



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 05:28 AM EDT

PDB ID : 4IOA / pdb_00004ioa
Title : Crystal structure of compound 4e bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.20 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

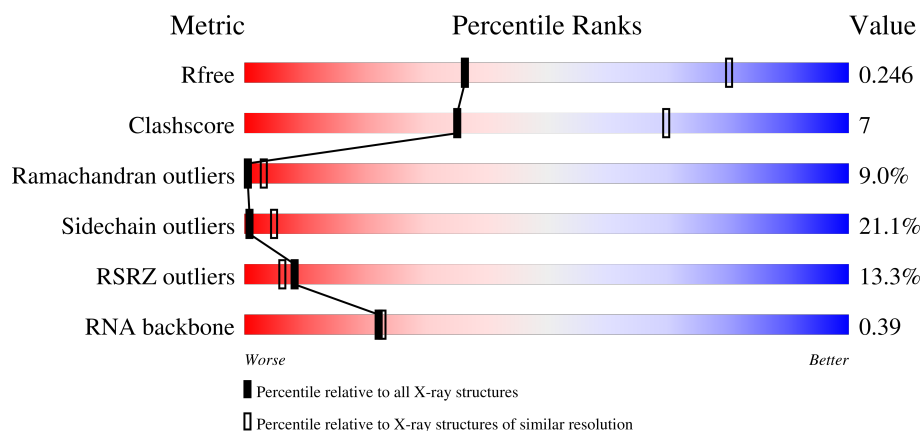
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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	X	2880	
2	Y	123	
3	A	274	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>84%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2904	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2930	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

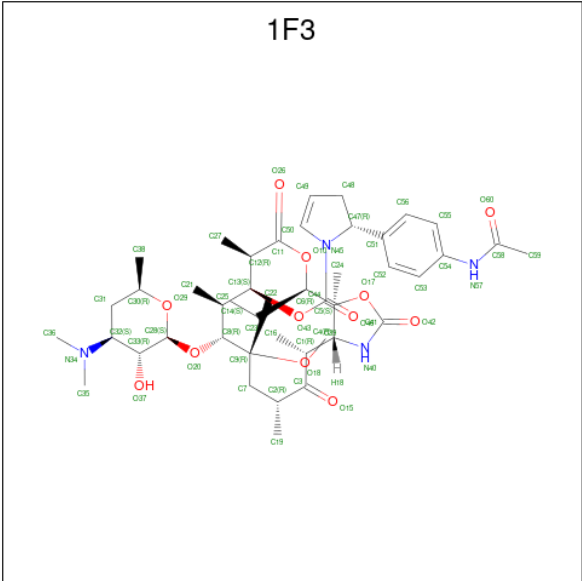
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

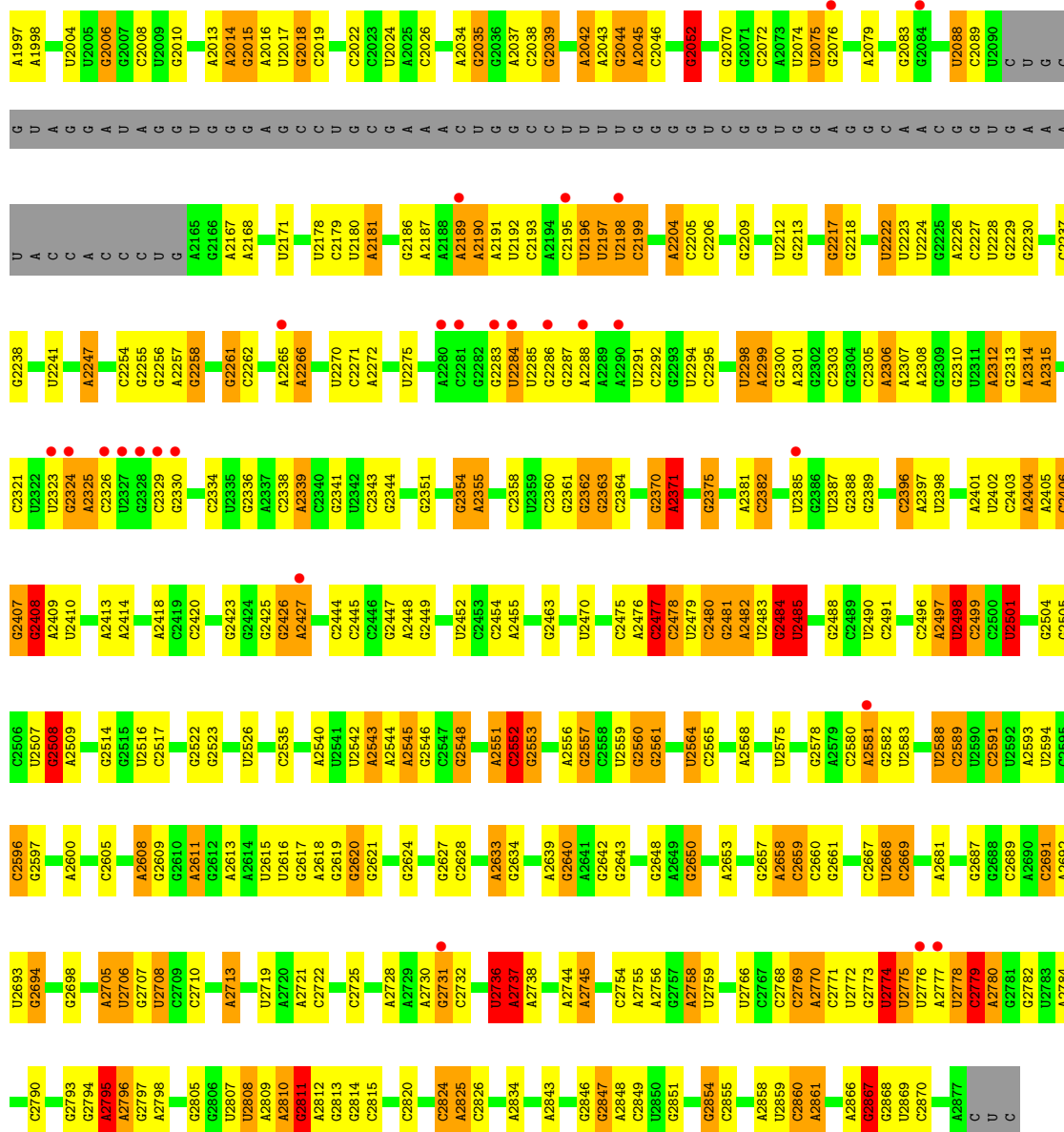
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-2-[4-(acetylamino)phenyl]-2,3-dihydro-1H-pyrrole-1-carboxylate (CCD ID: 1F3) (formula: C₄₄H₆₆N₄O₁₂).

