



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 05:32 AM EDT

PDB ID : 4IOA
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:

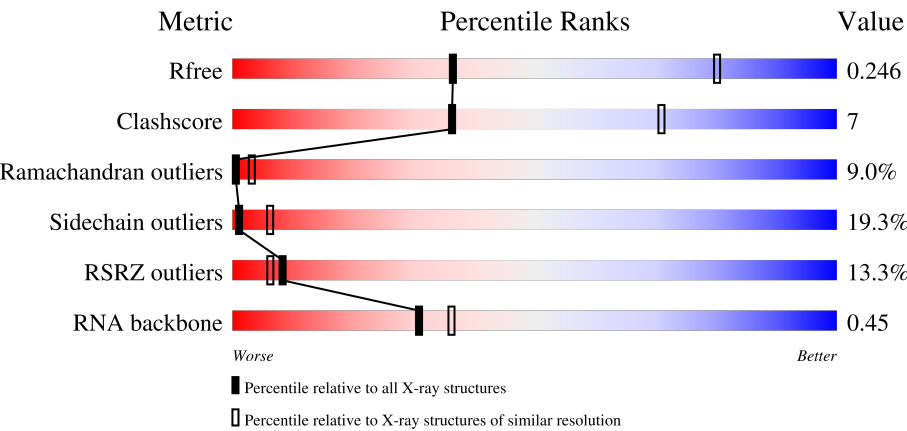
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	<div><div>4%</div><div>36%</div><div>34%</div><div>19%</div><div>7%</div></div>
2	Y	123	<div><div>7%</div><div>40%</div><div>42%</div><div>15%</div><div></div></div>
3	A	274	<div><div>18%</div><div>48%</div><div>30%</div><div>8%</div><div>12%</div></div>
4	B	211	<div><div>5%</div><div>67%</div><div>21%</div><div>9%</div><div></div></div>

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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>73%24%</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

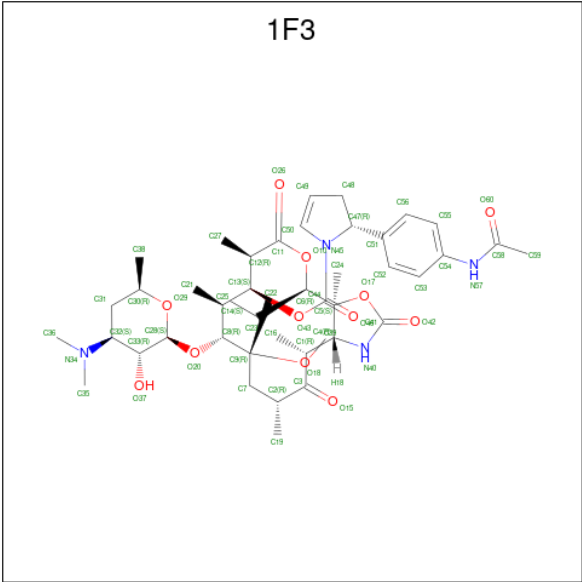
- Molecule 30 is a protein called 50S ribosomal protein L36.

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 (three-letter code: 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 (three-letter code: 1F3) (formula: C₄₄H₆₆N₄O₁₂).

