



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:19 PM BST

PDB ID : 4D61
EMDB ID: : EMD-2813
Title : Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors : Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on : 2014-11-07
Resolution : 9.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

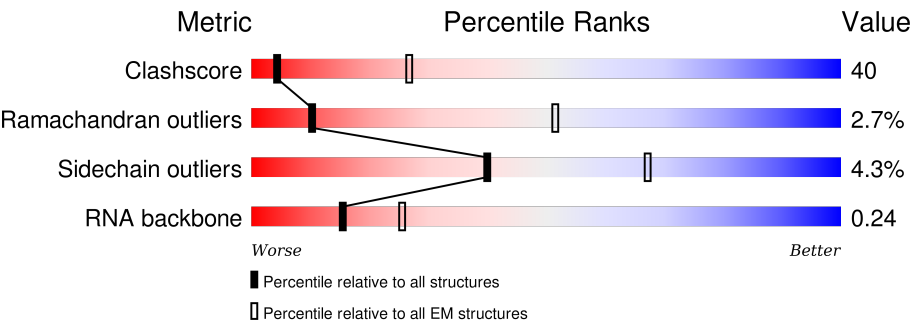
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 9.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.














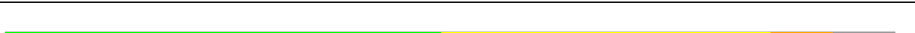













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	1869	<div><div>6%</div><div>38%</div><div>47%</div><div>• 7%</div></div>
2	A	295	<div><div>42%</div><div>31%</div><div>•</div><div>26%</div></div>
3	B	264	<div><div>33%</div><div>41%</div><div>6%</div><div>•</div><div>19%</div></div>
4	C	293	<div><div>49%</div><div>23%</div><div>•</div><div>24%</div></div>
5	D	243	<div><div>52%</div><div>34%</div><div>•</div><div>13%</div></div>
6	E	263	<div><div>54%</div><div>40%</div><div>•</div><div>•</div></div>
7	F	204	<div><div>49%</div><div>38%</div><div>6%</div><div>8%</div></div>
8	G	249	<div><div>51%</div><div>39%</div><div>•</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	

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Mol	Chain	Length	Quality of chain
34	g	317	<div><div></div><div>93%</div><div>5% •</div></div>
35	h	436	<div><div></div><div>97%</div><div>•</div></div>
36	i	426	<div><div></div><div>98%</div><div>•</div></div>
37	j	201	<div><div></div><div>45%</div><div>49%</div><div>6%</div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86384 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1742	Total	C	N	O	P	0	0
			37159	16589	6665	12164	1741		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	218	Total	C	N	O	S	0	0
			1719	1091	301	319	8		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	188	Total	C	N	O	S	0	0
			1486	930	283	266	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	191	Total	C	N	O	S	0	0
			1535	978	282	274	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	94	Total	C	N	O	S	0	0
			791	519	138	129	5		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	146	Total	C	N	O	S	0	0
			1199	764	224	205	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	137	Total	C	N	O	S	0	0
			1023	627	200	190	6		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	118	Total	C	N	O	S	0	0
			981	625	183	166	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			893	561	170	159	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	502	153	144	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	S	0	0
			605	387	112	105	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	96	Total	C	N	O	S	0	0
			767	476	159	127	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			490	298	99	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	51	Total	C	N	O	S	0	0
			412	258	90	63	1		

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	436	Total	C	N	O	S	0	0
			3450	2193	582	663	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	438	LEU	-	EXPRESSION TAG	UNP P62495
h	439	GLU	-	EXPRESSION TAG	UNP P62495
h	440	HIS	-	EXPRESSION TAG	UNP P62495

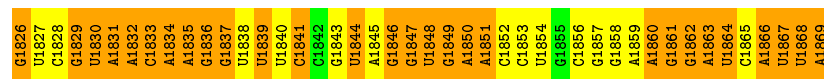
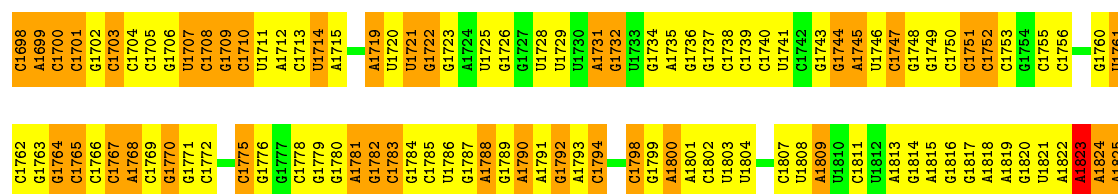
- Molecule 36 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUBUNIT ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	426	Total	C	N	O	S	0	0
			3357	2135	577	624	21		

