



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 11, 2017 – 02:05 AM EDT

PDB ID : 5TCU  
EMDB ID: : EMD-8402  
Title : Methicillin sensitive Staphylococcus aureus 70S ribosome  
Authors : Eyal, Z.; Ahmed, T.; Belousoff, N.; Mishra, S.; Matzov, D.; Bashan, A.; Zim-merman, E.; Lithgow, T.; Bhushan, S.; Yonath, A.  
Deposited on : unknown  
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

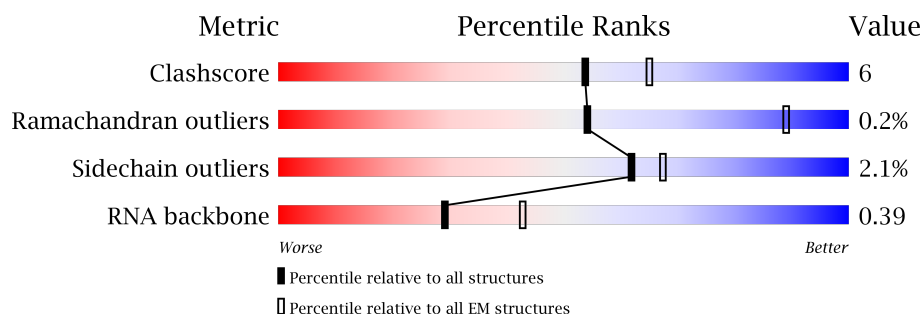
# 1 Overall quality at a glance

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.














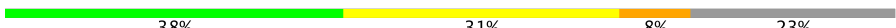








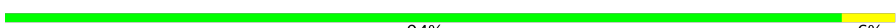




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	A	1555	38% 39% 15% 6%
2	SB	202	77% 23%
3	SC	198	92% 8%
4	SD	156	81% 19%
5	SE	95	75% 25%
6	SG	155	82% 17%
7	SF	130	72% 26%
8	SH	127	65% 31%









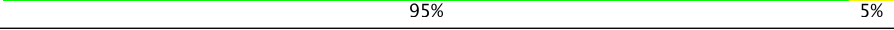


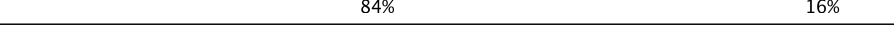







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Mol	Chain	Length	Quality of chain
9	S1	80	
10	S2	114	
11	S3	136	
12	S4	113	
13	S5	60	
14	S6	88	
15	S7	83	
16	S8	80	
17	S9	56	
18	SI	78	
19	SA	79	
20	X	13	
21	E	75	
22	D	76	
23	B	2923	
24	C	114	
25	L2	274	
26	LC	215	
27	LJ	205	
28	LK	166	
29	LL	174	
30	LM	145	
31	LN	122	
32	LO	145	
33	LP	136	

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Mol	Chain	Length	Quality of chain
34	LQ	119	 76% 24%
35	LR	113	 83% 16% .
36	L1	109	 90% 10%
37	L3	116	 81% 19%
38	L4	102	 83% 16% .
39	L5	112	 85% 15%
40	L6	89	 85% 15%
41	L7	103	 85% 15%
42	L8	93	 95% 5%
43	L9	82	 84% 16%
44	LA	58	 74% 22% .
45	LB	62	 84% 16%
46	LD	57	 89% 11%
47	LE	47	 91% 9%
48	LS	47	 83% 17%
49	LG	43	 79% 21%
50	LH	60	 85% 13% .
51	LI	37	 70% 30%
52	LF	74	 92% 8%

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 133876 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1464	Total	C	N	O	P	0	0
			31369	14007	5741	10159	1462		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	202	Total	C	N	O	S	0	0
			1551	979	293	278	1		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	SC	198	Total	C	N	O	0	0
			1058	634	211	213		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	156	Total	C	N	O	S	0	0
			1153	727	211	213	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	95	Total	C	N	O	S	0	0
			785	496	138	149	2		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	155	Total	C	N	O	S	0	0
			1164	724	220	217	3		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	130	Total	C	N	O	S	0	0
			1007	639	180	184	4		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	127	Total	C	N	O	S	0	0
			975	605	194	175	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S1	80	Total	C	N	O	0	0
			626	394	116	116		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S2	114	Total	C	N	O	S	0	0
			826	507	158	159	2		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S3	136	Total	C	N	O	S	0	0
			976	611	190	173	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	113	Total	C	N	O	S	0	0
			828	510	168	149	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S5	60	Total	C	N	O	S	0	0
			497	314	99	79	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S6	88	Total	C	N	O	S	0	0
			713	441	148	123	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S7	83	Total	C	N	O	S	0	0
			537	335	105	96	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S8	80	Total	C	N	O	0	0
			520	327	97	96		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S9	56	Total	C	N	O	S	0	0
			458	292	88	76	2		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SI	78	Total	C	N	O	S	0	0
			541	340	104	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SA	78	Total	C	N	O	S	0	0
			503	303	100	99	1		

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	10	Total	C	N	O	P	0	0
			213	96	39	68	10		

- Molecule 21 is a RNA chain called P-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	75	Total	C	N	O	P	0	0
			1600	713	285	527	75		

- Molecule 22 is a RNA chain called E-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 23 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	2755	Total	C	N	O	P	0	0
			59059	26368	10814	19122	2755		

- Molecule 24 is a RNA chain called 5S rRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	114	Total	C	N	O	P	0	0
			2430	1086	436	794	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L2	274	Total	C	N	O	S	0	0
			2066	1288	414	359	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	215	Total	C	N	O	S	0	0
			1570	987	295	283	5		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LJ	205	Total	C	N	O	S	0	0
			1514	953	282	277	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	LK	166	Total	C	N	O	S	0	0
			1026	635	185	204	2		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LL	174	Total	C	N	O	S	0	0
			1062	660	205	195	2		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LM	145	Total	C	N	O	S	0	0
			1124	703	205	213	3		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LN	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	LO	145	Total	C	N	O	0	0
			1020	631	207	182		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LP	136	Total	C	N	O	S	0	0
			1043	672	202	165	4		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LQ	119	Total	C	N	O	S	0	0
			898	551	176	170	1		

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	LR	113	Total	C	N	O	0	0
			765	474	145	146		

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L1	109	Total	C	N	O	0	0
			832	529	169	134		

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L3	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L4	102	Total	C	N	O	S	0	0
			749	474	140	134	1		

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L5	112	Total	C	N	O	S	0	0
			837	526	163	146	2		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L6	89	Total	C	N	O	S	0	0
			694	436	126	128	4		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	L7	103	Total	C	N	O	0	0
			734	462	137	135		

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	L8	93	Total	C	N	O	0	0
			648	411	115	122		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	L9	82	Total	C	N	O	0	0
			615	382	122	111		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	LA	58	Total	C	N	O	0	0
			443	276	96	71		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LB	62	Total	C	N	O	0	0
			493	304	93	96		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LD	57	Total	C	N	O	0	0
			436	272	83	81		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LE	47	Total	C	N	O	S	0	0
			356	218	77	59	2		

- Molecule 48 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LS	47	Total	C	N	O	S	0	0
			380	233	75	68	4		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LG	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	60	Total	C	N	O	S	0	0
			446	277	92	75	2		

