



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:43 AM UTC

PDB ID : 4KZX / pdb_00004kzx
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

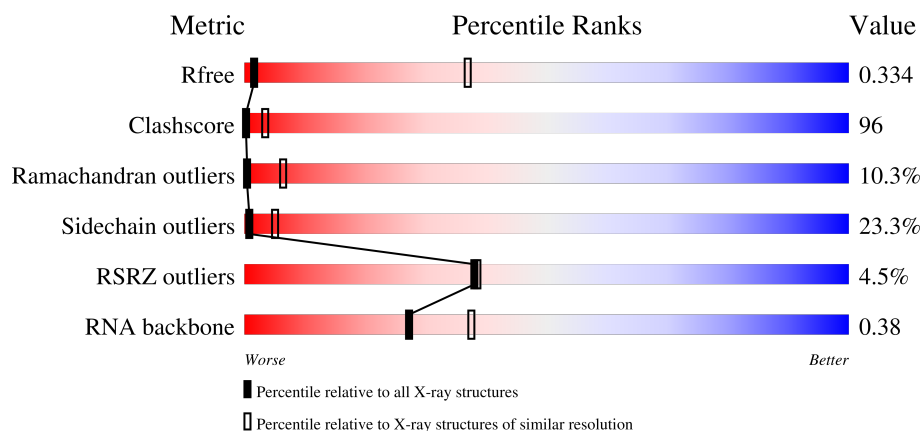
1 Overall quality at a glance

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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)
RNA backbone	3983	1057 (11.50-3.10)

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 of 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	
2	B	264	
3	C	278	
4	D	243	

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Mol	Chain	Length	Quality of chain
5	E	263	
6	F	204	
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	

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Mol	Chain	Length	Quality of chain
30	d	56	
31	e	133	
32	f	156	
33	g	317	
34	i	1863	
35	l	113	

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			

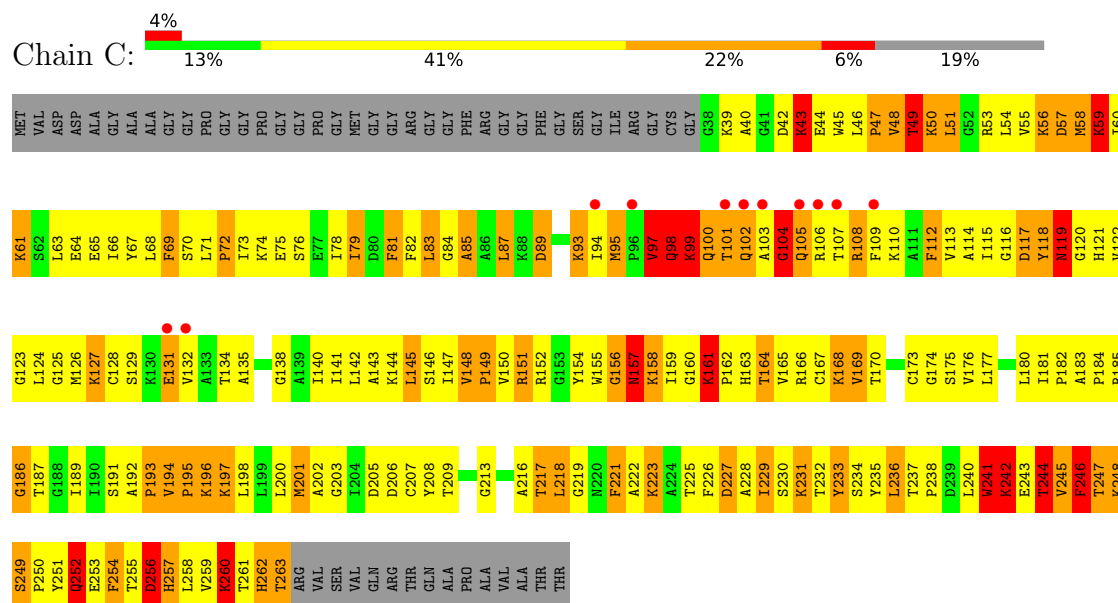
- Molecule 34 is a RNA chain called 18S ribosomal RNA.

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

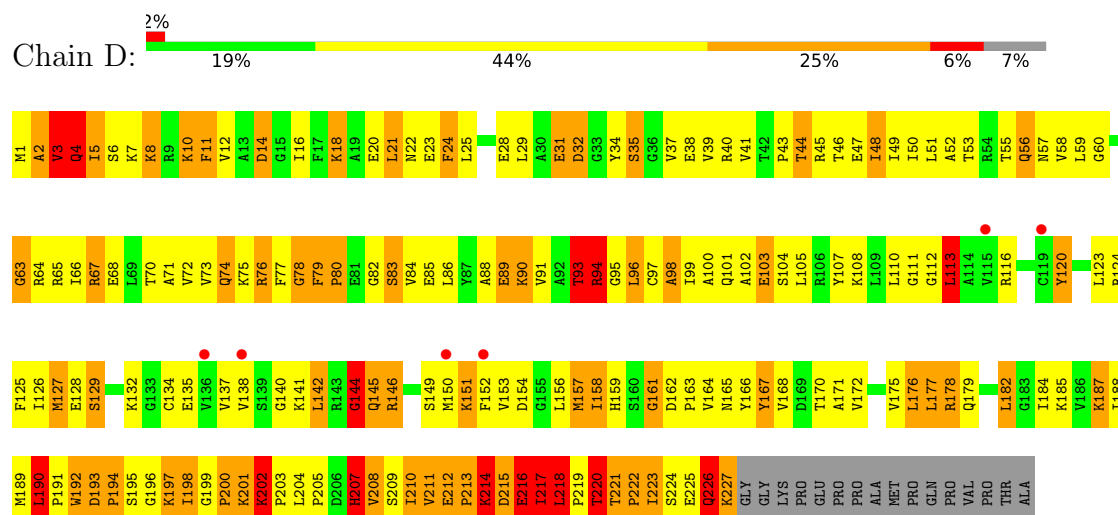
- Molecule 35 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1	85	Total	C	N	O	S	0	0	0
			691	438	125	126	2			

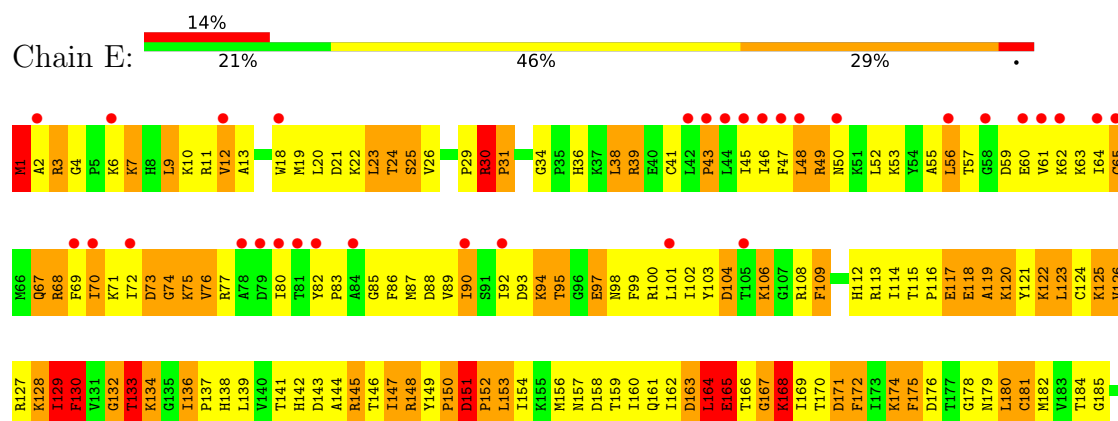
• Molecule 3: 40S ribosomal protein S2

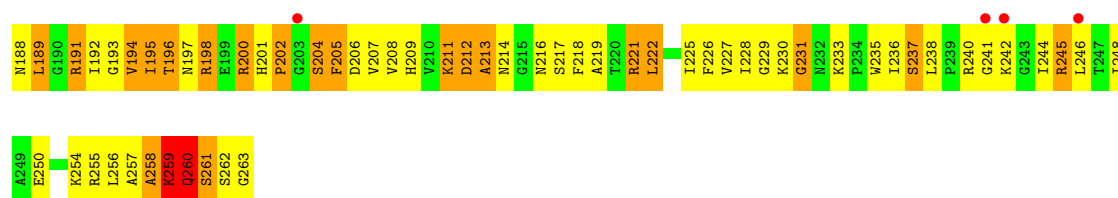


• Molecule 4: 40S ribosomal protein S3

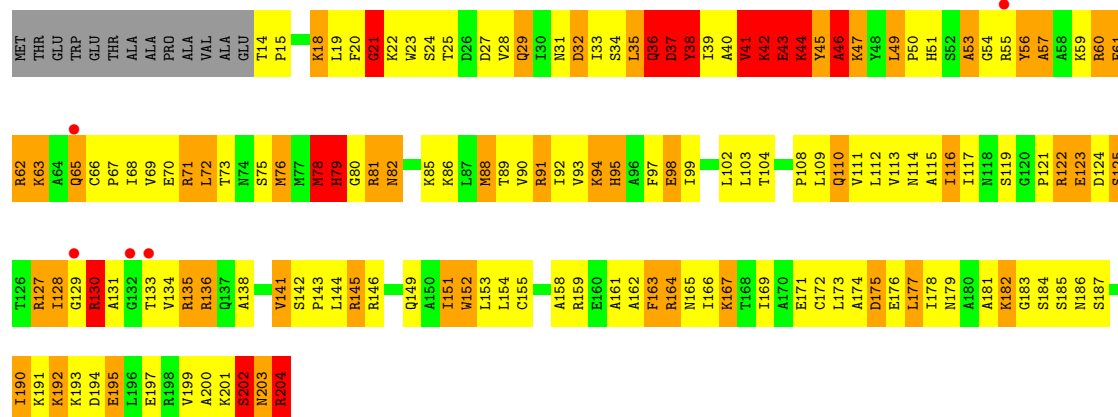
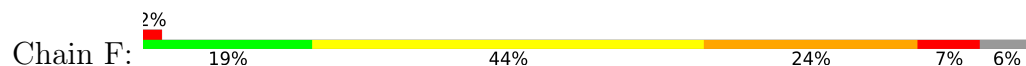