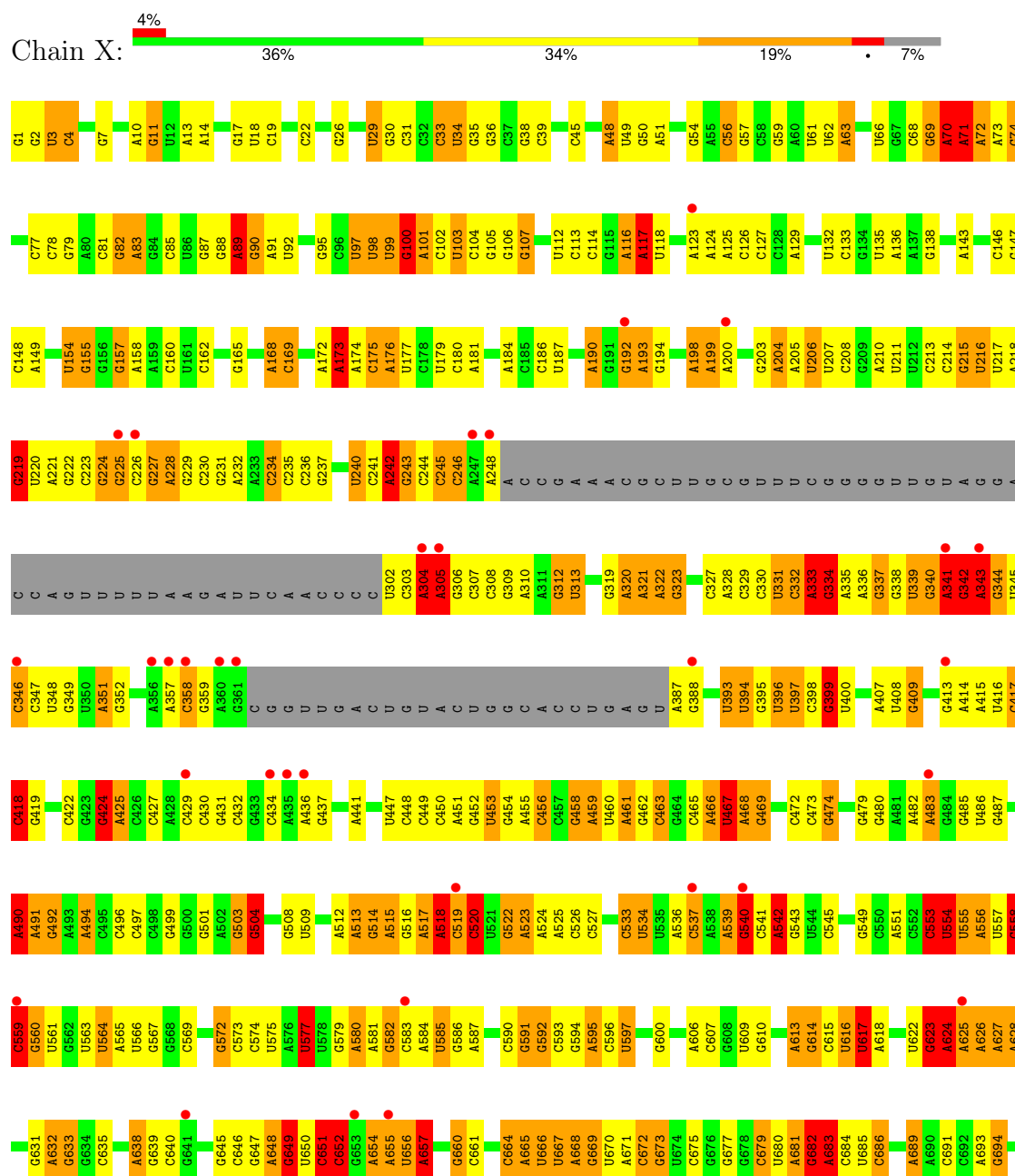


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

3 Residue-property plots

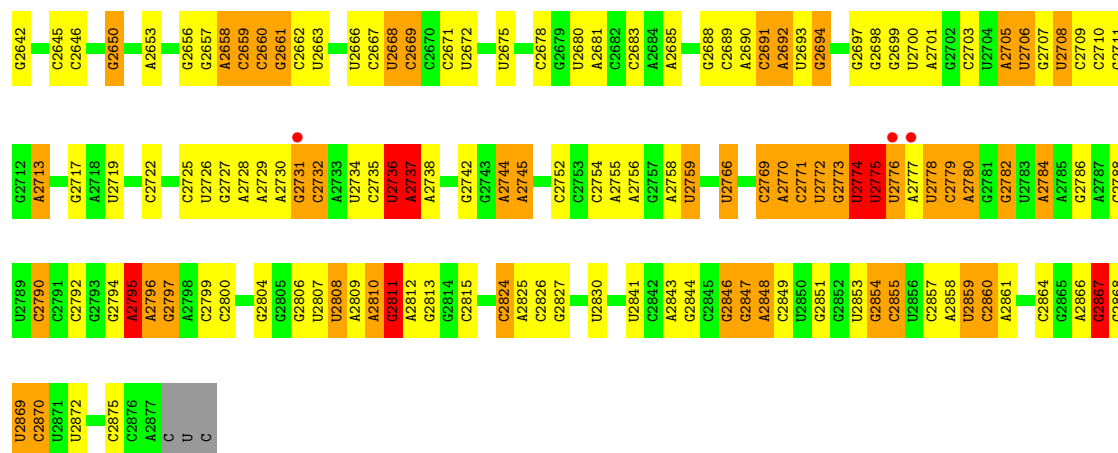
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

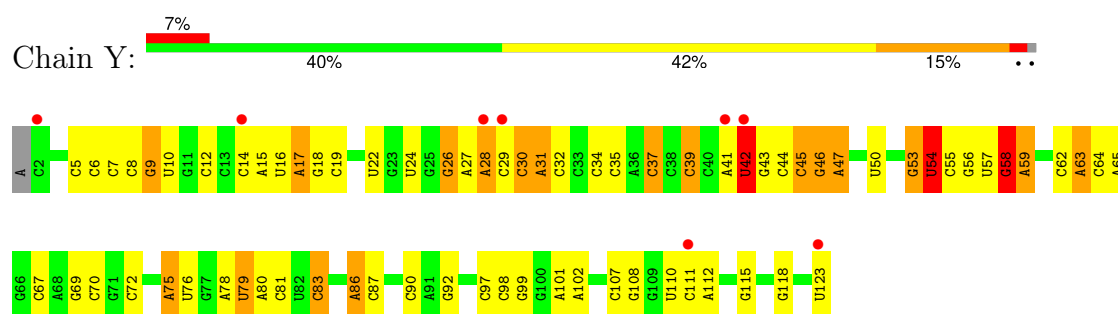


U1647	C1648	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1579	C1580	C1581	A1582	C1583	C1584	C1585	A1586	A1587	A1588	C1593	C1594	C1595	C1596	C1597	C1598	C1599	U1600	U1601	G1602	A1603	A1607	U1608	G1613	C1617	U1618	U1619	C1621	G1622	C1623	A1624	C1625	A1626	C1627	C1628	C1629	U1630	C1631	A1632	C1633	A1634	G1635	G1636	U1637	C1644	U1645	A1646
U1496	C1497	C1498	A1499	U1500	U1505	C1506	A1507	G1508	A1509	A1510	U1513	C1514	C1515	C1516	U1519	U1520	U1521	C1522	C1523	C1524	C1525	U1526	G1527	C1528	C1529	U1530	C1531	A1532	C1533	A1534	C1535	U1539	C1540	C1541	G1542	G1543	C1544	C1545	C1546	U1547	U1548	C1549	C1550	C1551	C1552	C1553	C1554	U1559	A1560	A1561	A1562	C1563	U1564			
C1422	U1426	G1427	G1428	A1429	G1430	U1431	G1432	A1433	U1434	A1437	G1438	A1441	C1442	G1443	C1444	A1445	U1446	U1447	A1448	C1451	U1454	U1458	U1459	G1460	C1461	G1465	C1466	C1467	A1468	U1469	G1470	C1471	C1472	C1473	U1474	U1475	G1476	U1477	U1478	U1482	C1483	C1487	G1488	C1489	U1490	C1491	A1492	A1493	G1494	C1495						
C1346	C1347	G1350	G1351	G1352	A1353	A1354	A1355	G1356	U1357	C1358	C1363	C1364	U1365	A1366	A1367	G1368	G1373	A1378	A1379	C1380	G1381	G1384	C1385	C1388	C1389	C1390	A1391	C1392	G1393	C1396	A1397	G1398	C1399	U1403	C1404	A1405	A1406	U1407	U1408	U1409	U1410	C1411	C1412	U1413	C1414	C1415	A1416	C1417	C1418	U1421						
U1276	G1277	A1278	G1279	U1280	A1281	A1282	C1283	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	A1292	A1297	G1298	A1299	A1300	U1301	C1302	U1303	U1304	C1305	U1306	U1307	C1310	C1311	C1312	U1313	A1314	A1315	C1319	G1324	U1325	U1326	C1327	C1328	U1329	G1330	G1333	A1334	A1335	G1336	G1337	G1338	U1339	C1340	G1341	U1342	C1343	C1344	G1345		
G1121	A1122	U1123	U1124	C1127	C1128	A1129	U1130	G1131	C1132	G1133	C1134	C1135	G1136	A1137	A1138	A1139	U1140	U1141	G1142	A1143	U1144	C1145	G1146	G1149	C1150	U1151	C1152	A1153	A1154	G1155	U1161	C1164	A1167	G1168	C1169	U1170	A1171	U1172	G1173	G1174	C1181	U1182	C1183	G1184	C1185	G1186	A1187	A1188	G1189	C1190	G1191	A1192	C1193			
A1055	U1056	A1057	G1058	A1059	C1060	C1063	C1064	G1067	A1068	A1069	G1070	U1071	U1072	G1073	G1074	C1075	U1076	U1077	A1078	A1081	C1082	C1083	A1084	G1085	C1086	C1087	U1015	C1088	C1089	C1090	C1091	U1092	U1093	C1094	A1095	A1096	A1097	G1098	A1099	G1100	G1104	U1105	A1108	A1109	G1110	C1111	C1112	C1113	A1114	C1115	U1116	G1117	U1118	U1119	C1120	
G983	A984	A985	A986	G989	A990	C993	A994	A995	C998	A999	G1000	A1001	C1002	C1003	A1004	U1005	C1006	G1007	G1008	C1009	U1010	A1011	A1012	G1013	C1014	C1015	C1016	C1017	C1018	U1019	A1022	U1023	G1024	G1028	C1029	U1030	C1031	A1032	G1033	C1034	G1035	U1036	U1037	U1038	A1043	U1044	C1049	G1050	U1051	C1052	C1054					
A774	U775	A776	A777	G778	U779	U780	G781	U784	A785	U786	G787	G788	G789	A790	U791	G792	G793	A794	A795	A796	A797	A798	G799	U800	A801	A802	C803	C804	G805	A806	C809	U810	C811	C812	A813	C814	A815	C816	U817	C818	C819	U820	A821	G822	U823	U824	C825	U826	C827	C828	C829	C830	G831	A832	A833	U835
A698	G699	C700	U701	A702	U707	C711	A712	G713	G714	A719	A720	C723	C724	C725	G728	A729	C730	A731	G732	G736	C737	G738	G739	G742	A743	G746	A747	A748	C749	C750	G751	G752	U753	U757	G758	C759	U760	A761	A762	A763	C764	A766	G767	U768	C769	U770	C771	G772	G773							