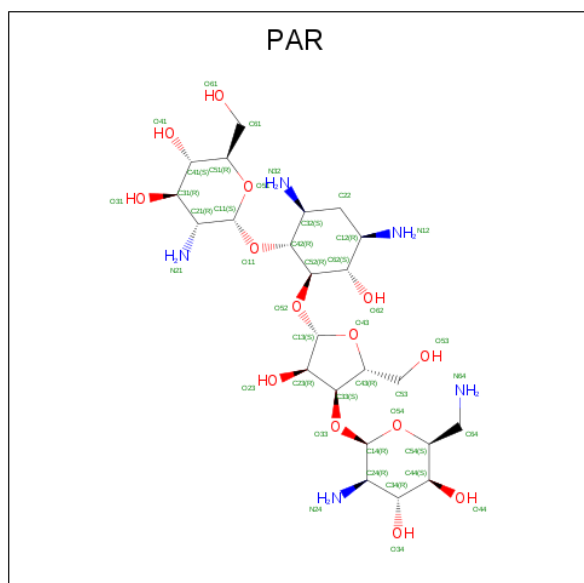
- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	37	Total	C	N	O	S	0	0
			272	170	57	40	5		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LF	74	Total	C	N	O	S	0	0
			447	269	86	91	1		

- Molecule 53 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			42	23	5	14	

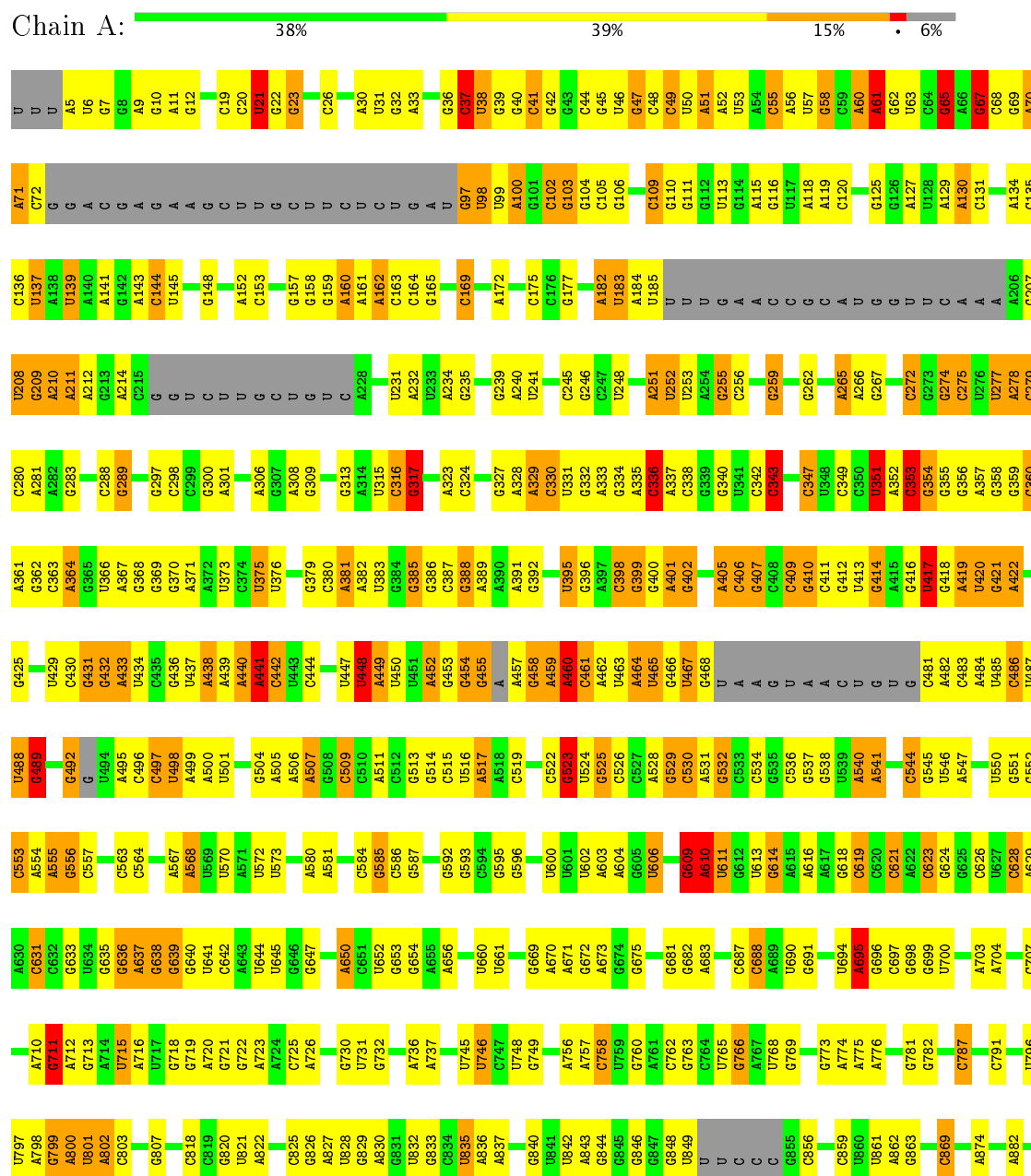
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

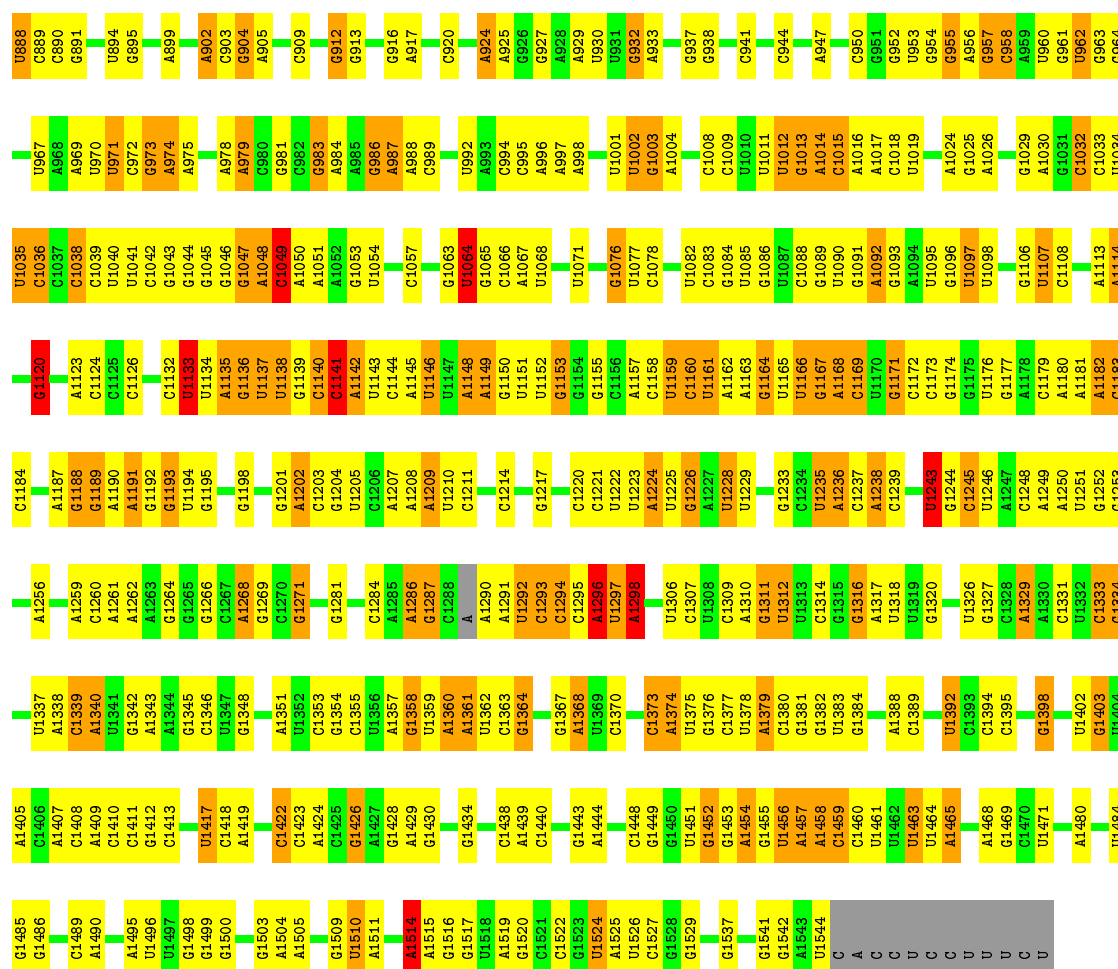
Mol	Chain	Residues	Atoms		AltConf
54	B	99	Total 99	Mg 99	0
54	A	27	Total 27	Mg 27	0
54	C	2	Total 2	Mg 2	0
54	SG	1	Total 1	Mg 1	0

