



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 12, 2019 – 08:19 AM EST

PDB ID : 5IMR
EMDB ID: : EMD-6585
Title : Structure of ribosome bound to cofactor at 5.7 angstrom resolution
Authors : Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.
Deposited on : 2016-03-06
Resolution : 5.70 Å (reported)
Based on PDB ID : 4W2E, 5AA0

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

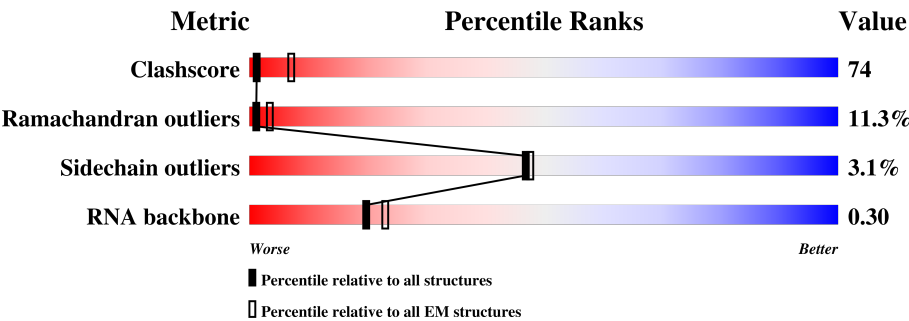
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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.



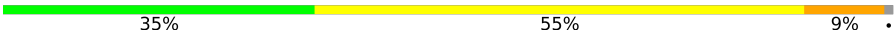

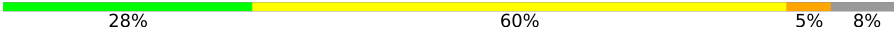

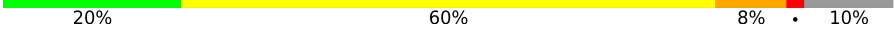




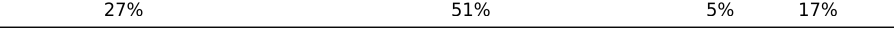
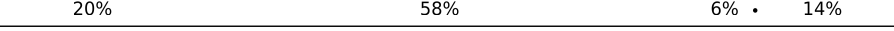
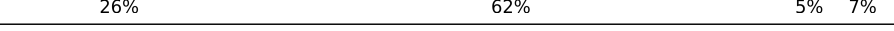
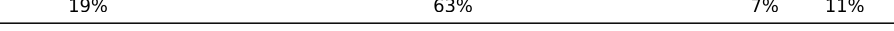






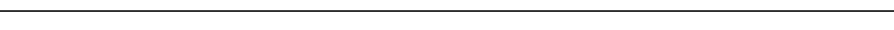

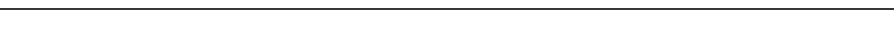
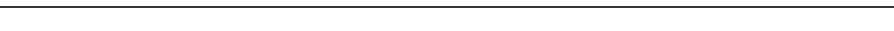


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	1522	<div><div>55%</div><div>41%</div><div>.</div></div>
2	F	256	<div><div>27%</div><div>60%</div><div>5%</div><div>9%</div></div>
3	G	239	<div><div>24%</div><div>59%</div><div>.</div><div>14%</div></div>
4	H	209	<div><div>27%</div><div>67%</div><div>6%</div></div>
5	I	162	<div><div>22%</div><div>68%</div><div>.</div><div>7%</div></div>
6	J	101	<div><div>26%</div><div>72%</div><div>.</div></div>
7	K	156	<div><div>33%</div><div>65%</div><div>..</div></div>
8	L	138	<div><div>21%</div><div>72%</div><div>7%</div></div>


















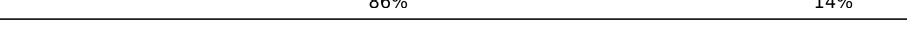





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Mol	Chain	Length	Quality of chain
9	M	128	
10	N	105	
11	O	129	
12	P	132	
13	Q	126	
14	R	61	
15	S	89	
16	T	88	
17	U	105	
18	V	88	
19	W	93	
20	X	106	
21	Y	27	
22	C	610	
23	D	2893	
24	E	123	
25	Z	229	
26	a	276	
27	b	206	
28	c	210	
29	d	182	
30	e	180	
31	f	140	
32	g	122	
33	h	150	

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Mol	Chain	Length	Quality of chain
34	i	141	 86% 10% . .
35	j	118	 92% 8% .
36	k	112	 89% 9% .
37	l	146	 70% 10% . 20%
38	m	118	 91% 8% .
39	n	101	 81% 18% .
40	o	113	 90% 6% . .
41	p	96	 91% 7% .
42	q	110	 78% 22%
43	r	206	 79% 8% 13%
44	s	85	 87% 6% 7%
45	t	67	 93% 7%
46	u	60	 92% 7% .
47	v	71	 76% 18% 6%
48	w	60	 82% 13% 5%
49	x	54	 69% 22% 9%
50	y	49	 86% 14%
51	z	65	 83% 14% . .
52	1	37	 30% 65% 5%
53	2	173	 50% 23% . 25%
54	3	147	 18% 48% 22% . 9%
55	4	77	 14% 51% 34% .
56	5	76	 5% 49% 45% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	GCP	C	701	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 152879 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1515	Total	C	N	O	P	0	0
			32554	14490	6022	10527	1515		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	73	Total	C	N	O	0	0
			597	380	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	570	Total	C	N	O	S	0	0
			4461	2858	768	826	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	272	Total	C	N	O	S	0	0
			2124	1339	424	358	3		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	182	Total	C	N	O	S	0	0
			1482	947	269	261	5		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	174	Total	C	N	O	S	0	0
			1328	844	248	235	1		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	p	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	79	Total	C	N	O	S	0	0
			625	387	131	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	u	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	130	Total	C	N	O	S	0	0
			641	381	130	130			

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

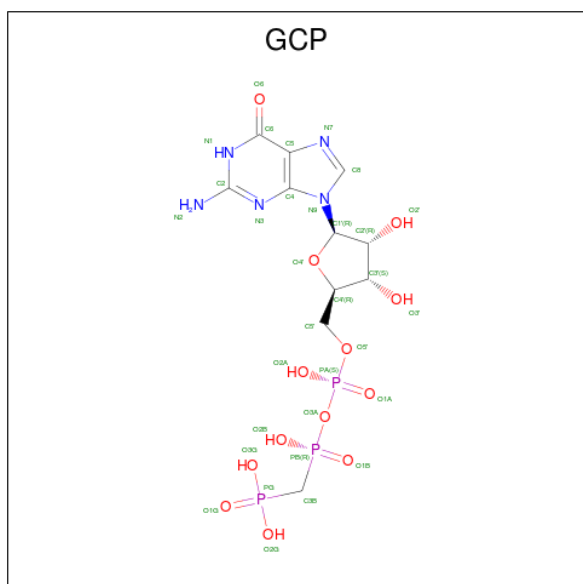
- Molecule 55 is a RNA chain called P site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called E site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).

