



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 01:43 AM EST

PDB ID : 6WU9  
EMDB ID : EMD-21907  
Title : 50S subunit of 70S Ribosome Enterococcus faecalis MultiBody refinement  
Authors : Jogl, G.; Khayat, R.  
Deposited on : 2020-05-04  
Resolution : 2.90 Å(reported)  
Based on initial models : 5LI0, 4YBB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

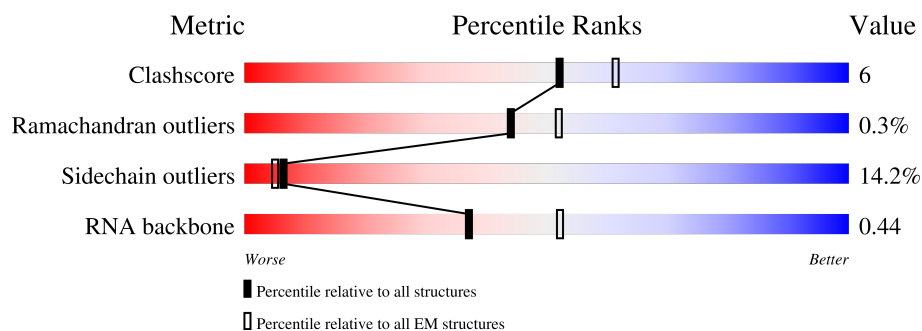
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.














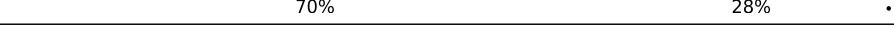

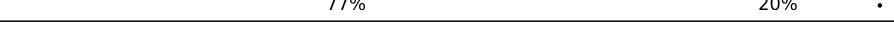






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	2908	60% 26% 7% • 6%
2	B	116	48% 31% 19% •
3	D	207	66% 29% 5%
4	E	206	74% 21% 5%
5	F	177	53% 42% 5% •
6	G	176	62% 31% 7%
7	K	145	79% 17% •

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Mol	Chain	Length	Quality of chain
8	L	122	 78% 20% .
9	M	146	 81% 16% .
10	N	141	 69% 26% 5%
11	O	124	 69% 26% 5%
12	P	117	 70% 25% 5%
13	Q	114	 77% 19% .
14	R	118	 82% 16% .
15	S	102	 74% 25% .
16	T	112	 73% 22% .
17	U	89	 70% 25% 6%
18	V	101	 70% 23% 7%
19	X	76	 70% 28% .
20	Y	54	 74% 20% 6%
21	Z	61	 77% 20% .
22	0	58	 76% 24%
23	2	56	 82% 14% .
24	3	49	 67% 33%
25	4	44	 70% 27% .
26	5	64	 80% 17% .
27	6	38	 76% 16% 8%

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 82295 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2739	Total	C	N	O	P	0	0
			58793	26244	10818	18992	2739		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	116	Total	C	N	O	P	0	0
			2480	1106	444	814	116		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	207	Total	C	N	O	S	0	0
			1579	994	292	289	4		

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	206	Total	C	N	O	S	0	0
			1574	984	290	298	2		

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total	C	N	O	S	0	0
			1345	842	244	255	4		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	145	Total	C	N	O	S	0	0
			1130	714	205	207	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	146	Total	C	N	O	S	0	0
			1095	677	212	205	1		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	141	Total	C	N	O	S	0	0
			1118	710	216	185	7		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	124	Total	C	N	O	S	0	0
			991	612	191	185	3		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	117	Total	C	N	O	S	0	0
			899	556	175	167	1		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	114	Total	C	N	O	0	0
			924	582	185	157		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	102	Total	C	N	O	S	0	0
			784	500	139	143	2		

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	112	Total	C	N	O	S	0	0
			849	532	156	159	2		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	89	Total	C	N	O	S	0	0
			720	458	127	132	3		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	76	Total	C	N	O	0	0
			572	351	109	112		

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	54	Total	C	N	O	S	0	0
			425	265	86	72	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	58	Total	C	N	O	S	0	0
			435	271	81	82	1		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 27 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