### 3 Residue-property plots

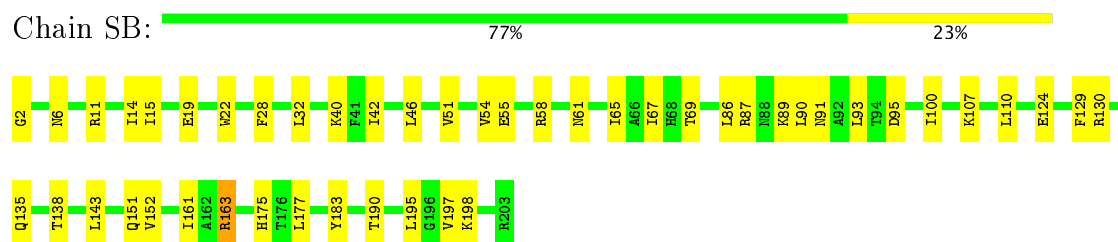
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 16S rRNA

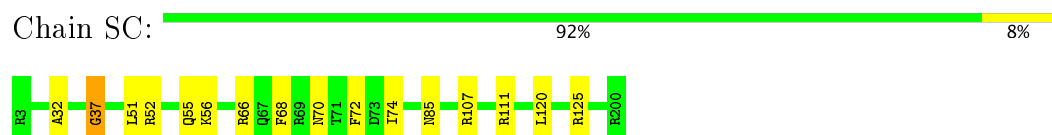




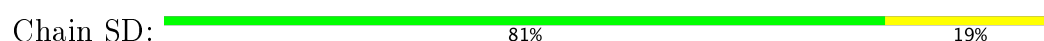
- Molecule 2: 30S ribosomal protein S3

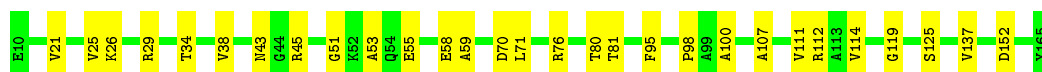


- Molecule 3: 30S ribosomal protein S4

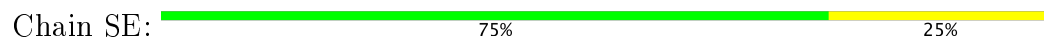


- Molecule 4: 30S ribosomal protein S5

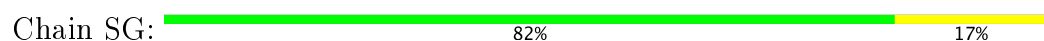




- Molecule 5: 30S ribosomal protein S6



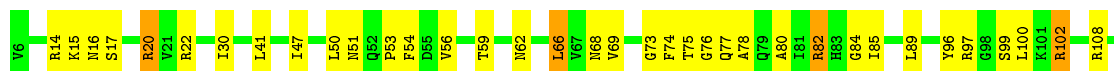
- Molecule 6: 30S ribosomal protein S7



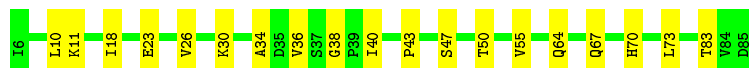
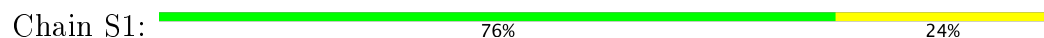
- Molecule 7: 30S ribosomal protein S8



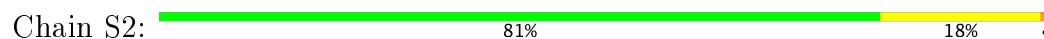
- Molecule 8: 30S ribosomal protein S9



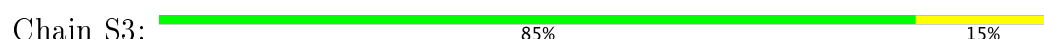
- Molecule 9: 30S ribosomal protein S10



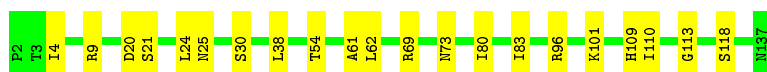
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

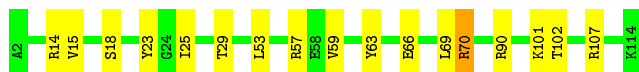






- Molecule 12: 30S ribosomal protein S13

Chain S4: 85% 14%



- Molecule 13: 30S ribosomal protein S14 type Z

Chain S5: 75% 25%



- Molecule 14: 30S ribosomal protein S15

Chain S6: 78% 22%



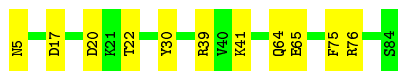
- Molecule 15: 30S ribosomal protein S16

Chain S7: 86% 14%



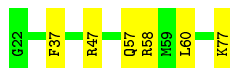
- Molecule 16: 30S ribosomal protein S17

