



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:26 AM UTC

PDB ID : 4V4I / pdb_00004v4i
Title : Crystal Structure of a 70S Ribosome-tRNA Complex Reveals Functional Interactions and Rearrangements.
Authors : Korostelev, A.; Trakhanov, S.; Laurberg, M.; Noller, H.F.
Deposited on : 2007-02-15
Resolution : 3.71 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

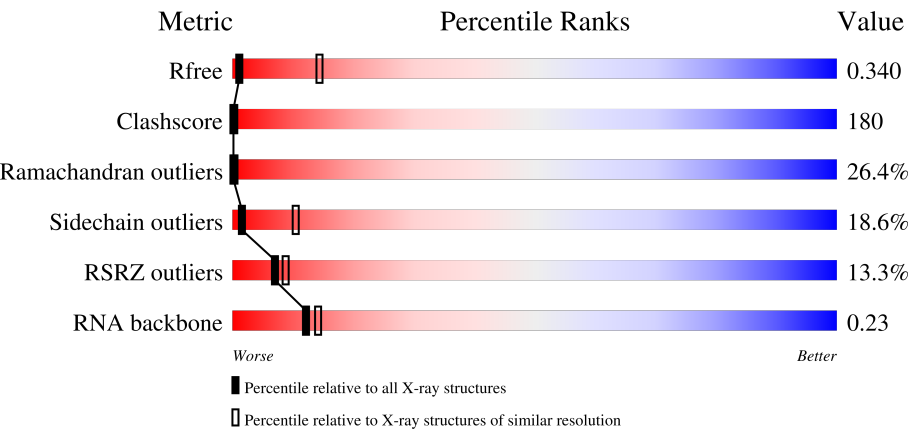
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	w	2889	11% 56% 38%
2	x	121	6% 62% 36%
3	A	229	5% 32% 16% 45%
4	B	276	25% 54% 36% 5%

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Mol	Chain	Length	Quality of chain
5	C	206	
6	D	205	
7	E	182	
8	F	180	
9	G	148	
10	H	163	
11	I	122	
12	J	150	
13	K	141	
14	L	118	
15	M	112	
16	N	146	
17	O	118	
18	P	101	
19	Q	113	
20	R	96	
21	S	110	
22	T	206	
23	U	85	
24	V	98	
25	W	72	
26	X	60	
27	Y	60	
28	Z	49	
29	a	65	

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Mol	Chain	Length	Quality of chain
30	b	37	
31	y	1522	
32	z	76	
33	0	76	
34	1	10	
35	c	256	
36	d	239	
37	e	209	
38	f	162	
39	g	101	
40	h	156	
41	i	138	
42	j	128	
43	k	105	
44	l	129	
45	m	132	
46	n	126	
47	o	61	
48	p	89	
49	q	88	
50	r	105	
51	s	88	
52	t	93	
53	u	106	
54	v	27	

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	2MG	y	1207	-	-	X	-
31	5MC	y	1400	-	-	X	-
31	4OC	y	1402	-	-	X	-
31	5MC	y	1407	-	-	X	-
31	UR3	y	1498	-	-	X	-
31	MA6	y	1518	-	-	X	-
31	MA6	y	1519	-	-	X	-
31	PSU	y	516	-	-	X	-
31	5MC	y	967	-	-	X	-
32	PSU	z	39	-	-	X	-
32	7MG	z	46	-	-	X	-
32	5MU	z	54	-	-	X	-
32	PSU	z	55	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 146532 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 LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	2889	Total	C	N	O	P	0	0	0
			62213	27690	11624	20011	2888			

- Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	x	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	127	Total	C	N	O	S	0	0	0
			996	627	184	184	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	201	Total	C	N	O	S	0	0	0
			1541	974	295	267	5			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	194	Total	C	N	O	S	0	0	0
			1517	969	283	263	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	180	Total	C	N	O	S	0	0	0
			1468	938	267	259	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	173	Total	C	N	O	S	0	0	0
			1319	839	245	234	1			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	148	Total	C	N	O	S	0	0	0
			1156	737	204	214	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1103	712	206	182	3			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	137	Total	C	N	O	S	0	0	0
			1089	698	207	177	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	106	Total	C	N	O	S	0	0	0
			846	534	168	144				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	109	Total	C	N	O	S	0	0	0
			868	547	170	150	1			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	103	Total	C	N	O	S	0	0	0
			793	510	151	126	6			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	185	Total	C	N	O	S	0	0	0
			1475	941	262	269	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	88	Total	C	N	O		0	0	0
			694	435	141	118				

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	56	Total	C	N	O	S	0	0	0
			436	275	84	72	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	a	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	b	35	Total	C	N	O	S	0	0	0
			294	181	66	44	3			

- Molecule 31 is a RNA chain called 16S SMALL SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1502	Total	C	N	O	P	0	0	0
			32302	14386	5984	10431	1501			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	450	G	C	conflict	GB 155076
y	516	PSU	U	modified residue	GB 155076
y	527	7MG	G	modified residue	GB 155076
y	966	M2G	G	modified residue	GB 155076
y	967	5MC	C	modified residue	GB 155076
y	1207	2MG	G	modified residue	GB 155076
y	1400	5MC	C	modified residue	GB 155076
y	1402	4OC	C	modified residue	GB 155076
y	1404	5MC	C	modified residue	GB 155076
y	1407	5MC	C	modified residue	GB 155076
y	1498	UR3	U	modified residue	GB 155076
y	1518	MA6	A	modified residue	GB 155076
y	1519	MA6	A	modified residue	GB 155076

- Molecule 32 is a RNA chain called P-site PHE-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	76	Total	C	N	O	P	0	0	0
			1628	731	290	530	75			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	8	4SU	U	modified residue	GB 174422
z	16	H2U	U	modified residue	GB 174422
z	20	H2U	U	modified residue	GB 174422
z	32	PSU	U	modified residue	GB 174422
z	37	MIA	A	modified residue	GB 174422
z	39	PSU	U	modified residue	GB 174422
z	46	7MG	G	modified residue	GB 174422
z	54	5MU	U	modified residue	GB 174422
z	55	PSU	U	modified residue	GB 174422

- Molecule 33 is a RNA chain called E-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	0	76	Total	C	N	O	P	0	0	0
			1621	725	293	528	75			

- Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1	6	Total	C	N	O	P	0	0	0
			122	56	19	42	5			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	c	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	d	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	e	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	f	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	g	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	h	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	i	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	j	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	k	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	l	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	m	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	n	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	o	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	p	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	q	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	r	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	s	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	t	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	u	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

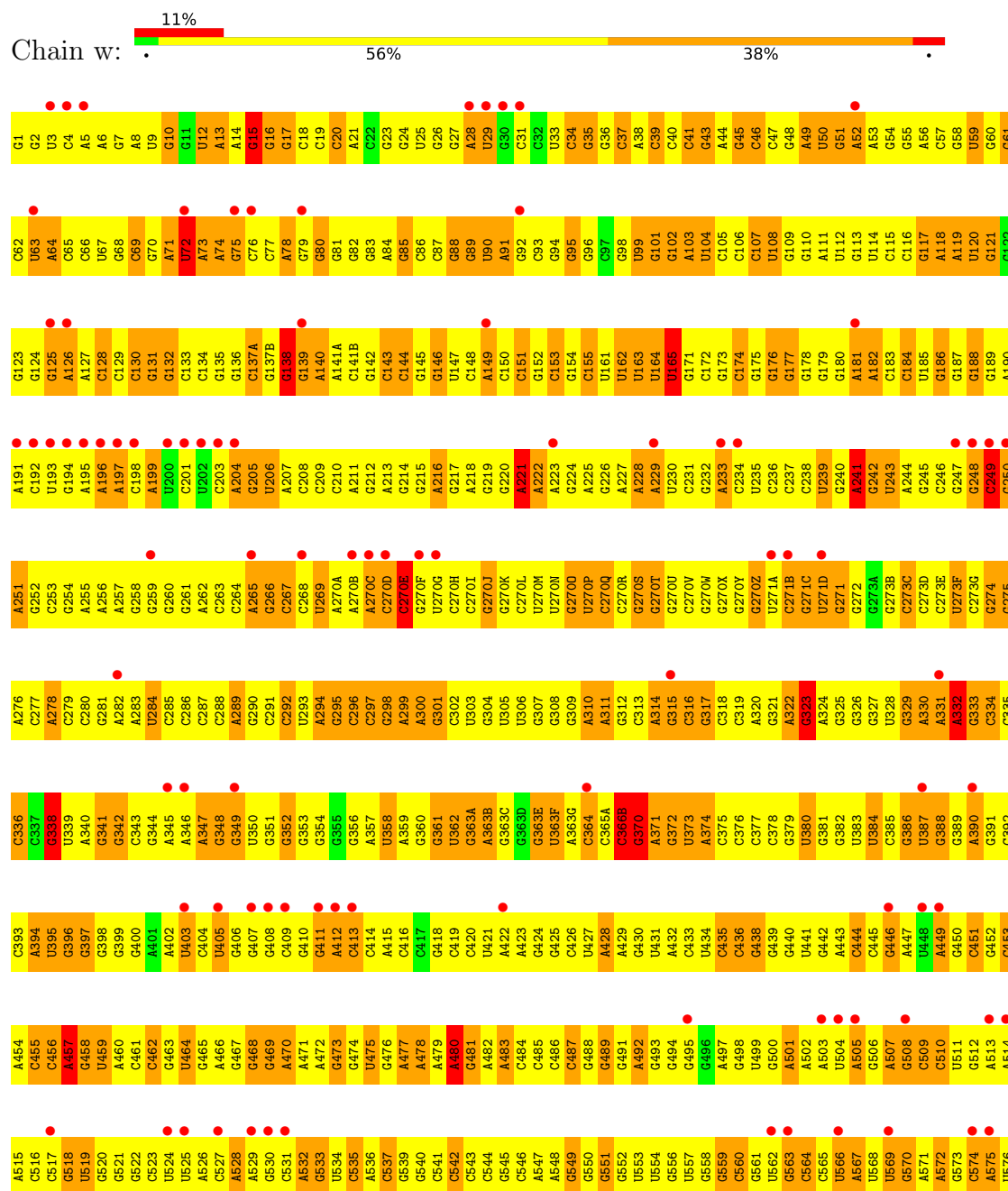
- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	v	24	Total	C	N	O	0	0	0
			208	128	50	30			

3 Residue-property plots [i](#)

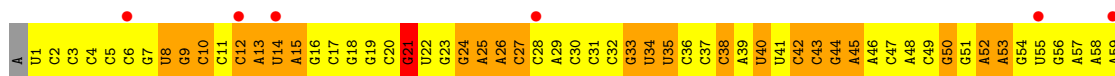
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

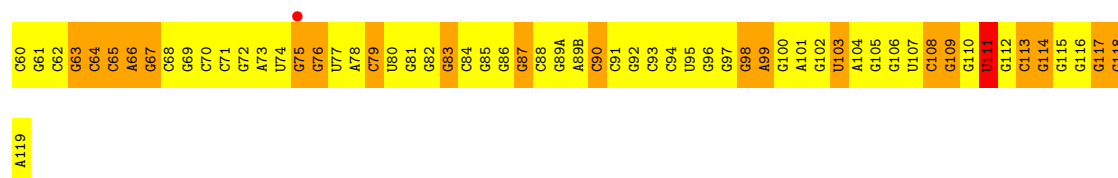
• Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