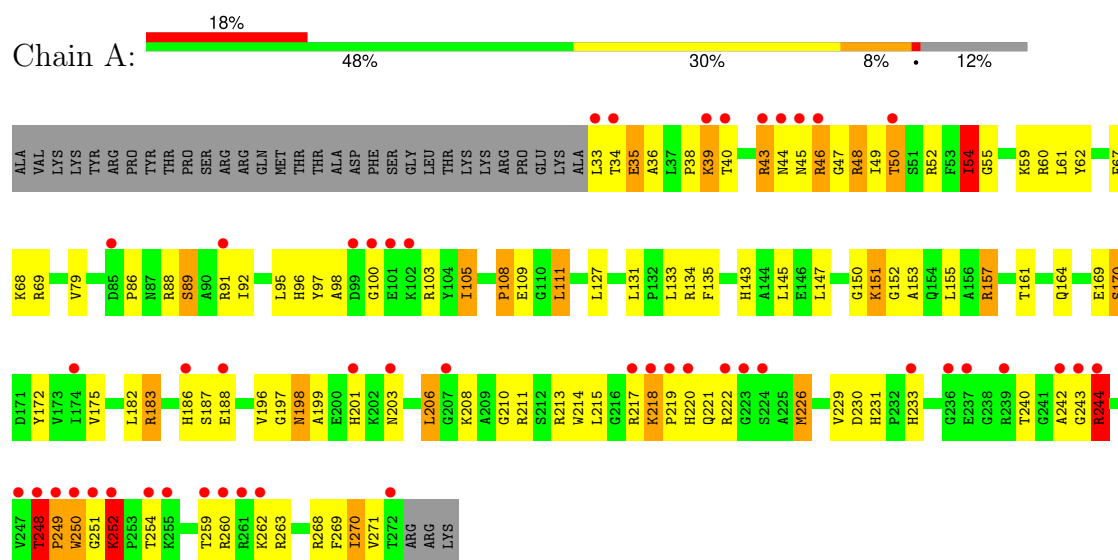




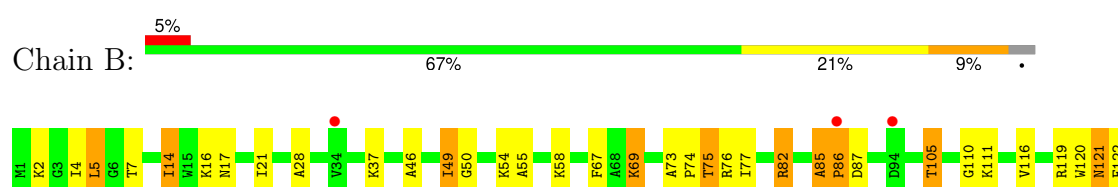
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

