



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 06:07 PM BST

PDB ID : 4KZX
Title : Rabbit 40S ribosomal subunit in complex with eIF1.
Authors : Lomakin, I.B.; Steitz, T.A.
Deposited on : 2013-05-30
Resolution : 7.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

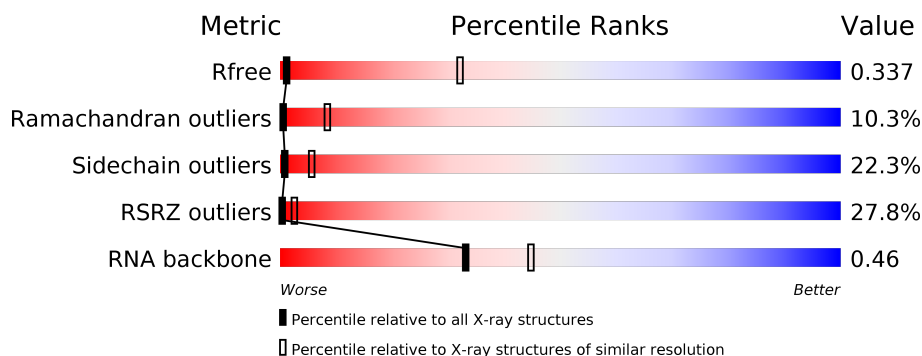
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.81 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)
RNA backbone	3102	1079 (11.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	<div> <div>6%</div> <div> <div>47%</div> <div>20%</div> <div>• •</div> <div>29%</div> </div> </div>
2	B	264	<div> <div>30%</div> <div> <div>56%</div> <div>22%</div> <div>•</div> <div>19%</div> </div> </div>
3	C	278	<div> <div>2%</div> <div> <div>57%</div> <div>21%</div> <div>• •</div> <div>19%</div> </div> </div>
4	D	243	<div> <div>32%</div> <div> <div>62%</div> <div>26%</div> <div>5%</div> <div>7%</div> </div> </div>
5	E	263	<div> <div>35%</div> <div> <div>67%</div> <div>29%</div> <div>•</div> </div> </div>
6	F	204	<div> <div>15%</div> <div> <div>67%</div> <div>21%</div> <div>• •</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	K	165	
12	L	158	
13	M	132	
14	N	151	
15	O	151	
16	P	145	
17	Q	146	
18	R	135	
19	S	152	
20	T	145	
21	U	119	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	Z	125	
27	a	115	
28	b	84	
29	c	69	
30	d	56	
31	e	133	

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Mol	Chain	Length	Quality of chain
32	f	156	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%19%17%8%54%</div></div>
33	g	317	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>14%74%20%</div></div>
34	i	1863	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>24%7%64%25%</div></div>
35	l	113	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%47%25%25%</div></div>

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 77211 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1642	1045	289	300	8			

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1741	1107	309	310	15			

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1742	1127	300	306	9			

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	0	0
			1764	1124	317	315	8			

- Molecule 5 is a protein called 40S ribosomal protein S4X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	263	Total	C	N	O	S	0	0	0
			2083	1329	385	359	10			

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	190	Total	C	N	O	S	0	0	0
			1530	975	281	273	1			

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	206	Total	C	N	O	S	0	0	0
			1679	1054	329	291	5			

- Molecule 10 is a protein called 40S Ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	182	Total	C	N	O	S	0	0	0
			1498	952	300	244	2			

- Molecule 11 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	158	Total	C	N	O	S	0	0	0
			1296	827	241	221	7			

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	124	Total	C	N	O	S	0	0	0
			950	594	169	179	8			

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	136	Total	C	N	O	S	0	0	0
			1016	621	199	190	6			

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	127	Total	C	N	O	S	0	0	0
			1060	673	201	179	7			

- Molecule 17 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	141	Total	C	N	O	S	0	0	0
			1124	715	212	194	3			

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	126	Total	C	N	O	S	0	0	0
			1019	639	188	187	5			

- Molecule 19 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	137	Total	C	N	O	S	0	0	0
			1139	714	231	193	1			

- Molecule 20 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	141	Total	C	N	O	S	0	0	0
			1112	701	213	195	3			

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	104	Total	C	N	O	S	0	0	0
			822	514	156	148	4			

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	82	Total	C	N	O	S	0	0	0
			619	378	117	119	5			

- Molecule 23 is a protein called 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			

- Molecule 24 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	142	Total	C	N	O	S	0	0	0
			1106	698	220	184	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	ALA	SEE REMARK 999	UNP G1SZ47

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	126	Total	C	N	O	S	0	0	0
			1021	645	198	173	5			

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	a	107	Total	C	N	O	S	0	0	0
			844	527	173	138	6			

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	b	84	Total	C	N	O	S	0	0	0
			659	413	122	116	8			

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	c	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	d	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	e	59	Total	C	N	O	S	0	0	0
			473	293	104	75	1			

- Molecule 32 is a protein called 40S ribosomal protein S27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	f	71	Total	C	N	O	S	0	0	0
			581	367	109	98	7			

- Molecule 33 is a protein called 40S ribosomal protein RACK1.

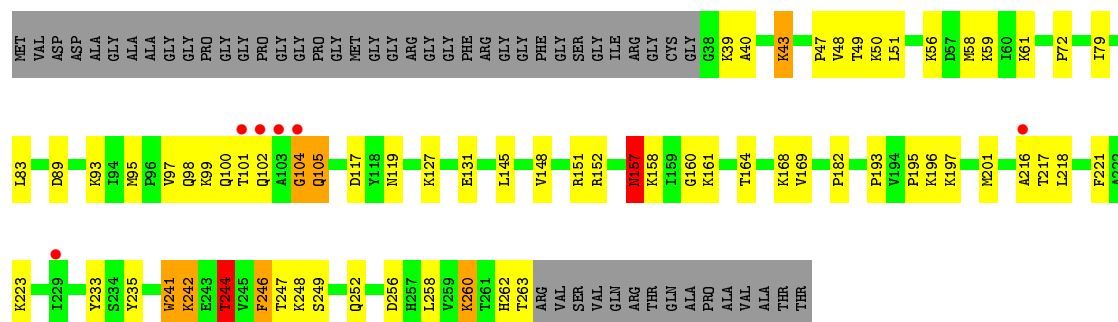
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	g	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

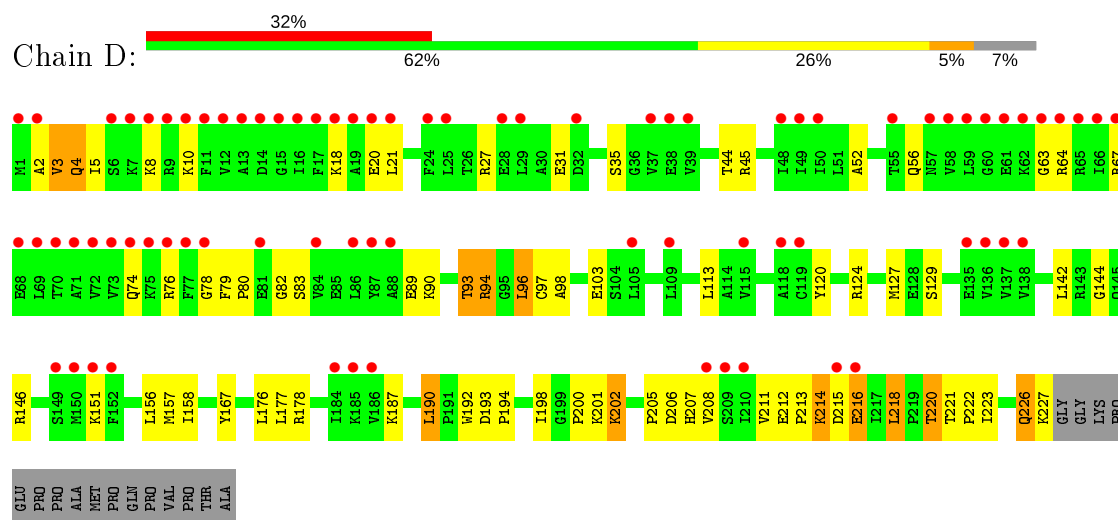
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	i	1797	Total	C	N	O	P	0	0	0
			37514	16712	6633	12373	1796			

- Molecule 35 is a protein called Eukaryotic translation initiation factor 1.