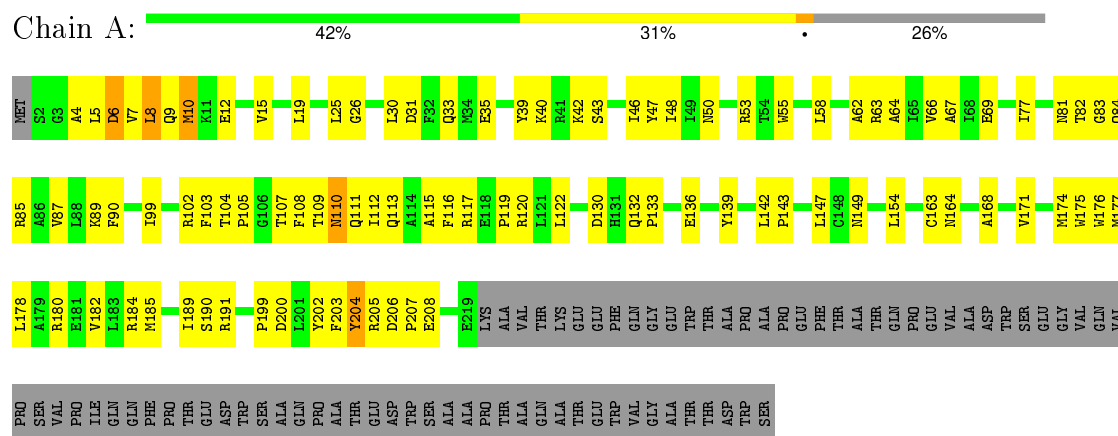
- Molecule 37 is a RNA chain called CRICKET PARALYSIS VIRUS IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	201	Total	C	N	O	P	0	0
			4257	1908	735	1413	201		

