



## wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 10:10 PM EDT

PDB ID : 5GAH  
EMDB ID: : EMD-8004  
Title : RNC in complex with SRP with detached NG domain  
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.  
Deposited on : 2015-11-26  
Resolution : 3.80 Å(reported)

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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) : rb-20027939

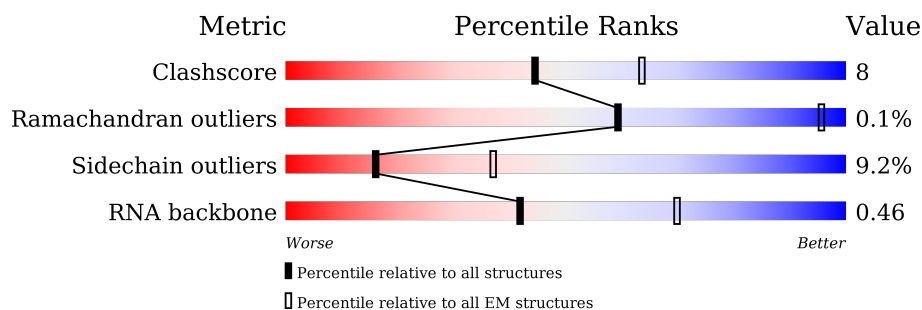
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.
























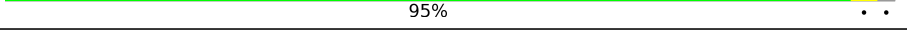



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	1	113	17% 18% . 62%
2	2	3	33% 33% 33%
3	A	2903	54% 37% 8% ..
4	B	120	74% 23% .
5	C	273	70% 26% ..
6	D	209	78% 20% .
7	E	201	77% 20% .
8	F	179	60% 35% ..

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Mol	Chain	Length	Quality of chain
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	
29	a	59	
30	b	57	
31	c	55	
32	d	46	
33	e	65	

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Mol	Chain	Length	Quality of chain
34	f	38	<div><div></div><div>92%</div><div>8%</div></div>
35	i	453	<div><div></div><div>26%</div><div></div><div>72%</div></div>
36	k	18	<div><div></div><div>89%</div><div>11%</div></div>

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 94027 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.



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

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	126	Total	C	N	O	S	0	0
			916	575	169	161	11		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	P	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	
37	B	11	Total	Mg	0
			11	11	
37	b	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	A	412	Total	Mg	0
			412	412	
37	2	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	

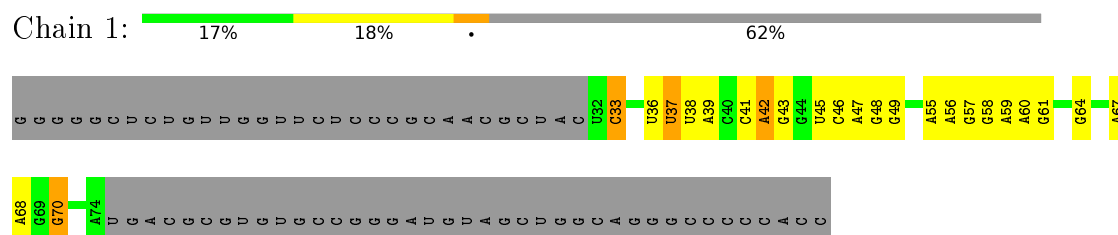
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	

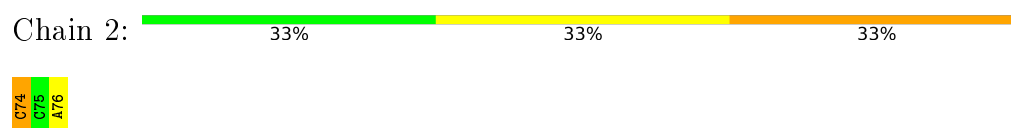
### 3 Residue-property plots

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.

