



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 9, 2017 – 11:01 am GMT

PDB ID : 5H1S
EMDB ID: : EMD-9572
Title : Structure of the large subunit of the chloro-ribosome
Authors : Ahmed, T.; Yin, Z.; Bhushan, S.
Deposited on : 2016-10-11
Resolution : 3.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
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) : recalc28906

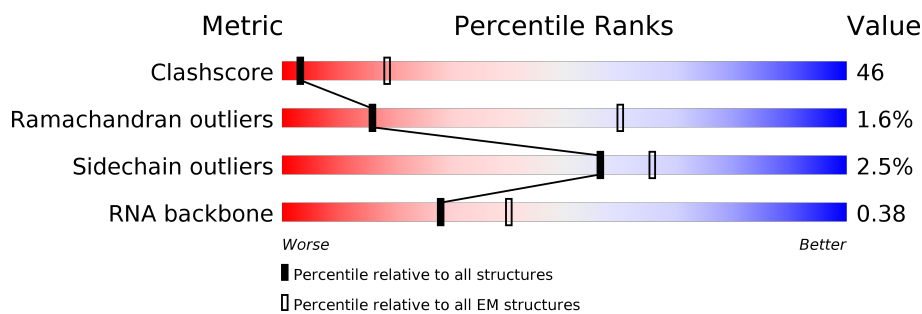
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.




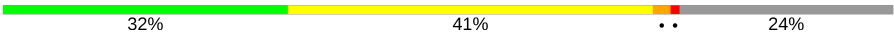
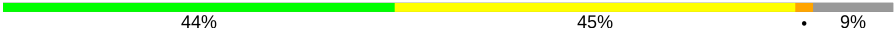
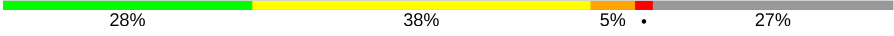
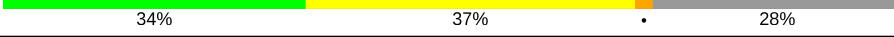
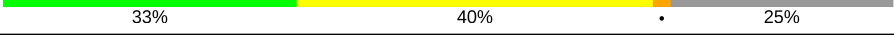
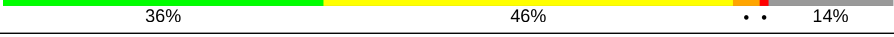
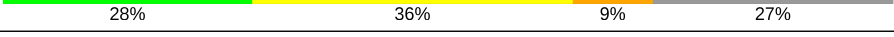
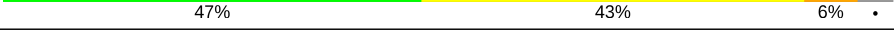

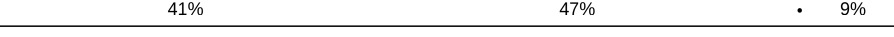




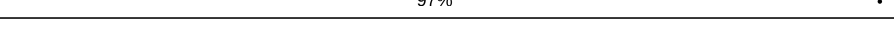

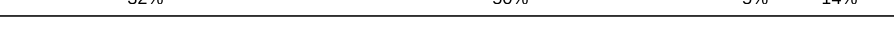
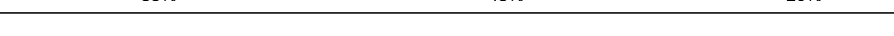
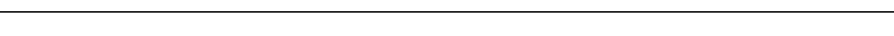
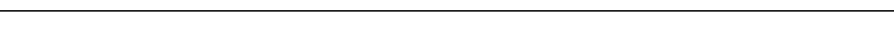
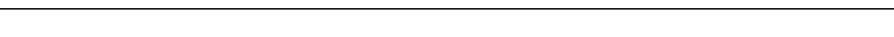
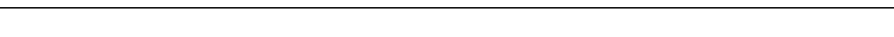

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	2810	29% 44% 26% .
2	C	106	9% 46% 37% . .
3	B	121	12% 44% 40% .
4	L	191	36% 39% . . 23%
5	M	121	54% 46%
6	N	192	31% 51% 9% . 8%
7	O	135	44% 54% . .
8	P	116	57% 43%

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Mol	Chain	Length	Quality of chain
9	Q	123	
10	R	156	
11	S	127	
12	T	201	
13	U	199	
14	V	122	
15	W	145	
16	X	137	
17	Y	77	
18	Z	109	
19	E	271	
20	b	56	
21	c	65	
22	d	60	
23	e	73	
24	f	37	
25	F	221	
26	G	243	
27	H	220	
28	I	182	
29	J	155	
30	g	142	
31	a	94	
32	h	116	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2799	Total	C	N	O	P	0	0
			60117	26819	11134	19365	2799		

- Molecule 2 is a RNA chain called Spinach chloroplast 4.5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	102	Total	C	N	O	P	0	0
			2187	977	403	705	102		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	117	Total	C	N	O	P	0	0
			2500	1116	452	815	117		

- Molecule 4 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	147	Total	C	N	O	S	0	0
			1184	754	225	202	3		

- Molecule 5 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	177	Total	C	N	O	S	0	0
			1342	836	264	236	6		

- Molecule 7 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	134	Total	C	N	O	S	0	0
			1067	672	217	173	5		

- Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 9 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	120	Total	C	N	O	S	0	0
			947	589	183	170	5		

- Molecule 10 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	118	Total	C	N	O	S	0	0
			953	610	186	156	1		

- Molecule 11 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	115	Total	C	N	O	S	0	0
			996	633	208	153	2		

- Molecule 12 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	T	147	Total	C	N	O	0	0
			1171	759	202	210		

- Molecule 13 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	144	Total	C	N	O	S	0	0
			1149	731	210	200	8		

- Molecule 14 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	92	Total	C	N	O	S	0	0
			740	477	129	132	2		

- Molecule 15 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	124	Total	C	N	O	S	0	0
			993	624	187	180	2		

- Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	100	Total	C	N	O	S	0	0
			810	511	159	140			

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	74	Total	C	N	O	S	0	0
			605	385	121	98	1		

