



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 4V4J / pdb_00004v4j
Title : Interactions and Dynamics of the Shine-Dalgarno Helix in the 70S Ribosome.
Authors : Korostelev, A.; Trakhanov, S.; Asahara, H.; Laurberg, M.; Noller, H.F.
Deposited on : 2007-07-18
Resolution : 3.83 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

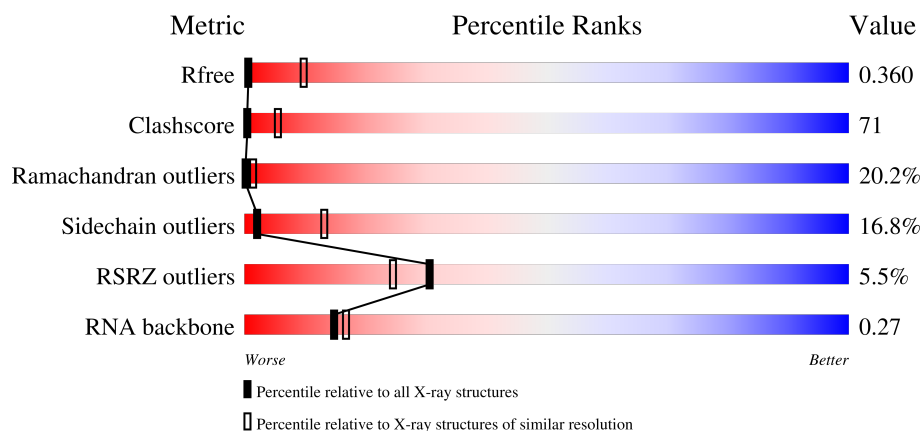
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

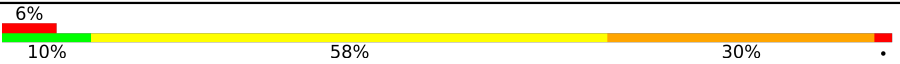
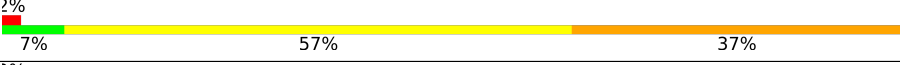
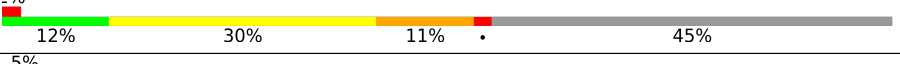
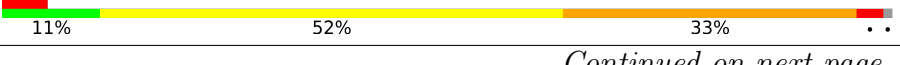
The reported resolution of this entry is 3.83 Å.

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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)
RNA backbone	3983	1010 (4.56-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	w	2889	
2	x	120	
3	A	229	
4	B	276	

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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	140	
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	77	
33	2	76	
34	3	18	
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	MA6	y	1518	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 147125 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	24	VAL	MET	conflict	UNP Q72IN1

- 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			
			725	471	131	123	0	0	0

- 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		
			793	510	151	126	6	0	0

- 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		
			1475	941	262	269	3	0	0

- 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		
			605	376	126	102	1	0	0

- Molecule 24 is a protein called LSU ribosomal protein L28P.

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

- 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		
			520	325	102	91	2	0	0

- Molecule 26 is a protein called LSU ribosomal protein L30P.

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

- 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 RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1514	Total	C	N	O	P	0	0	0
			32546	14494	6022	10517	1513			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	466	G	C	conflict	GB 155076

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2	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	3	18	Total	C	N	O	P	0	0	0
			390	176	80	117	17			

- 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	S	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 type Z.

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	81	Total	C	N	O	0	0	0
			668	423	135	110			

- 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			

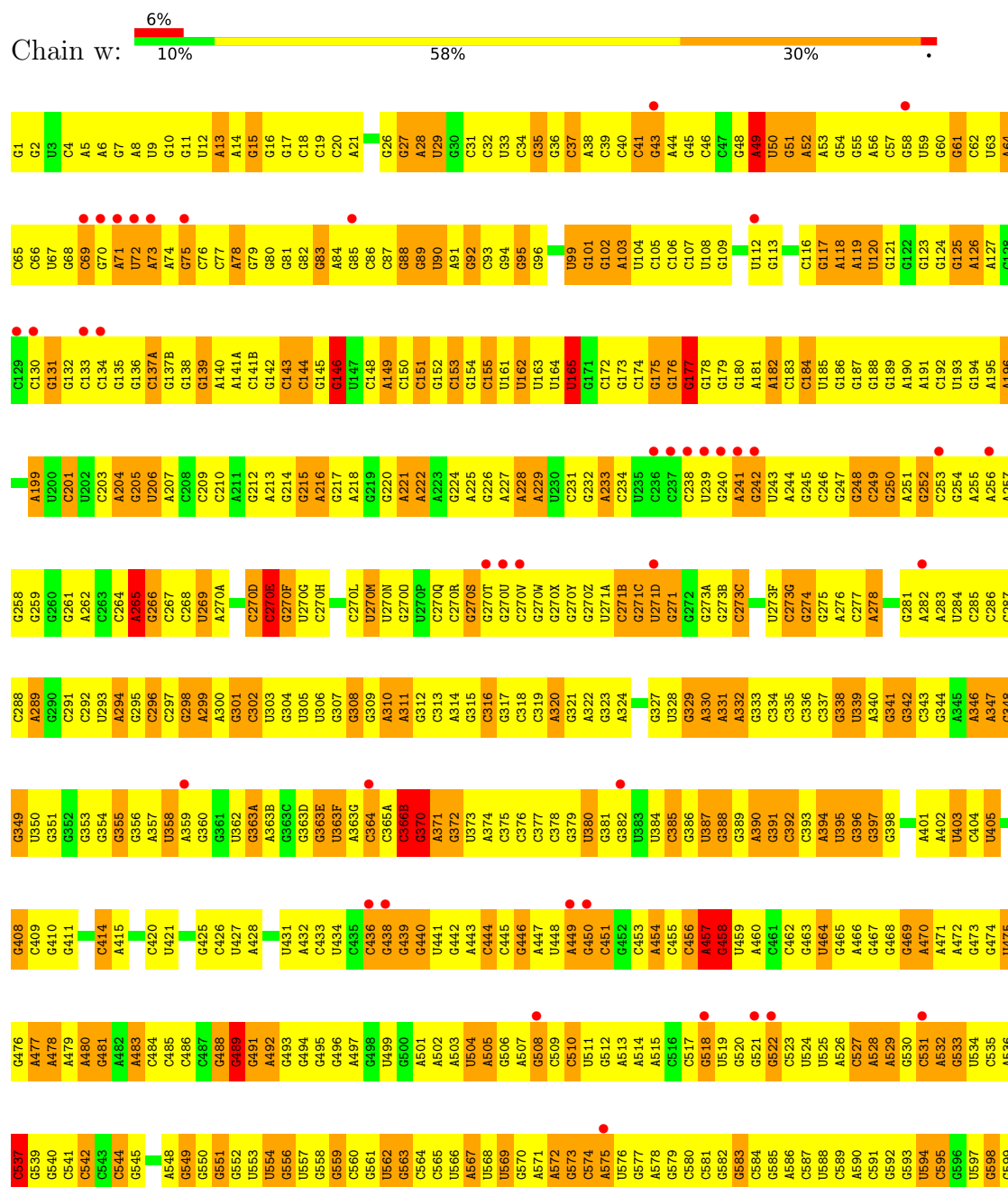
- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

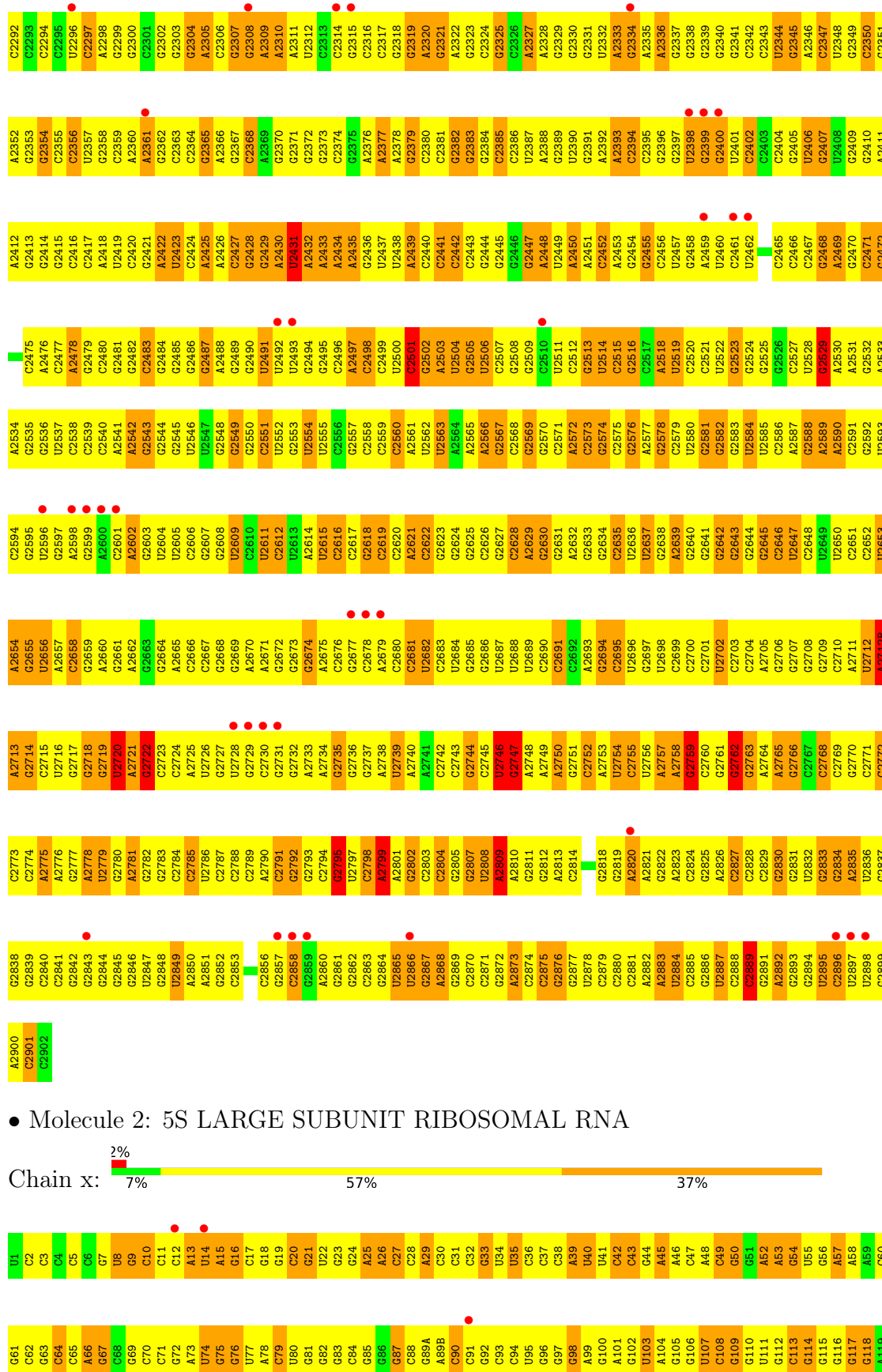
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

