



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 04:36 PM EDT

PDB ID : 4V4Z
Title : 70S Thermus thermophilus ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 4.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

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X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



Similar resolution
(#Entries, resolution range(Å))

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.

Quality of chain

Company	Good (%)	Bad (%)	Very bad (%)
Walmart	54%	34%	11%
Costco	49%	43%	8%
Amazon	37%	47%	13%
Target	19%	7%	74%
Home Depot	52%	22%	19%

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Mol	Chain	Length	Quality of chain
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	
9	AI	101	
10	AJ	156	
11	AK	138	
12	AL	128	
13	AM	105	
14	AN	129	
15	AO	132	
16	AP	126	
17	AQ	61	
18	AR	89	
19	AS	88	
20	AT	105	
21	AU	88	
22	AV	93	
23	AW	106	
24	AX	27	
25	BA	2916	
26	BB	123	
27	BC	229	
28	BD	276	
29	BE	206	

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Mol	Chain	Length	Quality of chain
30	BF	210	
31	BG	182	
32	BH	180	
33	BK	148	
34	BL	147	
35	BM	140	
36	BN	122	
37	BO	150	
38	BP	141	
39	BQ	118	
40	BR	112	
41	BS	146	
42	BT	118	
43	BU	101	
44	BV	113	
45	BW	96	
46	BX	110	
47	BY	206	
48	BZ	85	
49	B1	67	
50	B2	60	
51	B3	71	
52	B4	60	
53	B5	54	
54	B6	49	

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Mol	Chain	Length	Quality of chain
55	B7	65	<div><div></div><div>9%</div><div>46%</div><div>43%</div><div>9%</div><div></div></div>
56	B8	37	<div><div></div><div>5%</div><div>8%</div><div>46%</div><div>38%</div><div>8%</div><div></div></div>

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 149640 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	76	Total	C	N	O	P	0	0	0
			1624	723	295	530	76			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A1	27	Total	C	N	O	P	0	0	0
			596	267	127	175	27			

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	insertion	GB 48268

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 48271

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	U	-	insertion	GB 48271

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BR	110	Total	C	N	O			
			877	553	175	149	0	0	0

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BS	117	Total	C	N	O	S		
			976	614	197	164	1	0	0

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BV	110	Total	C	N	O	S		
			876	552	171	151	2	0	0

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BW	94	Total	C	N	O			
			742	483	133	126		0	0

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	110	Total	C	N	O	S		
			844	539	158	141	6	0	0

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

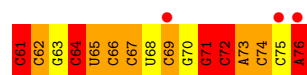
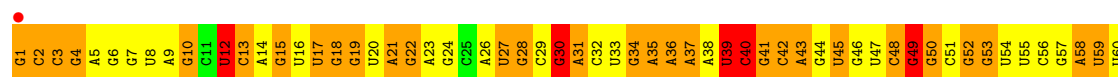
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 2: tRNA fMET (unmodified bases)

C1	C2	C3	C4	G5	G6	G7	G8	G9	G10	A11	G12	C13	A14	G15	C16	C17	G18	G19	U20	A21	G22	C23	U24	C25	G26	U27	C28	G29	G30	G31	C32	C33	U34	C35	A36	U36	A37	A38	C39	C40	C41	C42	A43	A44	G45	G46	U47	C48	G49	U50	C51	G52	G53	U54	U55	C56	A57	A58	A59	U60
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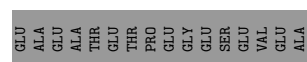
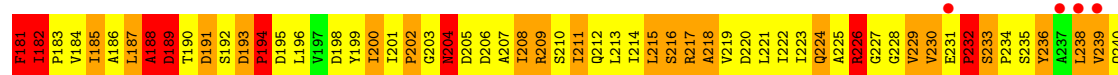
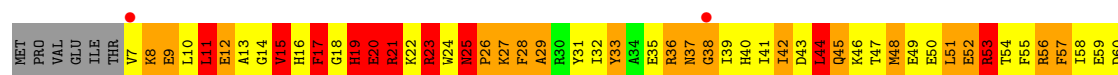
• Molecule 3: tRNA PHE (unmodified bases)