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	90	Total	C	N	O	S	0	0
			754	470	150	131	3		

- Molecule 19 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	247	Total	C	N	O	S	0	0
			1904	1181	390	327	6		

- Molecule 20 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	46	Total	C	N	O	S	0	0
			378	250	70	58			

- Molecule 21 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	51	Total	C	N	O	S	0	0
			415	258	83	70	4		

- Molecule 22 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	57	Total	C	N	O	S	0	0
			445	268	103	71	3		

- Molecule 23 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	e	69	Total	C	N	O	S	0	0
			563	353	119	90	1		

- Molecule 24 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	f	37	Total	C	N	O	S	0	0
			304	186	70	44	4		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	212	Total	C	N	O	S	0	0
			1620	1025	295	289	11		

- Molecule 26 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	210	Total	C	N	O	S	0	0
			1655	1052	308	292	3		

- Molecule 27 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	175	Total	C	N	O	S	0	0
			1351	862	233	248	8		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	173	Total	C	N	O	S	0	0
			1353	855	249	245	4		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	53	Total	C	N	O	S	0	0
			423	280	74	68	1		

- Molecule 30 is a protein called 50S ribosomal protein 5 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	43	Total	C	N	O	S	0	0
			345	218	65	59	3		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	38	Total	C	N	O	S	0	0
			300	187	49	62	2		

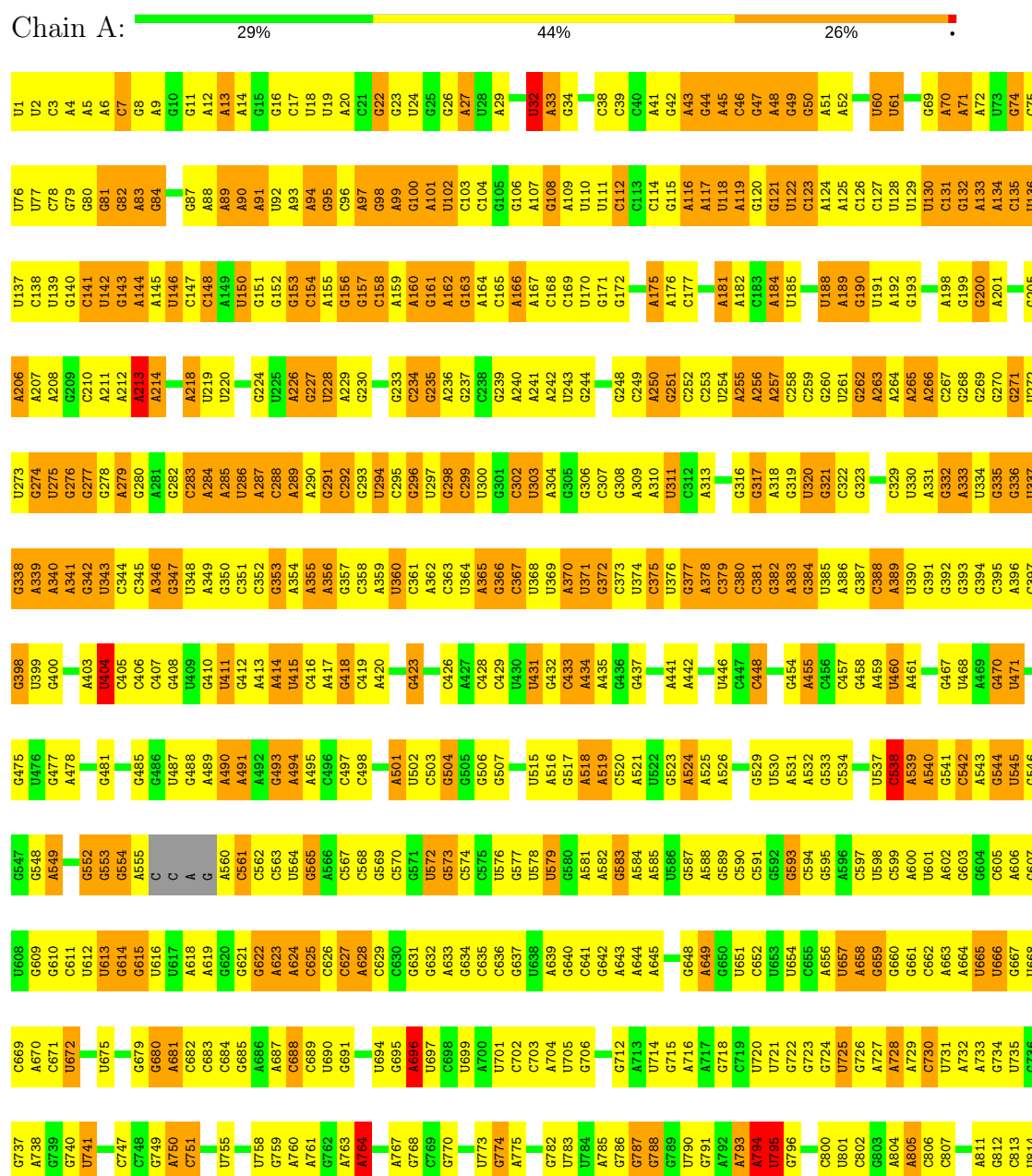
- Molecule 32 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