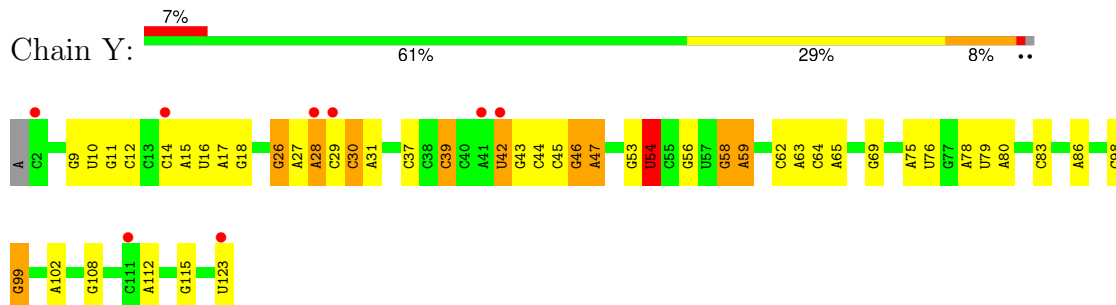


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

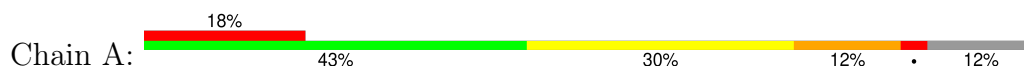
U1914	G1831	G1737	U1666	U1551	G1465	U1357	G1273	A1154	A1081	G1000	U	A802
G1918	G1832	G1742	U1657	C1552	C1466	C1388	C1274	G1155	G1082	A1001	A	C803
A1920	G1834	G1747	A1658	U1553	U1467	U1365	A1275	U1161	C1083	G0805	C	C804
A1921	A1240	G1753	G1660	G1554	U1469	A1366	U1276	C1169	G1085	A1004	A	A806
U1922	A1945	A1753	C1661	A1561	G1471	A1367	A1277	G1173	C1086	C1006	C	A807
U1923	A1945	G1754	G1662	U1562	C1472	G1368	G1278	G1173	A1087	A1007	U	G811
U1926	G1850	G1755	C1663	G1563	U1473	G1373	U1280	U1182	C1088	U1010	U	G812
U1927	G1850	C1756	G1664	U1564	A1474	A1378	A1281	U1182	C1090	A1011	A	A813
G1928	G1854	C1757	C1665	G1570	G1476	G1381	C1283	C1185	U1093	A1012	C	G814
A1935	A1859	A1764	G1666	G1571	U1481	G1384	A1285	G1186	C1094	G1014	A911	A815
U1938	A1860	C1765	A1669	A1574	U1482	G1385	U1286	A1187	A1095	U1015	A922	G818
U1939	U1938	A1771	A1670	C1575	G1483	U1392	A1287	A1188	A1096	C1016	A923	G822
A1943	U1963	C1772	C1673	G1576	U1490	U1403	A1289	G1189	A1097	U1019	C926	U823
U1946	G1865	A1774	C1675	C1581	A1493	A1404	A1290	G1191	A1099	G0939	C927	U824
G1947	C1866	A1775	U1676	A1582	G1494	A1405	A1291	A1192	G1100	A1022	G931	C825
U1950	A1872	A1776	G1677	A1583	G1495	U1406	A1297	G1193	G1104	U1023	G938	U826
G1951	A1873	C1777	U1678	G1584	G1496	A1407	A1299	U1194	G1108	G1024	G939	C828
A1952	C1874	C1778	U1680	A1587	C1497	A1408	A1300	U1195	A1109	C1028	G940	C830
A1953	U1881	U1787	G1683	A1588	U1505	A1409	U1301	C1218	U1112	U1030	G944	G831
G1955	C1882	C1788	G1684	U1594	C1506	U1410	C1302	C1219	C1113	C1031	U840	A832
G1958	A1883	G1790	A1685	U1600	A1507	U1411	U1307	G1220	C1114	A1032	G945	U841
U1959	C1884	C1791	A1686	U1601	G1508	A1412	A1313	A1224	C1115	U1034	U946	C842
A1960	C1885	C1792	U1688	G1602	A1509	U1413	A1314	A1233	U1116	G1035	C948	G843
G1961	G1886	A1793	U1689	A1603	A1510	U1414	A1315	C1234	G1117	U1037	G949	U852
A1962	U1887	U1798	U1690	A1607	U1513	U1421	C1319	C1235	U1119	U1038	G951	C853
G1963	C1888	A1800	A1692	U1608	C1514	C1422	G1324	A1238	G1121	U1044	A952	G858
U1964	G	G1803	A1693	G1613	A1516	G1428	U1328	G1240	A1122	G1050	U954	U859
U1965	C	U1804	A1699	U1618	G1519	A1429	C1328	G1248	C1127	U1051	G955	U868
U1974	C	G1805	C1702	U1618	G1520	U1431	U1329	G1249	G1128	C1052	A956	C869
G1975	U	G1806	U1702	C1623	U1521	G1432	G1330	A1250	A1129	G1053	G957	C870
U1976	A	A1807	C1702	C1623	C1522	A1433	A1334	G1251	U1130	C1054	A964	U871
C1979	C	C1808	U1710	A1624	A1523	U1434	A1335	C1252	U1134	A1055	G967	G872
A1980	U	G1809	C1711	A1625	C1524	A1437	A1336	C1253	G1136	U1056	C968	U873
G1983	U	U1810	G1712	A1626	A1525	U1438	G1337	G1254	C1137	A1057	U969	G874
A1984	A	U1811	G1713	C1627	C1528	A1441	U1338	G1255	G1138	A1058	A970	G875
G1985	A	A1812	G1716	G1628	C1531	C1442	C1340	U1257	A1138	C1060	A971	C878
G1986	C	A1813	A1717	A1630	A1532	G1443	G1341	G1258	A1139	G1067	C972	A879
G1987	C	U1816	U1723	A1632	G1533	U1444	A1342	A1259	U1140	A1068	U973	C880
A1988	G	U1817	C1724	C1633	G1541	A1448	G1343	G1261	U1141	G1069	U978	U890
C1989	U	G1820	C1725	A1634	G1542	U1449	C1344	G1264	A1142	G1070	A891	A891
U1990	C	A1821	C1726	G1635	G1543	U1451	G1345	G1265	A1143	U1071	G985	G
C1991	C	C1825	U1732	G1636	G1544	U1451	G1345	G1266	U1144	U1072	A986	G
G1992	U1909	U1826	U1733	G1644	G1545	U1459	A1353	G1268	G1145	G1073	A990	G
G1993	A1910	G1827	U1735	U1645	G1546	U1460	A1354	U1267	G1146	U1077	A994	G
U1994	A1911	G1827	G1735	U1646	C1547	U1460	A1355	U1268	C1152	A1078	A995	C
G1995	G1912	G1827	G1735	U1646	C1547	U1460	A1355	U1268	C1152	A1078	A995	C
A1996	G1913	C1830	C1736	C1648	U1548	U1460	A1356	G1269	C1152	A1078	A995	C