• Molecule 5: 40S ribosomal protein S4X

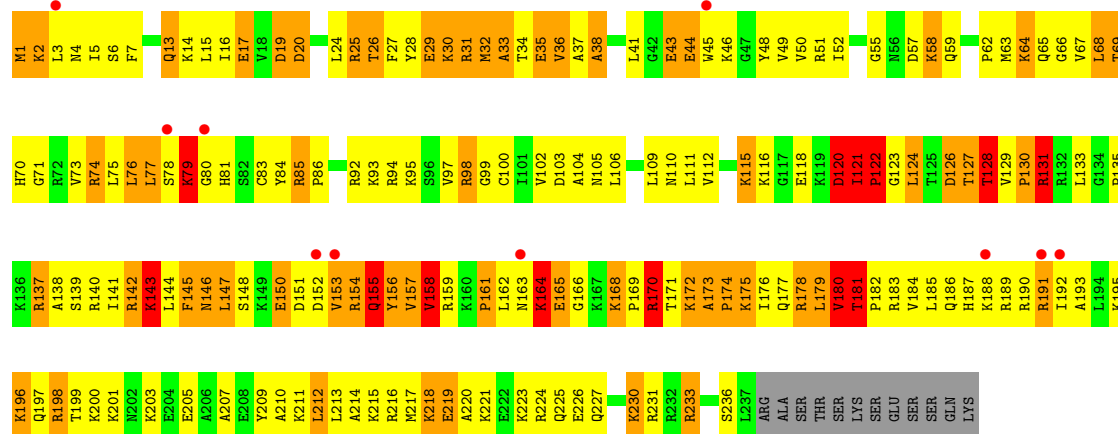
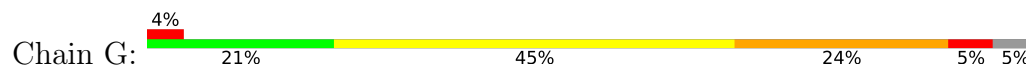




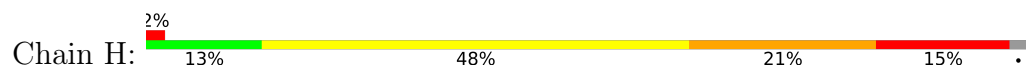
• Molecule 6: 40S ribosomal protein S5

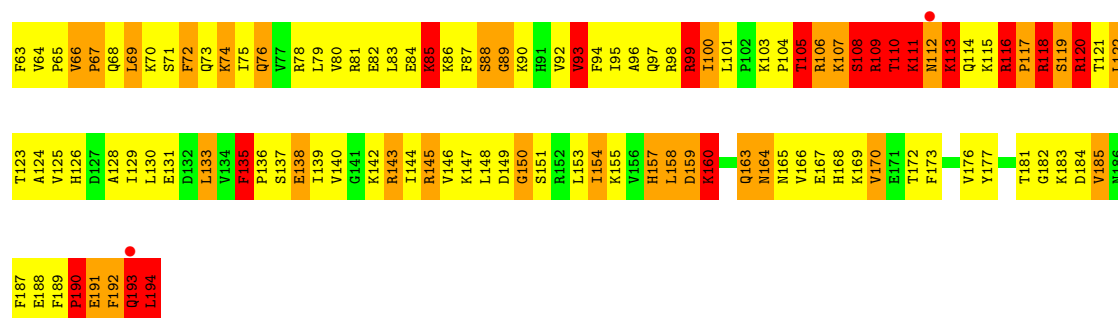


• Molecule 7: 40S ribosomal protein S6

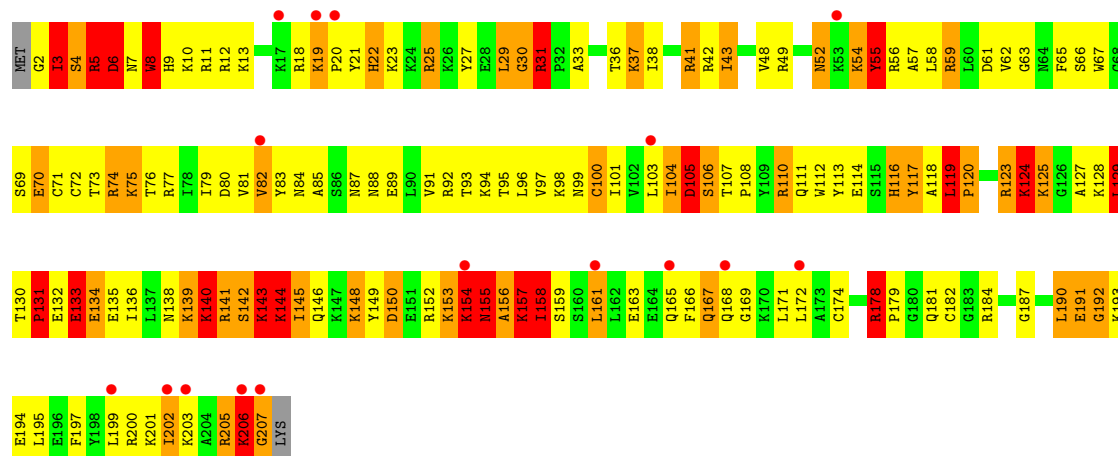
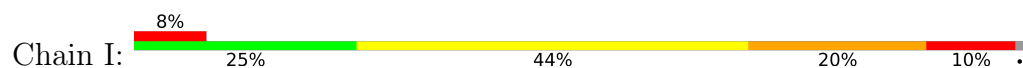


• Molecule 8: 40S ribosomal protein S7

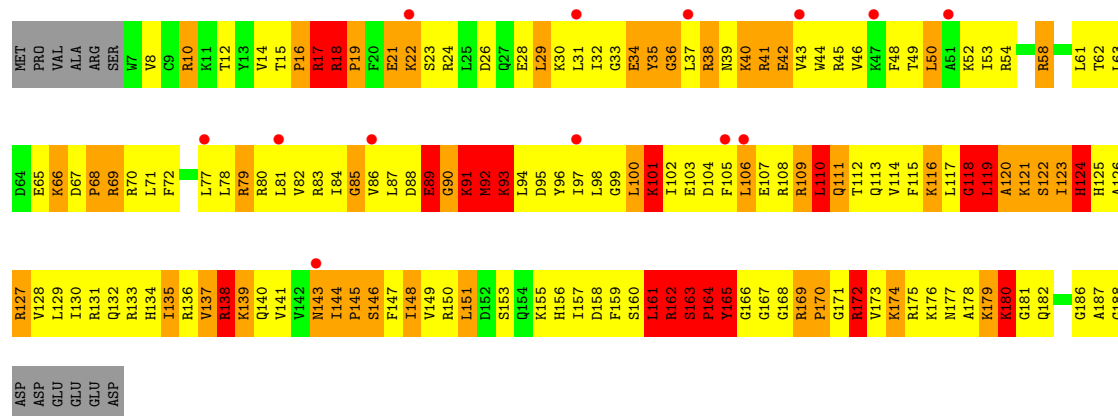
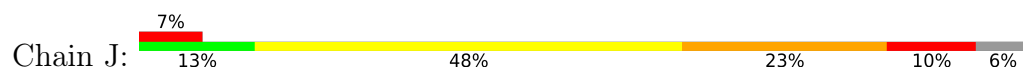