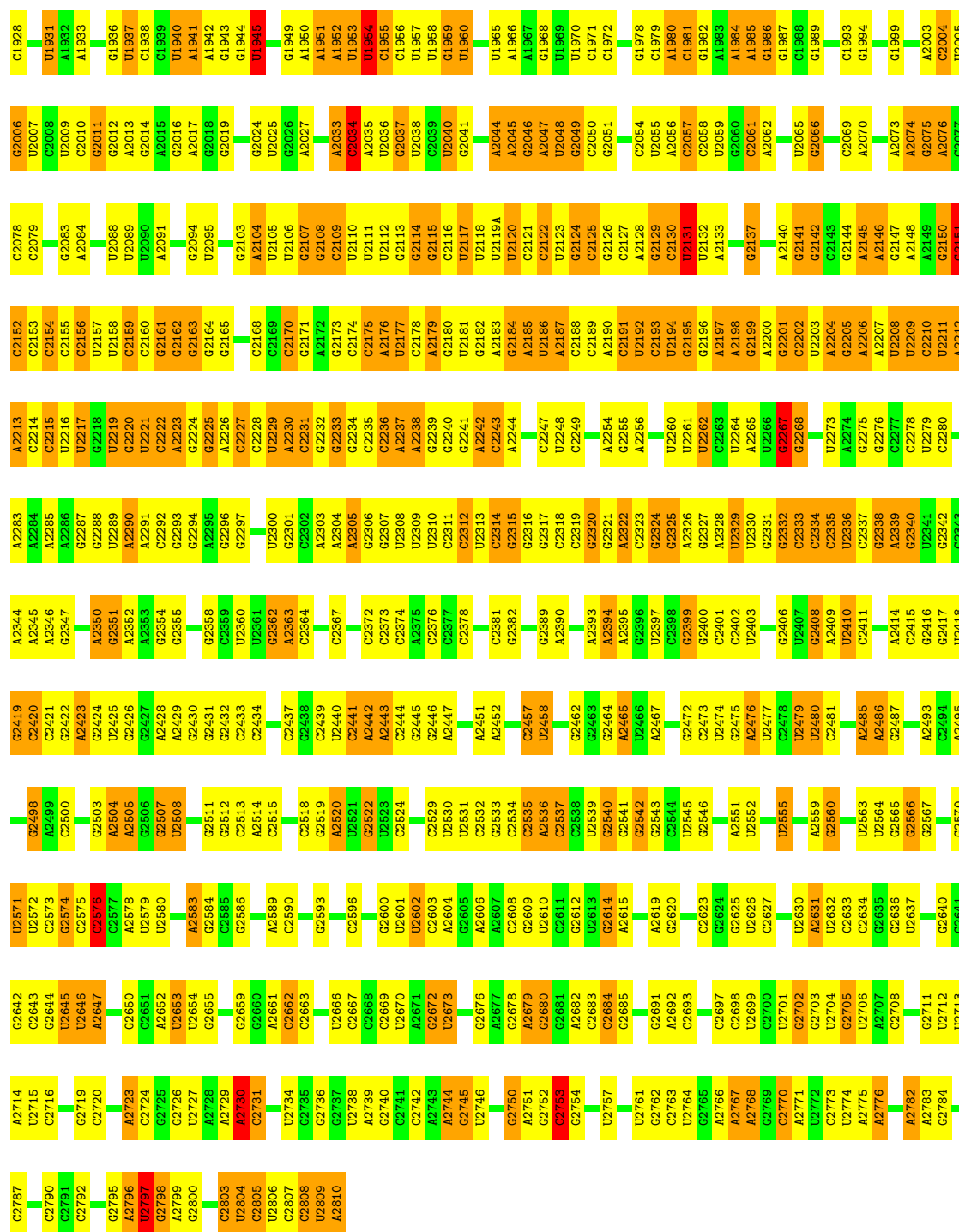
3 Residue-property plots

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

• Molecule 1: 23S rRNA

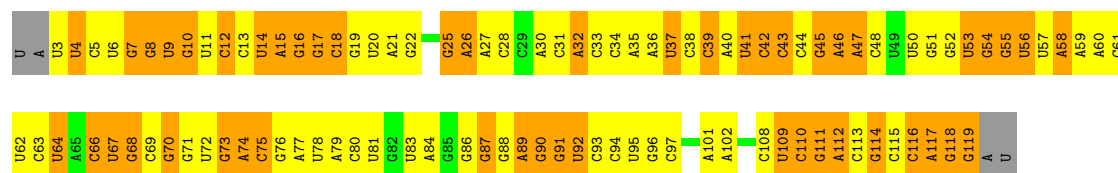


A1849	G1782	U1632	C1572	G1443	G1351	G1277	A1204	G1141	U1069	G1005	U942	U880	A1815
G1850	A1783	A1633	C1573	A1444	C1352	U1278	G1207	G1142	G1070	G1006	C943	U881	G816
U1851	G1786	C1635	G1574	A1448	A1353	G1281	G1208	U1143	C1071	A1007	C944	U882	C817
C1853	U1789	U1636	C1575	G1449	U1361	U1283	U1209	U1144	G1072	A1008	A945	C883	U818
A1857	G1793	G1637	U1576	G1450	U1362	U1284	A1210	U1145	A1074	A1009	A946	G884	G819
A1858	A1794	G1643	A1578	G1451	A1363	G1285	G1211	U1147	G1075	C1010	U948	U885	G820
G1859	U1795	A1644	G1517	A1452	C1366	U1286	U1219	G1150	A1076	G1012	A949	U886	U821
G1860	A1796	A1645	G1518	G1453	U1373	G1287	U1220	U1151	C1077	C1013	A950	G887	U822
U1861	G1797	C1647	A1519	G1454	A1374	U1288	U1224	G1153	A1078	G1016	A952	C888	C823
G1866	C1798	G1648	A1520	G1457	U1375	A1289	U1225	A1154	G1079	G1017	A954	G889	U824
A1867	A1799	C1649	A1522	U1459	G1376	C1291	U1227	A1155	C1080	A1018	C952	G891	C825
A1868	C1800	A1650	A1523	G1458	U1377	A1290	G1231	G1156	G1081	U1019	G955	C892	C828
G1869	A1801	C1651	G1524	G1461	C1379	A1294	A1232	A1157	G1082	G1020	G956	C893	G829
G1870	G1802	A1652	U1588	G1462	U1385	A1295	G1233	U1158	U1083	A1021	U957	G894	A830
U1871	C1803	C1653	G1589	G1463	A1386	A1296	A1234	A1159	C1084	C1022	C958	G895	A831
G1872	A1804	U1654	C1590	U1464	A1387	C1297	G1235	A1160	G1085	C1023	G959	G896	A832
G1873	C1805	G1655	C1591	A1465	A1388	U1298	A1236	A1161	G1086	A1024	A960	G898	G836
U1874	U1806	A1662	A1592	G1466	U1389	C1299	A1237	C1162	U1088	G1025	G961	A899	U837
G1875	G1807	A1663	U1593	C1467	A1390	U1299	G1238	G1163	U1090	A1028	G962	G900	U838
A1876	C1808	G1664	A1594	G1468	G1391	U1300	G1239	G1164	U1091	A1029	U963	C901	G839
G1877	G1809	U1665	G1595	G1469	C1392	U1301	G1240	G1165	U1092	G1030	G964	G902	A840
C1878	C1810	A1666	A1596	A1470	G1393	G1305	G1241	G1166	A1097	G1031	G965	U903	G841
U1879	A1811	G1667	C1597	A1471	U1394	A1307	G1242	U1168	A1098	G1032	C967	A905	C843
G1880	A1812	C1668	C1598	G1472	A1395	A1308	G1243	U1169	A1099	C1033	C968	C906	G844
A1881	C1813	A1669	A1536	G1473	C1397	U1309	U1245	A1170	C1103	G1034	A969	C907	C845
U1882	G1814	G1670	U1537	A1474	U1398	C1310	G1246	G1171	C1104	C1035	G970	A908	A846
G1883	C1815	A1671	G1602	G1475	A1399	A1312	U1247	G1172	U1107	U1036	G972	A909	G850