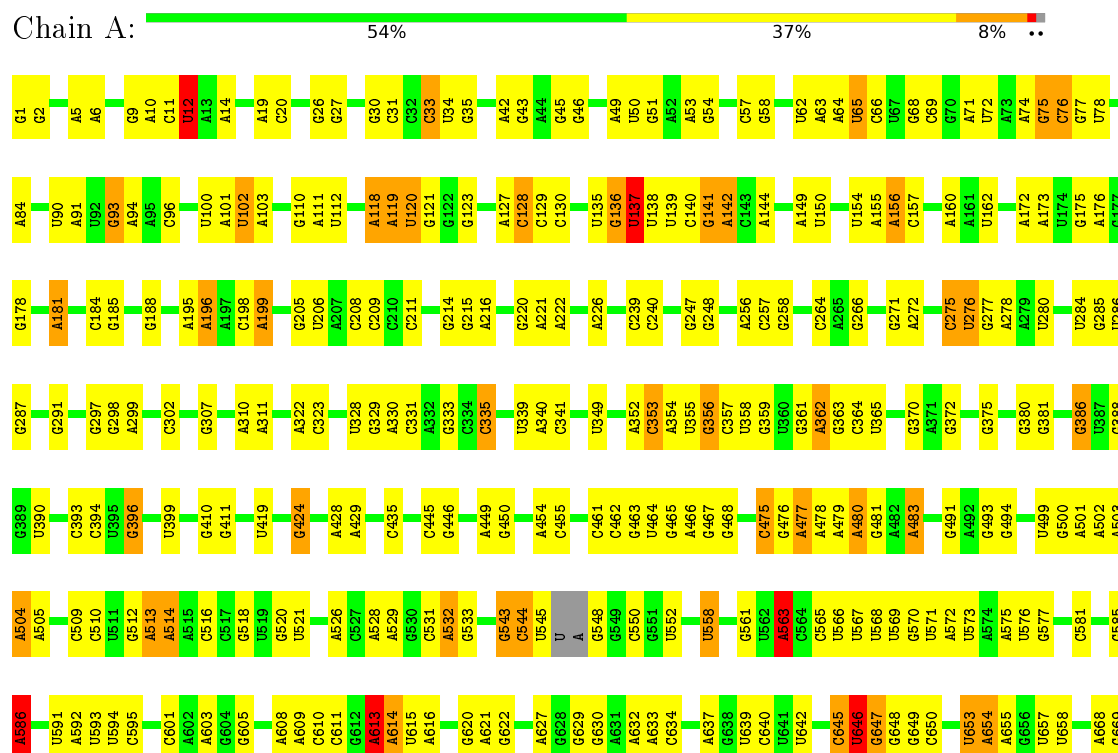
#### • Molecule 1: SRP 4.5S RNA



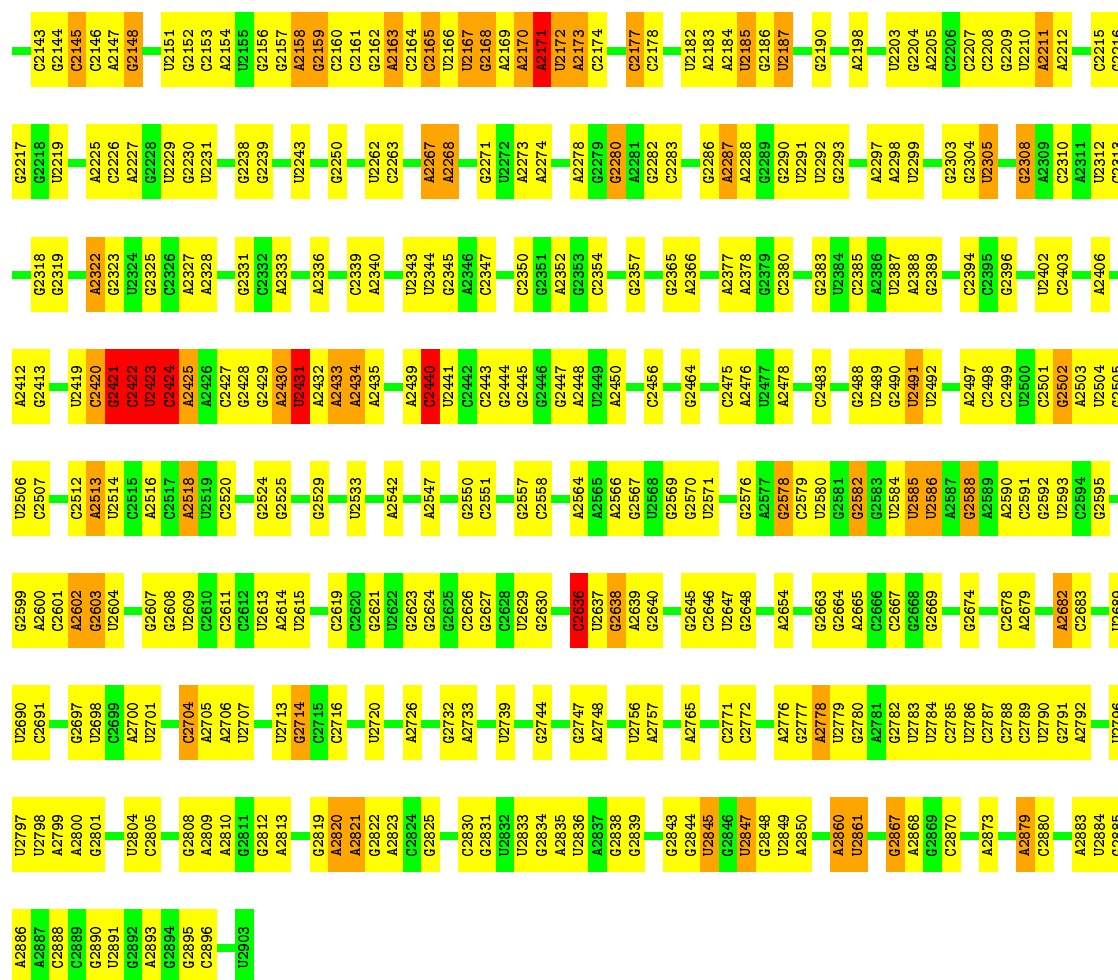
#### • Molecule 2: tRNA CCAend



#### • Molecule 3: 23S rRNA

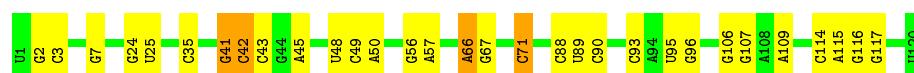


G2066	A1960	C1870	G1774	U1578	G1492	G1440	U199	G1300	U1023	U931	A845	G776	A670
A2060	C1961	A1871	U1775	G1581	C1493	G1414	A1205	U1101	G1024	U932	U846	G777	C671
G2061	U1963	G1873	A1780	C1582	A1494	C1415	G1206	A1102	G1025	A933	U847	G778	G672
A2062	U1966	U1874	U1781	U1583	A1496	G1416	G1210	G1104	A1027	C946	A849	U779	G673
G2069	C1967	G1875	U1782	U1584	U1497	G1417	G1211	U1105	A1028	A947	U850	G780	G674
A2070	A1970	A1876	A1785	C1585	C1498	G1418	G1212	G1106	U1033	C948	U851	A781	A677
A2071	A1977	A1877	A1786	A1590	C1499	A1419	G1218	G1110	G1038	G949	G857	A782	C676
C2072	U1971	U1878	A1787	A1591	A1500	A1420	G1218	A1111	G1039	G953	G858	A783	C678
C2073	G1972	U1880	A1789	C1592	A1501	G1421	U1329	G1112	A1038	G957	U859	G784	C679
U2074	G1973	C1881	C1790	A1597	U1506	G1422	A1230	G1115	A1040	U958	A861	G785	G681
A2077	C1974	G1888	A1791	A1598	C1507	G1424	U1231	G1116	U1044	G959	A862	A788	A685
U2086	G1980	A1794	A1700	A1598	C1508	G1425	G1236	G1125	C1044	A960	A863	U790	U686
G2087	A1981	C1795	A1603	A1508	A1509	G1426	G1237	G1126	A1045	C961	U864	C791	A706
U2088	U1982	C1604	G1706	G1426	A1510	A1427	G1238	A1126	A1047	A973	A794	A793	G707
A2090	G1983	G1707	G1707	G1605	G1511	A1428	C1243	A1127	A1048	C968	G869	A794	A711
G2093	U1991	C1708	C1708	C1606	A1515	G1432	A1247	A1128	G1056	U970	U870	C795	G712
U2097	G1992	G1710	A1608	C1607	G1516	A1433	U1248	A1129	A1057	A972	U871	G796	G713
A2097	U1993	A1711	A1609	A1610	G1517	A1434	U1249	U1130	A1058	A974	U872	G797	U714
G2101	C1997	G1715	A1614	A1615	G1524	G1436	G1250	A1133	U1060	A975	A877	G798	A717
G2102	C2000	G1721	G1615	C1526	A1525	U1438	G1251	A1134	U1061	A976	A878	A800	A718
C2103	G2012	A1722	A1616	G1527	A1528	A1439	G1252	G1135	G1062	A977	A879	A801	C719
U2105	A2013	U1725	C1617	A1528	G1529	A1443	A1253	G1136	G1064	A981	G880	A804	U720
U2106	U2106	U1725	A1617	A1529	U1443	U1443	U1254	U1139	U1066	A982	G881	C806	A722
G2107	G2018	U1729	G1627	G1530	C1531	U1446	C1257	G1140	A1067	A983	U807	U807	G729