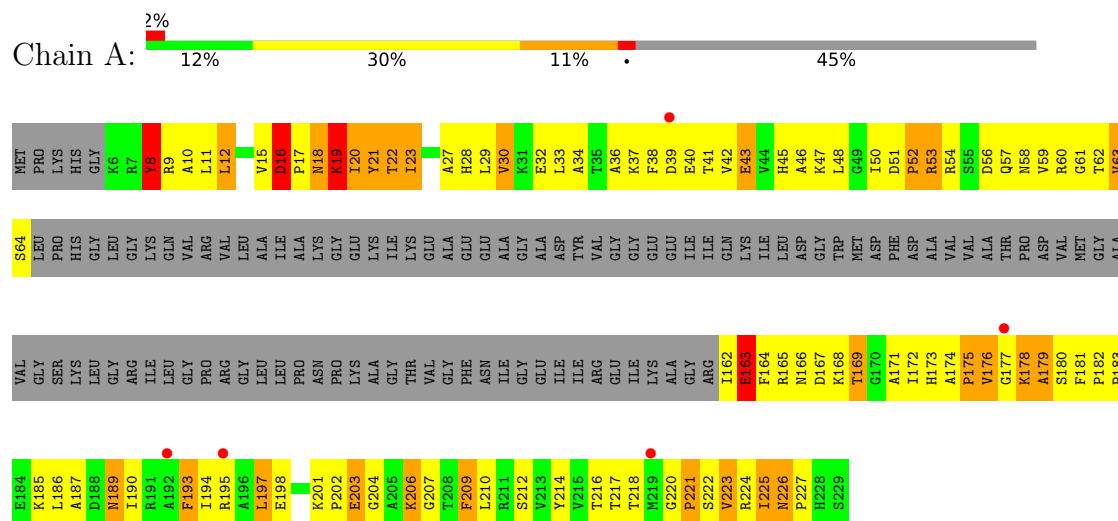


U1397	G1337	A1275	G1216	G1153	A1088	A1027	G906	G842	G780	C719	C658	G600
C1398	G1338	A1276	C1217	G1154	G1089	A1028	U907	G843	A781	C720	C659	C601
G1399	G1339	G1277	G1218	A1155	C1092	A1029	C908		A782	G860	G860	C602
G1400	G1340	A1156	G1219	A1157	C1093	G1030	A909		A783	C661	G861	A603
G1401	G1341	G1279	A1220	G1158	U1094	G1031	A910	C846	A784	G662	G662	G604
C1402	G1342	G1280	C1221	G1159	U1095	A1032	C912	C848	G785	G724	G663	C605
C1403	G1343	G1281	C1222	G1160	A1096	G1033	C913	G849	C786	G725	C664	U606
C1404	G1344	U1282	G1223	G1161	A1097	G974A	U913	A849	U787	G726	C665	U607
U1405	G1345	G1283	G1224	G1162	A1098	C374B	C914	C850	A788	A727	C666	A608
U1406	G1346	G1284	G1225	G1163	G1099	C976	C915	U851	A789	G728	U667	A609A
C1407	G1347	G1285	G1226	G1164	G1099	C977	G916	U852	C790	G729	G668	G609B
C1408	G1348	A1286	A1226	U1165	C1100	G978	A917	C853	G791	G730	G669	C610
C1409	G1349	A1287	G1227	U1166	U1101	G979	A918	C854	G792	C731	A670	C611
G1410	C1350	U1288	G1228	C1166	C1102	C1040	G919	G855	A793	C732	C671	G612
G1411	U1351	C1289			G1042	C1041	G920	C856	G794	G733	C672	U613
A1412	U1352		G1230	G1169	C1043	C921	G920	C857	A794	A734	C673	U614
G1413	G1231	G1170	G1231	G1171	G1104	G1044	G921	C858	C795	A735	G674	G615
G1414	C1293	G1171	G1232	G1172	U1105	A1045	U922	U858	C796	A736	A675	A616
U1415	U1294	G1173	C1233	G1174	G1110	A1046	C923	U860	C797	C737	G676	G617
G1416	C1295	A1174	U1234	A1175	A1111	G1047	C924	A861	G798	G738	A677	G618A
G1417	G1296	U1175	U1235	G1176	G1112	A1048	C925	G862	G799	G739	C678	C618B
G1418	C1297	G1176	G1236	U1177	U1113	C1049	A926	A863	U740	U740	C679	G619
A1419	U1298	A1177	A1237	G1178	G1114	A1050	G929	A864	A802	G741	G680	G620
U1420	C1299	G1178	G1238	C1179	G1115	U1051	U930	C865	U803	G742	G681	A621
G1421	U1300	C1179	G1239	G1180	C1116	C1052	G931	A866	A804	G743	G682	G622
G1422	C1362	C1180	U1240	C1181	G1117	C1053	G932	C867	G805	G744	C683	G623
G1423	C1363	A1241	A1241	C1182	C1118	G1054	A933	U868	G884	G745	C624	G624
G1424	G1364	G1303	A1242	U1182	C1119	G1055	G934	G869	U807	A746	A685	G625
G1425	A1365	G1183	G1243	U1188	G1120	C1056	C935	A870	G808	U747	G686	U626
G1426	G1366	G1184	G1244	C1121	C1121	A1057	C936	U871	G809	G748	C687	A627
A1427	A1367	G1185	G1245	G1186	G1122	G1058	U937	A872	U810	C749	U688	G628
G1428	G1368	C1306	U1246	G1186	C1123	G1059	G938	G873	U811	A750	A689	G629
G1429	G1369	A1307	A1247	G1187	C1124	U1060		G874	C812	A751	G690	G630
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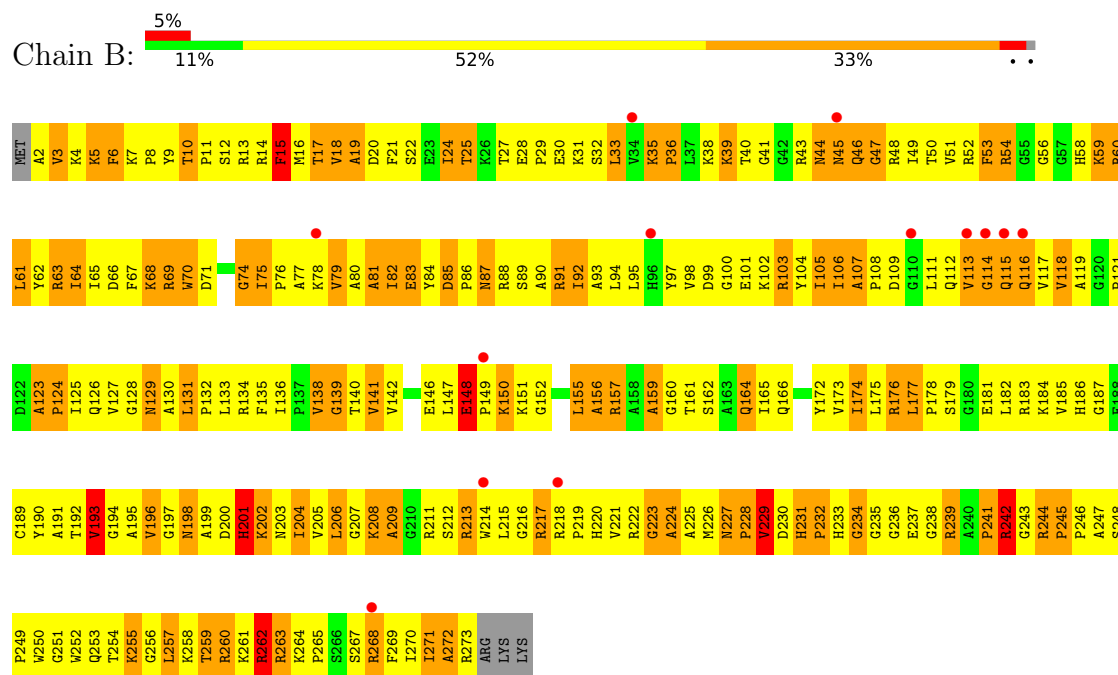
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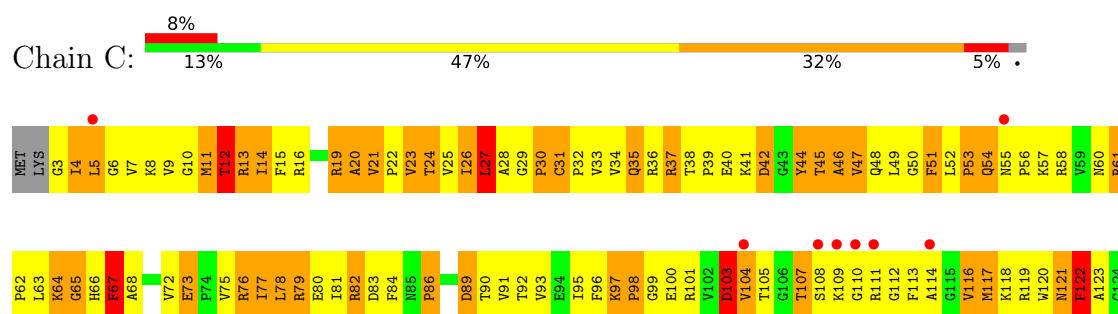
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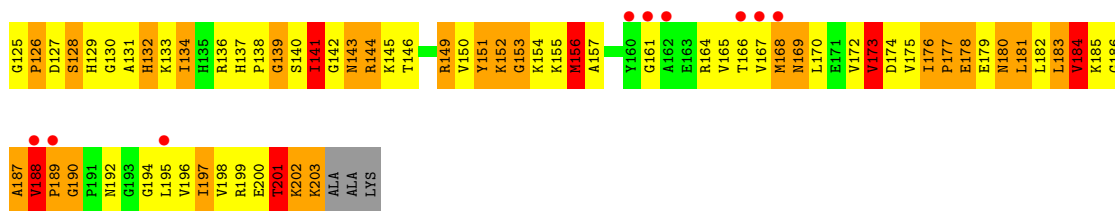


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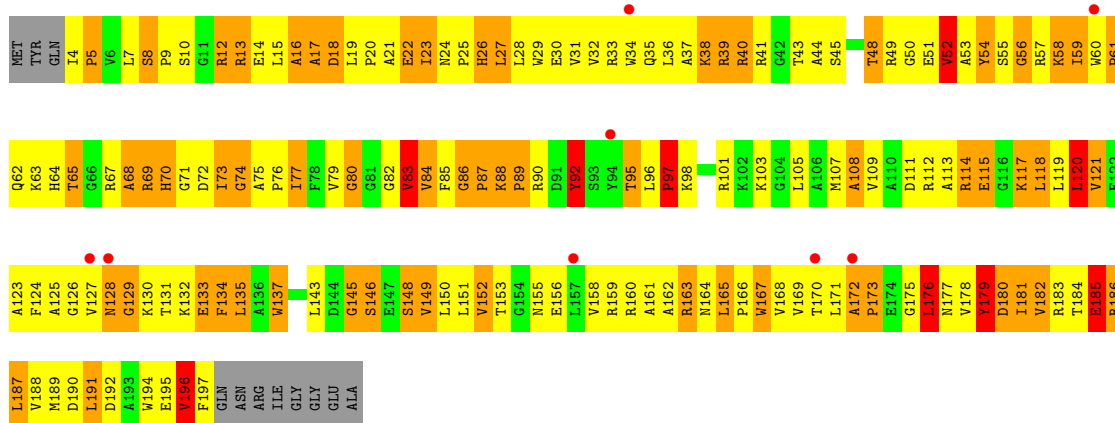
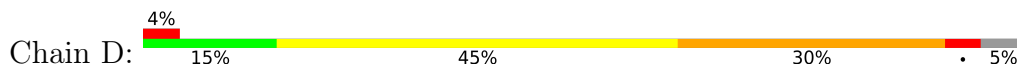