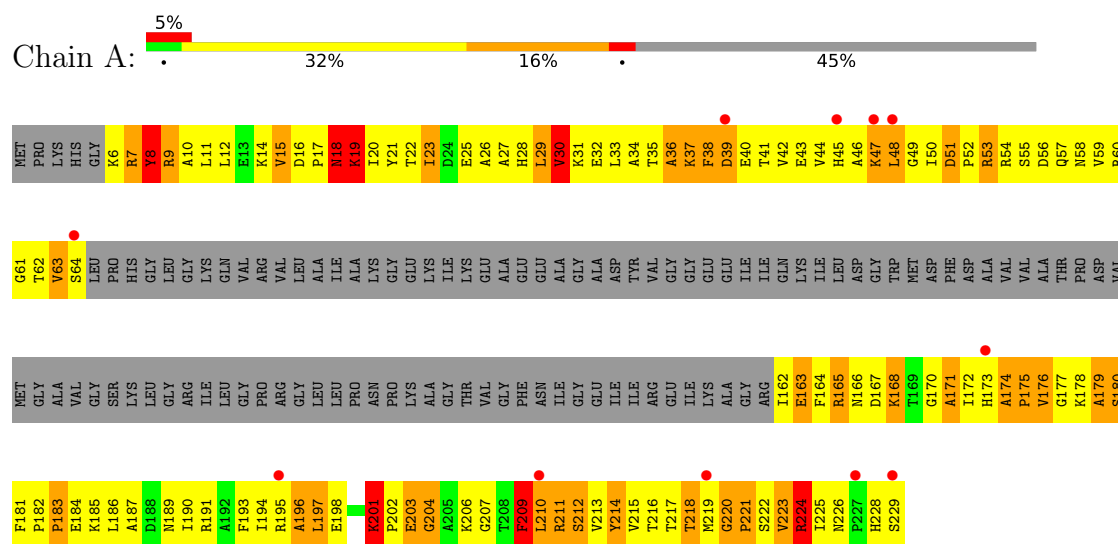
G1356	G1296	G1236	A1177	G1116	G1056	A996	U937	G875	G815	C755	G695	G635	G577
U1357	C1297	A1237	C1178	G1117	A1057	G997	G938	C876	C816	C756	G696	G636	A578
G1358	C1298	G1238	C1179	C1118	G1058	G998	G939	U877	C817	C757	G697	A837	G579
A1359	G1299	G1239	C1180	C1119	G1059	U999	G940	U878	G818	C758	C698	C580	C580
G1360	U1300	A1240	C1181	G1120	U1060	A1000	A941	G879	A819	G759	A699	U639	C581
G1361	A1301	A1241	A1182	G1121	U1061	A1001	G942	G880	A820	G760	G700	C640	G582
C1362	A1302	A1242	G1183	G1122	G1062	G1002	U943	C881	A821	A761	G701	C641	G583
G1363	G1303	G1243	G1184	C1123	G1063	G1003	G944	G882	U822	U762	G702	G642	C584
G1364	C1304	G1244	C1185	G1124	G1064	C1004	A945	G883	G823	G763	U703	A643	G585
A1365	G1305	A1125	G1186	U1065	G1065	C1005	G946	C884	A824	A764	G704	A644	A586
A1366	C1306	A1246	G1187	A1126	U1066	C1006	G947	C885	G825	G765	A705	C587	C587
G1367	A1307	A1247	U1188	A1127	A1067	C1007	G948	C886	U826	G766	A706	A646	U588
G1368	A1308	G1248	A1189	A1128	G1068	C1008	C949	A887	U827	U767	G707	G647	C589
G1369	G1309	U1249	G1190	A1129	A1069	A1009	G950	C888	U828	G768	C708	G648	A590
C1370	G1310	G1250	G1191	U1130	A1070	A1010	C951	C889	A829	G769	U709	G649	C591
G1371	G1311	C1251	G1192	G1131	G1071	G1011	G952	A890	G830	G770	G710	C850	G592
U1372	U1312	G1252	G1193	A1132	C1072	U1012	A953	G892	G831	G771	G711	G651	G593
A1373	U1313	A1253	A1194	U1133	A1073	C1013	G954	C893	G832	C772	G712	U652	U594
G1374	C1314	A1254	G1195	C1135	G1074	U1014	C955	C894	U833	U773	G713	C653	C595
C1375	C1315	U1255	C1196	G1136	C1075	G1015	G956	U895	C834	A774	G714	U654	G596
G1376	U1316	G1256	G1197	G1137	C1076	A957	G957	A896	A835	G775	G715	A655	U597
A1377	A1317	C1257	U1198	G1138	A1077	G1017	A958	C897	G836	G776	A716	G656	G598
G1378	C1318	C1258	U1199	G1139	U1078	C1018	A959	C898	C837	A777	G717	U657	G599
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A1384	G1324	G1264	U1205	G1145	A1084	G1024	C965	G904	G843	A783	C723	G663	C605
G1385	G1325	A1265	G1206	C1146	A1085	U1025	G966	U905	C844	A784	U724	C664	C606
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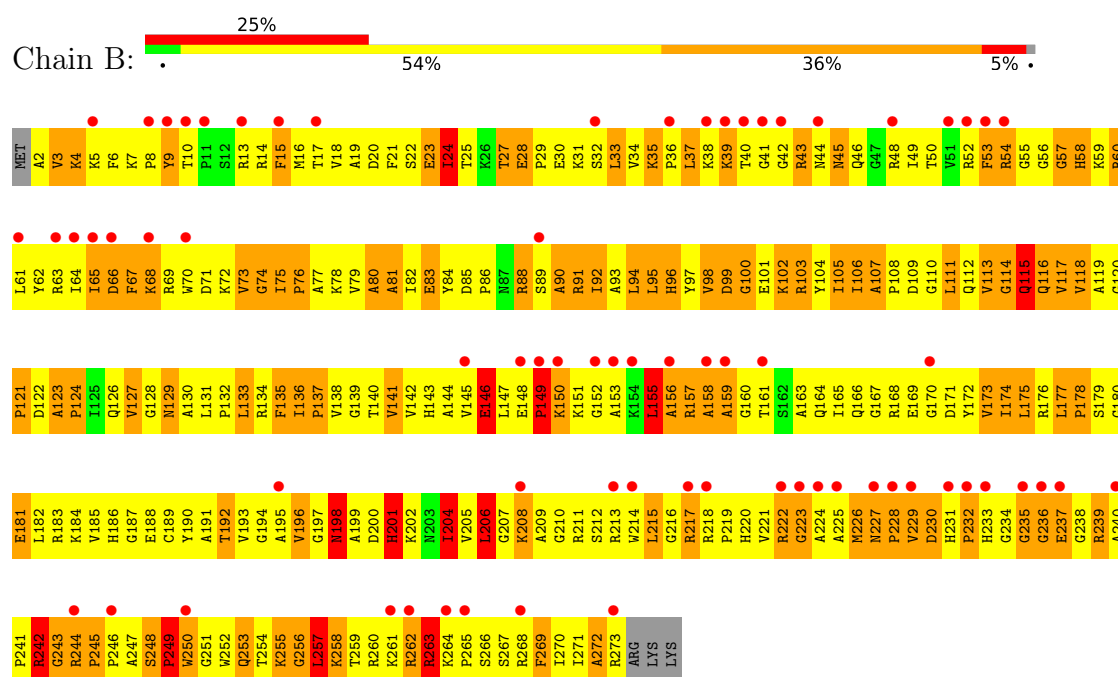