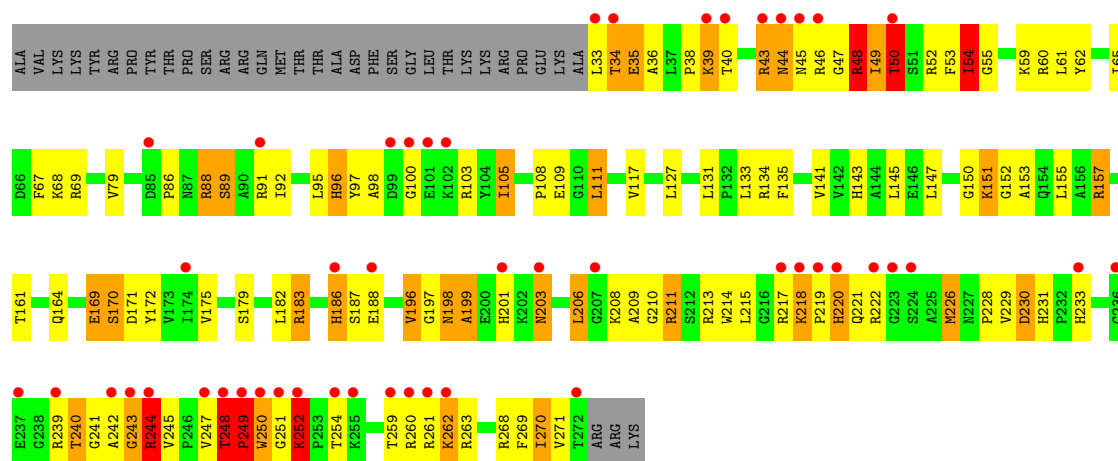


• Molecule 2: 5S ribosomal RNA

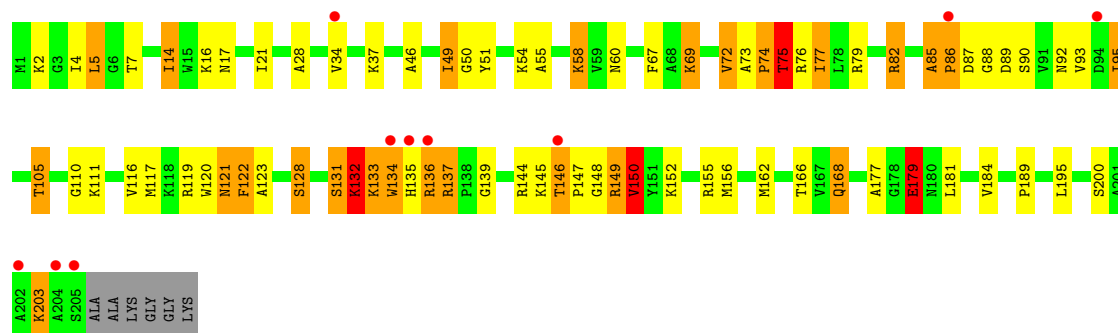


• Molecule 3: 50S ribosomal protein L2

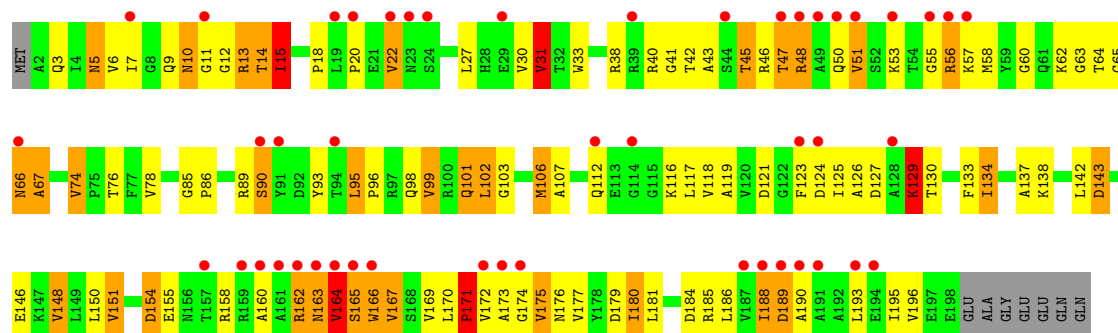
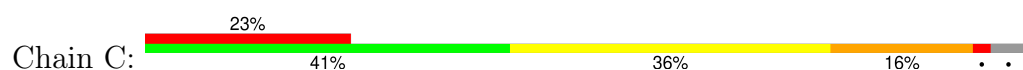




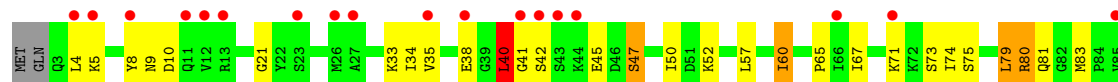
• Molecule 4: 50S ribosomal protein L3

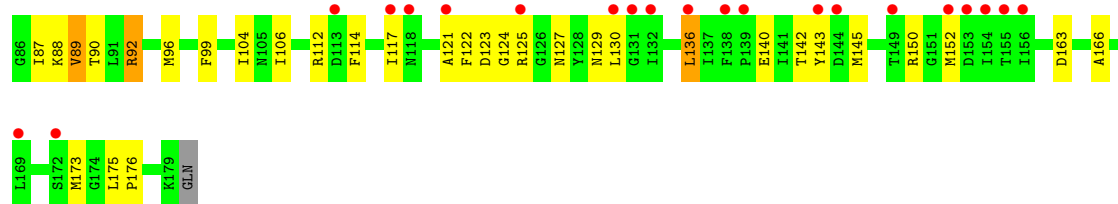


• Molecule 5: 50S ribosomal protein L4

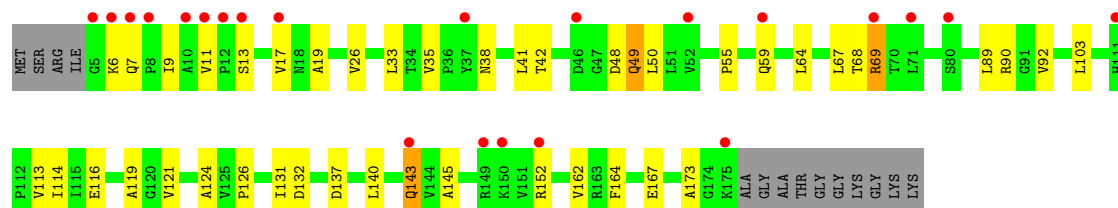


• Molecule 6: 50S ribosomal protein L5

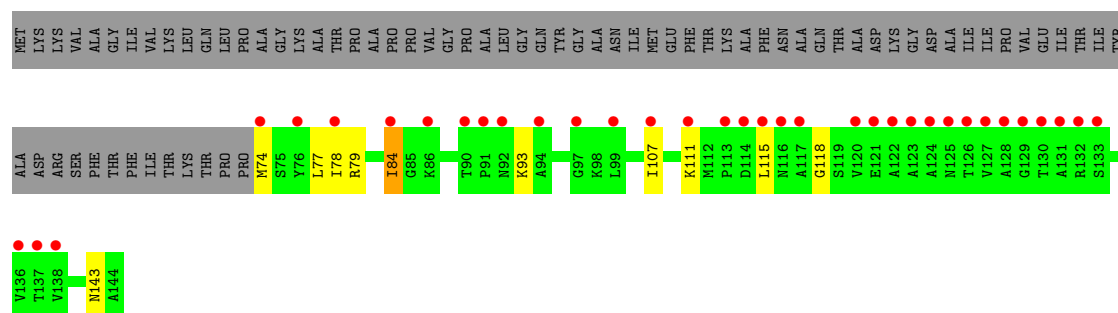
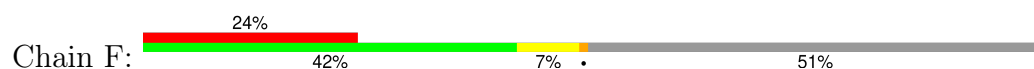




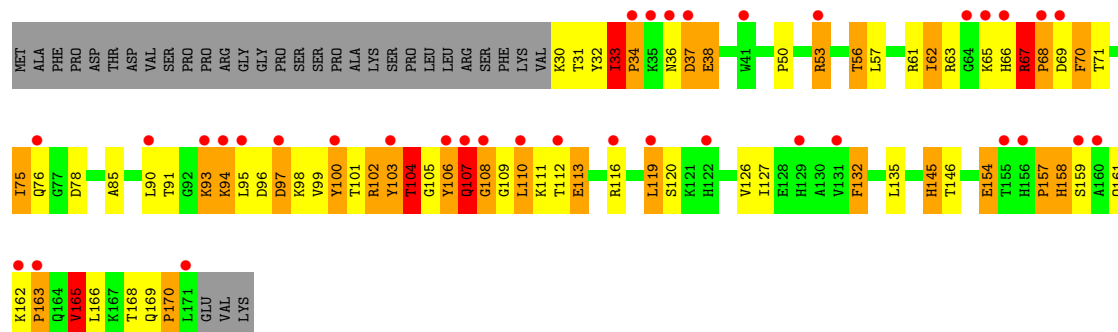
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L11

