



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:15 PM BST

PDB ID : 3J7Z
EMDB ID: : EMD-6057
Title : Structure of the E. coli 50S subunit with ErmCL nascent chain
Authors : Arenz, S.; Meydan, S.; Starosta, A.L.; Berninghausen, O.; Beckmann, R.;
Vazquez-Laslop, N.; Wilson, D.N.
Deposited on : 2014-08-27
Resolution : 3.90 Å(reported)
Based on PDB ID : 4KIX

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

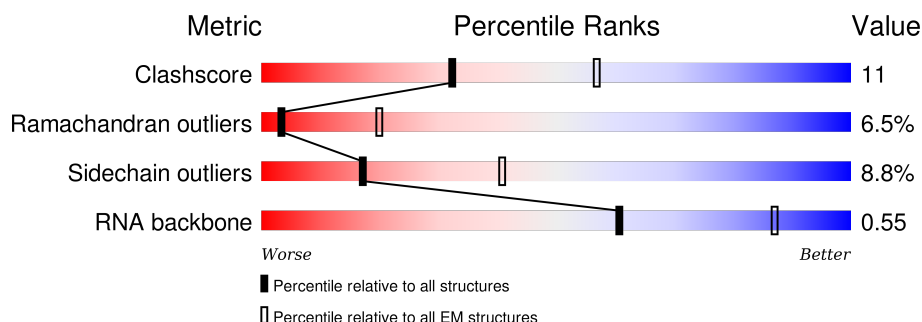
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.

























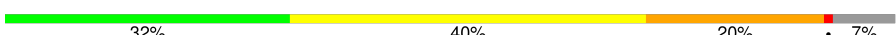


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	0	57	75% 19% . .
2	1	55	58% 25% 7% 9%
3	2	46	78% 20% .
4	3	65	77% 17% 5% .
5	4	38	55% 39% . .
6	5	165	25% 38% 18% 8% 10%
7	6	121	17% 6% . 75%
8	7	3	100%

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Mol	Chain	Length	Quality of chain
9	A	2903	
10	B	118	
11	C	273	
12	D	209	
13	E	201	
14	F	179	
15	G	177	
16	H	149	
17	I	142	
18	J	142	
19	K	123	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	115	
25	Q	118	
26	R	103	
27	S	110	
28	T	100	
29	U	104	
30	V	94	
31	W	85	
32	X	78	
33	Y	63	

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Mol	Chain	Length	Quality of chain
34	Z	59	<div><div></div><div>54%</div><div>34%</div><div>8%</div><div></div></div>
35	a	19	<div><div></div><div>32%</div><div>5%</div><div>63%</div><div></div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 90700 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	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 7 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 8 is a RNA chain called P-tRNA CCA-end.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	3	Total	C	N	O	P	0	0
			58	28	11	17	2		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 18 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 20 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 21 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 22 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 23 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 27 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 28 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 29 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 33 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

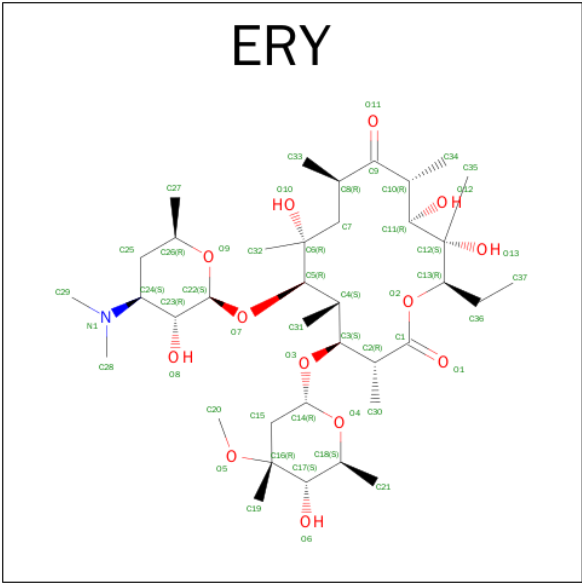
- Molecule 34 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 35 is a protein called ErmCL nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	a	7	Total	C	N	O	0	3
			36	27	4	5		

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).

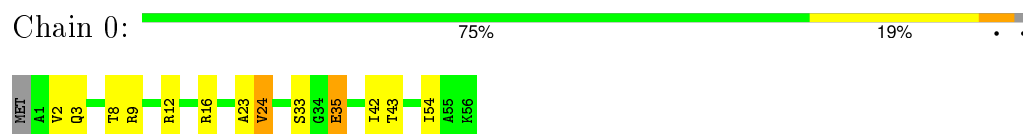


Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	N	O	0
			51	37	1	13	

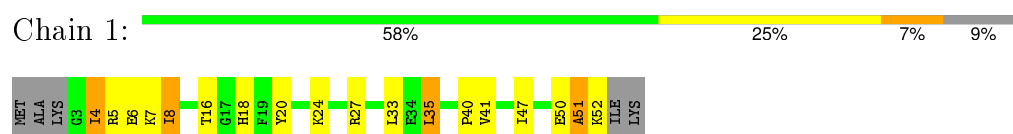
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