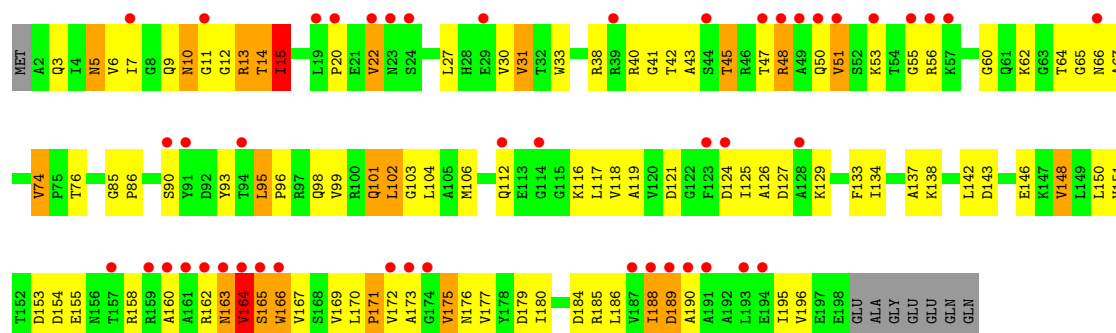


• Molecule 4: 50S ribosomal protein L3

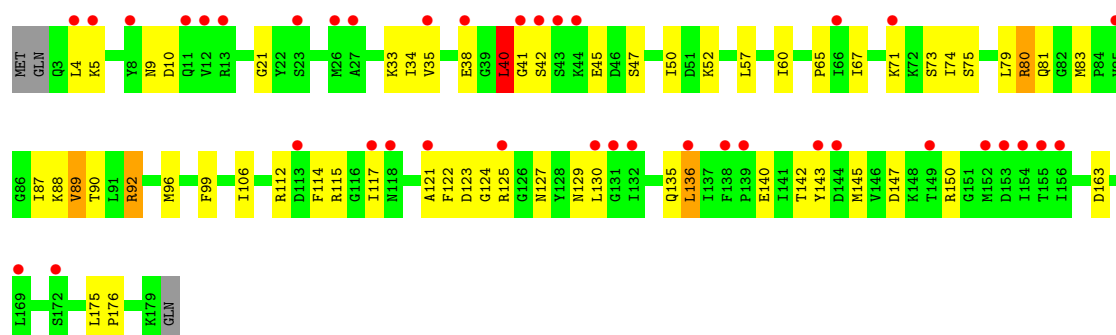




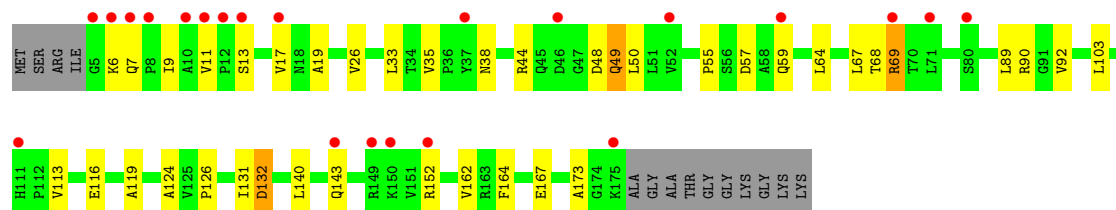
• Molecule 5: 50S ribosomal protein L4



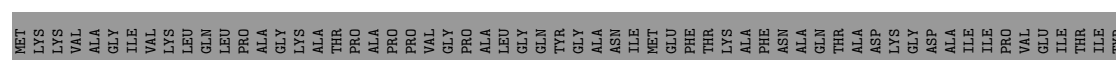
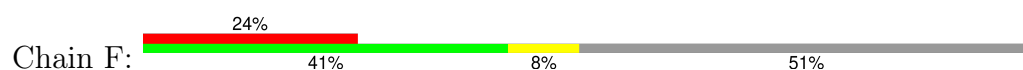
• Molecule 6: 50S ribosomal protein L5

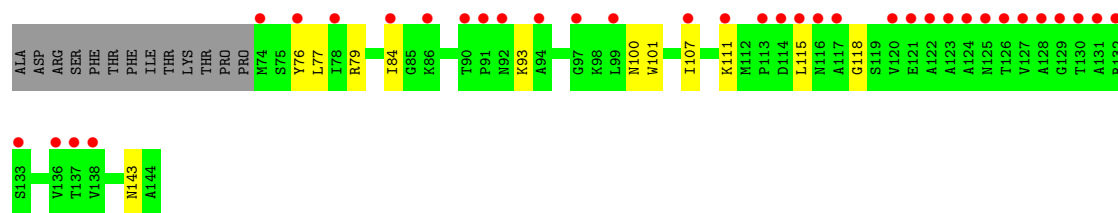


• Molecule 7: 50S ribosomal protein L6

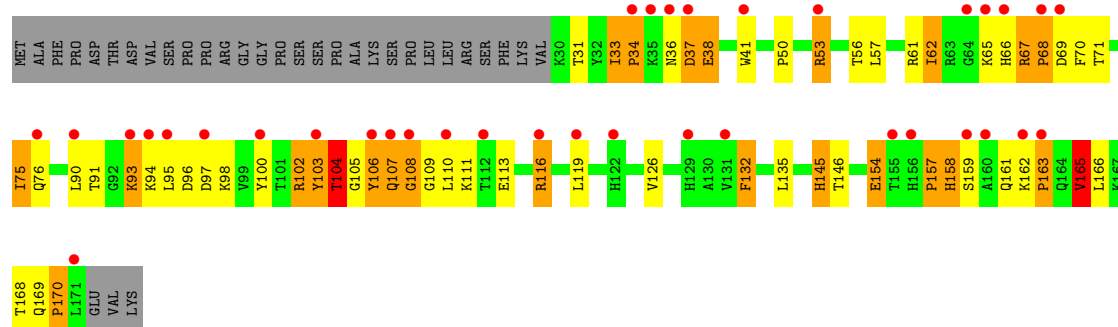


• Molecule 8: 50S ribosomal protein L11

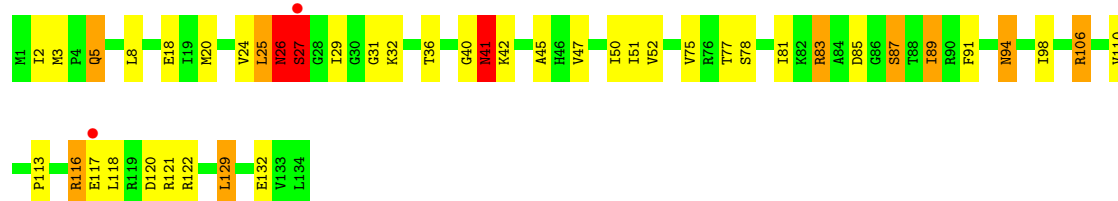




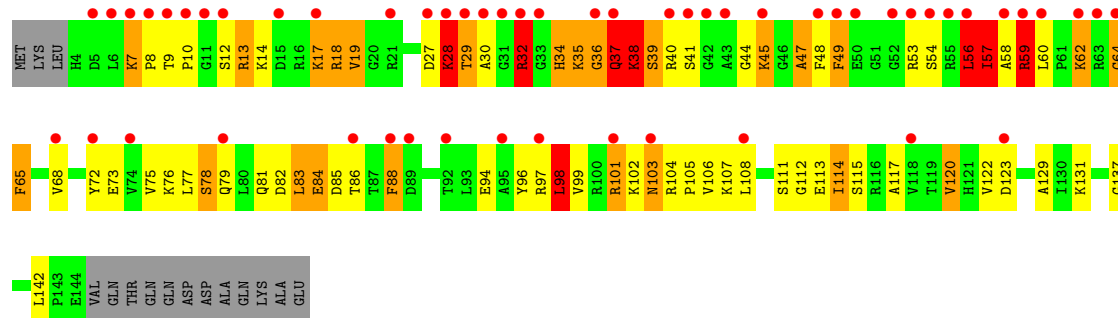
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