A2108	U2109	G1730	G1628	A1532	A1533	C1446	U1258	U1141	G1068	A984	U808	G808	A730
U2109	C2021	G1731	G1631	A1533	C1534	C1447	U1259	A1142	A1070	C987	U809	U810	G733
G2110	U2022	C1732	G1632	A1534	G1448	G1449	A1260	A1143	G1071	A990	U811	C812	G738
U2111	G2023	G1735	A1634	A1535	G1449	A1365	C1261	G1149	C1072	C991	U813	U813	G738
G2112	G2024	U1736	A1637	A1536	G1450	A1366	A1262	C1150	A1073	C992	C814	C814	G738
U2113	C2025	G1737	C1637	G1537	G1451	A1367	A1262	G1154	G1074	G993	C815	C815	U741
A2114	U2036	G1737	C1638	G1537	G1452	G1374	G1266	A1155	C1075	C994	C816	C816	A742
G2115	G2027	G1738	C1639	U1542	A1463	U1379	U1267	A1156	C1076	C995	A819	A743	A743
G2116	A2030	G1743	G1642	G1543	C1463	U1383	A1268	G1168	U1077	A996	U894	U746	U746
U2117	U2031	A1744	G1643	A1544	G1464	A1383	A1269	A1169	C1078	C997	U895	U747	U747
A2119	G2032	A1744	G1644	A1545	G1465	G1386	G1270	C1170	A896	C998	A896	G822	A753
G2120	A2033	U1761	G1645	G1546	U1466	A1387	A1272	G1171	U1082	U999	C897	G823	U754
G2121	C2037	C1762	C1646	U1554	U1467	G1388	A1275	C1172	U1083	A1000	C898	U824	U754
G2122	G2038	C1762	U1647	U1554	U1468	U1388	A1275	U1173	A1084	A1001	A899	A825	U755
G2123	U2039	G1756	U1648	G1560	A1469	U1394	A1287	U	A1085	G1002	U906	U826	G756
A2126	G2040	A1757	G1649	U1563	A1470	U1395	A1287	A	G1086	C1005	G907	U827	A756
G2127	U2041	U1758	U1758	C1564	U1563	U1396	G1288	U	G1087	C1006	G908	U828	G757
G2128	C2042	A1759	A1652	C1565	C1565	U1397	C1289	G1177	A1088	C1007	C908	A829	C758
G2129	C2043	C1761	G1653	A1566	U1468	U1398	C1290	C1178	A1089	U1008	A909	G830	G759
U2130	C2047	A1762	A1654	A1566	G1482	U1399	U1294	G1179	A1090	A1009	A911	G831	G763
U2131	C2050	G1763	A1655	A1569	G1483	C1399	U1294	U1180	G1093	A1010	A911	U832	A764
G2133	U2051	C1764	G1660	A1570	U1484	U1400	G1300	U1181	U1094	G1011	G914	A833	C765
A2134	A2052	G1765	G1661	A1571	U1485	U1402	G1301	G1182	A1095	U1012	C915	G834	G765
G2135	G2053	A1664	A1664	A1572	U1489	A1403	A1302	G1187	A1096	C1013	G916	C835	C772
A2136	U2054	U1770	A1664	U1576	A1490	C1404	G1303	U1188	U1097	A1021	A917	U839	U773
G2138	C2055	A1773	G1667	C1577	G1491	U1406	A1308	U1198	G1099	G1022	U930	C840	G775