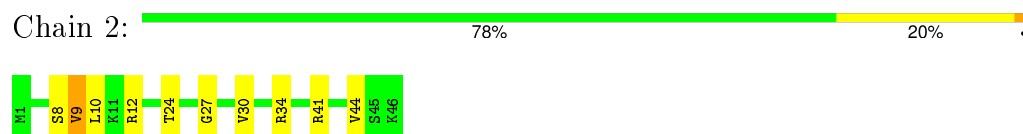
- Molecule 1: 50S ribosomal protein L32



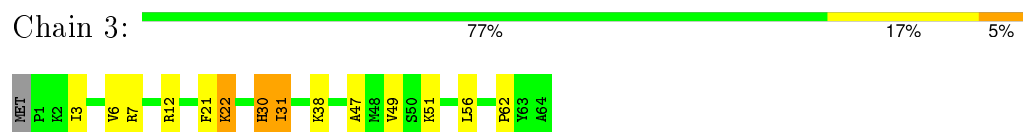
- Molecule 2: 50S ribosomal protein L33



- Molecule 3: 50S ribosomal protein L34



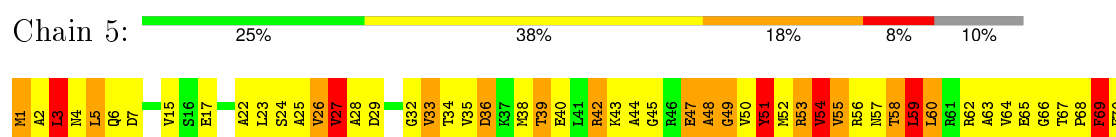
- Molecule 4: 50S ribosomal protein L35

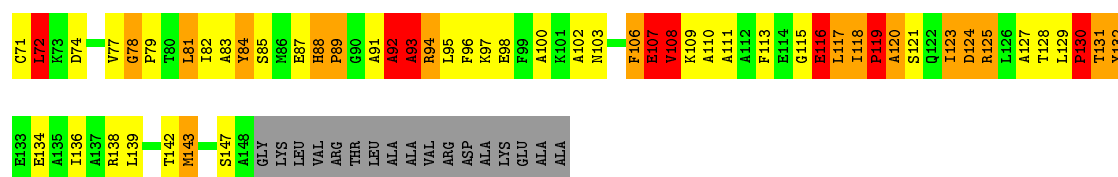


- Molecule 5: 50S ribosomal protein L36



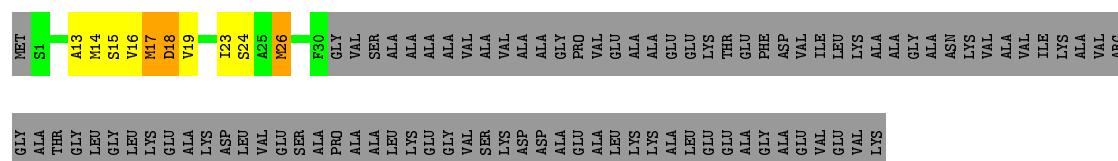
- Molecule 6: 50S ribosomal protein L10





- Molecule 7: 50S ribosomal protein L7/L12

Chain 6: 17% 6% 75%



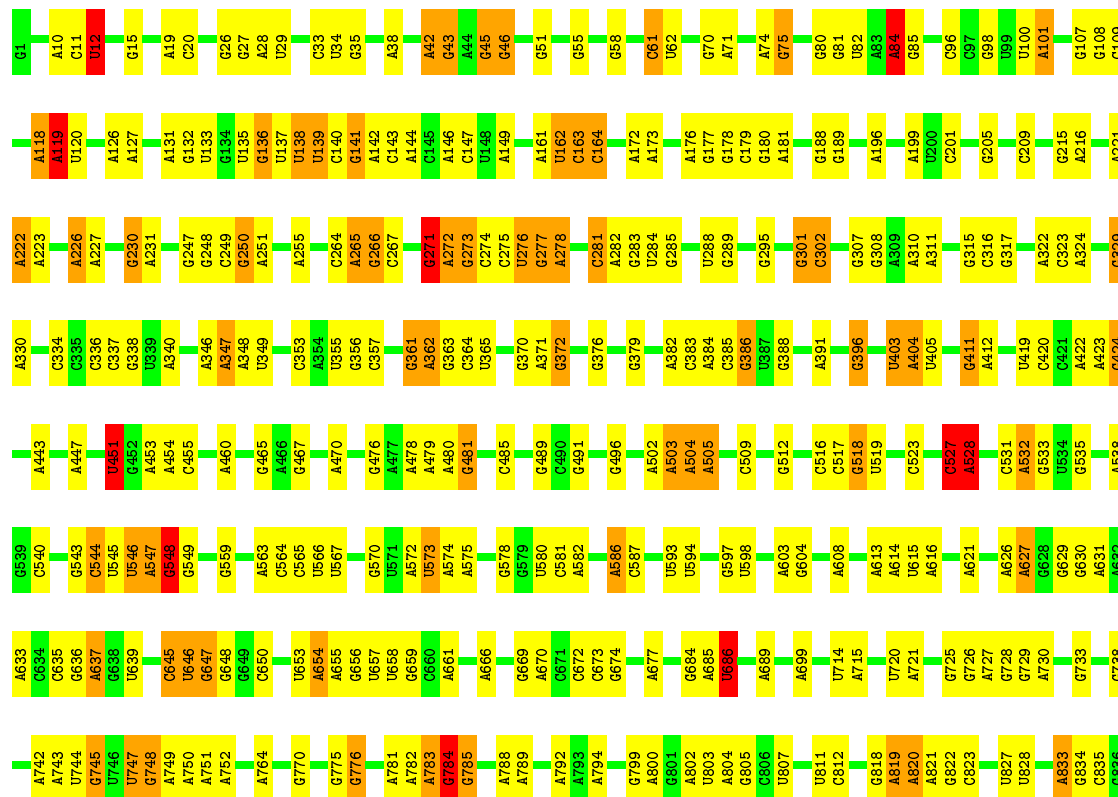
- Molecule 8: P-tRNA CCA-end

Chain 7: 100%

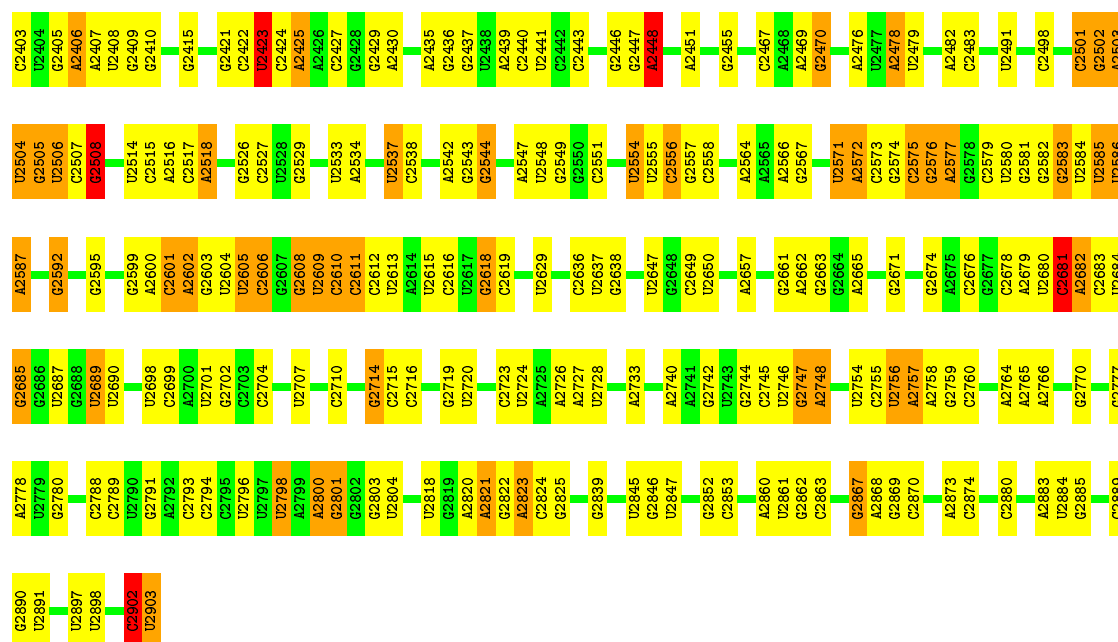


- Molecule 9: 23S rRNA

Chain A: 58% 30% 9%



A2311	U2210	U2139	C2055	U1965	A1819	U1747	A1618	A1509	C1398	G1309	U1199	G1124	A1046	C837
U2312	A2211	G2141	G2056	U1966	U1820	C1748	G1622	G1510	A1403	G1310	U1203	G1125	G1047	C838
C2313	A2212	G2142	A2057	C1967	G1824	G1750	G1622	G1514	C1404	U1312	A1204	A1129	G1051	U839
A2314	U2213	C2143	A2059	C1967	G1824	G1750	G1622	A1515	C1404	U1313	G1206	U1130	C1052	C841
G2318	C2214	C2144	A2060	A1960	A1829	G1753	A1754	U1523	C1414	C1314	C1207	U1132	C1053	A845
U2319	A2225	C2145	G2061	U1963	G1830	A1757	C1638	G1524	U1415	G1317	U1219	A1134	A1057	U846
U2320	C2226	C2146	A2062	U1963	G1831	A1757	C1639	G1524	G1416	U1322	U1224	A1134	U1058	U847
U2321	A2227	G2148	C2063	A1966	G1832	A1758	G1643	C1533	A1418	A1322	G1223	G1135	U1059	G855
U2322	U2228	U2149	C2064	C1967	G1833	A1759	G1644	U1534	A1419	G1323	U1224	G1136	U1060	G856
G2323	U2229	C2150	A2069	G1968	C1837	C1760	G1645	A1535	A1420	G1324	U1224	U1141	U1061	G859
U2324	G2230	U2151	G2070	A1969	C1838	C1761	G1646	C1536	A1420	U1327	C1229	C1140	G1062	G860
G2325	U2231	A2152	A2071	A1970	G1839	A1762	U1647	G1537	C1428	A1327	U1229	U1142	G1063	A861
C2326	C2232	C2153	C2072	U1971	C1843	C1764	U1648	G1538	G1429	U1328	G1232	A1142	U1064	G861
A2327	G2238	A2154	C2073	G1972	C1844	C1764	G1649	U1542	G1430	C1330	G1233	U1149	U1066	G864
U2328	U2239	U2155	U2074	U1979	G1847	G1770	A1652	G1543	G1435	A1336	G1233	G1149	A1067	G865
U2329	U2240	G2157	U2075	G1980	A1847	C1771	A1652	U1543	G1436	G1337	G1233	C1150	G1068	G866
G2330	A2241	A	C2091	G1980	A1848	A1772	G1653	A1553	C1437	G1337	G1233	A1151	A1069	A877
C2331	G2244	G	U2092	G1983	A1848	A1772	G1653	A1553	C1437	G1337	G1233	C1151	A1070	A878
U2332	U2244	C	C2093	C	G1857	C1774	A1654	C1565	A1439	U1339	A1247	G1153	G1071	G882
U2333	U2244	C	A2094	U1991	A1858	U1775	A1655	A1566	A1440	U1340	G1248	G1154	G1072	G883
U2334	U2244	C	A2094	U1991	A1858	U1775	A1655	A1566	A1440	U1340	G1248	G1154	G1072	G884