• Molecule 3: 50S ribosomal protein L1

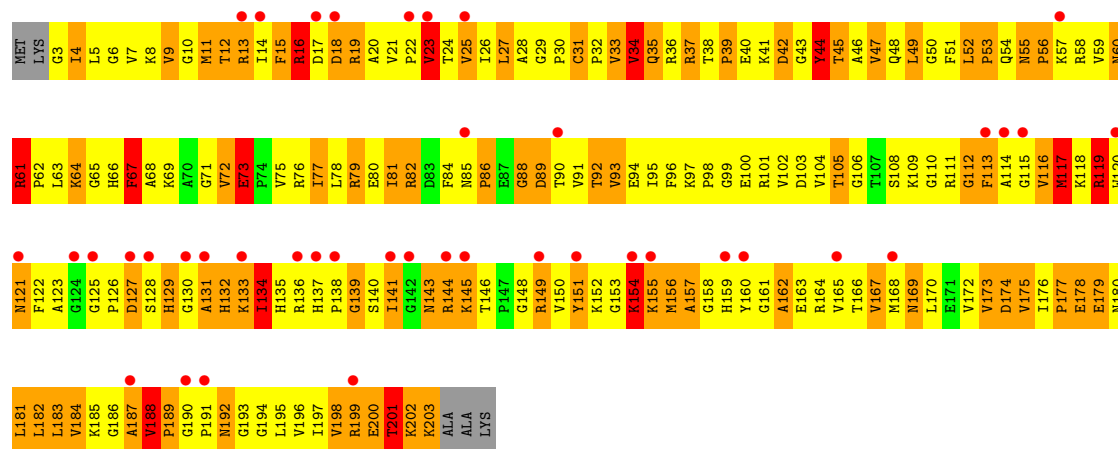


• Molecule 4: 50S ribosomal protein L2

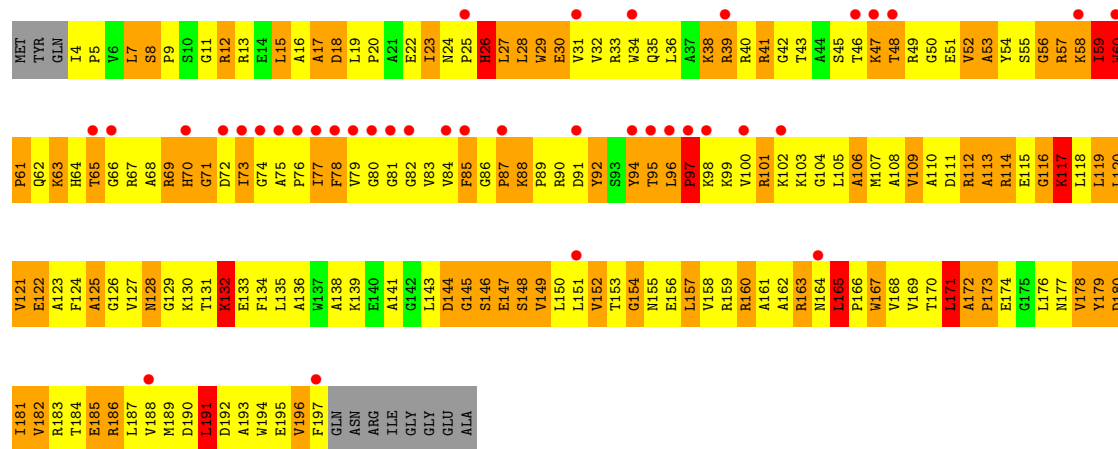


• Molecule 5: 50S ribosomal protein L3

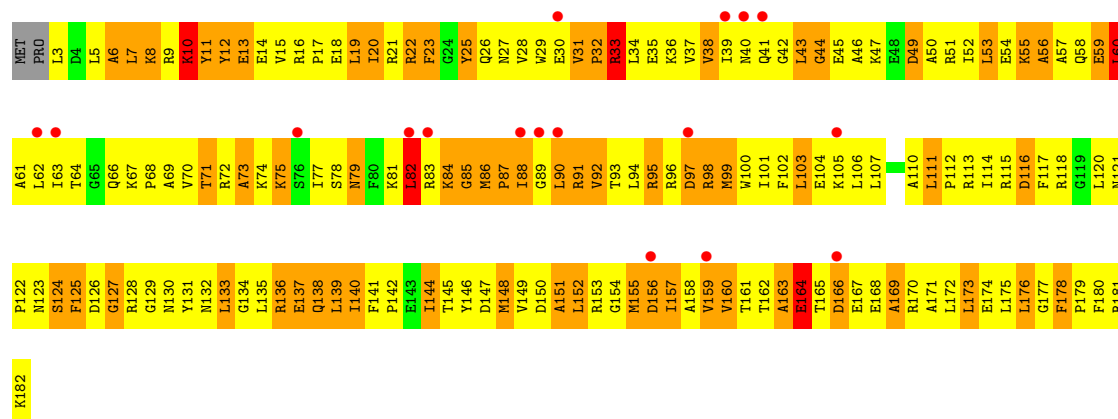




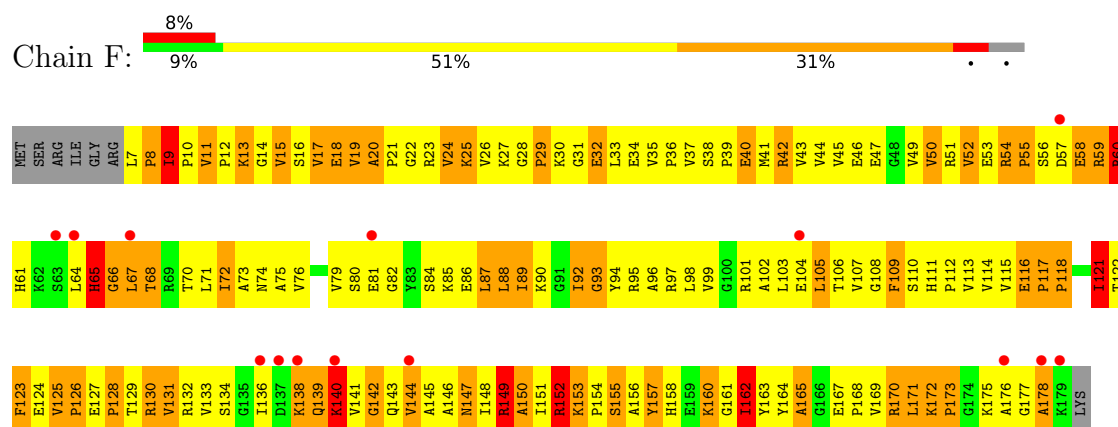
• Molecule 6: 50S ribosomal protein L4



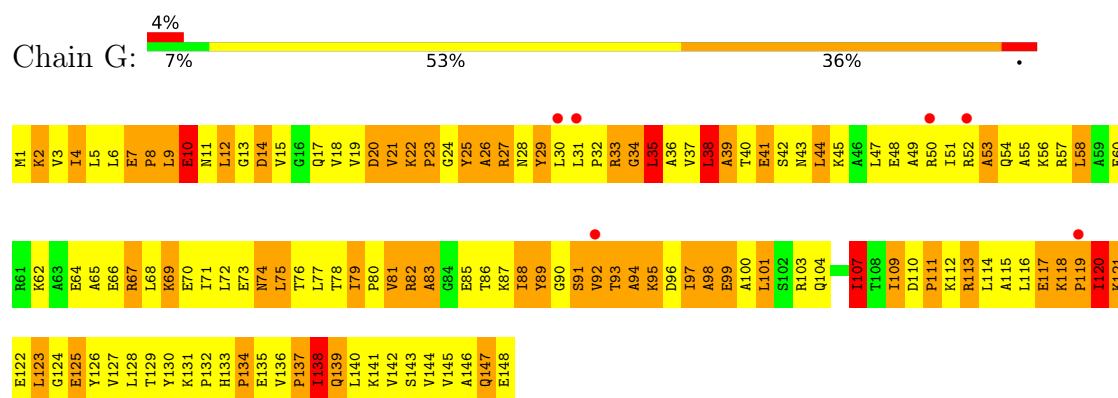
• Molecule 7: 50S ribosomal protein L5



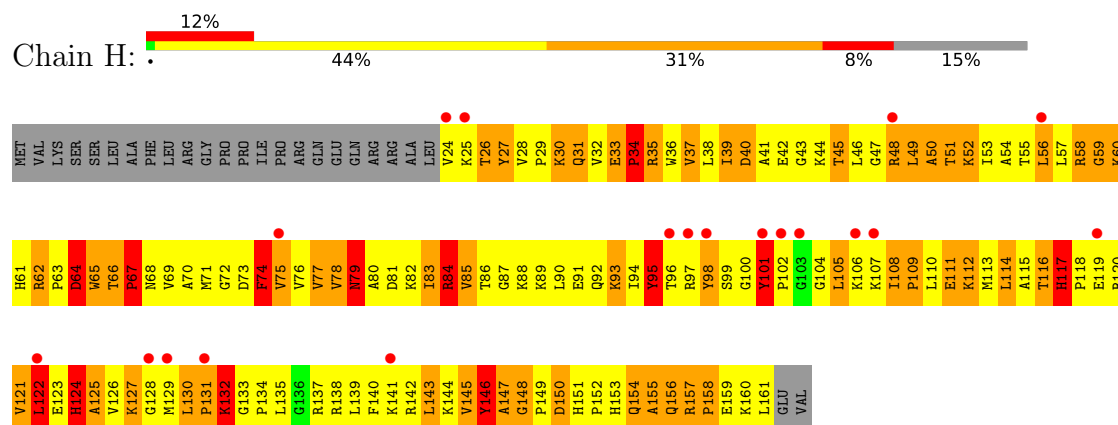
• Molecule 8: 50S ribosomal protein L6



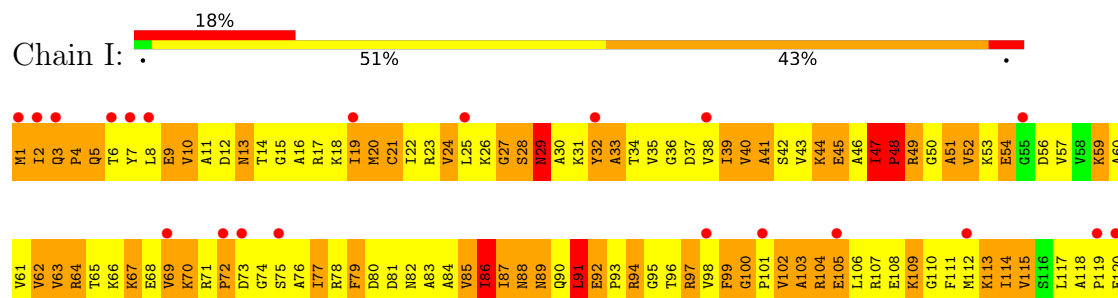
- Molecule 9: 50S ribosomal protein L9



- Molecule 10: 50S ribosomal protein L13

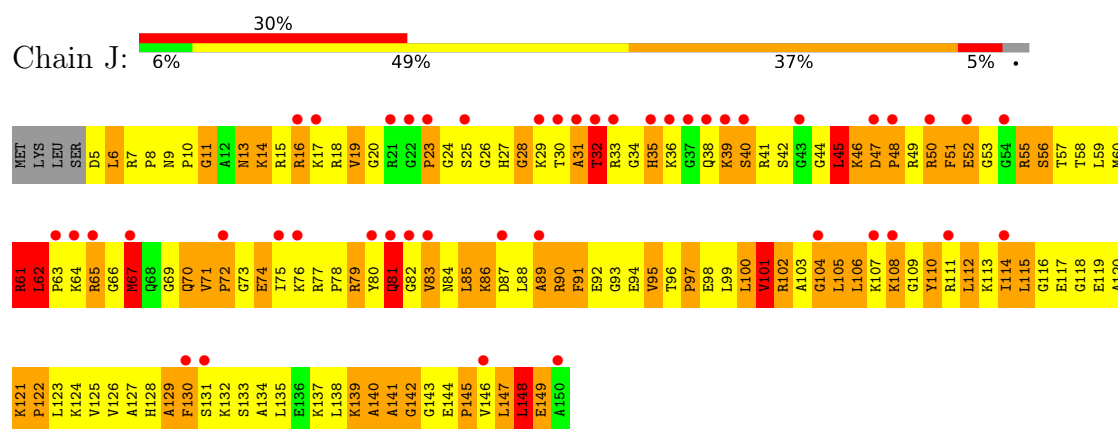


- Molecule 11: 50S ribosomal protein L14

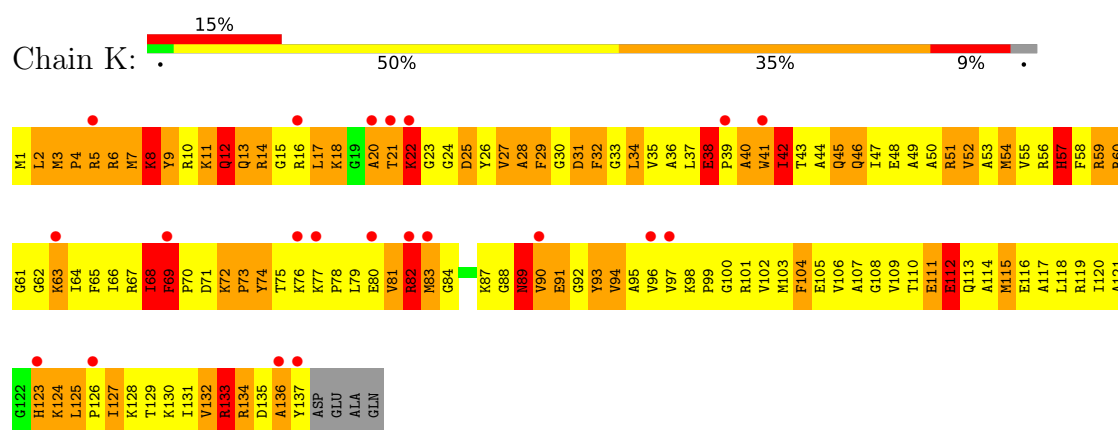


V121
L122

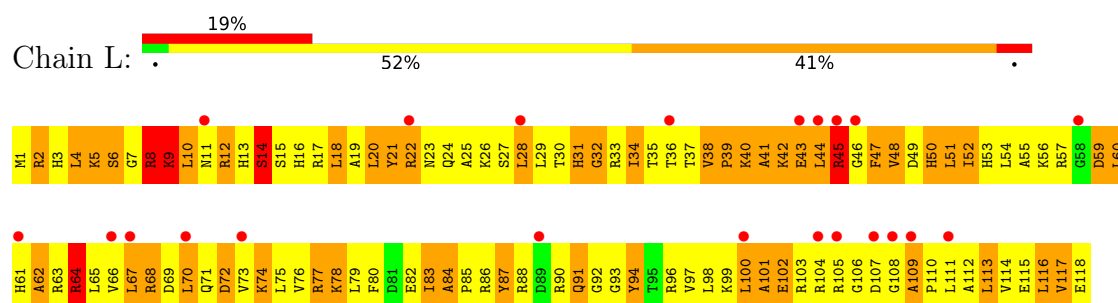
• Molecule 12: 50S ribosomal protein L15



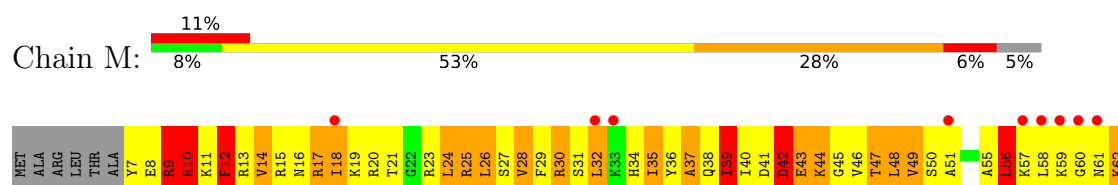
• Molecule 13: 50S ribosomal protein L16

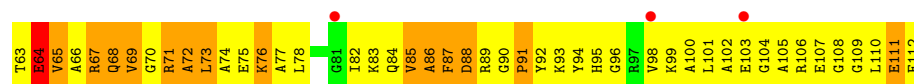


• Molecule 14: 50S ribosomal protein L17

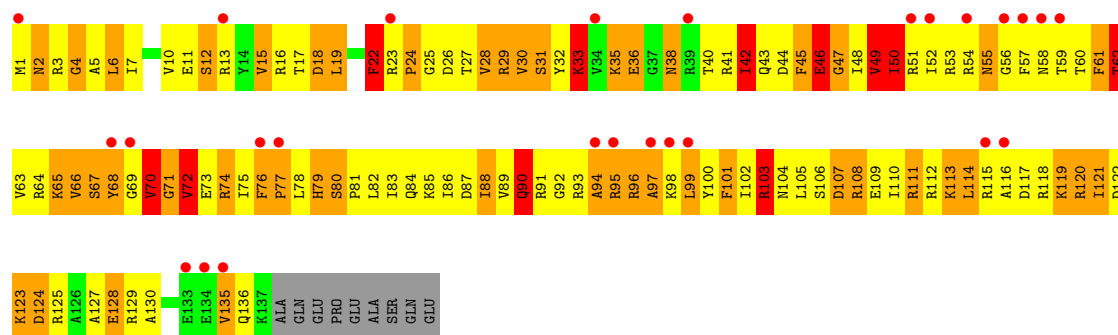


• Molecule 15: 50S ribosomal protein L18

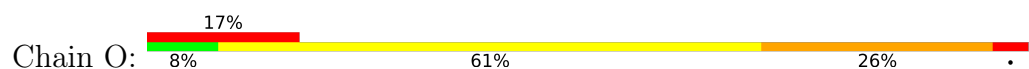




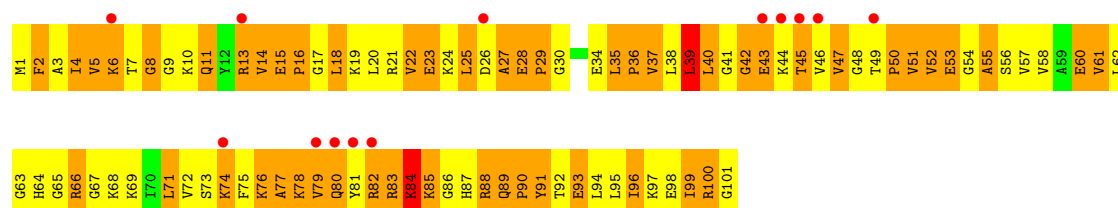
• Molecule 16: 50S ribosomal protein L19



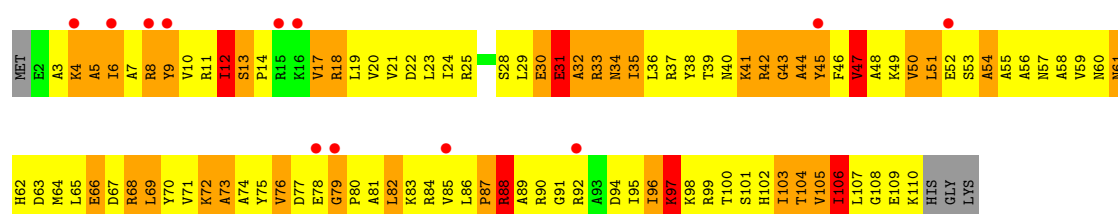
• Molecule 17: 50S ribosomal protein L20



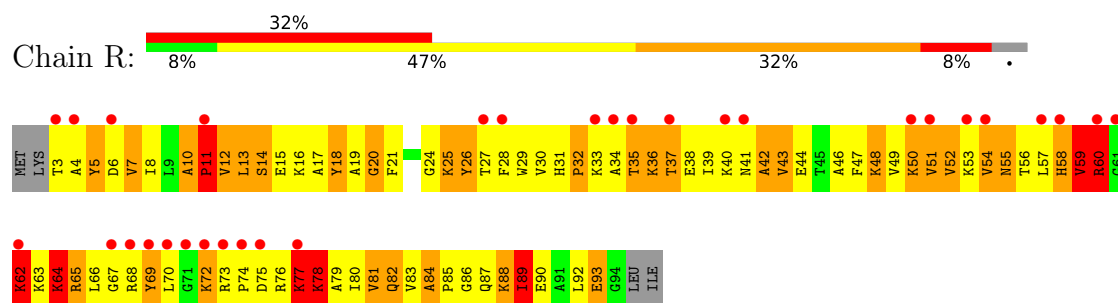
• Molecule 18: 50S ribosomal protein L21



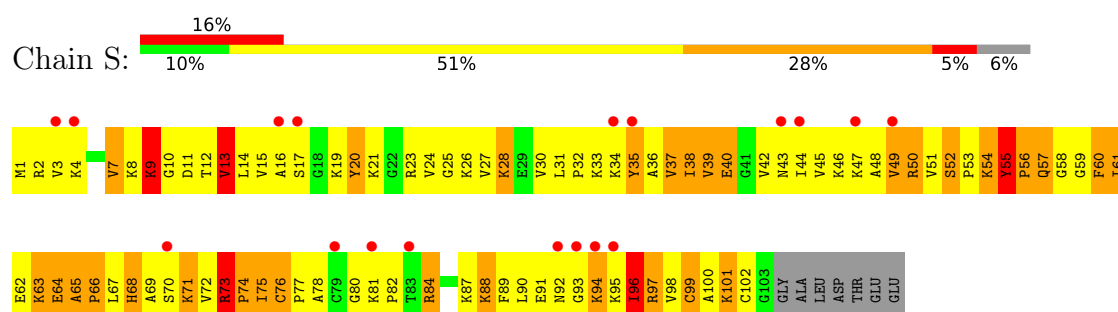
• Molecule 19: 50S ribosomal protein L22



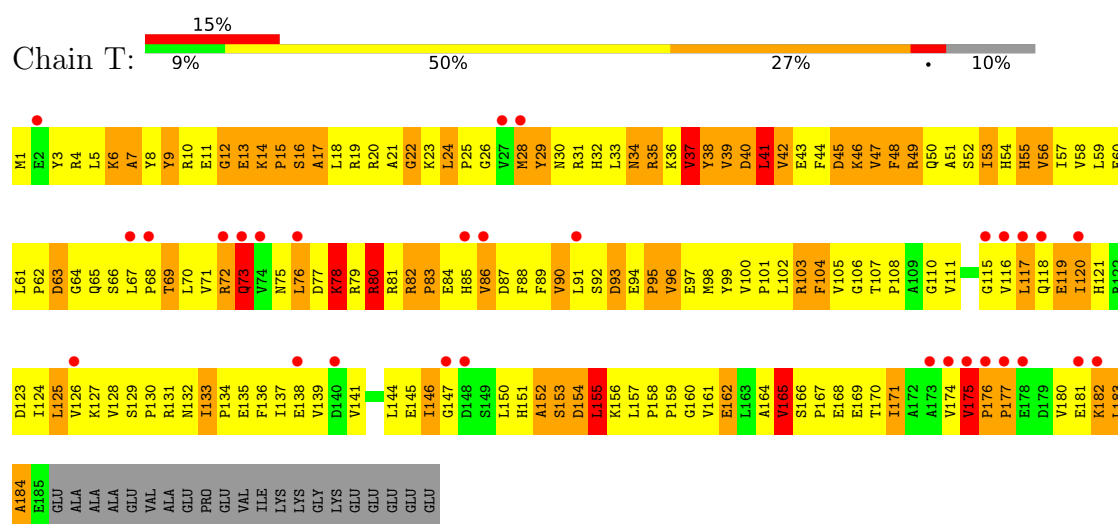
- Molecule 20: 50S ribosomal protein L23