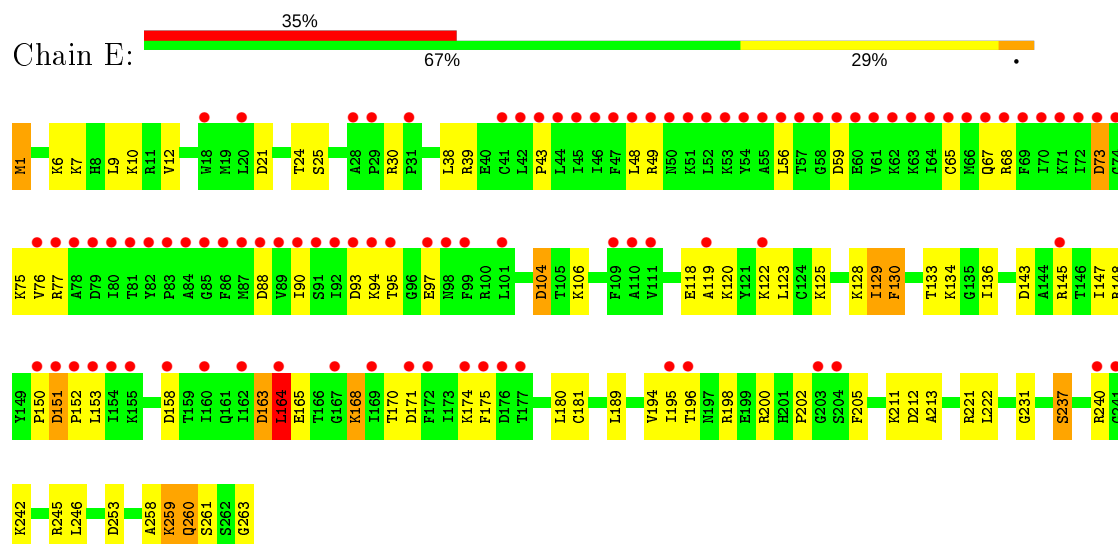
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	l	85	Total	C	N	O	S	0	0	0
			691	438	125	126	2			