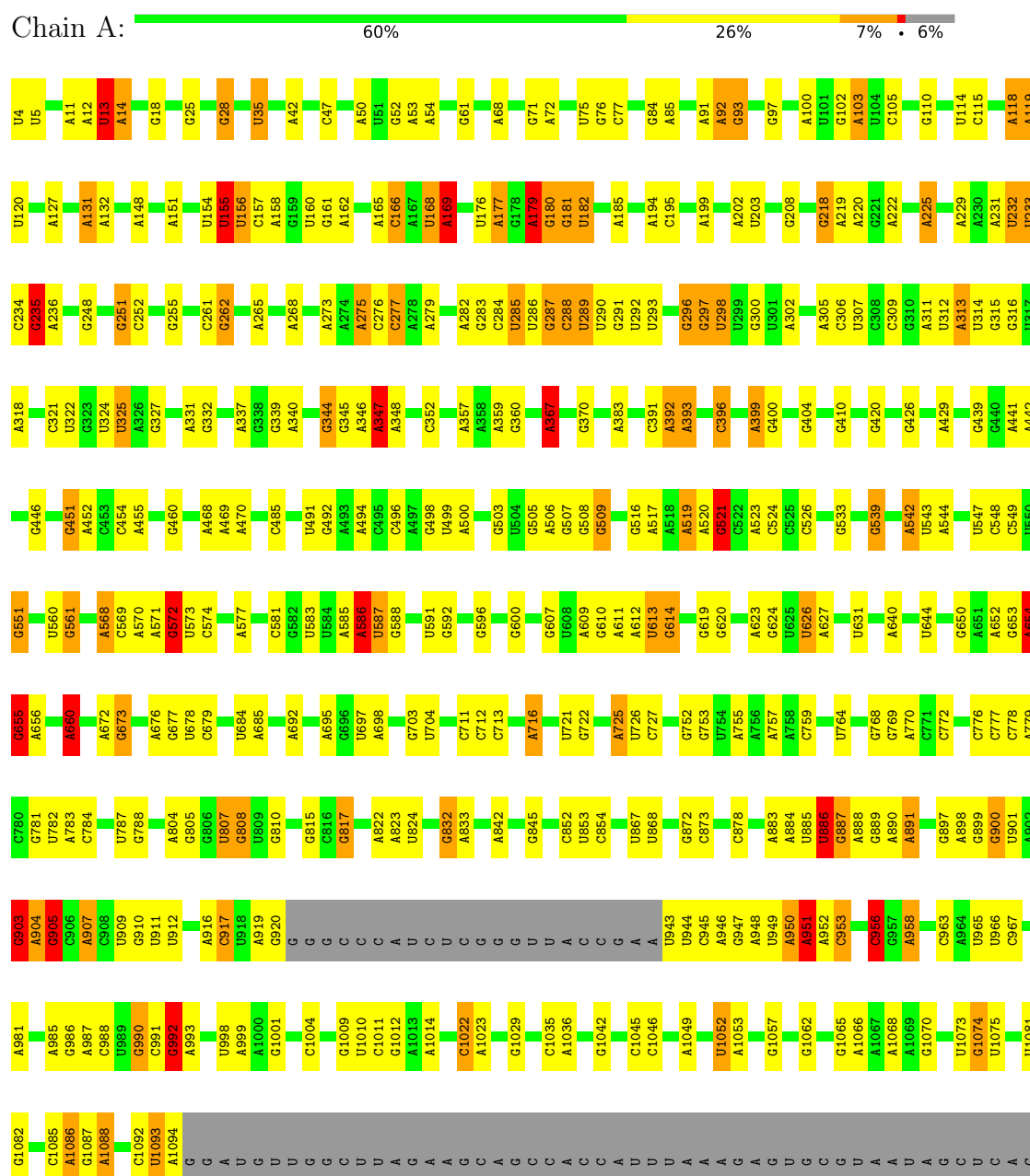
Mol	Chain	Residues	Atoms		AltConf
28	2	1	Total	Zn	0
			1	1	
28	3	1	Total	Zn	0
			1	1	
28	6	1	Total	Zn	0
			1	1	



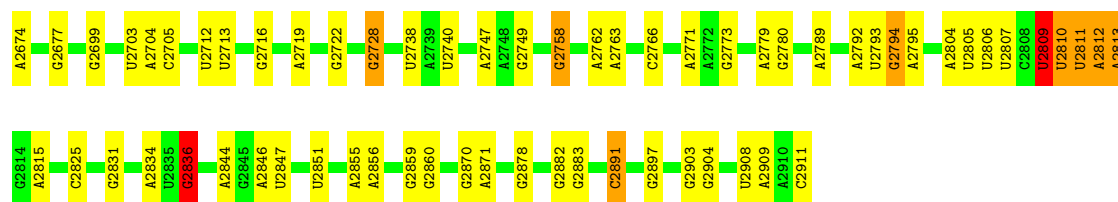
### 3 Residue-property plots

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. 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. 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.