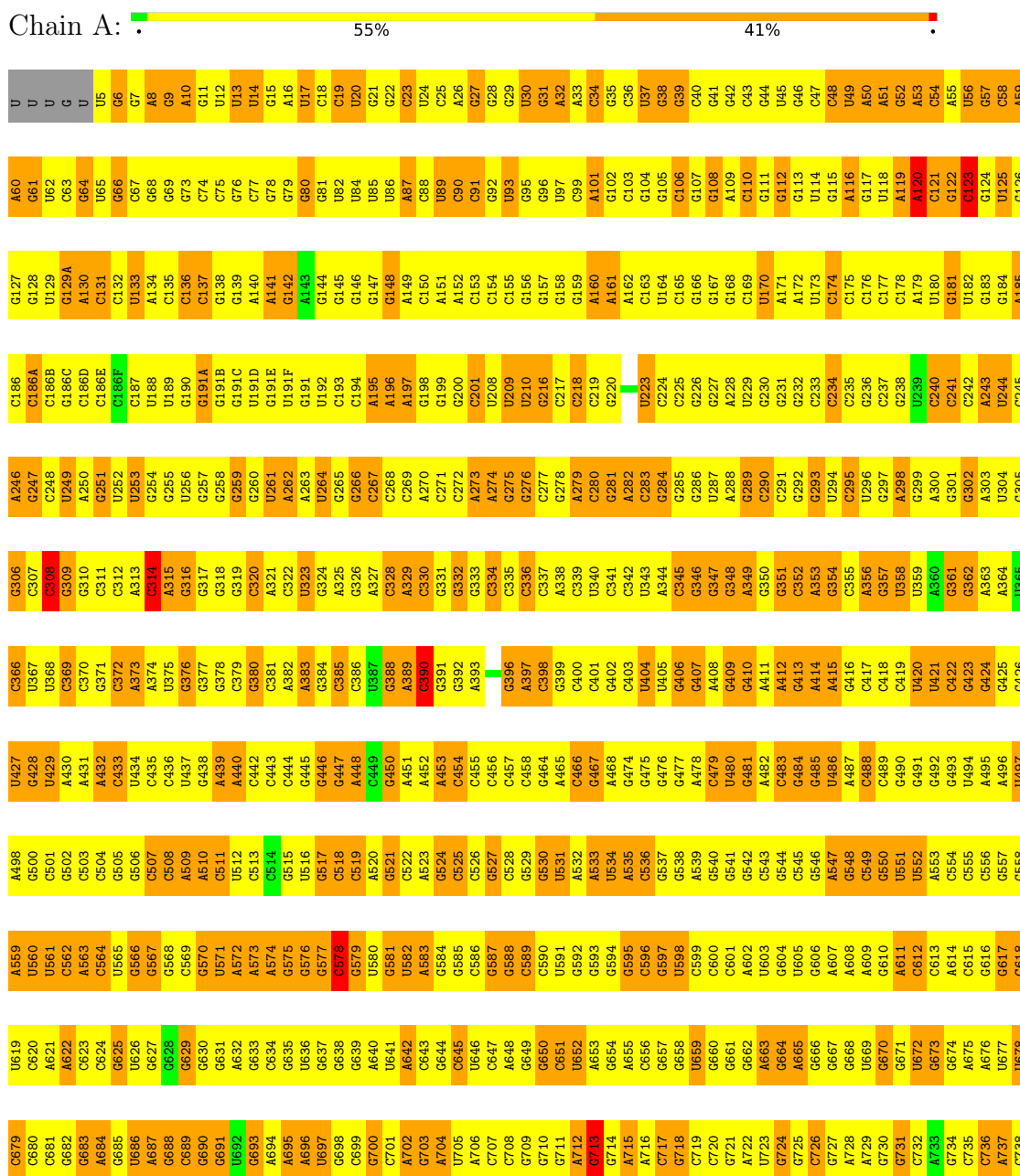


Mol	Chain	Residues	Atoms					AltConf
57	C	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

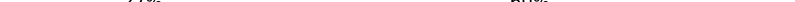
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

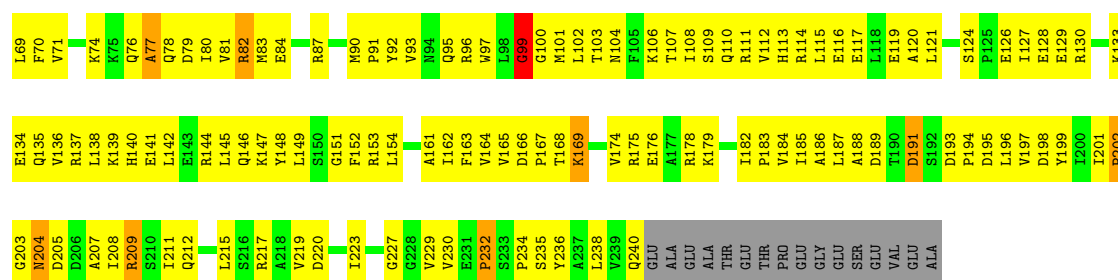


C1527	C1466	C1401	C1342	C1282	C1222	C1161	A1101	A1041	C985	C925	A865	G799	C739
U1528	C1467	C1402	C1343	C1283	C1223	C1162	A1102	C1042	A986	G926	C866	G800	C740
C1529	A1468	C1403	C1344	C1284	C1224	C1163	C1103	C1043	C987	G927	C867	U801	C741
C1530	C1469	C1404	U1345	C1285	C1225	C1164	C1104	C1044	C988	G928	C868	A802	C742
A1531	C1470	C1405	A1346	A1286	A1226	C1165	A1105	C1045	C989	G929	C869	G803	C743
C1532	C1471	C1406	C1347	A1287	A1227	C1166	C1106	A1046	C990	C930	U870	U804	C744
C1533	A1473	C1407	U1348	A1288	C1228	A1167	C1107	C1047	U991	C931	U871	C805	C745
A1534	C1474	A1408	A1349	A1289	A1229	A1169	C1108	C1048	U992	C932	A872	C806	A746
C1535	C1475	C1409	A1350	C1290	C1230	C1170	C1109	U1049	C993	C933	A873	A807	C747
C1536	C1476	C1410	U1351	C1291	C1231	C1171	A1110	C1050	A994	C934	C874	C808	C748
U1537	C1477	C1411	C1352	C1292	U1232	C1172	C1111	C1051	C995	A935	C875	C809	C749
C1538	C1478	C1412	C1353	C1293	C1233	C1173	C1112	U1052	C996	C936	C876	C810	C750
C1539	C1479	A1413	C1354	C1294	C1234	C1174	C1113	C1053	C998	A937	C877	C811	U751
U1540	C1480	U1414	C1355	C1295	U1235	C1175	C1114	C1054	C999A	A938	C878	C812	C752
U1541	C1481	C1415	C1356	A1296	A1236	A1176	C1115	U1055	U999	C939	C879	U813	A753
U1542	C1482	C1416	A1357	C1297	C1237	C1177	C1116	U1056	A1000	C940	C880	A814	C754
C	C1483	C1417	C1358	C1298	A1238	C1178	C1117	C1057	G1001	G941	C881	A815	C755
U	C1484	A1418	C1359	A1299	A1239	A1179	C1118	C1058	G1002	G942	C882	A816	C756
U	U1485	C1419	A1360	G1300	U1240	C1180	C1119	C1059	C1003	U943	C883	C817	U757
C1486	C1486	C1420	C1361	C1301	C1241	C1181	C1120	C1060	A1004	G944	U884	C818	C758
C1487	C1487	C1421	C1362	U1302	C1242	C1182	C1121	G1061	A1005	G945	C885	A819	A759
C1488	C1488	C1422	C1362A	C1303	C1243	A1183	U1122	U1062	C1006	A946	C886	U820	C760
C1489	C1489	C1423	A1363	C1304	C1244	C1184	C1123	C1063	C1007	G947	C887	C821	C761
C1490	C1490	C1424	C1364	C1305	A1245	C1185	A1224	C1064	C1008	C948	C888	C822	C762
C1491	U1425	U1426	C1365	A1306	C1246	C1186	U1125	U1065	G1009	A949	A889	C823	C763
A1492	C1427	C1427	C1366	U1307	U1247	C1187	U1126	C1066	G1010	U950	C890	C824	C764
A1493	C1427	C1427	C1367	U1308	A1248	A1188	C1127	A1067	G1011	G951	U891	C825	C765
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C1496	C1430	C1311	C1370	G1311	A1251	A1191	A1130	U1070	A1014	G954	C894	A828	A768
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A1500	A1434	A1374	C1374	C1315	C1265	C1195	C1134	C1074	C1018	A958	C898	C832	C772
C1501	C1435	A1375	A1375	C1316	A1266	U1196	C1135	C1075	C1019	A959	C899	U833	C773
A1502	U1436	U1376	C1376	C1317	U1267	C1197	U1136	C1076	U1020	U960	A900	C834	C774
A1503	C1437	A1377	A1377	C1318	C1268	C1198	C1137	C1077	A901	U961	A901	U835	C775
C1504	C1438	C1378	C1378	A1319	C1269	U1199	C1138	U1078	G1022	C962	G902	C836	C776
C1505	C1439	C1379	C1379	C1320	C1270	C1200	C1139	C1079	G1023	C963	G903	C837	C777
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A1507	C1441	U1381	C1381	C1322	C1262	C1202	C1141	U1081	U1025	A965	U905	U841	C779
C1508	C1442	C1382	C1382	C1323	C1263	C1203	C1142	C1082	G1026	C966	C906	C842	A780
C1509	C1443	C1383	C1383	A1324	C1264	A1204	C1143	U1083	C1027	C967	A907	U843	A781
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C1511	C1447	C1385	C1385	C1326	C1266	C1206	C1145	U1085	C1028A	A969	A909	C849	C783
U1512	C1448	C1386	C1386	C1327	C1267	C1207	C1146	U1086	C1028B	C970	C910	U850	C784
A1513	C1449	C1387	C1387	C1328	A1268	C1208	C1147	C1087	G1029	C971	U911	C851	C785
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C1517	C1453	C1391	C1391	A1332	C1272	U1212	A1151	U1091	C1032A	A975	A915	C855	U789
A1518	C1454	C1392	C1392	A1333	C1273	A1152	A1093	C1032B	G1033	C976	G916	C856	A790
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C1525	C1464	C1399	C1399	A1340	A1280	C1220	U1159	C1099	U1039	A983	C923	U863	C797
C1526	C1465	C1400	C1400	U1341	U1281	C1221	C1160	C1100	C1040	C984	A924	U864	C798