• Molecule 5: 50S ribosomal protein L3

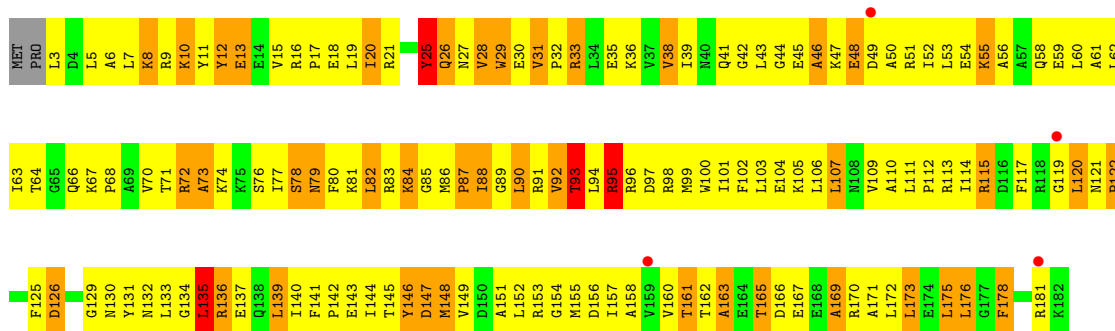
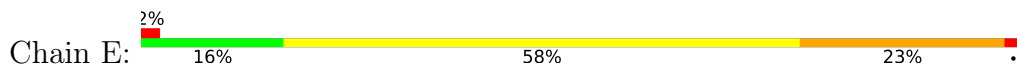




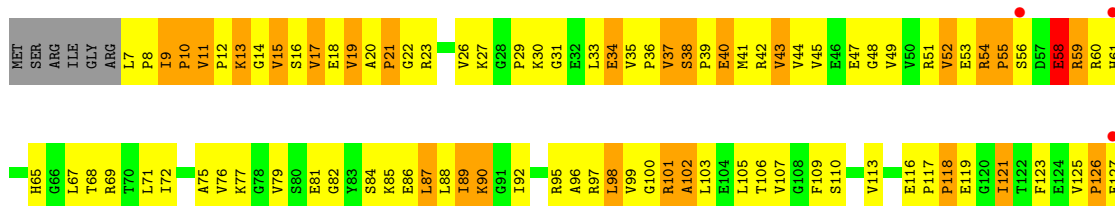
• Molecule 6: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L5

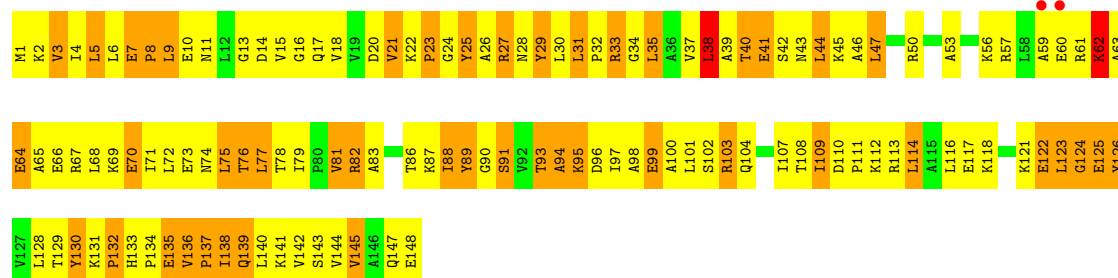
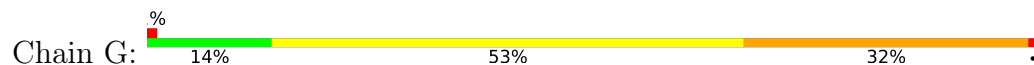


• Molecule 8: 50S ribosomal protein L6

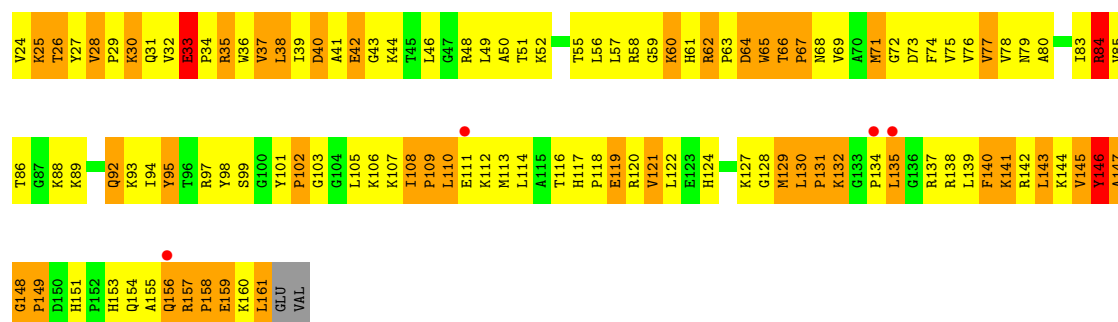
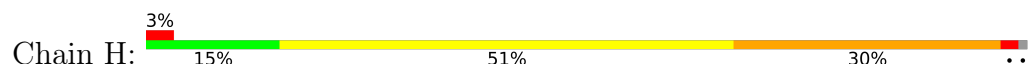




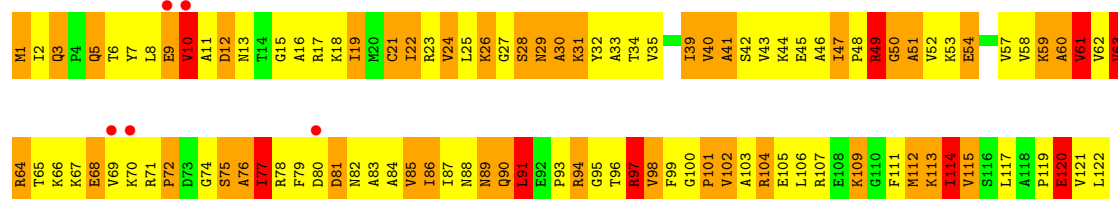
• Molecule 9: 50S ribosomal protein L9



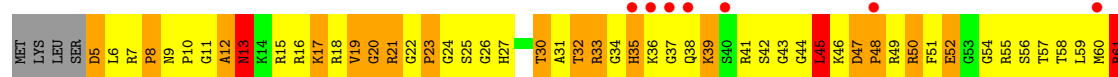
• Molecule 10: 50S ribosomal protein L13

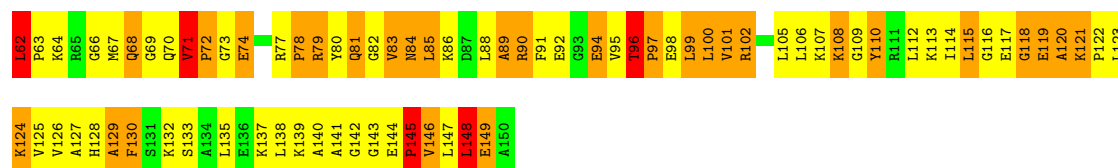


• Molecule 11: 50S ribosomal protein L14

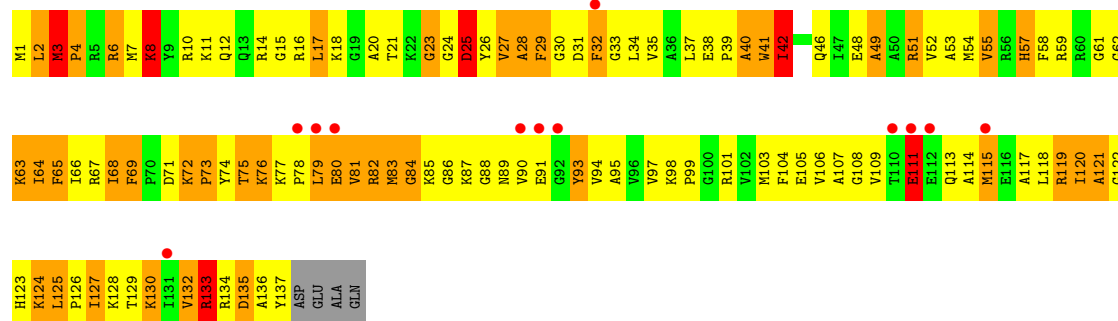
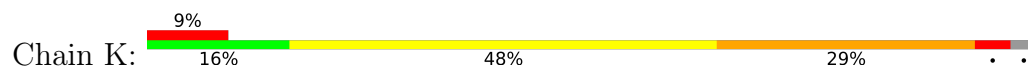


• Molecule 12: 50S ribosomal protein L15

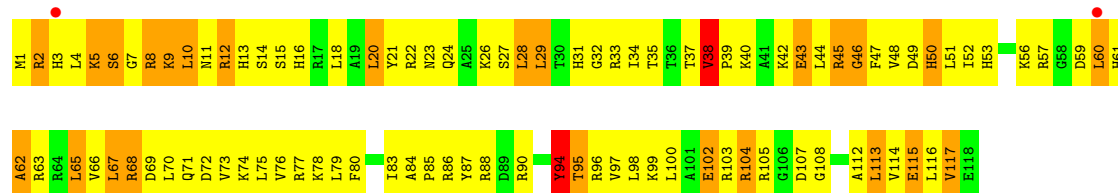




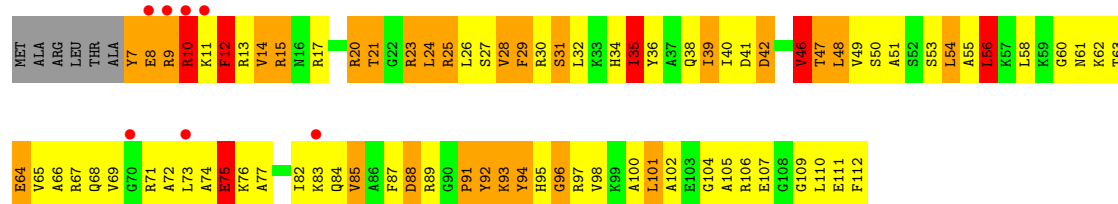
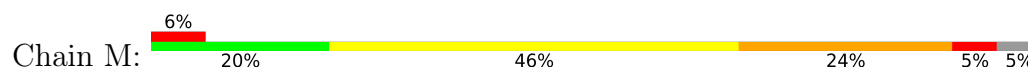
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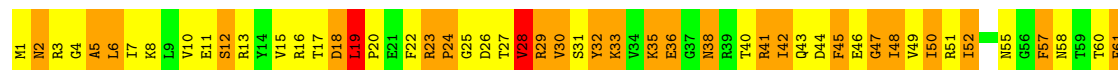
• Molecule 14: 50S ribosomal protein L17