A1884	G1816	U1672	C1539	G1476	U1400	A1313	G1248	G1173	C1108	A1037	A973	A910	U851
G1885	C1817	A1673	C1540	G1477	G1401	A1314	G1251	U1174	C1109	A1038	G974	C912	U852
A1886	U1818	G1674	U1541	U1478	A1406	C1315	G1252	U1175	U1109	U1040	A975	G913	G853
G1887	A1819	C1675	G1542	U1479	U1407	A1316	G1253	G1176	U1110	C1041	C976	A914	A854
G1888	C1820	U1676	A1544	U1481	A1408	C1317	U1254	G1177	G1111	A1042	G977	G915	C855
U1889	A1821	G1677	G1545	G1482	U1409	C1318	U1255	G1178	A1112	C1043	A978	G916	U856
G1890	C1822	C1608	G1546	G1483	U1410	C1319	G1256	C1180	U1113	C1044	U979	C917	G857
A1891	G1823	G1682	C1547	G1484	A1413	G1320	U1257	G1181	A1114	G1045	G980	A918	G858
G1892	C1824	C1683	U1547	U1485	U1414	A1321	G1258	U1182	G1115	C1046	G981	A919	A859
G1895	U1825	G1684	G1548	G1486	U1415	A1322	G1259	A1183	U1116	U1047	G982	A920	C860
G1896	G1826	U1687	A1549	U1487	U1416	A1323	U1260	G1184	G1117	C1048	G983	C921	A861
C1897	U1827	G1688	U1551	C1487	U1417	U1333	G1261	C1185	U1118	A1049	G984	U922	U862
G1898	A1828	C1689	U1552	U1488	U1418	U1334	A1262	U1186	G1119	G1050	A985	C923	C863
U1899	C1829	A1690	U1553	A1489	U1419	C1335	A1263	G1187	U1122	U1051	U986	U924	U864
G1902	G1830	G1682	A1554	G1494	U1425	C1336	A1264	U1188	U1125	A1052	A987	A927	A865
G1905	A1831	C1683	G1555	C1495	U1426	U1337	G1265	G1189	U1126	A1053	G988	U928	G866
U1906	C1832	G1684	U1556	A1496	U1427	C1338	G1266	A1192	U1130	A1054	G989	A929	C867
G1910	G1833	U1693	G1557	A1497	C1428	U1339	U1267	U1193	C1131	A1056	C993	A932	G868
A1914	C1834	C1694	U1558	G1498	C1429	C1340	A1268	G1194	U1132	A1057	A994	A933	U870
A1915	U1837	U1697	A1559	G1499	U1430	C1341	G1269	U1195	U1133	A1060	G997	A934	A871
G1916	C1838	C1698	U1560	U1500	C1431	A1342	U1270	A1196	G1134	G1061	U998	U935	A872
U1917	A1839	U1699	G1501	G1501	U1432	G1343	G1271	A1197	U1135	G1062	C999	U936	A873
G1920	G1840	A1701	U1502	A1502	U1433	G1344	G1272	A1198	U1136	U1063	G1000	U937	G874
G1921	C1841	G1702	C1504	C1504	U1435	U1345	A1271	A1199	U1137	A1064	A1001	G937	C875
U1925	G1842	U1666	C1505	C1505	U1436	U1347	G1273	A1200	C1137	G1065	A1002	G938	A876
A1926	C1847	U1568	U1506	G1506	U1437	C1348	A1274	A1201	G1138	A1066	G1003	A939	C877
U1927	C1848	G1571	G1507	U1507	G1438	G1349	U1275	A1202	U1139	G1066	A1004	C940	U878
			U	U		U1350	U1276	C1203	G1140			C941	G879



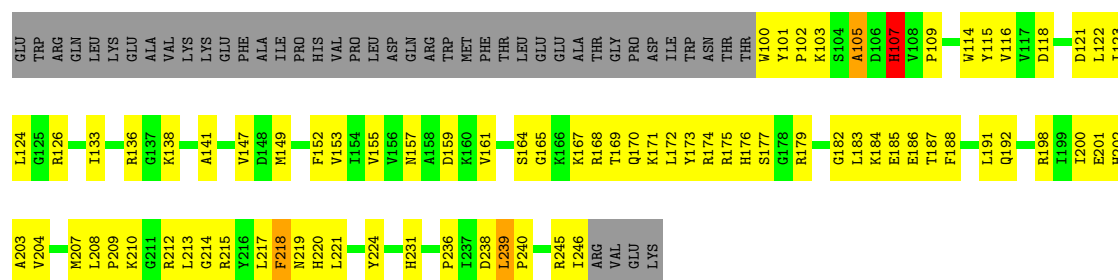
- Molecule 3: 5S rRNA

Chain B: 



- Molecule 4: 50S ribosomal protein L13, chloroplastic

Chain L: 