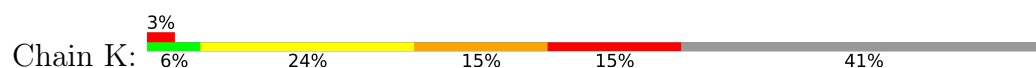
• Molecule 9: 40S ribosomal protein S8

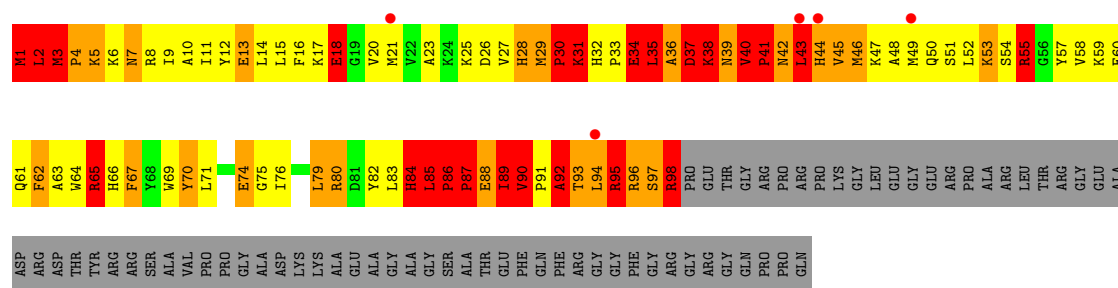


• Molecule 10: 40S Ribosomal protein S9

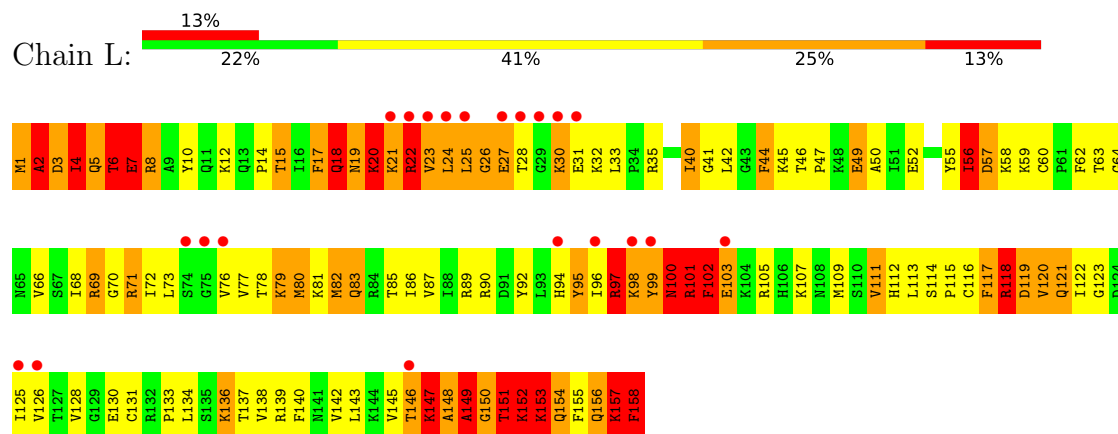


• Molecule 11: 40S ribosomal protein S10

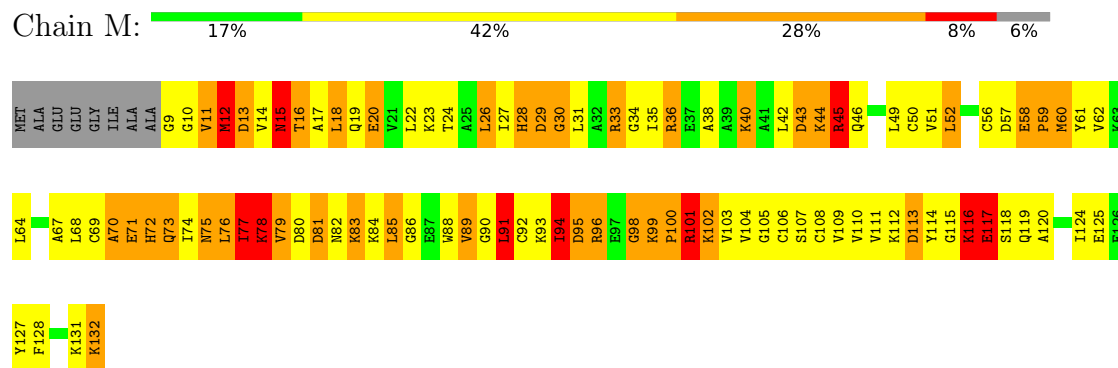




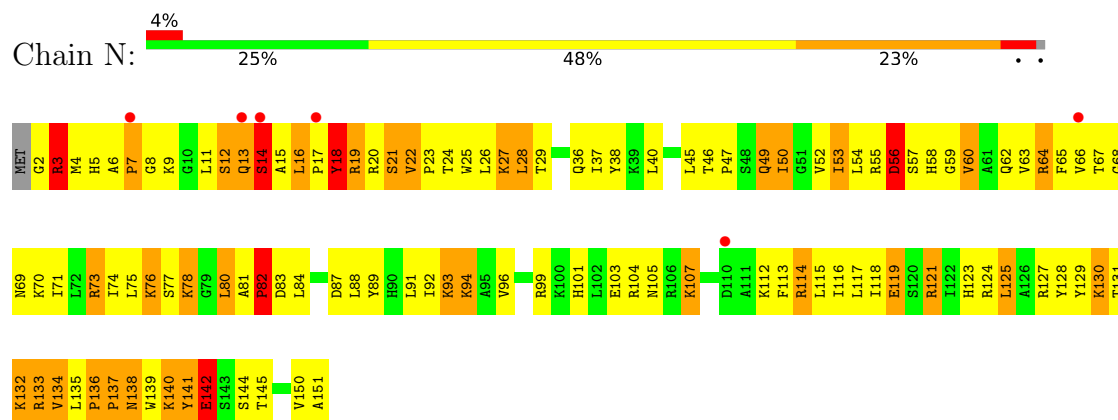
• Molecule 12: 40S ribosomal protein S11



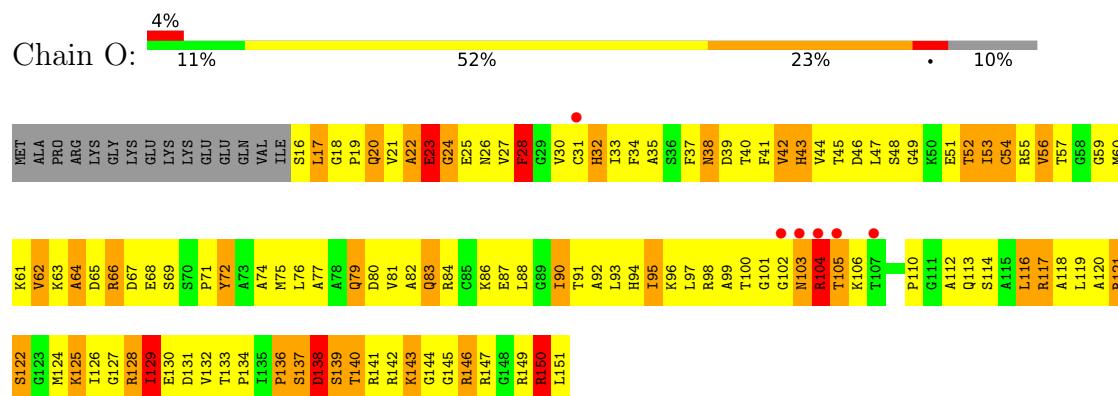
• Molecule 13: 40S ribosomal protein S12



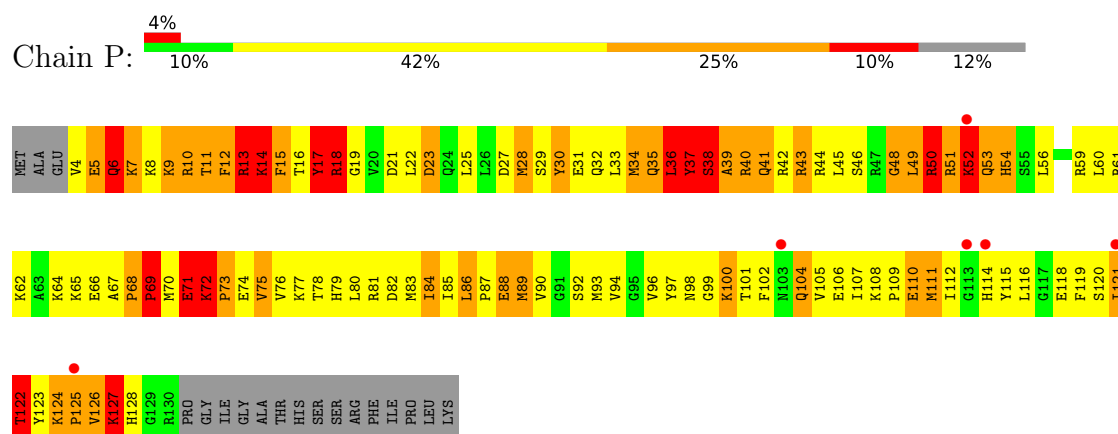
• Molecule 14: 40S ribosomal protein S13