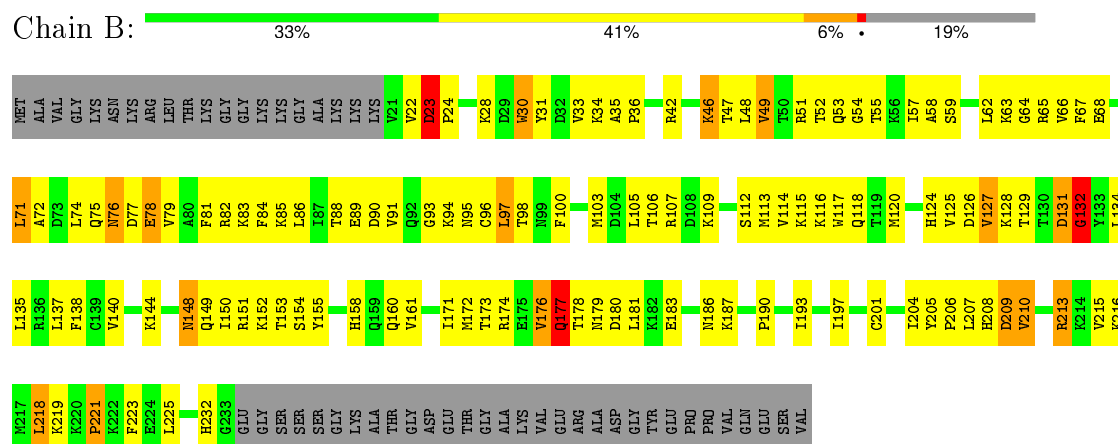
G1633	U1576	G1517	A1396	G1334	C1272	G1212	U1152	G1092	A1030	U968	G907	G846	C
G1639	A1579	C1518	U1397	G1336	C1273	C1213	C1153	A1093	A1031	U969	A908	A847	G
A1640	A1580	G1519	G1398	C1337	G1274	A1214	U1154	C1094	G1032	G970	G	U848	C
A1641	C1581	G1520	C1399	C1338	G1275	C1215	U1155	C1095	G1033	G971	C911	A849	C
G1642	C1582	A1400	U1400	G1339	C1276	C1216	U1156	G1096	A1034	A972	A912	C850	C
G1643	C1583	A1401	A1402	U1340	C1277	A1217	G1157	G1097	A1035	C973	A913	C851	G
C1644	G1584	C1522	A1403	C1341	C1278	C1218	G1158	C1098	A1036	C974	U914	C852	U
C1645	U1585	C1523	C1403	U1342	C1279	C1219	U1159	C1099	G1037	G975	G915	C853	C
G1646	U1586	G1526	U1404	C1343	G1280	A1220	G1160	A1100	U1038	G976	A916	C854	C
A1647	G1587	C1527	A1405	U1343	G1281	G1221	U1161	G1101	C1039	C977	U917	C855	C
G1648	A1588	G1528	G1406	A1344	A1282	C1222	C1162	G1102	G1040	G978	U918	C856	G
U1649	A1589	C1529	A1407	G1345	C1283	A1223	G1163	G1103	G1041	C979	A919	U857	G
A1650	U1590	U1530	A1469	U1346	C1284	G1224	G1164	G1104	A1042	A980	A920	A858	G
A1651	C1591	A1531	A1409	U1347	G1285	U1225	G1165	G1105	G1043	A981	G921	G859	G
G1652	C1592	C1532	C1471	G1348	G1286	G1226	G1166	C1106	A1044	G982	A922	G860	C
U1653	C1593	G1533	G1411	G1349	A1287	G1227	G1167	A1107	U1045	A983	G923	A861	C
G1654	A1594	C1534	C1412	U1350	U1288	A1228	G1168	G1108	U1046	C984	G924	A862	C
C1655	U1595	U1535	G1413	G1351	U1289	G1229	G1169	C1109	C1047	G985	G925	A863	C
G1656	U1596	G1536	A1414	G1352	G1290	C1230	A1170	G1110	G1048	G986	A926	A864	C
G1657	C1597	A1537	C1415	A1353	A1291	C1231	U1171	U1111	A1049	A987	C927	A865	C
G1658	U1598	C1538	G1416	G1354	C1292	U1232	U1172	U1112	A1050	C988	G928	U866	C
U1659	U1599	U1539	C1417	C1355	U1296	G1233	U1173	A1113	G1051	C989	G929	A867	C
C1660	G1600	G1540	C1418	G1356	G1297	C1234	U1174	U1114	A1052	A990	G930	G868	C
A1661	A1601	C1541	G1419	A1357	U1297	G1235	G1175	U1115	C1053	G991	C931	A869	C
U1662	U1602	G1542	G1420	U1358	G1298	G1236	G1176	U1116	G1054	A992	G932	A870	C
A1663	G1603	U1543	A1421	U1359	A1299	C1237	U1177	C1117	A1055	C993	G933	U871	C
A1664	G1604	C1544	G1422	U1360	U1300	U1238	U1178	C1118	U1056	C994	G934	A872	C
G1665	A1605	A1545	C1423	G1361	A1301	U1239	G1179	C1119	C1057	C995	G935	A873	C
C1666	G1606	G1546	U1485	G1362	G1302	A1240	U1180	U1120	A1058	G996	G936	G874	C
U1667	A1607	C1547	A1486	C1363	C1303	A1241	C1181	G1121	G1059	G999	C937	A875	C
G1668	U1608	G1548	U1426	U1364	U1304	U1242	A1182	A1122	A1060	A938	C938	C876	C
C1669	G1609	U1549	C1427	U1368	C1305	U1243	A1183	C1123	U1061	A1003	U939	C877	C
U1670	G1610	G1550	G1428	A1369	U1306	U1244	G1184	C1124	A1062	U1002	U940	G878	C
G1671	G1611	U1551	G1429	A1370	U1307	G1245	C1185	C1125	C1063	U1003	C941	C879	C
U1672	G1612	C1552	G1430	A1371	U1308	A1246	U1186	G1126	C1064	U1004	G942	U820	C
G1673	G1613	C1553	G1431	U1372	C1309	C1247	G1187	C1127	G1065	G1005	U943	G821	C
A1674	A1614	C1554	U1432	U1373	U1310	U1248	A1188	C1128	U1066	A944	A944	U822	C
U1675	U1615	U1555	C1433	C1373	C1311	C1249	A1189	G1129	C1067	C1007	U945	U823	C
U1676	U1616	A1556	G1434	C1374	G1312	A1250	A1190	G1130	G1068	A1008	U946	C884	C
U1677	G1617	C1557	C1435	G1375	A1313	A1251	C1191	G1131	U1069	A1009	G947	U885	C
A1678	C1618	C1558	G1436	A1376	U1314	C1252	U1192	C1132	A1070	G1010	C948	A836	C
A1679	A1619	C1559	C1437	U1377	U1315	A1253	U1193	A1133	G1071	A1011	G949	U887	C
G1680	A1620	U1560	A1438	A1378	C1316	C1254	A1194	G1134	U1069	A1012	C950	U889	C
U1681	U1621	A1561	A1439	A1379	G1317	G1255	A1195	C1135	G1074	U1013	C951	U890	C
C1682	U1622	C1562	C1440	C1380	G1318	G1256	A1196	U1136	C1075	G1014	G952	G891	C
C1683	A1623	G1563	U1441	G1381	U1319	G1257	U1197	U1137	G1076	U1015	G953	U892	C
C1684	C1624	C1564	U1442	A1382	G1320	A1258	G1198	C1138	C1079	U1016	U954	U893	C
U1685	U1625	U1504	C1443	A1383	G1321	A1259	A1199	C1139	A1080	U1017	A955	G894	C
G1686	C1626	G1565	U1444	C1384	G1322	A1260	A1200	G1140	A1081	U1018	G956	G895	C
C1687	G1627	G1566	U1445	G1385	U1323	C1261	U1201	G1141	U1081	C1019	A957	U896	C
C1688	C1628	C1567	A1446	A1386	G1324	C1262	U1202	G1142	A1082	A1020	G958	U897	C
G1689	C1629	A1568	G1447	G1387	G1325	U1263	G1203	A1143	U1083	U1021	G959	U898	C
U1690	U1630	G1570	A1448	A1388	U1326	C1264	A1204	U1144	A1084	U1022	U960	U899	C
U1691	U1631	G1571	G1449	C1389	G1327	A1265	C1205	A1145	C1085	A1023	G961	C900	C
U1692	G1632	C1572	U1511	U1390	G1328	C1266	G1206	C1146	G1086	A1024	A962	G901	C
G1693	A1633	G1573	G1451	C1391	U1329	C1267	G1207	C1147	A1087	U1025	A963	G902	C
U1694	A1634	C1574	A1452	U1392	G1330	C1268	A1208	A1148	U1088	C1026	A964	A903	C
A1695	C1635	G1575	C1453	G1393	C1331	C1269	A1209	U1149	G1089	A1027	U965	A904	C
G1696	G1636	G1576	A1454	G1394	A1332	G1270	A1150	A1150	C1090	U1028	U966	U844	C
A1697	A1637	G1577	A1455	C1395	U1333	C1271	G1211	G1151	C1091	G1029	C967	U906	C