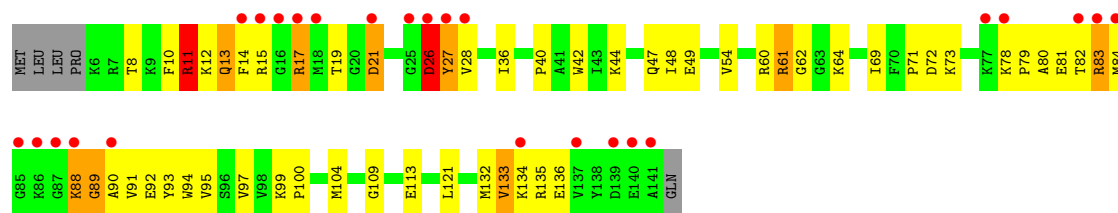


• Molecule 11: 50S ribosomal protein L15

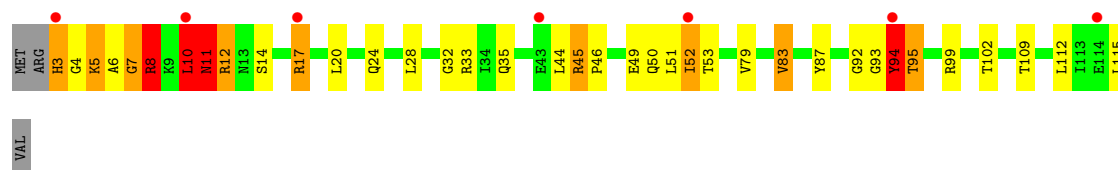


• Molecule 12: 50S ribosomal protein L16

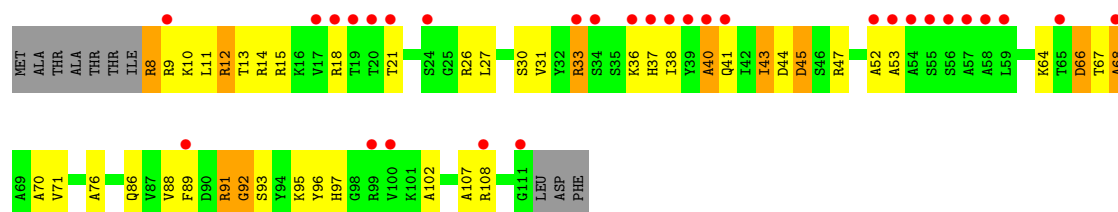




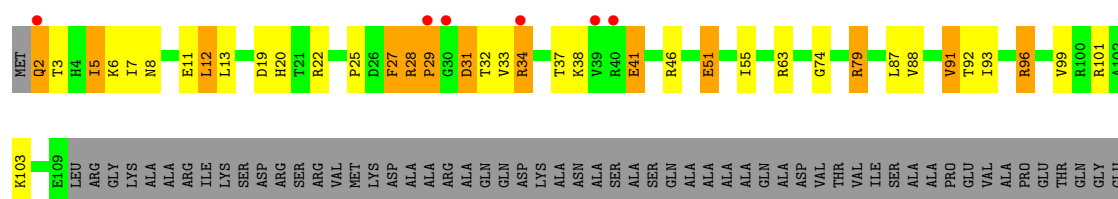
• Molecule 13: 50S ribosomal protein L17



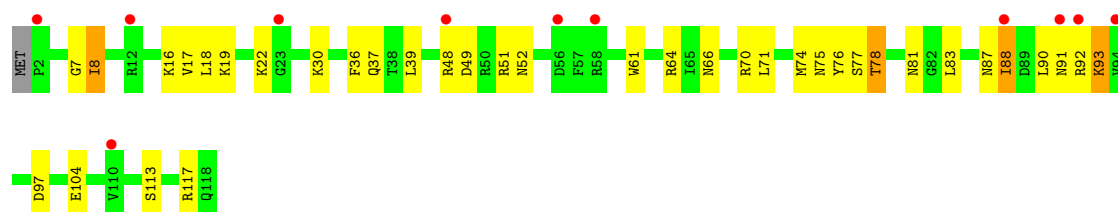
• Molecule 14: 50S ribosomal protein L18



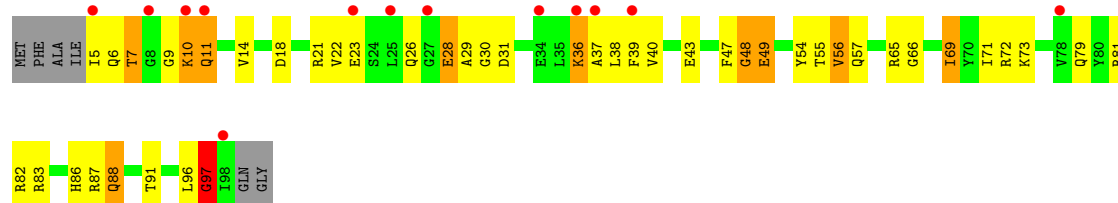
• Molecule 15: 50S ribosomal protein L19



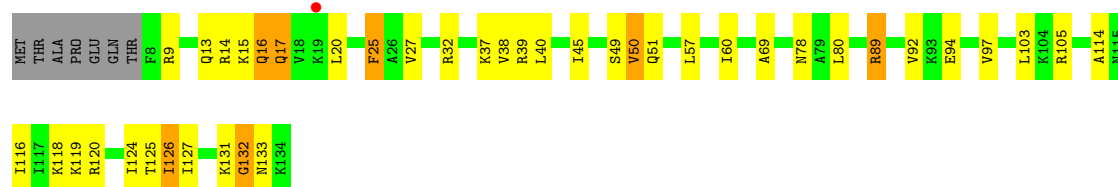
• Molecule 16: 50S ribosomal protein L20



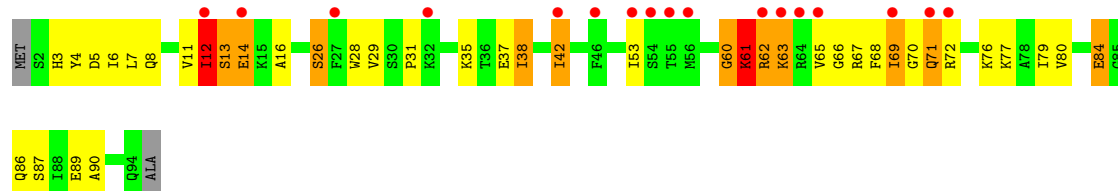
• Molecule 17: 50S ribosomal protein L21



