



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 07:48 AM EDT

PDB ID : 5LMV
EMDB ID: : EMD-4083
Title : Structure of bacterial 30S-IF1-IF2-IF3-mRNA-tRNA translation pre-initiation complex(state-III)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : unknown
Resolution : 4.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

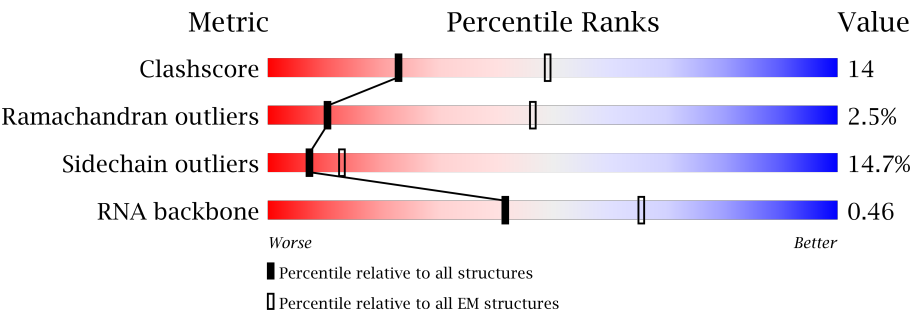
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.90 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.











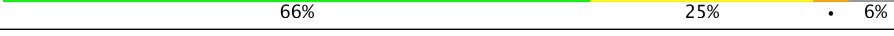

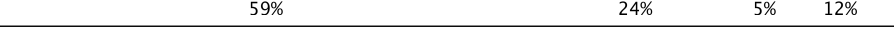


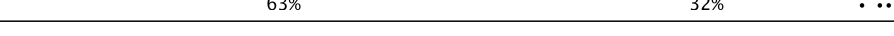




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	31% 54% 14%
2	B	256	57% 27% 5% 9%
3	C	239	59% 25% 14%
4	D	209	61% 32% 7%
5	E	162	55% 31% 6% 7%
6	F	101	63% 30% 6%
7	G	156	80% 19%
8	H	138	70% 26%

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	
26	a	571	

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
27	ZN	D	300	-	-	X	-
27	ZN	N	101	-	-	X	-
29	FME	Z	101	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 59470 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
			32548	14490	6022	10523	1513		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	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	C	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	D	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	E	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	F	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	G	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	H	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	I	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	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	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	L	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	M	118	Total	C	N	O	S	0	0
			937	579	193	163	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	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	O	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	P	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	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			655	419	120	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	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	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 25 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

- Molecule 26 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	502	Total	C	N	O	S	0	0
			3774	2365	679	718	12		

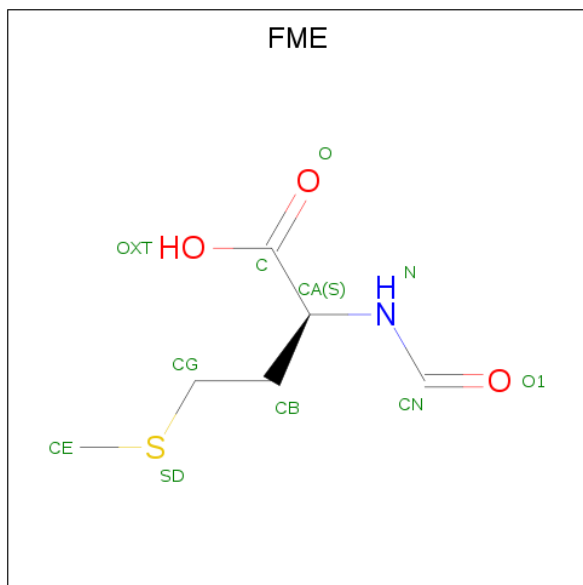
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Zn	0
			1	1	
27	N	1	Total	Zn	0
			1	1	

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	W	1	Total	Mg	0
			1	1	
28	Z	1	Total	Mg	0
			1	1	