• Molecule 4: 40S ribosomal protein S3

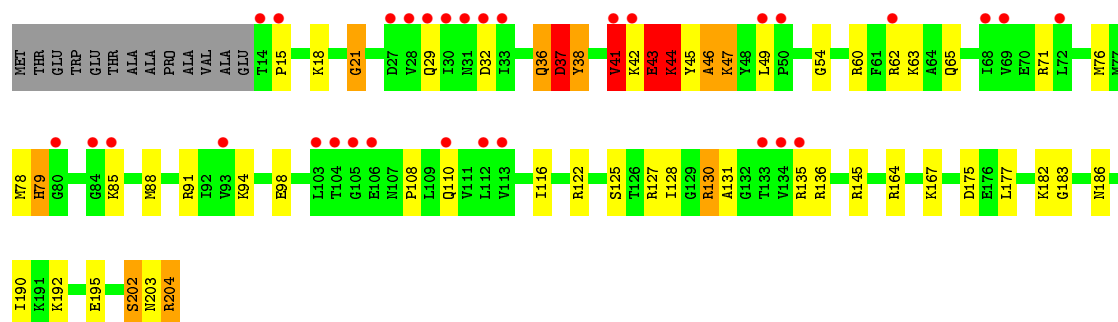


• Molecule 5: 40S ribosomal protein S4X

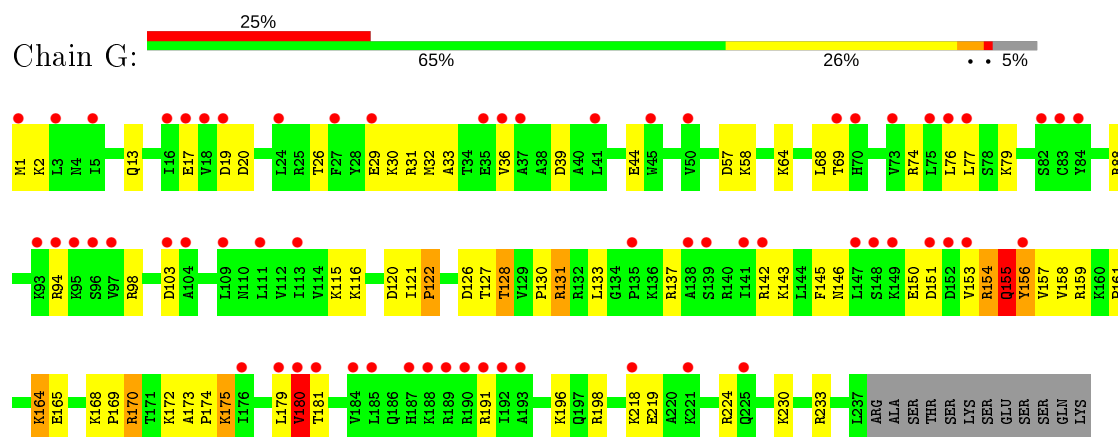


• Molecule 6: 40S ribosomal protein S5

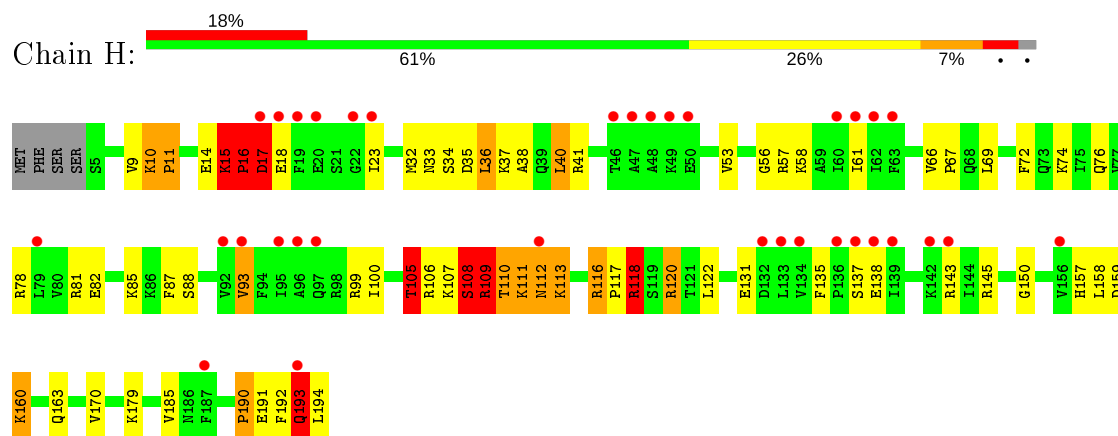




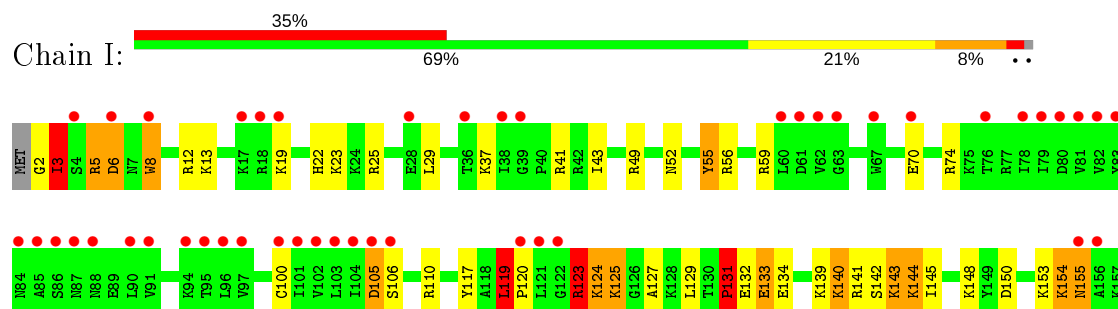
• Molecule 7: 40S ribosomal protein S6



• Molecule 8: 40S ribosomal protein S7

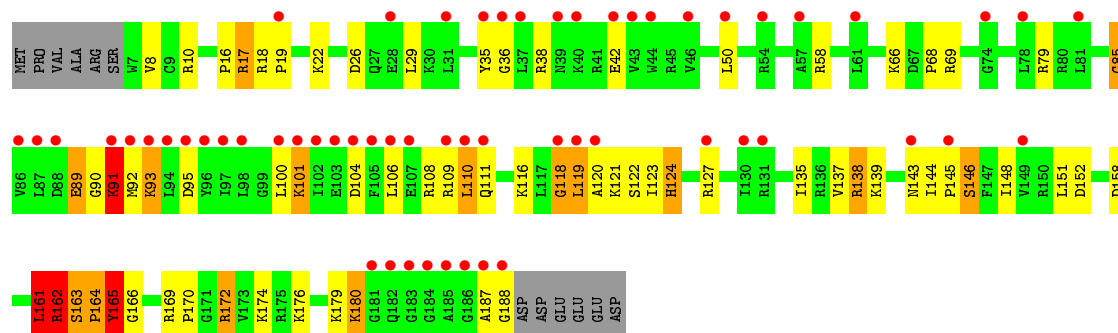


• Molecule 9: 40S ribosomal protein S8

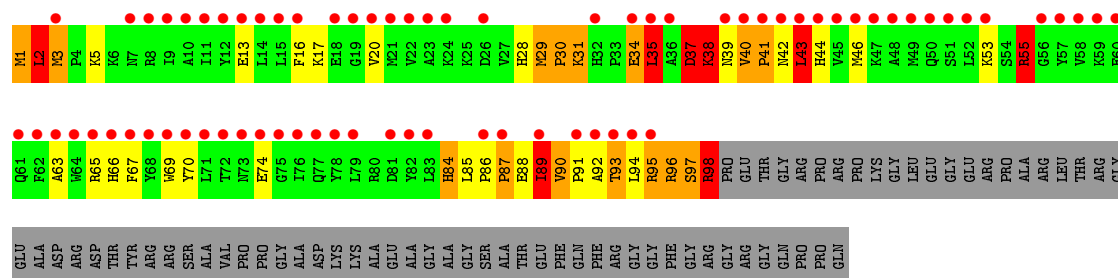
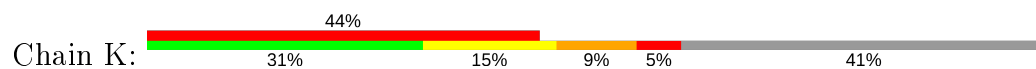




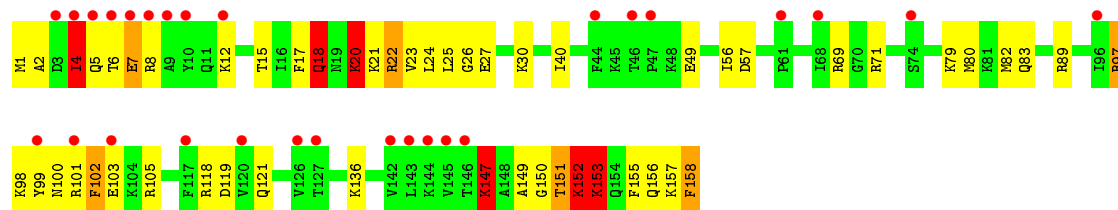
• Molecule 10: 40S Ribosomal protein S9



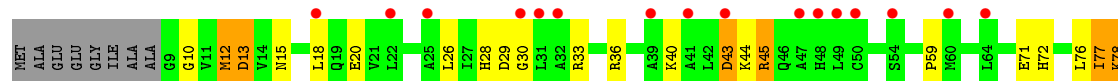
• Molecule 11: 40S ribosomal protein S10

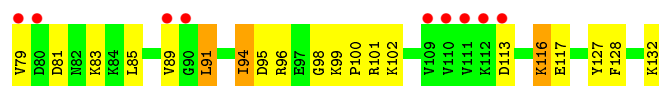


• Molecule 12: 40S ribosomal protein S11

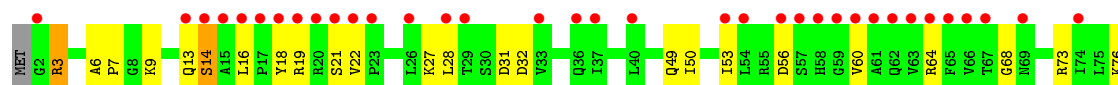


• Molecule 13: 40S ribosomal protein S12

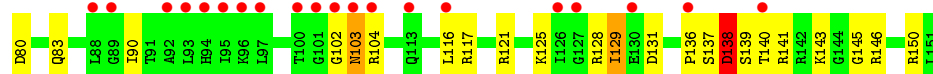
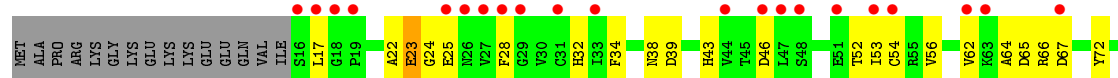




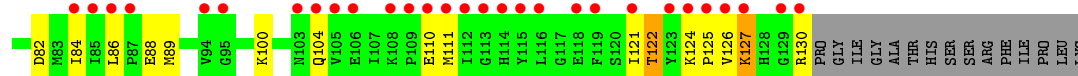
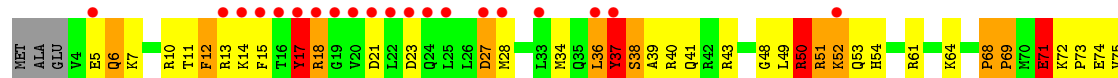
- Molecule 14: 40S ribosomal protein S13



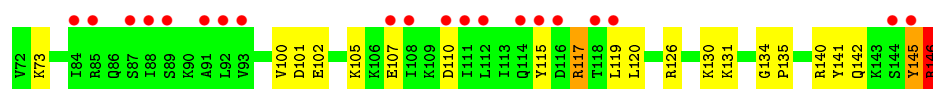
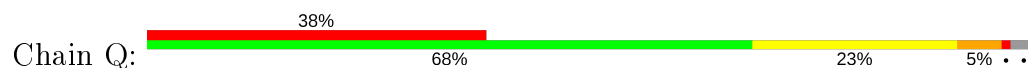
- Molecule 15: 40S ribosomal protein S14