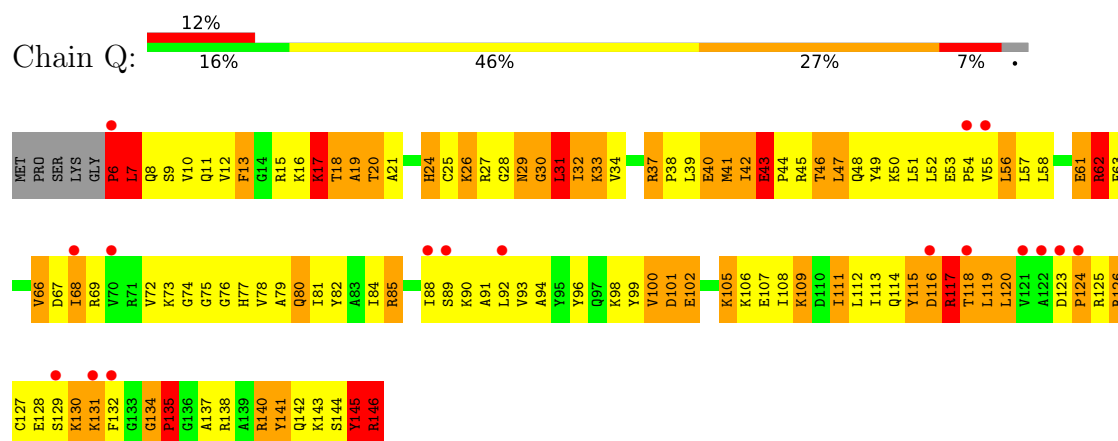
- Molecule 15: 40S ribosomal protein S14



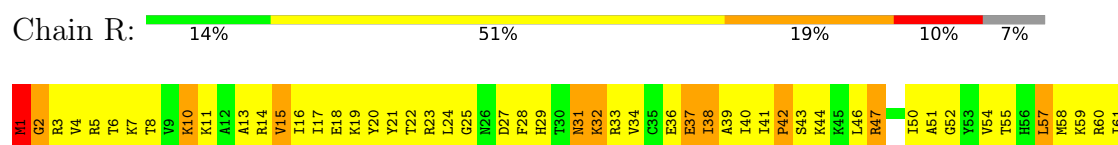
- Molecule 16: 40S ribosomal protein S15

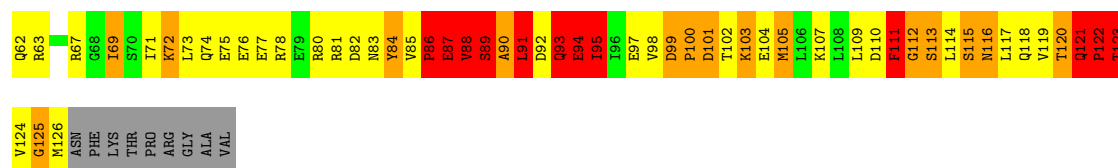


- Molecule 17: 40S ribosomal protein S16

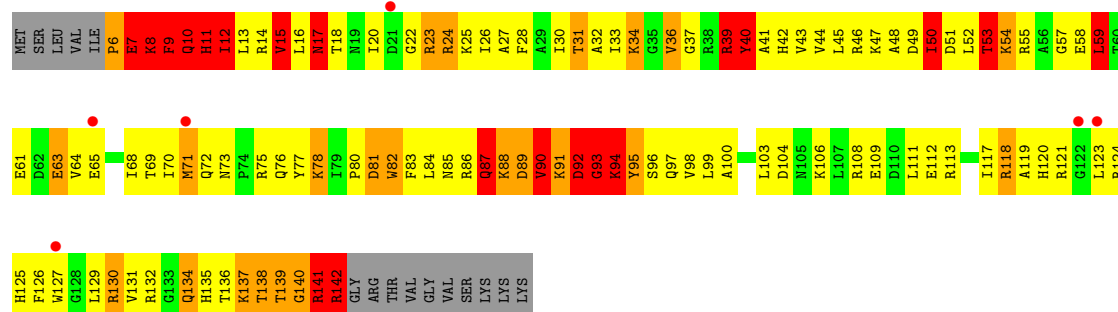
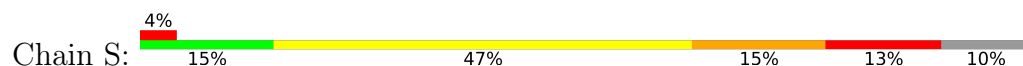


- Molecule 18: 40S ribosomal protein S17

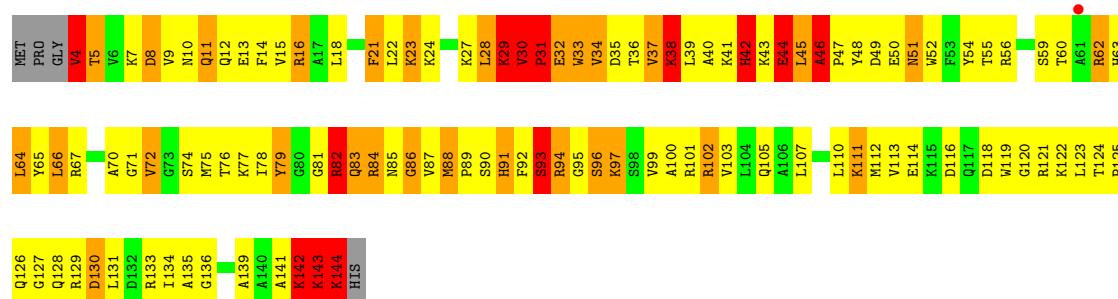
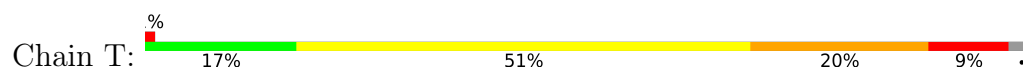




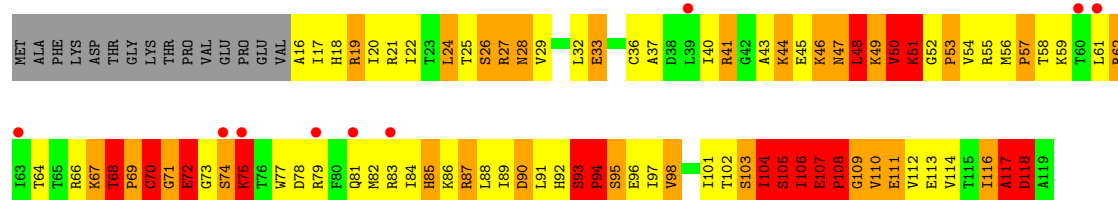
• Molecule 19: 40S ribosomal protein S18



• Molecule 20: 40S ribosomal protein S19

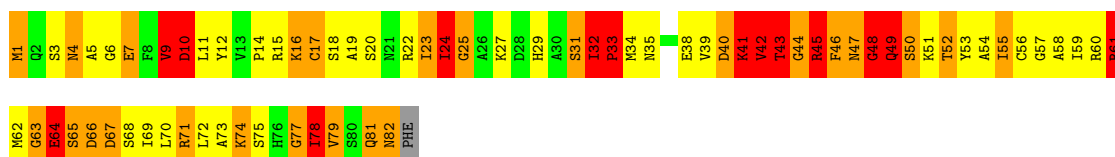


• Molecule 21: 40S ribosomal protein S20

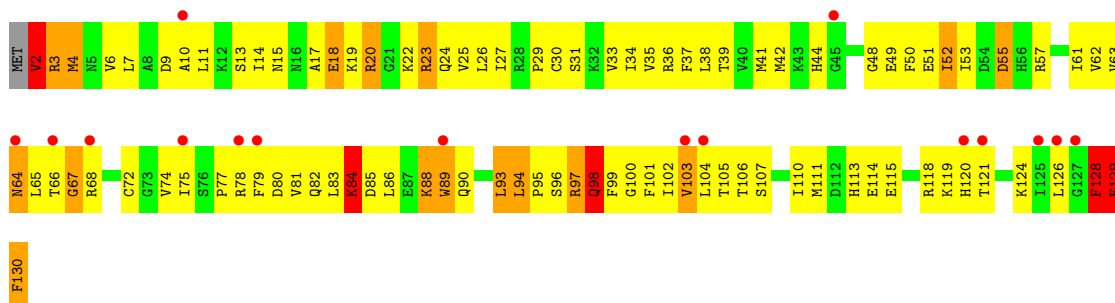


• Molecule 22: 40S ribosomal protein S21

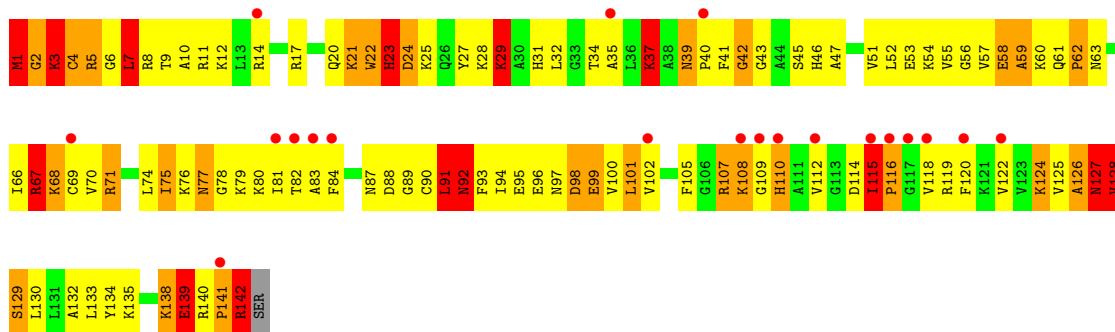
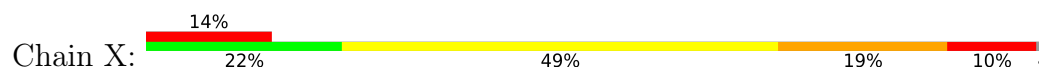