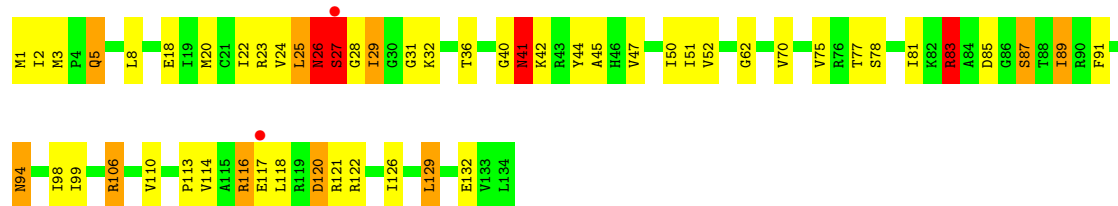


• Molecule 9: 50S ribosomal protein L13

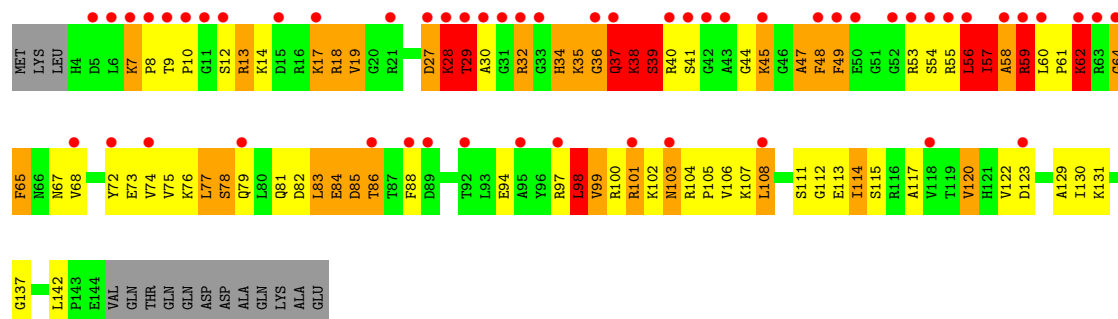


• Molecule 10: 50S ribosomal protein L14

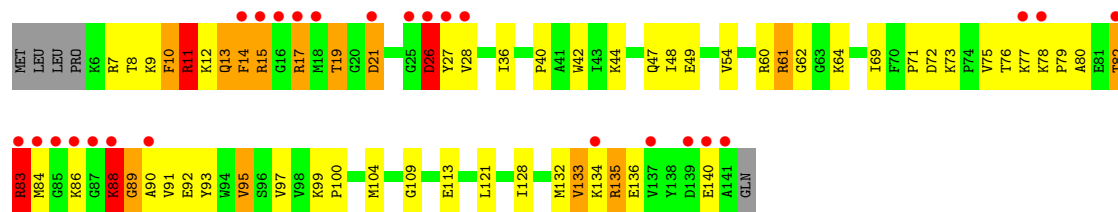




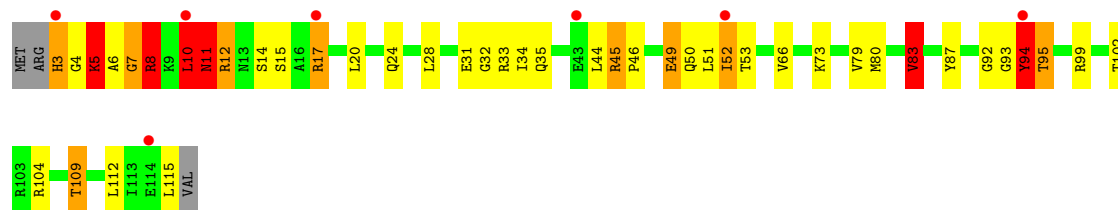
• Molecule 11: 50S ribosomal protein L15



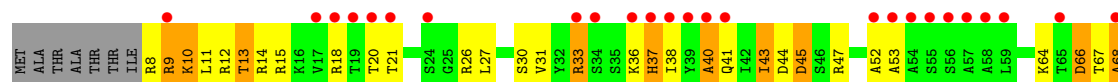
• Molecule 12: 50S ribosomal protein L16

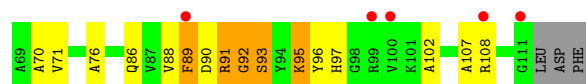


• Molecule 13: 50S ribosomal protein L17

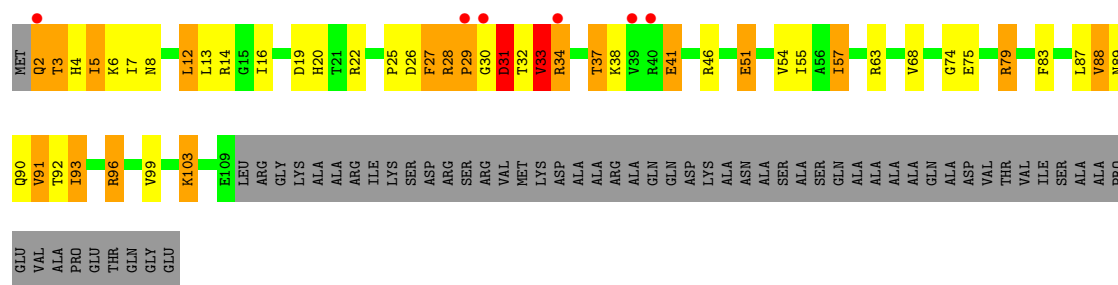
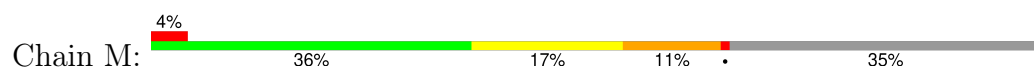


• Molecule 14: 50S ribosomal protein L18

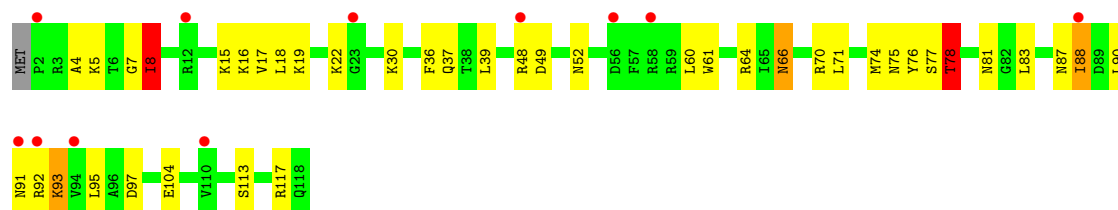




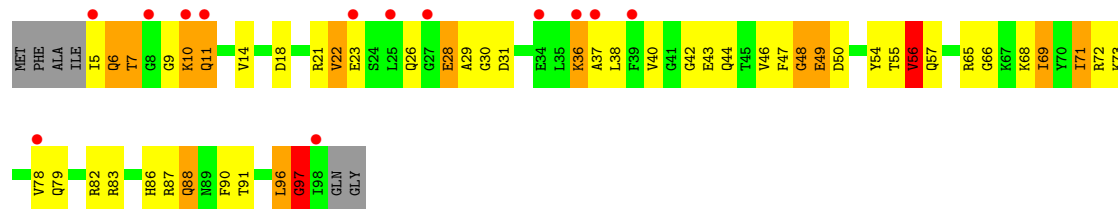
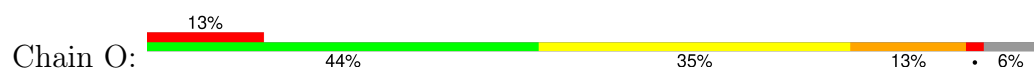
• Molecule 15: 50S ribosomal protein L19