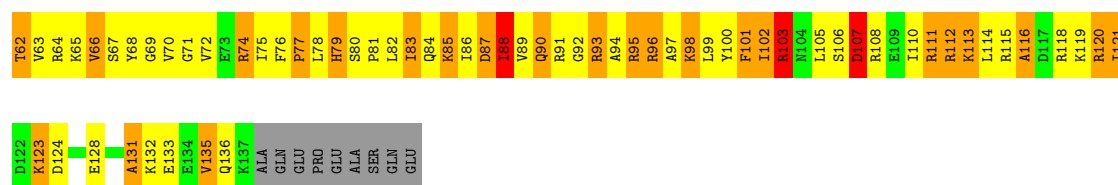


• Molecule 15: 50S ribosomal protein L18

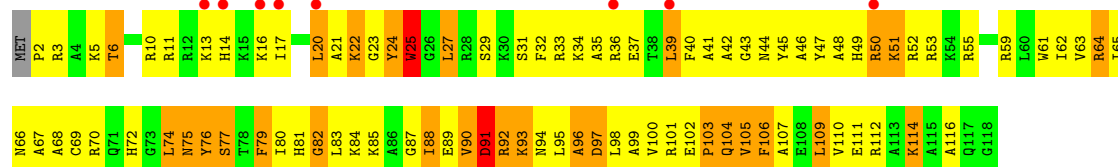


• Molecule 16: 50S ribosomal protein L19

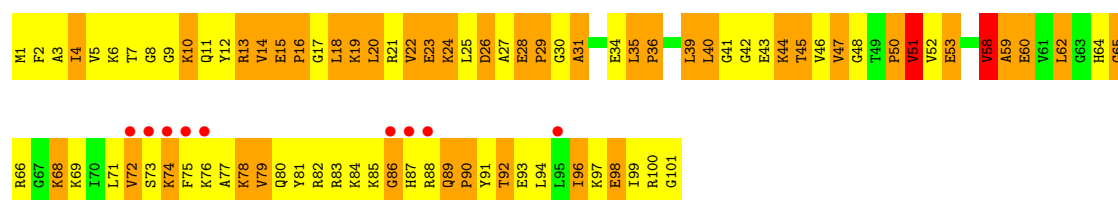




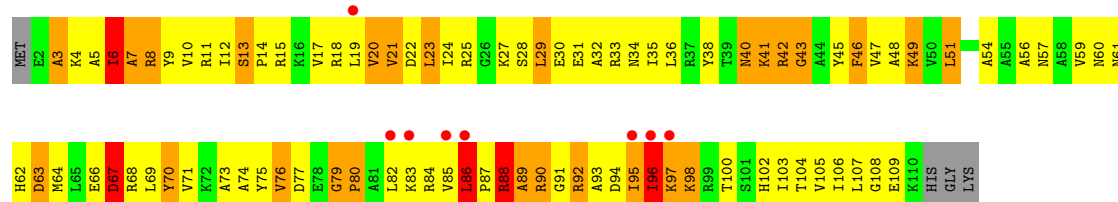
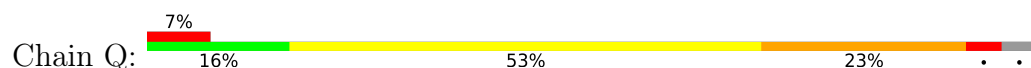
• Molecule 17: 50S ribosomal protein L20



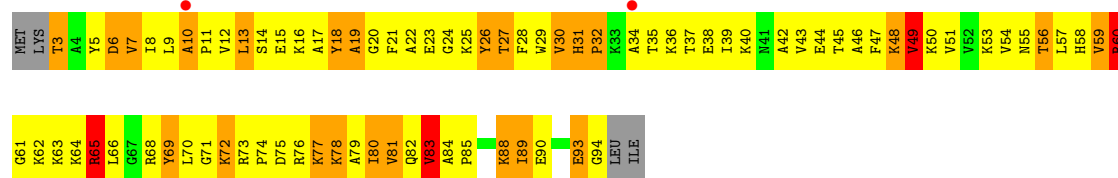
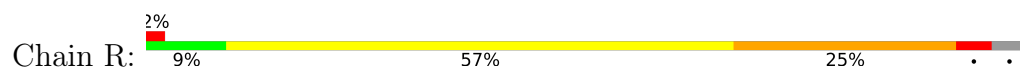
• Molecule 18: 50S ribosomal protein L21



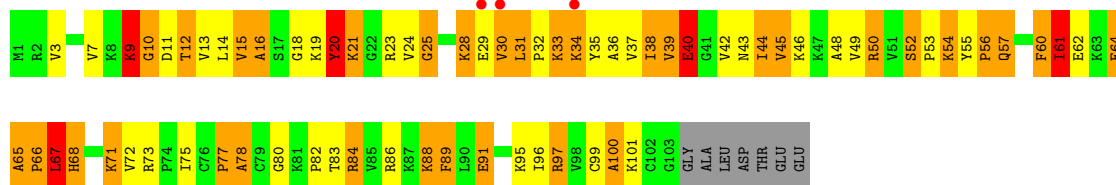
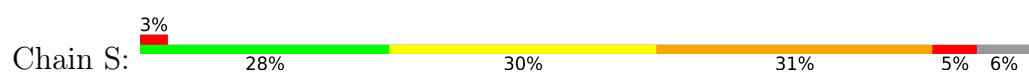
• Molecule 19: 50S ribosomal protein L22



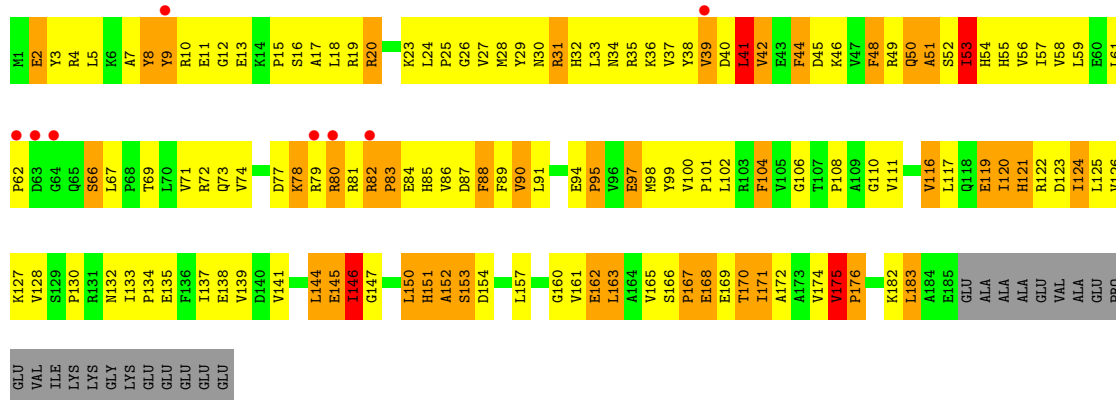
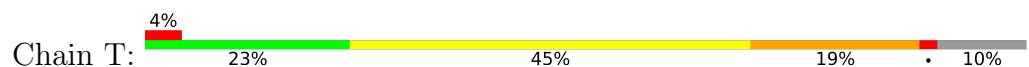
• Molecule 20: 50S ribosomal protein L23



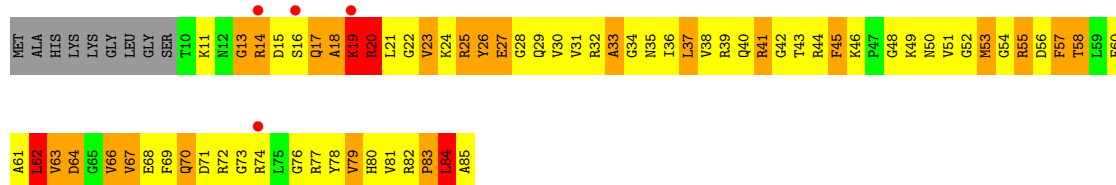
• Molecule 21: 50S ribosomal protein L24



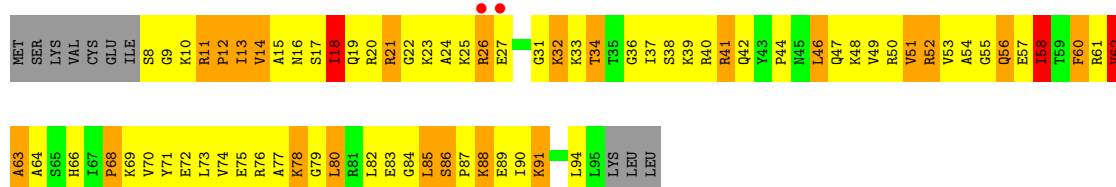
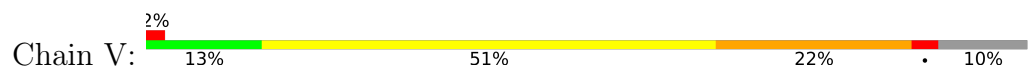
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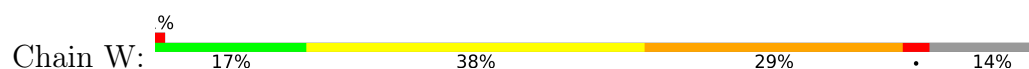
• Molecule 23: 50S ribosomal protein L27



• Molecule 24: LSU ribosomal protein L28P

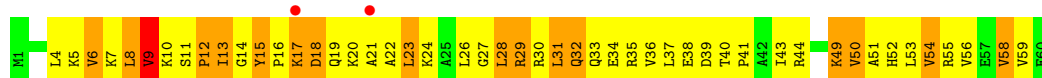
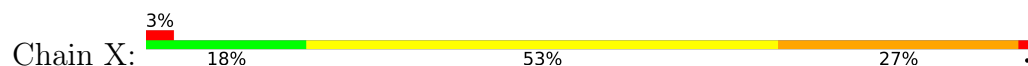


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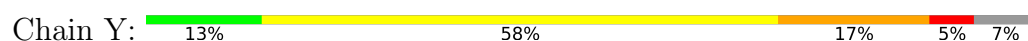




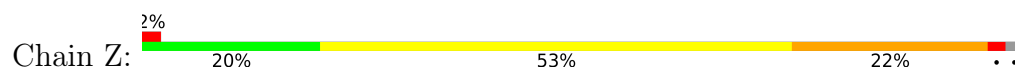
- Molecule 26: LSU ribosomal protein L30P



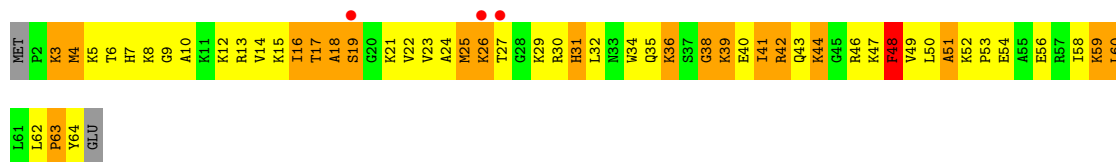
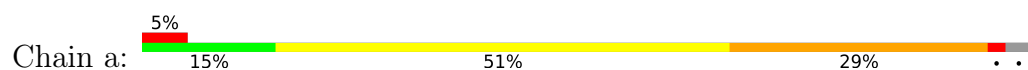
- Molecule 27: 50S ribosomal protein L32



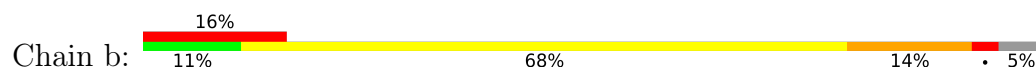
- Molecule 28: 50S ribosomal protein L34



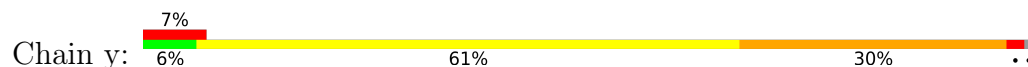
- Molecule 29: 50S ribosomal protein L35