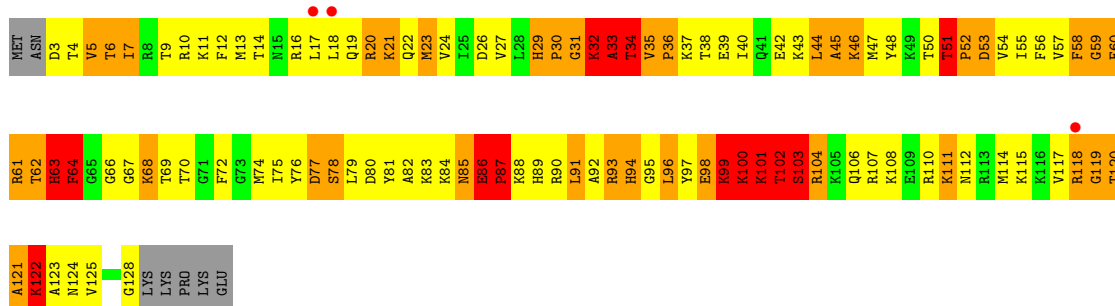
• Molecule 23: 40S ribosomal protein S15A



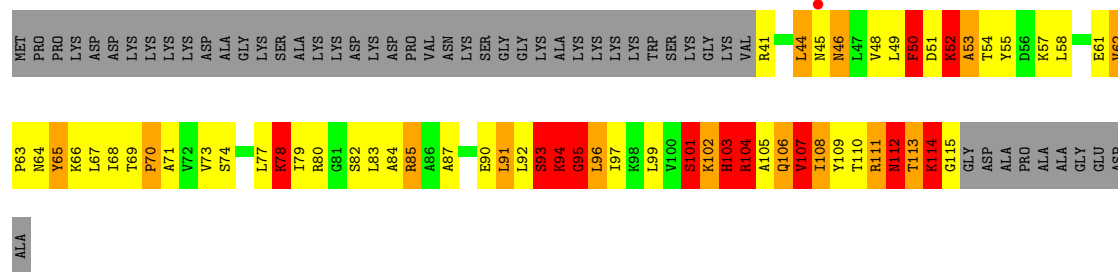
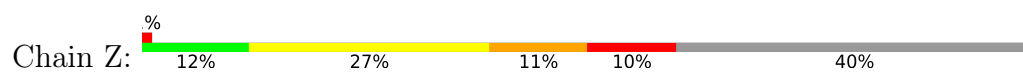
• Molecule 24: 40S ribosomal protein S23



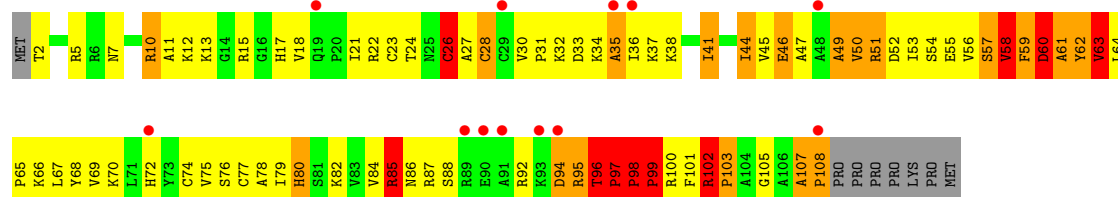
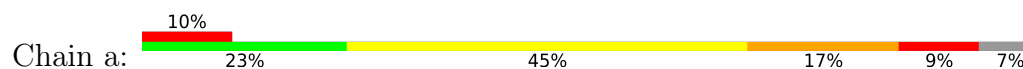
• Molecule 25: 40S ribosomal protein S24



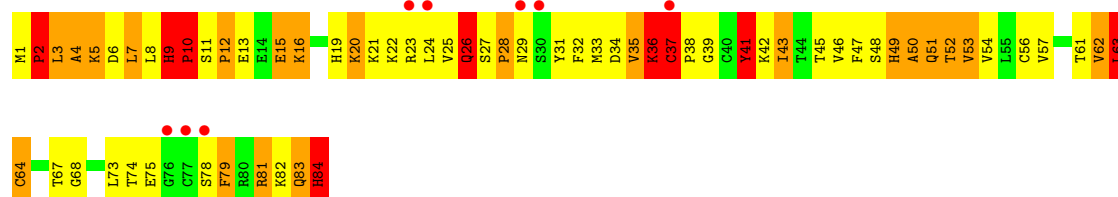
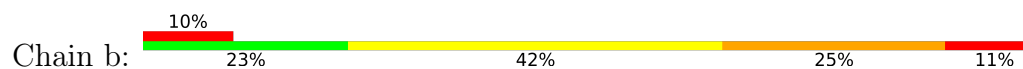
• Molecule 26: 40S ribosomal protein S25



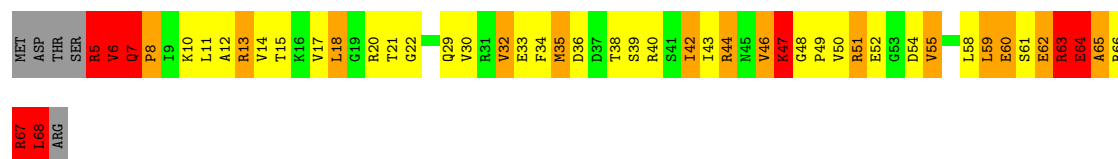
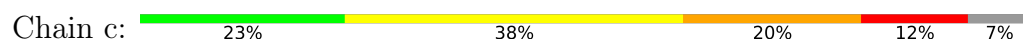
• Molecule 27: 40S ribosomal protein S26



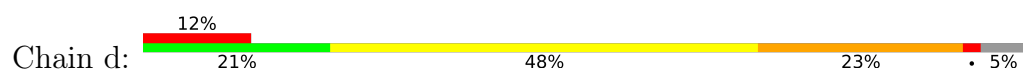
• Molecule 28: 40S ribosomal protein S27



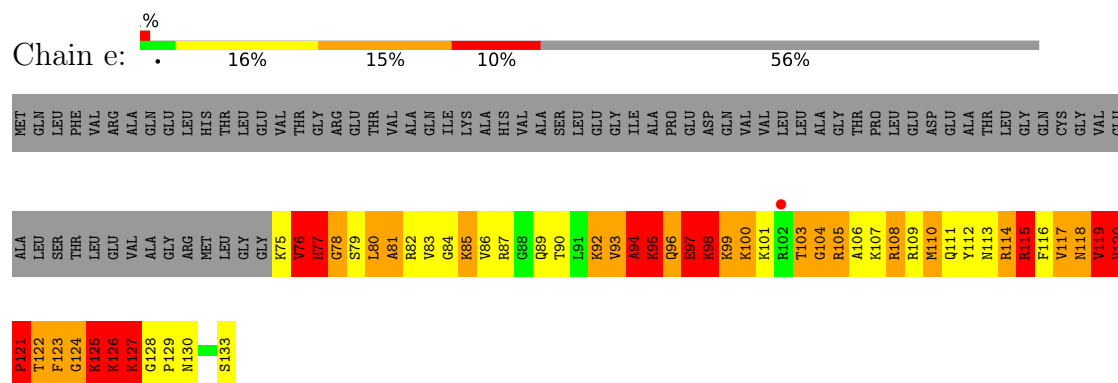
• Molecule 29: 40S ribosomal protein S28



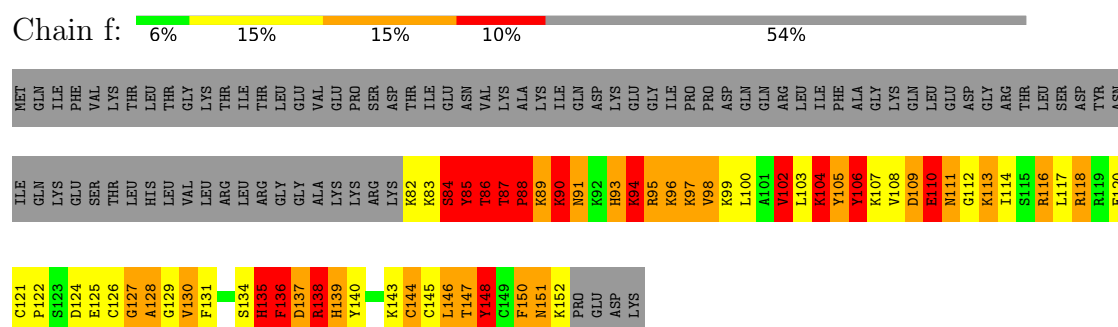
• Molecule 30: 40S ribosomal protein S29