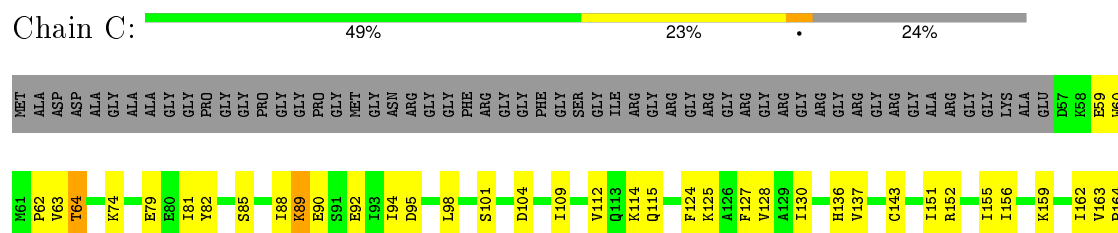
• Molecule 2: 40S RIBOSOMAL PROTEIN SA



• Molecule 3: 40S RIBOSOMAL PROTEIN S3A



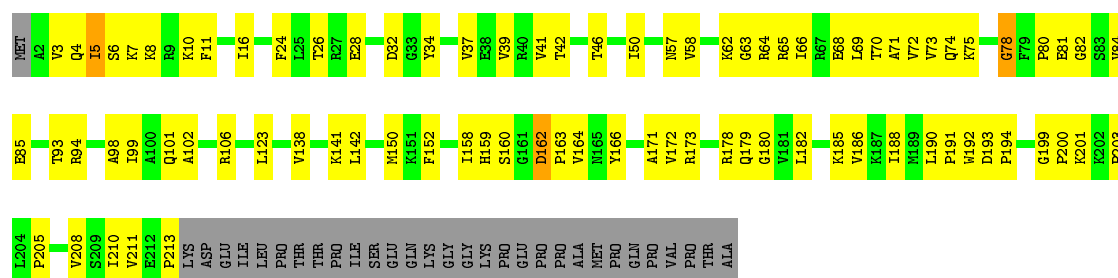
• Molecule 4: 40S RIBOSOMAL PROTEIN S2





- Molecule 5: 40S RIBOSOMAL PROTEIN S3

Chain D: 52% 34% 13%



- Molecule 6: 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1

Chain E: 54% 40% 6%



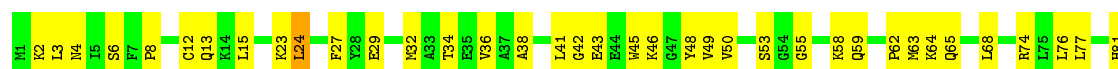
- Molecule 7: 40S RIBOSOMAL PROTEIN S5

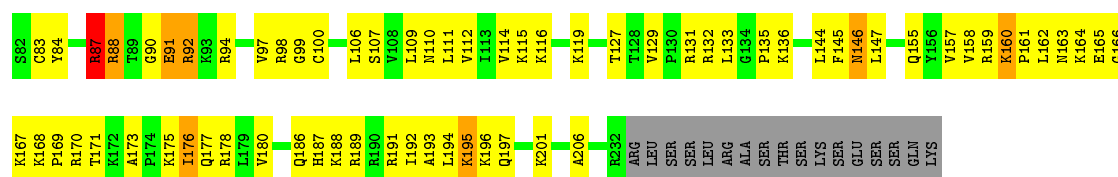
Chain F: 49% 38% 6% 8%



- Molecule 8: 40S RIBOSOMAL PROTEIN S6

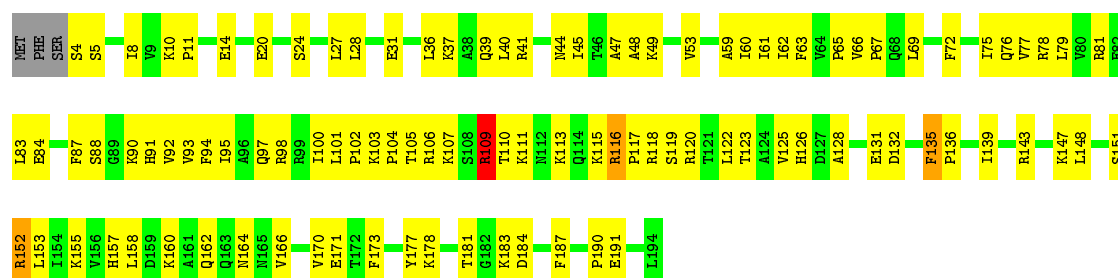
Chain G: 51% 39% 7%





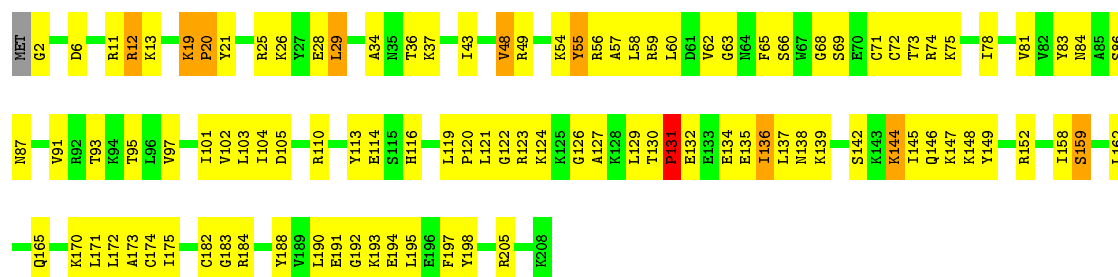