A2335	G2250	G	C2103	U1992	U1864	G1776	G1659	G1567	G1441	A1342	U1249	A1155	G1074	A
U2336	G2251	A	C2104	U1993	U1864	G1776	G1659	G1567	G1441	A1342	U1249	A1155	G1074	C
G2337	G2252	C	C2104	U1993	U1864	G1776	G1659	G1567	G1441	A1342	U1249	A1155	G1074	C
U2341	U2259	U	U2105	C1996	G1867	U1778	U1662	A1570	U1444	U1344	G1250	G1157	G1075	C
U2342	U2259	C	U2106	C1997	C1868	U1778	U1662	A1570	U1444	U1344	G1250	G1157	G1075	C
U2343	U2262	U	G2107	A1998	G1869	U1782	C1670	A1571	G1445	C1349	G1252	G1160	A1077	A
U2344	C2263	U	A2108	U2011	A1870	A1784	C1670	A1571	G1445	C1349	G1252	G1160	A1077	U
G2345	U2263	A	U2109	U2011	A1871	A1784	C1670	A1571	G1445	C1349	G1252	G1160	A1077	C
U2346	A2267	A	C2110	A2015	A1872	A1785	G1674	U1578	G1452	C1350	G1256	A1169	A1080	C
U2347	A2268	U	U	U2016	A1873	A1786	A1677	U1580	U1458	U1352	A1262	C1170	U1083	C
U2348	U2271	U	U	U2017	G1884	U1790	A1677	C1581	C1459	A1353	A1263	C1171	A1084	G
A2352	C	C	A	G2018	C1905	C1790	G1681	U1583	G1465	A1354	A1264	U1173	A1085	
G2353	A2274	C	G	A2019	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C994
C2354	G2275	A	G	A2020	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C995
G2355	C2276	C	A	C2021	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C996
U2361	A2277	C	U	U2022	A1913	U1795	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C997
G2362	G2278	U	A	C2023	C1914	U1797	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C998
U2363	G2279	U	G	G2024	U1915	U1797	G1681	U1584	U1466	G1355	A1265	U1174	A1086	C999
G2365	G2282	U	U	A2030	A1927	C1800	G1703	U1591	U1474	A1365	A1269	C1177	A1089	A899
C2368	C2283	G	G	A2031	A1928	A1801	G1703	U1592	U1475	A1365	A1269	C1177	A1089	A910
U2383	A2284	G	G	G2032	G1929	A1802	G1703	U1593	A1477	A1378	A1272	U1181	U1094	A911
G2383	G2285	G	G	A2033	G1930	A1803	G1715	U1594	G1478	U1379	U1273	U1183	A1096	C912
U2384	G2286	A	A	G2037	G1935	A1805	G1722	U1606	G1482	G1382	G1281	G1186	A1098	C913
C2385	A2287	U	U	C2038	A1936	A1805	G1722	U1607	U1485	A1384	A1284	U1188	G1022	C914
A2386	G2288	C	C	U2039	A1937	A1805	G1722	U1608	U1486	A1385	A1284	U1188	G1022	C915
U2387	G2289	U	U	G2040	A1938	A1805	G1722	U1609	U1487	C1386	A1284	U1188	G1022	C916
G2388	A2297	U	U	C2043	U1939	G1811	G1722	U1610	U1487	A1387	A1284	U1188	G1022	C917
U2389	A2298	U	U	C2043	U1939	G1811	G1722	U1610	U1487	A1387	A1284	U1188	G1022	C918
U2393	U2305	U	U	C2043	U1939	G1811	G1722	U1610	U1487	A1387	A1284	U1188	G1022	C919
G2396	G2307	U	U	C2043	U1939	G1811	G1722	U1610	U1487	A1387	A1284	U1188	G1022	C920
U2402	G2308	U	U	C2043	U1939	G1811	G1722	U1610	U1487	A1387	A1284	U1188	G1022	C921