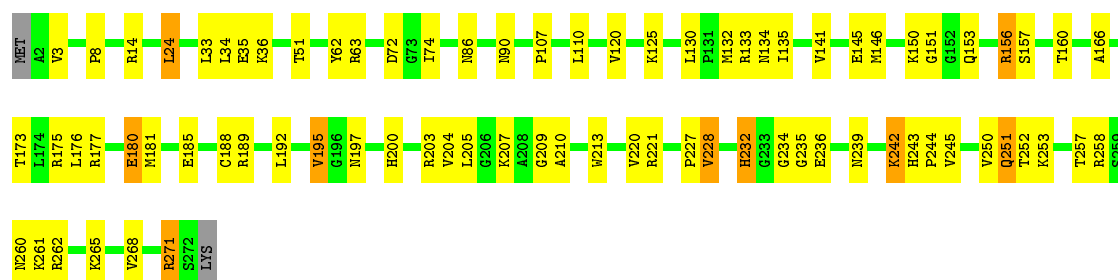
- Molecule 4: 5S rRNA

Chain B: 74% 23%

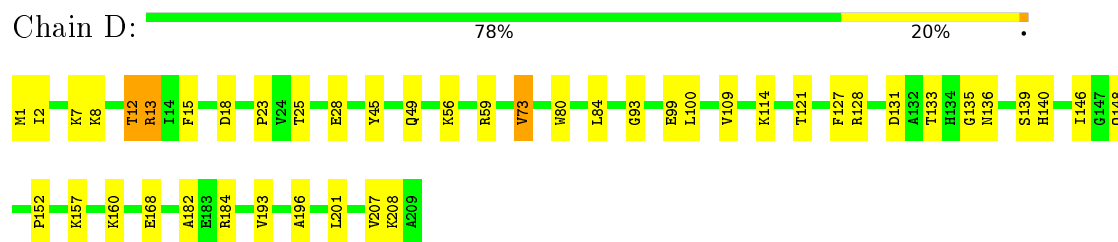


- Molecule 5: 50S ribosomal protein L2

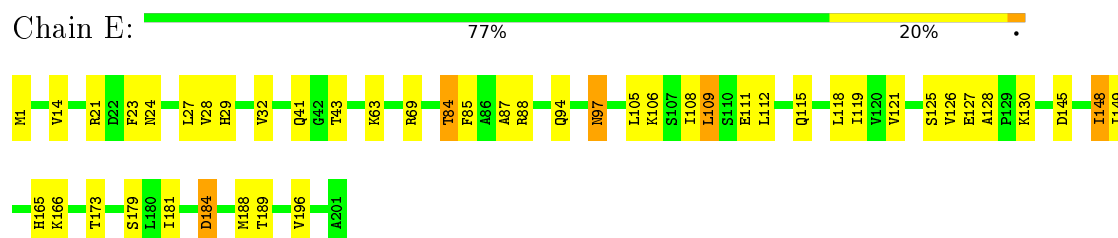
Chain C: 70% 26%



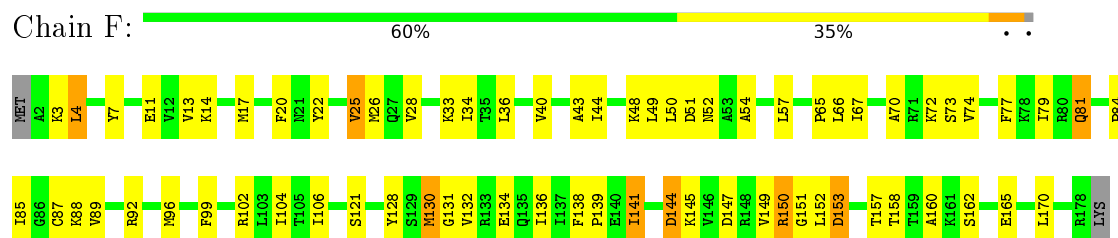
- Molecule 6: 50S ribosomal protein L3



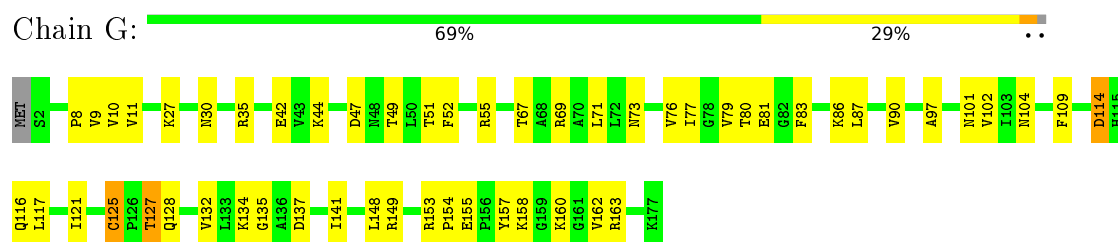
- Molecule 7: 50S ribosomal protein L4



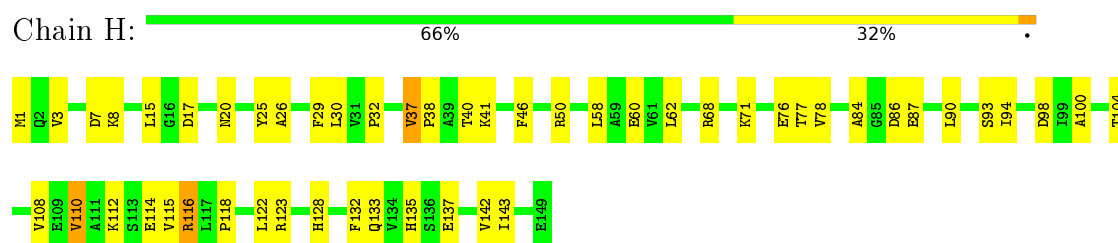