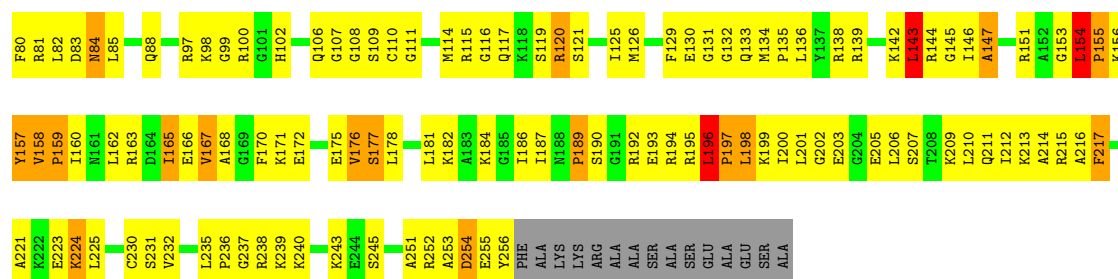
- Molecule 5: 50S ribosomal protein L14, chloroplastic

Chain M: 



- Molecule 6: 50S ribosomal protein L15

Chain N: 



- Molecule 7: 50S ribosomal protein L16, chloroplastic

Chain O: 





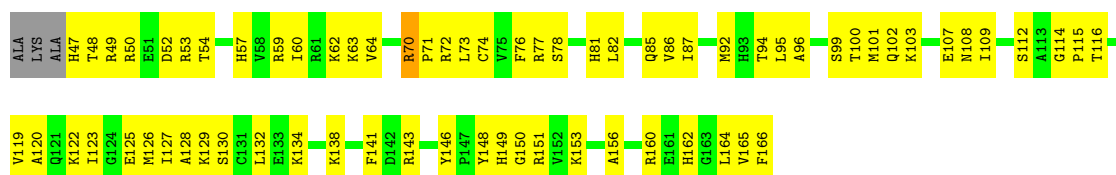
• Molecule 8: 50S ribosomal protein L17

Chain P: 57% 43%



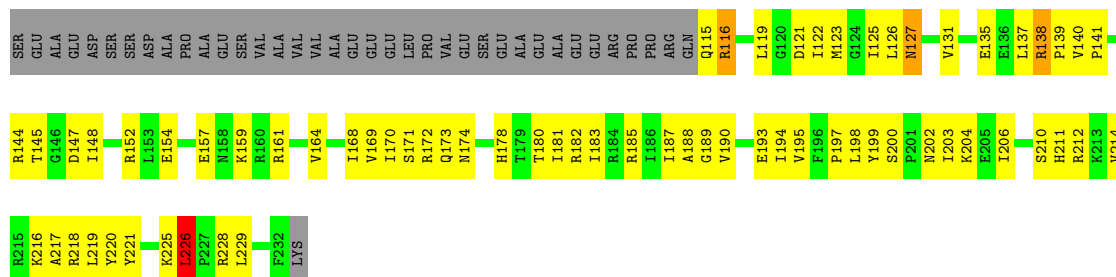
• Molecule 9: 50S ribosomal protein L18

Chain Q: 41% 55%



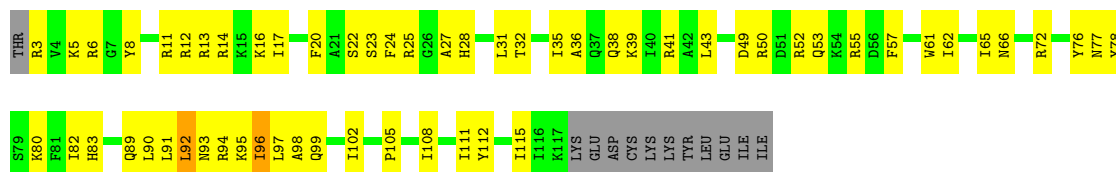
• Molecule 10: 50S ribosomal protein L19, chloroplastic

Chain R: 32% 41% 24%



• Molecule 11: 50S ribosomal protein L20, chloroplastic

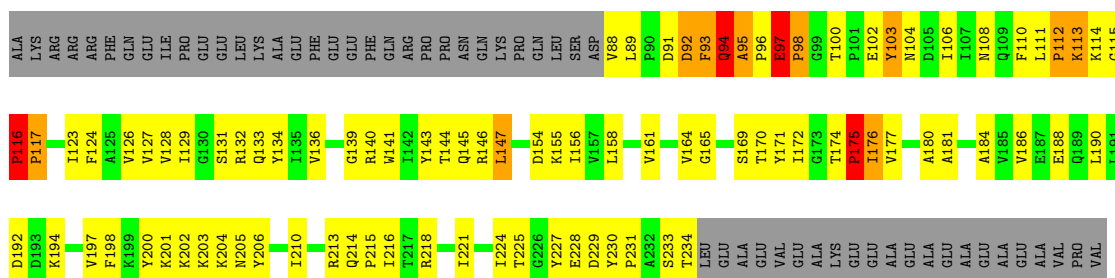
Chain S: 44% 45% 9%



• Molecule 12: 50S ribosomal protein L21, chloroplastic

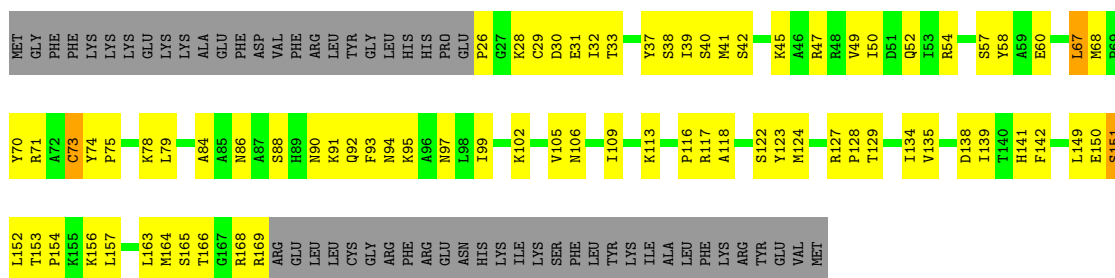
Chain T: 28% 38% 5% 27%





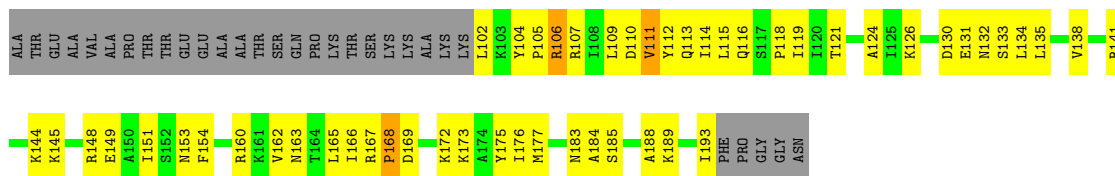
• Molecule 13: 50S ribosomal protein L22, chloroplastic