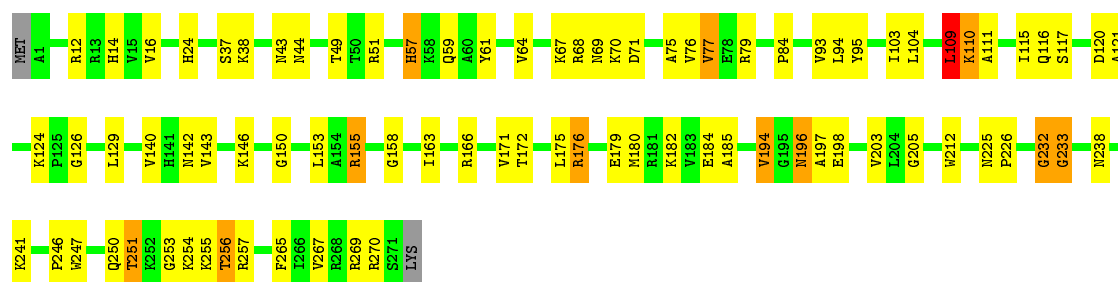
- Molecule 10: 5S rRNA

Chain B: 68% 25% 8%



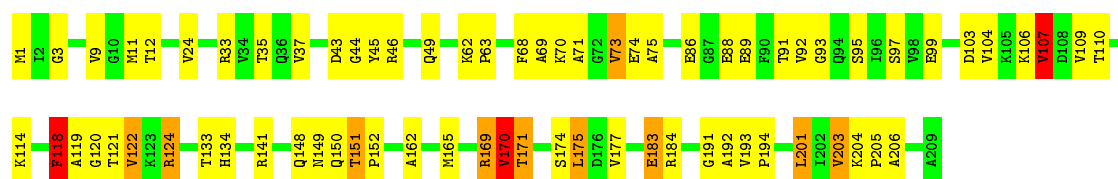
- Molecule 11: 50S ribosomal protein L2

Chain C: 68% 27% 5%

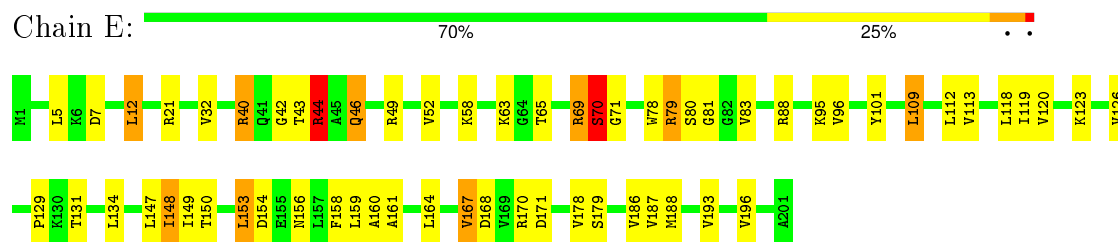


- Molecule 12: 50S ribosomal protein L3

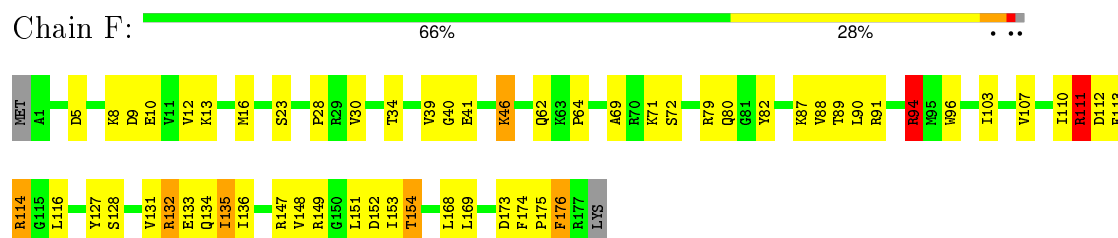
Chain D: 66% 28% 5%



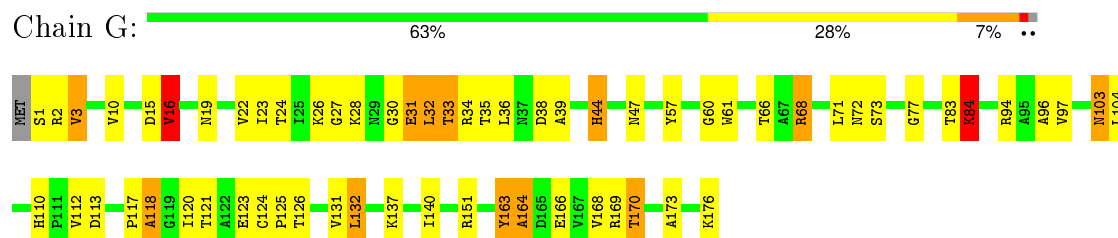
- Molecule 13: 50S ribosomal protein L4