- Molecule 8: 50S ribosomal protein L5



- Molecule 9: 50S ribosomal protein L6

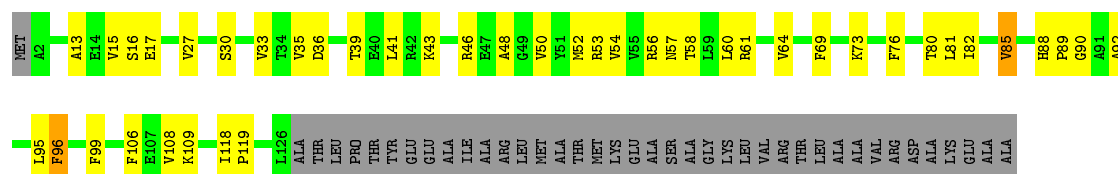


- Molecule 10: 50S ribosomal protein L9



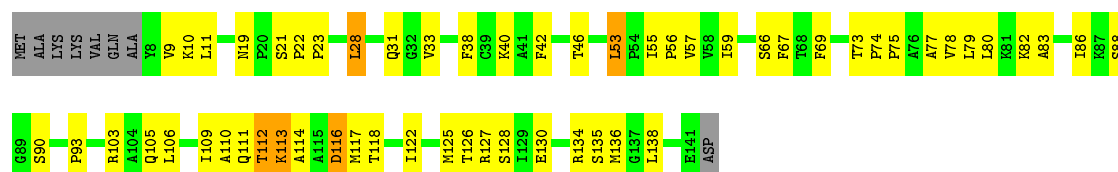
- Molecule 11: 50S ribosomal protein L10





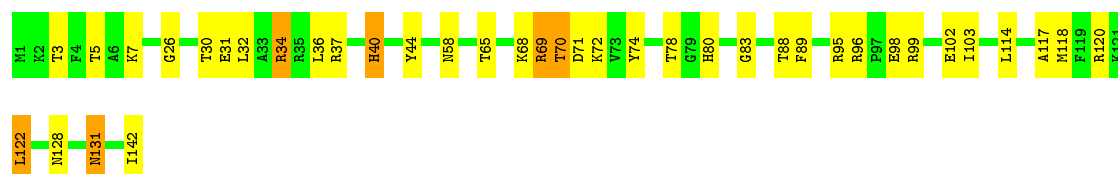
- Molecule 12: 50S ribosomal protein L11

Chain J: 54% 37% 6%



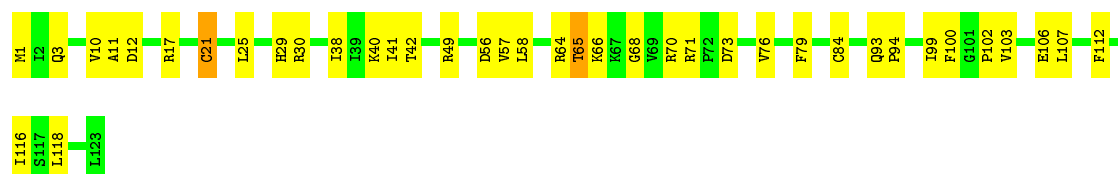
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 23% 4%