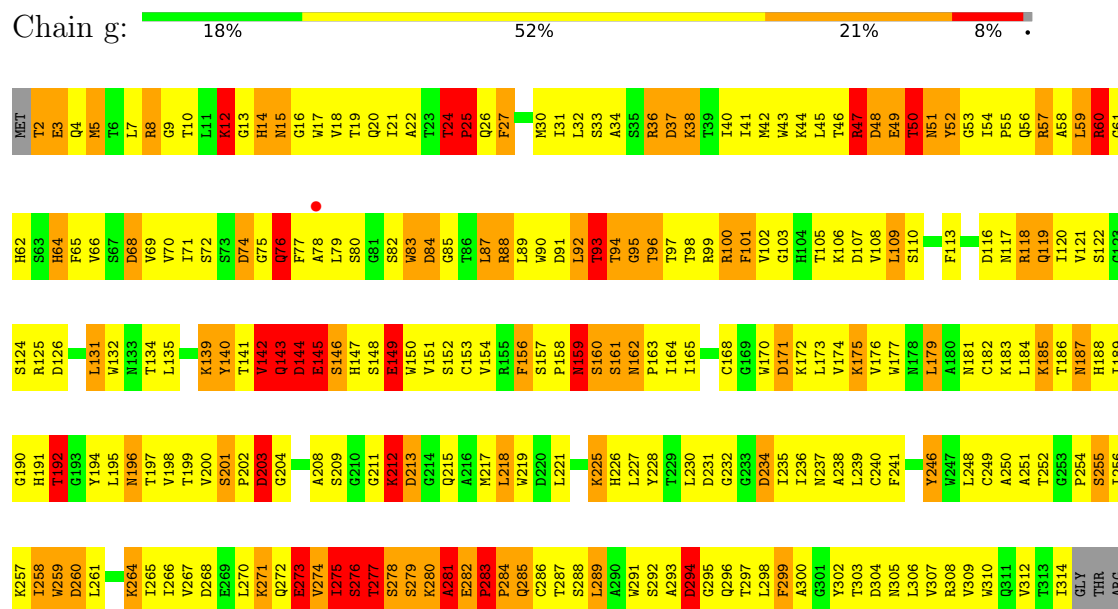
- Molecule 31: 40S ribosomal protein S30



- Molecule 32: 40S ribosomal protein S27A



- Molecule 33: 40S ribosomal protein RACK1

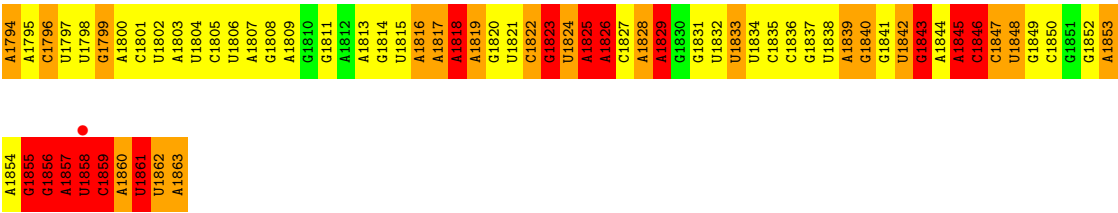


- Molecule 34: 18S ribosomal RNA

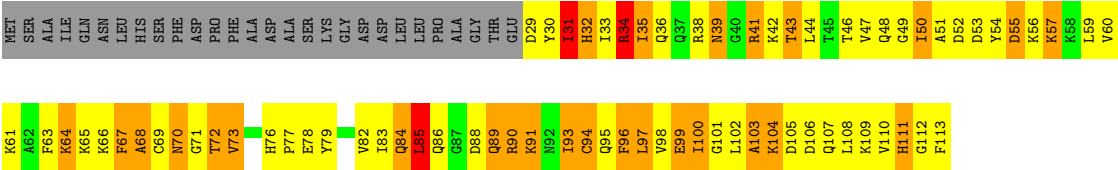




C1733	C1734	C1735	U1736	C1737	G1738	G1739	A1740	C1741	C1742	G1743	U1744	C1745	C1746	C1747	G1748	C1749	C1750	G1751	A1752	C1753	G1754	U1755	C1756	C1757	C1758	C1759	C1760	C1761	A1762	C1763	G1764	G1765	C1766	C1767	C1768	U1769	A1770	C1771	C1772	C1773	G1774	A1775	C1776	C1777	G1778	U1779	U1780	C1781	A1782	G1783	A1784	U1785	G1786	A1787	C1788	G1789	G1790	U1791	C1792	G1793		
U1670	U1671	U1672	U1673	U1674	G1675	U1676	U1677	C1678	C1679	U1680	G1681	C1682	C1683	C1684	U1685	U1686	U1687	U1688	U1689	A1690	C1691	A1692	C1693	A1694	C1695	C1696	C1697	C1698	C1699	C1700	G1701	U1702	C1703	G1704	C1705	U1706	A1707	C1708	U1709	A1710	C1711	G1712	G1713	U1714	U1715	U1716	U1717	G1718	U1719	U1720	U1721	G1722	U1723	U1724	U1725	A1726	U1727	G1728	U1729	A1730	U1731	C1732
U1610	U1611	G1612	C1613	A1614	A1615	U1616	U1617	A1618	U1619	U1620	C1621	C1622	C1623	C1624	A1625	U1626	G1627	A1628	A1629	C1630	G1631	A1632	G1633	A1634	C1635	U1636	U1637	U1638	C1639	C1640	C1641	A1642	G1643	U1644	A1645	A1646	G1647	U1648	U1649	C1650	G1651	G1652	G1653	U1654	C1655	A1656	U1657	U1658	A1659	U1660	C1661	U1662	U1663	G1664	C1665	G1666	U1667	U1668	G1669			
C1549	U1550	A1551	C1552	C1553	C1554	U1555	U1556	C1557	U1558	C1559	C1560	G1561	G1562	C1563	A1564	G1565	G1566	C1567	C1568	C1569	U1570	G1571	G1572	U1573	A1574	U1575	C1576	C1577	C1578	U1579	U1580	U1581	G1582	A1583	A1584	C1585	C1586	U1587	C1588	C1589	U1590	U1591	C1592	U1593	C1594	U1595	A1596	U1597	U1598	G1599	U1600	G1601	A1602	U1603	C1604	G1605	U1606	U1607				
C1489	U1490	G1491	U1492	G1493	A1494	U1495	U1496	C1497	U1498	C1499	U1500	U1501	A1502	G1503	A1504	U1505	G1506	U1507	C1508	U1509	G1510	C1511	G1512	U1513	U1514	G1515	C1516	U1517	C1518	U1519	C1520	G1521	C1522	G1523	A1524	U1525	A1526	C1527	A1528	C1529	U1530	G1531	A1532	C1533	U1534	G1535	C1536	U1537	A1538	U1539	A1540	G1541	C1542	G1543	U1544	G1545	U1546	C1547	U1548			
U1428	C1429	C1430	U1431	C1432	C1433	A1434	A1435	C1436	U1437	U1438	C1439	U1440	U1441	A1442	G1443	A1444	G1445	G1446	C1447	C1448	C1449	C1450	A1451	G1452	U1453	U1454	C1455	G1456	U1457	U1458	U1459	C1460	A1461	G1462	C1463	A1464	A1465	C1466	C1467	C1468	U1469	A1470	C1471	A1472	U1473	U1474	G1475	A1476	C1477	C1478	A1479	A1480	U1481	A1482	C1483	A1484	A1485	G1486	C1487	U1488		
A1365	A1366	U1367	U1368	C1369	C1370	G1371	U1372	U1373	A1374	A1375	C1376	G1377	A1378	U1379	U1380	G1381	A1382	G1383	A1384	C1385	U1386	C1387	U1388	G1389	C1390	C1391	A1392	U1393	G1394	C1395	U1396	U1397	A1398	U1399	U1400	A1401	C1402	U1403	A1404	A1405	C1406	C1407	C1408	G1409	A1410	C1411	C1412	C1413	C1414	C1415	G1416	A1417	C1418	C1419	U1420	C1421	C1422	U1423	C1424	G1425	C1426	C1427
U1304	C1305	U1306	C1307	C1308	A1309	U1310	U1311	C1312	U1313	G1314	U1315	G1316	G1317	U1318	U1319	C1320	G1321	U1322	G1323	C1324	U1325	G1326	C1327	A1328	U1329	G1330	C1331	G1332	C1333	U1334	U1335	U1336	C1337	U1338	U1339	A1340	G1341	U1342	U1343	G1344	G1345	U1346	G1347	G1348	A1349	G1350	C1351	A1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	G1361	U1362	U1363	U1364		
G1183	A1184	A1185	A1186	C1187	U1188	U1189	A1190	A1191	A1192	G1193	G1194	A1195	U1198	U1199	C1199	A1200	C1201	G1202	G1203	A1204	A1205	G1206	G1207	U1208	C1209	A1210	C1211	C1212	A1213	C1214	G1215	A1216	G1217	G1218	A1219	G1220	G1221	G1222	G1223	A1224	G1225	C1226	C1227	U1228	G1229	C1230	G1231	G1232	U1233	U1234	U1235	A1236	A1237	U1238	U1239	U1240	G1241	C1242	C1243			
U1244	C1245	A1246	A1247	C1248	U1249	C1250	G1251	G1252	G1253	U1254	A1255	A1256	C1257	C1258	U1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	C1268	C1269	G1270	C1271	C1272	C1273	A1274	C1275	G1276	G1277	A1278	C1279	A1280	G1281	G1282	U1283	U1284	U1285	G1286	A1287	C1288	U1289	G1290	A1291	U1292	U1293	G1294	U1295	U1296	A1297	G1298	C1299	U1300	C1301	A1302	U1303			
G1122	C1123	C1124	G1125	U1126	G1127	C1128	A1129	G1130	C1131	U1132	U1133	C1134	C1135	C1136	G1137	G1138	A1139	A1140	A1141	C1142	C1143	A1144	A1145	A1146	C1149	U1150	U1151	U1152	G1153	G1154	G1155	U1156	U1157	C1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	A1166	G1167	U1168	A1169	U1170	U1171	G1172	U1173	G1174	G1175	C1176	A1177	U1178	A1179	G1180	C1181	U1182				
U999	U1000	G1001	C1002	C1003	A1004	A1005	G1006	U1007	A1008	U1009	G1010	U1011	U1012	U1013	U1014	C1015	U1018	A1019	A1020	U1021	A1022	A1023	A1024	G1025	A1026	U1027	C1028	G1029	U1030	A1031	A1032	G1033	U1034	G1036	G1037	A1038	G1039	G1040	U1041	U1042	C1043	G1044	A1045	A1046	U1047	A1048	U1049	A1050	A1051	U1052	C1053	G1054	A1055	A1056	U1057	A1058	C1059					
C937	G938	U939	A940	U941	U942	G943	C944	G945	C946	C947	G948	C949	U950	A951	G952	A953	G954	G955	U956	G957	A958	A959	G960	U961	U962	G963	U964	U965	G966	G967	A968	C969	C970	G971	G972	C973	G974	C975	A976	A977	C980	G981	G982	A983	C984	C985	A986	G987	A988	C989	C990	G991	A994	G995	C996	A997	U998					