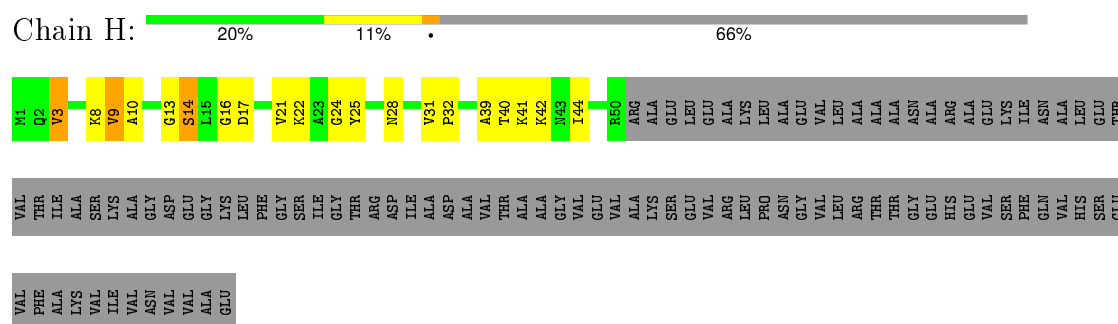
- Molecule 14: 50S ribosomal protein L5



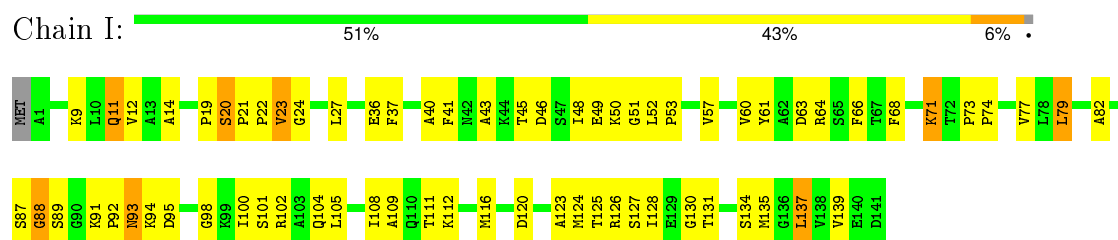
- Molecule 15: 50S ribosomal protein L6



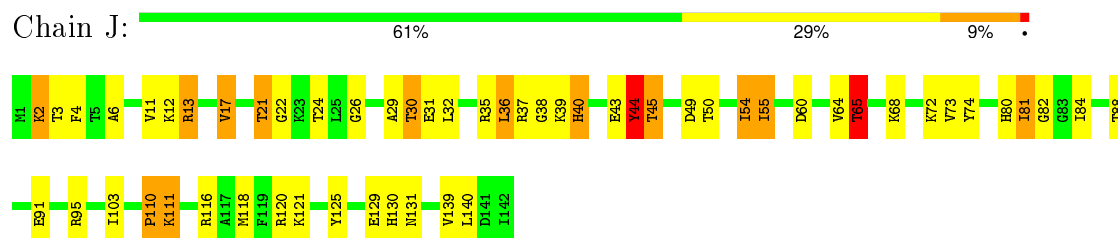
- Molecule 16: 50S ribosomal protein L9



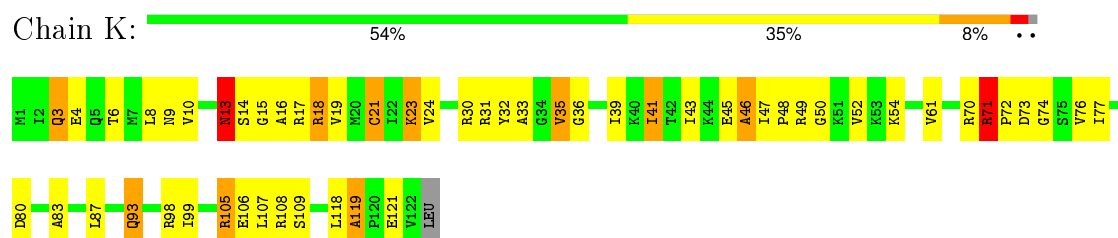
- Molecule 17: 50S ribosomal protein L11



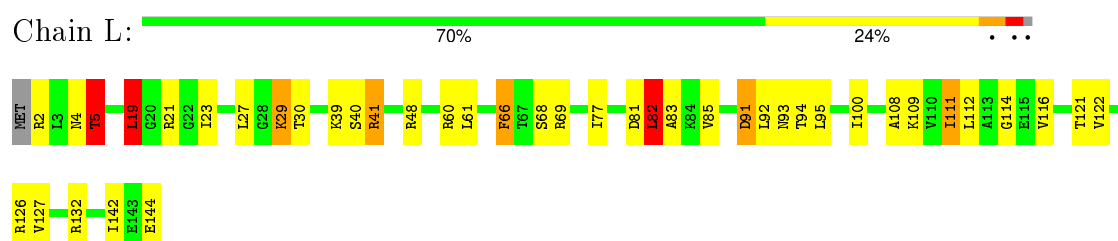
- Molecule 18: 50S ribosomal protein L13



