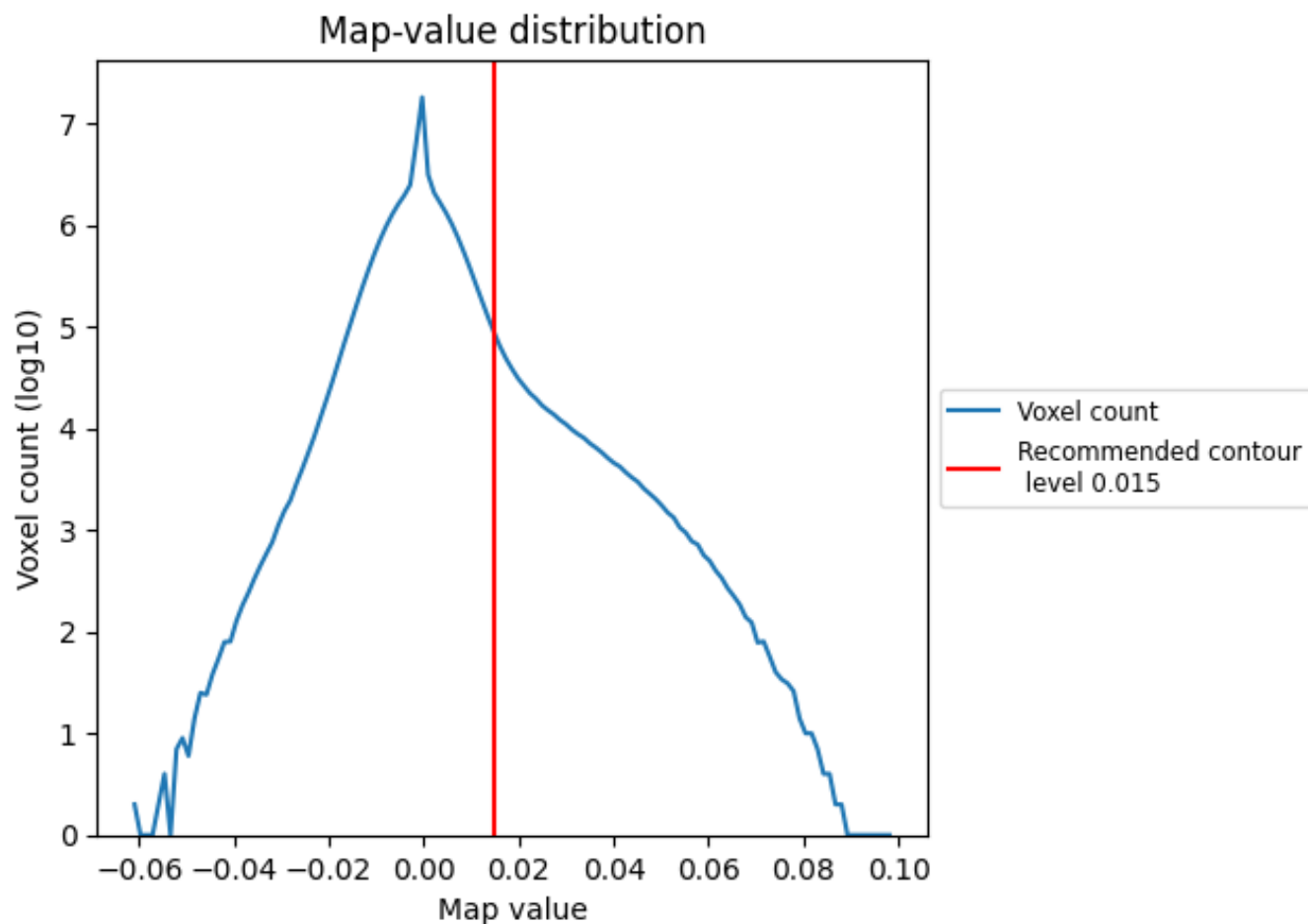
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

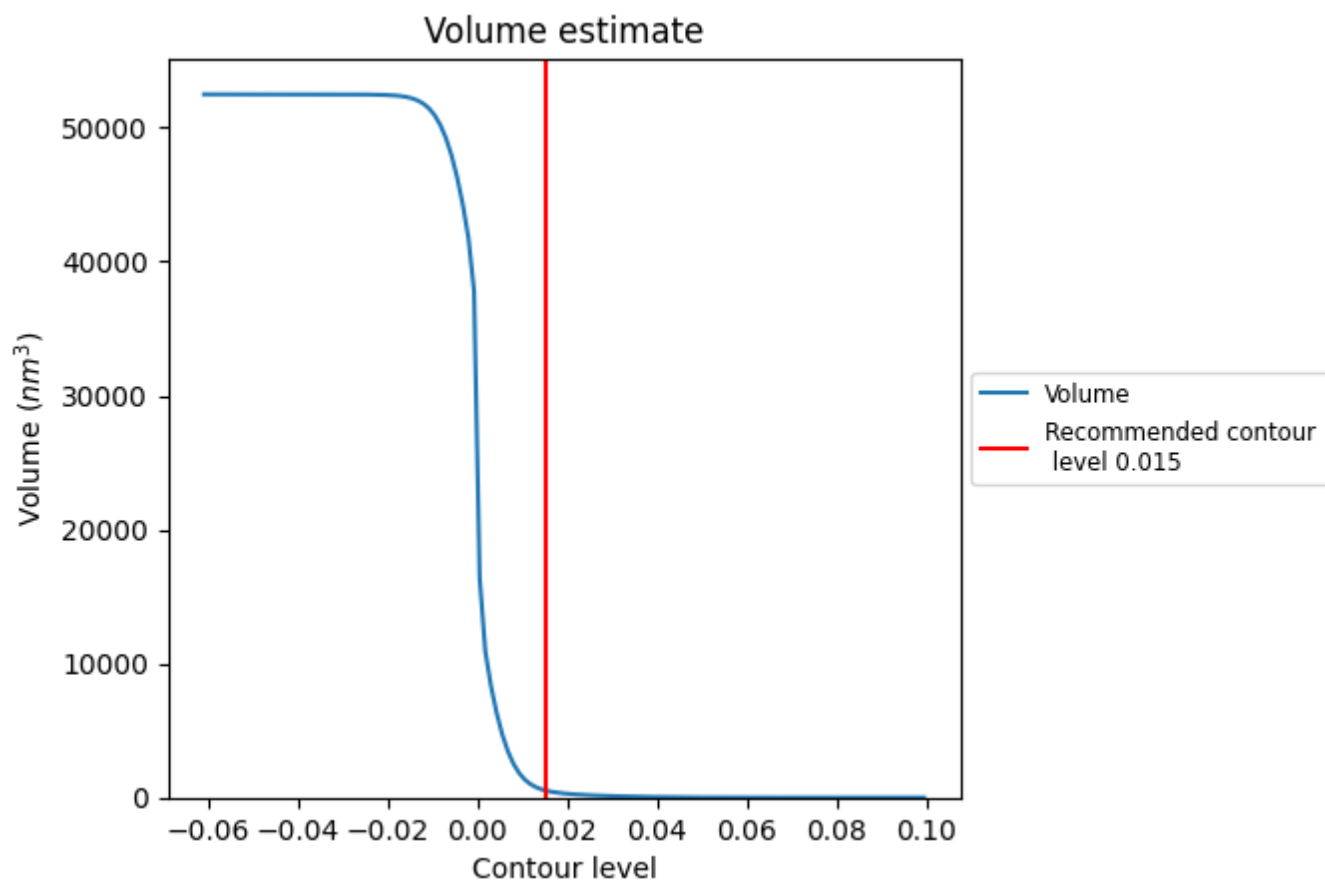
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

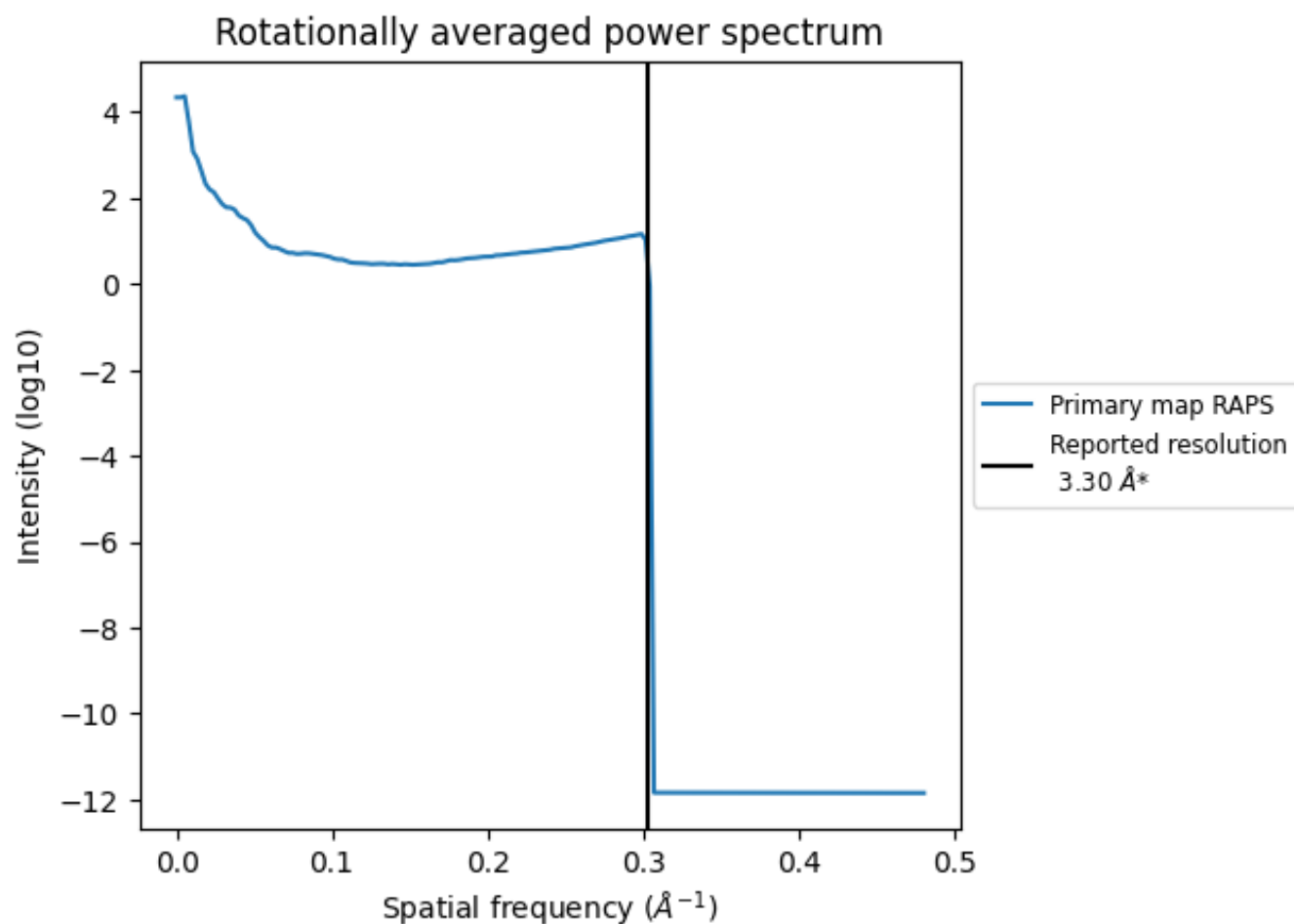
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 540 