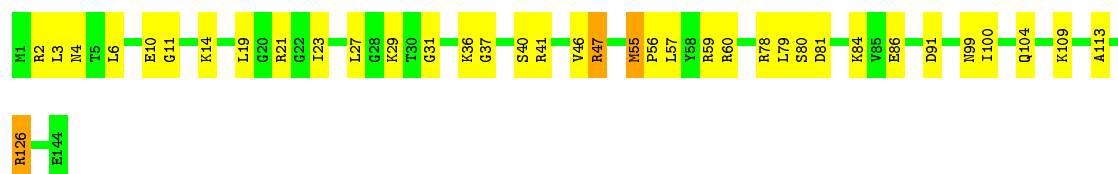
- Molecule 14: 50S ribosomal protein L14

Chain L: 68% 30% 2%



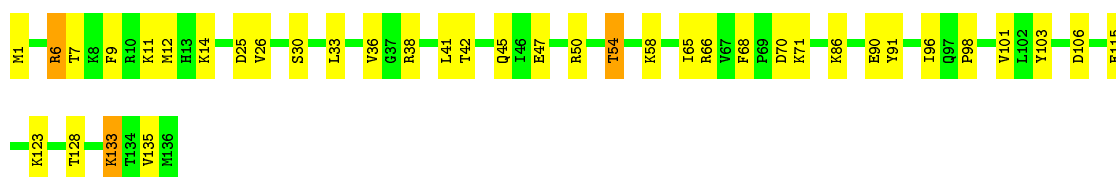
- Molecule 15: 50S ribosomal protein L15

Chain M: 74% 24% 2%



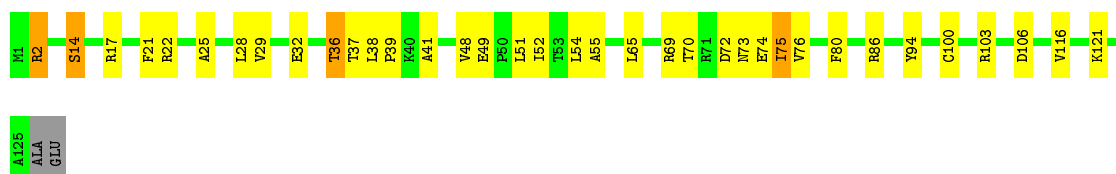
- Molecule 16: 50S ribosomal protein L16

Chain N: 72% 26% 2%



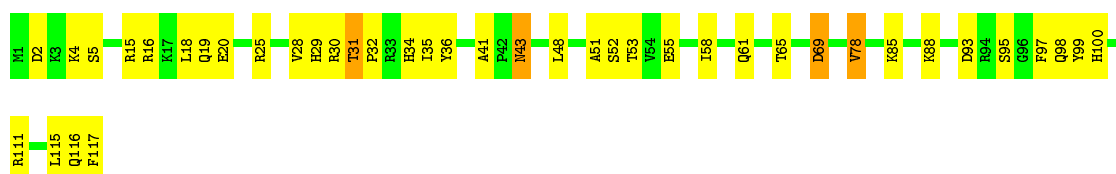
- Molecule 17: 50S ribosomal protein L17

Chain O: 70% 25%



- Molecule 18: 50S ribosomal protein L18

Chain P: 65% 32%



- Molecule 19: 50S ribosomal protein L19

Chain Q: 74% 24%



- Molecule 20: 50S ribosomal protein L20

Chain R: 74% 21%



- Molecule 21: 50S ribosomal protein L21

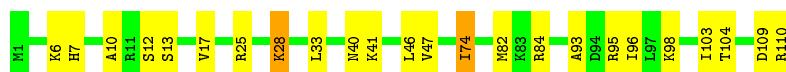
Chain S: 70% 28%



- Molecule 22: 50S ribosomal protein L22

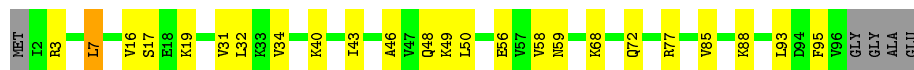
Chain T: 78% 20%





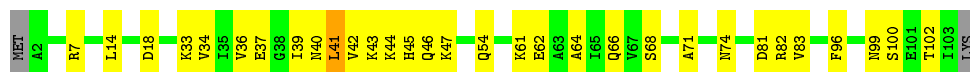
- Molecule 23: 50S ribosomal protein L23

Chain U: 71% 23% 5%



- Molecule 24: 50S ribosomal protein L24

Chain V: 68% 29% 2%



- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 24% 2%



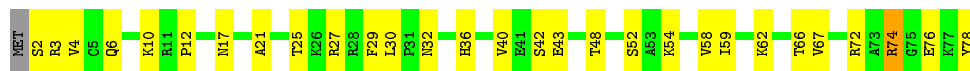
- Molecule 26: 50S ribosomal protein L27