Chain S8: 86% 14%



- Molecule 17: 30S ribosomal protein S18

Chain S9: 89% 11%

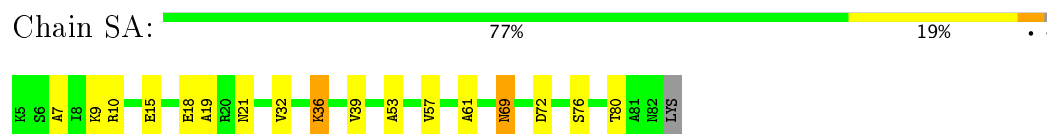


- Molecule 18: 30S ribosomal protein S19

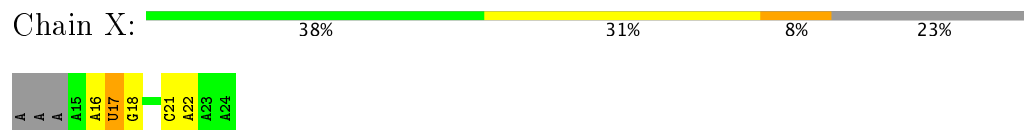
Chain SI: 79% 18%



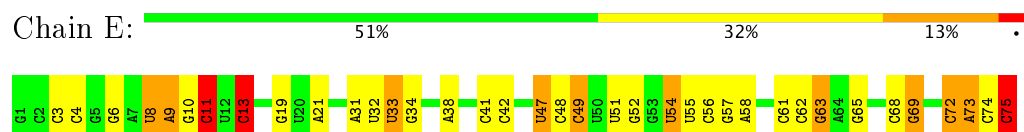
- Molecule 19: 30S ribosomal protein S20