Chain U: 34% 37% 28%



• Molecule 14: 50S ribosomal protein L23, chloroplastic

Chain V: 33% 40% 25%



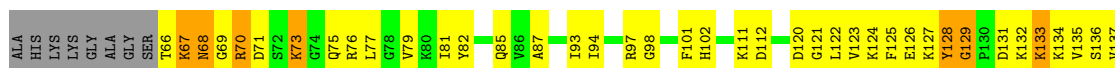
• Molecule 15: 50S ribosomal protein L24, chloroplastic

Chain W: 36% 46% 14%



• Molecule 16: 50S ribosomal protein L27

Chain X: 28% 36% 9% 27%





• Molecule 17: 50S ribosomal protein L28



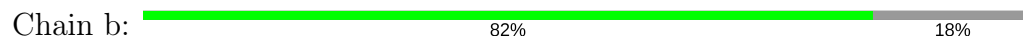
• Molecule 18: 50S ribosomal protein L29



• Molecule 19: 50S ribosomal protein L2, chloroplastic




• Molecule 20: 50S ribosomal protein L32, chloroplastic



• Molecule 21: 50S ribosomal protein L33, chloroplastic



• Molecule 22: 50S ribosomal protein L34, chloroplastic

Chain d: 



- Molecule 23: 50S ribosomal protein L35, chloroplastic

Chain e: 



- Molecule 24: 50S ribosomal protein L36, chloroplastic

Chain f: 



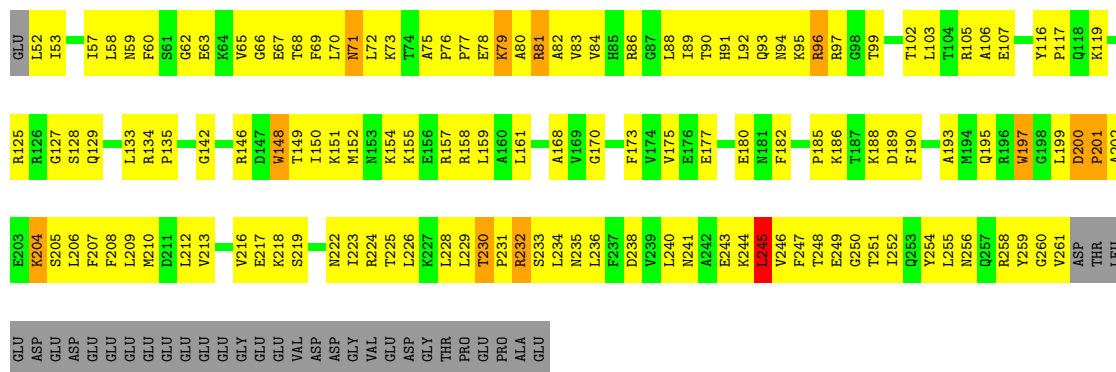
- Molecule 25: 50S ribosomal protein L3

Chain F: 



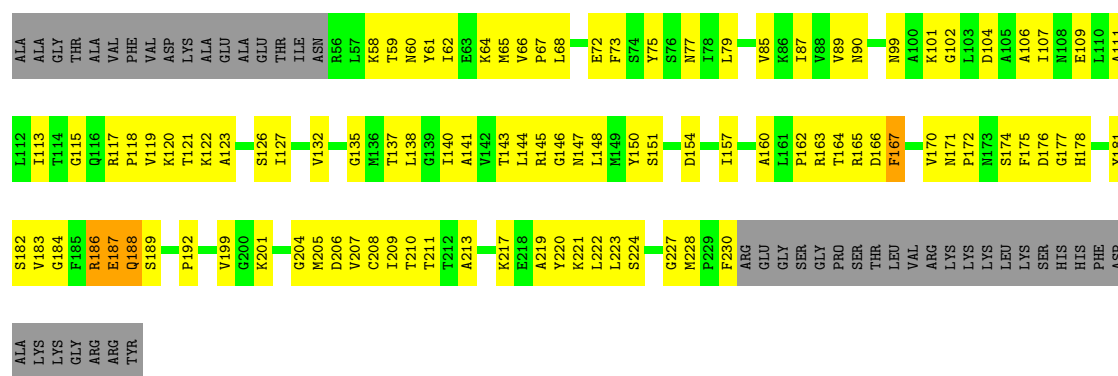
- Molecule 26: 50S ribosomal protein L4, chloroplastic

Chain G: 



- Molecule 27: 50S ribosomal protein L5, chloroplastic

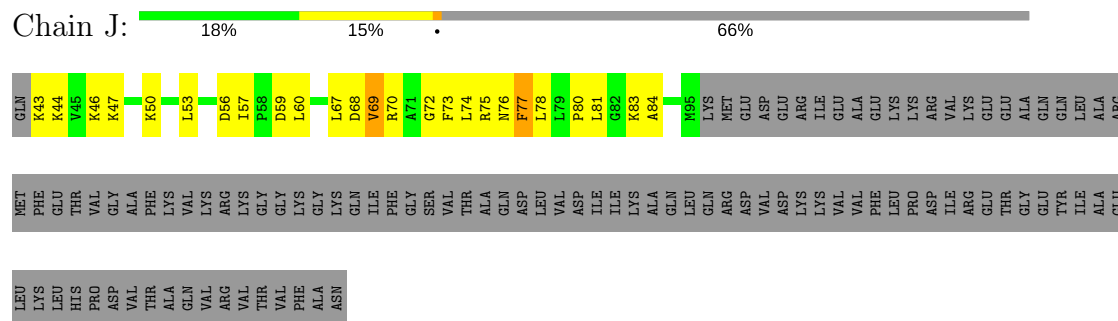
Chain H: 