Chain X: 59% 28% 11%



- Molecule 27: 50S ribosomal protein L28

Chain Y: 62% 36% 2%



- Molecule 28: 50S ribosomal protein L29

Chain Z: 67% 27% 5%

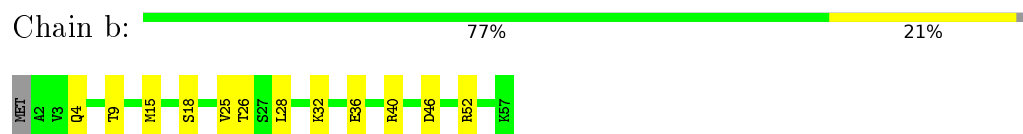


- Molecule 29: 50S ribosomal protein L30

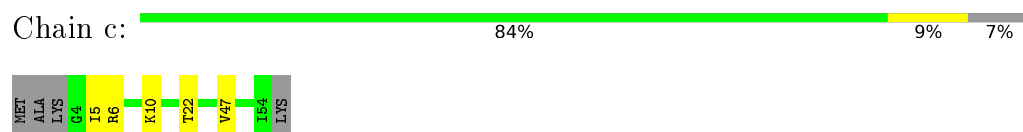
Chain a: 95% 5% 0%



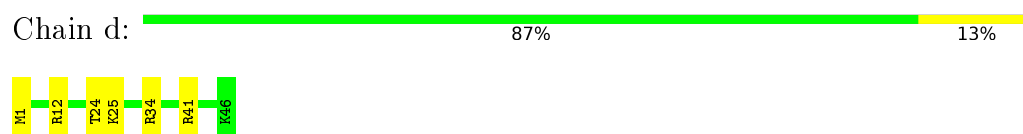
- Molecule 30: 50S ribosomal protein L32



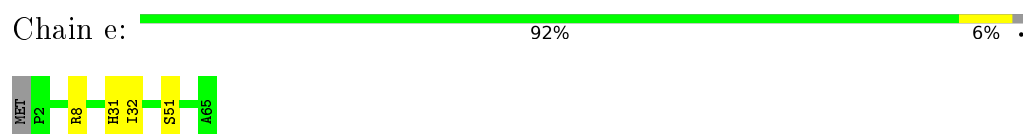
- Molecule 31: 50S ribosomal protein L33



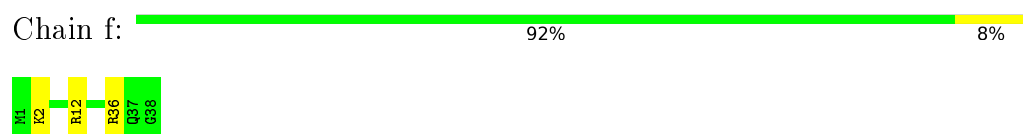
- Molecule 32: 50S ribosomal protein L34



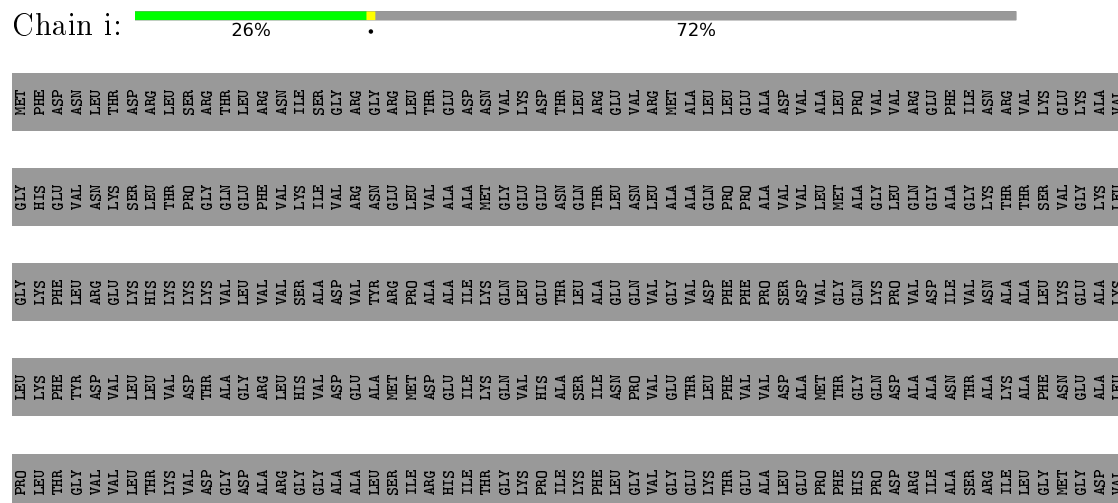
- Molecule 33: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L36

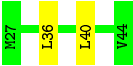
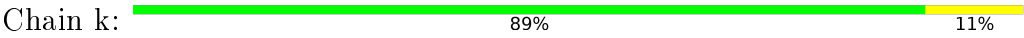


- Molecule 35: Signal recognition particle protein Ffh





● Molecule 36: 1A9L SS



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	46409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	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	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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  >2	RMSZ	# Z  >2
1	1	0.79	0/1037	1.29	7/1616 (0.4%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
2	2	0.57	0/68	1.25	1/103 (1.0%)
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.45	0/763	0.61	0/1021
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.41	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
3	A	0.68	14/69329 (0.0%)	1.17	187/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.44	0/672	0.56	0/883
36	k	0.62	0/137	0.85	0/186
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2121	0.65	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.63	14/101562 (0.0%)	1.05	199/152181 (0.1%)