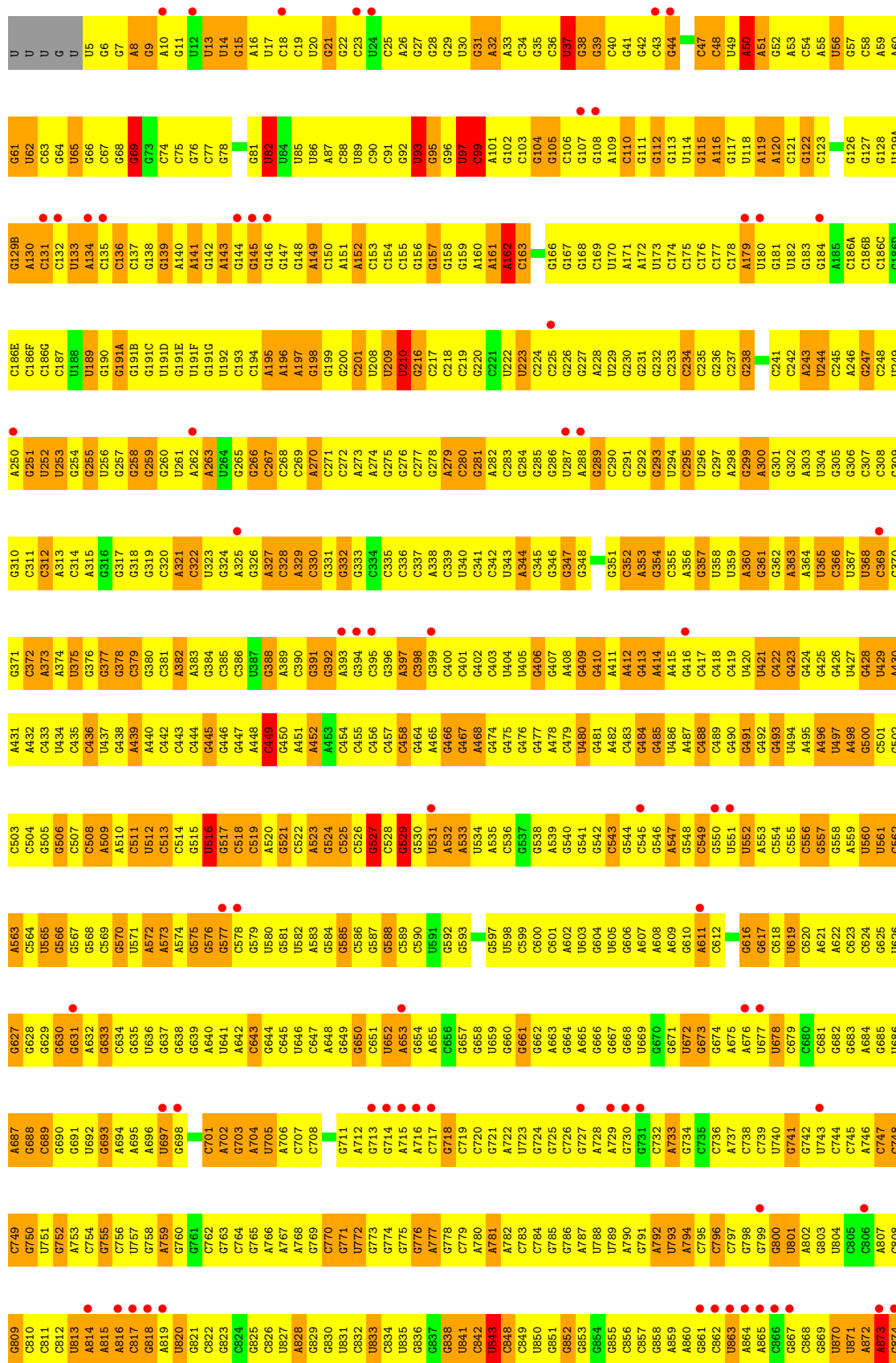


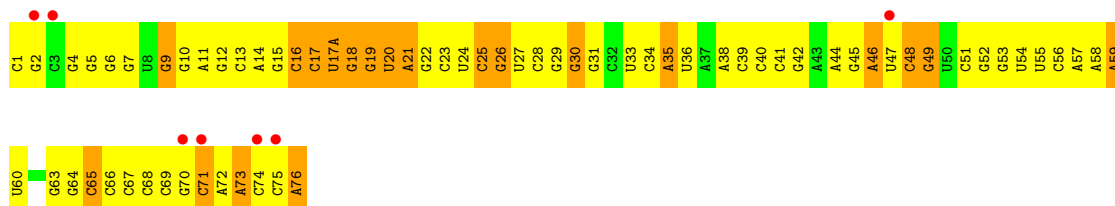
- Molecule 30: 50S ribosomal protein L36