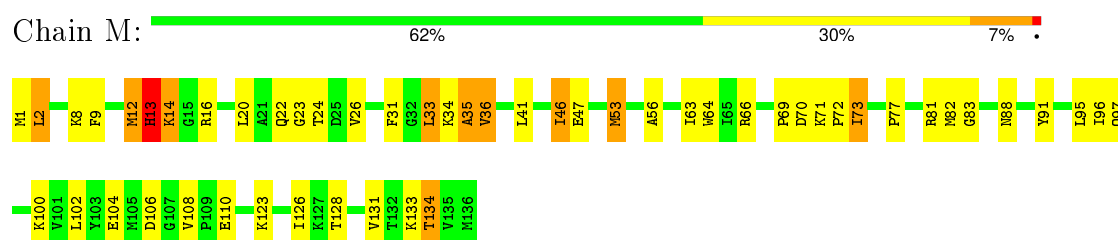
- Molecule 19: 50S ribosomal protein L14



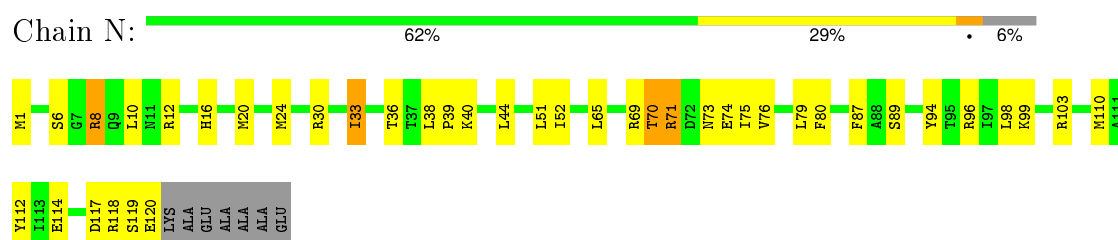
- Molecule 20: 50S ribosomal protein L15



- Molecule 21: 50S ribosomal protein L16

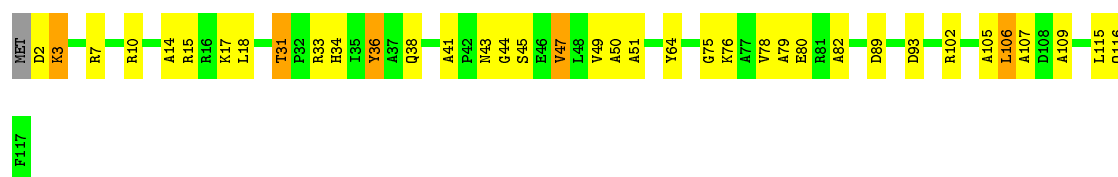


- Molecule 22: 50S ribosomal protein L17



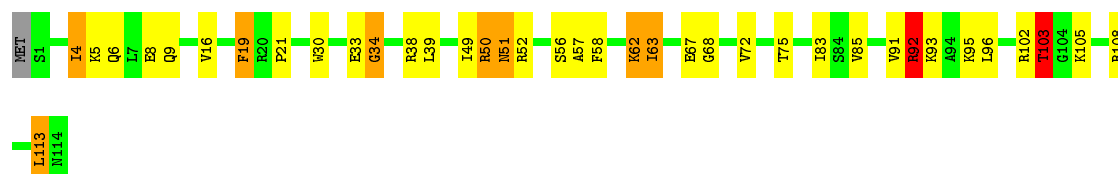
- Molecule 23: 50S ribosomal protein L18





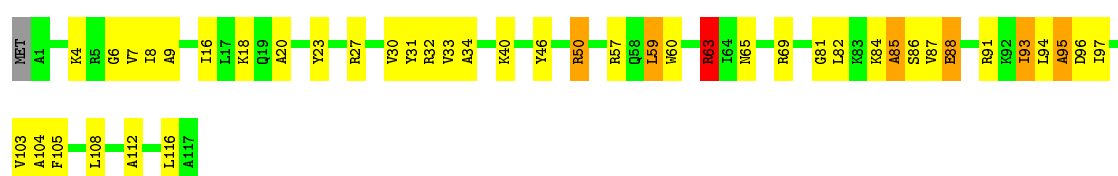
- Molecule 24: 50S ribosomal protein L19

Chain P: 66% 24% 7% ..



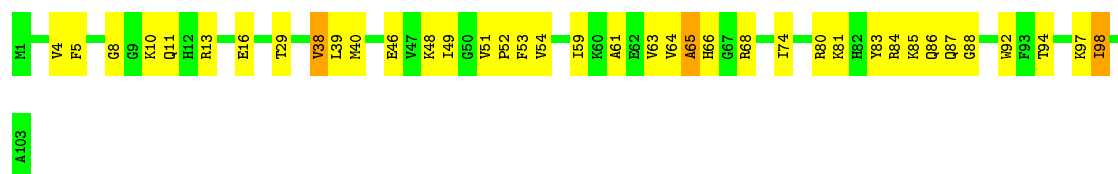
- Molecule 25: 50S ribosomal protein L20

Chain Q: 63% 31% 5% ..



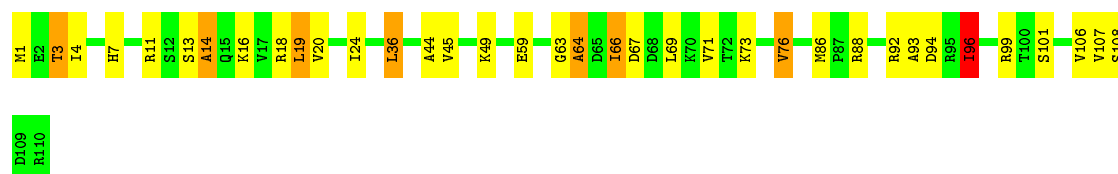
- Molecule 26: 50S ribosomal protein L21

Chain R: 63% 34% 3% .



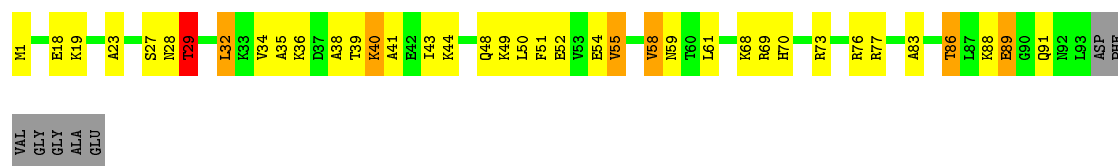
- Molecule 27: 50S ribosomal protein L22

Chain S: 67% 25% 6% .