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
12	J	0	1
5	C	0	1
9	G	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.90	1.33	1.37
3	A	1254	A	N9-C4	-6.39	1.34	1.37
3	A	1321	A	N9-C4	6.27	1.41	1.37
3	A	1490	A	N9-C4	6.00	1.41	1.37
3	A	2114	A	N9-C4	5.98	1.41	1.37

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.25	113.65	121.00
3	A	1838	C	C6-N1-C2	9.39	124.06	120.30
3	A	2422	C	O4'-C1'-N1	9.31	115.65	108.20
3	A	2423	U	C5-C6-N1	8.80	127.10	122.70
3	A	1584	U	C2-N1-C1'	8.52	127.92	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide

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Mol	Chain	Res	Type	Group
12	J	19	ASN	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	1	926	0	467	10	0
2	2	62	0	34	1	0
3	A	61902	0	31133	683	0
4	B	2569	0	1301	19	0
5	C	2082	0	2154	51	0
6	D	1565	0	1616	32	0
7	E	1552	0	1619	27	0
8	F	1410	0	1444	42	0
9	G	1323	0	1371	35	0
10	H	1110	0	1148	23	0
11	I	946	0	978	31	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	23	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	14	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	916	0	944	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	412	0	0	0	0
37	B	11	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	94027	0	62510	1167	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 8.

The worst 5 of 1167 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)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
3:A:276:U:O2	3:A:278:A:N6	2.08	0.87
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86

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	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	26	72
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	84/453 (18%)	84 (100%)	0	0	100	100
36	k	16/18 (89%)	12 (75%)	4 (25%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3532/4045 (87%)	3415 (97%)	115 (3%)	2 (0%)	59 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	H	118	PRO
11	I	108	VAL

### 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
5	C	216/218 (99%)	192 (89%)	24 (11%)	8 39
6	D	164/164 (100%)	154 (94%)	10 (6%)	23 65
7	E	165/165 (100%)	152 (92%)	13 (8%)	15 55
8	F	148/150 (99%)	130 (88%)	18 (12%)	6 34
9	G	137/138 (99%)	129 (94%)	8 (6%)	25 66
10	H	114/114 (100%)	100 (88%)	14 (12%)	6 34
11	I	95/123 (77%)	89 (94%)	6 (6%)	22 63
12	J	104/110 (94%)	93 (89%)	11 (11%)	8 41
13	K	116/116 (100%)	105 (90%)	11 (10%)	11 46
14	L	104/104 (100%)	94 (90%)	10 (10%)	10 46
15	M	103/103 (100%)	94 (91%)	9 (9%)	13 50
16	N	109/109 (100%)	100 (92%)	9 (8%)	14 52
17	O	102/103 (99%)	95 (93%)	7 (7%)	19 60
18	P	87/87 (100%)	75 (86%)	12 (14%)	4 30
19	Q	99/100 (99%)	90 (91%)	9 (9%)	12 48
20	R	89/90 (99%)	82 (92%)	7 (8%)	15 55
21	S	84/84 (100%)	76 (90%)	8 (10%)	11 46
22	T	93/93 (100%)	88 (95%)	5 (5%)	27 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	82/84 (98%)	77 (94%)	5 (6%)	23	65
24	V	83/85 (98%)	76 (92%)	7 (8%)	14	52
25	W	78/78 (100%)	72 (92%)	6 (8%)	16	56
26	X	57/63 (90%)	51 (90%)	6 (10%)	8	41
27	Y	67/68 (98%)	63 (94%)	4 (6%)	24	65
28	Z	54/55 (98%)	47 (87%)	7 (13%)	5	32
29	a	48/49 (98%)	46 (96%)	2 (4%)	36	74
30	b	47/48 (98%)	35 (74%)	12 (26%)	1	6
31	c	45/49 (92%)	40 (89%)	5 (11%)	8	39
32	d	38/38 (100%)	32 (84%)	6 (16%)	3	23
33	e	51/52 (98%)	47 (92%)	4 (8%)	16	55
34	f	34/34 (100%)	31 (91%)	3 (9%)	12	50
35	i	71/341 (21%)	65 (92%)	6 (8%)	13	52
36	k	17/17 (100%)	15 (88%)	2 (12%)	6	35
All	All	2901/3232 (90%)	2635 (91%)	266 (9%)	16	48

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	L	58	LEU
17	O	75	ILE
32	d	1	MET
14	L	106	GLU
16	N	7	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
14	L	89	ASN
18	P	100	HIS
35	i	332	ASN
16	N	3	GLN
19	Q	52	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	13 (30%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	545 (17%)	19 (0%)

5 of 545 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	36	U
1	1	37	U
1	1	38	U
1	1	39	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	1344	U
3	A	1721	G
3	A	2424	C
3	A	1110	G
3	A	2430	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](#)

Of 432 ligands modelled in this entry, 432 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.