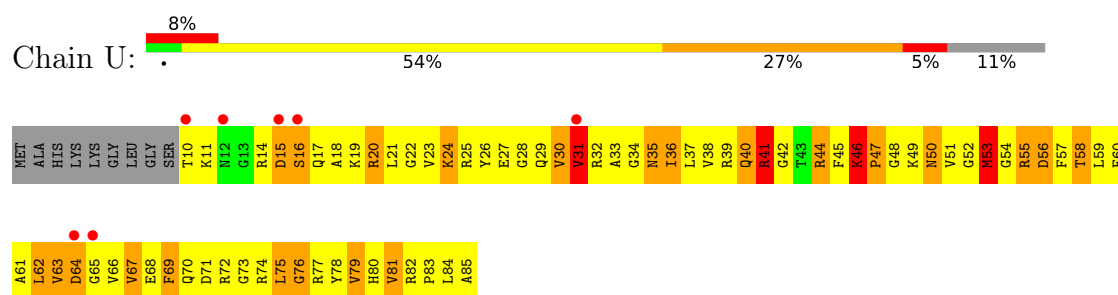
- Molecule 21: 50S ribosomal protein L24



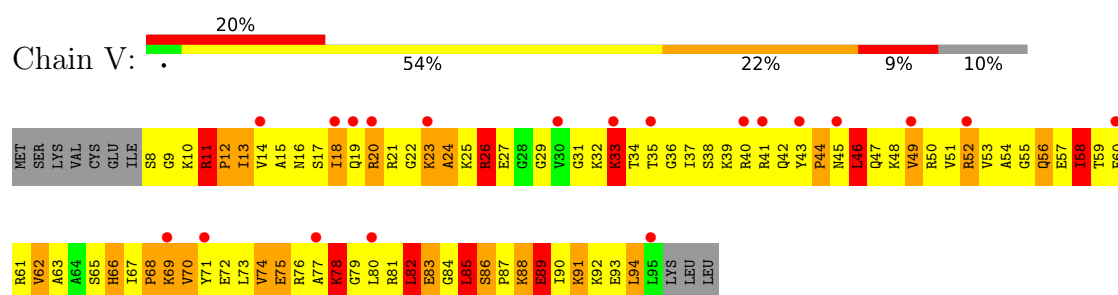
- Molecule 22: 50S ribosomal protein L25



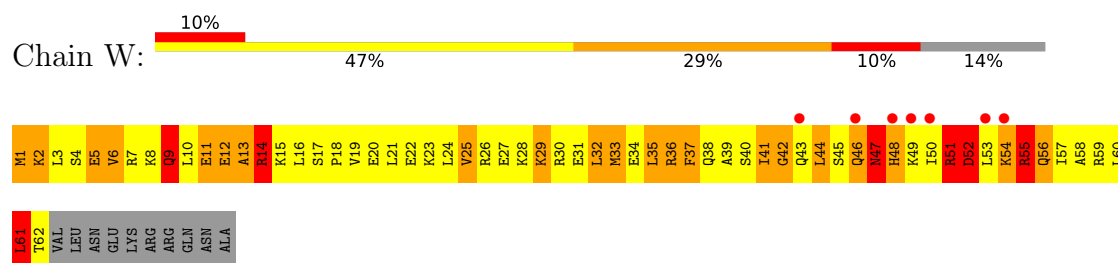
- Molecule 23: 50S ribosomal protein L27



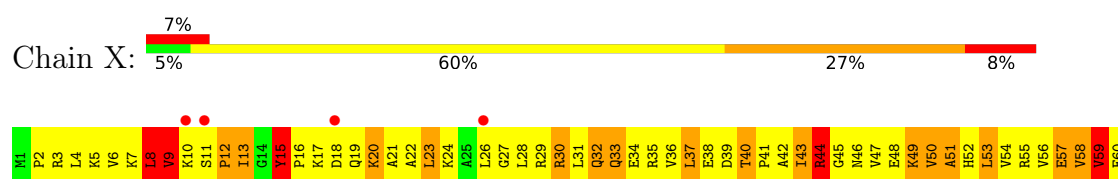
- Molecule 24: 50S ribosomal protein L28



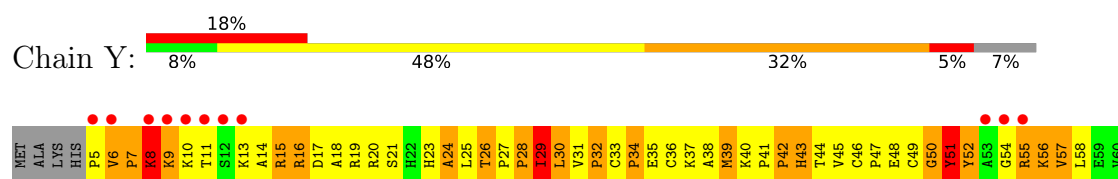
• Molecule 25: 50S ribosomal protein L29



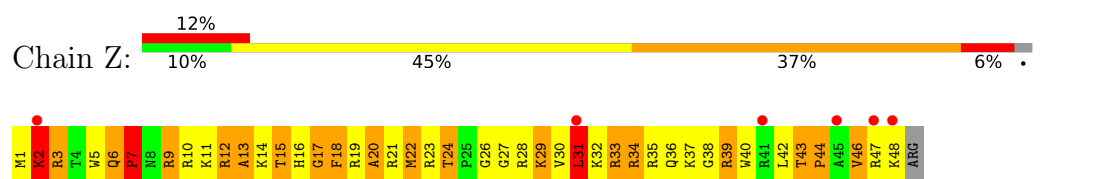
• Molecule 26: 50S ribosomal protein L30



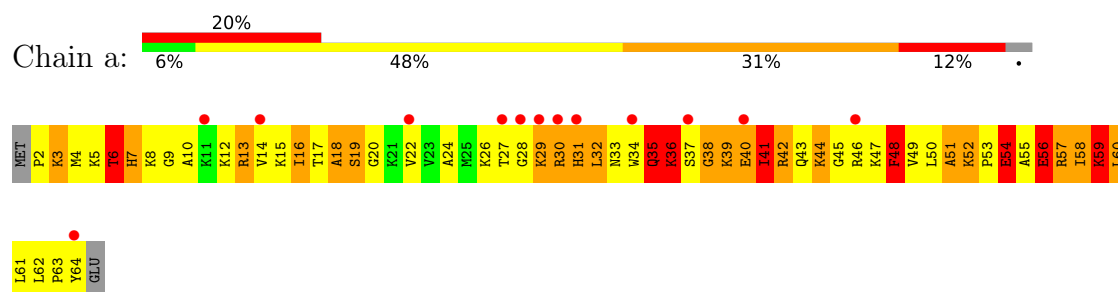
• Molecule 27: 50S ribosomal protein L32



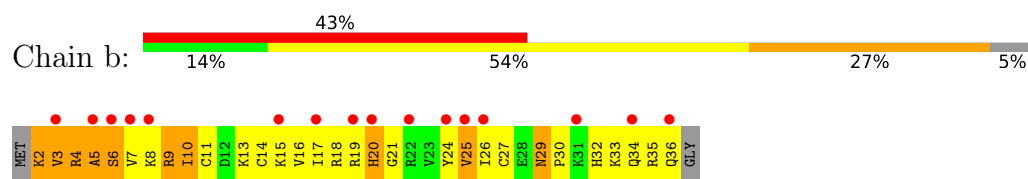
• Molecule 28: 50S ribosomal protein L34



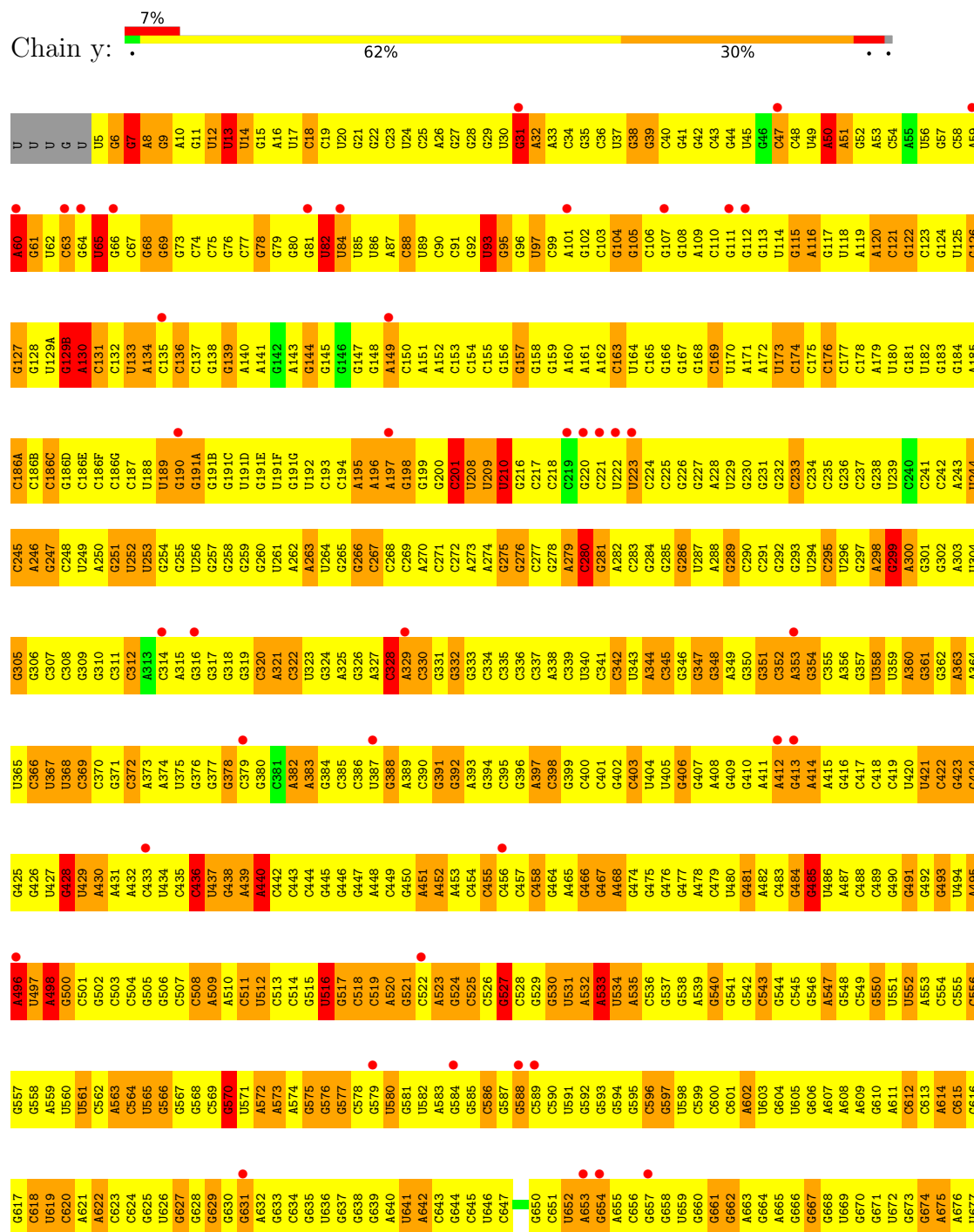
• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



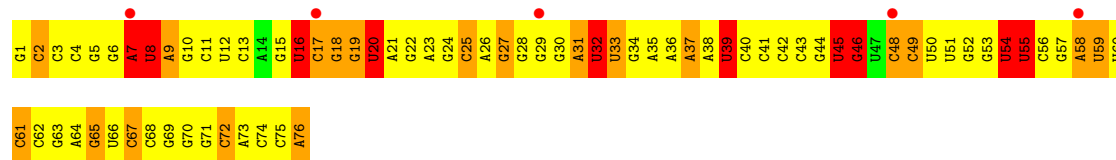
• Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA