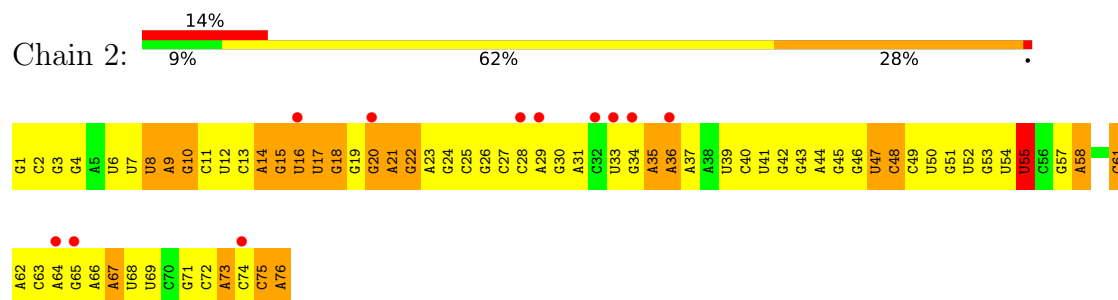
- Molecule 31: 16S RNA



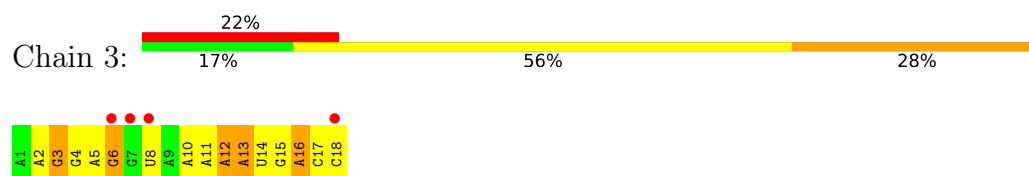




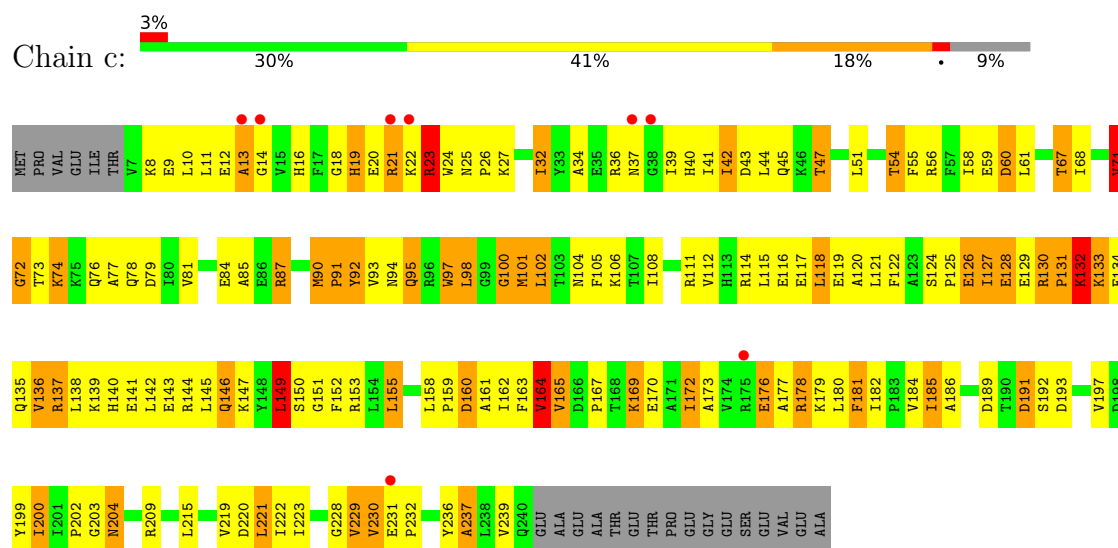
- Molecule 33: E-site tRNA

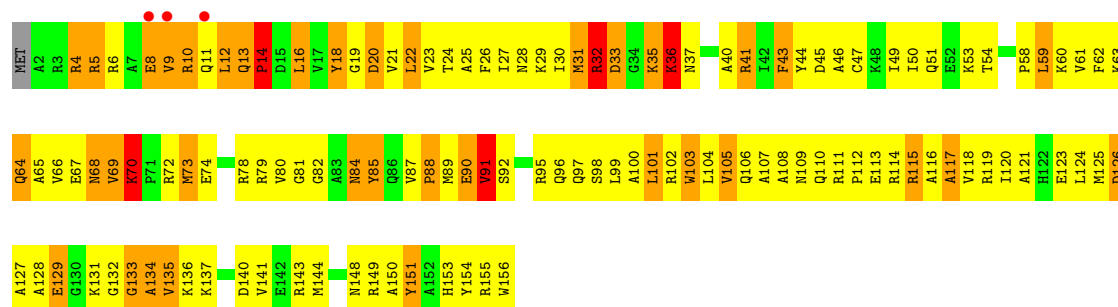


- Molecule 34: MRNA

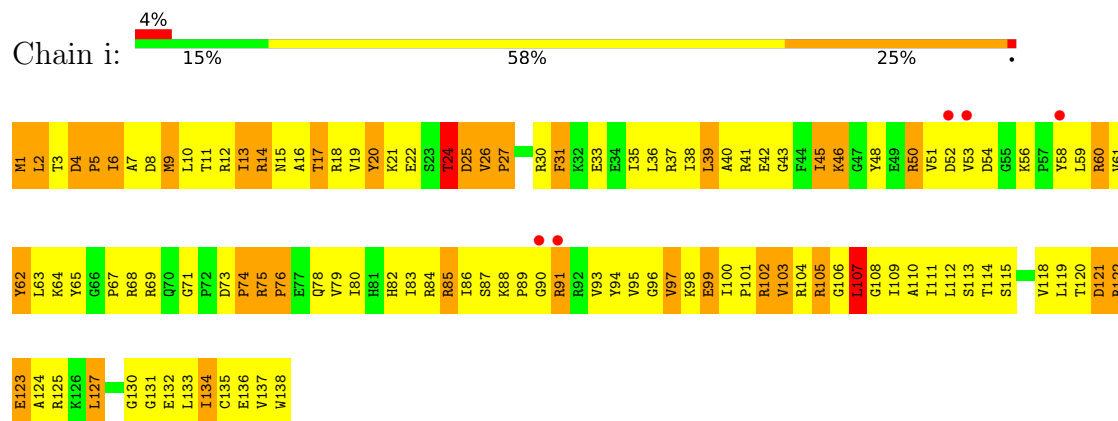


- Molecule 35: 30S ribosomal protein S2

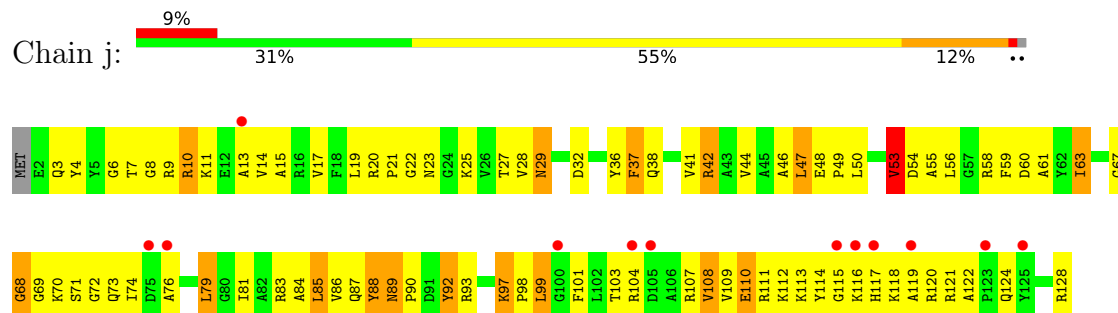




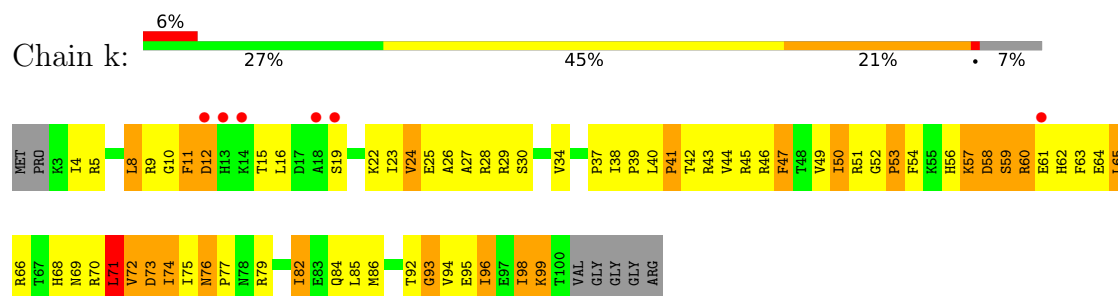
• Molecule 41: 30S ribosomal protein S8



• Molecule 42: 30S ribosomal protein S9

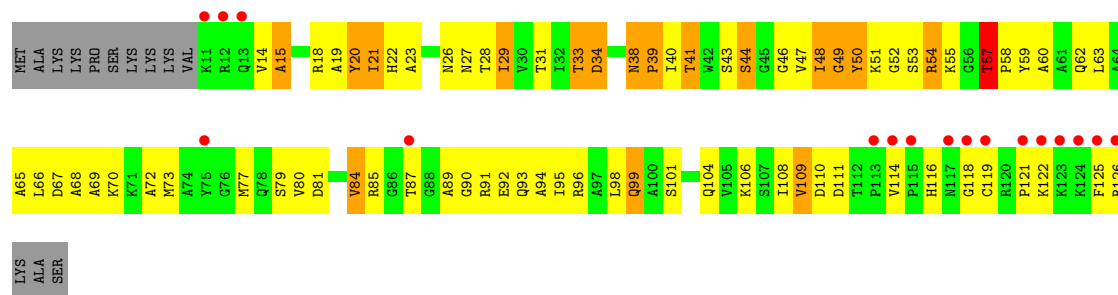


• Molecule 43: 30S ribosomal protein S10

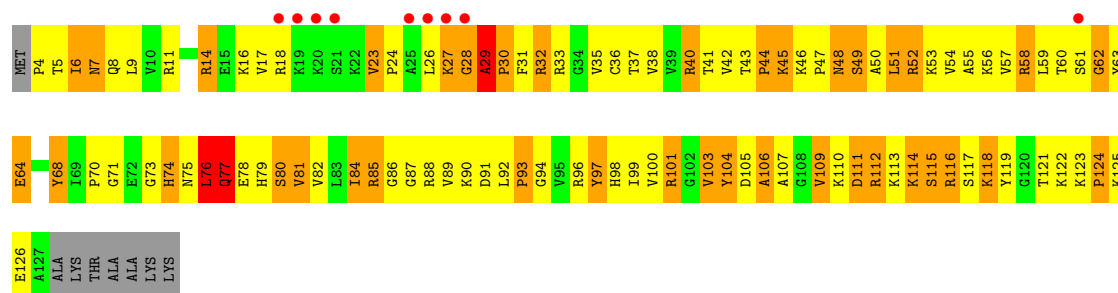
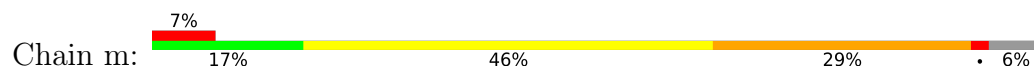


• Molecule 44: 30S ribosomal protein S11

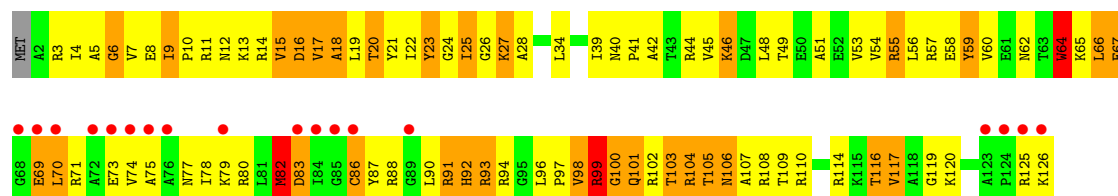




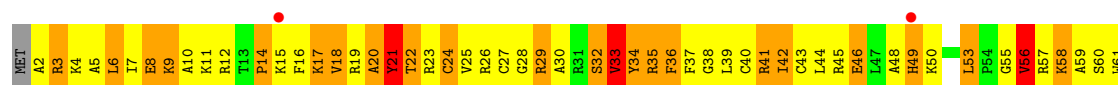
• Molecule 45: 30S ribosomal protein S12



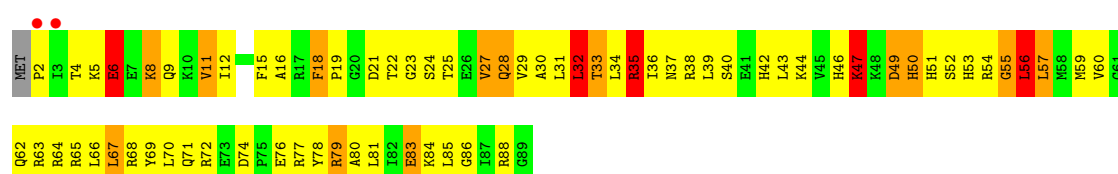
• Molecule 46: 30S ribosomal protein S13



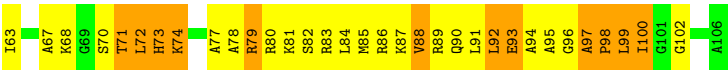
• Molecule 47: 30S ribosomal protein S14 type Z



• Molecule 48: 30S ribosomal protein S15



- [illegible]



- 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	507.21Å 507.21Å 692.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.83 30.00 – 3.83	Depositor EDS
% Data completeness (in resolution range)	81.7 (30.00-3.83) 73.9 (30.00-3.83)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.327 , 0.351 0.340 , 0.360	Depositor DCC
R_{free} test set	10300 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.54 , 365.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.22$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.267 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.260 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	0.82	EDS
Total number of atoms	147125	wwPDB-VP
Average B, all atoms (Å ²)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.08% 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: PSU, MA6, 7MG, 5MC, 2MG, M2G

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	45/69679 (0.1%)	0.91	101/108779 (0.1%)
2	x	0.56	0/2878	0.82	0/4490
3	A	0.70	0/1015	1.05	7/1369 (0.5%)
4	B	0.71	0/2165	1.05	17/2919 (0.6%)
5	C	0.76	0/1574	1.06	10/2125 (0.5%)
6	D	0.74	0/1551	1.05	8/2101 (0.4%)
7	E	0.73	0/1492	1.04	8/2006 (0.4%)
8	F	0.79	0/1345	1.12	9/1819 (0.5%)
9	G	0.67	0/1171	1.06	4/1583 (0.3%)
10	H	0.67	0/1130	1.10	10/1525 (0.7%)
11	I	0.76	0/942	1.16	8/1268 (0.6%)
12	J	0.77	1/1131 (0.1%)	1.09	8/1504 (0.5%)
13	K	0.75	0/1110	1.08	7/1483 (0.5%)
14	L	0.61	0/982	0.96	1/1312 (0.1%)
15	M	0.65	0/856	0.94	3/1138 (0.3%)
16	N	0.72	0/1157	1.12	11/1544 (0.7%)
17	O	0.61	0/982	0.97	3/1306 (0.2%)
18	P	0.80	0/790	1.06	6/1057 (0.6%)
19	Q	0.68	0/878	1.08	7/1179 (0.6%)
20	R	0.81	0/739	1.10	9/993 (0.9%)
21	S	0.88	0/806	1.02	2/1074 (0.2%)
22	T	0.72	0/1507	1.04	12/2045 (0.6%)
23	U	0.70	0/613	1.06	4/816 (0.5%)
24	V	0.80	0/701	1.05	2/932 (0.2%)
25	W	0.66	0/522	1.04	2/690 (0.3%)
26	X	0.65	0/482	1.08	3/646 (0.5%)
27	Y	0.75	0/449	1.17	1/606 (0.2%)
28	Z	0.63	0/426	1.02	3/561 (0.5%)
29	a	0.77	0/515	1.07	2/679 (0.3%)
30	b	0.87	0/297	0.96	0/392
31	y	0.61	27/36178 (0.1%)	0.87	37/56463 (0.1%)
32	z	0.53	0/1831	0.84	0/2853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.54	0/1791	0.80	1/2791 (0.0%)
34	3	0.59	1/439 (0.2%)	0.79	0/684
35	c	0.70	0/1935	1.04	14/2609 (0.5%)
36	d	0.63	0/1636	0.97	2/2205 (0.1%)
37	e	0.67	0/1733	1.02	11/2318 (0.5%)
38	f	0.76	0/1162	1.08	9/1564 (0.6%)
39	g	0.67	0/856	1.15	14/1154 (1.2%)
40	h	0.67	0/1276	1.09	9/1709 (0.5%)
41	i	0.65	0/1136	0.99	2/1527 (0.1%)
42	j	0.68	0/1029	0.99	4/1378 (0.3%)
43	k	0.83	0/807	1.02	3/1085 (0.3%)
44	l	0.76	0/879	1.03	6/1187 (0.5%)
45	m	0.70	0/986	1.20	10/1320 (0.8%)
46	n	0.66	0/1008	1.06	2/1347 (0.1%)
47	o	0.65	0/501	1.01	1/664 (0.2%)
48	p	0.62	0/745	1.03	6/992 (0.6%)
49	q	0.67	0/716	1.06	6/963 (0.6%)
50	r	0.75	0/870	1.07	6/1159 (0.5%)
51	s	0.72	0/675	1.00	2/894 (0.2%)
52	t	0.76	0/661	1.06	5/890 (0.6%)
53	u	0.54	0/764	0.97	2/1006 (0.2%)
54	v	0.64	0/212	0.81	0/277
All	All	0.72	74/159711 (0.0%)	0.94	420/238980 (0.2%)

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	41	C	O3'-P	34.69	2.13	1.61
1	w	1506	C	O3'-P	32.07	2.09	1.61
1	w	489	G	O3'-P	31.78	2.08	1.61
1	w	1448(B)	A	O3'-P	30.89	2.07	1.61
1	w	436	C	O3'-P	29.30	2.05	1.61

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2712(B)	A	P-O3'-C3'	-18.77	92.04	120.20
1	w	489	G	P-O3'-C3'	-15.31	97.23	120.20
31	y	97	U	P-O3'-C3'	-13.87	99.40	120.20
1	w	2746	U	P-O5'-C5'	-12.79	101.71	120.90
1	w	41	C	P-O3'-C3'	-12.56	101.35	120.20

There are no chirality outliers.