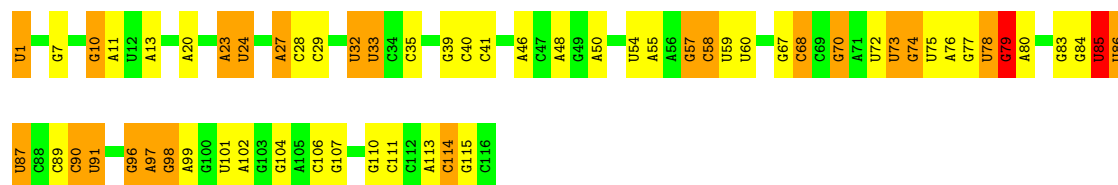
#### • Molecule 1: 23S rRNA



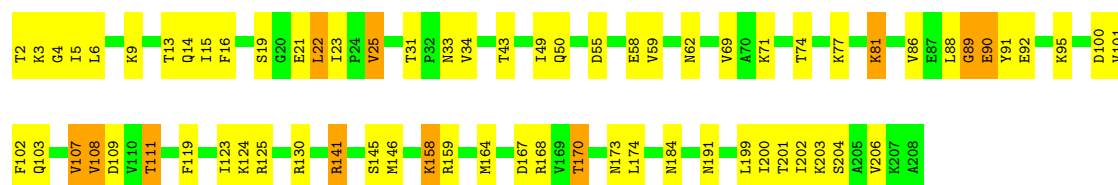
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A2556	A2449	G2339	G2239	A2102	C2008	A1890	U1793	U1551	U1551	C1459	U1365	A1241	G
G2563	A2453	U2340	A2241	U2106	A2011	U1894	U1796	A1652	A1552	A1460	G1373	U1247	C1149
U2566	C2454	A2341	G2252	A2108	C2020	C1895	C1796	A1653	A1559	A1461	U1376	G1256	G1150
U2570	C2455	A2342	G2253	G2109	U2021	A1896	A1798	A1653	G1560	U1462	U1376	A1257	A1151
C2571	G2458	G2344	G2252	U2110	C2022	G1897	A1799	C1658	C1567	A1469	U1379	G1262	G1165
C2572	A2461	G2345	G2264	U2111	G2035	A1898	A1800	G1669	C1568	C1470	U1380	A1263	A1167
A2575	G2462	G2348	G2267	U2112	U2036	A1899	U1800	G1669	G1570	G1471	U1380	A1264	A1169
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C2581	A2464	A2360	C2272	G	C2038	A1910	A1805	G1674	A1572	U1475	A1390	U1278	U1171
U2587	U2474	C2361	C2277	U	C2039	U2040	G1807	G1686	A1577	A1486	C1393	A1284	A1173
C2588	G2475	G2362	G2280	C	G2041	G1920	C1809	G1686	A1578	U1487	G1394	G1285	C1174
U2592	C2476	A2364	A2281	A	A2042	A1927	C1814	A1689	A1576	C1488	C1393	U1286	U1172
G2596	U2477	G2365	A2281	C	A2045	U1928	A1815	C1690	A1577	C1489	G1397	U1286	G1178
C2597	A2478	A2366	A2282	A	G2046	G1929	A1816	C1691	A1578	U1491	C1398	G1287	G1179
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A2601	G2481	G2368	A2284	U	U2048	U1931	A1817	C1699	U	G1494	G1400	G1289	G1181
G2602	A2483	U2371	A2285	A	C2050	A1933	A1823	U1700	A1583	A1495	A1401	A1290	A1182
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C2624	U2488	A2383	A2290	U	C2055	G1944	A1837	G1724	A1590	U1501	A1408	G1301	G1194
U2627	A2489	G2384	A2291	G	A2056	A1950	G1842	A1725	A1591	G1502	A1409	A1305	A1195
A2628	C2490	U2385	A2292	A	G2057	U1959	A1843	C1726	G1592	G1503	G1410	G1308	G1196
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G2632	C2492	A2387	A2294	G	G2059	U1960	A1843	C1734	G1600	U1507	U1415	A1310	G1202
U2633	U2493	G2388	A2295	A	C2060	U1961	A1843	C1734	G1601	G1508	A1420	G1203	G1203
C2636	A2494	U2389	A2296	C	U2061	U1962	A1843	G1746	A1604	C1510	A1421	U1206	U1206