- Molecule 2: 30S ribosomal protein S2

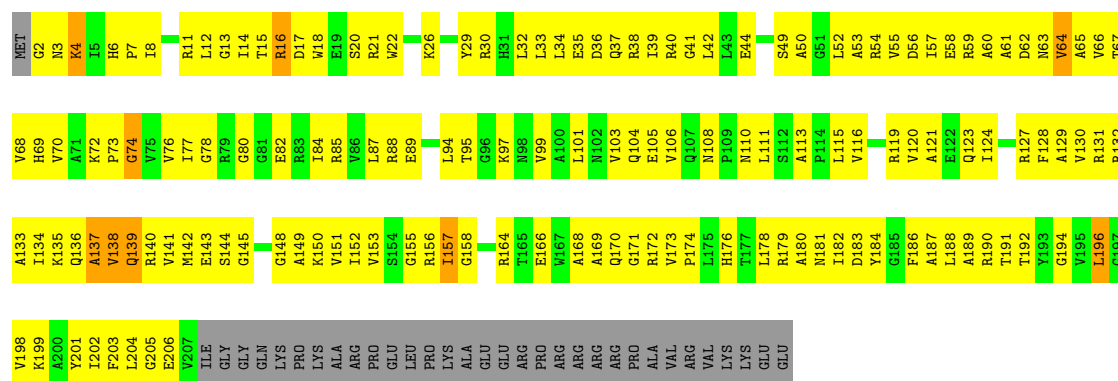
Chain F:  27% 60% 5% 9%

MET	PRO	VAL	GLU	ILE	THR	V7	V8	E9	L10	L11	V15	H16	F17	G18	H19	E20	K21	K22	R23	W24	F28	A29	I32	Y33	A34	E35	R36	N37	G38	I39	H40	I41	I42	D43	L44	L44	K46	T47	M48	E49	E50	L51	F52	R53	T54	F55	R56	F57	F58	E59	D60	L61	R64	F68
-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