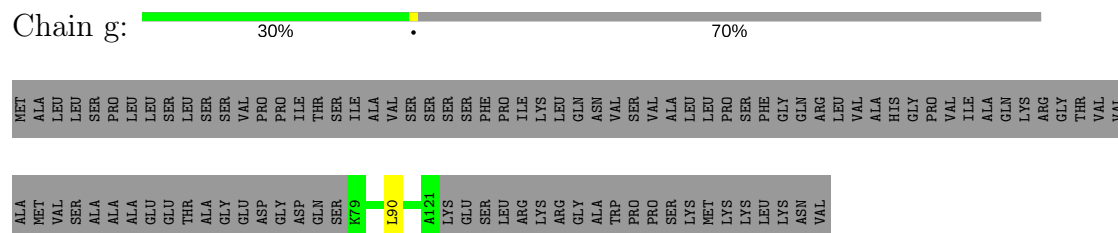
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9

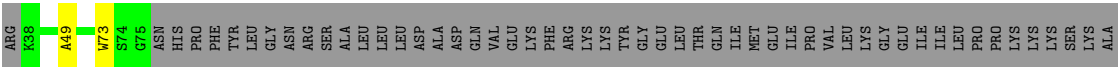


• Molecule 30: 50S ribosomal protein 5 alpha, chloroplastic

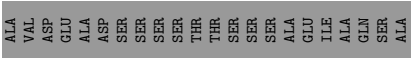
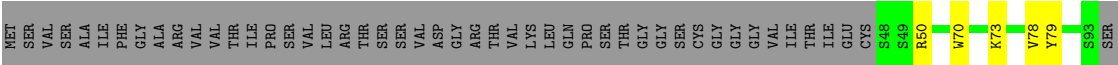


• Molecule 31: 50S ribosomal protein L31





- Molecule 32: 50S ribosomal protein 6, chloroplastic



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	174949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	109375	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.80	18/67340 (0.0%)	0.94	109/105056 (0.1%)
10	R	0.61	0/967	0.79	2/1300 (0.2%)
11	S	0.77	0/1013	0.82	1/1351 (0.1%)
12	T	0.73	0/1199	0.88	3/1633 (0.2%)
13	U	0.60	1/1168 (0.1%)	0.69	0/1566
14	V	0.53	0/749	0.65	0/1006
15	W	0.49	0/1006	0.67	2/1343 (0.1%)
16	X	0.66	0/825	0.80	2/1099 (0.2%)
17	Y	0.65	0/615	0.78	2/819 (0.2%)
18	Z	0.52	0/762	0.71	0/1012
19	E	0.60	0/1938	0.78	1/2603 (0.0%)
2	C	3.05	9/2449 (0.4%)	1.30	26/3817 (0.7%)
20	b	0.72	0/387	0.65	0/513
21	c	0.55	0/422	0.85	1/564 (0.2%)
22	d	0.45	0/447	0.63	0/588
23	e	0.72	0/569	0.82	1/752 (0.1%)
24	f	0.57	0/306	0.78	0/403
25	F	0.66	0/1646	0.74	1/2201 (0.0%)
26	G	0.65	2/1687 (0.1%)	0.78	1/2271 (0.0%)
27	H	0.37	0/1372	0.60	0/1848
28	I	0.49	0/1374	0.63	1/1849 (0.1%)
29	J	0.33	0/427	0.65	0/568
3	B	0.78	0/2796	0.87	2/4357 (0.0%)
30	g	0.44	0/345	0.85	1/455 (0.2%)
31	a	0.29	0/306	0.60	0/413
32	h	0.70	1/382 (0.3%)	0.81	2/520 (0.4%)
4	L	0.67	0/1212	0.68	1/1634 (0.1%)
5	M	0.60	0/951	0.69	1/1282 (0.1%)
6	N	0.40	0/1361	0.77	3/1806 (0.2%)
7	O	0.63	1/1089 (0.1%)	0.71	1/1461 (0.1%)
8	P	0.63	0/959	0.76	0/1280
9	Q	0.52	0/963	0.67	0/1293
All	All	0.88	32/99032 (0.0%)	0.90	164/148663 (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
10	R	0	1
11	S	0	3
13	U	0	1
19	E	0	3
24	f	0	1
25	F	0	1
26	G	0	2
27	H	0	1
32	h	0	2
9	Q	0	1
All	All	0	16

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	A	N3-C4	76.76	1.80	1.34
2	C	95	A	C6-N1	71.09	1.85	1.35
2	C	95	A	C5-C4	50.90	1.74	1.38
2	C	95	A	C2-N3	47.29	1.76	1.33
2	C	95	A	N1-C2	47.04	1.76	1.34

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	95	A	N1-C2-N3	-28.24	115.18	129.30
2	C	95	A	C2-N3-C4	24.30	122.75	110.60
2	C	95	A	N7-C8-N9	14.45	121.03	113.80
6	N	196	LEU	C-N-CD	-14.44	88.83	120.60
2	C	95	A	C4-C5-N7	-13.30	104.05	110.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	Q	70	ARG	Peptide
10	R	190	VAL	Peptide
11	S	24	PHE	Peptide
11	S	82	ILE	Peptide

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Mol	Chain	Res	Type	Group
11	S	96	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	60117	0	30254	3962	0
2	C	2187	0	1099	306	0
3	B	2500	0	1263	331	0
4	L	1184	0	1221	135	0
5	M	942	0	996	51	0
6	N	1342	0	1413	392	0
7	O	1067	0	1120	103	0
8	P	944	0	1004	68	0
9	Q	947	0	966	87	0
10	R	953	0	1044	80	0
11	S	996	0	1060	122	0
12	T	1171	0	1216	216	0
13	U	1149	0	1220	98	0
14	V	740	0	795	103	0
15	W	993	0	1054	127	0
16	X	810	0	847	185	0
17	Y	605	0	652	51	0
18	Z	754	0	804	99	0
19	E	1904	0	1982	219	0
20	b	378	0	413	0	0
21	c	415	0	434	0	0
22	d	445	0	501	0	0
23	e	563	0	621	0	0
24	f	304	0	342	0	0
25	F	1620	0	1699	174	0
26	G	1655	0	1723	238	0
27	H	1351	0	1407	136	0
28	I	1353	0	1416	90	0
29	J	423	0	488	39	0
30	g	345	0	395	0	0
31	a	300	0	279	0	0
32	h	368	0	386	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	90825	0	60114	6418	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 46.