● 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 58.11 – 7.81	Depositor EDS
% Data completeness (in resolution range)	94.8 (58.11-7.81) 94.7 (58.11-7.81)	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 0.331 , 0.334	Depositor DCC
R_{free} test set	1305 reflections (4.76%)	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)	0.25 , 133.5	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	0.87	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	1.05	15/1679 (0.9%)	1.62	46/2283 (2.0%)
2	B	0.94	8/1769 (0.5%)	1.64	44/2367 (1.9%)
3	C	1.38	23/1778 (1.3%)	1.88	54/2399 (2.3%)
4	D	1.57	9/1792 (0.5%)	1.97	56/2412 (2.3%)
5	E	0.90	8/2125 (0.4%)	1.48	47/2856 (1.6%)
6	F	1.29	10/1531 (0.7%)	1.77	40/2059 (1.9%)
7	G	1.30	27/1946 (1.4%)	1.76	48/2590 (1.9%)
8	H	1.48	20/1553 (1.3%)	2.04	61/2079 (2.9%)
9	I	1.58	20/1708 (1.2%)	1.98	50/2278 (2.2%)
10	J	1.86	27/1522 (1.8%)	2.13	75/2031 (3.7%)
11	K	1.72	19/851 (2.2%)	2.31	60/1147 (5.2%)
12	L	1.45	14/1319 (1.1%)	1.99	56/1761 (3.2%)
13	M	1.38	6/960 (0.6%)	1.79	27/1287 (2.1%)
14	N	1.01	8/1232 (0.6%)	1.27	15/1656 (0.9%)
15	O	0.89	6/1029 (0.6%)	1.55	25/1380 (1.8%)
16	P	1.03	8/1079 (0.7%)	1.85	51/1437 (3.5%)
17	Q	0.84	1/1142 (0.1%)	1.67	40/1528 (2.6%)
18	R	1.61	17/1031 (1.6%)	1.99	47/1383 (3.4%)
19	S	1.76	25/1157 (2.2%)	2.17	59/1548 (3.8%)
20	T	1.31	10/1132 (0.9%)	1.70	28/1517 (1.8%)
21	U	1.22	7/832 (0.8%)	2.34	53/1117 (4.7%)
22	V	1.13	5/626 (0.8%)	1.82	29/839 (3.5%)
23	W	1.10	4/1051 (0.4%)	1.38	15/1406 (1.1%)
24	X	1.49	16/1124 (1.4%)	1.97	36/1500 (2.4%)
25	Y	1.15	6/1038 (0.6%)	1.82	37/1380 (2.7%)
26	Z	1.17	6/604 (1.0%)	1.89	29/810 (3.6%)
27	a	1.32	11/860 (1.3%)	2.24	30/1156 (2.6%)
28	b	1.26	7/673 (1.0%)	2.20	33/902 (3.7%)
29	c	1.05	4/508 (0.8%)	1.77	20/680 (2.9%)
30	d	0.98	2/455 (0.4%)	1.23	3/603 (0.5%)
31	e	2.07	11/478 (2.3%)	2.14	21/628 (3.3%)
32	f	1.21	3/593 (0.5%)	2.01	34/786 (4.3%)
33	g	1.29	12/2493 (0.5%)	1.86	80/3394 (2.4%)
34	i	1.92	1351/41880 (3.2%)	1.94	2110/65161 (3.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
35	l	1.24	7/701 (1.0%)	1.39	8/936 (0.9%)
All	All	1.65	1733/82251 (2.1%)	1.90	3467/119296 (2.9%)

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 1733 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	ILE	C-N	37.63	1.82	1.33
34	i	1683	C	O3'-P	32.89	2.10	1.61
31	e	95	LYS	C-N	30.57	1.76	1.33
10	J	85	GLY	C-N	-30.25	0.95	1.33
10	J	118	GLY	C-N	28.19	1.73	1.33

The worst 5 of 3467 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1683	C	P-O3'-C3'	-37.84	63.44	120.20
27	a	97	PRO	N-CA-C	32.73	150.64	110.70
34	i	1774	G	P-O3'-C3'	30.14	165.42	120.20
4	D	5	ILE	O-C-N	-29.06	97.69	122.97
8	H	109	ARG	NE-CZ-NH2	-28.48	93.57	119.20

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 [i](#)

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	1642	0	1642	652	0
2	B	1741	0	1809	510	3
3	C	1742	0	1830	620	6
4	D	1764	0	1858	621	9
5	E	2083	0	2189	543	0
6	F	1509	0	1559	552	0
7	G	1923	0	2086	566	33
8	H	1530	0	1624	509	0
9	I	1679	0	1762	472	31
10	J	1498	0	1596	632	0
11	K	827	0	853	365	34
12	L	1296	0	1370	420	0
13	M	950	0	969	282	0
14	N	1208	0	1294	324	0
15	O	1016	0	1039	388	0
16	P	1060	0	1120	507	0
17	Q	1124	0	1193	500	0
18	R	1019	0	1070	380	0
19	S	1139	0	1188	462	23
20	T	1112	0	1149	428	0
21	U	822	0	887	234	0
22	V	619	0	620	282	0
23	W	1034	0	1079	311	0
24	X	1106	0	1177	334	0
25	Y	1021	0	1083	512	0
26	Z	598	0	652	215	0
27	a	844	0	895	186	0
28	b	659	0	681	265	0
29	c	506	0	536	185	0
30	d	445	0	441	141	0
31	e	473	0	521	212	32
32	f	581	0	598	193	0
33	g	2436	0	2388	709	0
34	i	37514	0	18810	1229	116
35	l	691	0	704	164	19
All	All	77211	0	60272	13123	168

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 96.

The worst 5 of 13123 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)
33:g:5:MET:SD	33:g:312:VAL:HG22	1.20	1.78
28:b:64:CYS:SG	28:b:73:LEU:HD23	1.11	1.68
9:I:141:ARG:CB	9:I:144:LYS:HB2	1.24	1.68
3:C:197:LYS:HA	3:C:200:LEU:CD2	1.22	1.66
17:Q:135:PRO:HD3	17:Q:141:TYR:CE1	1.16	1.66

The worst 5 of 168 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:125:LYS:NZ	35:l:56:LYS:N[4_555]	0.47	1.73
31:e:123:PHE:CE1	34:i:1758:G:C3'[3_564]	0.56	1.64
7:G:155:GLN:NE2	11:K:98:ARG:N[2_665]	0.61	1.59
19:S:108:ARG:NE	34:i:724:C:OP1[5_664]	0.68	1.52
34:i:136:C:C5'	34:i:533:C:N3[2_665]	0.71	1.49