There are no planarity outliers.

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	31375	5674	0
2	x	2573	0	1306	326	0
3	A	996	0	1013	149	0
4	B	2115	0	2195	524	0
5	C	1541	0	1599	417	0
6	D	1517	0	1565	287	0
7	E	1468	0	1529	267	0
8	F	1319	0	1399	167	0
9	G	1156	0	1239	206	6
10	H	1103	0	1177	231	0
11	I	932	0	994	203	0
12	J	1114	0	1187	252	0
13	K	1089	0	1156	242	0
14	L	968	0	1033	193	0
15	M	846	0	902	192	0
16	N	1143	0	1211	206	0
17	O	964	0	1022	202	0
18	P	779	0	852	172	0
19	Q	868	0	929	146	0
20	R	725	0	778	128	0
21	S	793	0	890	87	0
22	T	1475	0	1504	217	0
23	U	605	0	628	191	0
24	V	694	0	764	161	0
25	W	520	0	575	80	0
26	X	477	0	529	89	0
27	Y	436	0	460	81	0
28	Z	418	0	467	106	0
29	a	507	0	576	99	0
30	b	294	0	323	58	0
31	y	32546	0	16450	4133	6
32	z	1639	0	837	159	0
33	2	1621	0	821	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	3	390	0	198	24	0
35	c	1900	0	1951	189	0
36	d	1612	0	1677	307	0
37	e	1703	0	1767	357	0
38	f	1146	0	1207	185	0
39	g	843	0	857	75	0
40	h	1257	0	1296	231	0
41	i	1116	0	1177	222	0
42	j	1011	0	1043	138	0
43	k	794	0	840	109	0
44	l	864	0	881	127	0
45	m	970	0	1057	208	0
46	n	997	0	1072	144	0
47	o	492	0	533	164	0
48	p	734	0	771	112	0
49	q	700	0	720	172	0
50	r	857	0	930	202	0
51	s	668	0	748	89	0
52	t	647	0	673	100	0
53	u	762	0	859	174	0
54	v	208	0	221	52	0
All	All	147125	0	99763	17210	6

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 71.

The worst 5 of 17210 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:2746:U:O5'	1:w:2746:U:C5'	1.70	1.40
1:w:2784:C:C2'	1:w:2785:C:H5''	1.61	1.31
1:w:568:U:H2'	1:w:570:G:OP2	1.31	1.26
1:w:2588:G:H2'	1:w:2589:A:O4'	1.31	1.26
31:y:66:G:H4'	31:y:173:U:O4	1.36	1.25

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:10:GLU:O	31:y:436:C:OP1[4_555]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:89:TYR:O	31:y:357:G:O2'[4_555]	2.00	0.20
9:G:90:GLY:O	31:y:368:U:OP2[4_555]	2.11	0.09
9:G:90:GLY:O	31:y:368:U:OP1[4_555]	2.14	0.06
9:G:91:SER:O	31:y:368:U:OP1[4_555]	2.17	0.03

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%)	72 (58%)	31 (25%)	20 (16%)	0	2
4	B	270/276 (98%)	134 (50%)	64 (24%)	72 (27%)	0	0
5	C	199/206 (97%)	99 (50%)	47 (24%)	53 (27%)	0	0
6	D	192/205 (94%)	91 (47%)	45 (23%)	56 (29%)	0	0
7	E	178/182 (98%)	97 (54%)	55 (31%)	26 (15%)	0	3
8	F	171/180 (95%)	90 (53%)	40 (23%)	41 (24%)	0	1
9	G	146/148 (99%)	83 (57%)	35 (24%)	28 (19%)	0	2
10	H	136/140 (97%)	62 (46%)	45 (33%)	29 (21%)	0	1
11	I	120/122 (98%)	62 (52%)	24 (20%)	34 (28%)	0	0
12	J	144/150 (96%)	63 (44%)	46 (32%)	35 (24%)	0	1
13	K	135/141 (96%)	56 (42%)	41 (30%)	38 (28%)	0	0
14	L	116/118 (98%)	64 (55%)	30 (26%)	22 (19%)	0	2
15	M	104/112 (93%)	58 (56%)	22 (21%)	24 (23%)	0	1
16	N	135/146 (92%)	56 (42%)	40 (30%)	39 (29%)	0	0
17	O	115/118 (98%)	66 (57%)	28 (24%)	21 (18%)	0	2
18	P	99/101 (98%)	39 (39%)	28 (28%)	32 (32%)	0	0
19	Q	107/113 (95%)	64 (60%)	23 (22%)	20 (19%)	0	2
20	R	90/96 (94%)	29 (32%)	36 (40%)	25 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	101/110 (92%)	28 (28%)	31 (31%)	42 (42%)	0	0
22	T	183/206 (89%)	115 (63%)	45 (25%)	23 (13%)	0	4
23	U	74/85 (87%)	31 (42%)	21 (28%)	22 (30%)	0	0
24	V	86/98 (88%)	41 (48%)	29 (34%)	16 (19%)	0	2
25	W	60/72 (83%)	33 (55%)	11 (18%)	16 (27%)	0	0
26	X	58/60 (97%)	31 (53%)	20 (34%)	7 (12%)	0	4
27	Y	54/60 (90%)	27 (50%)	16 (30%)	11 (20%)	0	1
28	Z	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	0	6
29	a	61/65 (94%)	28 (46%)	20 (33%)	13 (21%)	0	1
30	b	33/37 (89%)	16 (48%)	10 (30%)	7 (21%)	0	1
35	c	232/256 (91%)	142 (61%)	59 (25%)	31 (13%)	0	3
36	d	204/239 (85%)	102 (50%)	60 (29%)	42 (21%)	0	1
37	e	206/209 (99%)	120 (58%)	60 (29%)	26 (13%)	0	4
38	f	148/162 (91%)	102 (69%)	32 (22%)	14 (10%)	0	9
39	g	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	11
40	h	153/156 (98%)	96 (63%)	30 (20%)	27 (18%)	0	2
41	i	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	3
42	j	125/128 (98%)	81 (65%)	29 (23%)	15 (12%)	0	4
43	k	96/105 (91%)	55 (57%)	25 (26%)	16 (17%)	0	2
44	l	114/129 (88%)	74 (65%)	28 (25%)	12 (10%)	0	7
45	m	122/132 (92%)	67 (55%)	35 (29%)	20 (16%)	0	2
46	n	123/126 (98%)	70 (57%)	35 (28%)	18 (15%)	0	3
47	o	58/61 (95%)	30 (52%)	16 (28%)	12 (21%)	0	1
48	p	86/89 (97%)	51 (59%)	24 (28%)	11 (13%)	0	4
49	q	81/88 (92%)	34 (42%)	25 (31%)	22 (27%)	0	0
50	r	102/105 (97%)	54 (53%)	24 (24%)	24 (24%)	0	1
51	s	79/88 (90%)	45 (57%)	21 (27%)	13 (16%)	0	2
52	t	78/93 (84%)	30 (38%)	26 (33%)	22 (28%)	0	0
53	u	97/106 (92%)	47 (48%)	35 (36%)	15 (16%)	0	2
54	v	22/27 (82%)	8 (36%)	6 (27%)	8 (36%)	0	0
All	All	5697/6163 (92%)	3030 (53%)	1515 (27%)	1152 (20%)	0	1

5 of 1152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	8	TYR
3	A	16	ASP
3	A	63	VAL
3	A	176	VAL
3	A	179	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	106/181 (59%)	89 (84%)	17 (16%)	2	14
4	B	214/218 (98%)	180 (84%)	34 (16%)	2	14
5	C	163/166 (98%)	128 (78%)	35 (22%)	1	6
6	D	154/162 (95%)	129 (84%)	25 (16%)	2	14
7	E	154/156 (99%)	132 (86%)	22 (14%)	3	17
8	F	142/148 (96%)	126 (89%)	16 (11%)	5	23
9	G	124/124 (100%)	97 (78%)	27 (22%)	1	6
10	H	117/119 (98%)	96 (82%)	21 (18%)	2	12
11	I	100/100 (100%)	73 (73%)	27 (27%)	0	3
12	J	112/116 (97%)	87 (78%)	25 (22%)	1	6
13	K	108/111 (97%)	88 (82%)	20 (18%)	1	11
14	L	101/101 (100%)	86 (85%)	15 (15%)	3	16
15	M	84/88 (96%)	70 (83%)	14 (17%)	2	13
16	N	121/128 (94%)	102 (84%)	19 (16%)	2	15
17	O	93/94 (99%)	81 (87%)	12 (13%)	4	20
18	P	82/82 (100%)	67 (82%)	15 (18%)	2	11
19	Q	89/92 (97%)	73 (82%)	16 (18%)	2	12
20	R	74/78 (95%)	65 (88%)	9 (12%)	5	21
21	S	86/91 (94%)	74 (86%)	12 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	T	163/179 (91%)	134 (82%)	29 (18%)	2	12
23	U	61/67 (91%)	51 (84%)	10 (16%)	2	13
24	V	73/83 (88%)	62 (85%)	11 (15%)	3	16
25	W	58/67 (87%)	47 (81%)	11 (19%)	1	10
26	X	52/52 (100%)	43 (83%)	9 (17%)	2	12
27	Y	49/52 (94%)	41 (84%)	8 (16%)	2	14
28	Z	41/42 (98%)	34 (83%)	7 (17%)	2	12
29	a	53/55 (96%)	44 (83%)	9 (17%)	2	13
30	b	33/34 (97%)	31 (94%)	2 (6%)	17	43
35	c	202/220 (92%)	169 (84%)	33 (16%)	2	14
36	d	160/188 (85%)	132 (82%)	28 (18%)	2	12
37	e	180/181 (99%)	150 (83%)	30 (17%)	2	13
38	f	115/123 (94%)	100 (87%)	15 (13%)	4	19
39	g	90/90 (100%)	78 (87%)	12 (13%)	4	19
40	h	126/127 (99%)	105 (83%)	21 (17%)	2	13
41	i	119/119 (100%)	98 (82%)	21 (18%)	2	12
42	j	98/99 (99%)	91 (93%)	7 (7%)	13	40
43	k	88/92 (96%)	76 (86%)	12 (14%)	3	18
44	l	88/99 (89%)	81 (92%)	7 (8%)	11	36
45	m	104/109 (95%)	81 (78%)	23 (22%)	1	6
46	n	100/101 (99%)	75 (75%)	25 (25%)	0	4
47	o	49/50 (98%)	34 (69%)	15 (31%)	0	2
48	p	79/80 (99%)	68 (86%)	11 (14%)	3	17
49	q	72/74 (97%)	58 (81%)	14 (19%)	1	9
50	r	96/97 (99%)	82 (85%)	14 (15%)	3	16
51	s	71/77 (92%)	62 (87%)	9 (13%)	4	20
52	t	71/80 (89%)	53 (75%)	18 (25%)	0	3
53	u	76/82 (93%)	62 (82%)	14 (18%)	1	11
54	v	19/22 (86%)	17 (90%)	2 (10%)	6	26
All	All	4810/5096 (94%)	4002 (83%)	808 (17%)	2	13

5 of 808 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	Z	29	LYS
38	f	57	LYS
53	u	51	GLU
30	b	25	VAL
28	Z	15	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
40	h	109	ASN
51	s	63	GLN
41	i	70	GLN
46	n	40	ASN
15	M	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	984 (34%)	0
2	x	119/120 (99%)	47 (39%)	0
31	y	1513/1522 (99%)	509 (33%)	0
32	z	76/77 (98%)	20 (26%)	0
33	2	75/76 (98%)	22 (29%)	0
34	3	17/18 (94%)	5 (29%)	0
All	All	4688/4702 (99%)	1587 (33%)	0

5 of 1587 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	13	A
1	w	15	G
1	w	27	G
1	w	28	A

There are no RNA pucker outliers to report.