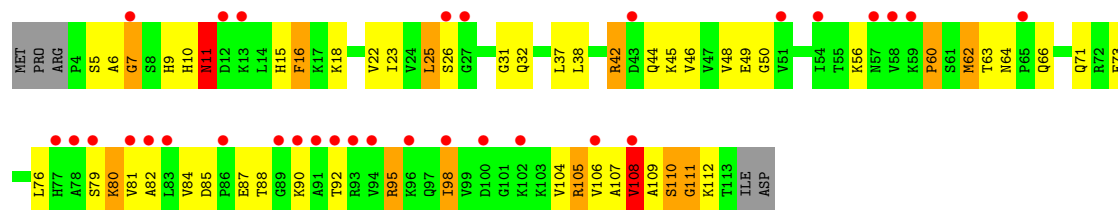
- Molecule 18: 50S ribosomal protein L22



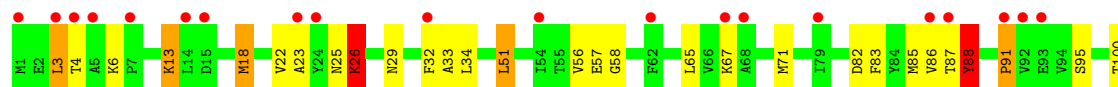
- Molecule 19: 50S ribosomal protein L23

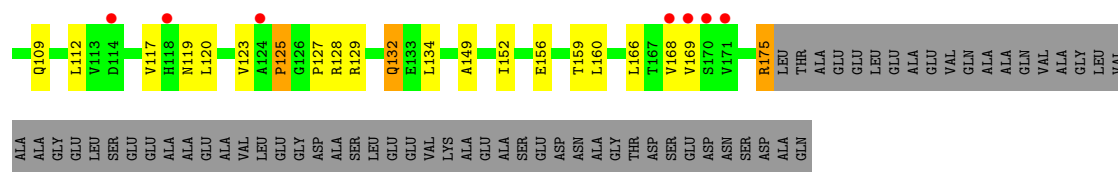


- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

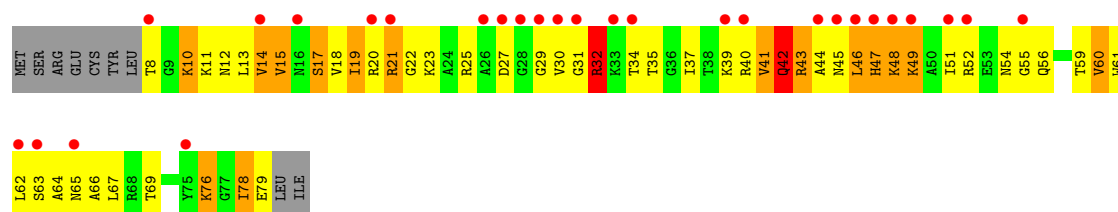




• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



• Molecule 25: 50S ribosomal protein L30

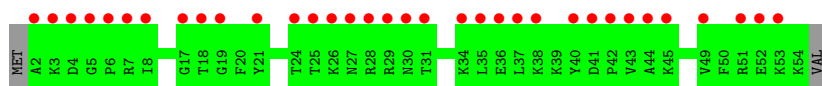


• Molecule 26: 50S ribosomal protein L32

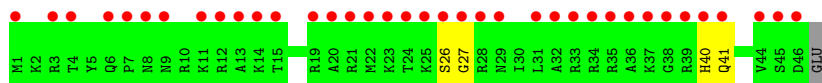
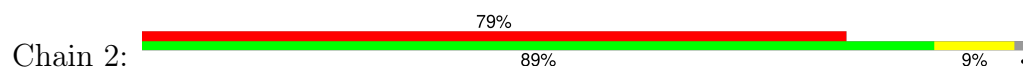


• Molecule 27: 50S ribosomal protein L33

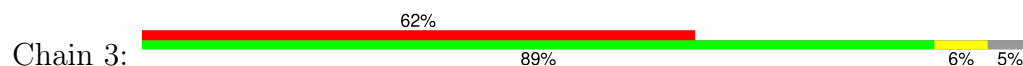




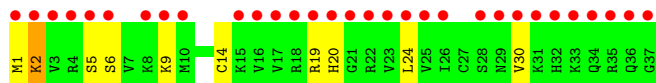
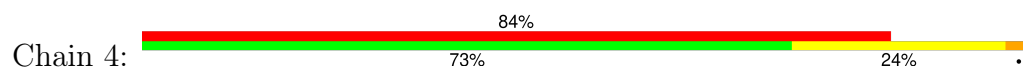
- Molecule 28: 50S ribosomal protein L34



- 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 , 84.0	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: 1F3, MG

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	1.00	38/64561 (0.1%)	1.86	1965/100708 (2.0%)
2	Y	1.02	0/2904	1.68	66/4525 (1.5%)
3	A	0.62	0/1862	0.96	2/2510 (0.1%)
4	B	0.60	0/1567	0.96	2/2105 (0.1%)
5	C	0.63	0/1529	0.95	1/2070 (0.0%)
6	D	0.47	0/1419	0.67	0/1903
7	E	0.44	0/1308	0.68	0/1771
8	F	0.47	0/508	0.64	0/683
9	G	0.64	0/1138	1.01	4/1539 (0.3%)
10	H	0.55	0/1007	0.84	1/1352 (0.1%)
11	I	0.73	0/1081	1.11	8/1448 (0.6%)
12	J	0.65	0/1113	0.92	2/1486 (0.1%)
13	K	0.80	2/886 (0.2%)	0.99	3/1188 (0.3%)
14	L	0.57	0/785	0.95	1/1048 (0.1%)
15	M	0.65	1/884 (0.1%)	0.98	2/1186 (0.2%)
16	N	0.51	0/994	0.78	0/1323
17	O	0.56	0/750	0.96	1/1000 (0.1%)
18	P	0.56	0/1027	0.82	0/1373
19	Q	0.62	0/737	1.04	4/988 (0.4%)
20	R	0.64	0/835	0.99	0/1121
21	S	0.49	0/1370	0.73	0/1862
22	T	0.53	0/633	0.85	0/838
23	U	0.75	0/556	1.12	2/741 (0.3%)
24	V	0.47	0/537	0.69	0/714
25	W	0.46	0/426	0.79	0/568
26	Z	0.65	0/469	0.97	0/629
30	4	0.48	0/298	0.72	0/390
All	All	0.91	41/91184 (0.0%)	1.68	2064/137069 (1.5%)