- Molecule 29 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

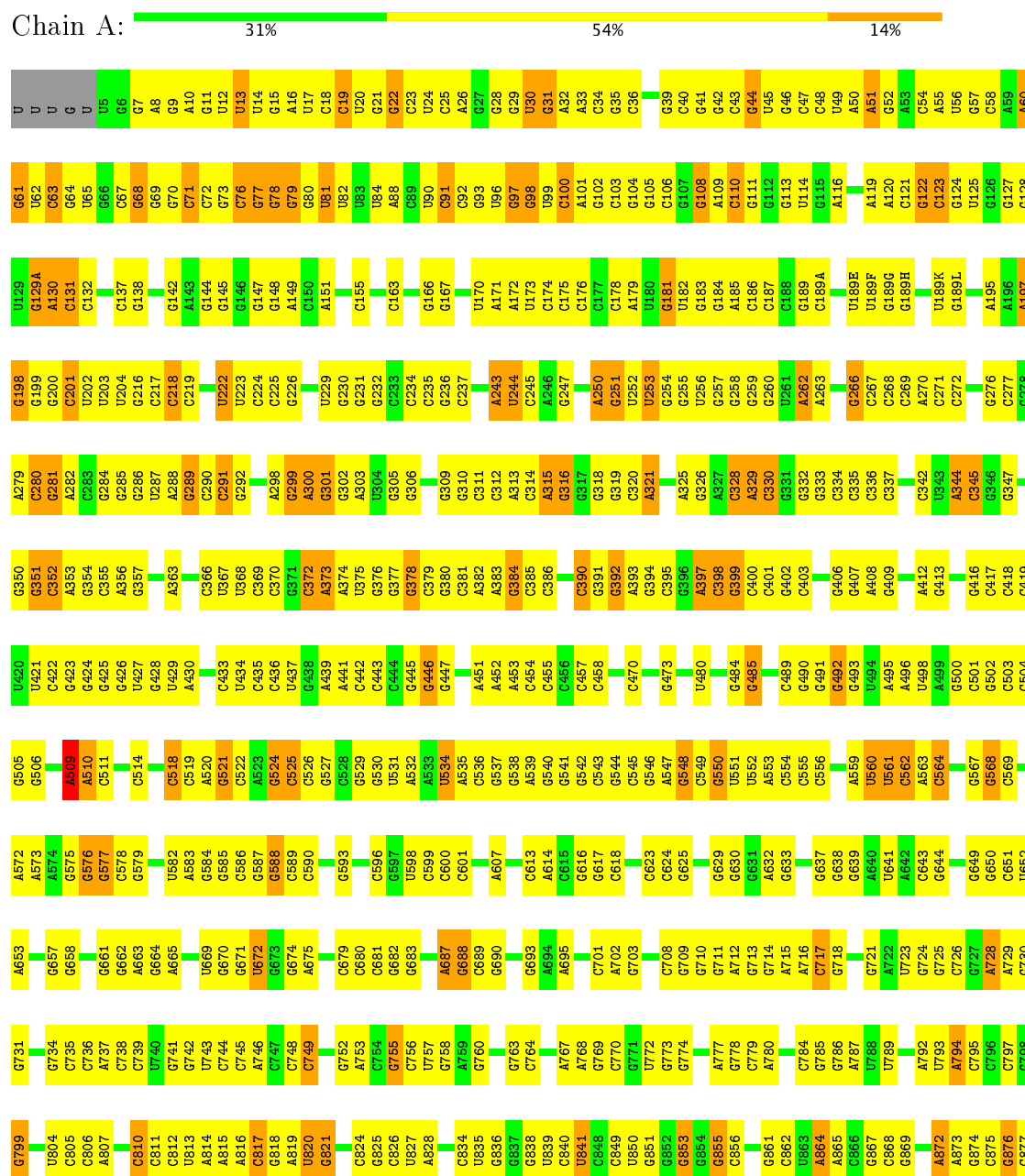


Mol	Chain	Residues	Atoms					AltConf
29	Z	1	Total	C	N	O	S	0
			9	6	1	1	1	

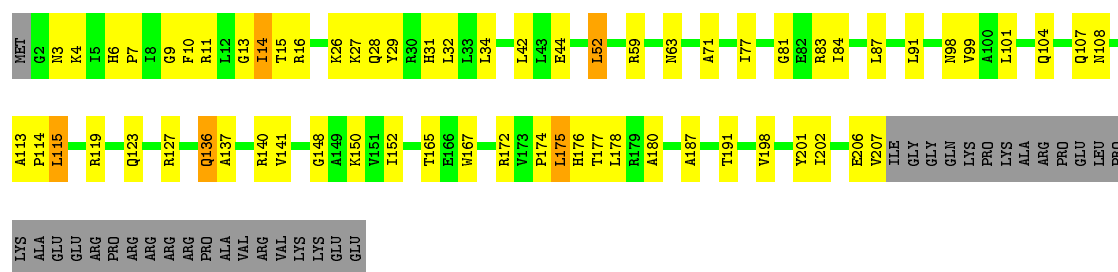
3 Residue-property plots

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

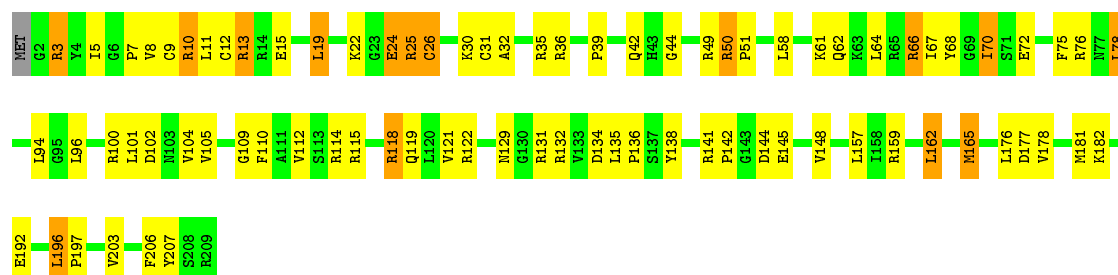


C1514	C1517	A1518	A1519	A1520	A1521	G1526	G1527	G1528	G1529	G1530	A1531	A1532	C1533	A1534	C1535	C1536	C1539	U1540	U1541	U1542	C	U																																																																																																																																																																																																																																																																																																																																																																																																																		
G1378	G1379	U1380	U1381	G1384	G1385	G1386	G1387	G1388	G1389	G1390	U1391	G1392	U1393	A1394	C1395	C1396	G1397	A1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1430	G1431	G1432	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	A1502	A1503	G1504	G1505	U1506	U1507	A1508	G1509	U1510	G1511	U1512	A1513																																																																																																																																																																																																																																																																																																																																																														
A1426	C1427	A1428	A1429	U1430	U1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	A1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	C1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	A1492	A1493	G1494	G1497	U1498	A1499	A1500	A1501	G1502	G1503	G1504	G1505	U1506	U1507	A1508	G1509	U1510	G1511	U1512	A1513																																																																																																																																																																																																																																																																																																																																																			
G1312	U1313	U1314	U1315	G1316	A1317	A1318	A1319	A1320	A1321	A1322	G1323	A1324	A1325	A1326	A1327	A1328	G1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	U1372	A1373	A1374	A1375	A1376	A1377																																																																																																																																																																																																																																																																																																																																																																							