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

11 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	MA6	y	1518	31	23,26,27	1.75	6 (26%)	33,38,41	2.39	15 (45%)
31	M2G	y	966	31	24,27,28	1.19	3 (12%)	33,40,43	1.13	3 (9%)
33	PSU	2	55	33	18,21,22	1.84	3 (16%)	21,30,33	2.18	7 (33%)
31	5MC	y	1404	31	19,22,23	1.10	1 (5%)	26,32,35	1.51	4 (15%)
31	5MC	y	1400	31	19,22,23	0.97	1 (5%)	26,32,35	0.95	1 (3%)
31	7MG	y	527	31	23,26,27	2.86	4 (17%)	27,39,42	1.81	6 (22%)
31	5MC	y	1407	31	19,22,23	0.90	1 (5%)	26,32,35	1.27	3 (11%)
31	5MC	y	967	31	19,22,23	0.95	2 (10%)	26,32,35	1.28	3 (11%)
31	2MG	y	1207	31	23,26,27	1.40	3 (13%)	33,38,41	1.68	3 (9%)
31	PSU	y	516	31	18,21,22	2.04	4 (22%)	21,30,33	1.94	6 (28%)
31	MA6	y	1519	31	23,26,27	1.97	8 (34%)	33,38,41	2.56	17 (51%)

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	MA6	y	1518	31	-	2/11/29/30	0/3/3/3
31	M2G	y	966	31	-	2/11/29/30	0/3/3/3
33	PSU	2	55	33	-	2/7/25/26	0/2/2/2
31	5MC	y	1404	31	-	2/7/25/26	0/2/2/2
31	5MC	y	1400	31	-	0/7/25/26	0/2/2/2
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	5MC	y	1407	31	-	0/7/25/26	0/2/2/2
31	5MC	y	967	31	-	0/7/25/26	0/2/2/2
31	2MG	y	1207	31	-	2/9/27/28	0/3/3/3
31	PSU	y	516	31	-	0/7/25/26	0/2/2/2
31	MA6	y	1519	31	-	3/11/29/30	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	527	7MG	C8-N9	-12.42	1.37	1.45
33	2	55	PSU	O2-C2	5.14	1.34	1.23
31	y	516	PSU	O2-C2	5.00	1.34	1.23
31	y	516	PSU	C6-C5	4.82	1.40	1.35
33	2	55	PSU	C6-C5	4.35	1.40	1.35

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1519	MA6	C2'-C1'-N9	-6.58	96.96	113.30
31	y	527	7MG	N9-C8-N7	6.39	112.42	103.37
31	y	1207	2MG	C4'-O4'-C1'	-6.15	95.89	109.47
31	y	1518	MA6	N1-C6-N6	5.53	123.59	116.86
33	2	55	PSU	N1-C2-N3	5.10	120.55	115.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	y	1518	MA6	O4'-C4'-C5'-O5'
31	y	1519	MA6	C5-C6-N6-C9
33	2	55	PSU	C2'-C1'-C5-C4
31	y	1518	MA6	C3'-C4'-C5'-O5'
31	y	966	M2G	O4'-C1'-N9-C8

There are no ring outliers.

11 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	y	1518	MA6	16	0
31	y	966	M2G	6	0
33	2	55	PSU	3	0
31	y	1404	5MC	4	0
31	y	1400	5MC	3	0
31	y	527	7MG	2	0
31	y	1407	5MC	6	0
31	y	967	5MC	5	0
31	y	1207	2MG	3	0
31	y	516	PSU	1	0
31	y	1519	MA6	5	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	w	35
31	y	9

The worst 5 of 44 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	41:C	O3'	43:G	P	2.13
1	w	1506:C	O3'	1508:A	P	2.09
1	w	489:G	O3'	491:G	P	2.08
1	w	1448(B):A	O3'	1449:G	P	2.07
1	w	436:C	O3'	438:G	P	2.05

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%)	-0.41	183 (6%) 26 22	1, 1, 1, 1	0
2	x	120/120 (100%)	-0.78	3 (2%) 58 40	1, 1, 1, 1	0
3	A	127/229 (55%)	-0.84	5 (3%) 43 31	1, 1, 1, 1	0
4	B	272/276 (98%)	-0.37	13 (4%) 35 27	1, 1, 1, 1	0
5	C	201/206 (97%)	-0.17	17 (8%) 16 17	1, 1, 1, 1	0
6	D	194/205 (94%)	-0.50	8 (4%) 41 30	1, 1, 1, 1	0
7	E	180/182 (98%)	-0.64	4 (2%) 62 44	1, 1, 1, 1	0
8	F	173/180 (96%)	-0.91	5 (2%) 53 37	1, 1, 1, 1	0
9	G	148/148 (100%)	-0.97	2 (1%) 73 52	1, 1, 1, 1	0
10	H	138/140 (98%)	-0.57	4 (2%) 53 37	1, 1, 1, 1	0
11	I	122/122 (100%)	-0.45	5 (4%) 41 30	1, 1, 1, 1	0
12	J	146/150 (97%)	-0.51	7 (4%) 35 27	1, 1, 1, 1	0
13	K	137/141 (97%)	-0.24	12 (8%) 15 16	1, 1, 1, 1	0
14	L	118/118 (100%)	-0.91	2 (1%) 69 48	1, 1, 1, 1	0
15	M	106/112 (94%)	-0.45	7 (6%) 24 21	1, 1, 1, 1	0
16	N	137/146 (93%)	-0.60	0 100 100	1, 1, 1, 1	0
17	O	117/118 (99%)	-0.49	8 (6%) 23 21	1, 1, 1, 1	0
18	P	101/101 (100%)	-0.25	9 (8%) 15 16	1, 1, 1, 1	0
19	Q	109/113 (96%)	-0.40	8 (7%) 21 19	1, 1, 1, 1	0
20	R	92/96 (95%)	-0.63	2 (2%) 62 44	1, 1, 1, 1	0
21	S	103/110 (93%)	-0.50	3 (2%) 53 37	1, 1, 1, 1	0
22	T	185/206 (89%)	-0.72	8 (4%) 40 29	1, 1, 1, 1	0
23	U	76/85 (89%)	-0.53	4 (5%) 32 25	1, 1, 1, 1	0
24	V	88/98 (89%)	-0.49	2 (2%) 61 43	1, 1, 1, 1	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	62/72 (86%)	-0.73	1 (1%) 70 49	1, 1, 1, 1	0
26	X	60/60 (100%)	-0.69	2 (3%) 49 34	1, 1, 1, 1	0
27	Y	56/60 (93%)	-0.80	0 100 100	1, 1, 1, 1	0
28	Z	48/49 (97%)	-0.68	1 (2%) 63 44	1, 1, 1, 1	0
29	a	63/65 (96%)	-0.06	3 (4%) 35 27	1, 1, 1, 1	0
30	b	35/37 (94%)	0.69	6 (17%) 4 7	1, 1, 1, 1	0
31	y	1504/1522 (98%)	-0.40	101 (6%) 24 21	1, 1, 1, 1	0
32	z	77/77 (100%)	-0.26	7 (9%) 15 16	1, 1, 1, 1	0
33	2	75/76 (98%)	0.14	11 (14%) 6 9	1, 1, 1, 1	0
34	3	18/18 (100%)	2.00	4 (22%) 2 4	1, 1, 1, 1	0
35	c	234/256 (91%)	-0.72	8 (3%) 48 34	1, 1, 1, 1	0
36	d	206/239 (86%)	-0.62	9 (4%) 39 29	1, 1, 1, 1	0
37	e	208/209 (99%)	-0.61	8 (3%) 44 32	1, 1, 1, 1	0
38	f	150/162 (92%)	-0.29	12 (8%) 18 18	1, 1, 1, 1	0
39	g	101/101 (100%)	-0.69	1 (0%) 79 58	1, 1, 1, 1	0
40	h	155/156 (99%)	-0.61	3 (1%) 66 46	1, 1, 1, 1	0
41	i	138/138 (100%)	-0.83	5 (3%) 46 33	1, 1, 1, 1	0
42	j	127/128 (99%)	-0.14	12 (9%) 14 16	1, 1, 1, 1	0
43	k	98/105 (93%)	-0.38	6 (6%) 27 23	1, 1, 1, 1	0
44	l	116/129 (89%)	0.25	17 (14%) 6 9	1, 1, 1, 1	0
45	m	124/132 (93%)	-0.42	9 (7%) 21 19	1, 1, 1, 1	0
46	n	125/126 (99%)	0.05	18 (14%) 6 9	1, 1, 1, 1	0
47	o	60/61 (98%)	-0.48	2 (3%) 49 34	1, 1, 1, 1	0
48	p	88/89 (98%)	-0.83	2 (2%) 61 43	1, 1, 1, 1	0
49	q	83/88 (94%)	-0.55	1 (1%) 76 55	1, 1, 1, 1	0
50	r	104/105 (99%)	-0.61	1 (0%) 79 58	1, 1, 1, 1	0
51	s	81/88 (92%)	-0.92	2 (2%) 58 40	1, 1, 1, 1	0
52	t	80/93 (86%)	-0.81	2 (2%) 58 40	1, 1, 1, 1	0
53	u	99/106 (93%)	-0.52	3 (3%) 52 36	1, 1, 1, 1	0
54	v	24/27 (88%)	-0.02	2 (8%) 17 17	1, 1, 1, 1	0
All	All	10478/10865 (96%)	-0.47	580 (5%) 30 24	1, 1, 1, 1	0

The worst 5 of 580 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	3	7	G	17.0
31	y	145	G	11.8
1	w	1983	C	11.2
44	l	125	PHE	10.8
5	C	167	VAL	10.7

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

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($\text{\AA}^2$)	Q<0.9
33	PSU	2	55	20/21	0.94	0.10	1,1,1,1	0
31	7MG	y	527	24/25	0.98	0.13	1,1,1,1	0
31	M2G	y	966	25/26	0.98	0.07	1,1,1,1	0
31	5MC	y	1400	21/22	0.98	0.12	1,1,1,1	0
31	5MC	y	1404	21/22	0.98	0.10	1,1,1,1	0
31	PSU	y	516	20/21	0.98	0.07	1,1,1,1	0
31	5MC	y	1407	21/22	0.99	0.06	1,1,1,1	0
31	MA6	y	1518	24/25	0.99	0.04	1,1,1,1	0
31	MA6	y	1519	24/25	0.99	0.05	1,1,1,1	0
31	5MC	y	967	21/22	0.99	0.08	1,1,1,1	0
31	2MG	y	1207	24/25	1.00	0.03	1,1,1,1	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.