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 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	540	G	C2-N3	9.96	1.40	1.32
1	X	774	A	C5-C4	9.11	1.45	1.38
1	X	774	A	N7-C5	-7.92	1.34	1.39
1	X	2018	G	N9-C8	7.57	1.43	1.37
1	X	542	A	N7-C5	-7.47	1.34	1.39

The worst 5 of 2064 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-38.76	78.89	109.90
1	X	1288	A	C5'-C4'-O4'	20.93	134.22	109.10
1	X	1716	G	P-O3'-C3'	19.09	142.60	119.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	2808	U	O4'-C1'-N1	17.91	122.53	108.20

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	431	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	62	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	22	0
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	63	0
10	H	997	0	1046	24	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	28	0
14	L	779	0	820	17	0
15	M	871	0	894	29	0
16	N	978	0	1020	25	0
17	O	741	0	756	30	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	23	0
20	R	825	0	881	28	0
21	S	1345	0	1372	21	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	4	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	5	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	969	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 969 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%)	144 (78%)	41 (22%)	1	4
4	B	155/157 (99%)	135 (87%)	20 (13%)	3	17
5	C	157/163 (96%)	125 (80%)	32 (20%)	1	5
6	D	153/156 (98%)	129 (84%)	24 (16%)	2	10
7	E	136/144 (94%)	117 (86%)	19 (14%)	3	14
8	F	51/107 (48%)	46 (90%)	5 (10%)	6	27
9	G	118/146 (81%)	95 (80%)	23 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	5
11	I	108/121 (89%)	72 (67%)	36 (33%)	0	0
12	J	110/115 (96%)	93 (84%)	17 (16%)	2	10
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%)	75 (80%)	19 (20%)	1	5
16	N	96/97 (99%)	81 (84%)	15 (16%)	2	10
17	O	75/79 (95%)	60 (80%)	15 (20%)	1	5
18	P	109/115 (95%)	94 (86%)	15 (14%)	3	14
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	5
20	R	91/96 (95%)	71 (78%)	20 (22%)	1	4
21	S	149/192 (78%)	126 (85%)	23 (15%)	2	11
22	T	62/67 (92%)	53 (86%)	9 (14%)	2	13
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	44 (82%)	10 (18%)	1	7
25	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
26	Z	51/53 (96%)	37 (72%)	14 (28%)	0	1
30	4	35/35 (100%)	31 (89%)	4 (11%)	4	21
All	All	2436/2715 (90%)	1967 (81%)	469 (19%)	1	6

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	64	LYS
25	W	9	VAL
15	M	37	THR
24	V	41	HIS
22	T	16	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
17	O	11	GLN
18	P	81	HIS
26	Z	43	HIS

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Mol	Chain	Res	Type
17	O	79	GLN
18	P	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	638 (23%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)
All	All	2802/3003 (93%)	666 (23%)	243 (8%)

5 of 666 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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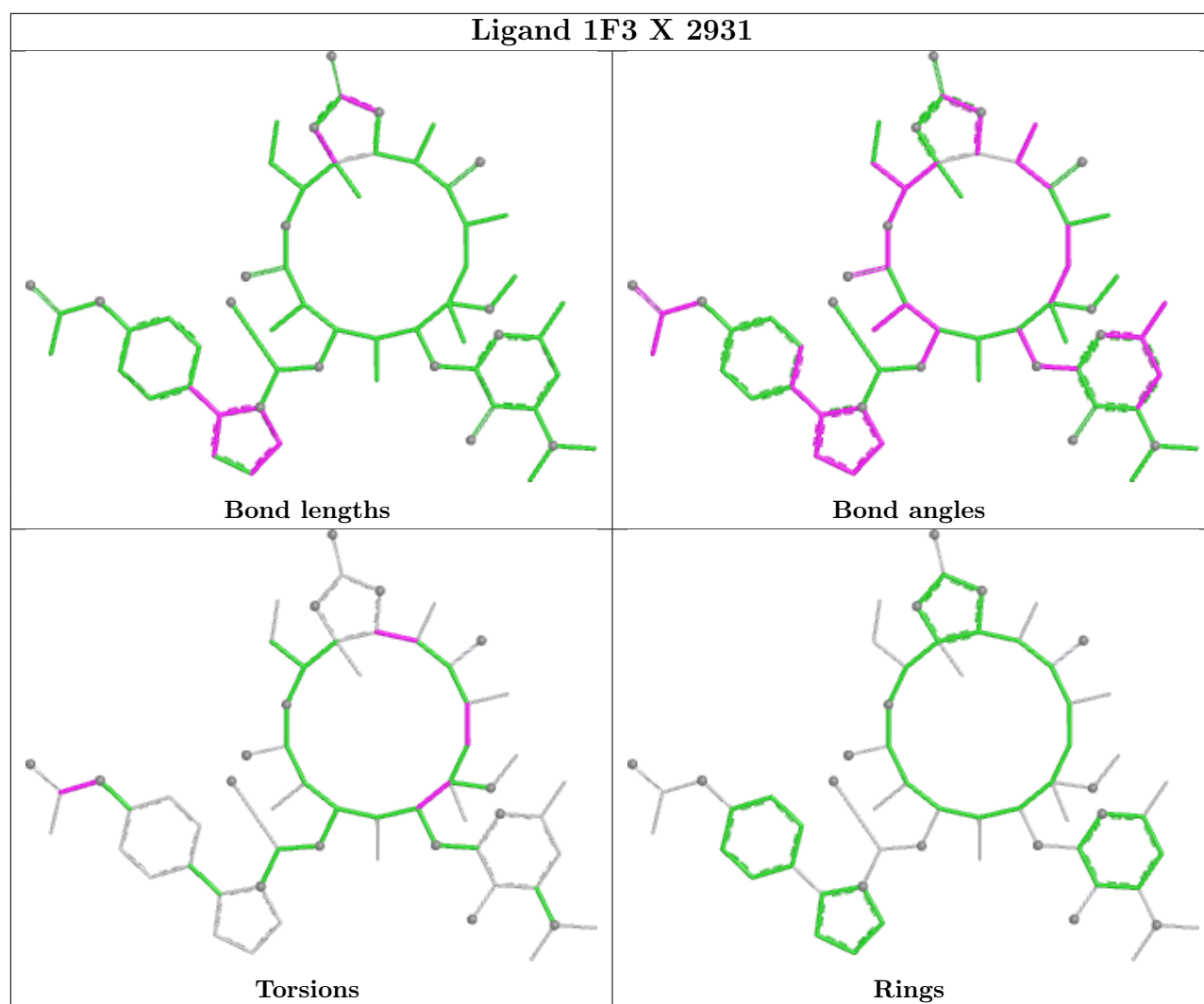
Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	O60-C58-N57-C54
32	X	2931	1F3	C16-C1-C4-N40
32	X	2931	1F3	O20-C8-C9-C7
32	X	2931	1F3	C3-C2-C7-C9