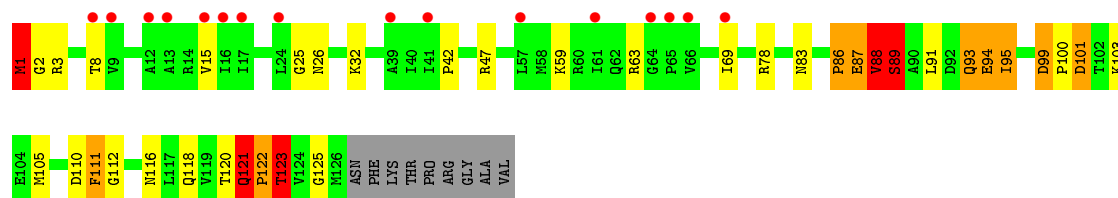
- Molecule 16: 40S ribosomal protein S15



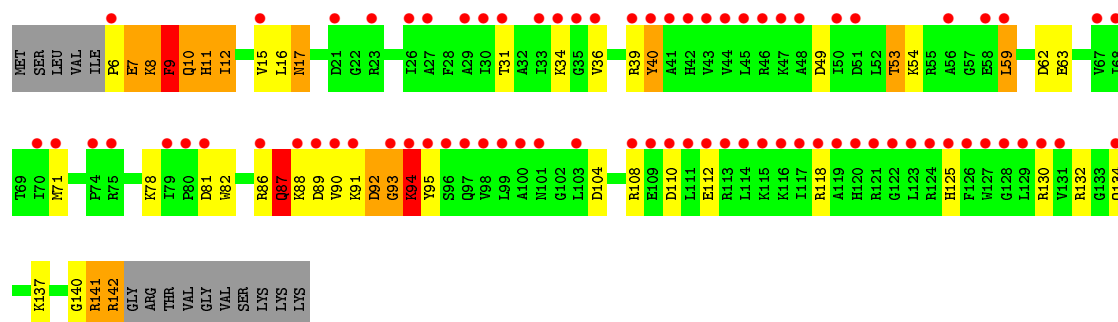
- Molecule 17: 40S ribosomal protein S16



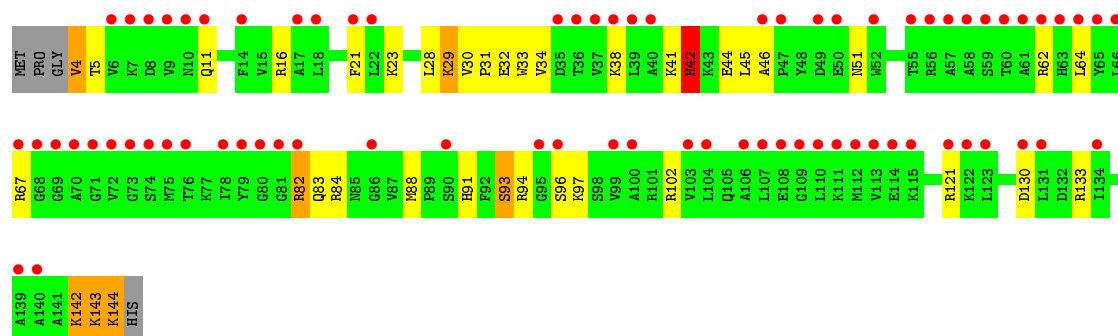
- Molecule 18: 40S ribosomal protein S17



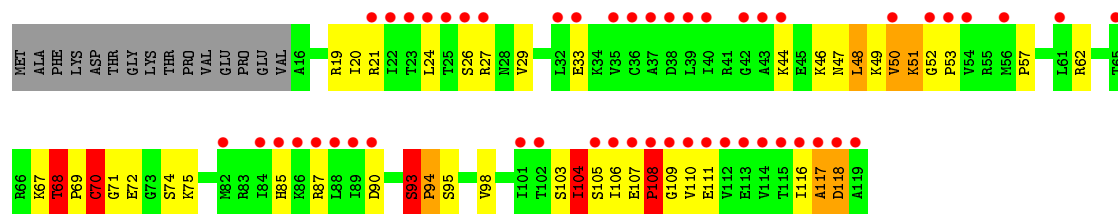
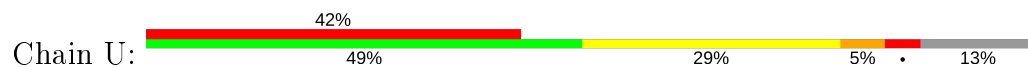
- Molecule 19: 40S ribosomal protein S18



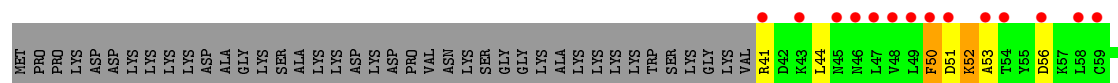
- Molecule 20: 40S ribosomal protein S19

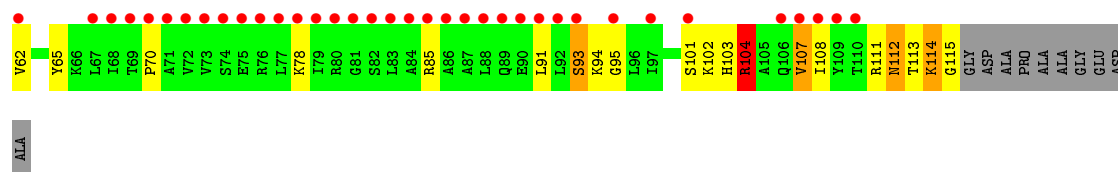


- Molecule 21: 40S ribosomal protein S20

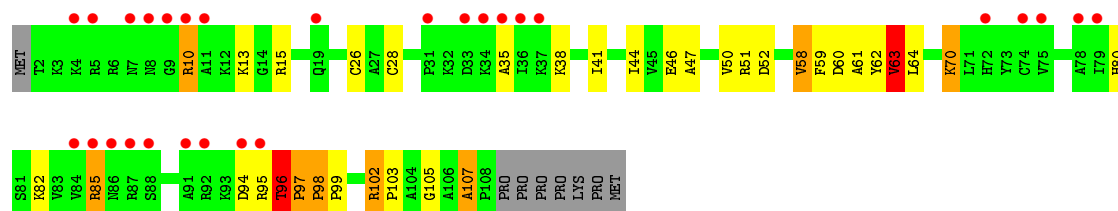


- Molecule 22: 40S ribosomal protein S21

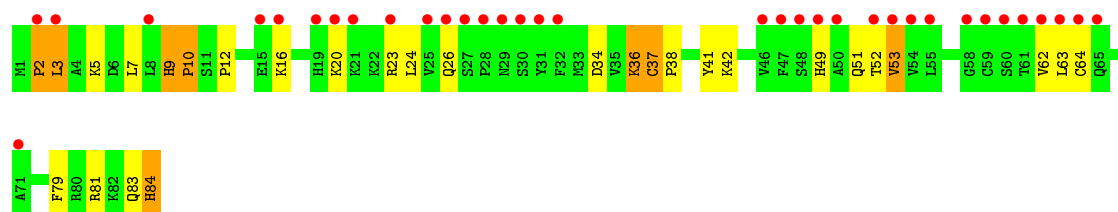
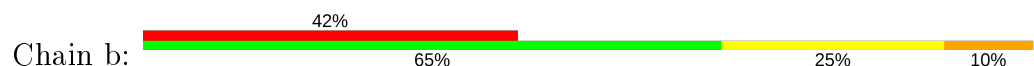