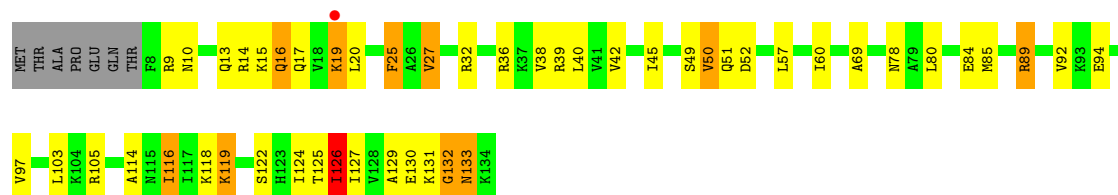
• Molecule 16: 50S ribosomal protein L20



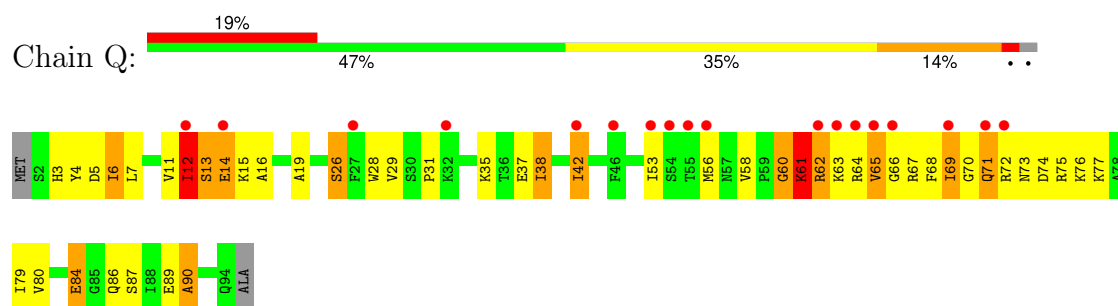
• Molecule 17: 50S ribosomal protein L21



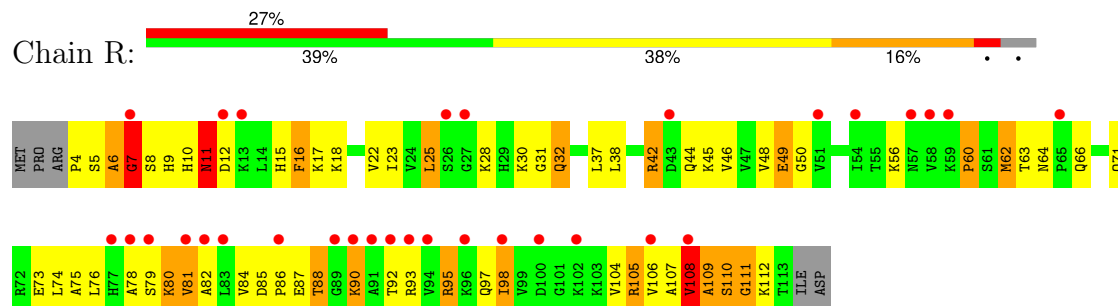
• Molecule 18: 50S ribosomal protein L22



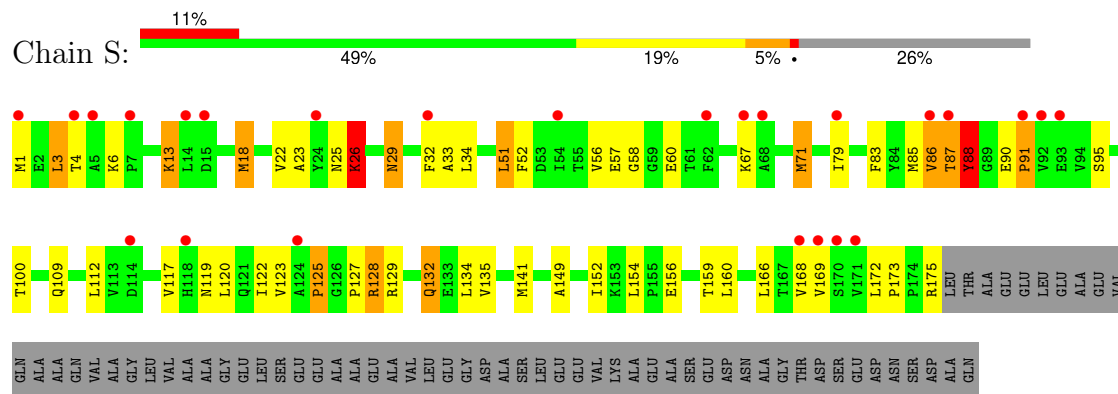
• Molecule 19: 50S ribosomal protein L23



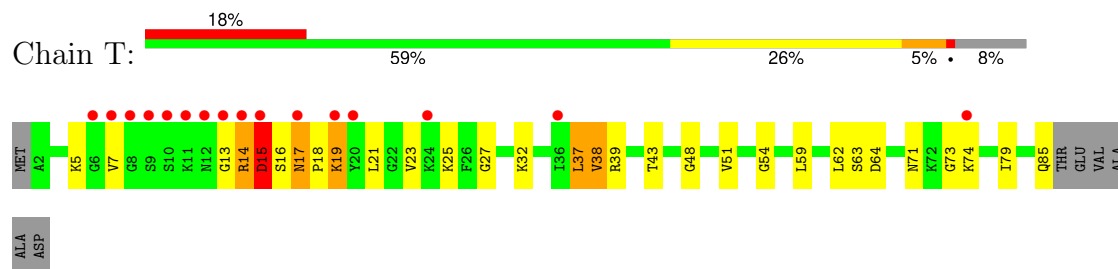
• Molecule 20: 50S ribosomal protein L24



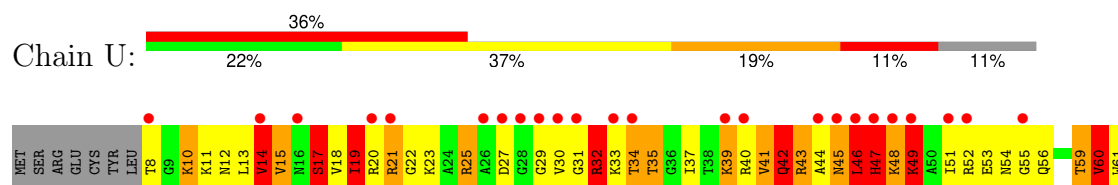
• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28





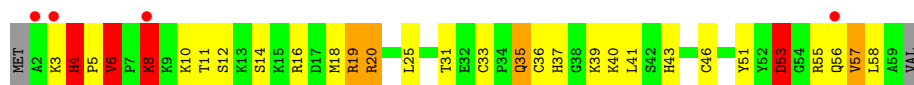
- Molecule 24: 50S ribosomal protein L29



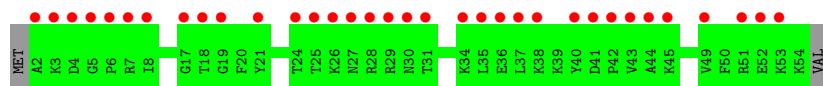
- Molecule 25: 50S ribosomal protein L30