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C2639	A2497	U2392	A2299	A	G2064	U1965	A1843	G1746	A1606	G1514	A1423	A1320	A1209
G2645	U2498	G2393	A2300	C	U2065	U1966	A1843	G1746	A1606	G1514	A1423	G1321	C1210
U2650	C2499	A2394	A2301	G	A2066	U1967	A1843	G1746	A1606	G1514	A1423	A1322	G1211
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A2679	U2527	U2422	A2329	G	A2094	U1995	A1843	G1746	A1606	G1514	A1423		
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G2681	U2529	U2424	A2331	C	U2096	U1997	A1843	G1746	A1606	G1514	A1423		
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C2689	C2537	U2432	A2339	G	U2104	U2005	A1843	G1746	A1606	G1514	A1423		
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U2697	C2545	U2440	A2347	C	U2110	U2013	A1843	G1746	A1606	G1514	A1423		
A2698	U2546	G2441	A2348	U	U2111	U2014	A1843	G1746	A1606	G1514	A1423		
C2699	C2547	U2442	A2349	C	U2112	U2015	A1843	G1746	A1606	G1514	A1423		
U2700	U2548	G2443	A2350	A	U2113	U2016	A1843	G1746	A1606	G1514	A1423		
C2701	C2549	U2444	A2351	C	U2114	U2017	A1843	G1746	A1606	G1514	A1423		
U2702	U2550	G2445	A2352	G	G	U2018	A1843	G1746	A1606	G1514	A1423		
A2703	C2551	U2446	A2353	U	U	U2019	A1843	G1746	A1606	G1514	A1423		
C2704	U2552	G2447	A2354	C	U	U2020	A1843	G1746	A1606	G1514	A1423		
U2705	C2553	U2448	A2355	A	U	U2021	A1843	G1746	A1606	G1514	A1423		
A2706	U2554	G2449	A2356	C	U	U2022	A1843	G1746	A1606	G1514	A1423		
C2707	C2555	U2450	A2357	G	U	U2023	A1843	G1746	A1606	G1514	A1423		
U2708	U2556	G2451	A2358	A	A	U2024	A1843	G1746	A1606	G1514	A1423		
A2709	C2557	U2452	A2359	C	C	A2025	A1843	G1746	A1606	G1514	A1423		
C2710	U2558	G2453	A2360	U	A	G2026	A1843	G1746	A1606	G1514	A1423		
U2711	C2559	U2454	A2361	C	C	U2027	A1843	G1746	A1606	G1514	A1423		
A2712	U2560	G2455	A2362	A	G	U2028	A1843	G1746	A1606	G1514	A1423		
C2713	C2561	U2456	A2363	C	U	U2029	A1843	G1746	A1606	G1514	A1423		
U2714	U2562	G2457	A2364	G	A	G2030	A1843	G1746	A1606	G1514	A1423		
A2715	C2563	U2458	A2365	A	C	U2031	A1843	G1746	A1606	G1514	A1423		
C2716	U2564	G2459	A2366	C	C	A2032							