- Molecule 27: 40S ribosomal protein S26



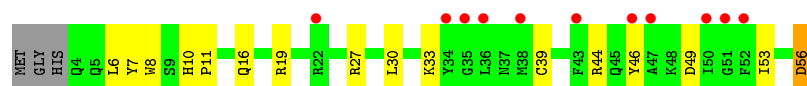
- Molecule 28: 40S ribosomal protein S27



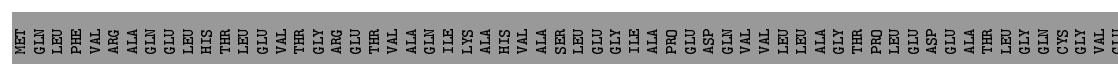
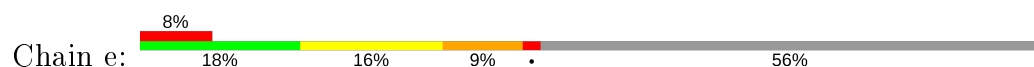
- Molecule 29: 40S ribosomal protein S28

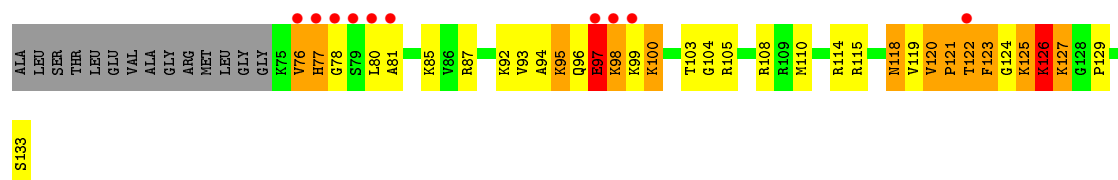


- Molecule 30: 40S ribosomal protein S29

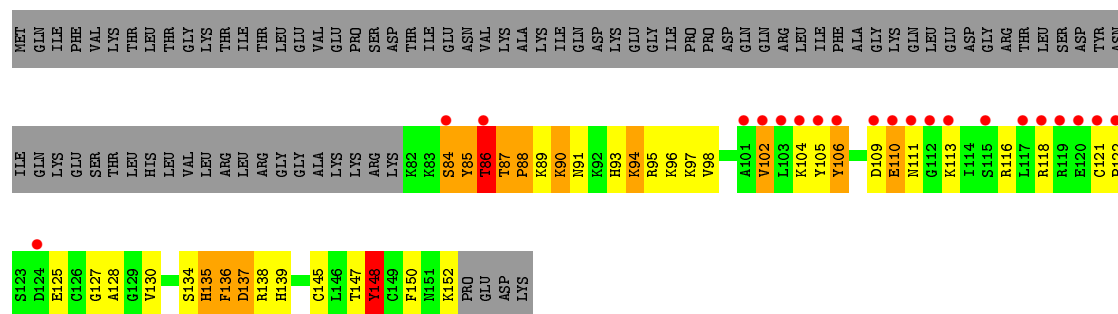
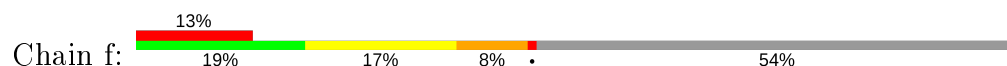


- Molecule 31: 40S ribosomal protein S30

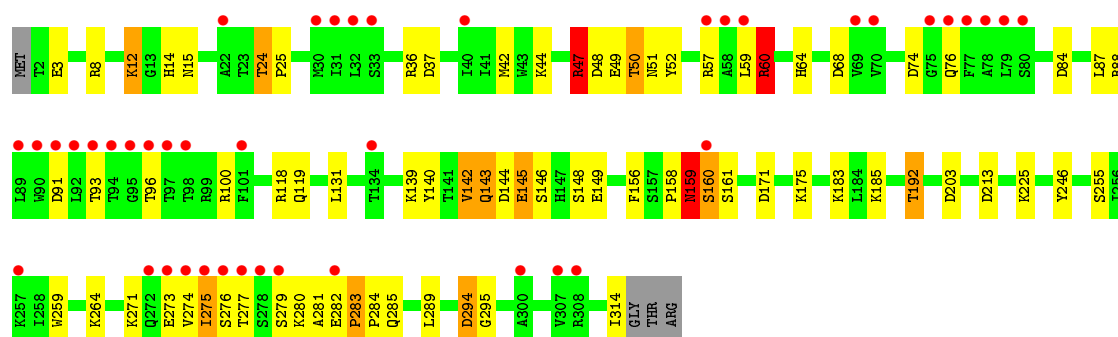
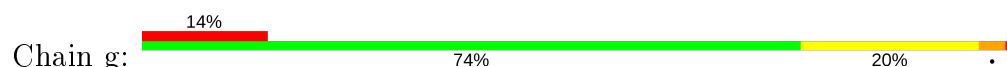




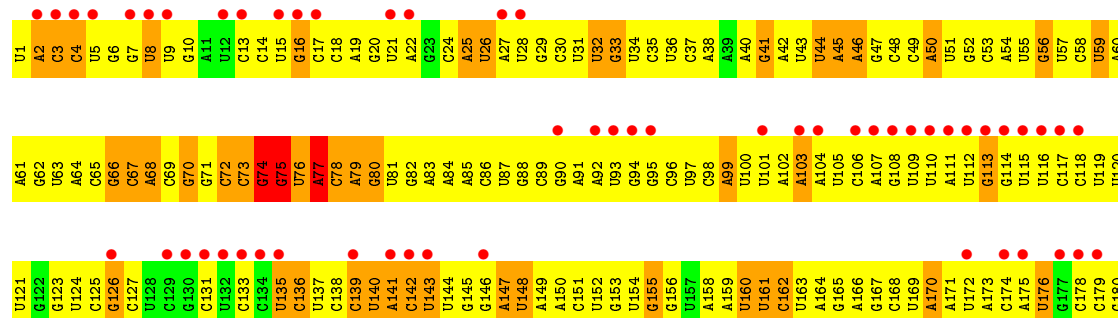
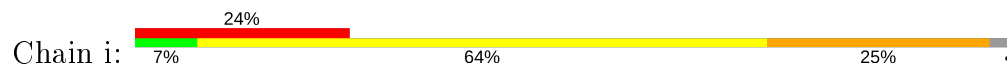
- Molecule 32: 40S ribosomal protein S27A