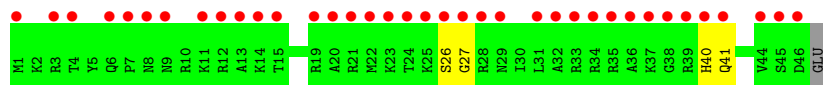
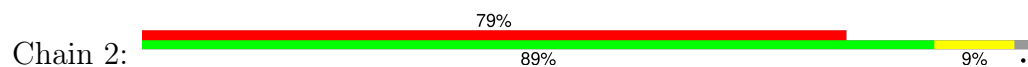
- Molecule 26: 50S ribosomal protein L32



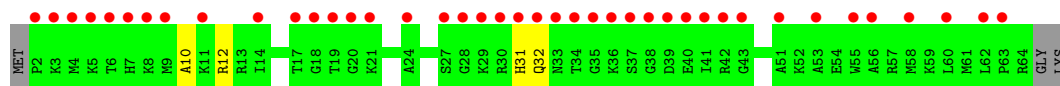
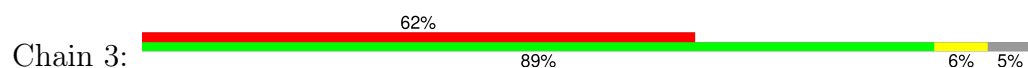
- Molecule 27: 50S ribosomal protein L33



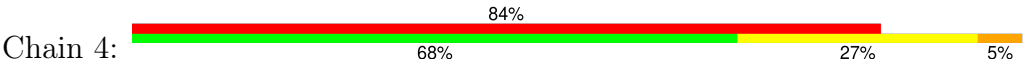
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.7 (30.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 3.24Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.197 , 0.230 0.210 , 0.246	Depositor DCC
R_{free} test set	17364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1F3

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	X	0.69	21/64561 (0.0%)	1.38	832/100708 (0.8%)
2	Y	0.69	0/2904	1.24	12/4525 (0.3%)
3	A	1.07	9/1862 (0.5%)	1.62	31/2510 (1.2%)
4	B	1.01	3/1567 (0.2%)	1.55	21/2105 (1.0%)
5	C	1.04	3/1529 (0.2%)	1.70	41/2070 (2.0%)
6	D	0.86	0/1419	1.31	4/1903 (0.2%)
7	E	0.82	0/1308	1.33	4/1771 (0.2%)
8	F	0.92	0/508	1.38	0/683
9	G	1.01	2/1138 (0.2%)	1.71	29/1539 (1.9%)
10	H	0.94	1/1007 (0.1%)	1.48	12/1352 (0.9%)
11	I	1.25	9/1081 (0.8%)	1.83	32/1448 (2.2%)
12	J	1.10	2/1113 (0.2%)	1.61	17/1486 (1.1%)
13	K	1.25	4/886 (0.5%)	1.76	21/1188 (1.8%)
14	L	0.97	0/785	1.75	12/1048 (1.1%)
15	M	1.06	5/884 (0.6%)	1.60	15/1186 (1.3%)
16	N	0.86	0/994	1.55	6/1323 (0.5%)
17	O	0.94	0/750	1.60	14/1000 (1.4%)
18	P	0.93	0/1027	1.47	10/1373 (0.7%)
19	Q	1.05	1/737 (0.1%)	1.70	18/988 (1.8%)
20	R	1.12	1/835 (0.1%)	1.68	23/1121 (2.1%)
21	S	0.92	0/1370	1.40	10/1862 (0.5%)
22	T	0.92	0/633	1.44	11/838 (1.3%)
23	U	1.33	3/556 (0.5%)	1.92	22/741 (3.0%)
24	V	0.83	0/537	1.56	5/714 (0.7%)
25	W	0.79	0/426	1.48	7/568 (1.2%)
26	Z	1.07	1/469 (0.2%)	1.69	11/629 (1.7%)
30	4	0.95	0/298	1.31	0/390
All	All	0.79	65/91184 (0.1%)	1.43	1220/137069 (0.9%)

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	X	0	6

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	38	LYS	CA-C	11.43	1.62	1.52
13	K	52	ILE	CG1-CD1	10.65	1.93	1.51
26	Z	53	ASP	CA-C	8.64	1.64	1.52
15	M	29	PRO	CA-C	8.60	1.64	1.52
11	I	29	THR	CA-C	8.14	1.63	1.52

The worst 5 of 1220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.81	78.89	109.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	1288	A	C5'-C4'-O4'	16.75	134.22	109.10
11	I	64	GLY	N-CA-C	15.62	126.04	111.67
1	X	1716	G	P-O3'-C3'	14.94	142.60	120.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	Sidechain

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	X	57651	0	29049	437	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	63	0
4	B	1539	0	1600	67	0
5	C	1506	0	1525	58	0
6	D	1400	0	1481	23	0
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	64	0
10	H	997	0	1046	23	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	29	0
14	L	779	0	820	17	0
15	M	871	0	894	30	0
16	N	978	0	1020	26	0
17	O	741	0	756	31	0
18	P	1014	0	1096	22	0
19	Q	726	0	753	23	0
20	R	825	0	881	29	0
21	S	1345	0	1372	23	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	5	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0
30	4	297	0	330	6	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	994	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 7.

The worst 5 of 994 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)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HG3	15:M:79:ARG:HH11	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09

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 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	
3	A	238/274 (87%)	170 (71%)	39 (16%)	29 (12%)	0	1
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1	7
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0	1
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1	6
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	2	14
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	3	24
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	0	2
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2	15
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0	0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1	4
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1	6
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	0	3
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	2	18
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	20
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0	0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	2	15
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0	2
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0	0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	1	8
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1	6
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	11
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	0	3

5 of 268 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA

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	
3	A	185/215 (86%)	139 (75%)	46 (25%)	0	2
4	B	155/157 (99%)	129 (83%)	26 (17%)	1	8
5	C	157/163 (96%)	123 (78%)	34 (22%)	1	4
6	D	153/156 (98%)	128 (84%)	25 (16%)	2	9
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	11
8	F	51/107 (48%)	46 (90%)	5 (10%)	6	27
9	G	118/146 (81%)	92 (78%)	26 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	76 (74%)	27 (26%)	0	1
11	I	108/121 (89%)	71 (66%)	37 (34%)	0	0
12	J	110/115 (96%)	90 (82%)	20 (18%)	1	7
13	K	90/93 (97%)	73 (81%)	17 (19%)	1	6
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	1
15	M	94/134 (70%)	69 (73%)	25 (27%)	0	1
16	N	96/97 (99%)	79 (82%)	17 (18%)	1	8
17	O	75/79 (95%)	61 (81%)	14 (19%)	1	6
18	P	109/115 (95%)	93 (85%)	16 (15%)	2	12
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	5
20	R	91/96 (95%)	70 (77%)	21 (23%)	0	3
21	S	149/192 (78%)	123 (83%)	26 (17%)	1	8
22	T	62/67 (92%)	54 (87%)	8 (13%)	3	17
23	U	57/66 (86%)	31 (54%)	26 (46%)	0	0
24	V	54/55 (98%)	46 (85%)	8 (15%)	2	12
25	W	48/48 (100%)	36 (75%)	12 (25%)	0	2
26	Z	51/53 (96%)	36 (71%)	15 (29%)	0	1
30	4	35/35 (100%)	29 (83%)	6 (17%)	1	8
All	All	2436/2715 (90%)	1923 (79%)	513 (21%)	1	5