• Molecule 9: 40S RIBOSOMAL PROTEIN S7

Chain H: 46% 51%



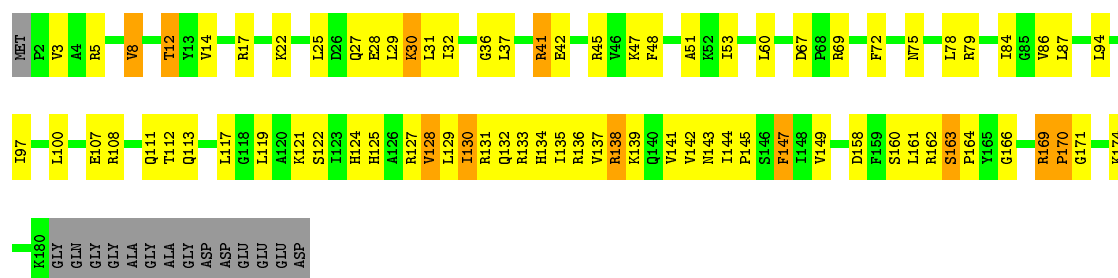
• Molecule 10: 40S RIBOSOMAL PROTEIN S8

Chain I: 50% 45%



• Molecule 11: 40S RIBOSOMAL PROTEIN S9

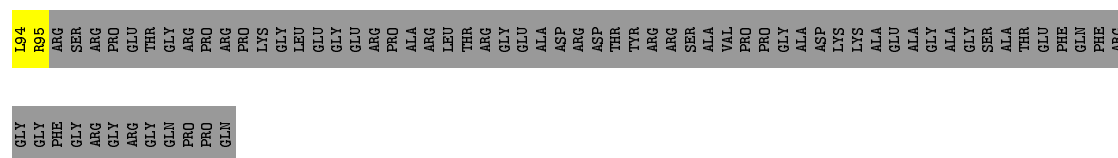
Chain J: 52% 35% 6% 8%



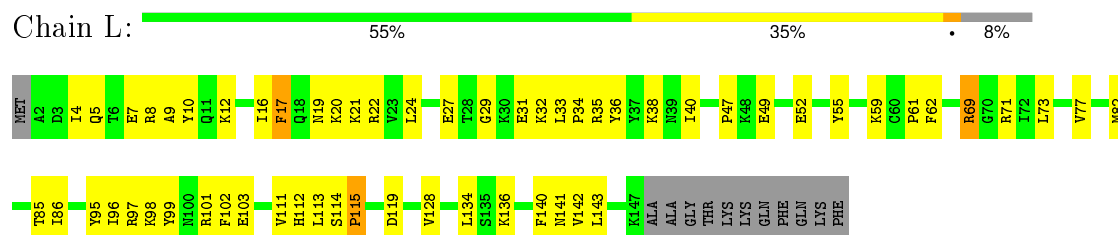
• Molecule 12: 40S RIBOSOMAL PROTEIN S10

Chain K: 32% 22% 43%

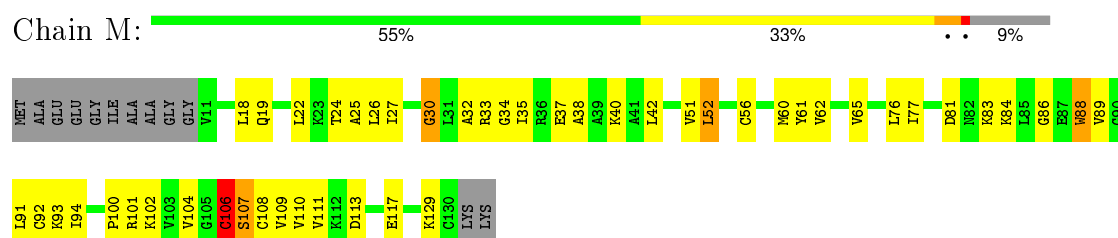




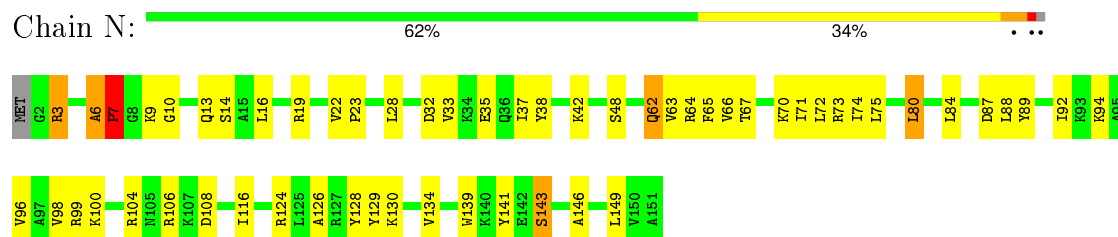
• Molecule 13: 40S RIBOSOMAL PROTEIN S11



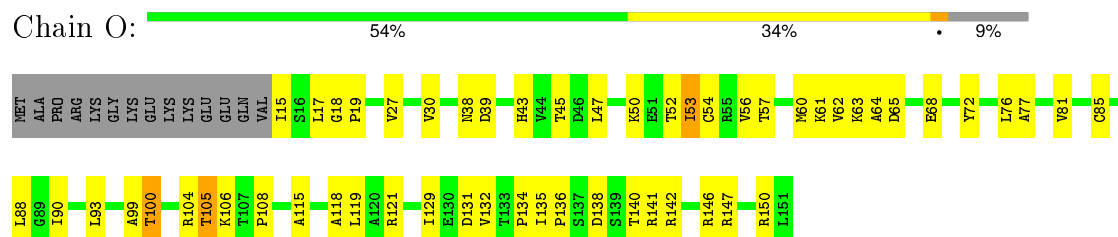
• Molecule 14: 40S RIBOSOMAL PROTEIN S12



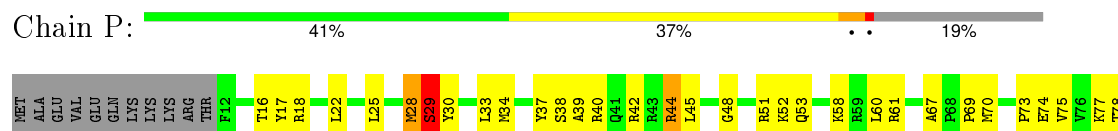
• Molecule 15: 40S RIBOSOMAL PROTEIN S13