- Molecule 33: 40S ribosomal protein RACK1

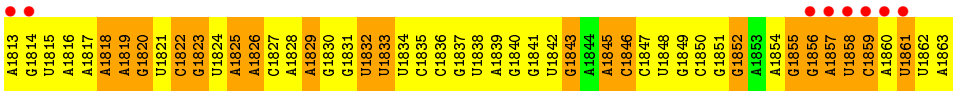


- Molecule 34: 18S ribosomal RNA





G1753	G1693	G1633	G1572	G1512	G1452	G1392	G1332	A1272	C1212	U1150	C1090	A1030
G1754	A1694	G1634	U1573	C1513	U1453	U1393	C1333	G1273	A1213	U1151	U1091	A1031
U1755	A1695	A1635	A1574	U1514	G1454	G1394	G1334	G1274	C1214	U1152	G1092	A1032
C1756	C1696	A1636	A1575	G1515	G1455	C1395	U1335	C1275	C1215	G1153	G1093	G1033
G1757	G1697	U1637	C1576	G1516	C1456	U1396	U1336	G1276	A1216	G1154	C1094	U1034
G1758	C1698	U1638	G1577	A1517	G1457	A1397	C1337	G1277	G1217		G1095	U1035
C1759	C1699	C1639	C1578	C1518	U1458	A1398	U1338	A1278	G1218	U1157	A1096	G1036
C1760	C1700	C1640	C1579	G1519	U1459	C1399	U1339	C1279	A1219	C1158	U1097	G1037
G1701	G1701	C1641	U1580	C1520	U1460	U1400	A1340	C1280	G1220	C1159	G1098	A1038
U1702	U1702	A1642	U1581	G1521	A1461	A1401	G1341	G1281	U1221	G1160	G1099	G1039
C1703	C1703	G1643	G1582	C1522	G1462	G1402	U1342	G1282	U1222	G1161	G1100	G1040
G1704	G1704	U1644	A1583	G1523	C1463	U1403	U1343	G1283	G1223	G1162	G1101	U1041
G1705	G1705	A1645	A1584	C1524	C1464	U1404	G1344	U1284	A1224	G1163	C1102	U1042
G1765	G1765	A1646	C1585	U1525	A1465	A1405	G1345	U1285	G1225	G1164	G1103	C1043
C1766	C1766	C1647	C1586	A1526	C1466	C1406	U1346	G1286	C1226	G1165	G1104	A1044
A1707	A1707	U1648	C1587	C1527	G1467	G1407	G1347	U1287	C1227	A1166	C1105	A1045
C1768	C1768	U1649	C1588	A1528	C1468	C1408	G1348	C1288	U1228	G1167	G1106	A1046
U1709	U1709	G1649	C1589	C1529	C1469	A1349	A1349	A1289	G1229	U1168	U1107	G1047
G1710	G1710	C1650	U1590	U1530	A1470	A1410	G1350	G1290	C1230	A1169	U1108	A1048
G1711	G1711	G1651	U1591	G1531	G1471	C1411	C1351	A1291	G1231	U1170	A1109	C1049
C1712	C1712	G1652	U1592	A1532	G1472	C1412	G1352	U1292	G1232	G1171	U1110	G1050
G1713	G1713	G1653	C1593	C1533	U1473	C1413	A1353	U1293	C1233	G1172	U1111	A1051
A1714	A1714	U1654	G1594	U1534	U1474	C1414	U1354	G1294	U1234	U1173	C1112	U1052
U1715	U1715	C1655	U1595	G1535	G1475	C1415	U1355	A1295	A1235	U1174	C1113	C1053
U1716	U1716	A1656	G1596	G1536	A1476	G1416	U1356	U1296	A1236	G1175	C1114	A1054
G1717	G1717	U1657	U1597	C1537	G1477	A1417	G1357	A1297	A1237	C1176	A1115	G1055
G1718	G1718	A1658	U1598	U1538	C1478	G1418	U1358	G1298	U1238	A1177	U1116	A1056
C1719	C1719	G1659	G1599	C1539	C1479	C1419	C1359	C1299	U1239	A1178	G1117	U1057
U1720	U1720	G1660	G1600	A1540	U1480	G1420	U1360	U1300	U1240		A1118	A1058
G1721	G1721	U1661	G1601	G1541	U1481	G1421	G1361	C1301	G1241		G1119	C1059
C1722	C1722	U1662	G1602	C1542	A1482	U1422	G1362	U1302	A1242		C1120	C1060
U1723	U1723	G1663	A1603	G1543	A1483	C1423	U1363	U1303	C1243		C1121	G1061
U1724	U1724	U1664	C1604	U1544	G1484	G1424	U1364	U1304	U1244		G1122	U1062
U1725	U1725	C1665	G1605	U1545	A1485	G1425	A1365	C1305	C1245		C1123	C1063
G1786	G1786	U1666	G1606	U1546	G1486	C1426	A1366	U1306	A1246		C1124	G1064
A1787	A1787	U1667	G1607	G1547	G1487	G1427	U1367	C1307	A1247		G1125	U1065
C1788	C1788	U1668	G1608	C1548	U1488	U1428	U1368	G1308	C1248		G1126	A1066
G1789	G1789	G1669	C1609	C1549	C1489	C1429	G1369	A1309	A1249		G1127	G1067
U1730	U1730	A1670	A1609	U1550	U1490	C1430	C1370	U1310	C1250		C1128	U1068
G1731	G1731	U1671	U1610	A1551	G1491	C1431	G1371	U1311	G1251		A1190	U1069
C1732	C1732	U1672	U1611	C1552	U1492	C1432	A1372	C1312	G1252		A1191	C1070
G1793	G1793	A1673	G1612	C1553	G1493	C1433	U1373	U1313	G1253		G1192	C1071
A1794	A1794	A1674	C1613	C1554	A1494	A1434	A1374	G1314	A1254		C1131	C1072
C1735	C1735	G1675	A1614	U1555	U1495	A1435	A1375	U1315	A1255		U1132	A1073
U1736	U1736	C1676	U1615	A1556	G1496	C1436	C1376	G1316	A1256		C1133	C1074
C1737	C1737	U1677	U1616	C1557	C1497	U1437	G1377	G1317	C1257		G1134	A1075
G1738	G1738	C1678	U1617	G1558	C1498	U1438	A1378	G1318	C1258		G1135	C1076
C1739	C1739	U1679	C1618	C1559	C1499	C1439	A1379	U1319	U1259		G1136	U1077
A1800	A1800	U1680	A1618				G1380	G1320	C1260		G1137	U1077
C1801	C1801	U1681	C1621	C1560	U1500	U1440	G1381	G1321	A1261		G1138	A1078
U1802	U1802	C1682	G1622	G1561	U1501	U1441	G1382	G1322	C1262		A1139	A1079
A1803	A1803	C1683	C1623	G1562	A1502	A1442	A1382	U1323	C1263		A1140	A1080
G1744	G1744	C1684	C1624	C1563	G1493	G1443	G1383	G1324	G1264		C1141	C1081
C1745	C1745	U1685	A1625	A1564	A1504	A1444	A1384	G1325	G1265		C1142	G1082
U1806	U1806	U1686	U1626	G1565	U1505	G1445	C1385	U1326	G1266		C1143	A1083
C1746	C1746	G1687	G1627	G1566	G1506	G1446	U1386	G1326	G1267		A1144	U1084
A1807	A1807	U1688	A1628	C1567	U1507	G1447	C1387	C1327	C1268		A1145	G1085
G1808	G1808	U1689	A1629	G1568	C1508	A1448	U1388	A1328	G1269		A1146	C1086
A1809	A1809	U1690	C1630	U1569	G1509	C1449	G1389	U1329	C1270		G1147	G1087
C1750	C1750	G1691	G1631	G1570	A1450	A1450	G1390	U1330	G1271		A1148	U1088
G1811	G1811											
A1812	A1812											