nm³; this corresponds to an approximate mass of 488 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

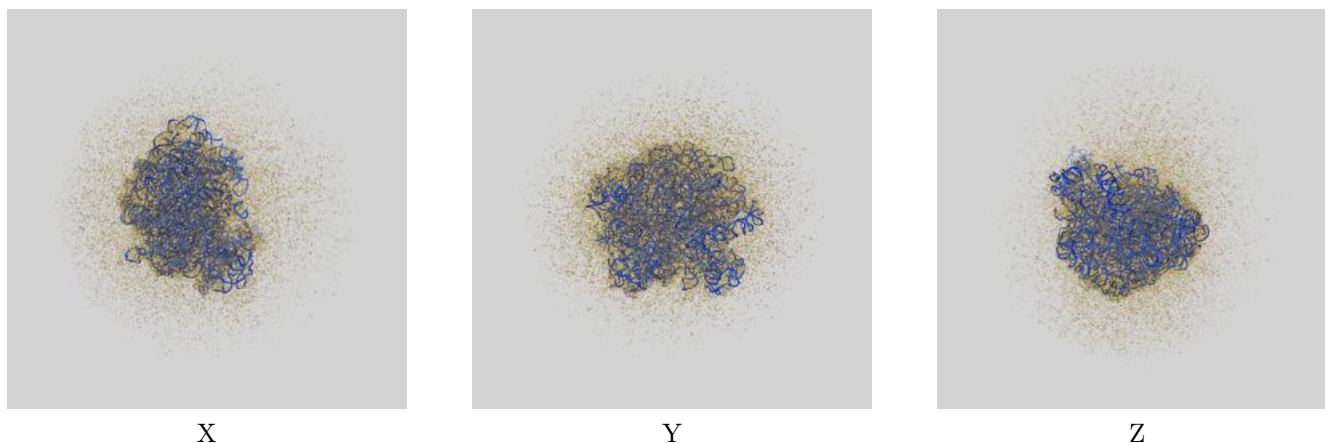
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

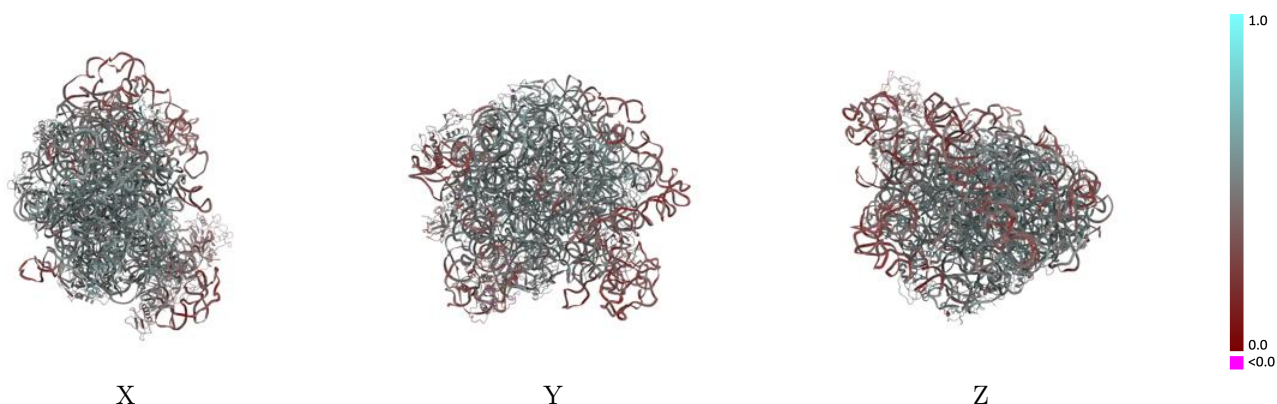
This section contains information regarding