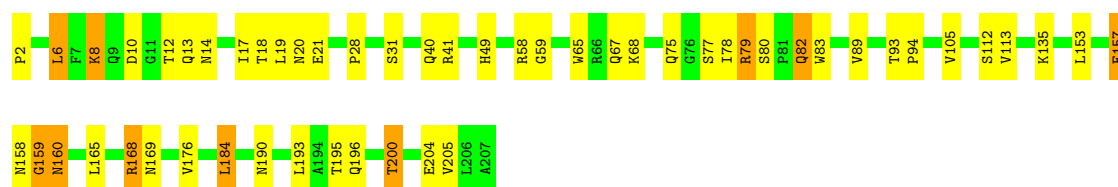
• Molecule 2: 5S rRNA



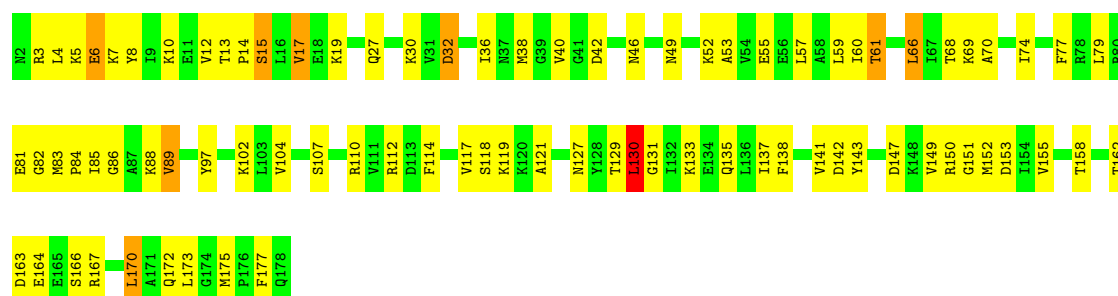
• Molecule 3: 50S ribosomal protein L3



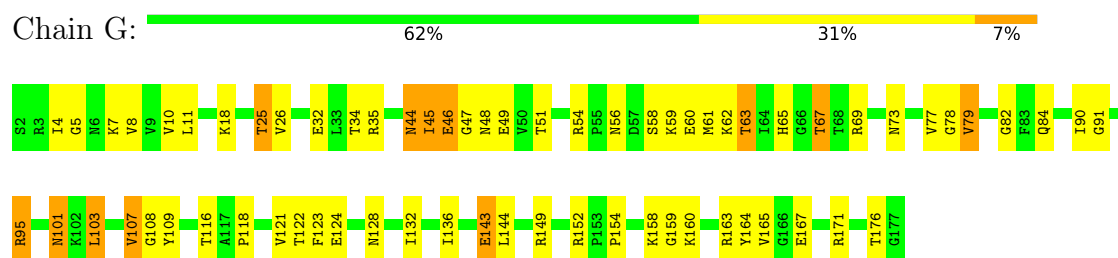
• Molecule 4: 50S ribosomal protein L4



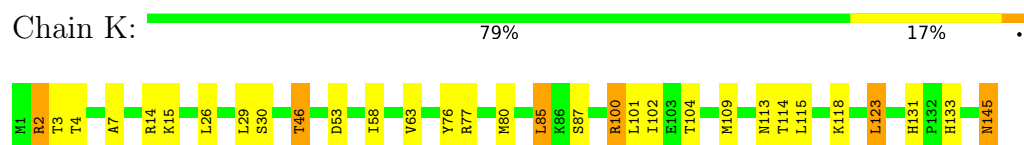
• Molecule 5: 50S ribosomal protein L5



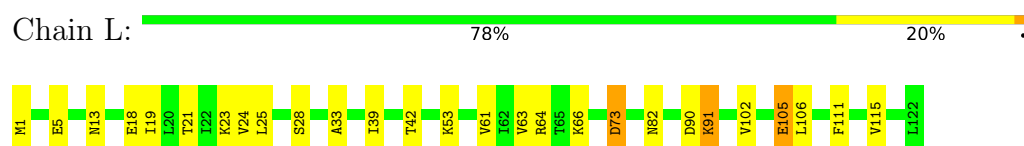
- Molecule 6: 50S ribosomal protein L6



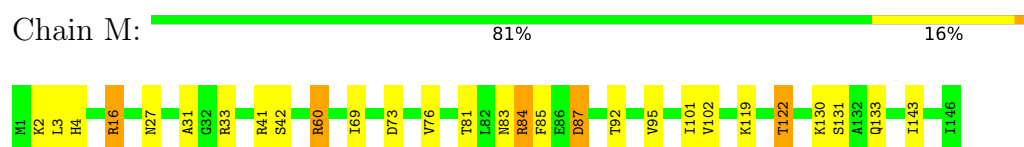
- Molecule 7: 50S ribosomal protein L13



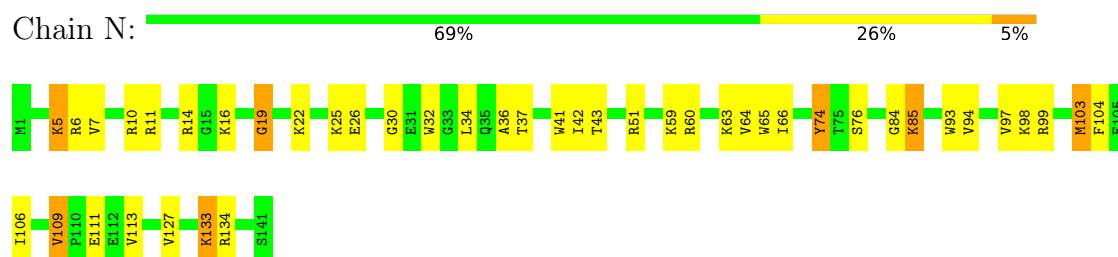
- Molecule 8: 50S ribosomal protein L14



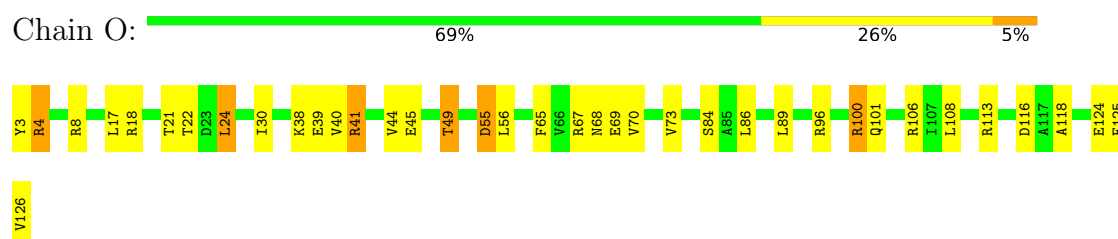
- Molecule 9: 50S ribosomal protein L15



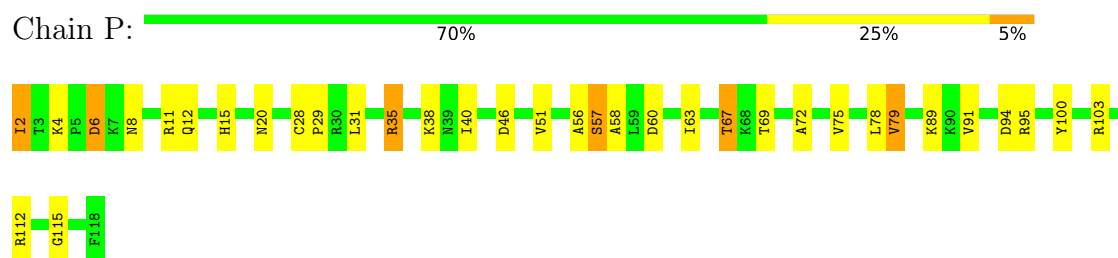
- Molecule 10: 50S ribosomal protein L16