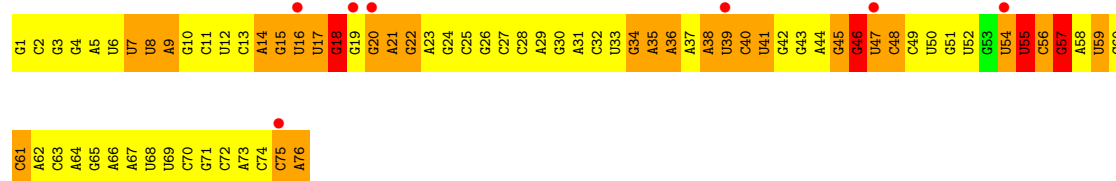
C1466	G1467	A1468	A1469	G1470	G1471	G1472	A1473	G1474	G1475	G1476	C1477	C1478	C1479	G1480	U1481	G1482	U1483	A1484	G1485	C1486	G1487	G1488	G1489	C1490	G1491	A1492	A1493	C1494	U1495	C1496	G1497	U1498	A1499	A1500	G1436	A1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509	U1510	G1511	U1512	A1513	C1514	C1515	G1516	G1517	A1518	A1519	C1520	G1521	G1522	A1523	G1524	G1525		
G1401	C1402	C1403	A1404	G1405	U1406	C1407	A1408	C1409	G1410	C1411	C1412	C1413	C1414	G1415	G1416	U1417	U1418	G1419	C1420	G1421	C1422	G1423	C1424	U1425	C1426	U1427	A1428	C1429	C1430	C1431	G1432	A1433	A1434	G1435	U1436	C1437	G1438	C1439	C1440	G1441	G1442	G1443	A1446	G1447	C1448	C1449	U1450	A1451	C1452	G1453	G1454	C1455	C1456	A1457	C1458	G1459	A1460	G1461	G1462	C1463	U1464	C1465
C1342	G1343	C1344	U1345	A1346	G1347	U1348	A1349	G1350	U1351	C1352	G1353	C1354	G1355	G1356	A1357	U1358	C1359	A1360	G1361	C1362	C1363	C1364	U1365	C1366	C1367	G1368	C1369	G1370	C1371	U1372	G1373	A1374	G1375	U1376	A1377	C1378	G1379	U1380	C1381	C1382	C1383	C1384	G1385	G1386	C1387	C1388	C1389	U1390	U1391	G1392	U1393	A1394	C1395	A1396	C1397	A1398	C1399	C1400				
C1282	G1283	C1284	A1285	A1286	G1287	A1288	A1289	G1290	G1291	U1292	U1293	G1294	G1295	C1296	C1297	C1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	U1306	U1307	U1308	G1309	G1310	G1311	A1252	C1312	U1313	C1314	U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	U1329	U1330	G1331	A1332	C1333	G1334	C1335	C1336	G1337	G1338	A1339	G1340	U1341		
G1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	G1233	C1234	U1235	A1236	C1237	A1238	U1239	U1240	G1241	C1242	C1243	C1244	A1245	C1246	U1247	A1248	C1249	A1250	A1251	A1252	C1253	G1254	C1255	A1256	U1257	C1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	C1269	C1270	G1271	U1272	G1273	G1274	A1275	G1276	C1277	U1278	A1279	A1280	U1281			
C1161	C1162	C1163	G1164	C1165	G1166	A1167	A1169	A1170	G1171	C1172	G1173	G1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	C1182	A1183	G1184	G1185	G1186	U1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	U1218	U1219	G1220	C1221			
A1101	A1102	C1103	A1104	C1105	G1106	C1107	G1108	C1109	A1110	C1111	C1112	C1113	C1114	C1115	G1116	G1117	C1118	C1119	G1120	U1121	U1122	A1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	U1131	C1132	G1133	U1134	U1135	U1136	C1137	G1138	C1139	C1140	G1141	C1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	U1155	C1156	A1157	C1158	U1159	G1160			
A1041	G1042	C1043	A1044	C1045	U1046	G1047	G1048	U1049	U1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	C1058	G1059	A1060	G1061	U1062	C1063	U1064	U1065	C1066	A1067	G1068	U1069	U1070	C1071	G1072	U1073	G1074	C1075	C1076	G1077	U1078	U1079	A1080	G1081	C1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	C1093	G1094	U1095	C1096	C1097	C1098	C1099	U1100			
C984	C985	A986	G987	C988	G989	C990	U991	U992	G993	A994	C995	A996	U997	A1000	G999	C994	G941	G942	U943	G944	A945	C946	G947	C948	A949	U950	G951	U952	C953	G954	U955	U956	G1017	C1018	A958	A959	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	G1034	U1035	C1036	U1037	C1038	U1040		
G924	G925	G926	G927	C928	G929	C930	C931	C932	G933	C934	A935	C936	A937	A938	G939	C940	G941	G942	U943	G944	A945	C946	G947	C948	A949	U950	G951	U952	C953	G954	U955	U956	G1017	C1018	A958	A959	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	G1034	U1035	C1036	U1037	C1038	U1040		
C738	C739	U740	G741	G742	G743	U744	C745	U746	C747	C748	C749	G750	U751	G752	A753	C754	G755	C756	U757	G758	A759	G760	G761	C762	C763	C764	U765	A766	C767	U768	G769	C770	G771	U772	C773	G774	G775	G776	A777	C778	C779	U780	A781	A782	C783	C784	G785	G786	C787	U788	U789	A790	G791	C792	A793	U794	C795	G796	C797			
U678	C679	G680	C681	G682	G683	U684	C685	U686	C687	C688	C689	G690	C691	U692	G693	A694	A695	A696	U697	G698	C699	G700	C701	A702	G703	U704	U705	A706	C707	U708	G709	G710	G711	A712	G713	G714	A715	A716	C717	G718	C719	G720	G721	A722	U723	G724	G725	C726	C727	U728	A729	G730	C731	A732	U733	G734	C735	G736	A737			



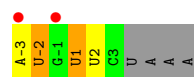
• Molecule 32: P-site PHE-tRNA



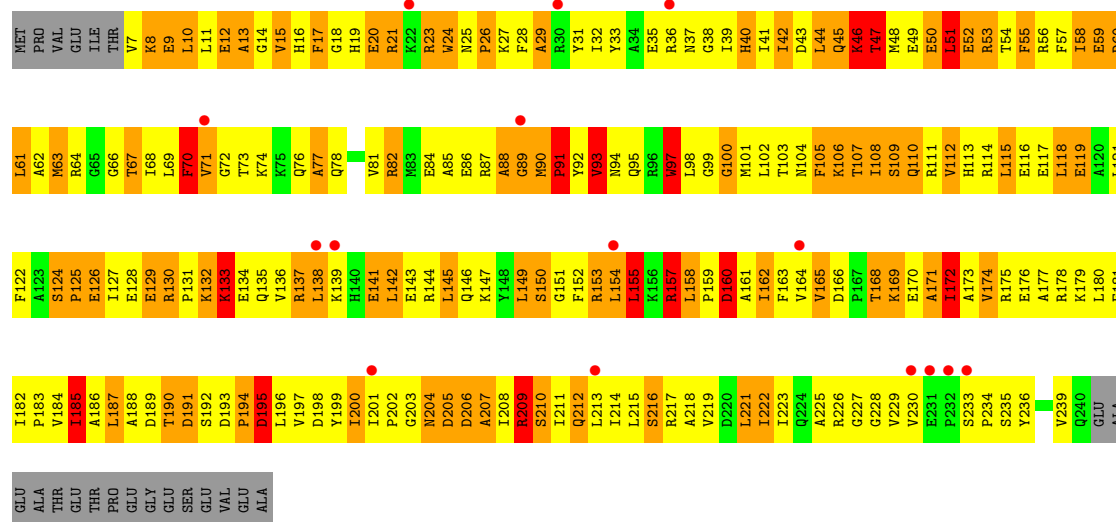
• Molecule 33: E-TRNA



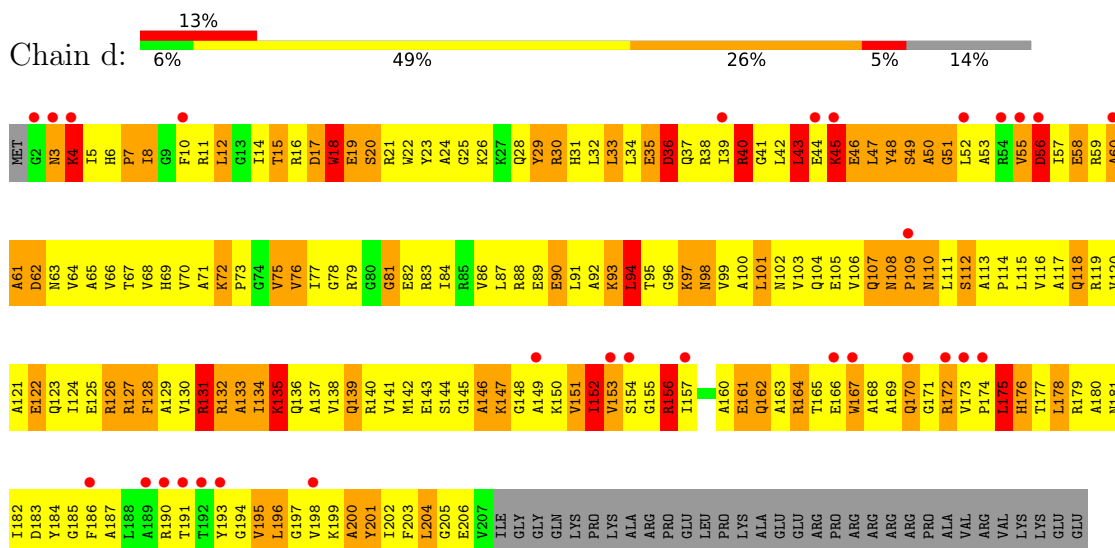
• Molecule 34: MRNA



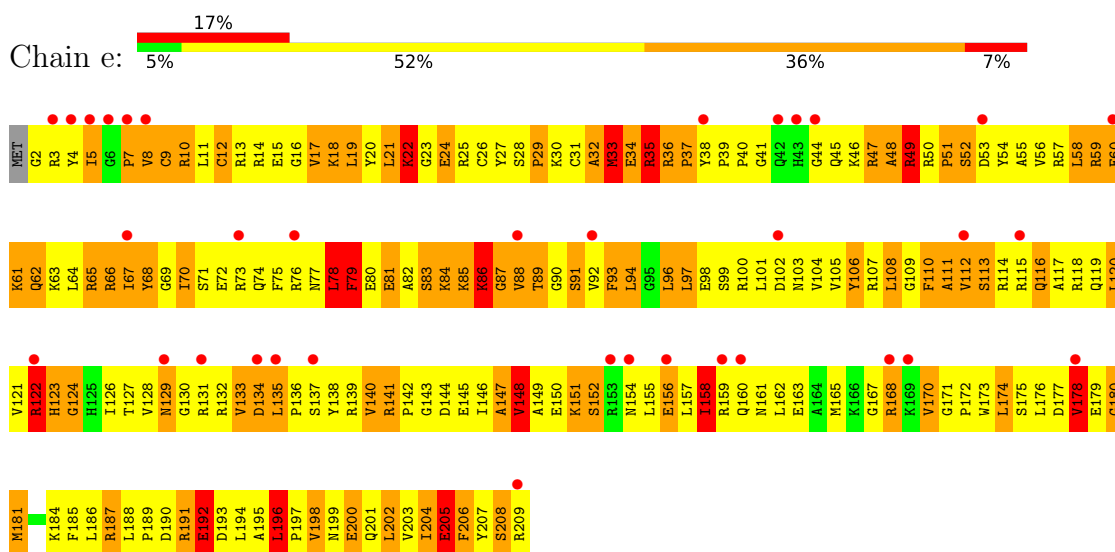
• Molecule 35: 30S ribosomal protein S2



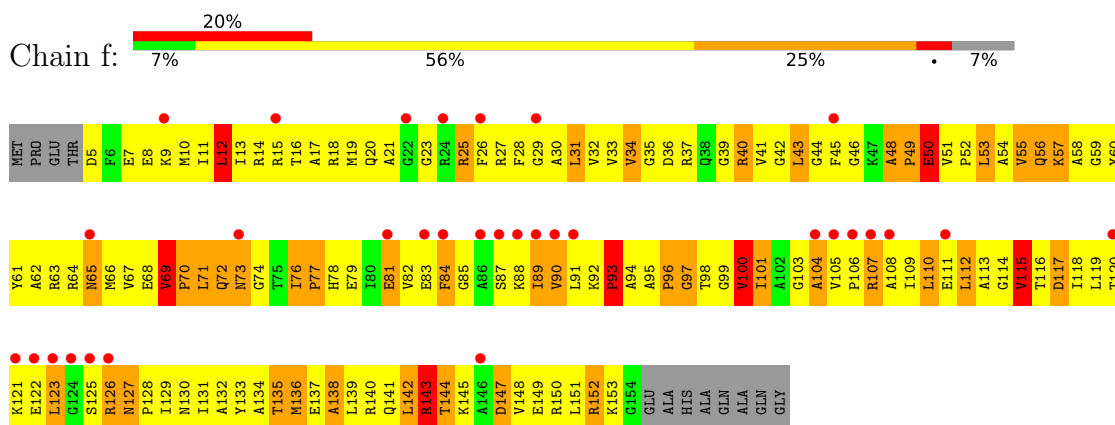
- Molecule 36: 30S ribosomal protein S3



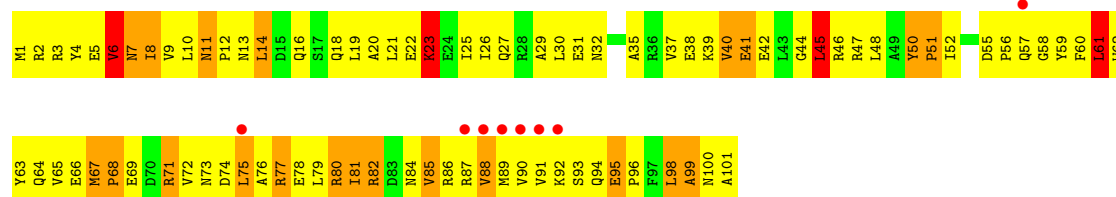
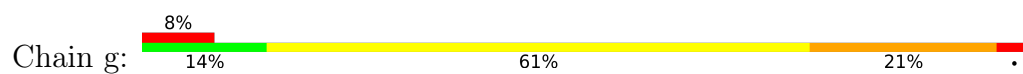
- Molecule 37: 30S ribosomal protein S4



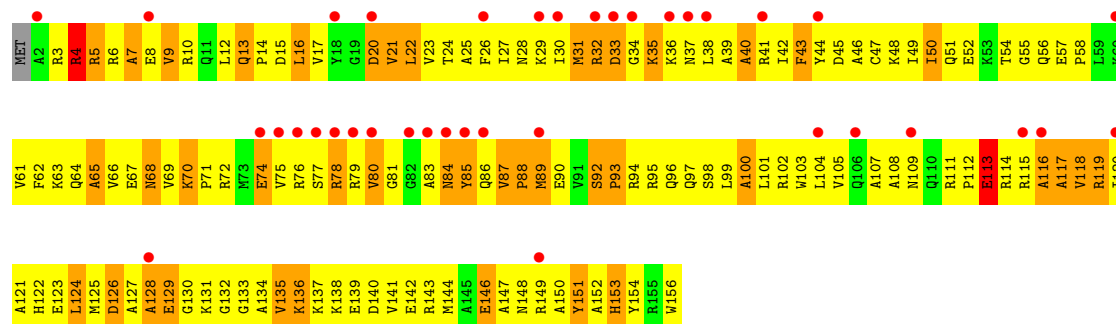
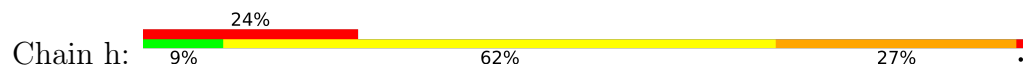
- Molecule 38: 30S ribosomal protein S5