the fit between EMDB map EMD-31398 and PDB model 7F0D. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



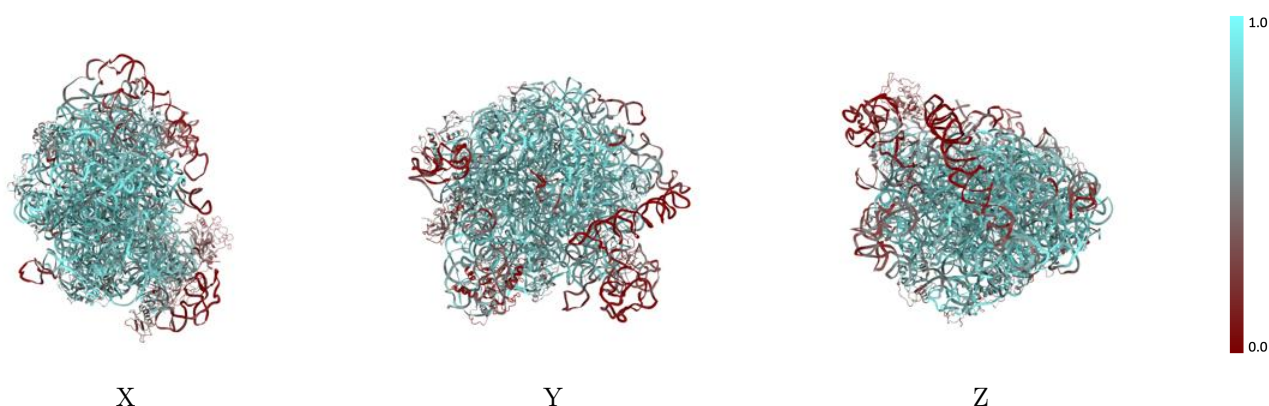
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



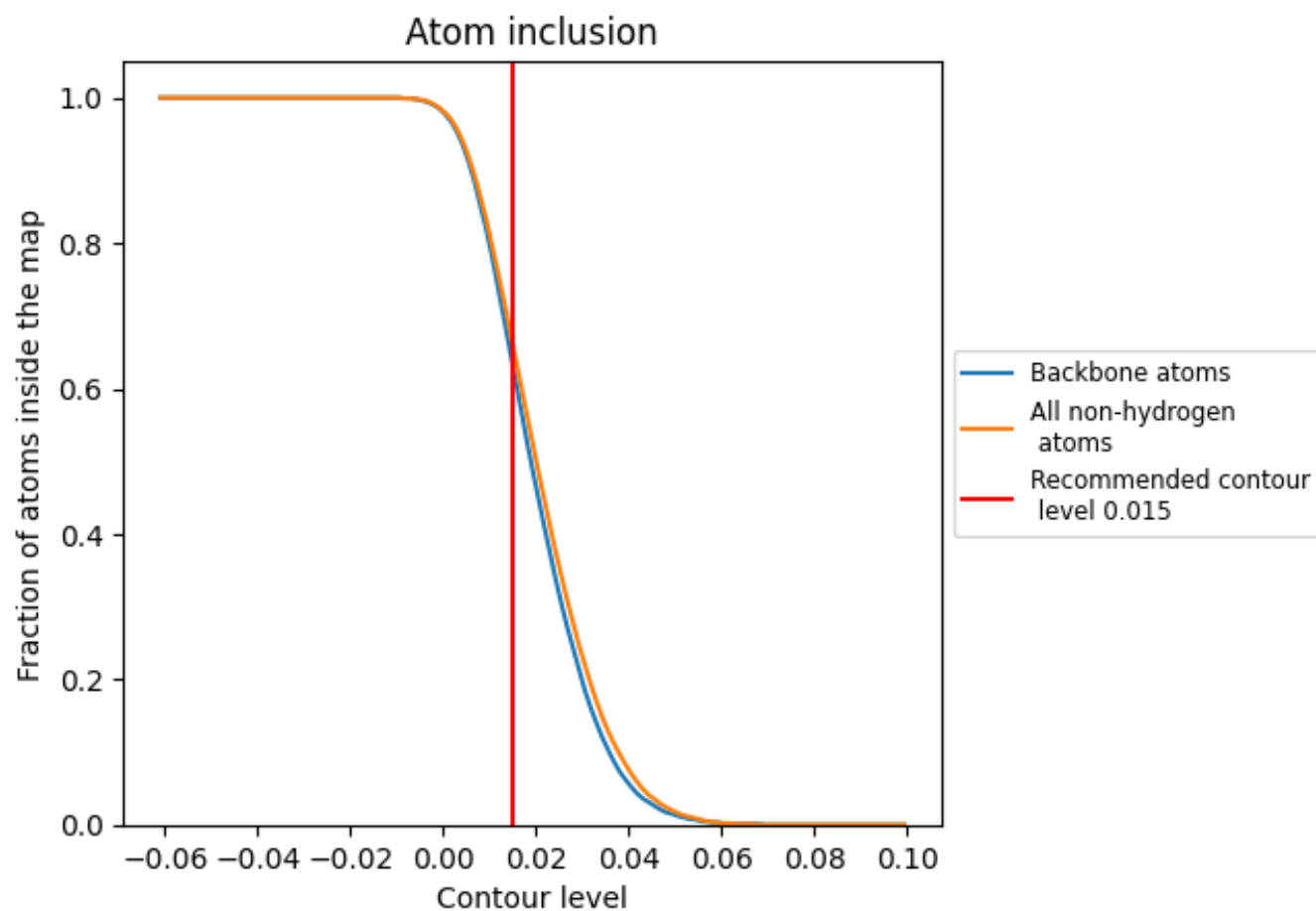
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.4730
0	 0.6690	 0.5050
1	 0.4240	 0.4770
2	 0.8020	 0.5440
3	 0.7030	 0.5260
4	 0.4910	 0.5000
6	 0.0210	 0.3140
A	 0.6920	 0.4670
B	 0.6430	 0.4180
C	 0.7070	 0.5280
D	 0.6960	 0.5250
E	 0.6670	 0.5160
F	 0.1740	 0.3720
G	 0.4060	 0.4200
H	 0.1110	 0.4110
J	 0.6880	 0.5270
K	 0.6580	 0.5160
L	 0.6390	 0.5100
M	 0.6130	 0.5030
N	 0.7420	 0.5420
O	 0.5220	 0.4550
P	 0.5640	 0.4960
Q	 0.7610	 0.5390
R	 0.6860	 0.5240
S	 0.7270	 0.5380
T	 0.6300	 0.5130
U	 0.5840	 0.4850
V	 0.3410	 0.4230
W	 0.6860	 0.5230
X	 0.6810	 0.5110
Y	 0.6250	 0.4870
Z	 0.6660	 0.5160