5 of 513 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	49	LYS
24	V	25	LEU
23	U	46	LEU
10	H	41	ASN
10	H	26	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
21	S	105	GLN
30	4	13	ASN
21	S	132	GLN

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Mol	Chain	Res	Type
25	W	15	ASN
10	H	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	664 (24%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)
All	All	2802/3003 (93%)	692 (24%)	243 (8%)

5 of 692 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A

5 of 243 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1249	G
1	X	2705	A
1	X	1581	C
1	X	2669	C
1	X	2854	G

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	1F3	X	2931	-	63,64,64	1.32	7 (11%)	83,96,96	1.87	19 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F3	X	2931	-	-	9/78/119/119	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C50-C49	4.20	1.50	1.34
32	X	2931	1F3	C48-C47	-4.14	1.51	1.54
32	X	2931	1F3	C50-N45	3.34	1.44	1.38
32	X	2931	1F3	O17-C5	-3.08	1.43	1.47
32	X	2931	1F3	C47-N45	-2.63	1.43	1.47

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C59-C58-N57	-5.48	106.72	114.95
32	X	2931	1F3	C28-O20-C8	-4.96	107.83	116.26
32	X	2931	1F3	C23-C6-C5	-4.94	108.42	115.23
32	X	2931	1F3	O60-C58-N57	3.83	128.31	123.06
32	X	2931	1F3	C47-N45-C50	3.52	113.23	109.61

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	C59-C58-N57-C54

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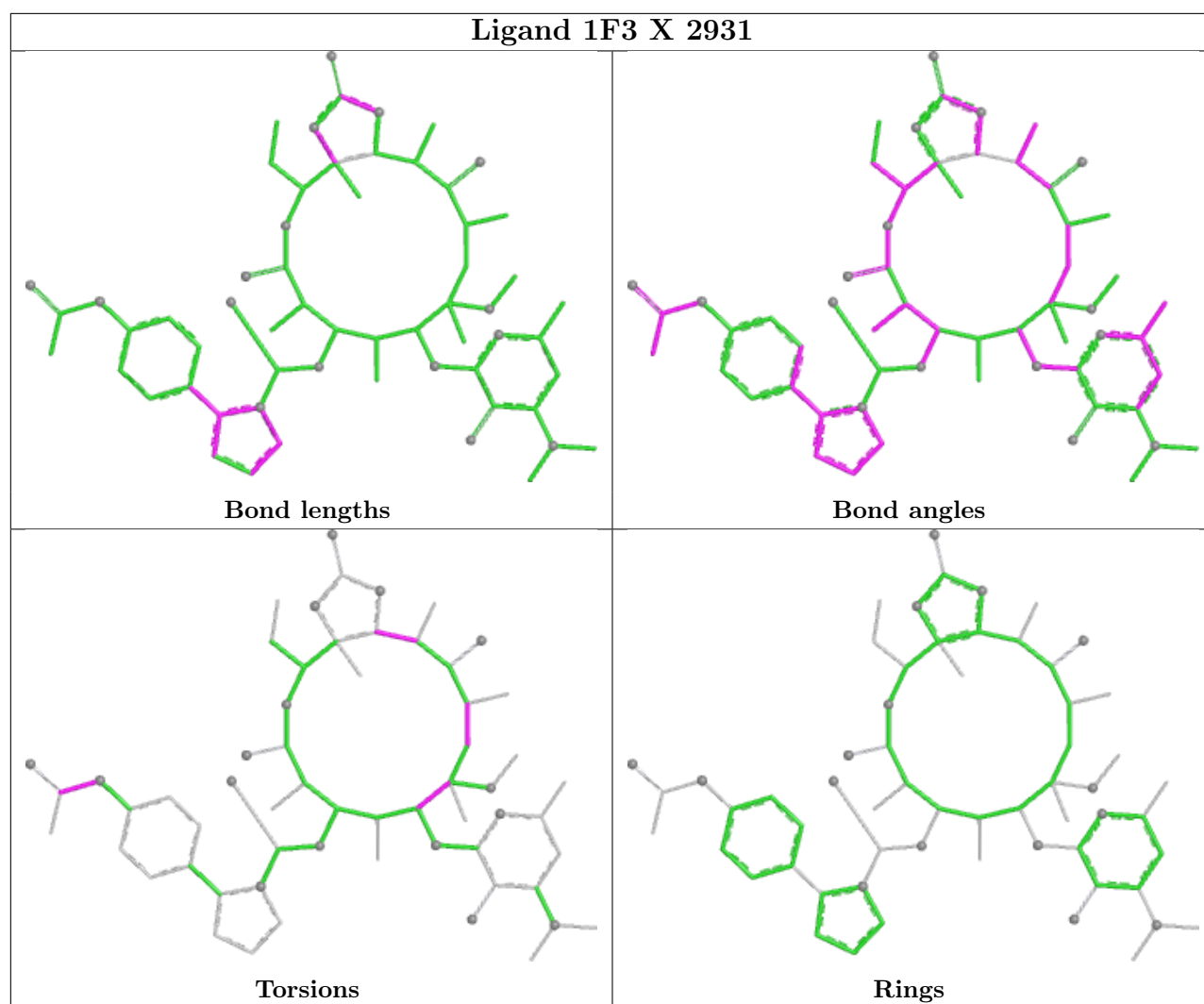
Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	O60-C58-N57-C54
32	X	2931	1F3	C16-C1-C4-N40
32	X	2931	1F3	O20-C8-C9-C7
32	X	2931	1F3	C3-C2-C7-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	X	2686/2880 (93%)	0.16	128 (4%) 36 25	43, 87, 194, 279	0
2	Y	122/123 (99%)	0.62	8 (6%) 26 17	82, 129, 165, 187	0
3	A	240/274 (87%)	1.19	48 (20%) 3 3	63, 107, 137, 156	0
4	B	205/211 (97%)	0.15	10 (4%) 36 25	38, 68, 99, 145	0
5	C	197/205 (96%)	1.26	47 (23%) 2 2	55, 107, 150, 178	0
6	D	177/180 (98%)	1.17	39 (22%) 3 2	148, 178, 210, 216	0
7	E	171/185 (92%)	0.82	22 (12%) 9 6	98, 139, 178, 188	0
8	F	71/144 (49%)	2.39	35 (49%) 0 1	221, 234, 251, 259	0
9	G	142/174 (81%)	1.18	36 (25%) 2 2	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.10	2 (1%) 71 56	49, 62, 88, 110	0
11	I	141/156 (90%)	2.11	54 (38%) 1 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.91	25 (18%) 4 3	83, 106, 147, 172	0
13	K	113/116 (97%)	0.01	7 (6%) 28 18	37, 53, 71, 99	0
14	L	104/114 (91%)	1.41	30 (28%) 1 1	91, 122, 149, 166	0
15	M	108/166 (65%)	0.13	6 (5%) 31 20	44, 64, 106, 128	0
16	N	117/118 (99%)	0.54	11 (9%) 15 11	54, 86, 124, 152	0
17	O	94/100 (94%)	0.80	13 (13%) 8 5	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.15	1 (0%) 82 70	48, 64, 103, 143	0
19	Q	93/95 (97%)	1.00	18 (19%) 4 3	69, 101, 156, 193	0
20	R	110/115 (95%)	1.46	31 (28%) 1 1	84, 113, 170, 173	0
21	S	175/237 (73%)	0.93	25 (14%) 7 5	119, 154, 178, 190	0
22	T	84/91 (92%)	1.06	16 (19%) 4 3	72, 103, 176, 195	0
23	U	72/81 (88%)	1.97	29 (40%) 1 1	86, 122, 146, 182	0
24	V	66/67 (98%)	0.71	8 (12%) 10 7	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.14	0	100 100	76, 96, 123, 161	0
26	Z	58/60 (96%)	0.46	4 (6%)	24 17	47, 64, 96, 108	0
27	1	53/55 (96%)	5.65	34 (64%)	0 1	6, 28, 62, 73	0
28	2	46/47 (97%)	5.10	37 (80%)	0 0	3, 10, 27, 42	0
29	3	63/66 (95%)	5.52	41 (65%)	0 1	3, 18, 41, 84	0
30	4	37/37 (100%)	5.54	31 (83%)	0 0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.71	796 (13%)	8 6	3, 96, 193, 279	0