● Molecule 35: Eukaryotic translation initiation factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	292.12Å 292.12Å 477.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.11 – 7.81 64.21 – 7.81	Depositor EDS
% Data completeness (in resolution range)	94.8 (58.11-7.81) 94.9 (64.21-7.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 7.40Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.347 , 0.347 0.334 , 0.337	Depositor DCC
R_{free} test set	1305 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	667.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.120 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	77211	wwPDB-VP
Average B, all atoms (Å ²)	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	2/1679 (0.1%)	1.06	16/2283 (0.7%)
2	B	0.79	6/1769 (0.3%)	1.08	20/2367 (0.8%)
3	C	0.97	7/1778 (0.4%)	1.19	19/2399 (0.8%)
4	D	1.03	6/1792 (0.3%)	1.30	22/2412 (0.9%)
5	E	0.76	4/2125 (0.2%)	0.98	23/2856 (0.8%)
6	F	1.00	5/1531 (0.3%)	1.21	17/2059 (0.8%)
7	G	0.97	15/1946 (0.8%)	1.23	25/2590 (1.0%)
8	H	1.09	9/1553 (0.6%)	2.19	29/2079 (1.4%)
9	I	1.11	7/1708 (0.4%)	1.51	33/2278 (1.4%)
10	J	1.27	19/1522 (1.2%)	1.51	42/2031 (2.1%)
11	K	1.21	7/851 (0.8%)	1.78	32/1147 (2.8%)
12	L	1.10	6/1319 (0.5%)	1.40	17/1761 (1.0%)
13	M	1.00	3/960 (0.3%)	1.23	7/1287 (0.5%)
14	N	0.83	3/1232 (0.2%)	1.00	12/1656 (0.7%)
15	O	0.61	0/1029	1.05	12/1380 (0.9%)
16	P	0.75	1/1079 (0.1%)	1.43	32/1437 (2.2%)
17	Q	0.70	3/1142 (0.3%)	1.12	15/1528 (1.0%)
18	R	1.23	10/1031 (1.0%)	1.64	30/1383 (2.2%)
19	S	1.21	11/1157 (1.0%)	1.61	36/1548 (2.3%)
20	T	0.95	3/1132 (0.3%)	1.25	13/1517 (0.9%)
21	U	0.96	1/832 (0.1%)	1.59	28/1117 (2.5%)
22	V	0.75	1/626 (0.2%)	1.39	15/839 (1.8%)
23	W	0.85	4/1051 (0.4%)	0.86	9/1406 (0.6%)
24	X	1.00	8/1124 (0.7%)	1.24	21/1500 (1.4%)
25	Y	0.93	3/1038 (0.3%)	1.42	20/1380 (1.4%)
26	Z	1.04	5/604 (0.8%)	1.35	17/810 (2.1%)
27	a	0.89	4/860 (0.5%)	1.60	21/1156 (1.8%)
28	b	1.02	2/673 (0.3%)	1.36	12/902 (1.3%)
29	c	0.80	1/508 (0.2%)	1.18	8/680 (1.2%)
30	d	0.89	2/455 (0.4%)	0.79	3/603 (0.5%)
31	e	1.46	5/478 (1.0%)	1.43	11/628 (1.8%)
32	f	1.10	4/593 (0.7%)	1.49	15/786 (1.9%)
33	g	0.91	1/2493 (0.0%)	1.29	26/3394 (0.8%)
34	i	2.42	1848/41880 (4.4%)	2.22	2570/65161 (3.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
35	l	1.00	3/701 (0.4%)	1.11	4/936 (0.4%)
All	All	1.85	2019/82251 (2.5%)	1.87	3232/119296 (2.7%)

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	11
2	B	0	4
3	C	1	5
4	D	0	5
5	E	1	2
6	F	0	3
7	G	0	1
8	H	0	10
9	I	0	8
10	J	1	11
11	K	0	11
12	L	0	7
13	M	0	1
14	N	0	4
15	O	0	1
16	P	0	10
17	Q	0	4
18	R	1	5
19	S	1	10
20	T	1	6
21	U	0	8
22	V	0	9
23	W	0	2
24	X	0	4
25	Y	1	6
26	Z	0	6
27	a	0	2
28	b	0	3
31	e	0	5
32	f	0	6
33	g	0	13
34	i	6	0
All	All	13	183

The worst 5 of 2019 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1683	C	O3'-P	41.12	2.10	1.61
34	i	1322	U	C2'-C1'	-25.29	1.25	1.53
34	i	66	G	C2'-C1'	-24.37	1.26	1.53
34	i	858	A	C2'-C1'	-23.82	1.27	1.53
34	i	652	G	C2'-C1'	-23.61	1.27	1.53

The worst 5 of 3232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	109	ARG	NE-CZ-NH2	-53.46	93.57	120.30
34	i	1683	C	P-O3'-C3'	-46.88	63.44	119.70
8	H	109	ARG	NE-CZ-NH1	42.70	141.65	120.30
34	i	1774	G	P-O3'-C3'	38.10	165.42	119.70
34	i	1114	C	O4'-C1'-N1	35.28	136.42	108.20

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	157	ASN	CA
5	E	171	ASP	CA
10	J	138	ARG	CA
18	R	3	ARG	CA
19	S	92	ASP	CA

5 of 183 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ALA	Mainchain
1	A	23	THR	Mainchain
1	A	4	ALA	Peptide
1	A	63	ARG	Sidechain
1	A	97	THR	Mainchain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
1	A	206/295 (70%)	156 (76%)	23 (11%)	27 (13%)	0	5
2	B	213/264 (81%)	173 (81%)	25 (12%)	15 (7%)	1	14
3	C	224/278 (81%)	200 (89%)	13 (6%)	11 (5%)	2	20
4	D	225/243 (93%)	180 (80%)	23 (10%)	22 (10%)	0	10
5	E	261/263 (99%)	209 (80%)	28 (11%)	24 (9%)	1	11
6	F	189/204 (93%)	162 (86%)	15 (8%)	12 (6%)	1	17
7	G	235/249 (94%)	201 (86%)	19 (8%)	15 (6%)	1	16
8	H	188/194 (97%)	146 (78%)	11 (6%)	31 (16%)	0	3
9	I	204/208 (98%)	169 (83%)	12 (6%)	23 (11%)	0	7
10	J	180/194 (93%)	138 (77%)	18 (10%)	24 (13%)	0	5
11	K	96/165 (58%)	67 (70%)	11 (12%)	18 (19%)	0	2
12	L	156/158 (99%)	132 (85%)	10 (6%)	14 (9%)	1	11
13	M	122/132 (92%)	85 (70%)	16 (13%)	21 (17%)	0	3
14	N	148/151 (98%)	124 (84%)	18 (12%)	6 (4%)	3	23
15	O	134/151 (89%)	101 (75%)	14 (10%)	19 (14%)	0	4
16	P	125/145 (86%)	92 (74%)	16 (13%)	17 (14%)	0	4
17	Q	139/146 (95%)	109 (78%)	20 (14%)	10 (7%)	1	14
18	R	124/135 (92%)	96 (77%)	13 (10%)	15 (12%)	0	6
19	S	135/152 (89%)	106 (78%)	20 (15%)	9 (7%)	1	15
20	T	139/145 (96%)	119 (86%)	10 (7%)	10 (7%)	1	14
21	U	102/119 (86%)	76 (74%)	10 (10%)	16 (16%)	0	3
22	V	80/83 (96%)	55 (69%)	11 (14%)	14 (18%)	0	3
23	W	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	9	44
24	X	140/143 (98%)	121 (86%)	11 (8%)	8 (6%)	1	18
25	Y	124/133 (93%)	91 (73%)	15 (12%)	18 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	73/125 (58%)	52 (71%)	12 (16%)	9 (12%)	0	5
27	a	105/115 (91%)	72 (69%)	14 (13%)	19 (18%)	0	3
28	b	82/84 (98%)	57 (70%)	14 (17%)	11 (13%)	0	5
29	c	62/69 (90%)	44 (71%)	13 (21%)	5 (8%)	1	12
30	d	51/56 (91%)	46 (90%)	3 (6%)	2 (4%)	3	23
31	e	57/133 (43%)	37 (65%)	7 (12%)	13 (23%)	0	2
32	f	69/156 (44%)	38 (55%)	13 (19%)	18 (26%)	0	1
33	g	311/317 (98%)	271 (87%)	23 (7%)	17 (6%)	2	19
35	l	83/113 (74%)	49 (59%)	24 (29%)	10 (12%)	0	6
All	All	4909/5648 (87%)	3884 (79%)	520 (11%)	505 (10%)	0	8