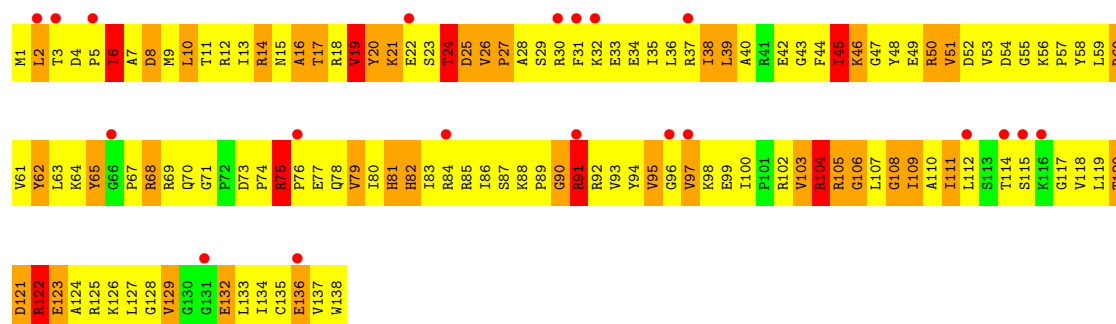
- Molecule 39: 30S ribosomal protein S6



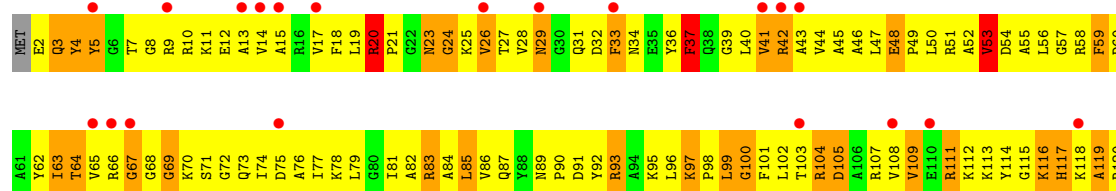
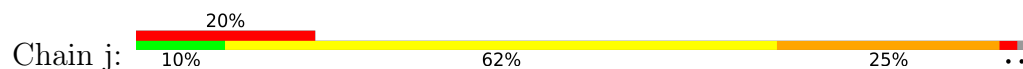
• Molecule 40: 30S ribosomal protein S7

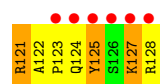


• Molecule 41: 30S ribosomal protein S8

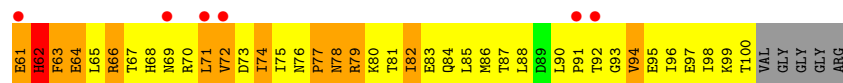


• Molecule 42: 30S ribosomal protein S9

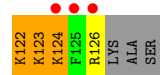
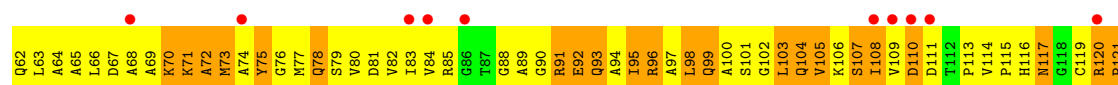
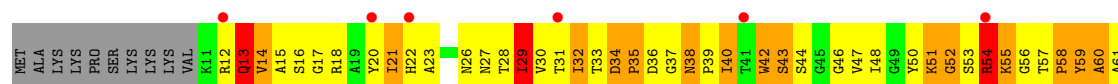




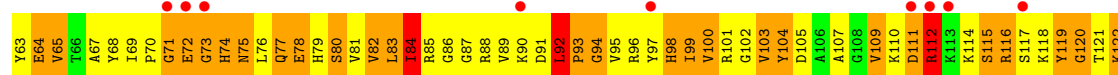
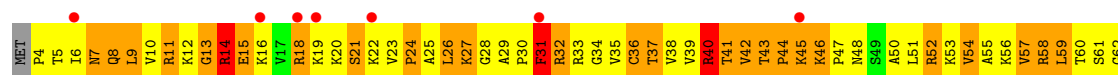
• Molecule 43: 30S ribosomal protein S10



• Molecule 44: 30S ribosomal protein S11

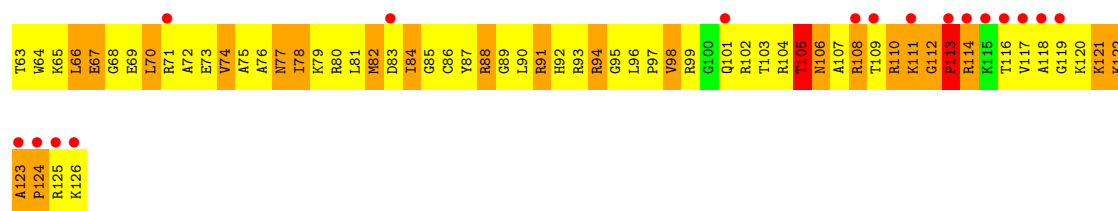


• Molecule 45: 30S ribosomal protein S12

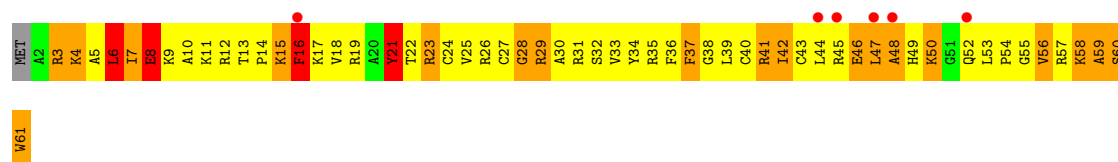


• Molecule 46: 30S ribosomal protein S13

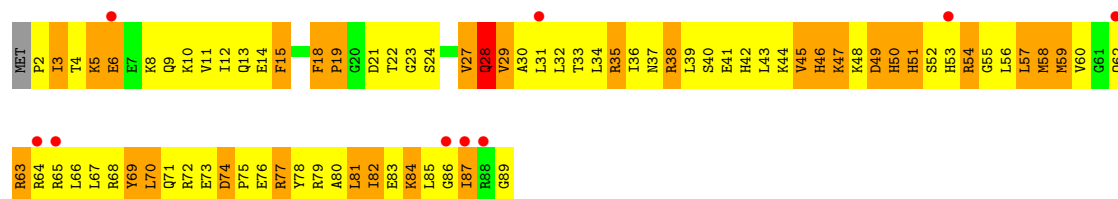
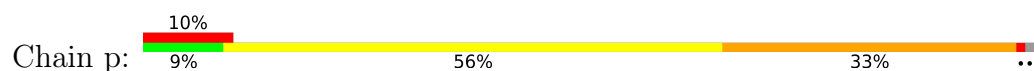




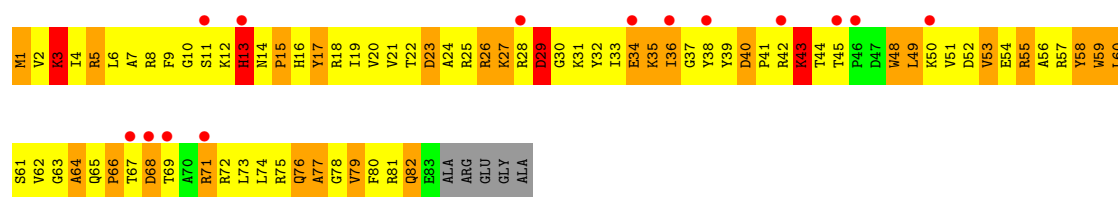
• Molecule 47: 30S ribosomal protein S14



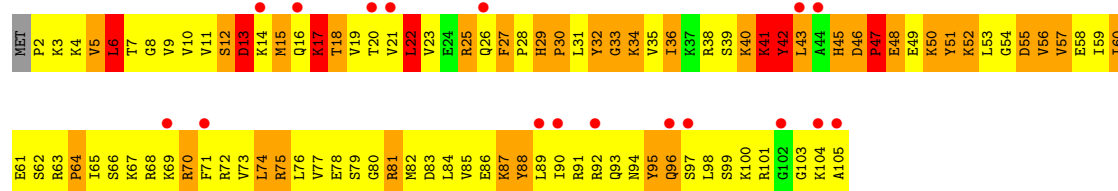
• Molecule 48: 30S ribosomal protein S15



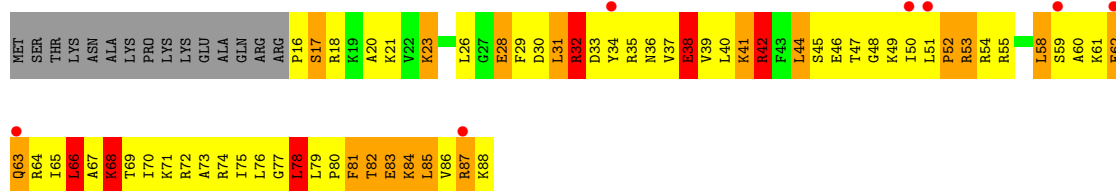
• Molecule 49: 30S ribosomal protein S16



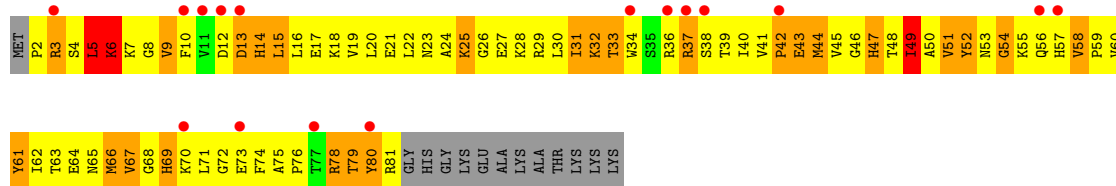
• Molecule 50: 30S ribosomal protein S17



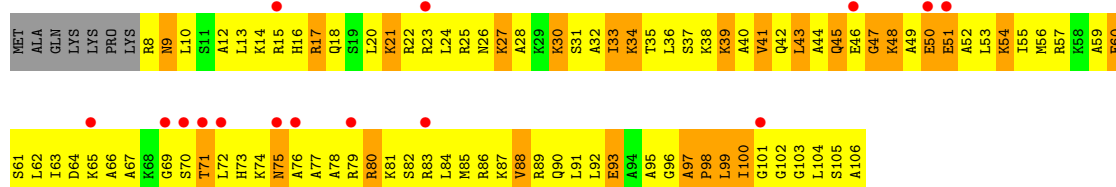
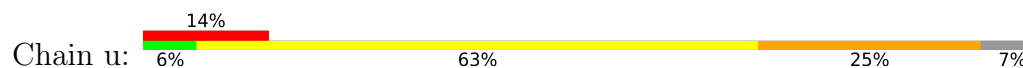
• Molecule 51: 30S ribosomal protein S18



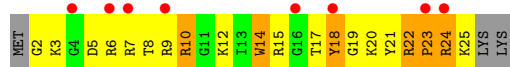
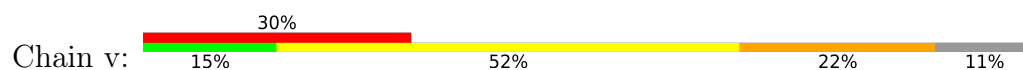
• Molecule 52: 30S ribosomal protein S19



• Molecule 53: 30S ribosomal protein S20



• Molecule 54: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	507.81Å 507.81Å 689.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.71 30.00 – 3.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.71) 97.7 (30.00-3.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.348 , 0.353 0.334 , 0.340	Depositor DCC
R_{free} test set	11428 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.228 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.219 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	146532	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.09% 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: 4SU, MA6, MIA, 2MG, M2G, H2U, UR3, PSU, 5MU, 4OC, 5MC, 7MG

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	w	0.79	35/69679 (0.1%)	1.00	197/108779 (0.2%)
2	x	0.70	0/2878	0.93	11/4490 (0.2%)
3	A	0.67	0/1015	0.96	9/1369 (0.7%)
4	B	0.63	0/2165	1.02	12/2919 (0.4%)
5	C	0.73	0/1574	1.08	9/2125 (0.4%)
6	D	0.75	0/1551	0.99	7/2101 (0.3%)
7	E	0.76	1/1492 (0.1%)	1.00	7/2006 (0.3%)
8	F	0.73	0/1345	1.08	10/1819 (0.5%)
9	G	0.68	0/1171	1.01	6/1583 (0.4%)
10	H	0.61	0/1130	0.89	6/1525 (0.4%)
11	I	0.72	0/942	1.10	12/1268 (0.9%)
12	J	0.63	0/1131	0.91	4/1504 (0.3%)
13	K	0.80	0/1110	1.12	11/1483 (0.7%)
14	L	0.74	2/982 (0.2%)	1.03	11/1312 (0.8%)
15	M	0.69	0/856	0.86	0/1138
16	N	0.63	0/1157	1.00	5/1544 (0.3%)
17	O	0.66	0/982	1.06	4/1306 (0.3%)
18	P	0.73	0/790	1.01	10/1057 (0.9%)
19	Q	0.74	0/878	1.08	8/1179 (0.7%)
20	R	0.88	1/739 (0.1%)	1.12	6/993 (0.6%)
21	S	0.80	0/806	1.09	7/1074 (0.7%)
22	T	0.75	0/1507	1.12	18/2045 (0.9%)
23	U	0.76	0/613	0.99	4/816 (0.5%)
24	V	0.67	0/701	0.89	1/932 (0.1%)
25	W	0.64	0/522	0.98	2/690 (0.3%)
26	X	0.71	0/482	1.33	8/646 (1.2%)
27	Y	0.66	0/449	1.08	5/606 (0.8%)
28	Z	1.04	0/426	1.20	7/561 (1.2%)
29	a	0.67	0/515	1.04	4/679 (0.6%)
30	b	0.73	0/297	1.04	1/392 (0.3%)
31	y	0.73	11/35859 (0.0%)	0.97	80/55966 (0.1%)
32	z	0.72	1/1603 (0.1%)	0.96	7/2497 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	0	0.67	0/1791	0.87	3/2791 (0.1%)
34	1	0.82	0/135	0.95	0/208
35	c	0.71	0/1935	0.94	9/2609 (0.3%)
36	d	0.66	0/1636	0.94	5/2205 (0.2%)
37	e	0.65	0/1733	0.97	9/2318 (0.4%)
38	f	0.66	0/1162	1.03	12/1564 (0.8%)
39	g	0.77	0/856	1.13	7/1154 (0.6%)
40	h	0.67	0/1276	1.08	12/1709 (0.7%)
41	i	0.68	0/1136	1.03	6/1527 (0.4%)
42	j	0.59	0/1029	0.95	6/1378 (0.4%)
43	k	0.71	0/807	0.91	3/1085 (0.3%)
44	l	0.69	0/879	1.06	11/1187 (0.9%)
45	m	0.77	0/986	1.12	10/1320 (0.8%)
46	n	0.66	0/1008	1.01	12/1347 (0.9%)
47	o	0.61	0/501	0.85	1/664 (0.2%)
48	p	0.61	0/745	1.04	5/992 (0.5%)
49	q	0.63	0/716	1.00	6/963 (0.6%)
50	r	0.70	0/870	0.92	2/1159 (0.2%)
51	s	0.64	0/604	0.98	4/801 (0.5%)
52	t	0.69	0/661	0.96	3/890 (0.3%)
53	u	0.24	0/764	0.70	1/1006 (0.1%)
54	v	0.69	0/212	0.76	0/277
All	All	0.75	51/158789 (0.0%)	1.00	616/237558 (0.3%)