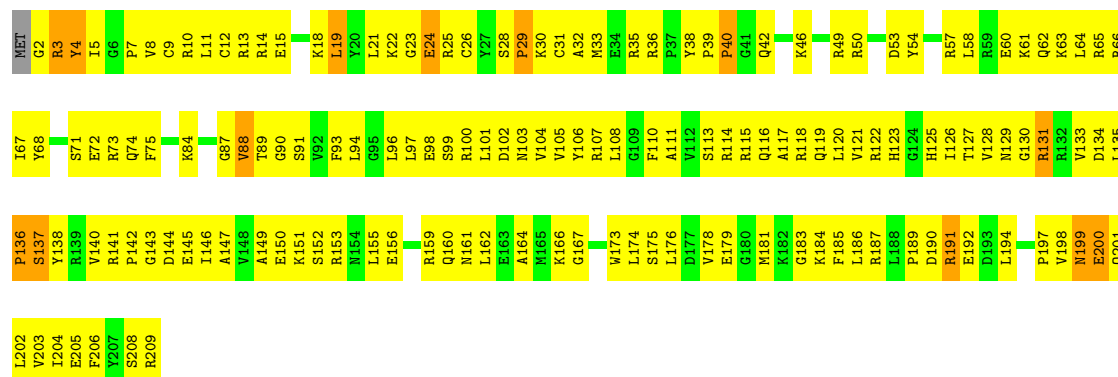
• Molecule 3: 30S ribosomal protein S3

Chain G: 24% 59% 14%



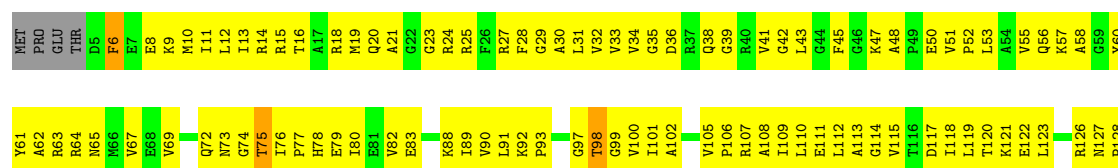
• Molecule 4: 30S ribosomal protein S4

Chain H: 27% 67% 6%



• Molecule 5: 30S ribosomal protein S5

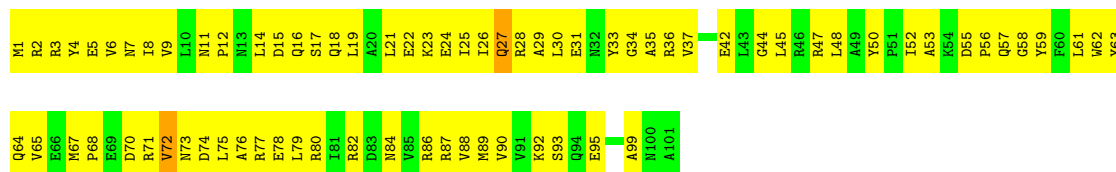
Chain I: 22% 68% 7%





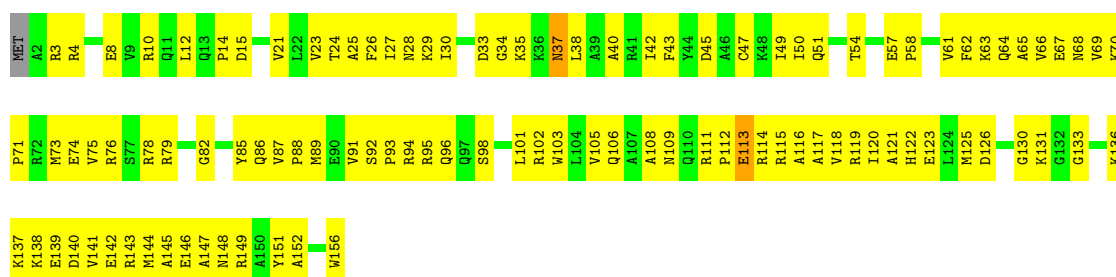
- Molecule 6: 30S ribosomal protein S6

Chain J:  26% 72%



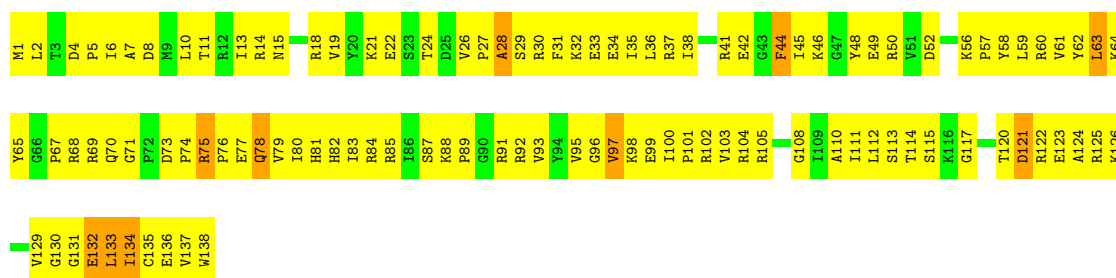
- Molecule 7: 30S ribosomal protein S7

Chain K: 33% 65%



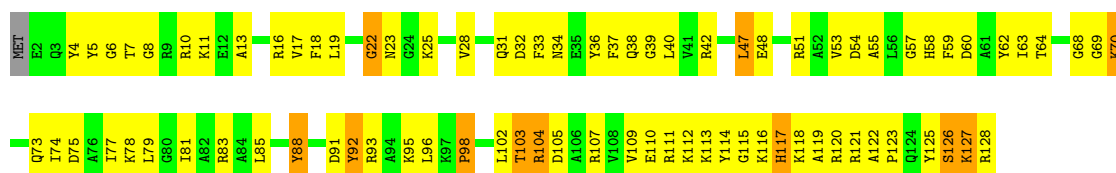
- Molecule 8: 30S ribosomal protein S8

Chain L:  21% 72% 7%



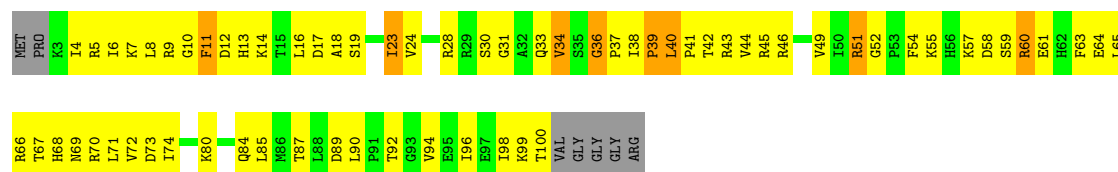
- Molecule 9: 30S ribosomal protein S9

Chain M: 35% 55% 9%



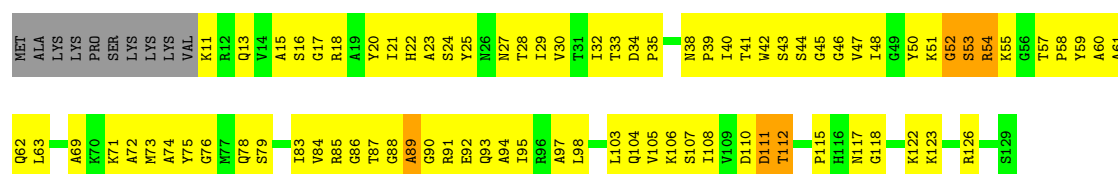
- Molecule 10: 30S ribosomal protein S10

Chain N: 

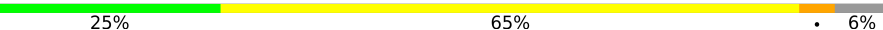


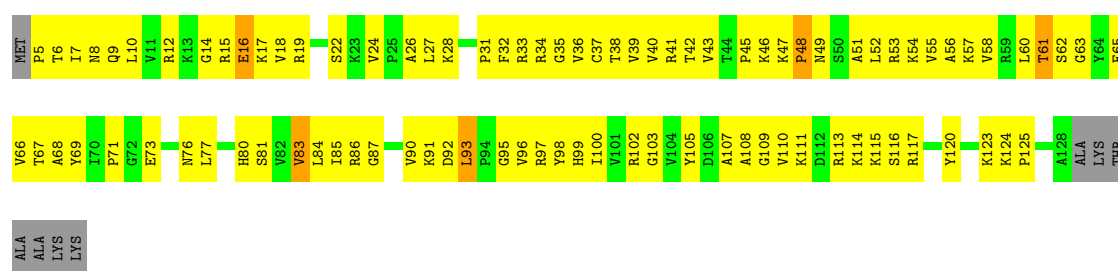
• Molecule 11: 30S ribosomal protein S11

Chain O: 



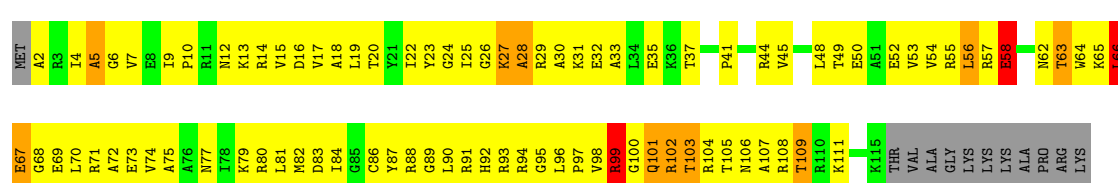
• Molecule 12: 30S ribosomal protein S12

Chain P: 



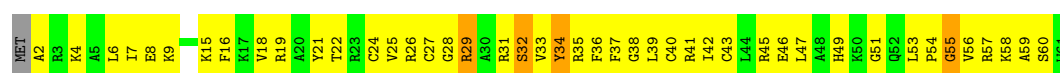
• Molecule 13: 30S ribosomal protein S13

Chain Q: 



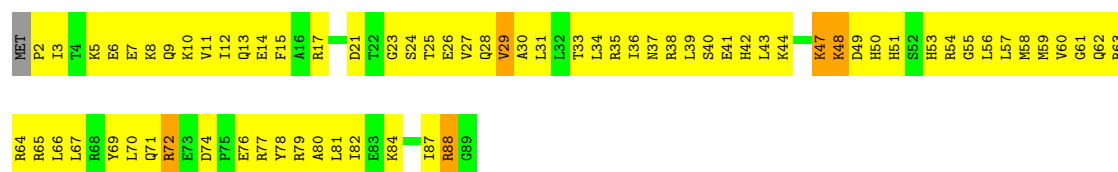
• Molecule 14: 30S ribosomal protein S14 type Z

Chain R: 



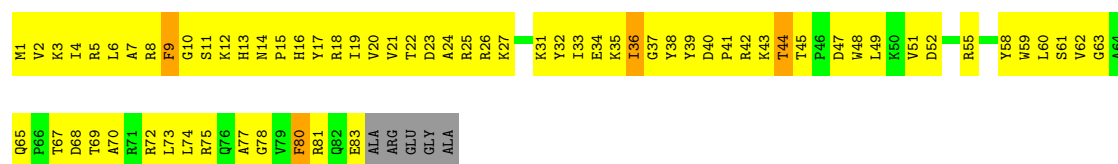
• Molecule 15: 30S ribosomal protein S15

Chain S: 



• Molecule 16: 30S ribosomal protein S16

Chain T: 17% 73% 5% 6%



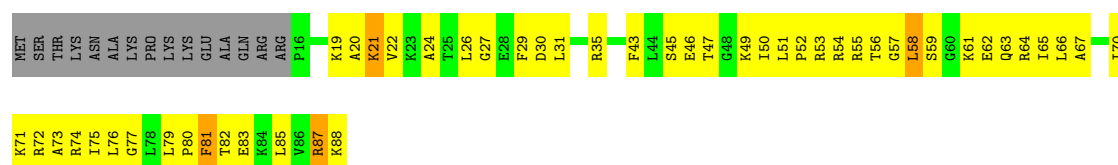
• Molecule 17: 30S ribosomal protein S17

Chain U: 16% 78% 5%



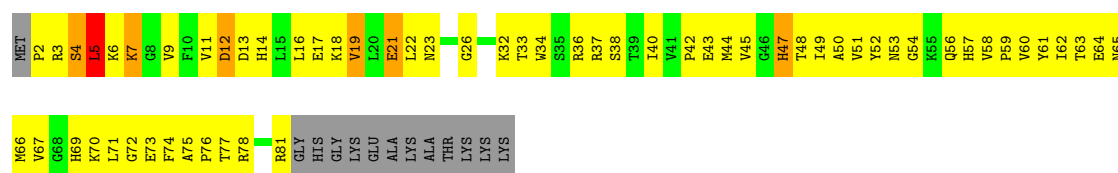
• Molecule 18: 30S ribosomal protein S18