• Molecule 16: 40S RIBOSOMAL PROTEIN S14

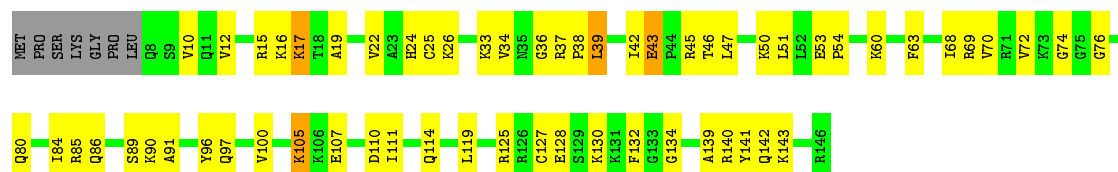


• Molecule 17: 40S RIBOSOMAL PROTEIN S15

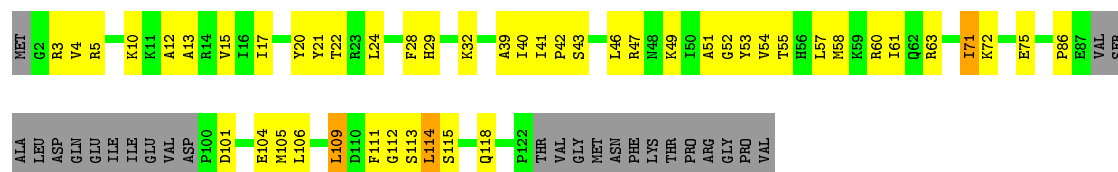




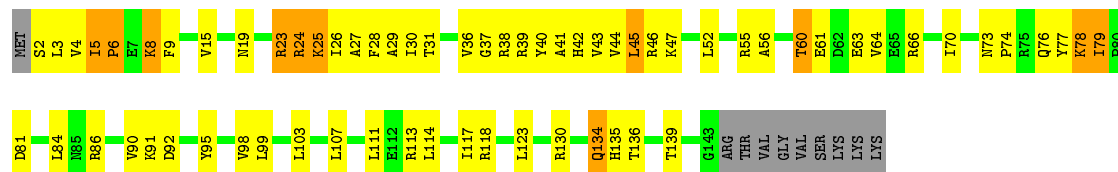
• Molecule 18: 40S RIBOSOMAL PROTEIN S16



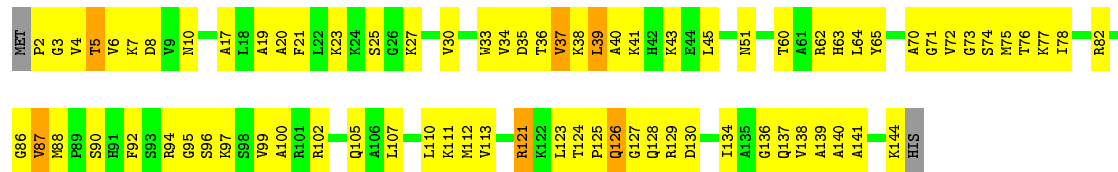
• Molecule 19: 40S RIBOSOMAL PROTEIN S17



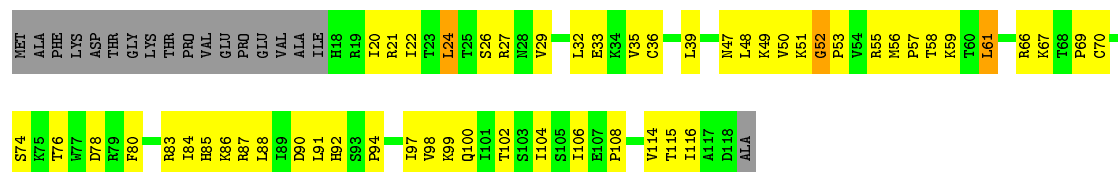
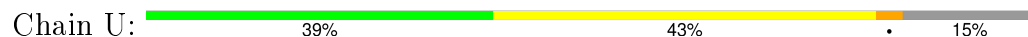
• Molecule 20: 40S RIBOSOMAL PROTEIN S18




• Molecule 21: 40S RIBOSOMAL PROTEIN S19



• Molecule 22: 40S RIBOSOMAL PROTEIN S20




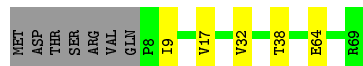
- Molecule 29: 40S RIBOSOMAL PROTEIN S27

Chain b:  90% 5% 5%




- Molecule 30: 40S RIBOSOMAL PROTEIN S28

Chain c:  83% 7% 10%




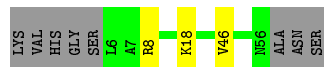
- Molecule 31: 40S RIBOSOMAL PROTEIN S29

Chain d:  88% 7% 5%



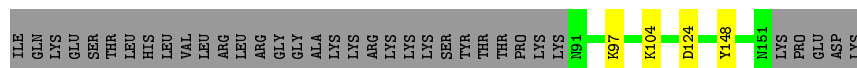
- Molecule 32: 40S RIBOSOMAL PROTEIN S30