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	w	0	24
2	x	2	0
31	y	0	8
All	All	2	32

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	926	A	O3'-P	24.06	1.97	1.61
1	w	1506	C	O3'-P	23.84	1.97	1.61
1	w	1171	G	O3'-P	22.48	1.94	1.61
1	w	890	A	O3'-P	22.42	1.94	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	1481	U	O3'-P	19.31	1.90	1.61

The worst 5 of 616 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	149	ARG	N-CA-C	-17.44	92.35	111.36
1	w	1822	G	N9-C1'-C2'	-14.88	89.67	112.00
1	w	1577	C	N1-C1'-C2'	-12.03	93.96	112.00
1	w	712(B)	A	P-O3'-C3'	-11.74	102.58	120.20
4	B	23	GLU	N-CA-C	-11.38	100.91	112.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	x	14	U	C3'
2	x	24	G	C3'

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	w	138	G	Sidechain
1	w	241	A	Sidechain
1	w	338	G	Sidechain
1	w	566	U	Sidechain
1	w	74	A	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	w	62213	0	31360	16110	1
2	x	2573	0	1306	734	0
3	A	996	0	1013	374	0
4	B	2115	0	2195	1159	0
5	C	1541	0	1599	910	0
6	D	1517	0	1565	743	0
7	E	1468	0	1529	682	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1319	0	1399	522	0
9	G	1156	0	1239	569	2
10	H	1103	0	1177	668	0
11	I	932	0	994	519	0
12	J	1114	0	1187	593	0
13	K	1089	0	1156	605	0
14	L	968	0	1033	556	0
15	M	846	0	902	405	0
16	N	1143	0	1211	557	0
17	O	964	0	1022	474	0
18	P	779	0	852	404	0
19	Q	868	0	929	438	0
20	R	725	0	778	323	0
21	S	793	0	890	268	0
22	T	1475	0	1504	551	0
23	U	605	0	628	427	0
24	V	694	0	764	441	0
25	W	520	0	575	210	0
26	X	477	0	529	253	0
27	Y	436	0	460	217	0
28	Z	418	0	467	222	0
29	a	507	0	576	282	0
30	b	294	0	323	143	0
31	y	32302	0	16327	8640	2
32	z	1628	0	844	343	0
33	0	1621	0	821	294	0
34	1	122	0	65	17	0
35	c	1900	0	1951	678	0
36	d	1612	0	1677	711	0
37	e	1703	0	1767	829	0
38	f	1146	0	1207	455	0
39	g	843	0	857	236	0
40	h	1257	0	1296	484	0
41	i	1116	0	1177	587	0
42	j	1011	0	1043	339	0
43	k	794	0	840	254	0
44	l	864	0	881	349	0
45	m	970	0	1057	537	0
46	n	997	0	1072	413	0
47	o	492	0	533	269	0
48	p	734	0	771	279	0
49	q	700	0	720	339	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	r	857	0	930	418	0
51	s	598	0	670	225	0
52	t	647	0	673	247	0
53	u	762	0	859	271	0
54	v	208	0	221	98	0
All	All	146532	0	99421	43508	3

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 180.

The worst 5 of 43508 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:1458:C:H1'	1:w:1459:G:C2	1.35	1.60
1:w:1699:G:C3'	1:w:1700:A:H5''	1.33	1.56
31:y:701:C:C5'	31:y:703:G:H5'	1.38	1.53
1:w:2743:C:C2'	1:w:2744:G:H5''	1.34	1.52
31:y:1518:MA6:H8	31:y:1518:MA6:C5'	1.35	1.52

All (3) 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)
1:w:1457:A:OP1	1:w:1457:A:OP1[6_555]	1.38	0.82
9:G:89:TYR:O	31:y:357:G:O2'[4_555]	2.01	0.19
9:G:91:SER:O	31:y:368:U:OP1[4_555]	2.19	0.01

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	
3	A	123/229 (54%)	54 (44%)	39 (32%)	30 (24%)	0	0
4	B	270/276 (98%)	103 (38%)	84 (31%)	83 (31%)	0	0
5	C	199/206 (97%)	89 (45%)	48 (24%)	62 (31%)	0	0
6	D	192/205 (94%)	76 (40%)	54 (28%)	62 (32%)	0	0
7	E	178/182 (98%)	84 (47%)	53 (30%)	41 (23%)	0	0
8	F	171/180 (95%)	76 (44%)	53 (31%)	42 (25%)	0	0
9	G	146/148 (99%)	75 (51%)	30 (20%)	41 (28%)	0	0
10	H	136/163 (83%)	48 (35%)	40 (29%)	48 (35%)	0	0
11	I	120/122 (98%)	50 (42%)	37 (31%)	33 (28%)	0	0
12	J	144/150 (96%)	59 (41%)	39 (27%)	46 (32%)	0	0
13	K	135/141 (96%)	52 (38%)	44 (33%)	39 (29%)	0	0
14	L	116/118 (98%)	60 (52%)	28 (24%)	28 (24%)	0	0
15	M	104/112 (93%)	40 (38%)	31 (30%)	33 (32%)	0	0
16	N	135/146 (92%)	59 (44%)	36 (27%)	40 (30%)	0	0
17	O	115/118 (98%)	64 (56%)	27 (24%)	24 (21%)	0	1
18	P	99/101 (98%)	30 (30%)	32 (32%)	37 (37%)	0	0
19	Q	107/113 (95%)	49 (46%)	30 (28%)	28 (26%)	0	0
20	R	90/96 (94%)	28 (31%)	29 (32%)	33 (37%)	0	0
21	S	101/110 (92%)	36 (36%)	34 (34%)	31 (31%)	0	0
22	T	183/206 (89%)	104 (57%)	41 (22%)	38 (21%)	0	1
23	U	74/85 (87%)	35 (47%)	23 (31%)	16 (22%)	0	1
24	V	86/98 (88%)	30 (35%)	31 (36%)	25 (29%)	0	0
25	W	60/72 (83%)	28 (47%)	12 (20%)	20 (33%)	0	0
26	X	58/60 (97%)	32 (55%)	15 (26%)	11 (19%)	0	1
27	Y	54/60 (90%)	22 (41%)	12 (22%)	20 (37%)	0	0
28	Z	46/49 (94%)	25 (54%)	9 (20%)	12 (26%)	0	0
29	a	61/65 (94%)	20 (33%)	22 (36%)	19 (31%)	0	0
30	b	33/37 (89%)	22 (67%)	5 (15%)	6 (18%)	0	1
35	c	232/256 (91%)	109 (47%)	66 (28%)	57 (25%)	0	0
36	d	204/239 (85%)	98 (48%)	49 (24%)	57 (28%)	0	0
37	e	206/209 (99%)	99 (48%)	44 (21%)	63 (31%)	0	0
38	f	148/162 (91%)	89 (60%)	33 (22%)	26 (18%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	g	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	3
40	h	153/156 (98%)	84 (55%)	40 (26%)	29 (19%)	0	1
41	i	136/138 (99%)	71 (52%)	35 (26%)	30 (22%)	0	0
42	j	125/128 (98%)	73 (58%)	31 (25%)	21 (17%)	0	2
43	k	96/105 (91%)	50 (52%)	24 (25%)	22 (23%)	0	0
44	l	114/129 (88%)	59 (52%)	28 (25%)	27 (24%)	0	0
45	m	122/132 (92%)	51 (42%)	32 (26%)	39 (32%)	0	0
46	n	123/126 (98%)	53 (43%)	35 (28%)	35 (28%)	0	0
47	o	58/61 (95%)	22 (38%)	19 (33%)	17 (29%)	0	0
48	p	86/89 (97%)	46 (54%)	23 (27%)	17 (20%)	0	1
49	q	81/88 (92%)	37 (46%)	28 (35%)	16 (20%)	0	1
50	r	102/105 (97%)	46 (45%)	31 (30%)	25 (24%)	0	0
51	s	71/88 (81%)	42 (59%)	12 (17%)	17 (24%)	0	0
52	t	78/93 (84%)	26 (33%)	31 (40%)	21 (27%)	0	0
53	u	97/106 (92%)	42 (43%)	37 (38%)	18 (19%)	0	1
54	v	22/27 (82%)	11 (50%)	7 (32%)	4 (18%)	0	1
All	All	5689/6186 (92%)	2619 (46%)	1567 (28%)	1503 (26%)	0	0

5 of 1503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	VAL
3	A	179	ALA
3	A	180	SER
3	A	201	LYS
3	A	203	GLU

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	106/181 (59%)	89 (84%)	17 (16%)	2	15
4	B	214/218 (98%)	171 (80%)	43 (20%)	1	8
5	C	163/166 (98%)	124 (76%)	39 (24%)	1	5
6	D	154/162 (95%)	125 (81%)	29 (19%)	1	10
7	E	154/156 (99%)	126 (82%)	28 (18%)	2	11
8	F	142/148 (96%)	118 (83%)	24 (17%)	2	13
9	G	124/124 (100%)	100 (81%)	24 (19%)	1	9
10	H	117/139 (84%)	91 (78%)	26 (22%)	1	7
11	I	100/100 (100%)	78 (78%)	22 (22%)	1	7
12	J	112/116 (97%)	89 (80%)	23 (20%)	1	8
13	K	108/111 (97%)	79 (73%)	29 (27%)	0	4
14	L	101/101 (100%)	77 (76%)	24 (24%)	1	6
15	M	84/88 (96%)	69 (82%)	15 (18%)	2	12
16	N	121/128 (94%)	94 (78%)	27 (22%)	1	6
17	O	93/94 (99%)	79 (85%)	14 (15%)	3	16
18	P	82/82 (100%)	69 (84%)	13 (16%)	2	15
19	Q	89/92 (97%)	74 (83%)	15 (17%)	2	13
20	R	74/78 (95%)	62 (84%)	12 (16%)	2	14
21	S	86/91 (94%)	75 (87%)	11 (13%)	4	21
22	T	163/179 (91%)	138 (85%)	25 (15%)	3	16
23	U	61/67 (91%)	48 (79%)	13 (21%)	1	7
24	V	73/83 (88%)	59 (81%)	14 (19%)	1	9
25	W	58/67 (87%)	42 (72%)	16 (28%)	0	3
26	X	52/52 (100%)	42 (81%)	10 (19%)	1	9
27	Y	49/52 (94%)	43 (88%)	6 (12%)	5	22
28	Z	41/42 (98%)	32 (78%)	9 (22%)	1	7
29	a	53/55 (96%)	39 (74%)	14 (26%)	0	4
30	b	33/34 (97%)	30 (91%)	3 (9%)	9	32
35	c	202/220 (92%)	153 (76%)	49 (24%)	1	5
36	d	160/188 (85%)	129 (81%)	31 (19%)	1	9
37	e	180/181 (99%)	142 (79%)	38 (21%)	1	7
38	f	115/123 (94%)	93 (81%)	22 (19%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	g	90/90 (100%)	77 (86%)	13 (14%)	3	18
40	h	126/127 (99%)	112 (89%)	14 (11%)	6	25
41	i	119/119 (100%)	100 (84%)	19 (16%)	2	15
42	j	98/99 (99%)	82 (84%)	16 (16%)	2	14
43	k	88/92 (96%)	77 (88%)	11 (12%)	4	21
44	l	88/99 (89%)	73 (83%)	15 (17%)	2	13
45	m	104/109 (95%)	84 (81%)	20 (19%)	1	9
46	n	100/101 (99%)	83 (83%)	17 (17%)	2	13
47	o	49/50 (98%)	39 (80%)	10 (20%)	1	8
48	p	79/80 (99%)	65 (82%)	14 (18%)	2	12
49	q	72/74 (97%)	59 (82%)	13 (18%)	2	12
50	r	96/97 (99%)	76 (79%)	20 (21%)	1	8
51	s	64/77 (83%)	53 (83%)	11 (17%)	2	13
52	t	71/80 (89%)	63 (89%)	8 (11%)	5	25
53	u	76/82 (93%)	69 (91%)	7 (9%)	8	32
54	v	19/22 (86%)	17 (90%)	2 (10%)	6	28
All	All	4803/5116 (94%)	3908 (81%)	895 (19%)	1	10