Chain V: 27% 51% 5% 17%



• Molecule 19: 30S ribosomal protein S19

Chain W: 20% 58% 6% 14%



• Molecule 20: 30S ribosomal protein S20

Chain X: 26% 62% 5% 7%

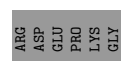
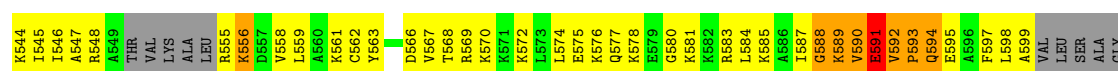
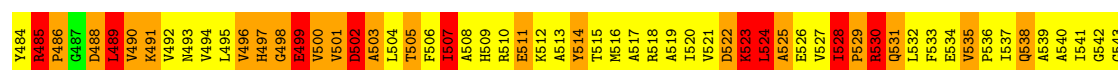
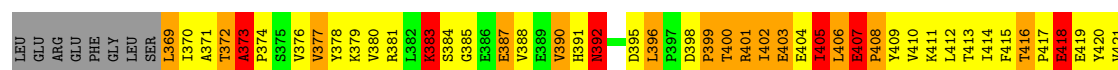
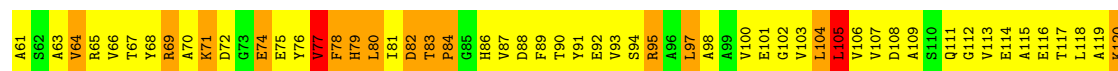




- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: Elongation factor 4



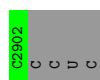
- Molecule 23: 23S ribosomal RNA





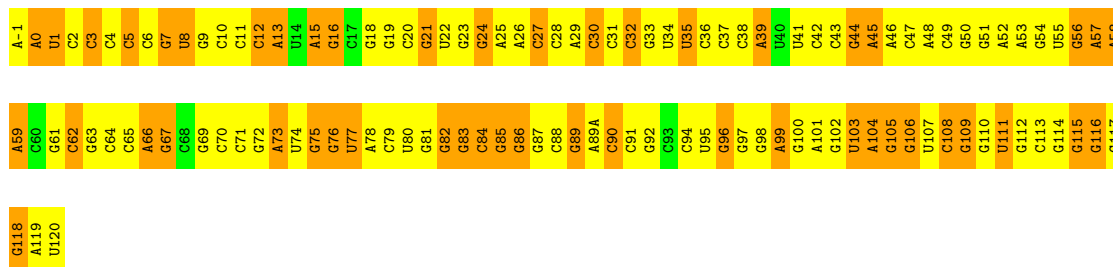

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C1798	C1799	G1730	C1660	U1541	U1542	G1479	A1420	G1361	U1300	U1240	C1180	C1120	U1060	A1000
C1800	C1801	A1731	C1661	U1602	G1543	G1480	G1421	G1362	A1301	A1241	C1181	C1121	U1061	A1001
G1861	G1862	G1732	C1662	C1603	C1544	U1482	G1422	C1363	G1302	A1242	A1182	C1122	G1062	G1002
A1802	A1803	G1733	C1663	C1604	C1545	G1483	G1423	G1364	G1303	G1243	G1183	C1123	G1063	G1003
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A1804	A1805	C1735	A1665	G1606	A1545A	G1485	G1425	A1365	C1305	G1245	G1185	G1125	U1065	C1005
G1865	G1866	C1741	G1666	C1607	C1546	G1486	G1426	A1366	C1306	A1246	G1186	A1126	U1066	C1006
G1867	G1868	G1742	A1667	A1608	C1547	G1487	A1427	A1367	A1307	A1247	G1187	A1127	G1067	C1007
G1869	G1870	G1743	A1668	A1609	C1548	G1488	G1428	G1368	A1308	G1248	U1188	A1128	G1068	C1008
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G1871	G1872	G1747	C1670	C1611	C1550	A1490	G1430	C1370	G1310	G1250	A1190	U1130	A1070	A1010
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G1810	G1811	G1750	A1673	A1614	A1553	C1493	U1433	A1373	U1313	A1253	G1193	A1133	A1073	U1013
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G1924	G1925	A1791	G1717	G1654	C1595	C1533	A1472	G1413	A1353	U1293	G1233	G1172	C1053	C1053
U1922	U1923	G1792	G1718	A1655	G1596	G1534	G1473	G1414	A1354	U1294	U1234	A1174	A1054	A1054
C1924	C1925	C1793	G1725	C1656	A1597	C1537	G1474	U1415	G1355	C1295	G1235	U1175	G1055	G1055
A1854	A1855	U1794	U1727	C1657	C1598	G1538	C1476	C1417	U1357	C1297	A1237	A1177	G1117	A1057



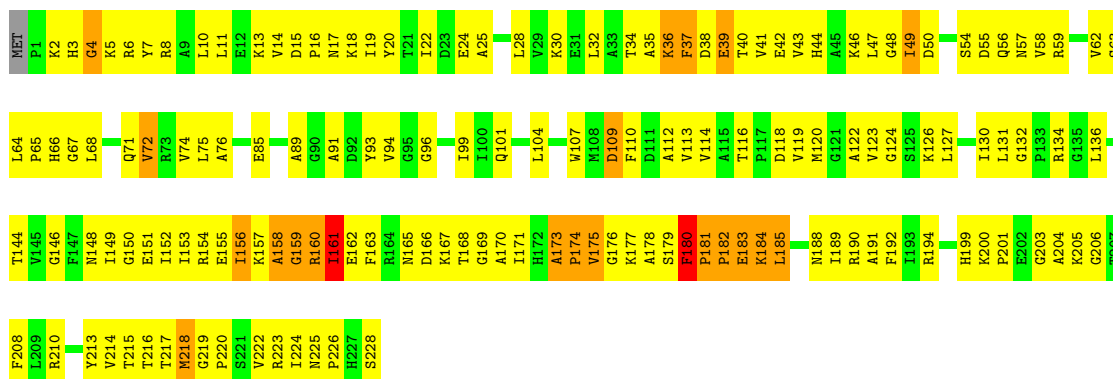
- Molecule 24: 5S ribosomal RNA

Chain E: 5% 55% 40%



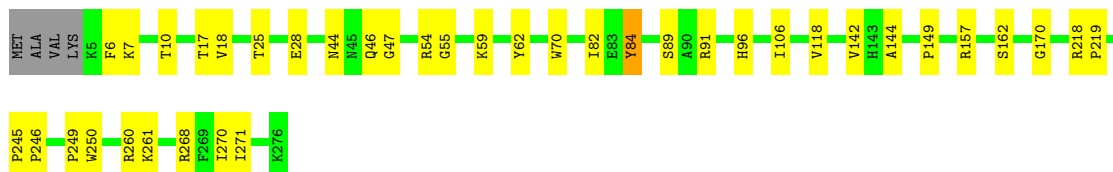
- Molecule 25: 50S ribosomal protein L1

Chain Z: 33% 57% 9%



- Molecule 26: 50S ribosomal protein L2

Chain a: 84% 14%




- Molecule 27: 50S ribosomal protein L3

Chain b: 85% 15%



- Molecule 28: 50S ribosomal protein L4

Chain c:  90% 9% .




- Molecule 29: 50S ribosomal protein L5

Chain d:  86% 13% .




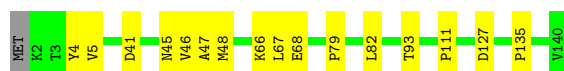
- Molecule 30: 50S ribosomal protein L6

Chain e:  82% 13% . .




- Molecule 31: 50S ribosomal protein L13

Chain f:  88% 11% .




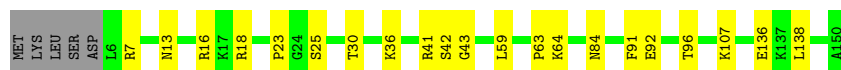
- Molecule 32: 50S ribosomal protein L14

Chain g:  89% 11%




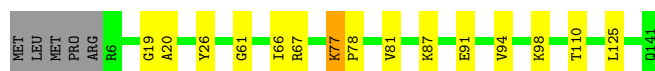
- Molecule 33: 50S ribosomal protein L15

Chain h:  83% 14% .




- Molecule 34: 50S ribosomal protein L16

Chain i:  86% 10% . .



- Molecule 35: 50S ribosomal protein L17

Chain j:  92% 8% .