The worst 5 of 6418 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2351:G:C4	9:Q:64:VAL:HG21	1.27	1.61
2:C:95:A:C6	2:C:95:A:C5	1.79	1.59
16:X:128:TYR:CB	16:X:134:LYS:CD	1.78	1.58
11:S:91:LEU:CD1	12:T:175:PRO:HB3	1.30	1.55
1:A:274:G:C6	1:A:433:C:C6	1.94	1.54

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	
4	L	145/191 (76%)	120 (83%)	21 (14%)	4 (3%)	6	39
5	M	119/121 (98%)	97 (82%)	22 (18%)	0	100	100
6	N	175/192 (91%)	156 (89%)	6 (3%)	13 (7%)	1	14
7	O	132/135 (98%)	107 (81%)	23 (17%)	2 (2%)	12	52
8	P	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
9	Q	118/123 (96%)	99 (84%)	19 (16%)	0	100	100
10	R	116/156 (74%)	89 (77%)	26 (22%)	1 (1%)	20	63
11	S	113/127 (89%)	91 (80%)	22 (20%)	0	100	100
12	T	145/201 (72%)	108 (74%)	28 (19%)	9 (6%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	U	142/199 (71%)	117 (82%)	24 (17%)	1 (1%)	25	68
14	V	90/122 (74%)	79 (88%)	9 (10%)	2 (2%)	8	44
15	W	122/145 (84%)	95 (78%)	25 (20%)	2 (2%)	11	50
16	X	98/137 (72%)	87 (89%)	7 (7%)	4 (4%)	3	29
17	Y	72/77 (94%)	61 (85%)	11 (15%)	0	100	100
18	Z	88/109 (81%)	85 (97%)	3 (3%)	0	100	100
19	E	245/271 (90%)	187 (76%)	57 (23%)	1 (0%)	38	77
20	b	44/56 (79%)	35 (80%)	9 (20%)	0	100	100
21	c	49/65 (75%)	34 (69%)	15 (31%)	0	100	100
22	d	55/60 (92%)	47 (86%)	6 (11%)	2 (4%)	4	33
23	e	67/73 (92%)	50 (75%)	16 (24%)	1 (2%)	12	52
24	f	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
25	F	210/221 (95%)	173 (82%)	37 (18%)	0	100	100
26	G	208/243 (86%)	166 (80%)	40 (19%)	2 (1%)	18	61
27	H	173/220 (79%)	145 (84%)	27 (16%)	1 (1%)	28	70
28	I	171/182 (94%)	142 (83%)	27 (16%)	2 (1%)	15	57
29	J	51/155 (33%)	41 (80%)	9 (18%)	1 (2%)	9	46
30	g	41/142 (29%)	36 (88%)	5 (12%)	0	100	100
31	a	36/94 (38%)	26 (72%)	9 (25%)	1 (3%)	6	39
32	h	44/116 (38%)	31 (70%)	12 (27%)	1 (2%)	7	43
All	All	3218/4086 (79%)	2630 (82%)	538 (17%)	50 (2%)	16	50

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	107	HIS
6	N	143	LEU
6	N	147	ALA
6	N	154	LEU
6	N	155	PRO

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	
4	L	125/165 (76%)	124 (99%)	1 (1%)	85	94
5	M	101/101 (100%)	101 (100%)	0	100	100
6	N	135/144 (94%)	126 (93%)	9 (7%)	19	57
7	O	107/108 (99%)	107 (100%)	0	100	100
8	P	96/96 (100%)	96 (100%)	0	100	100
9	Q	99/100 (99%)	99 (100%)	0	100	100
10	R	104/135 (77%)	101 (97%)	3 (3%)	48	78
11	S	102/114 (90%)	102 (100%)	0	100	100
12	T	129/174 (74%)	122 (95%)	7 (5%)	26	63
13	U	126/176 (72%)	125 (99%)	1 (1%)	85	94
14	V	81/103 (79%)	80 (99%)	1 (1%)	75	90
15	W	112/129 (87%)	109 (97%)	3 (3%)	50	80
16	X	85/111 (77%)	74 (87%)	11 (13%)	5	25
17	Y	64/67 (96%)	61 (95%)	3 (5%)	30	67
18	Z	83/97 (86%)	79 (95%)	4 (5%)	30	67
19	E	195/216 (90%)	189 (97%)	6 (3%)	45	78
20	b	39/49 (80%)	39 (100%)	0	100	100
21	c	48/59 (81%)	47 (98%)	1 (2%)	59	84
22	d	47/49 (96%)	45 (96%)	2 (4%)	33	70
23	e	59/62 (95%)	58 (98%)	1 (2%)	66	87
24	f	34/34 (100%)	34 (100%)	0	100	100
25	F	174/182 (96%)	170 (98%)	4 (2%)	56	82
26	G	176/205 (86%)	169 (96%)	7 (4%)	36	71
27	H	148/183 (81%)	146 (99%)	2 (1%)	71	89
28	I	147/154 (96%)	147 (100%)	0	100	100
29	J	47/134 (35%)	46 (98%)	1 (2%)	59	84
30	g	39/121 (32%)	39 (100%)	0	100	100
31	a	33/83 (40%)	32 (97%)	1 (3%)	46	78
32	h	40/96 (42%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2775/3447 (80%)	2707 (98%)	68 (2%)	56 81

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	X	146	ASN
17	Y	131	LYS
26	G	232	ARG
16	X	150	TYR
16	X	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
15	W	68	HIS
18	Z	77	ASN
26	G	257	GLN
15	W	121	GLN
15	W	133	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2796/2810 (99%)	962 (34%)	0
2	C	101/106 (95%)	45 (44%)	0
3	B	116/121 (95%)	54 (46%)	0
All	All	3013/3037 (99%)	1061 (35%)	0

5 of 1061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	C
1	A	13	A
1	A	22	G
1	A	27	A
1	A	32	U

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

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.