5 of 505 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	31	ASP
1	A	45	GLY
1	A	103	PHE
1	A	164	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
1	A	174/244 (71%)	140 (80%)	34 (20%)	1	8
2	B	196/231 (85%)	155 (79%)	41 (21%)	1	6
3	C	187/215 (87%)	147 (79%)	40 (21%)	1	6
4	D	190/202 (94%)	144 (76%)	46 (24%)	0	4
5	E	225/225 (100%)	173 (77%)	52 (23%)	1	4
6	F	161/170 (95%)	117 (73%)	44 (27%)	0	3
7	G	207/218 (95%)	157 (76%)	50 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	170/174 (98%)	124 (73%)	46 (27%)	0	3
9	I	177/179 (99%)	142 (80%)	35 (20%)	1	8
10	J	157/168 (94%)	128 (82%)	29 (18%)	1	9
11	K	89/136 (65%)	61 (68%)	28 (32%)	0	2
12	L	142/142 (100%)	105 (74%)	37 (26%)	0	3
13	M	101/108 (94%)	78 (77%)	23 (23%)	1	5
14	N	130/131 (99%)	103 (79%)	27 (21%)	1	6
15	O	106/119 (89%)	87 (82%)	19 (18%)	2	10
16	P	116/130 (89%)	84 (72%)	32 (28%)	0	3
17	Q	117/121 (97%)	89 (76%)	28 (24%)	0	4
18	R	114/121 (94%)	90 (79%)	24 (21%)	1	6
19	S	119/132 (90%)	95 (80%)	24 (20%)	1	7
20	T	113/116 (97%)	87 (77%)	26 (23%)	1	4
21	U	94/107 (88%)	74 (79%)	20 (21%)	1	6
22	V	67/68 (98%)	50 (75%)	17 (25%)	0	3
23	W	112/113 (99%)	98 (88%)	14 (12%)	4	19
24	X	114/115 (99%)	91 (80%)	23 (20%)	1	7
25	Y	108/115 (94%)	85 (79%)	23 (21%)	1	6
26	Z	66/103 (64%)	53 (80%)	13 (20%)	1	8
27	a	91/99 (92%)	76 (84%)	15 (16%)	2	12
28	b	76/76 (100%)	63 (83%)	13 (17%)	2	11
29	c	57/62 (92%)	46 (81%)	11 (19%)	1	8
30	d	47/49 (96%)	35 (74%)	12 (26%)	0	3
31	e	49/106 (46%)	26 (53%)	23 (47%)	0	0
32	f	64/140 (46%)	43 (67%)	21 (33%)	0	2
33	g	272/275 (99%)	224 (82%)	48 (18%)	2	11
35	l	74/96 (77%)	57 (77%)	17 (23%)	1	4
All	All	4282/4806 (89%)	3327 (78%)	955 (22%)	1	5

5 of 955 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	55	ARG

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Mol	Chain	Res	Type
15	O	28	PHE
32	f	116	ARG
11	K	98	ARG
13	M	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	156	GLN
16	P	53	GLN
33	g	119	GLN
13	M	28	HIS
14	N	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	i	1721/1863 (92%)	498 (28%)	0

5 of 498 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	i	2	A
34	i	3	C
34	i	4	C
34	i	8	U
34	i	16	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	i	11
10	J	3
4	D	2
19	S	2
7	G	1
31	e	1
9	I	1
3	C	1
21	U	1
18	R	1

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	326:A	O3'	327:C	P	8.42
1	i	309:A	O3'	310:G	P	7.21
1	i	304:A	O3'	305:U	P	5.77
1	i	209:C	O3'	210:G	P	5.60
1	i	1826:A	O3'	1827:C	P	5.04

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/295 (70%)	0.01	19 (9%) 9 11	173, 263, 322, 332	0
2	B	215/264 (81%)	1.79	78 (36%) 0 1	128, 196, 242, 252	0
3	C	226/278 (81%)	0.12	6 (2%) 54 48	82, 160, 268, 295	0
4	D	227/243 (93%)	1.58	78 (34%) 0 2	167, 217, 294, 337	0
5	E	263/263 (100%)	2.15	93 (35%) 0 2	117, 216, 286, 299	0
6	F	191/204 (93%)	0.91	31 (16%) 1 4	191, 263, 305, 317	0
7	G	237/249 (95%)	1.13	63 (26%) 0 2	164, 242, 325, 343	0
8	H	190/194 (97%)	0.75	34 (17%) 1 4	187, 326, 368, 385	0
9	I	206/208 (99%)	1.83	73 (35%) 0 2	89, 239, 276, 287	0
10	J	182/194 (93%)	1.34	58 (31%) 0 2	89, 166, 231, 276	0
11	K	98/165 (59%)	4.84	73 (74%) 0 0	222, 291, 316, 323	0
12	L	158/158 (100%)	0.71	28 (17%) 1 4	77, 176, 261, 270	0
13	M	124/132 (93%)	1.14	25 (20%) 1 3	298, 378, 406, 431	0
14	N	150/151 (99%)	1.33	39 (26%) 0 2	87, 150, 275, 297	0
15	O	136/151 (90%)	1.25	41 (30%) 0 2	92, 194, 256, 272	0
16	P	127/145 (87%)	1.69	49 (38%) 0 1	234, 305, 340, 361	0
17	Q	141/146 (96%)	2.31	55 (39%) 0 1	166, 287, 321, 331	0
18	R	126/135 (93%)	0.64	16 (12%) 3 7	174, 225, 322, 329	0
19	S	137/152 (90%)	3.00	77 (56%) 0 1	217, 311, 344, 357	0
20	T	141/145 (97%)	3.25	75 (53%) 0 1	238, 311, 341, 349	0
21	U	104/119 (87%)	2.89	50 (48%) 0 1	167, 266, 306, 317	0
22	V	82/83 (98%)	-0.22	2 (2%) 59 52	164, 218, 318, 328	0
23	W	129/130 (99%)	2.24	66 (51%) 0 1	107, 159, 204, 218	0
24	X	142/143 (99%)	3.83	86 (60%) 0 0	50, 90, 134, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	126/133 (94%)	0.67	16 (12%) 3 7	156, 205, 243, 261	0
26	Z	75/125 (60%)	2.90	50 (66%) 0 0	292, 320, 350, 360	0
27	a	107/115 (93%)	1.20	28 (26%) 0 2	87, 129, 234, 249	0
28	b	84/84 (100%)	1.75	35 (41%) 0 1	164, 223, 303, 334	0
29	c	64/69 (92%)	-0.06	2 (3%) 49 42	175, 224, 274, 287	0
30	d	53/56 (94%)	1.00	11 (20%) 1 3	183, 212, 290, 295	0
31	e	59/133 (44%)	0.59	10 (16%) 1 4	103, 158, 182, 189	0
32	f	71/156 (45%)	1.07	21 (29%) 0 2	213, 332, 401, 415	0
33	g	313/317 (98%)	0.57	43 (13%) 3 6	235, 304, 346, 364	0
34	i	1797/1863 (96%)	1.41	446 (24%) 0 2	49, 184, 371, 475	0
35	l	85/113 (75%)	0.08	3 (3%) 44 39	223, 235, 250, 253	0
All	All	6774/7511 (90%)	1.43	1880 (27%) 0 2	49, 228, 347, 475	0

The worst 5 of 1880 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	i	252	C	72.0
34	i	251	C	49.1
34	i	250	G	45.1
34	i	249	C	31.8
24	X	83	ALA	23.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.