5 of 895 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	36	ILE
53	u	21	LYS
35	c	132	LYS
51	s	78	LEU
46	n	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
37	e	42	GLN
44	l	22	HIS
37	e	201	GLN
40	h	28	ASN
45	m	74	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	1140 (39%)	0
2	x	119/121 (98%)	42 (35%)	0
31	y	1501/1522 (98%)	506 (33%)	0
32	z	75/76 (98%)	29 (38%)	0
33	0	75/76 (98%)	30 (40%)	5 (6%)
34	1	5/10 (50%)	2 (40%)	0
All	All	4663/4694 (99%)	1749 (37%)	5 (0%)

5 of 1749 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	12	U
1	w	13	A
1	w	15	G
1	w	16	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	0	7	U
33	0	9	A
33	0	46	G
33	0	48	C
33	0	56	C

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
31	UR3	y	1498	31	19,22,23	1.64	2 (10%)	26,32,35	1.57	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	H2U	z	16	32	18,21,22	0.98	1 (5%)	19,30,33	0.97	1 (5%)
31	5MC	y	1407	31	19,22,23	0.92	1 (5%)	26,32,35	1.48	5 (19%)
31	MA6	y	1518	31	23,26,27	1.71	6 (26%)	33,38,41	2.39	14 (42%)
31	5MC	y	967	31	19,22,23	0.89	2 (10%)	26,32,35	1.17	3 (11%)
32	PSU	z	55	32	18,21,22	1.97	4 (22%)	21,30,33	2.08	6 (28%)
33	PSU	0	55	33	18,21,22	3.40	6 (33%)	21,30,33	2.16	5 (23%)
32	4SU	z	8	32	18,21,22	1.82	3 (16%)	25,30,33	2.38	9 (36%)
32	MIA	z	37	32	28,31,32	2.10	8 (28%)	38,44,47	2.09	5 (13%)
31	7MG	y	527	31	23,26,27	3.19	4 (17%)	27,39,42	1.77	6 (22%)
31	MA6	y	1519	31	23,26,27	1.80	6 (26%)	33,38,41	2.38	16 (48%)
32	PSU	z	32	32	18,21,22	2.04	3 (16%)	21,30,33	2.19	6 (28%)
31	2MG	y	1207	31	23,26,27	1.26	2 (8%)	33,38,41	1.82	8 (24%)
32	5MU	z	54	32	19,22,23	1.77	1 (5%)	27,32,35	1.54	5 (18%)
31	5MC	y	1404	31	19,22,23	1.11	2 (10%)	26,32,35	1.53	5 (19%)
32	PSU	z	39	32	18,21,22	2.31	4 (22%)	21,30,33	1.92	7 (33%)
31	PSU	y	516	31	18,21,22	1.90	4 (22%)	21,30,33	1.99	7 (33%)
32	H2U	z	20	32	18,21,22	0.76	0	19,30,33	0.92	1 (5%)
31	M2G	y	966	31	24,27,28	1.59	3 (12%)	33,40,43	1.35	5 (15%)
31	5MC	y	1400	31	19,22,23	1.09	2 (10%)	26,32,35	1.47	4 (15%)
31	4OC	y	1402	31	20,23,24	1.38	3 (15%)	25,32,35	1.57	5 (20%)
32	7MG	z	46	32	23,26,27	3.05	5 (21%)	27,39,42	1.91	6 (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
31	UR3	y	1498	31	-	5/7/25/26	0/2/2/2
32	H2U	z	16	32	-	2/7/38/39	0/2/2/2
31	5MC	y	1407	31	-	0/7/25/26	0/2/2/2
31	MA6	y	1518	31	-	2/11/29/30	0/3/3/3
31	5MC	y	967	31	-	0/7/25/26	0/2/2/2
32	PSU	z	55	32	-	2/7/25/26	0/2/2/2
33	PSU	0	55	33	-	2/7/25/26	0/2/2/2
32	4SU	z	8	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MIA	z	37	32	-	5/15/33/34	0/3/3/3
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	MA6	y	1519	31	-	1/11/29/30	0/3/3/3
32	PSU	z	32	32	-	3/7/25/26	0/2/2/2
31	2MG	y	1207	31	-	1/9/27/28	0/3/3/3
32	5MU	z	54	32	-	0/7/25/26	0/2/2/2
31	5MC	y	1404	31	-	2/7/25/26	0/2/2/2
32	PSU	z	39	32	-	4/7/25/26	0/2/2/2
31	PSU	y	516	31	-	4/7/25/26	0/2/2/2
32	H2U	z	20	32	-	2/7/38/39	0/2/2/2
31	M2G	y	966	31	-	2/11/29/30	0/3/3/3
31	5MC	y	1400	31	-	0/7/25/26	0/2/2/2
31	4OC	y	1402	31	-	3/9/29/30	0/2/2/2
32	7MG	z	46	32	-	0/7/37/38	0/3/3/3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	527	7MG	C8-N9	-14.14	1.36	1.45
32	z	46	7MG	C8-N9	-13.24	1.37	1.45
33	0	55	PSU	O2-C2	11.91	1.48	1.23
32	z	54	5MU	O4-C4	6.90	1.36	1.23
32	z	39	PSU	O2-C2	6.87	1.38	1.23

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	z	37	MIA	C12-C13-C14	-9.14	110.60	127.01
31	y	1207	2MG	C4'-O4'-C1'	-5.72	96.83	109.47
31	y	1518	MA6	N1-C6-N6	5.68	123.78	116.86
31	y	527	7MG	N9-C8-N7	5.67	111.41	103.37
32	z	8	4SU	C5-C4-S4	-5.59	117.92	124.31

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	y	516	PSU	C2'-C1'-C5-C4
31	y	516	PSU	C2'-C1'-C5-C6
31	y	1402	4OC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
31	y	1518	MA6	O4'-C4'-C5'-O5'
32	z	16	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	y	1498	UR3	10	0
32	z	16	H2U	3	0
31	y	1407	5MC	9	0
31	y	1518	MA6	37	0
31	y	967	5MC	15	0
32	z	55	PSU	11	0
33	0	55	PSU	5	0
32	z	8	4SU	6	0
31	y	527	7MG	5	0
31	y	1519	MA6	12	0
32	z	32	PSU	4	0
31	y	1207	2MG	16	0
32	z	54	5MU	8	0
31	y	1404	5MC	1	0
32	z	39	PSU	7	0
31	y	516	PSU	10	0
32	z	20	H2U	2	0
31	y	966	M2G	8	0
31	y	1400	5MC	12	0
31	y	1402	4OC	16	0
32	z	46	7MG	12	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	w	31
31	y	5

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	926:A	O3'	928:G	P	1.97
1	w	1506:C	O3'	1508:A	P	1.96
1	w	890:A	O3'	892:G	P	1.94
1	w	1171:G	O3'	1173:G	P	1.94
1	w	1481:U	O3'	1483:G	P	1.90

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	w	2889/2889 (100%)	0.53	309 (10%) 11 12	5, 5, 117, 159	0
2	x	120/121 (99%)	0.14	7 (5%) 29 20	5, 13, 95, 127	0
3	A	127/229 (55%)	0.28	11 (8%) 16 14	5, 50, 148, 151	0
4	B	272/276 (98%)	1.13	70 (25%) 1 2	5, 60, 148, 155	0
5	C	201/206 (97%)	1.08	41 (20%) 3 3	5, 49, 148, 159	0
6	D	194/205 (94%)	1.02	38 (19%) 3 4	5, 55, 148, 165	0
7	E	180/182 (98%)	0.57	17 (9%) 14 13	5, 58, 148, 156	0
8	F	173/180 (96%)	0.38	14 (8%) 18 14	5, 67, 148, 160	0
9	G	148/148 (100%)	-0.06	6 (4%) 41 26	5, 43, 148, 151	0
10	H	138/163 (84%)	0.77	19 (13%) 6 8	5, 52, 147, 152	0
11	I	122/122 (100%)	0.85	22 (18%) 3 5	5, 35, 142, 148	0
12	J	146/150 (97%)	1.41	45 (30%) 1 1	5, 90, 150, 160	0
13	K	137/141 (97%)	0.79	21 (15%) 5 7	5, 24, 148, 152	0
14	L	118/118 (100%)	0.85	22 (18%) 3 4	5, 44, 148, 148	0
15	M	106/112 (94%)	0.55	12 (11%) 10 11	5, 48, 148, 160	0
16	N	137/146 (93%)	0.75	26 (18%) 3 4	5, 74, 150, 167	0
17	O	117/118 (99%)	1.04	20 (17%) 4 5	5, 35, 114, 148	0
18	P	101/101 (100%)	0.68	13 (12%) 7 9	5, 79, 148, 159	0
19	Q	109/113 (96%)	0.41	12 (11%) 10 11	5, 33, 137, 149	0
20	R	92/96 (95%)	1.47	31 (33%) 1 1	5, 73, 148, 161	0
21	S	103/110 (93%)	0.73	18 (17%) 4 5	5, 86, 160, 163	0
22	T	185/206 (89%)	0.77	30 (16%) 4 6	5, 50, 148, 161	0
23	U	76/85 (89%)	0.62	7 (9%) 14 13	5, 57, 151, 166	0
24	V	88/98 (89%)	1.07	20 (22%) 2 3	5, 91, 148, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	62/72 (86%)	0.68	7 (11%) 10 11	5, 88, 149, 155	0
26	X	60/60 (100%)	0.22	4 (6%) 24 17	5, 36, 148, 150	0
27	Y	56/60 (93%)	0.79	11 (19%) 3 4	7, 77, 164, 168	0
28	Z	48/49 (97%)	0.65	6 (12%) 8 10	5, 5, 42, 126	0
29	a	63/65 (96%)	1.16	13 (20%) 2 3	5, 50, 151, 157	0
30	b	35/37 (94%)	2.19	16 (45%) 0 1	5, 102, 149, 153	0
31	y	1490/1522 (97%)	0.33	109 (7%) 21 16	5, 9, 113, 163	0
32	z	67/76 (88%)	0.35	5 (7%) 20 15	5, 6, 82, 117	0
33	0	75/76 (98%)	0.58	7 (9%) 14 13	5, 37, 128, 148	0
34	1	6/10 (60%)	1.76	2 (33%) 1 1	5, 5, 54, 67	0
35	c	234/256 (91%)	0.27	15 (6%) 25 18	5, 50, 151, 164	0
36	d	206/239 (86%)	0.51	30 (14%) 6 8	5, 57, 148, 151	0
37	e	208/209 (99%)	0.88	35 (16%) 4 6	5, 50, 148, 157	0
38	f	150/162 (92%)	1.18	32 (21%) 2 3	5, 62, 148, 154	0
39	g	101/101 (100%)	0.52	8 (7%) 18 15	5, 72, 148, 156	0
40	h	155/156 (99%)	1.04	37 (23%) 2 2	5, 73, 155, 163	0
41	i	138/138 (100%)	0.61	20 (14%) 6 8	5, 43, 148, 149	0
42	j	127/128 (99%)	1.16	26 (20%) 2 3	5, 85, 150, 154	0
43	k	98/105 (93%)	1.10	21 (21%) 2 3	5, 83, 151, 164	0
44	l	116/129 (89%)	0.81	19 (16%) 4 6	5, 71, 150, 162	0
45	m	124/132 (93%)	0.61	16 (12%) 7 9	5, 30, 148, 152	0
46	n	125/126 (99%)	1.17	27 (21%) 2 3	5, 74, 148, 162	0
47	o	60/61 (98%)	0.65	6 (10%) 12 13	5, 66, 151, 161	0
48	p	88/89 (98%)	0.64	9 (10%) 12 12	5, 57, 148, 163	0
49	q	83/88 (94%)	0.78	14 (16%) 4 6	5, 50, 148, 148	0
50	r	104/105 (99%)	0.56	17 (16%) 4 6	5, 52, 148, 158	0
51	s	73/88 (82%)	0.70	7 (9%) 13 13	5, 69, 149, 157	0
52	t	80/93 (86%)	0.78	16 (20%) 3 4	5, 52, 148, 159	0
53	u	99/106 (93%)	0.91	15 (15%) 5 7	10, 66, 199, 199	0
54	v	24/27 (88%)	1.23	8 (33%) 1 1	5, 47, 139, 142	0
All	All	10434/10880 (95%)	0.64	1389 (13%) 7 9	5, 32, 148, 199	0

The worst 5 of 1389 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	n	118	ALA	18.5
1	w	1061	U	15.8
1	w	896	A	14.1
42	j	14	VAL	14.1
22	T	173	ALA	13.3

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

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
32	H2U	z	20	20/21	0.66	0.12	124,124,133,133	0
31	5MC	y	967	21/22	0.69	0.24	124,124,133,133	0
32	H2U	z	16	20/21	0.73	0.16	80,92,93,95	0
31	PSU	y	516	20/21	0.77	0.16	137,138,148,148	0
32	PSU	z	55	20/21	0.79	0.13	40,50,52,53	0
32	4SU	z	8	20/21	0.85	0.18	5,5,5,5	0
32	MIA	z	37	29/30	0.86	0.26	20,26,32,32	0
32	PSU	z	32	20/21	0.86	0.16	42,52,58,59	0
33	PSU	0	55	20/21	0.86	0.12	36,36,36,36	0
31	5MC	y	1404	21/22	0.89	0.19	5,6,8,9	0
31	M2G	y	966	25/26	0.92	0.11	15,16,20,31	0
32	PSU	z	39	20/21	0.92	0.12	5,5,5,5	0
31	4OC	y	1402	22/23	0.93	0.10	10,13,16,16	0
31	7MG	y	527	24/25	0.93	0.10	7,10,24,26	0
31	MA6	y	1518	24/25	0.93	0.14	31,39,52,53	0
31	MA6	y	1519	24/25	0.93	0.14	5,5,6,8	0
32	7MG	z	46	24/25	0.94	0.09	5,5,12,12	0
31	2MG	y	1207	24/25	0.94	0.09	21,22,26,26	0
31	5MC	y	1407	21/22	0.94	0.09	25,28,30,30	0
31	UR3	y	1498	21/22	0.95	0.12	5,5,5,5	0
32	5MU	z	54	21/22	0.95	0.08	5,5,5,5	0
31	5MC	y	1400	21/22	0.96	0.09	5,5,5,5	0

6.3 Carbohydrates ⓘ

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.