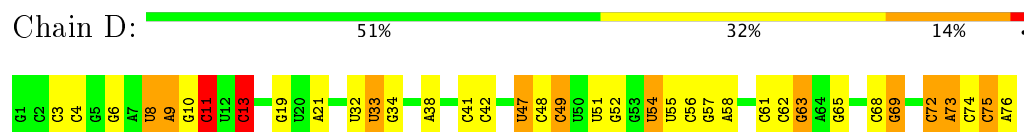
- Molecule 20: mRNA



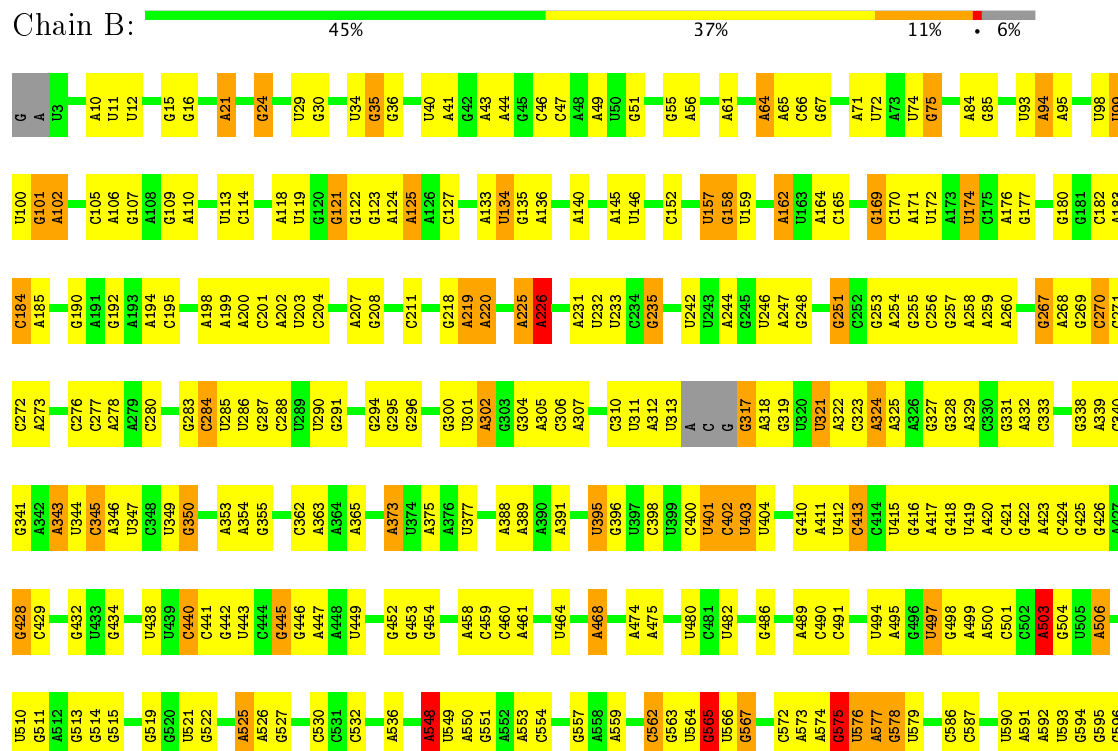
- Molecule 21: P-site tRNA CHAIN



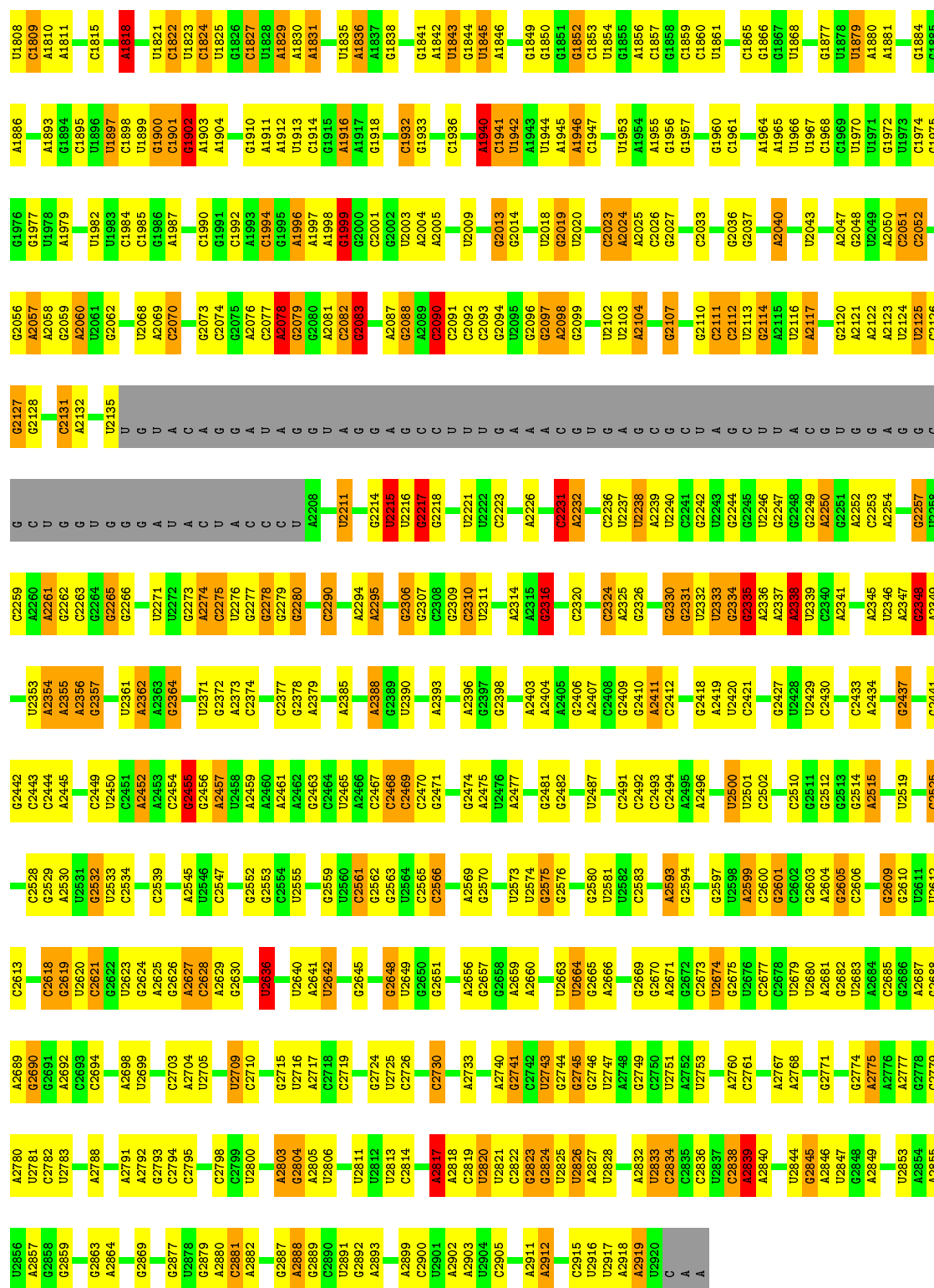
- Molecule 22: E-site tRNA CHAIN

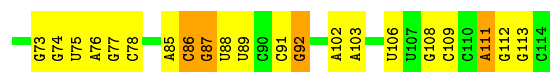


- Molecule 23: 23S RRNA



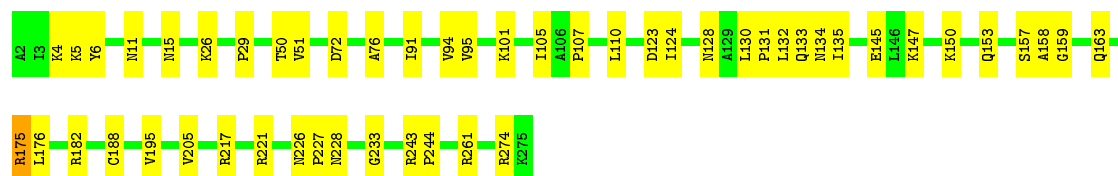
A1712	A1626	G1559	U1498	G1429	U1350	A1269	A1177	A	G1046	U970	G903	A833	U759	C674	U597
A1713	G1627	A1500	U1499	A1430	C1351	U1270	C1178	G	G1047	U971	G904	A834	U759	C675	U598
C1714	A1628	G1561	G1500	U1431	C1352	G1271	C1179	A	U1048	A972	U905	U835	A761	A676	G596
U1715	U1629	G1574	G1501	A1432	A1353			A	C1049	A973	A906	C836	A760	A677	G602
C1716	A1630	U1503	A1502	U1433	G1354	G1274	G1183	G	G1050	U974	G907	G837	C762	G678	C603
C1719	G1631	U1503	U1503	U1434	G1355	A1275	G1184	C	C1051	U975	A908	A838	A763	G679	G604
A1720	A1635	U1506	U1504	C1435	G1356	G1276	U1185	A	A1052	U976	U913	A839	C764	C680	U605
A1723	U1636	G1507	G1506	A1440	G1357	C1277	A1186	G	A1053	A977		C840	U765	G681	G606
U1737	G1638	G1571	C1507	C1441	A1358	G1278	A1187	C	U1057	U981	U916	U842	U766	G682	G607
C1738	U1639	U1508	C1508	C1442	G1360			A	A1058	U982	G919	U845	U767	C683	U608
G1739	U1640	U1510	G1509	A1443	G1361	U1287	U1193	U	A1059	U983	G920	G846	U768	U609	
G1740	G1641	A1575	U1511	C1444	C1362	U1288	U1194	C	U1060	U984	G921	G847	U769	U610	
C1741	C1642	A1576	U1512	U1447	U1363	G1289	A1195	A	U1063	U985	G922	U848			U611
A1742	G1643	G1577	A1513	A1447	C1364	C1290	C1197	U	A1064	U986	G923	A849	G774	G693	U612
	G1651	C1578	A1514	U1448	C1368	A1291	U1205	U	G1065	U988	G924	G850	G775	G694	G613
G1747	A1652	A1579	G1515	U1449	A1292	U1293	U1206	A	A1066	U989	G925	G854	A778	C695	A615
G1748	A1653	A	A1516	A1450	U1378	U1294	G1207	A	U1067	U990	G	U855	A780	G696	A616
G1749	U1654	U	A1517	U1451	A1379	G1294	G1208	A	G1068	A991	C	U856	C781	U698	
C1750	C1655	U	G1518	G1452	G1380		U1209	G	G1069	A992	C	C857	C782	U699	
U1755	C1656	G	U1519	G1453	U1381	G1298	U1210	A	A1070	C993	C	C861	C783	U702	A621
A1758	G1657	A	A1520	U	G1382	A1303	G1211	U	A1071	A994	C	C862	C784	A703	C623
A1759	U1658	U1586	U1521	U	G1383	G1304	U1212	C	G1074	G997	U	C863	C785	U704	C624
G1760	G1659	C1587	C1524	U	G1384		C1213	C	U1077			U864	C786	U705	
G1761	U1660	U1588	U1525	A	U1389	C1308	G1214	G	U1078	A1001	U	A865	A789	G706	G628
U1762	C1661	U1589	G1526	A1459	U1390	G1309	U1215	U	G1079	U1002	C	U866	C790	U707	A629
U1763	A1662	C1590	A1527	U1460	C1392	A1310	U1216	A	U1080	A1003	G	U867	C792	C710	G630
	G1663	G1591	G1528	C1461	C1393	A1311	U1217	A	G1081	A1004	G	U868	C793		U631
	A1666	U1592	U1529	G1462	U1397	A1312	G1218	U	C1082	G1005	U	C869	A797	U713	U632
G1766	G1667	G1593	A1530		G1398	C1315	G1219	A	G1083	G1012	U	C870	C794	A714	A633
G1767	U1668	U1594	U	G1465	C1399	G1320	A1220	G	U1084		A	U871	C802	G714	C634
C1768	A1673	C1595	U1525	G1466	C1400	G1321	C1221	C	U1085	G1016	C942	U872	C805	C716	G635
C1769	U1674	G1596	A	G1467	C1401	A1321	U1222	U	G1086	A1017	C943	U873	A806	C717	U639
C1770	G1675	U1597	G	G1468	A1402	G1322	G1225	A	C1087	A1018	G944	A874			
A1771	U1676	U1598	C	G1469	A1403	G1323	G1226	C	C1088	A1019	A945	C875	A806		
G1772	G1682	G1599	U	G1470	G1405	U1324	U1227		C1089	G1020	U946	G876		A720	A646
	A1686	U1600	A	A1471	G1406	U1325	A1228		A1090	A1024	U947	C877	A809	A721	A647
C1781	A1690	A1601	A	C1472	C1407	C1326	G1229	U1149	G1091	A1025	U948	C878	A810	A722	
U1784	G1691	U1602	U1539	G1473	C1408	C1327	G1230	G1151	A1092	C1026		C879	C811	C723	U650
G1785	C1692	A1604	C1541	U1477	U1409	C1328	G1234	C1153	G1093	A1027	G951	U879	U812	C724	A651
A1786	G1693	C1606	G1543	A1478	G1411	G1332	C1235	G1154	A1094	G1028	A952	A880	G813	A725	
	A1694	G1607	G1544	U1482	G1412	C1332	G1235	A1155	A1095			C883	A814	C726	G654
A1789	G1695	C1608	U1545	U1483		C1333	A1241	G1156	C1096		A955	U894	G816	G727	A655
G1790	C1696	A1546	A1483	G1484	A1415	C1334	A1242	U1157	U1097	C1031	A956	C885		A730	G656
G1791	A1698	U1547	C1542	U1487	U1416	G1335	A1243	G1158	A1098	A1032	C957	C886	C821	U731	U657
	U1699	G1612	U1548	A1488	G1417	U1337	U1248	A1159	G1099	C1035	U958	U888	C822	C732	A658
C1794	A1795	G1614	C1549	A1489	U1420	U1338	U1249	C1160	G	C1036	C960	A891	G823	C736	A660
A1796	U1700	U1615	U	G1490	A1421	C1342	G1253	U1163	U	C1037	G961	U892	A824	C737	G662
A1800	U1703	A1616	U1550	C1491	A1422	U1343	C1254	C1168	U	C1038	A962	U895	A826	C738	A666
	U1707	U1618	A	U1492	A1423	A1344	A1255	U	U	C1039	U964	U896	A827	G741	
G1803	U1708	C1622	G1555	U1493	A1424	A1345	G1265	A1172	G	G1041	G965	A897	C828		C669
U1806	G1710	U1623	G1556	G1494	G1425	G1346	G1266	A1173	G	C1042	C966	G900	U829	G752	G670
A1807	G1711	U1625	U1558	G1495	G1426	U1347	G1267	U1174	C	U1043	C967	G901	U830	U753	U671
				U1497	U1428	U1349	C1268	G1175	U	A1044	A968	U892	U831	C755	A672
								U1176	U	A1045	A969	A902	C832		A673