A1236	C1237	A1238	A1239	U1240	U1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	G1289	G1290	G1291	G1292	G1293	G1294	A1295	A1296	A1297	A1298	A1299	G1300	U1301	U1302	C1303	C1304	C1305	C1306	C1307	U1308	G1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	U1372	A1373	A1374	A1375	A1376	A1377																																																																																																																																																																																																																																																																																											
G1163	G1164	G1165	U1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	G1222	G1223	G1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	G1289	G1290	G1291	G1292	G1293	G1294	A1295	A1296	A1297	A1298	A1299	G1300	U1301	U1302	C1303	C1304	C1305	C1306	C1307	U1308	G1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	U1372	A1373	A1374	A1375	A1376	A1377																																																																																																																																																																																																																		
C1100	A1101	A1102	C1103	G1104	A1105	A1106	C1107	G1108	G1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	G1222	G1223	G1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	G1289	G1290	G1291	G1292	G1293	G1294	A1295	A1296	A1297	A1298	A1299	G1300	U1301	U1302	C1303	C1304	C1305	C1306	C1307	U1308	G1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	U1372	A1373	A1374	A1375	A1376	A1377																																																																																																																																																			
G953	G954	U955	U956	U957	C958	A959	U960	U961	A962	A963	A964	A965	A966	A967	A968	A969	C970	G971	C972	G973	A974	A975	G976	G977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	U1000	A1001	G1002	G1003	A1004	A1005	C1006	G1007	C1008	G1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	G1222	G1223	G1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	G1289	G1290	G1291	G1292	G1293	G1294	A1295	A1296	A1297	A1298	A1299	G1300	U1301	U1302	C1303	C1304	C1305	C1306	C1307	U1308	G1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	U1372	A1373	A1374	A1375	A1376	A1377
G878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	U891	A892	C893	C894	A895	A896	A897	A898	A899	A900	A901	G902	G903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A9																																																																																																																																																																																																																																																																																																																																																																																				