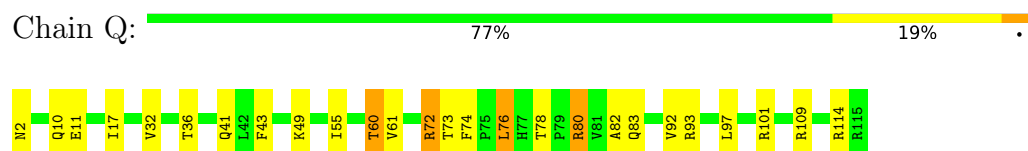
- Molecule 11: 50S ribosomal protein L17



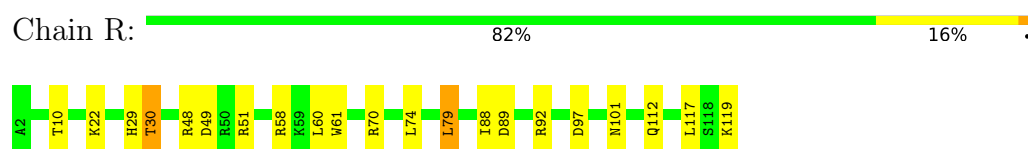
- Molecule 12: 50S ribosomal protein L18



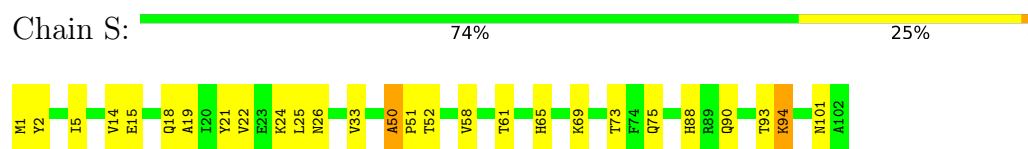
- Molecule 13: 50S ribosomal protein L19



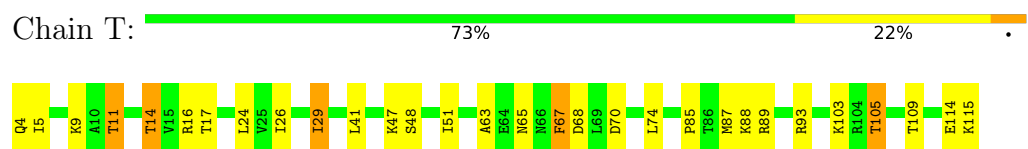
- Molecule 14: 50S ribosomal protein L20



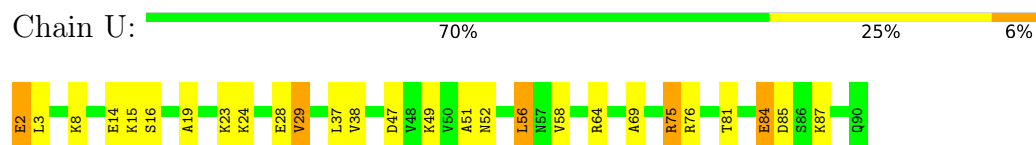
- Molecule 15: 50S ribosomal protein L21



- Molecule 16: 50S ribosomal protein L22



- Molecule 17: 50S ribosomal protein L23

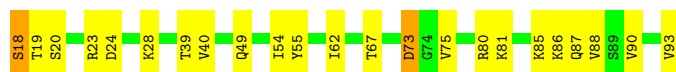


- Molecule 18: 50S ribosomal protein L24





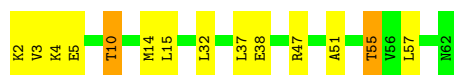
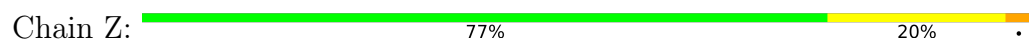
- Molecule 19: 50S ribosomal protein L27