Chain e:  81% 5% 14%



- Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

Chain f:  37% 61%



- Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

Chain g:  93% 5%



- Molecule 35: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1

Chain h:  97%



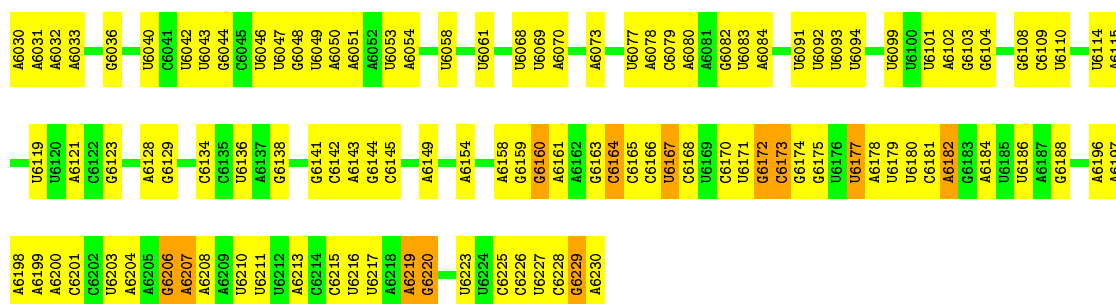
• Molecule 36: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUB-UNIT ERF3A

Chain i:  98%



• Molecule 37: CRICKET PARALYSIS VIRUS IRES RNA

Chain j:  45%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	115000	Depositor
Image detector	TVIPS TEMCAM F416	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
10	I	0.48	0/1724	0.72	0/2298
11	J	0.45	0/1520	0.77	0/2030
12	K	0.48	0/815	0.68	0/1101
13	L	0.45	0/1220	0.72	0/1633
14	M	0.48	0/941	0.72	0/1264
15	N	0.43	0/1231	0.73	1/1656 (0.1%)
16	O	0.46	0/1036	0.71	0/1391
17	P	0.43	0/1000	0.67	0/1335
18	Q	0.43	0/1125	0.66	0/1506
19	R	0.42	0/904	0.67	0/1208
2	A	0.51	0/1756	0.68	0/2386
20	S	0.42	0/1190	0.68	0/1594
21	T	0.44	0/1131	0.69	0/1515
22	U	0.50	0/813	0.70	0/1092
23	V	0.47	0/643	0.71	0/860
24	W	0.44	0/1050	0.69	0/1406
25	X	0.46	0/1063	0.70	0/1421
26	Y	0.45	0/1019	0.70	0/1354
27	Z	0.46	0/611	0.71	0/820
28	a	0.48	0/778	0.75	1/1041 (0.1%)
29	b	0.48	0/637	0.68	0/854
3	B	0.51	0/1756	0.75	1/2350 (0.0%)
30	c	0.46	0/492	0.74	0/657
31	d	0.51	0/454	0.77	0/603
32	e	0.45	0/417	0.69	0/548
33	f	0.53	0/507	0.84	1/673 (0.1%)
34	g	0.45	0/2497	0.67	0/3399
35	h	0.35	0/3506	0.56	0/4709
36	i	0.37	0/3418	0.55	0/4600
37	j	1.42	85/4752 (1.8%)	1.74	207/7383 (2.8%)
4	C	0.42	0/1761	0.65	0/2379
5	D	0.41	0/1672	0.66	0/2250
6	E	0.47	0/2072	0.70	0/2793

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	F	0.43	0/1507	0.74	0/2026
8	G	0.48	0/1907	0.74	0/2538
9	H	0.46	0/1558	0.74	1/2087 (0.0%)
All	All	0.52	87/92033 (0.1%)	0.83	218/133523 (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
1	1	0	24
37	j	0	1
All	All	0	25

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	j	6173	C	O3'-P	-20.14	1.36	1.61
37	j	6229	G	O3'-P	19.64	1.84	1.61
37	j	6079	C	N3-C4	19.19	1.47	1.33
37	j	6177	U	O3'-P	-18.39	1.39	1.61
37	j	6219	A	O3'-P	-15.97	1.42	1.61

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	j	6079	C	C5-C6-N1	19.25	130.62	121.00
37	j	6114	U	C4-C5-C6	-18.58	108.55	119.70
37	j	6114	U	N3-C4-C5	17.39	125.03	114.60
37	j	6077	U	C2-N3-C4	-15.00	118.00	127.00
37	j	6161	A	N1-C2-N3	-15.00	121.80	129.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	111	A	Sidechain
1	1	44	U	Sidechain
1	1	77	A	Sidechain
1	1	84	A	Sidechain

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Mol	Chain	Res	Type	Group
1	1	88	G	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	37159	0	18774	3646	0
2	A	1719	0	1717	129	0
3	B	1729	0	1803	135	0
4	C	1724	0	1808	63	0
5	D	1646	0	1736	81	0
6	E	2031	0	2138	116	0
7	F	1486	0	1545	99	0
8	G	1884	0	2044	151	0
9	H	1535	0	1632	130	0
10	I	1695	0	1785	113	0
11	J	1495	0	1615	89	0
12	K	791	0	811	45	0
13	L	1199	0	1269	69	0
14	M	931	0	961	40	0
15	N	1207	0	1294	63	0
16	O	1023	0	1050	51	0
17	P	981	0	1026	55	0
18	Q	1108	0	1174	73	0
19	R	893	0	946	57	0
20	S	1172	0	1229	77	0
21	T	1112	0	1146	116	0
22	U	803	0	866	68	0
23	V	636	0	637	42	0
24	W	1033	0	1080	61	0
25	X	1046	0	1110	68	0
26	Y	1002	0	1075	65	0
27	Z	605	0	665	58	0
28	a	767	0	816	0	0
29	b	625	0	642	0	0
30	c	490	0	520	0	0
31	d	444	0	442	0	0
32	e	412	0	463	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	f	497	0	497	0	0
34	g	2440	0	2396	0	0
35	h	3450	0	3446	0	0
36	i	3357	0	3398	0	0
37	j	4257	0	2143	0	0
All	All	86384	0	67699	5137	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 40.