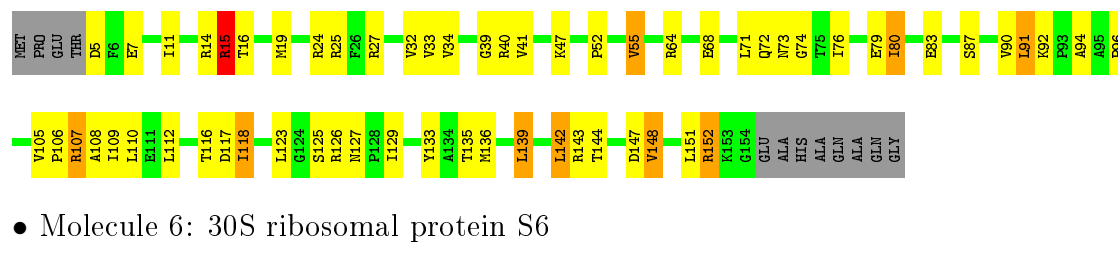
- Molecule 4: 30S ribosomal protein S4

Chain D: 61% 32% 7%



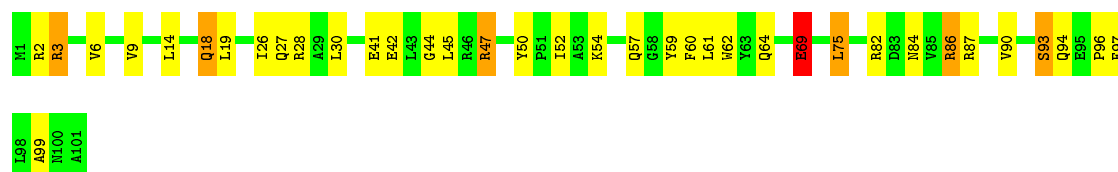
- Molecule 5: 30S ribosomal protein S5

Chain E: 55% 31% 6% 7%



- Molecule 6: 30S ribosomal protein S6

Chain F: 63% 30% 6%



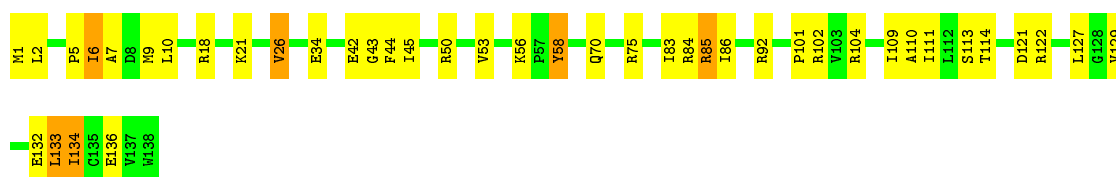
- Molecule 7: 30S ribosomal protein S7

Chain G: 80% 19%



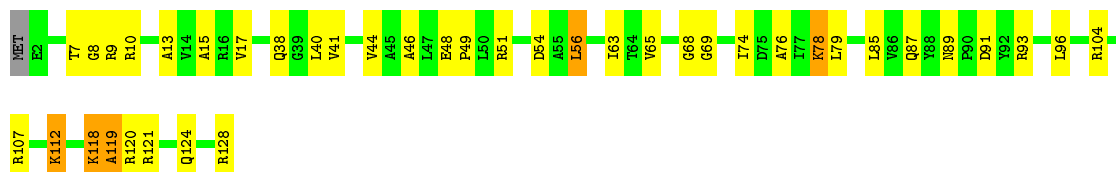
- Molecule 8: 30S ribosomal protein S8

Chain H: 70% 26%



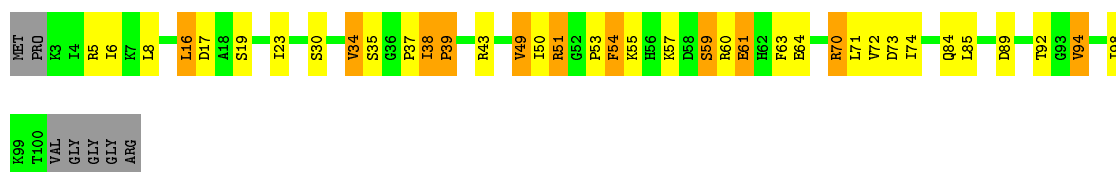
- Molecule 9: 30S ribosomal protein S9

Chain I: 68% 27%



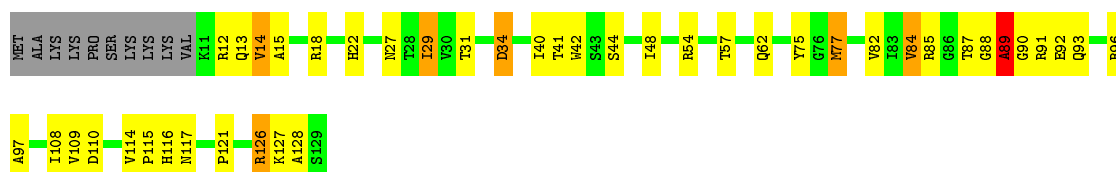
- Molecule 10: 30S ribosomal protein S10