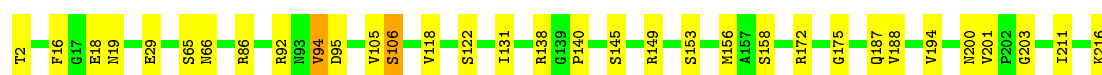
- Molecule 25: 50S ribosomal protein L2

Chain L2: 81% 18%



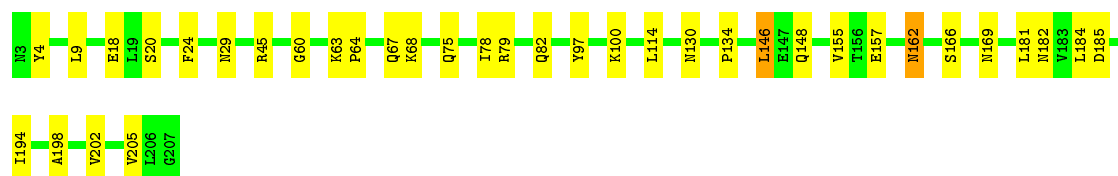
- Molecule 26: 50S ribosomal protein L3

Chain LC: 85% 14%



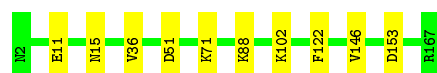
- Molecule 27: 50S ribosomal protein L4

Chain LJ: 82% 17%



- Molecule 28: 50S ribosomal protein L5

Chain LK: 94% 6%



- Molecule 29: 50S ribosomal protein L6

Chain LL: 94% 6%




- Molecule 30: 50S ribosomal protein L13

Chain LM: 81% 18%




- Molecule 31: 50S ribosomal protein L14

Chain LN:  87% 11%




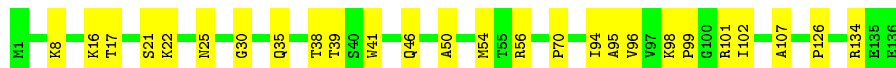
- Molecule 32: 50S ribosomal protein L15

Chain LO:  82% 17%




- Molecule 33: 50S ribosomal protein L16

Chain LP:  81% 19%




- Molecule 34: 50S ribosomal protein L17

Chain LQ:  76% 24%



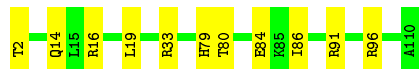
- Molecule 35: 50S ribosomal protein L18

Chain LR:  83% 16%




- Molecule 36: 50S ribosomal protein L19

Chain L1:  90% 10%




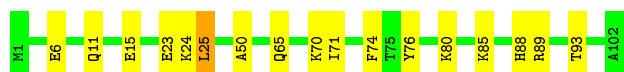
- Molecule 37: 50S ribosomal protein L20

Chain L3:  81% 19%




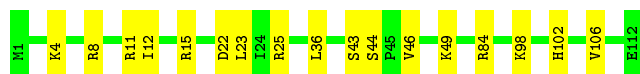
- Molecule 38: 50S ribosomal protein L21

Chain L4:  83% 16%




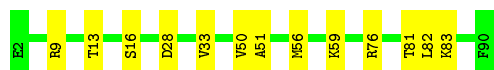
- Molecule 39: 50S ribosomal protein L22

Chain L5:  85% 15%




- Molecule 40: 50S ribosomal protein L23

Chain L6:  85% 15%



- Molecule 41: 50S ribosomal protein L24

Chain L7:  85% 15%




- Molecule 42: 50S ribosomal protein L25

Chain L8:  95% 5%




- Molecule 43: 50S ribosomal protein L27

Chain L9:  84% 16%




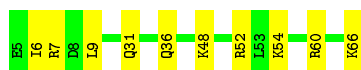
- Molecule 44: 50S ribosomal protein L28

Chain LA:  74% 22%



- Molecule 45: 50S ribosomal protein L29

Chain LB:  84% 16%



- Molecule 46: 50S ribosomal protein L30

Chain LD: 89% 11%



- Molecule 47: 50S ribosomal protein L32

Chain LE: 91% 9%



- Molecule 48: 50S ribosomal protein L33 1

Chain LS: 83% 17%



- Molecule 49: 50S ribosomal protein L34

Chain LG: 79% 21%



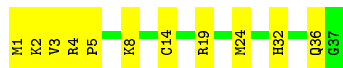
- Molecule 50: 50S ribosomal protein L35

Chain LH: 85% 13% .



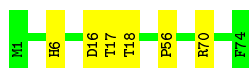
- Molecule 51: 50S ribosomal protein L36