The worst 5 of 5137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1431:G:H2'	1:1:1432:U:C6	1.77	1.18
1:1:377:G:H4'	10:1:97:VAL:HG13	1.24	1.18
1:1:571:U:H3'	1:1:572:U:C5'	1.77	1.15
1:1:569:A:H2'	1:1:570:C:H5''	1.24	1.14
1:1:1547:C:H3'	1:1:1548:G:H5''	1.29	1.14

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	A	216/295 (73%)	209 (97%)	5 (2%)	2 (1%)	21	67
3	B	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1	19
4	C	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	8	48
5	D	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	7	47
6	E	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	186/204 (91%)	163 (88%)	13 (7%)	10 (5%)	2	29
8	G	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	4	36
9	H	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	9	50
10	I	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	5	40
11	J	177/194 (91%)	168 (95%)	6 (3%)	3 (2%)	11	55
12	K	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1	20
13	L	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3	34
14	M	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	2	30
15	N	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	5	40
16	O	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	8	49
17	P	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	3	34
18	Q	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	13	57
19	R	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	10	52
20	S	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	2	28
21	T	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	14	58
22	U	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	19	65
23	V	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	7	46
24	W	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	12	56
25	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2	29
26	Y	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	5	40
27	Z	74/125 (59%)	71 (96%)	0	3 (4%)	3	35
28	a	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	3	34
29	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
30	c	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	5	40
31	d	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
32	e	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	9	51
33	f	59/156 (38%)	53 (90%)	6 (10%)	0	100	100
34	g	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	8	49
35	h	428/436 (98%)	410 (96%)	14 (3%)	4 (1%)	21	67
36	i	414/426 (97%)	403 (97%)	9 (2%)	2 (0%)	34	77
All	All	5553/6338 (88%)	5186 (93%)	215 (4%)	152 (3%)	10	45

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	76	ASN
3	B	132	GLY
3	B	148	ASN
3	B	154	SER
3	B	176	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	181/243 (74%)	176 (97%)	5 (3%)	51	78
3	B	194/231 (84%)	183 (94%)	11 (6%)	25	62
4	C	188/225 (84%)	181 (96%)	7 (4%)	41	73
5	D	175/202 (87%)	166 (95%)	9 (5%)	29	66
6	E	220/225 (98%)	208 (94%)	12 (6%)	27	63
7	F	158/170 (93%)	151 (96%)	7 (4%)	35	69
8	G	202/218 (93%)	195 (96%)	7 (4%)	43	74
9	H	171/174 (98%)	167 (98%)	4 (2%)	58	83
10	I	179/180 (99%)	167 (93%)	12 (7%)	20	57
11	J	160/168 (95%)	150 (94%)	10 (6%)	22	59
12	K	85/136 (62%)	82 (96%)	3 (4%)	43	74
13	L	133/142 (94%)	131 (98%)	2 (2%)	72	88
14	M	102/108 (94%)	97 (95%)	5 (5%)	31	67
15	N	130/131 (99%)	128 (98%)	2 (2%)	72	88
16	O	107/119 (90%)	100 (94%)	7 (6%)	21	58
17	P	107/130 (82%)	102 (95%)	5 (5%)	32	68
18	Q	115/121 (95%)	111 (96%)	4 (4%)	43	74
19	R	99/122 (81%)	94 (95%)	5 (5%)	29	66
20	S	123/132 (93%)	114 (93%)	9 (7%)	17	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	T	113/115 (98%)	106 (94%)	7 (6%)	23	60
22	U	93/107 (87%)	89 (96%)	4 (4%)	35	70
23	V	67/67 (100%)	66 (98%)	1 (2%)	72	88
24	W	112/113 (99%)	107 (96%)	5 (4%)	34	69
25	X	108/115 (94%)	103 (95%)	5 (5%)	33	68
26	Y	107/115 (93%)	101 (94%)	6 (6%)	26	62
27	Z	67/103 (65%)	63 (94%)	4 (6%)	24	60
28	a	83/98 (85%)	76 (92%)	7 (8%)	14	48
29	b	72/76 (95%)	68 (94%)	4 (6%)	26	62
30	c	55/62 (89%)	52 (94%)	3 (6%)	27	63
31	d	47/49 (96%)	43 (92%)	4 (8%)	13	48
32	e	42/48 (88%)	40 (95%)	2 (5%)	31	67
33	f	54/140 (39%)	51 (94%)	3 (6%)	26	62
34	g	272/275 (99%)	260 (96%)	12 (4%)	35	69
35	h	376/376 (100%)	368 (98%)	8 (2%)	61	84
36	i	371/371 (100%)	364 (98%)	7 (2%)	65	86
All	All	4868/5407 (90%)	4660 (96%)	208 (4%)	40	70

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	N	7	PRO
19	R	118	GLN
34	g	289	LEU
16	O	45	THR
17	P	40	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	43	HIS
20	S	85	ASN
35	h	266	GLN
17	P	35	GLN
18	Q	80	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1738/1869 (92%)	1037 (59%)	152 (8%)
37	j	195/201 (97%)	50 (25%)	0
All	All	1933/2070 (93%)	1087 (56%)	152 (7%)

5 of 1087 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	C
1	1	4	C
1	1	5	U
1	1	6	G

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	834	C
1	1	1150	A
1	1	1721	U
1	1	899	U
1	1	1021	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.