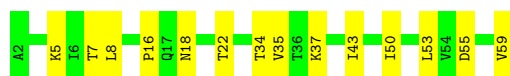
- Molecule 20: 50S ribosomal protein L28



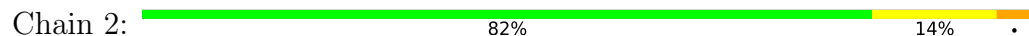
- Molecule 21: 50S ribosomal protein L29



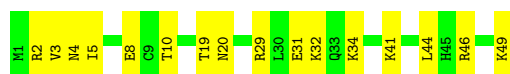
- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32



- Molecule 24: 50S ribosomal protein L33

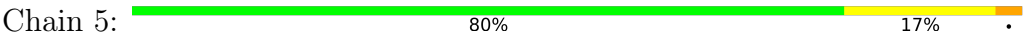


- Molecule 25: 50S ribosomal protein L34

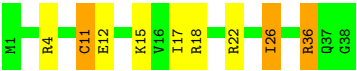




• Molecule 26: 50S ribosomal protein L35



• Molecule 27: 50S ribosomal protein L36



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	335675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	A	1.21	32/65858 (0.0%)	1.30	435/102721 (0.4%)
2	B	0.97	1/2773 (0.0%)	1.23	23/4320 (0.5%)
3	D	0.54	0/1601	0.67	0/2150
4	E	0.52	0/1596	0.63	0/2159
5	F	0.36	0/1411	0.58	1/1897 (0.1%)
6	G	0.39	0/1365	0.57	0/1839
7	K	0.53	0/1151	0.68	2/1554 (0.1%)
8	L	0.51	0/929	0.65	1/1247 (0.1%)
9	M	0.52	1/1105 (0.1%)	0.64	0/1474
10	N	0.49	0/1141	0.61	0/1519
11	O	0.55	0/1000	0.71	1/1341 (0.1%)
12	P	0.47	0/908	0.64	0/1216
13	Q	0.56	0/938	0.63	0/1262
14	R	0.59	0/963	0.64	2/1280 (0.2%)
15	S	0.54	0/796	0.62	0/1068
16	T	0.49	0/858	0.64	1/1157 (0.1%)
17	U	0.50	0/727	0.65	1/972 (0.1%)
18	V	0.46	0/772	0.63	0/1035
19	X	0.56	0/578	0.61	0/773
20	Y	0.57	1/431 (0.2%)	0.60	0/574
21	Z	0.42	0/505	0.57	0/672
22	0	0.47	0/437	0.63	0/589
23	2	0.55	0/436	0.63	0/578
24	3	0.46	0/423	0.60	0/563
25	4	0.48	0/377	0.61	0/491
26	5	0.43	0/528	0.62	0/689
27	6	0.47	0/309	0.67	0/409
All	All	1.08	35/89916 (0.0%)	1.19	467/135549 (0.3%)

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
3	D	0	1
10	N	0	2
11	O	0	2
15	S	0	1
16	T	0	1
18	V	0	1
All	All	0	8

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	903	G	C6-N1	-11.86	1.31	1.39
2	B	1	U	OP3-P	-10.45	1.48	1.61
1	A	769	G	N9-C4	-8.64	1.31	1.38
1	A	1492	G	N9-C4	-8.09	1.31	1.38
1	A	956	C	N3-C4	-7.24	1.28	1.33

The worst 5 of 467 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	956	C	N3-C4-N4	-30.89	96.38	118.00
1	A	956	C	C5-C4-N4	25.47	138.03	120.20
1	A	903	G	N1-C6-O6	-24.12	105.42	119.90
1	A	903	G	C5-C6-O6	22.01	141.81	128.60
1	A	1591	A	N1-C6-N6	-15.79	109.12	118.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	89	GLY	Peptide
10	N	16	LYS	Peptide
10	N	19	GLY	Peptide
11	O	4	ARG	Peptide
11	O	73	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	A	58793	0	29547	404	0
2	B	2480	0	1249	42	0
3	D	1579	0	1661	31	0
4	E	1574	0	1621	28	0
5	F	1392	0	1454	49	0
6	G	1345	0	1375	36	0
7	K	1130	0	1169	16	0
8	L	922	0	985	14	0
9	M	1095	0	1148	15	0
10	N	1118	0	1180	25	0
11	O	991	0	1028	21	0
12	P	899	0	932	26	0
13	Q	924	0	979	9	0
14	R	950	0	1009	11	0
15	S	784	0	826	12	0
16	T	849	0	906	13	0
17	U	720	0	772	13	0
18	V	763	0	824	15	0
19	X	572	0	580	9	0
20	Y	425	0	460	4	0
21	Z	504	0	538	5	0
22	0	435	0	472	6	0
23	2	429	0	444	3	0
24	3	419	0	435	9	0
25	4	374	0	424	9	0
26	5	522	0	576	5	0
27	6	304	0	337	6	0
28	2	1	0	0	0	0
28	3	1	0	0	0	0
28	6	1	0	0	0	0
All	All	82295	0	52931	757	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 6.