Chain J: 58% 25% 10% 7%



- Molecule 11: 30S ribosomal protein S11

Chain K: 59% 28% 5% 8%



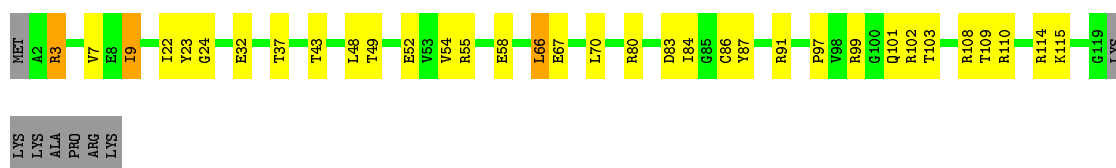
- Molecule 12: 30S ribosomal protein S12

Chain L: 61% 30% 6%



- Molecule 13: 30S ribosomal protein S13

Chain M: 67% 25% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 61% 36% . .



- Molecule 15: 30S ribosomal protein S15

Chain O: 69% 21% 9% .



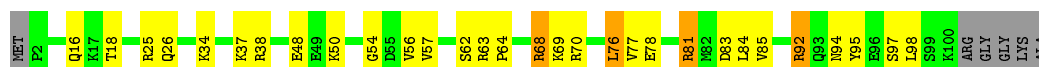
- Molecule 16: 30S ribosomal protein S16

Chain P: 66% 25% . 6%



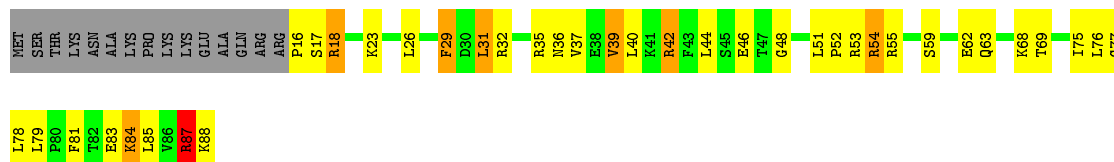
- Molecule 17: 30S ribosomal protein S17

Chain Q: 66% 25% . 6%



- Molecule 18: 30S ribosomal protein S18

Chain R: 40% 34% 8% 17%

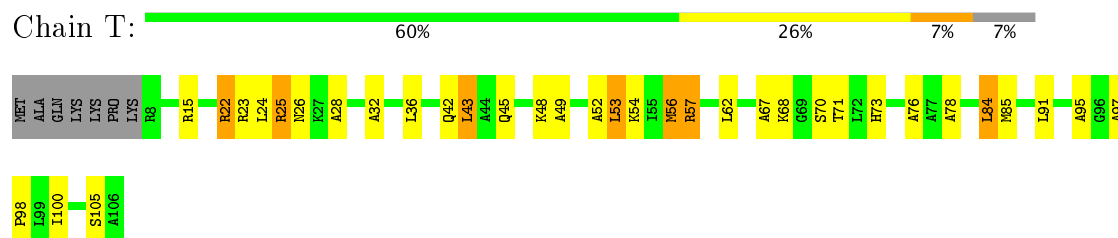


- Molecule 19: 30S ribosomal protein S19

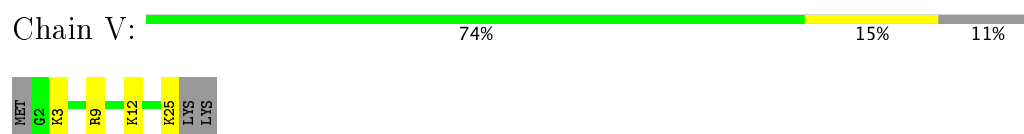
Chain S: 59% 24% 5% 12%



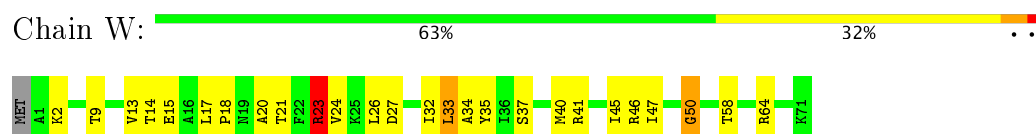
- Molecule 20: 30S ribosomal protein S20