- Molecule 36: 50S ribosomal protein L18

Chain k: 89% 9%



- Molecule 37: 50S ribosomal protein L19

Chain l: 70% 10% 20%



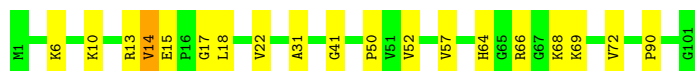
- Molecule 38: 50S ribosomal protein L20

Chain m: 91% 8%



- Molecule 39: 50S ribosomal protein L21

Chain n: 81% 18%



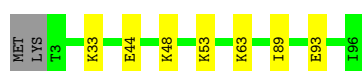
- Molecule 40: 50S ribosomal protein L22

Chain o: 90% 6%



- Molecule 41: 50S ribosomal protein L23

Chain p: 91% 7%




- Molecule 42: 50S ribosomal protein L24

Chain q: 78% 22%




- Molecule 43: 50S ribosomal protein L25

Chain r:  79% 8% 13%



- Molecule 44: 50S ribosomal protein L27

Chain s:  87% 6% 7%



- Molecule 45: 50S ribosomal protein L29

Chain t:  93% 7%



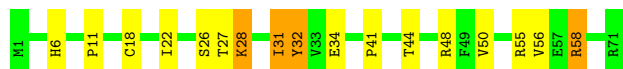
- Molecule 46: 50S ribosomal protein L30

Chain u:  92% 7% .




- Molecule 47: 50S ribosomal protein L31

Chain v:  76% 18% 6%



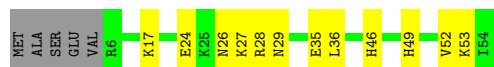
- Molecule 48: 50S ribosomal protein L32

Chain w:  82% 13% 5%




- Molecule 49: 50S ribosomal protein L33

Chain x:  69% 22% 9%



- Molecule 50: 50S ribosomal protein L34

Chain y:  86% 14%



- Molecule 51: 50S ribosomal protein L35

Chain z: 83% 14% ..



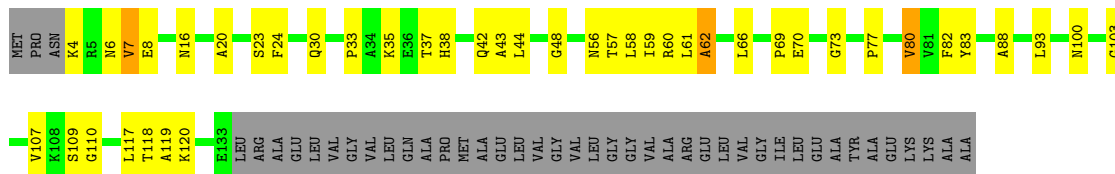
- Molecule 52: 50S ribosomal protein L36

Chain 1: 30% 65% 5%



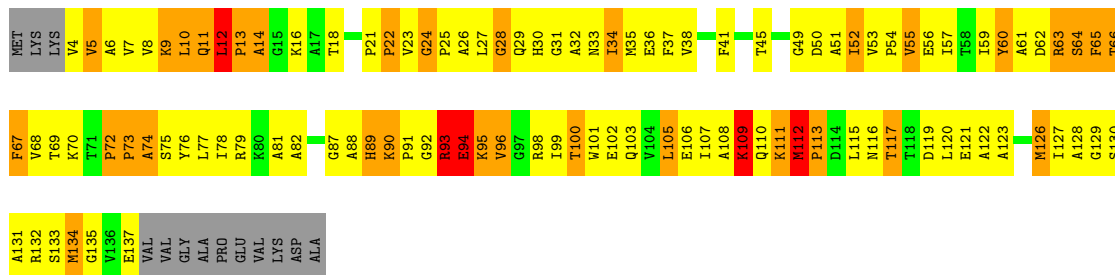
- Molecule 53: 50S ribosomal protein L10

Chain 2: 50% 23% 25%



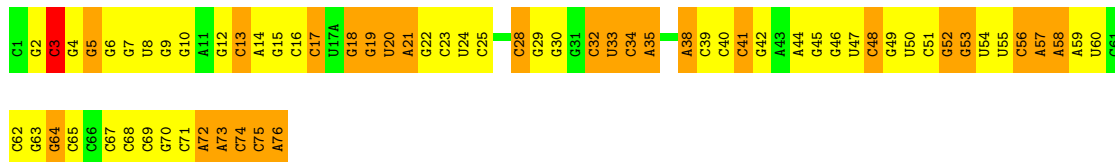
- Molecule 54: 50S ribosomal protein L11

Chain 3: 18% 48% 22% 9%



- Molecule 55: P site- tRNA

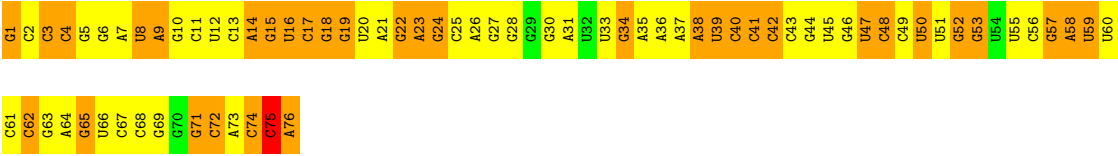
Chain 4: 14% 51% 34%



- Molecule 56: E site- tRNA



Chain 5: 5%49%45%.



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	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: GCP

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	0.78	1/36438 (0.0%)	1.10	50/56869 (0.1%)
10	N	0.34	0/807	0.67	0/1085
11	O	0.39	0/900	0.63	0/1213
12	P	0.54	0/986	0.79	0/1320
13	Q	0.35	0/924	0.67	1/1238 (0.1%)
14	R	0.42	0/501	0.69	0/664
15	S	0.56	0/745	0.78	0/992
16	T	0.53	0/716	0.75	0/963
17	U	0.48	0/870	0.71	0/1159
18	V	0.41	0/603	0.72	1/799 (0.1%)
19	W	0.39	0/661	0.67	0/890
2	F	0.44	0/1935	0.72	1/2609 (0.0%)
20	X	0.50	0/765	0.79	0/1007
21	Y	0.36	0/212	0.66	0/277
22	C	0.44	0/4545	0.57	25/6155 (0.4%)
23	D	0.97	10/69685 (0.0%)	1.24	293/108786 (0.3%)
24	E	0.82	1/2954 (0.0%)	1.09	2/4606 (0.0%)
25	Z	0.33	0/1775	0.58	2/2393 (0.1%)
26	a	0.57	1/2174 (0.0%)	0.80	1/2927 (0.0%)
27	b	0.54	0/1611	0.85	2/2171 (0.1%)
28	c	0.56	0/1660	0.78	0/2247
29	d	0.39	0/1507	0.73	2/2027 (0.1%)
3	G	0.42	0/1636	0.66	0/2205
30	e	0.47	0/1354	0.75	1/1831 (0.1%)
31	f	0.53	0/1140	0.79	2/1537 (0.1%)
32	g	0.52	0/942	0.80	0/1268
33	h	0.48	0/1123	0.85	1/1493 (0.1%)
34	i	0.55	0/1100	0.81	1/1470 (0.1%)
35	j	0.52	0/974	0.73	0/1302
36	k	0.48	0/887	0.78	0/1180
37	l	0.52	0/990	0.81	1/1325 (0.1%)
38	m	0.60	0/982	0.79	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.45	0/790	0.78	0/1057
4	H	0.49	0/1733	0.71	1/2318 (0.0%)
40	o	0.52	0/886	0.71	0/1189
41	p	0.47	0/756	0.71	0/1015
42	q	0.43	0/857	0.78	0/1142
43	r	0.41	0/1467	0.70	0/1992
44	s	0.48	0/633	0.71	0/843
45	t	0.50	0/569	0.72	0/751
46	u	0.56	0/474	0.77	0/635
47	v	0.51	0/594	0.85	1/795 (0.1%)
48	w	0.56	0/459	0.76	0/621
49	x	0.49	0/433	0.87	0/576
5	I	0.49	0/1162	0.76	0/1564
50	y	0.58	0/438	0.78	0/575
51	z	0.57	0/523	0.83	0/690
52	1	0.46	0/310	0.72	0/407
53	2	0.23	0/640	0.45	0/889
54	3	0.43	0/1012	0.70	2/1373 (0.1%)
55	4	0.57	0/1832	0.96	1/2855 (0.0%)
56	5	1.93	7/1813 (0.4%)	1.02	3/2823 (0.1%)
6	J	0.40	0/856	0.63	0/1154
7	K	0.38	0/1276	0.67	0/1709
8	L	0.48	0/1136	0.77	1/1527 (0.1%)
9	M	0.38	0/1029	0.65	0/1379
All	All	0.81	20/165780 (0.0%)	1.07	395/247193 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
26	a	0	5
28	c	0	3
30	e	0	1
31	f	0	1
32	g	0	1
37	l	0	2
38	m	0	1
39	n	0	1
40	o	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	p	0	1
42	q	0	1
46	u	0	1
47	v	0	1
49	x	0	1
51	z	0	1
54	3	0	2
8	L	0	1
All	All	0	26