The worst 5 of 757 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)
1:A:1571:G:N2	1:A:1591:A:H62	1.58	1.01
1:A:275:A:H62	1:A:296:G:N2	1.67	0.93
1:A:1571:G:H22	1:A:1591:A:H62	0.94	0.92
1:A:1871:G:N2	1:A:1899:A:H62	1.69	0.91
1:A:1871:G:H21	1:A:1899:A:H62	0.92	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	
3	D	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	29	61
4	E	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	15	45
5	F	175/177 (99%)	148 (85%)	27 (15%)	0	100	100
6	G	174/176 (99%)	145 (83%)	27 (16%)	2 (1%)	14	42
7	K	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
8	L	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	19	51
9	M	144/146 (99%)	118 (82%)	25 (17%)	1 (1%)	22	54
10	N	139/141 (99%)	119 (86%)	20 (14%)	0	100	100
11	O	122/124 (98%)	102 (84%)	20 (16%)	0	100	100
12	P	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
13	Q	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
14	R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
15	S	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	15	45
16	T	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
17	U	87/89 (98%)	73 (84%)	14 (16%)	0	100	100
18	V	99/101 (98%)	81 (82%)	18 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	X	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
20	Y	52/54 (96%)	43 (83%)	8 (15%)	1 (2%)	8	28
21	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
22	0	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
23	2	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
24	3	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
25	4	42/44 (96%)	42 (100%)	0	0	100	100
26	5	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
27	6	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
All	All	2647/2697 (98%)	2354 (89%)	284 (11%)	9 (0%)	44	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	90	GLU
9	M	16	ARG
4	E	13	GLN
8	L	25	LEU
20	Y	20	HIS

### 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	
3	D	170/170 (100%)	140 (82%)	30 (18%)	2	5
4	E	172/172 (100%)	144 (84%)	28 (16%)	2	7
5	F	154/154 (100%)	129 (84%)	25 (16%)	2	7
6	G	146/146 (100%)	123 (84%)	23 (16%)	2	8
7	K	122/122 (100%)	105 (86%)	17 (14%)	3	10
8	L	98/98 (100%)	87 (89%)	11 (11%)	6	18
9	M	112/112 (100%)	102 (91%)	10 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	N	112/112 (100%)	98 (88%)	14 (12%)	4	14
11	O	106/106 (100%)	92 (87%)	14 (13%)	4	12
12	P	91/91 (100%)	79 (87%)	12 (13%)	4	12
13	Q	97/97 (100%)	83 (86%)	14 (14%)	3	9
14	R	94/94 (100%)	87 (93%)	7 (7%)	13	38
15	S	83/83 (100%)	73 (88%)	10 (12%)	5	15
16	T	95/95 (100%)	82 (86%)	13 (14%)	3	11
17	U	80/80 (100%)	66 (82%)	14 (18%)	2	6
18	V	85/85 (100%)	71 (84%)	14 (16%)	2	7
19	X	61/61 (100%)	48 (79%)	13 (21%)	1	3
20	Y	47/47 (100%)	38 (81%)	9 (19%)	1	4
21	Z	55/55 (100%)	45 (82%)	10 (18%)	1	5
22	0	49/49 (100%)	44 (90%)	5 (10%)	7	22
23	2	46/46 (100%)	39 (85%)	7 (15%)	3	8
24	3	49/49 (100%)	46 (94%)	3 (6%)	18	48
25	4	39/39 (100%)	34 (87%)	5 (13%)	4	13
26	5	51/51 (100%)	44 (86%)	7 (14%)	3	11
27	6	35/35 (100%)	30 (86%)	5 (14%)	3	10
All	All	2249/2249 (100%)	1929 (86%)	320 (14%)	6	10

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	U	16	SER
21	Z	38	GLU
17	U	75	ARG
19	X	24	ASP
24	3	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
15	S	86	GLN
20	Y	23	ASN
15	S	88	HIS

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Mol	Chain	Res	Type
16	T	65	ASN
20	Y	34	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2733/2908 (93%)	536 (19%)	24 (0%)
2	B	115/116 (99%)	32 (27%)	3 (2%)
All	All	2848/3024 (94%)	568 (19%)	27 (0%)

5 of 568 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U
1	A	14	A
1	A	28	G
1	A	35	U
1	A	42	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1590	A
1	A	1605	C
2	B	32	U
1	A	1604	A
1	A	1861	A

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	60:ARG	C	61:LEU	N	1.18



## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21907. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.