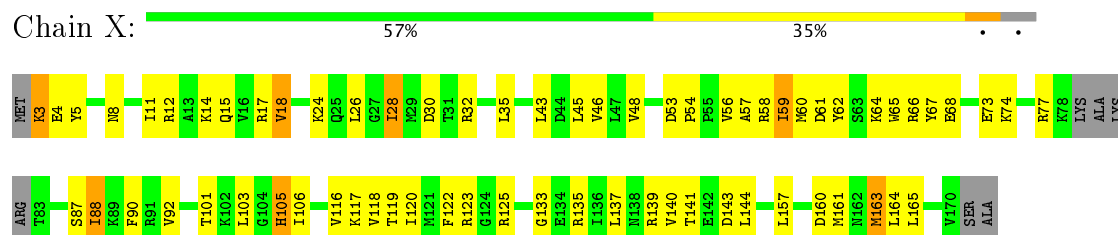
- Molecule 21: 30S ribosomal protein Thx



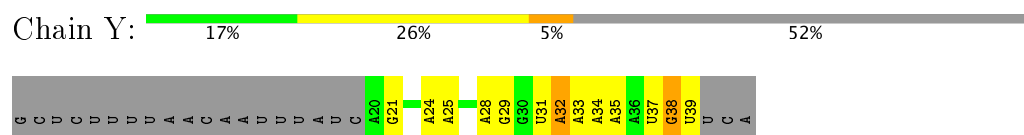
- Molecule 22: Translation initiation factor IF-1



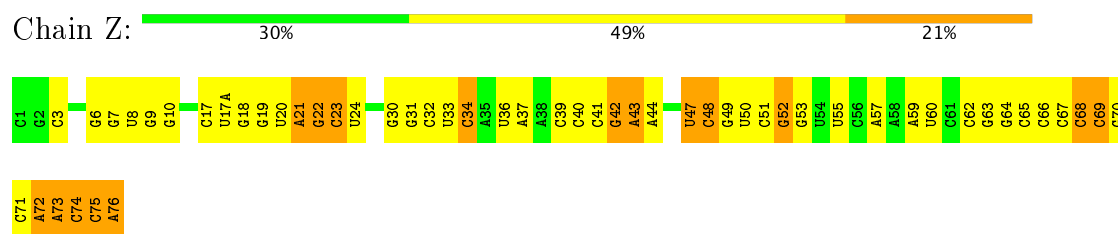
- Molecule 23: Translation initiation factor IF-3



- Molecule 24: mRNA

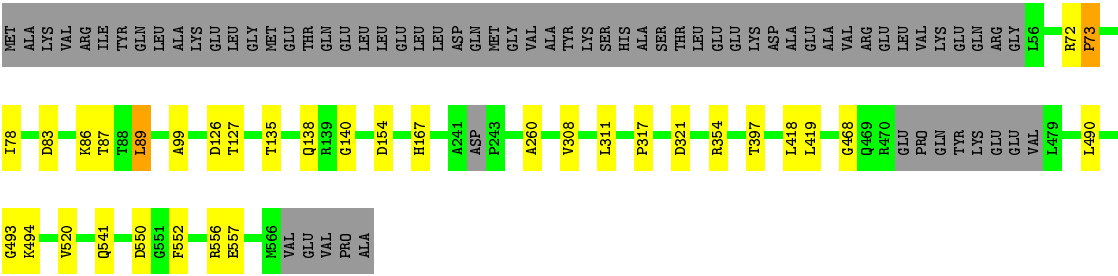


- Molecule 25: tRNAi



- Molecule 26: Translation initiation factor IF-2





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	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: OMC, 5MU, ZN, FME, G7M, MG, 4SU, PSU

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	0.29	1/36426 (0.0%)	0.70	10/56837 (0.0%)
10	J	0.39	0/805	0.74	1/1082 (0.1%)
11	K	0.41	0/900	0.90	2/1213 (0.2%)
12	L	0.35	0/986	0.76	0/1320
13	M	0.41	0/947	0.74	0/1270
14	N	0.40	0/501	0.78	0/664
15	O	0.41	0/745	0.83	0/992
16	P	0.39	0/716	0.73	0/963
17	Q	0.38	0/836	0.75	0/1117
18	R	0.40	0/604	0.85	0/801
19	S	0.42	0/670	0.70	0/903
2	B	0.44	0/1935	0.79	1/2609 (0.0%)
20	T	0.42	0/765	0.87	0/1007
21	V	0.43	0/212	0.69	0/277
22	W	0.48	0/580	1.07	5/782 (0.6%)
23	X	0.49	0/1354	0.74	1/1813 (0.1%)
24	Y	0.36	0/494	0.67	0/770
25	Z	0.34	0/1721	0.71	1/2682 (0.0%)
26	a	0.46	0/3824	0.70	2/5169 (0.0%)
3	C	0.39	0/1636	0.75	2/2205 (0.1%)
4	D	0.41	0/1733	0.80	1/2318 (0.0%)
5	E	0.41	0/1162	0.88	2/1564 (0.1%)
6	F	0.39	0/856	0.78	1/1154 (0.1%)
7	G	0.41	0/1276	0.73	0/1709
8	H	0.38	0/1136	0.76	0/1527
9	I	0.41	0/1029	0.78	1/1379 (0.1%)
All	All	0.35	1/63849 (0.0%)	0.73	30/94127 (0.0%)