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	127 (4%) 37 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%)	2.40	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%)	0.90	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	17 (18%) 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	27 (15%) 6 5	119, 154, 178, 190	0
22	T	84/91 (92%)	1.05	16 (19%) 4 3	72, 103, 176, 195	0
23	U	72/81 (88%)	1.96	28 (38%) 1 1	86, 122, 146, 182	0
24	V	66/67 (98%)	0.70	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%)	5.12	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%)	5.53	31 (83%)	0 0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.71	795 (13%)	8 6	3, 96, 193, 279	0

The worst 5 of 795 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	51.0
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.

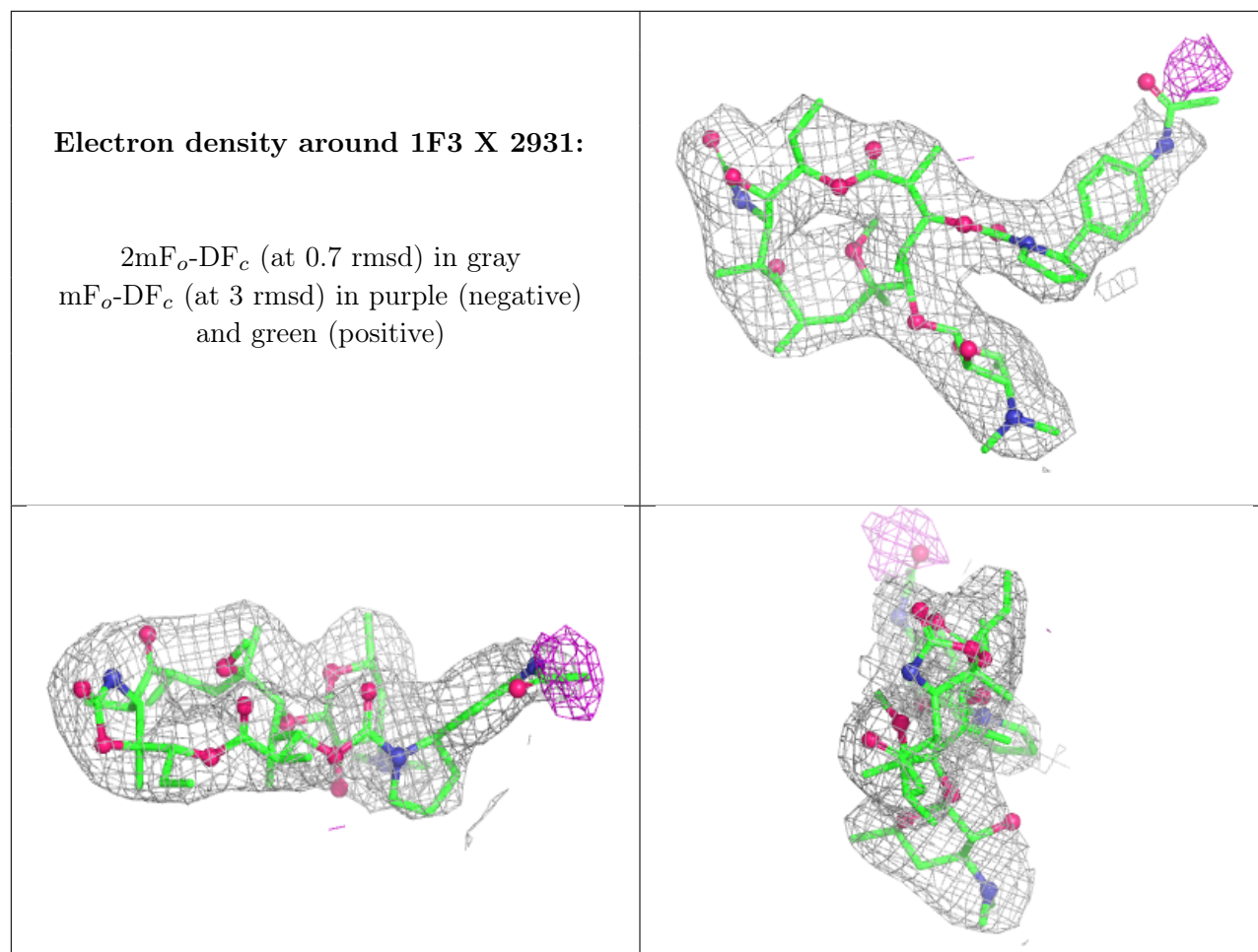
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2922	1/1	0.53	0.83	81,81,81,81	0
31	MG	X	2904	1/1	0.61	0.87	90,90,90,90	0
31	MG	X	2930	1/1	0.80	1.19	71,71,71,71	0
31	MG	X	2910	1/1	0.82	0.43	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	2912	1/1	0.84	0.31	60,60,60,60	0
31	MG	Y	205	1/1	0.84	0.12	77,77,77,77	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	2929	1/1	0.87	0.35	77,77,77,77	0
31	MG	X	2907	1/1	0.87	0.38	53,53,53,53	0
31	MG	X	2911	1/1	0.87	0.34	35,35,35,35	0
31	MG	X	2926	1/1	0.88	0.51	56,56,56,56	0
31	MG	X	2908	1/1	0.89	0.39	49,49,49,49	0
31	MG	Y	201	1/1	0.89	0.63	82,82,82,82	0
31	MG	X	2925	1/1	0.89	0.49	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.