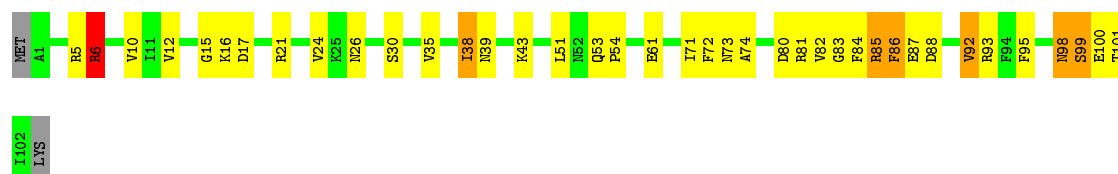
- Molecule 28: 50S ribosomal protein L23

Chain T: 55% 31% 6% • 7%



- Molecule 29: 50S ribosomal protein L24

Chain U: 61% 31% 6% ..



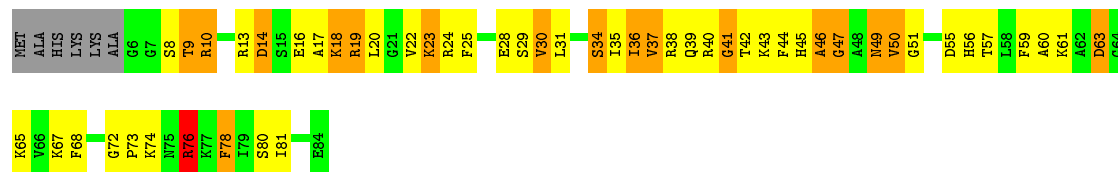
- Molecule 30: 50S ribosomal protein L25

Chain V: 79% 19% .



- Molecule 31: 50S ribosomal protein L27

Chain W: 32% 40% 20% 7% .



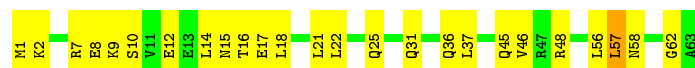
- Molecule 32: 50S ribosomal protein L28

Chain X: 71% 22% 5% ..



- Molecule 33: 50S ribosomal protein L29

Chain Y: 60% 38% .



- Molecule 34: 50S ribosomal protein L30

Chain Z: 54% 34% 8% ..



● Molecule 35: ErmCL nascent chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	269163	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	0	0.54	0/450	0.70	0/599
10	B	0.66	0/2828	1.10	2/4410 (0.0%)
11	C	0.54	0/2121	0.79	3/2852 (0.1%)
12	D	0.57	0/1586	0.77	1/2134 (0.0%)
13	E	0.53	0/1571	0.76	2/2113 (0.1%)
14	F	0.50	0/1434	0.71	1/1926 (0.1%)
15	G	0.55	0/1343	0.73	0/1816
16	H	0.53	0/389	0.73	0/523
17	I	0.62	0/1046	0.84	1/1410 (0.1%)
18	J	0.63	1/1152 (0.1%)	0.78	0/1551
19	K	0.65	1/947 (0.1%)	0.77	0/1268
2	1	0.53	0/416	0.74	0/554
20	L	0.56	0/1054	0.79	2/1403 (0.1%)
21	M	0.61	0/1093	0.77	0/1460
22	N	0.51	0/973	0.68	0/1301
23	O	0.46	0/902	0.70	0/1209
24	P	0.52	0/929	0.78	1/1242 (0.1%)
25	Q	0.62	0/960	0.71	1/1278 (0.1%)
26	R	0.61	1/829 (0.1%)	0.76	0/1107
27	S	0.54	0/864	0.73	0/1156
28	T	0.55	0/744	0.85	1/994 (0.1%)
29	U	0.56	0/787	0.78	0/1051
3	2	0.53	0/380	0.70	0/498
30	V	0.48	0/766	0.67	1/1025 (0.1%)
31	W	0.69	0/603	1.00	1/797 (0.1%)
32	X	0.50	0/635	0.79	1/848 (0.1%)
33	Y	0.46	0/510	0.75	0/677
34	Z	0.54	0/453	0.84	1/605 (0.2%)
35	a	0.86	0/32	1.43	1/40 (2.5%)
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	6	0.59	0/227	0.65	0/304
8	7	0.16	0/64	0.54	0/97
9	A	0.80	15/68626 (0.0%)	1.22	301/107056 (0.3%)
All	All	0.74	18/98661 (0.0%)	1.12	347/147901 (0.2%)

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
11	C	0	1
12	D	0	1
18	J	0	1
19	K	0	1
6	5	0	1
All	All	0	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	984	A	N9-C4	-8.36	1.32	1.37
9	A	528	A	N9-C4	-6.60	1.33	1.37
9	A	1142	A	N9-C4	-6.51	1.33	1.37
9	A	783	A	N9-C4	-6.27	1.34	1.37
9	A	1569	A	N9-C4	-6.16	1.34	1.37

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1073	A	N1-C6-N6	-20.00	106.60	118.60
9	A	1073	A	C5-C6-N6	14.06	134.95	123.70
9	A	2053	G	N1-C6-O6	13.89	128.23	119.90
9	A	984	A	C2-N3-C4	-12.15	104.53	110.60
9	A	961	C	O5'-P-OP2	-11.75	95.12	105.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide