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
1	A	0	1
11	K	1	0
23	X	0	1
26	a	0	1
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	C	O3'-P	-5.32	1.54	1.61

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	89	ALA	CB-CA-C	18.64	138.06	110.10
9	I	7	THR	CB-CA-C	-13.26	75.81	111.60
5	E	15	ARG	N-CA-C	-12.58	77.04	111.00
22	W	33	LEU	CB-CA-C	-12.05	87.30	110.20
22	W	23	ARG	N-CA-C	-10.10	83.72	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	K	89	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	C	Sidechain
23	X	53	ASP	Peptide
26	a	73	PRO	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	32548	0	16440	867	0
2	B	1900	0	1951	40	0
3	C	1612	0	1677	41	0
4	D	1703	0	1766	46	0
5	E	1146	0	1207	23	0
6	F	843	0	857	19	0
7	G	1257	0	1296	13	0
8	H	1116	0	1177	16	0
9	I	1010	0	1037	22	0
10	J	792	0	835	30	0
11	K	885	0	904	20	0
12	L	970	0	1057	24	0
13	M	937	0	995	18	0
14	N	492	0	530	18	0
15	O	734	0	771	11	0
16	P	700	0	720	13	0
17	Q	823	0	891	18	0
18	R	598	0	670	26	0
19	S	655	0	672	14	0
20	T	763	0	861	22	0
21	V	208	0	221	2	0
22	W	570	0	599	24	0
23	X	1336	0	1389	45	0
24	Y	439	0	218	10	0
25	Z	1646	0	843	71	0
26	a	3774	0	3747	0	0
27	D	1	0	0	2	0
27	N	1	0	0	2	0
28	W	1	0	0	0	0
28	Z	1	0	0	0	0
29	Z	9	0	10	6	0
All	All	59470	0	43341	1342	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 14.

The worst 5 of 1342 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)
25:Z:76:A:O3'	29:Z:101:FME:C	1.70	1.37
1:A:1358:U:H3	1:A:1363(A):A:N6	1.21	1.33
25:Z:76:A:C3'	29:Z:101:FME:C	2.09	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:O	3:C:32:LEU:HG	1.32	1.27
23:X:3:LYS:CB	23:X:66:ARG:NH2	2.02	1.20

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	B	232/256 (91%)	189 (82%)	32 (14%)	11 (5%)	3	29
3	C	204/239 (85%)	179 (88%)	19 (9%)	6 (3%)	5	39
4	D	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	12	53
5	E	148/162 (91%)	132 (89%)	13 (9%)	3 (2%)	9	47
6	F	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	5	38
7	G	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	9	47
8	H	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	12	53
9	I	125/128 (98%)	106 (85%)	17 (14%)	2 (2%)	11	52
10	J	96/105 (91%)	81 (84%)	10 (10%)	5 (5%)	2	26
11	K	117/129 (91%)	101 (86%)	12 (10%)	4 (3%)	4	36
12	L	122/132 (92%)	104 (85%)	14 (12%)	4 (3%)	4	37
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	26
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	81/88 (92%)	74 (91%)	7 (9%)	0	100	100
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
18	R	71/88 (81%)	66 (93%)	3 (4%)	2 (3%)	6	40
19	S	80/93 (86%)	70 (88%)	6 (8%)	4 (5%)	2	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	84 (87%)	9 (9%)	4 (4%)	3	31
21	V	22/27 (82%)	22 (100%)	0	0	100	100
22	W	69/72 (96%)	58 (84%)	9 (13%)	2 (3%)	5	39
23	X	160/171 (94%)	138 (86%)	20 (12%)	2 (1%)	14	56
26	a	496/571 (87%)	434 (88%)	48 (10%)	14 (3%)	6	40
All	All	3071/3352 (92%)	2698 (88%)	296 (10%)	77 (2%)	10	42