Chain LI: 70% 30%



- Molecule 52: 50S ribosomal protein L31 type B

Chain LF: 92% 8%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	126000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: PAR, 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	A	0.99	2/35118 (0.0%)	1.35	416/54749 (0.8%)
10	S2	0.40	0/840	0.63	0/1137
11	S3	0.44	0/991	0.80	2/1337 (0.1%)
12	S4	0.39	0/835	0.75	0/1123
13	S5	0.50	0/507	0.73	0/674
14	S6	0.46	0/721	0.70	1/964 (0.1%)
15	S7	0.36	0/541	0.68	0/733
16	S8	0.41	0/527	0.62	0/721
17	S9	0.41	0/465	0.67	0/620
18	SI	0.36	0/551	0.70	0/747
19	SA	0.31	0/502	0.50	0/679
2	SB	0.42	0/1573	0.67	0/2121
20	X	0.83	0/238	1.29	3/368 (0.8%)
21	E	0.55	0/1787	1.36	17/2784 (0.6%)
22	D	0.57	0/1809	1.35	17/2819 (0.6%)
23	B	1.36	83/66138 (0.1%)	1.38	823/103134 (0.8%)
24	C	1.01	0/2717	1.37	22/4232 (0.5%)
25	L2	0.64	0/2101	0.69	0/2823
26	LC	0.59	0/1593	0.73	0/2143
27	LJ	0.59	1/1536 (0.1%)	0.76	3/2078 (0.1%)
28	LK	0.40	0/1033	0.65	0/1412
29	LL	0.36	0/1074	0.56	0/1467
3	SC	0.34	1/1062 (0.1%)	0.61	0/1465
30	LM	0.55	0/1146	0.69	0/1546
31	LN	0.63	1/925 (0.1%)	0.76	1/1242 (0.1%)
32	LO	0.57	0/1034	0.76	2/1388 (0.1%)
33	LP	0.54	0/1067	0.65	0/1436
34	LQ	0.51	0/900	0.73	1/1205 (0.1%)
35	LR	0.45	0/770	0.69	1/1044 (0.1%)
36	L1	0.55	0/844	0.65	0/1134
37	L3	0.65	0/954	0.68	0/1264
38	L4	0.54	0/758	0.69	0/1014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	L5	0.59	0/845	0.71	1/1140 (0.1%)
4	SD	0.51	0/1167	0.68	0/1576
40	L6	0.63	0/701	0.71	0/939
41	L7	0.43	0/742	0.69	1/1001 (0.1%)
42	L8	0.37	0/655	0.69	0/888
43	L9	0.60	0/621	0.70	0/824
44	LA	0.48	0/449	0.65	0/600
45	LB	0.48	0/494	0.69	0/660
46	LD	0.49	0/438	0.70	0/591
47	LE	0.54	0/361	0.64	0/481
48	LS	0.48	0/385	0.65	0/518
49	LG	0.64	0/371	0.71	0/484
5	SE	0.47	0/796	0.65	0/1069
50	LH	0.49	0/450	0.76	0/597
51	LI	0.53	0/275	0.65	0/366
52	LF	0.30	0/454	0.58	0/624
6	SG	0.37	0/1180	0.63	0/1595
7	SF	0.49	0/1019	0.76	2/1371 (0.1%)
8	SH	0.38	0/990	0.77	1/1332 (0.1%)
9	S1	0.47	0/637	0.66	0/865
All	All	1.08	88/145687 (0.1%)	1.24	1314/219124 (0.6%)

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
10	S2	0	1
11	S3	0	1
13	S5	0	1
15	S7	0	1
18	SI	0	1
25	L2	0	1
26	LC	0	3
28	LK	0	1
30	LM	0	1
31	LN	0	1
33	LP	0	1
34	LQ	0	1
38	L4	0	2
42	L8	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	L9	0	1
48	LS	0	1
5	SE	0	1
50	LH	0	1
6	SG	0	1
All	All	0	23

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	2025	A	N9-C4	-9.99	1.31	1.37
23	B	559	A	N9-C4	-7.97	1.33	1.37
23	B	1979	A	N9-C4	-7.63	1.33	1.37
23	B	834	A	N9-C4	-7.45	1.33	1.37
23	B	902	A	N7-C5	-6.89	1.35	1.39

The worst 5 of 1314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	86	C	N1-C2-O2	14.88	127.83	118.90
24	C	86	C	C2-N1-C1'	13.72	133.89	118.80
24	C	86	C	N3-C2-O2	-12.99	112.81	121.90
1	A	1078	C	N1-C2-O2	12.78	126.56	118.90
23	B	317	G	OP1-P-O3'	-11.81	79.22	105.20

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	S2	40	ASN	Peptide
11	S3	54	THR	Peptide
13	S5	15	LYS	Peptide
5	SE	43	TRP	Peptide
6	SG	124	ILE	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	31369	0	15803	356	0
2	SB	1551	0	1570	31	0
3	SC	1058	0	568	8	0
4	SD	1153	0	1210	17	0
5	SE	785	0	781	16	0
6	SG	1164	0	1146	18	0
7	SF	1007	0	1050	22	0
8	SH	975	0	970	34	0
9	S1	626	0	628	12	0
10	S2	826	0	817	13	0
11	S3	976	0	966	11	0
12	S4	828	0	809	10	0
13	S5	497	0	512	12	0
14	S6	713	0	733	11	0
15	S7	537	0	462	9	0
16	S8	520	0	415	6	0
17	S9	458	0	496	6	0
18	SI	541	0	482	10	0
19	SA	503	0	451	13	0
20	X	213	0	108	0	0
21	E	1600	0	810	15	0
22	D	1619	0	822	13	0
23	B	59059	0	29695	453	0
24	C	2430	0	1229	28	0
25	L2	2066	0	2161	32	0
26	LC	1570	0	1593	20	0
27	LJ	1514	0	1540	20	0
28	LK	1026	0	797	7	0
29	LL	1062	0	808	5	0
30	LM	1124	0	1101	15	0
31	LN	918	0	981	8	0
32	LO	1020	0	998	18	0
33	LP	1043	0	1084	16	0
34	LQ	898	0	932	19	0
35	LR	765	0	720	11	0
36	L1	832	0	875	10	0
37	L3	942	0	1014	19	0
38	L4	749	0	730	10	0
39	L5	837	0	893	13	0
40	L6	694	0	705	6	0
41	L7	734	0	731	11	0
42	L8	648	0	598	1	0
43	L9	615	0	637	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	LA	443	0	461	8	0
45	LB	493	0	503	6	0
46	LD	436	0	474	4	0
47	LE	356	0	354	4	0
48	LS	380	0	379	3	0
49	LG	367	0	415	7	0
50	LH	446	0	465	5	0
51	LI	272	0	290	9	0
52	LF	447	0	289	5	0
53	A	42	0	44	0	0
54	A	27	0	0	0	0
54	B	99	0	0	0	0
54	C	2	0	0	0	0
54	SG	1	0	0	0	0
All	All	133876	0	85105	1251	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 1251 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)
23:B:1037:A:N7	23:B:1206:G:N1	2.02	1.08
23:B:1037:A:C5	23:B:1206:G:N1	2.22	1.07
1:A:251:A:C5	1:A:289:G:N2	2.26	1.03
23:B:497:U:C2	23:B:499:A:N7	2.27	1.02
23:B:420:A:H62	23:B:446:G:N2	1.62	0.98