The worst 5 of 796 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	50.7
27	1	4	ASP	44.3
29	3	60	LEU	38.8
28	2	46	ASP	21.7
27	1	3	LYS	19.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

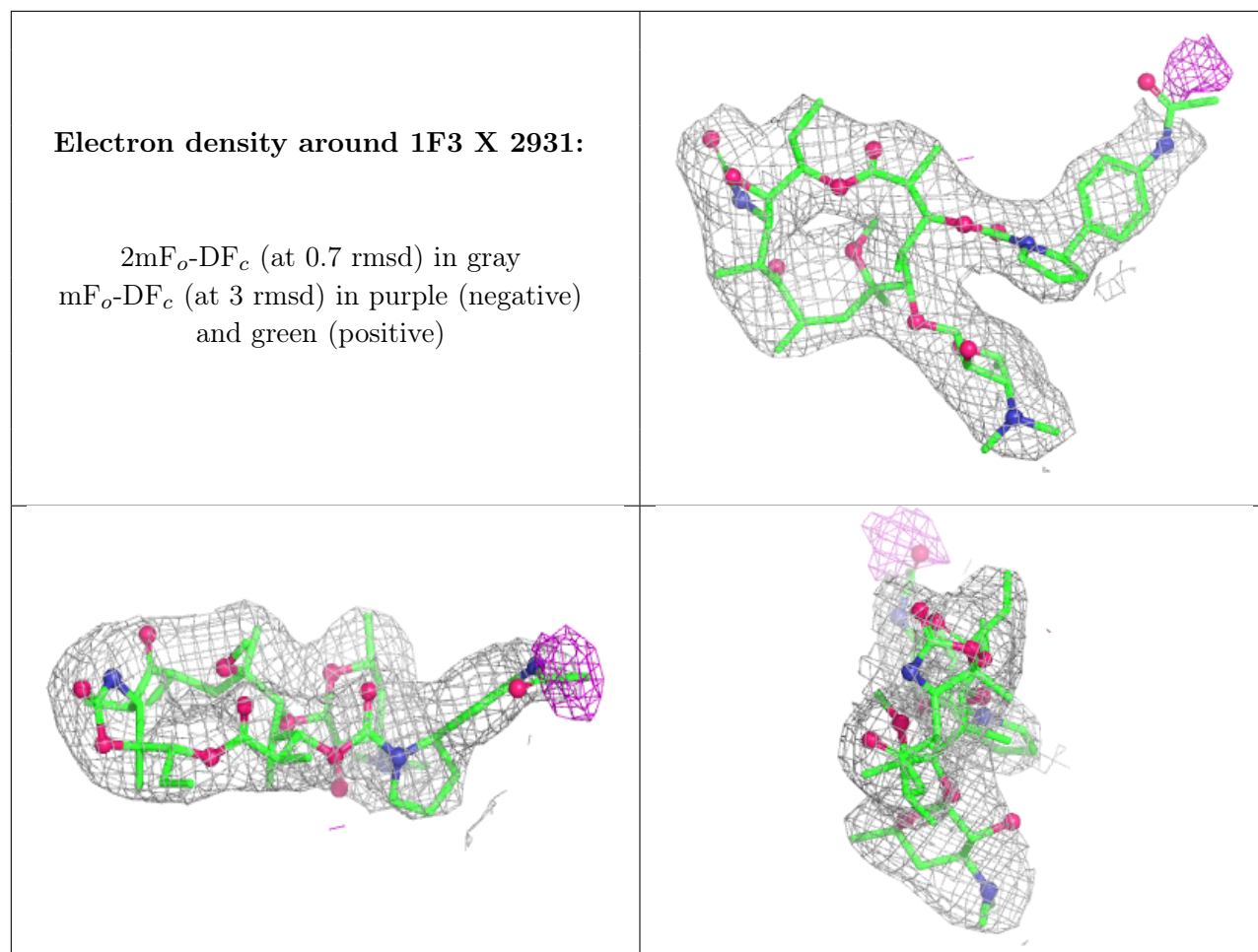
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2922	1/1	0.53	0.83	81,81,81,81	0
31	MG	X	2904	1/1	0.58	0.92	90,90,90,90	0
31	MG	X	2930	1/1	0.80	1.20	71,71,71,71	0
31	MG	X	2910	1/1	0.82	0.42	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	Y	205	1/1	0.84	0.12	77,77,77,77	0
31	MG	X	2912	1/1	0.85	0.31	60,60,60,60	0
31	MG	X	2906	1/1	0.86	0.85	79,79,79,79	0
31	MG	X	2901	1/1	0.86	0.62	110,110,110,110	0
31	MG	X	2911	1/1	0.87	0.34	35,35,35,35	0
31	MG	X	2929	1/1	0.87	0.35	77,77,77,77	0
31	MG	X	2926	1/1	0.88	0.51	56,56,56,56	0
31	MG	X	2907	1/1	0.88	0.38	53,53,53,53	0
31	MG	Y	201	1/1	0.89	0.63	82,82,82,82	0
31	MG	X	2908	1/1	0.89	0.39	49,49,49,49	0
31	MG	X	2925	1/1	0.90	0.50	39,39,39,39	0
31	MG	X	2913	1/1	0.91	0.45	66,66,66,66	0
31	MG	X	2905	1/1	0.92	0.22	104,104,104,104	0
31	MG	Y	203	1/1	0.92	0.47	87,87,87,87	0
31	MG	Y	204	1/1	0.92	0.16	67,67,67,67	0
31	MG	X	2923	1/1	0.92	0.63	74,74,74,74	0
31	MG	X	2916	1/1	0.93	0.50	53,53,53,53	0
31	MG	X	2903	1/1	0.93	0.17	82,82,82,82	0
31	MG	Y	202	1/1	0.93	0.34	54,54,54,54	0
31	MG	X	2920	1/1	0.94	0.56	38,38,38,38	0
31	MG	X	2927	1/1	0.94	0.20	106,106,106,106	0
31	MG	X	2919	1/1	0.94	0.60	56,56,56,56	0
31	MG	X	2924	1/1	0.95	0.42	39,39,39,39	0
32	1F3	X	2931	60/60	0.95	0.10	38,60,90,99	0
31	MG	X	2917	1/1	0.96	0.47	37,37,37,37	0
31	MG	X	2902	1/1	0.97	0.63	45,45,45,45	0
31	MG	X	2915	1/1	0.97	0.26	24,24,24,24	0
31	MG	X	2914	1/1	0.98	0.54	51,51,51,51	0
31	MG	X	2918	1/1	0.98	0.48	32,32,32,32	0
31	MG	X	2921	1/1	0.98	0.38	18,18,18,18	0
31	MG	X	2928	1/1	0.98	0.58	42,42,42,42	0
31	MG	X	2909	1/1	0.99	0.45	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.