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	5	75	C	N3-C4	39.72	1.61	1.33
56	5	75	C	N1-C6	36.95	1.59	1.37
56	5	75	C	C2-N3	36.64	1.65	1.35
56	5	75	C	C4-C5	26.84	1.64	1.43
56	5	75	C	N1-C2	25.86	1.66	1.40

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2075	U	N1-C2-O2	10.51	130.16	122.80
23	D	1498	C	C2-N1-C1'	10.33	130.16	118.80
23	D	2498	C	N1-C2-O2	9.67	124.70	118.90
23	D	2498	C	N3-C2-O2	-9.54	115.22	121.90
23	D	1937	A	N1-C6-N6	-9.37	112.98	118.60

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	99	GLY	Peptide
8	L	28	ALA	Peptide
26	a	46	GLN	Peptide
26	a	82	ILE	Peptide
26	a	96	HIS	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	32554	0	16432	3245	0
2	F	1900	0	1951	189	0
3	G	1612	0	1677	179	0
4	H	1703	0	1763	200	0
5	I	1146	0	1207	149	0
6	J	843	0	857	106	0
7	K	1257	0	1296	115	0
8	L	1116	0	1177	144	0
9	M	1010	0	1037	108	0
10	N	794	0	840	87	0
11	O	885	0	904	98	0
12	P	970	0	1057	130	0
13	Q	914	0	969	194	0
14	R	492	0	529	88	0
15	S	734	0	771	106	0
16	T	700	0	720	104	0
17	U	857	0	930	116	0
18	V	597	0	668	71	0
19	W	647	0	673	104	0
20	X	763	0	861	91	0
21	Y	208	0	221	33	0
22	C	4461	0	4547	2055	0
23	D	62218	0	31357	6741	0
24	E	2641	0	1337	210	0
25	Z	1742	0	1794	264	0
26	a	2124	0	2207	0	0
27	b	1578	0	1647	0	0
28	c	1625	0	1666	0	0
29	d	1482	0	1546	0	0
30	e	1328	0	1407	0	0
31	f	1113	0	1183	0	0
32	g	932	0	994	0	0
33	h	1106	0	1183	0	0
34	i	1080	0	1127	0	0
35	j	960	0	1021	0	0
36	k	877	0	938	0	0
37	l	976	0	1033	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	964	0	1022	0	0
39	n	779	0	852	0	0
40	o	876	0	941	0	0
41	p	742	0	800	0	0
42	q	844	0	930	0	0
43	r	1435	0	1463	0	0
44	s	625	0	647	0	0
45	t	567	0	621	0	0
46	u	469	0	518	0	0
47	v	581	0	576	0	0
48	w	445	0	459	0	0
49	x	426	0	452	0	0
50	y	430	0	480	0	0
51	z	515	0	587	0	0
52	1	307	0	335	52	0
53	2	641	0	309	31	0
54	3	993	0	1030	295	0
55	4	1640	0	837	128	0
56	5	1623	0	821	118	0
57	C	32	0	13	17	0
All	All	152879	0	105220	14755	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 74.

The worst 5 of 14755 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)
22:C:116:GLU:HB3	22:C:120:LYS:CE	1.19	1.66
22:C:41:MET:HB3	22:C:45:PHE:CD1	1.31	1.62
23:D:1064:C:C2	54:3:91:PRO:HD3	1.30	1.62
22:C:493:ASN:HA	22:C:505:THR:CG2	1.26	1.62
22:C:25:LEU:CD2	22:C:174:VAL:HG21	1.19	1.61

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	F	232/256 (91%)	181 (78%)	33 (14%)	18 (8%)	1	16
3	G	204/239 (85%)	157 (77%)	33 (16%)	14 (7%)	1	19
4	H	206/209 (99%)	168 (82%)	21 (10%)	17 (8%)	1	15
5	I	148/162 (91%)	122 (82%)	19 (13%)	7 (5%)	2	27
6	J	99/101 (98%)	85 (86%)	11 (11%)	3 (3%)	5	35
7	K	153/156 (98%)	130 (85%)	16 (10%)	7 (5%)	2	27
8	L	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	17
9	M	125/128 (98%)	96 (77%)	14 (11%)	15 (12%)	0	7
10	N	96/105 (91%)	73 (76%)	11 (12%)	12 (12%)	0	6
11	O	117/129 (91%)	96 (82%)	15 (13%)	6 (5%)	2	25
12	P	122/132 (92%)	79 (65%)	33 (27%)	10 (8%)	1	15
13	Q	112/126 (89%)	80 (71%)	19 (17%)	13 (12%)	0	7
14	R	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	10
15	S	86/89 (97%)	70 (81%)	9 (10%)	7 (8%)	1	15
16	T	81/88 (92%)	65 (80%)	10 (12%)	6 (7%)	1	17
17	U	102/105 (97%)	82 (80%)	13 (13%)	7 (7%)	1	19
18	V	71/88 (81%)	57 (80%)	9 (13%)	5 (7%)	1	18
19	W	78/93 (84%)	53 (68%)	17 (22%)	8 (10%)	0	10
20	X	97/106 (92%)	85 (88%)	7 (7%)	5 (5%)	2	24
21	Y	22/27 (82%)	17 (77%)	2 (9%)	3 (14%)	0	5
22	C	562/610 (92%)	244 (43%)	187 (33%)	131 (23%)	0	2
25	Z	226/229 (99%)	180 (80%)	26 (12%)	20 (9%)	1	14
26	a	270/276 (98%)	188 (70%)	51 (19%)	31 (12%)	0	7
27	b	204/206 (99%)	147 (72%)	29 (14%)	28 (14%)	0	5
28	c	206/210 (98%)	160 (78%)	29 (14%)	17 (8%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	180/182 (99%)	119 (66%)	39 (22%)	22 (12%)	0	6
30	e	172/180 (96%)	121 (70%)	27 (16%)	24 (14%)	0	5
31	f	137/140 (98%)	106 (77%)	18 (13%)	13 (10%)	1	13
32	g	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	11
33	h	143/150 (95%)	98 (68%)	25 (18%)	20 (14%)	0	5
34	i	134/141 (95%)	89 (66%)	30 (22%)	15 (11%)	0	9
35	j	115/118 (98%)	93 (81%)	13 (11%)	9 (8%)	1	16
36	k	108/112 (96%)	78 (72%)	20 (18%)	10 (9%)	1	13
37	l	115/146 (79%)	70 (61%)	32 (28%)	13 (11%)	0	8
38	m	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	16
39	n	99/101 (98%)	59 (60%)	21 (21%)	19 (19%)	0	3
40	o	108/113 (96%)	82 (76%)	18 (17%)	8 (7%)	1	17
41	p	92/96 (96%)	74 (80%)	12 (13%)	6 (6%)	1	21
42	q	108/110 (98%)	61 (56%)	24 (22%)	23 (21%)	0	2
43	r	178/206 (86%)	128 (72%)	33 (18%)	17 (10%)	1	12
44	s	77/85 (91%)	60 (78%)	12 (16%)	5 (6%)	1	21
45	t	65/67 (97%)	58 (89%)	2 (3%)	5 (8%)	1	17
46	u	57/60 (95%)	43 (75%)	11 (19%)	3 (5%)	2	24
47	v	69/71 (97%)	39 (56%)	14 (20%)	16 (23%)	0	2
48	w	55/60 (92%)	35 (64%)	12 (22%)	8 (14%)	0	5
49	x	47/54 (87%)	21 (45%)	15 (32%)	11 (23%)	0	2
50	y	47/49 (96%)	30 (64%)	10 (21%)	7 (15%)	0	4
51	z	62/65 (95%)	38 (61%)	14 (23%)	10 (16%)	0	4
52	1	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	2	23
53	2	128/173 (74%)	95 (74%)	21 (16%)	12 (9%)	1	13
54	3	132/147 (90%)	82 (62%)	20 (15%)	30 (23%)	0	2
All	All	6511/6972 (93%)	4639 (71%)	1137 (18%)	735 (11%)	1	8