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	
2	SB	200/202 (99%)	165 (82%)	34 (17%)	1 (0%)	32	73
3	SC	196/198 (99%)	151 (77%)	45 (23%)	0	100	100
4	SD	154/156 (99%)	135 (88%)	19 (12%)	0	100	100
5	SE	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
6	SG	153/155 (99%)	134 (88%)	19 (12%)	0	100	100
7	SF	128/130 (98%)	110 (86%)	18 (14%)	0	100	100
8	SH	125/127 (98%)	101 (81%)	24 (19%)	0	100	100
9	S1	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
10	S2	112/114 (98%)	85 (76%)	27 (24%)	0	100	100
11	S3	134/136 (98%)	98 (73%)	36 (27%)	0	100	100
12	S4	111/113 (98%)	87 (78%)	24 (22%)	0	100	100
13	S5	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
14	S6	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
15	S7	81/83 (98%)	60 (74%)	21 (26%)	0	100	100
16	S8	78/80 (98%)	58 (74%)	20 (26%)	0	100	100
17	S9	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
18	SI	76/78 (97%)	54 (71%)	21 (28%)	1 (1%)	14	57
19	SA	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
25	L2	272/274 (99%)	230 (85%)	42 (15%)	0	100	100
26	LC	213/215 (99%)	164 (77%)	46 (22%)	3 (1%)	13	55
27	LJ	203/205 (99%)	174 (86%)	27 (13%)	2 (1%)	18	61
28	LK	164/166 (99%)	120 (73%)	44 (27%)	0	100	100
29	LL	172/174 (99%)	136 (79%)	36 (21%)	0	100	100
30	LM	143/145 (99%)	118 (82%)	24 (17%)	1 (1%)	25	67
31	LN	120/122 (98%)	97 (81%)	22 (18%)	1 (1%)	22	65
32	LO	143/145 (99%)	107 (75%)	36 (25%)	0	100	100
33	LP	134/136 (98%)	114 (85%)	19 (14%)	1 (1%)	25	67
34	LQ	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
35	LR	111/113 (98%)	85 (77%)	25 (22%)	1 (1%)	20	63
36	L1	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
37	L3	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
38	L4	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	18	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	L5	110/112 (98%)	97 (88%)	13 (12%)	0	100	100
40	L6	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
41	L7	101/103 (98%)	80 (79%)	21 (21%)	0	100	100
42	L8	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
43	L9	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
44	LA	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
45	LB	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
46	LD	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
47	LE	45/47 (96%)	37 (82%)	8 (18%)	0	100	100
48	LS	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
49	LG	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
50	LH	58/60 (97%)	46 (79%)	12 (21%)	0	100	100
51	LI	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
52	LF	72/74 (97%)	46 (64%)	26 (36%)	0	100	100
All	All	5042/5135 (98%)	4153 (82%)	877 (17%)	12 (0%)	54	84

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	LR	71	GLU
2	SB	129	PHE
18	SI	9	PRO
27	LJ	67	GLN
26	LC	19	ASN

### 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	
2	SB	151/164 (92%)	147 (97%)	4 (3%)	51	78
3	SC	23/174 (13%)	22 (96%)	1 (4%)	33	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SD	120/122 (98%)	118 (98%)	2 (2%)	66	86
5	SE	82/83 (99%)	81 (99%)	1 (1%)	75	89
6	SG	115/131 (88%)	111 (96%)	4 (4%)	41	72
7	SF	107/111 (96%)	106 (99%)	1 (1%)	82	92
8	SH	96/105 (91%)	91 (95%)	5 (5%)	27	63
9	S1	67/73 (92%)	67 (100%)	0	100	100
10	S2	85/90 (94%)	83 (98%)	2 (2%)	54	79
11	S3	95/118 (80%)	93 (98%)	2 (2%)	59	82
12	S4	75/97 (77%)	73 (97%)	2 (3%)	50	77
13	S5	51/52 (98%)	51 (100%)	0	100	100
14	S6	74/80 (92%)	71 (96%)	3 (4%)	35	69
15	S7	36/70 (51%)	36 (100%)	0	100	100
16	S8	35/75 (47%)	34 (97%)	1 (3%)	48	75
17	S9	49/50 (98%)	49 (100%)	0	100	100
18	SI	45/69 (65%)	44 (98%)	1 (2%)	57	81
19	SA	37/66 (56%)	35 (95%)	2 (5%)	26	62
25	L2	212/221 (96%)	208 (98%)	4 (2%)	62	84
26	LC	158/173 (91%)	157 (99%)	1 (1%)	89	95
27	LJ	154/168 (92%)	149 (97%)	5 (3%)	44	74
28	LK	67/147 (46%)	67 (100%)	0	100	100
29	LL	61/152 (40%)	60 (98%)	1 (2%)	68	86
30	LM	117/123 (95%)	114 (97%)	3 (3%)	51	78
31	LN	100/100 (100%)	99 (99%)	1 (1%)	80	90
32	LO	91/111 (82%)	89 (98%)	2 (2%)	57	81
33	LP	101/113 (89%)	100 (99%)	1 (1%)	80	90
34	LQ	90/100 (90%)	89 (99%)	1 (1%)	78	89
35	LR	63/90 (70%)	61 (97%)	2 (3%)	44	74
36	L1	83/95 (87%)	82 (99%)	1 (1%)	75	89
37	L3	96/96 (100%)	92 (96%)	4 (4%)	34	68
38	L4	68/86 (79%)	67 (98%)	1 (2%)	70	87
39	L5	84/91 (92%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	L6	72/80 (90%)	70 (97%)	2 (3%)	49	76
41	L7	71/88 (81%)	71 (100%)	0	100	100
42	L8	58/82 (71%)	57 (98%)	1 (2%)	66	86
43	L9	61/64 (95%)	61 (100%)	0	100	100
44	LA	43/49 (88%)	37 (86%)	6 (14%)	4	27
45	LB	52/57 (91%)	51 (98%)	1 (2%)	62	84
46	LD	50/51 (98%)	50 (100%)	0	100	100
47	LE	35/43 (81%)	34 (97%)	1 (3%)	48	75
48	LS	42/45 (93%)	41 (98%)	1 (2%)	54	79
49	LG	39/39 (100%)	38 (97%)	1 (3%)	51	78
50	LH	44/52 (85%)	41 (93%)	3 (7%)	18	55
51	LI	29/35 (83%)	29 (100%)	0	100	100
52	LF	23/66 (35%)	23 (100%)	0	100	100
All	All	3507/4347 (81%)	3433 (98%)	74 (2%)	62	82

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	L2	15	ASN
29	LL	175	LYS
47	LE	7	ARG
25	L2	175	ARG
27	LJ	45	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
27	LJ	29	ASN
27	LJ	169	ASN
47	LE	40	HIS
27	LJ	40	GLN
27	LJ	130	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1455/1555 (93%)	522 (35%)	24 (1%)
20	X	9/13 (69%)	4 (44%)	1 (11%)
21	E	74/75 (98%)	25 (33%)	1 (1%)
22	D	75/76 (98%)	26 (34%)	1 (1%)
23	B	2746/2923 (93%)	817 (29%)	28 (1%)
24	C	113/114 (99%)	37 (32%)	1 (0%)
All	All	4472/4756 (94%)	1431 (31%)	56 (1%)

5 of 1431 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	U
1	A	9	A
1	A	10	G
1	A	21	U
1	A	23	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	E	32	U
23	B	660	A
23	B	2238	U
22	D	32	U
23	B	267	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 130 ligands modelled in this entry, 129 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
53	PAR	A	1601	1	45,45,45	0.28	0	60,67,67	1.02	5 (8%)

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
53	PAR	A	1601	1	-	0/18/94/94	0/4/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	PAR	O52-C13-O43	-3.46	107.69	111.43
53	A	1601	PAR	C13-C23-C33	-3.16	98.21	102.07
53	A	1601	PAR	O33-C14-C24	-2.62	103.24	108.20
53	A	1601	PAR	O11-C42-C32	-2.19	103.90	108.96
53	A	1601	PAR	O54-C14-C24	2.08	114.75	110.06

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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1460:C	O3'	1461:U	P	4.77