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	TRP
6	F	69	GLU
9	I	119	ALA
10	J	34	VAL
10	J	39	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	
2	B	202/220 (92%)	166 (82%)	36 (18%)	2	14
3	C	160/188 (85%)	143 (89%)	17 (11%)	8	32
4	D	180/181 (99%)	148 (82%)	32 (18%)	2	14
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	3
6	F	90/90 (100%)	76 (84%)	14 (16%)	3	19
7	G	126/127 (99%)	112 (89%)	14 (11%)	7	30
8	H	119/119 (100%)	96 (81%)	23 (19%)	1	11
9	I	98/99 (99%)	85 (87%)	13 (13%)	4	25
10	J	87/92 (95%)	75 (86%)	12 (14%)	4	24
11	K	90/99 (91%)	72 (80%)	18 (20%)	1	10
12	L	104/109 (95%)	89 (86%)	15 (14%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	94/101 (93%)	80 (85%)	14 (15%)	3	21
14	N	49/50 (98%)	42 (86%)	7 (14%)	4	23
15	O	79/80 (99%)	59 (75%)	20 (25%)	0	5
16	P	72/74 (97%)	64 (89%)	8 (11%)	7	30
17	Q	94/97 (97%)	85 (90%)	9 (10%)	10	36
18	R	64/77 (83%)	46 (72%)	18 (28%)	0	3
19	S	71/80 (89%)	60 (84%)	11 (16%)	3	19
20	T	76/82 (93%)	64 (84%)	12 (16%)	3	19
21	V	19/22 (86%)	16 (84%)	3 (16%)	3	19
22	W	62/63 (98%)	55 (89%)	7 (11%)	7	30
23	X	145/150 (97%)	125 (86%)	20 (14%)	4	24
26	a	374/460 (81%)	355 (95%)	19 (5%)	28	60
All	All	2570/2783 (92%)	2193 (85%)	377 (15%)	7	21

5 of 377 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	134	ILE
11	K	93	GLN
23	X	73	GLU
9	I	78	LYS
10	J	61	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	89	ASN
11	K	13	GLN
23	X	162	ASN
10	J	56	HIS
10	J	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	407 (26%)	89 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	Y	19/42 (45%)	7 (36%)	1 (5%)
25	Z	76/77 (98%)	27 (35%)	4 (5%)
All	All	1604/1641 (97%)	441 (27%)	94 (5%)

5 of 441 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G

5 of 94 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	703	G
1	A	965	A
1	A	1504	G
1	A	748	C
1	A	873	A

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

5 non-standard protein/DNA/RNA residues are 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
25	OMC	Z	32	25	15,22,23	0.76	1 (6%)	19,31,34	1.14	1 (5%)
25	G7M	Z	46	25	19,26,27	2.70	3 (15%)	19,39,42	2.25	5 (26%)
25	5MU	Z	54	25	14,22,23	0.80	0	16,32,35	2.84	3 (18%)
25	PSU	Z	55	25	16,21,22	1.11	1 (6%)	20,30,33	3.69	9 (45%)
25	4SU	Z	8	25	14,21,22	1.42	2 (14%)	15,30,33	1.75	4 (26%)

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
25	OMC	Z	32	25	-	0/5/27/28	0/2/2/2
25	G7M	Z	46	25	-	0/3/25/26	0/3/3/3
25	5MU	Z	54	25	-	0/3/25/26	0/2/2/2
25	PSU	Z	55	25	-	0/7/25/26	0/2/2/2
25	4SU	Z	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	8	4SU	C4-S4	-3.87	1.60	1.67
25	Z	55	PSU	C5-C1'	-2.93	1.49	1.52
25	Z	32	OMC	O4'-C1'	2.01	1.44	1.41
25	Z	8	4SU	O4'-C1'	2.02	1.44	1.41
25	Z	46	G7M	C6-C5	3.92	1.48	1.41

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	55	PSU	N1-C2-N3	-9.35	121.68	128.40
25	Z	55	PSU	C5-C4-N3	-7.70	119.11	125.43
25	Z	54	5MU	C5-C4-N3	-6.33	118.26	125.24
25	Z	46	G7M	C5-C6-N1	-5.28	115.97	123.48
25	Z	55	PSU	C5-C1'-C2'	-4.40	107.95	115.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	32	OMC	2	0
25	Z	8	4SU	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 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	$\# Z > 2$
29	FME	Z	101	-	8,8,10	0.49	0	7,8,11	1.05	1 (14%)

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
29	FME	Z	101	-	-	0/7/7/11	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
29	Z	101	FME	CB-CA-N	2.52	113.79	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Z	101	FME	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1442(A):G	O3'	1442(B):A	P	5.40
1	A	84:U	O3'	88:A	P	5.02
1	A	93:G	O3'	96:U	P	4.43
1	A	204:U	O3'	216:G	P	4.27
1	A	841:U	O3'	848:C	P	3.83