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Mol	Chain	Res	Type	Group
11	C	233	GLY	Peptide
12	D	9	VAL	Peptide
18	J	110	PRO	Peptide
19	K	71	ARG	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	444	0	461	16	0
2	1	409	0	440	15	0
3	2	377	0	418	5	0
4	3	504	0	574	10	0
5	4	302	0	340	14	0
6	5	1117	0	1155	123	0
7	6	227	0	237	6	0
8	7	58	0	33	12	0
9	A	61274	0	30817	801	0
10	B	2529	0	1281	20	0
11	C	2082	0	2157	54	0
12	D	1565	0	1616	52	0
13	E	1552	0	1619	40	0
14	F	1410	0	1447	44	0
15	G	1323	0	1374	37	0
16	H	384	0	405	12	0
17	I	1032	0	1088	53	0
18	J	1129	0	1162	50	0
19	K	938	0	1012	40	0
20	L	1045	0	1117	37	0
21	M	1074	0	1157	29	0
22	N	960	0	1000	30	0
23	O	892	0	923	21	0
24	P	917	0	965	38	0
25	Q	947	0	1022	52	0
26	R	816	0	839	35	0
27	S	857	0	922	28	0
28	T	738	0	807	33	0
29	U	779	0	834	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	753	0	780	12	0
31	W	596	0	610	80	0
32	X	625	0	655	18	0
33	Y	509	0	543	13	0
34	Z	449	0	491	15	0
35	a	36	0	34	0	0
36	A	51	0	67	8	0
All	All	90700	0	60402	1640	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 11.

The worst 5 of 1640 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)
9:A:912:C:OP1	21:M:8:LYS:NZ	1.79	1.15
9:A:2062:A:N6	36:A:9000:ERY:H273	1.64	1.13
9:A:2061:G:OP2	13:E:63:LYS:NZ	1.88	1.06
6:5:71:CYS:HB3	6:5:117:LEU:HD12	1.33	1.04
9:A:2579:C:H2'	9:A:2580:U:H5'	1.40	1.03

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	
1	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	21
2	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	2	26
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	18
6	5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	2
7	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	4	40
11	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	29
12	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	24
13	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3	31
14	F	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	8	50
15	G	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	1	14
16	H	48/149 (32%)	29 (60%)	14 (29%)	5 (10%)	1	12
17	I	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	26
18	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2	26
19	K	120/123 (98%)	95 (79%)	15 (12%)	10 (8%)	1	18
20	L	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	4	41
21	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	18
22	N	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	24	68
23	O	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	21	65
24	P	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	19
25	Q	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	41
26	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	44
27	S	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	3	33
28	T	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	10
29	U	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	13
30	V	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
31	W	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	2
32	X	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	4	37
33	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	25
34	Z	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	40
35	a	1/19 (5%)	1 (100%)	0	0	100	100
All	All	3385/3714 (91%)	2613 (77%)	553 (16%)	219 (6%)	3	26

5 of 219 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA

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	47/48 (98%)	46 (98%)	1 (2%)	61	85
2	1	45/49 (92%)	42 (93%)	3 (7%)	20	60
3	2	38/38 (100%)	35 (92%)	3 (8%)	15	54
4	3	51/52 (98%)	46 (90%)	5 (10%)	10	43
5	4	34/34 (100%)	31 (91%)	3 (9%)	12	48
6	5	112/123 (91%)	93 (83%)	19 (17%)	2	20
7	6	26/85 (31%)	22 (85%)	4 (15%)	3	24
11	C	216/218 (99%)	202 (94%)	14 (6%)	21	61
12	D	164/164 (100%)	151 (92%)	13 (8%)	15	54
13	E	165/165 (100%)	146 (88%)	19 (12%)	7	36
14	F	148/150 (99%)	138 (93%)	10 (7%)	20	59
15	G	137/138 (99%)	122 (89%)	15 (11%)	8	39
16	H	40/114 (35%)	39 (98%)	1 (2%)	55	82
17	I	109/110 (99%)	105 (96%)	4 (4%)	41	75
18	J	116/116 (100%)	100 (86%)	16 (14%)	4	29
19	K	103/104 (99%)	92 (89%)	11 (11%)	8	39
20	L	102/103 (99%)	95 (93%)	7 (7%)	19	59
21	M	109/109 (100%)	93 (85%)	16 (15%)	4	26
22	N	100/103 (97%)	93 (93%)	7 (7%)	19	58
23	O	86/87 (99%)	78 (91%)	8 (9%)	11	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	P	99/100 (99%)	91 (92%)	8 (8%)	15	53
25	Q	89/90 (99%)	81 (91%)	8 (9%)	12	47
26	R	84/84 (100%)	78 (93%)	6 (7%)	18	58
27	S	93/93 (100%)	84 (90%)	9 (10%)	10	43
28	T	80/84 (95%)	77 (96%)	3 (4%)	40	74
29	U	83/85 (98%)	76 (92%)	7 (8%)	14	51
30	V	78/78 (100%)	75 (96%)	3 (4%)	40	74
31	W	59/63 (94%)	53 (90%)	6 (10%)	9	41
32	X	67/68 (98%)	61 (91%)	6 (9%)	12	47
33	Y	55/55 (100%)	52 (94%)	3 (6%)	27	66
34	Z	48/49 (98%)	40 (83%)	8 (17%)	3	21
35	a	4/18 (22%)	4 (100%)	0	100	100
All	All	2787/2977 (94%)	2541 (91%)	246 (9%)	17	48

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	I	63	ASP
19	K	54	LYS
31	W	49	ASN
18	J	2	LYS
18	J	73	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
27	S	15	GLN
33	Y	41	HIS
30	V	44	HIS
14	F	26	GLN
30	V	80	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	117/118 (99%)	17 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	7	1/3 (33%)	0	0
9	A	2850/2903 (98%)	466 (16%)	43 (1%)
All	All	2968/3024 (98%)	483 (16%)	43 (1%)

5 of 483 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	12	U
9	A	15	G
9	A	34	U
9	A	35	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1110	G
9	A	1535	A
9	A	2601	C
9	A	1247	A
9	A	1378	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
36	ERY	A	9000	-	53,53,53	0.78	1 (1%)	82,82,82	1.64	15 (18%)

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
36	ERY	A	9000	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.18	1.59	1.55

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C25-C24-C23	-4.98	102.73	110.05
36	A	9000	ERY	O7-C5-C6	-4.64	100.47	106.45
36	A	9000	ERY	C3-C2-C1	-3.57	102.94	109.85
36	A	9000	ERY	O2-C1-O1	-3.43	117.24	123.88
36	A	9000	ERY	C15-C16-C17	-2.97	104.03	107.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	ERY	8	0

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.