5 of 735 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	191	ASP
2	F	209	ARG

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Mol	Chain	Res	Type
3	G	64	VAL
4	H	30	LYS
4	H	191	ARG

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	F	202/220 (92%)	202 (100%)	0	100	100
3	G	160/188 (85%)	160 (100%)	0	100	100
4	H	180/181 (99%)	180 (100%)	0	100	100
5	I	115/123 (94%)	115 (100%)	0	100	100
6	J	90/90 (100%)	90 (100%)	0	100	100
7	K	126/127 (99%)	126 (100%)	0	100	100
8	L	119/119 (100%)	119 (100%)	0	100	100
9	M	98/99 (99%)	98 (100%)	0	100	100
10	N	88/92 (96%)	88 (100%)	0	100	100
11	O	90/99 (91%)	90 (100%)	0	100	100
12	P	104/109 (95%)	103 (99%)	1 (1%)	78	89
13	Q	92/101 (91%)	87 (95%)	5 (5%)	24	55
14	R	49/50 (98%)	49 (100%)	0	100	100
15	S	79/80 (99%)	79 (100%)	0	100	100
16	T	72/74 (97%)	72 (100%)	0	100	100
17	U	96/97 (99%)	96 (100%)	0	100	100
18	V	64/77 (83%)	64 (100%)	0	100	100
19	W	71/80 (89%)	69 (97%)	2 (3%)	47	71
20	X	76/82 (93%)	76 (100%)	0	100	100
21	Y	19/22 (86%)	19 (100%)	0	100	100
22	C	473/505 (94%)	347 (73%)	126 (27%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Z	180/181 (99%)	174 (97%)	6 (3%)	41	67
26	a	215/218 (99%)	213 (99%)	2 (1%)	81	90
27	b	166/166 (100%)	165 (99%)	1 (1%)	87	93
28	c	164/166 (99%)	164 (100%)	0	100	100
29	d	156/156 (100%)	153 (98%)	3 (2%)	60	80
30	e	143/148 (97%)	141 (99%)	2 (1%)	69	85
31	f	118/119 (99%)	118 (100%)	0	100	100
32	g	100/100 (100%)	99 (99%)	1 (1%)	78	89
33	h	111/116 (96%)	111 (100%)	0	100	100
34	i	106/111 (96%)	106 (100%)	0	100	100
35	j	100/101 (99%)	100 (100%)	0	100	100
36	k	87/88 (99%)	87 (100%)	0	100	100
37	l	105/127 (83%)	105 (100%)	0	100	100
38	m	93/94 (99%)	93 (100%)	0	100	100
39	n	82/82 (100%)	82 (100%)	0	100	100
40	o	90/92 (98%)	90 (100%)	0	100	100
41	p	76/78 (97%)	76 (100%)	0	100	100
42	q	91/91 (100%)	91 (100%)	0	100	100
43	r	159/179 (89%)	159 (100%)	0	100	100
44	s	63/67 (94%)	63 (100%)	0	100	100
45	t	62/62 (100%)	62 (100%)	0	100	100
46	u	51/52 (98%)	51 (100%)	0	100	100
47	v	63/63 (100%)	60 (95%)	3 (5%)	28	58
48	w	50/52 (96%)	50 (100%)	0	100	100
49	x	48/52 (92%)	48 (100%)	0	100	100
50	y	42/42 (100%)	42 (100%)	0	100	100
51	z	54/55 (98%)	54 (100%)	0	100	100
52	1	34/34 (100%)	34 (100%)	0	100	100
54	3	101/111 (91%)	86 (85%)	15 (15%)	3	18
All	All	5373/5618 (96%)	5206 (97%)	167 (3%)	47	69

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	C	294	PHE
22	C	377	VAL
54	3	12	LEU
22	C	315	LYS
22	C	332	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
22	C	538	GLN
27	b	129	HIS
49	x	46	HIS
22	C	594	GLN
25	Z	172	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1514/1522 (99%)	640 (42%)	80 (5%)
23	D	2888/2893 (99%)	1464 (50%)	169 (5%)
24	E	122/123 (99%)	47 (38%)	4 (3%)
55	4	76/77 (98%)	30 (39%)	0
56	5	75/76 (98%)	36 (48%)	4 (5%)
All	All	4675/4691 (99%)	2217 (47%)	257 (5%)

5 of 2217 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U

5 of 257 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	D	574	C
23	D	973	A
23	D	2660	A
23	D	616	A

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Mol	Chain	Res	Type
23	D	822	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	GCP	C	701	-	26,34,34	3.73	11 (42%)	31,54,54	1.63	4 (12%)

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
57	GCP	C	701	-	-	10/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	701	GCP	C3'-C4'	-9.35	1.28	1.53
57	C	701	GCP	C4-N9	-8.71	1.36	1.47
57	C	701	GCP	C5-C6	-7.75	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	701	GCP	O4'-C4'	7.70	1.62	1.45
57	C	701	GCP	O4'-C1'	-4.36	1.31	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	701	GCP	PA-O3A-PB	-4.80	116.91	132.49
57	C	701	GCP	C4-C5-N7	4.30	108.16	102.46
57	C	701	GCP	O6-C6-N1	-2.73	119.03	122.68
57	C	701	GCP	C3'-C2'-C1'	2.66	106.49	101.44

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

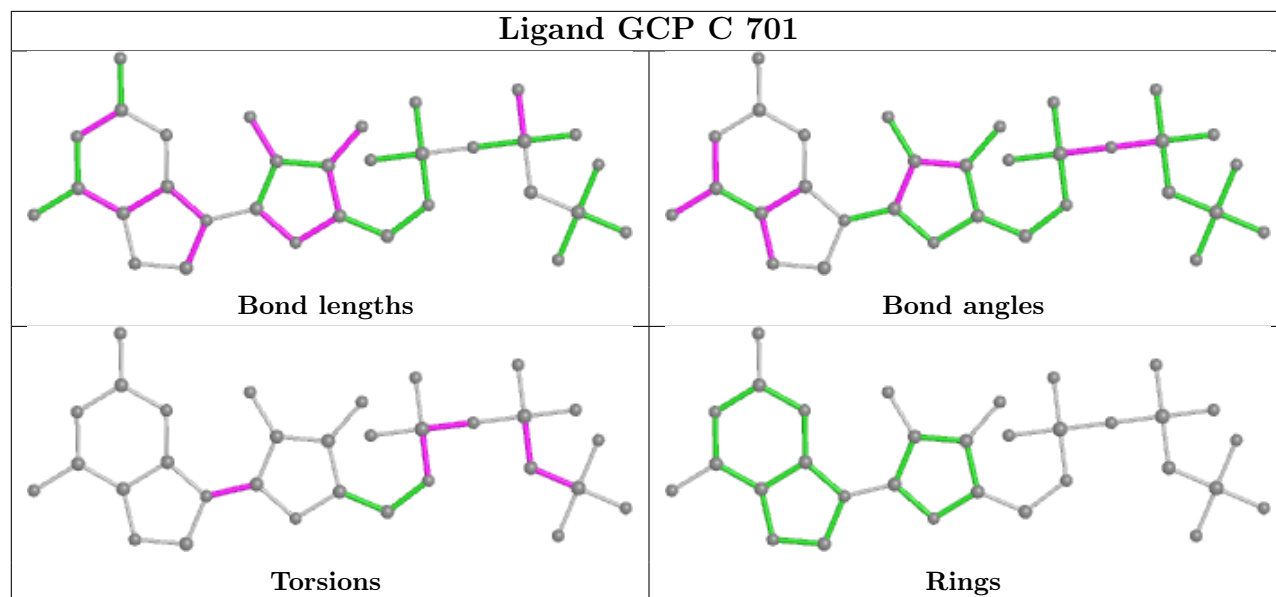
Mol	Chain	Res	Type	Atoms
57	C	701	GCP	PG-C3B-PB-O1B
57	C	701	GCP	PG-C3B-PB-O2B
57	C	701	GCP	PG-C3B-PB-O3A
57	C	701	GCP	C5'-O5'-PA-O3A
57	C	701	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	C	701	GCP	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.