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	4
2	B	213/264 (81%)	173 (81%)	25 (12%)	15 (7%)	1	11
3	C	224/278 (81%)	200 (89%)	13 (6%)	11 (5%)	1	16
4	D	225/243 (93%)	180 (80%)	23 (10%)	22 (10%)	0	7
5	E	261/263 (99%)	209 (80%)	28 (11%)	24 (9%)	0	8
6	F	189/204 (93%)	162 (86%)	15 (8%)	12 (6%)	1	13
7	G	235/249 (94%)	201 (86%)	19 (8%)	15 (6%)	1	12
8	H	188/194 (97%)	146 (78%)	11 (6%)	31 (16%)	0	2
9	I	204/208 (98%)	169 (83%)	12 (6%)	23 (11%)	0	5
10	J	180/194 (93%)	138 (77%)	18 (10%)	24 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	96/165 (58%)	67 (70%)	11 (12%)	18 (19%)	0	2
12	L	156/158 (99%)	132 (85%)	10 (6%)	14 (9%)	0	8
13	M	122/132 (92%)	85 (70%)	16 (13%)	21 (17%)	0	2
14	N	148/151 (98%)	124 (84%)	18 (12%)	6 (4%)	2	18
15	O	134/151 (89%)	101 (75%)	14 (10%)	19 (14%)	0	3
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	11
18	R	124/135 (92%)	96 (77%)	13 (10%)	15 (12%)	0	4
19	S	135/152 (89%)	106 (78%)	20 (15%)	9 (7%)	1	12
20	T	139/145 (96%)	119 (86%)	10 (7%)	10 (7%)	1	11
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	2
23	W	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	7	38
24	X	140/143 (98%)	121 (86%)	11 (8%)	8 (6%)	1	14
25	Y	124/133 (93%)	91 (73%)	15 (12%)	18 (14%)	0	3
26	Z	73/125 (58%)	52 (71%)	12 (16%)	9 (12%)	0	4
27	a	105/115 (91%)	72 (69%)	14 (13%)	19 (18%)	0	2
28	b	82/84 (98%)	57 (70%)	14 (17%)	11 (13%)	0	4
29	c	62/69 (90%)	44 (71%)	13 (21%)	5 (8%)	1	9
30	d	51/56 (91%)	46 (90%)	3 (6%)	2 (4%)	2	19
31	e	57/133 (43%)	37 (65%)	7 (12%)	13 (23%)	0	1
32	f	69/156 (44%)	38 (55%)	13 (19%)	18 (26%)	0	1
33	g	311/317 (98%)	271 (87%)	23 (7%)	17 (6%)	1	15
35	l	83/113 (74%)	49 (59%)	24 (29%)	10 (12%)	0	4
All	All	4909/5648 (87%)	3884 (79%)	520 (11%)	505 (10%)	0	6

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%)	141 (81%)	33 (19%)	1	8
2	B	196/231 (85%)	153 (78%)	43 (22%)	1	6
3	C	187/215 (87%)	142 (76%)	45 (24%)	1	4
4	D	190/202 (94%)	144 (76%)	46 (24%)	1	4
5	E	225/225 (100%)	170 (76%)	55 (24%)	1	4
6	F	161/170 (95%)	114 (71%)	47 (29%)	0	2
7	G	207/218 (95%)	157 (76%)	50 (24%)	1	4
8	H	170/174 (98%)	124 (73%)	46 (27%)	0	3
9	I	177/179 (99%)	137 (77%)	40 (23%)	1	6
10	J	157/168 (94%)	128 (82%)	29 (18%)	1	8
11	K	89/136 (65%)	63 (71%)	26 (29%)	0	2
12	L	142/142 (100%)	106 (75%)	36 (25%)	0	3
13	M	101/108 (94%)	78 (77%)	23 (23%)	1	6
14	N	130/131 (99%)	100 (77%)	30 (23%)	1	5
15	O	106/119 (89%)	88 (83%)	18 (17%)	2	10
16	P	116/130 (89%)	86 (74%)	30 (26%)	0	3
17	Q	117/121 (97%)	83 (71%)	34 (29%)	0	2
18	R	114/121 (94%)	87 (76%)	27 (24%)	1	4
19	S	119/132 (90%)	95 (80%)	24 (20%)	1	7
20	T	113/116 (97%)	84 (74%)	29 (26%)	0	3
21	U	94/107 (88%)	72 (77%)	22 (23%)	1	5
22	V	67/68 (98%)	47 (70%)	20 (30%)	0	2
23	W	112/113 (99%)	97 (87%)	15 (13%)	4	14
24	X	114/115 (99%)	90 (79%)	24 (21%)	1	6
25	Y	108/115 (94%)	85 (79%)	23 (21%)	1	6
26	Z	66/103 (64%)	53 (80%)	13 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	91/99 (92%)	76 (84%)	15 (16%)	2	10
28	b	76/76 (100%)	64 (84%)	12 (16%)	2	11
29	c	57/62 (92%)	43 (75%)	14 (25%)	1	4
30	d	47/49 (96%)	35 (74%)	12 (26%)	0	3
31	e	49/106 (46%)	27 (55%)	22 (45%)	0	0
32	f	64/140 (46%)	42 (66%)	22 (34%)	0	1
33	g	272/275 (99%)	219 (80%)	53 (20%)	1	7
35	l	74/96 (77%)	53 (72%)	21 (28%)	0	2
All	All	4282/4806 (89%)	3283 (77%)	999 (23%)	1	5

5 of 999 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	8	ARG
31	e	97	GLU
16	P	14	LYS
30	d	44	ARG
33	g	118	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	20	GLN
35	l	84	GLN
20	T	11	GLN
35	l	48	GLN
32	f	151	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	i	1722/1863 (92%)	500 (29%)	0

5 of 500 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	i	2	A

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Mol	Chain	Res	Type
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
31	e	1
9	I	1
21	U	1
3	C	1
7	G	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%)	-0.29	8 (3%) 44 42	173, 263, 322, 332	0
2	B	215/264 (81%)	-0.16	9 (4%) 40 40	128, 196, 242, 252	0
3	C	226/278 (81%)	-0.40	11 (4%) 35 36	82, 160, 268, 295	0
4	D	227/243 (93%)	-0.29	6 (2%) 57 49	167, 217, 294, 337	0
5	E	263/263 (100%)	0.64	36 (13%) 6 15	117, 216, 286, 299	0
6	F	191/204 (93%)	-0.37	5 (2%) 57 49	191, 263, 305, 317	0
7	G	237/249 (95%)	-0.22	10 (4%) 40 40	164, 242, 325, 343	0
8	H	190/194 (97%)	-0.47	3 (1%) 70 59	187, 326, 368, 385	0
9	I	206/208 (99%)	0.13	16 (7%) 19 25	89, 239, 276, 287	0
10	J	182/194 (93%)	0.01	13 (7%) 22 28	89, 166, 231, 276	0
11	K	98/165 (59%)	0.27	5 (5%) 33 35	222, 291, 316, 323	0
12	L	158/158 (100%)	0.23	21 (13%) 7 15	77, 176, 261, 270	0
13	M	124/132 (93%)	-0.65	0 100 100	298, 378, 406, 431	0
14	N	150/151 (99%)	-0.15	6 (4%) 42 41	87, 150, 275, 297	0
15	O	136/151 (90%)	-0.09	6 (4%) 39 39	92, 194, 256, 272	0
16	P	127/145 (87%)	-0.04	6 (4%) 36 37	234, 305, 340, 361	0
17	Q	141/146 (96%)	0.31	17 (12%) 8 17	166, 287, 321, 331	0
18	R	126/135 (93%)	-0.30	0 100 100	174, 225, 322, 329	0
19	S	137/152 (90%)	0.14	6 (4%) 39 39	217, 311, 344, 357	0
20	T	141/145 (97%)	-0.26	1 (0%) 84 74	238, 311, 341, 349	0
21	U	104/119 (87%)	0.00	9 (8%) 16 23	167, 266, 306, 317	0
22	V	82/83 (98%)	-0.59	0 100 100	164, 218, 318, 328	0
23	W	129/130 (99%)	0.44	16 (12%) 8 16	107, 159, 204, 218	0
24	X	142/143 (99%)	0.54	20 (14%) 6 15	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%)	-0.34	3 (2%) 59 52	156, 205, 243, 261	0
26	Z	75/125 (60%)	-0.36	1 (1%) 75 64	292, 320, 350, 360	0
27	a	107/115 (93%)	0.31	12 (11%) 10 18	87, 129, 234, 249	0
28	b	84/84 (100%)	0.56	8 (9%) 14 21	164, 223, 303, 334	0
29	c	64/69 (92%)	-0.62	0 100 100	175, 224, 274, 287	0
30	d	53/56 (94%)	0.38	7 (13%) 7 15	183, 212, 290, 295	0
31	e	59/133 (44%)	-0.34	1 (1%) 69 59	103, 158, 182, 189	0
32	f	71/156 (45%)	-0.69	0 100 100	213, 332, 401, 415	0
33	g	313/317 (98%)	-0.30	1 (0%) 90 82	235, 304, 346, 364	0
34	i	1797/1863 (96%)	-0.38	40 (2%) 62 53	49, 184, 371, 475	0
35	l	85/113 (75%)	-0.67	0 100 100	223, 235, 250, 253	0
All	All	6774/7511 (90%)	-0.17	303 (4%) 38 38	49, 228, 347, 475	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	80	ILE	21.4
5	E	70	ILE	16.5
5	E	44	LEU	15.0
12	L	23	VAL	12.0
34	i	230	C	9.8

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 oligosaccharides 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.