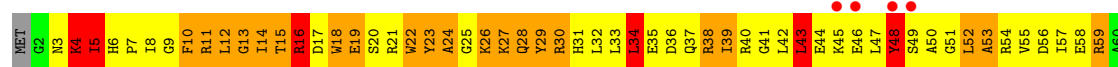
• Molecule 4: mRNA

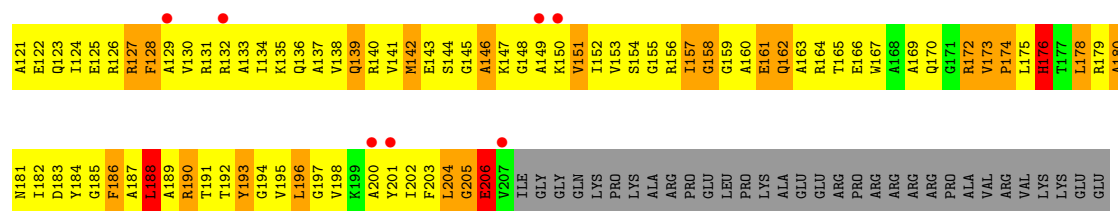


• Molecule 5: 30S ribosomal protein S2

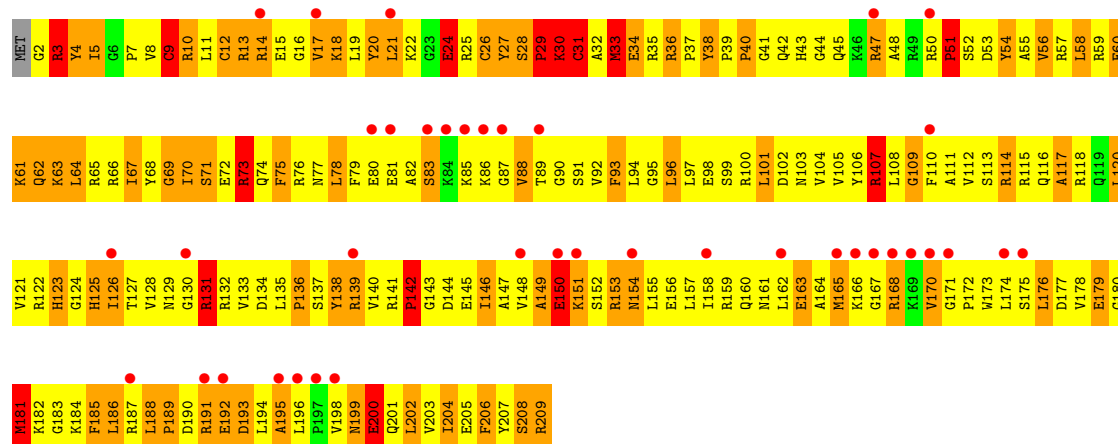


• Molecule 6: 30S ribosomal protein S3

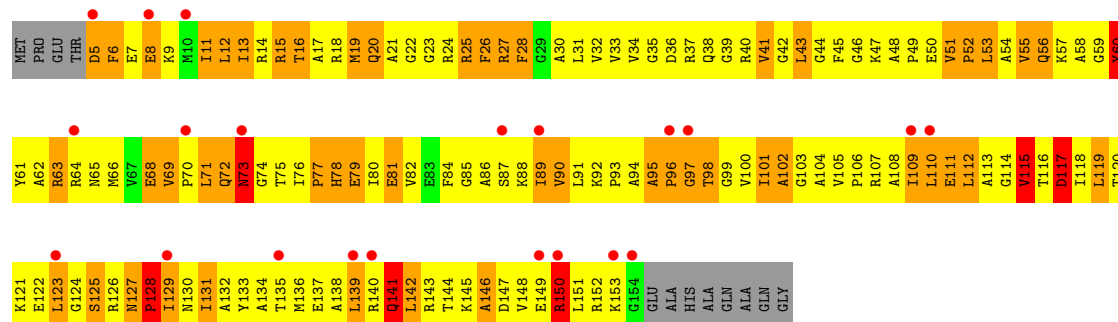




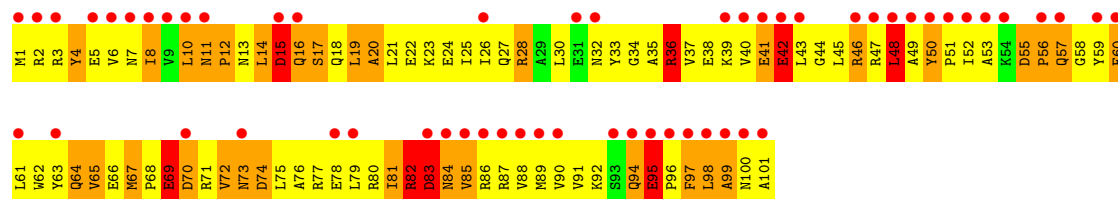
• Molecule 7: 30S ribosomal protein S4



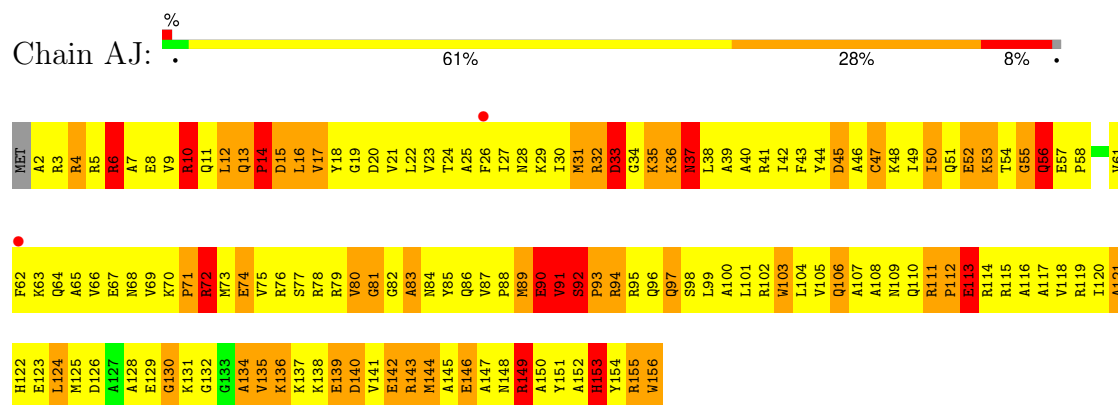
• Molecule 8: 30S ribosomal protein S5



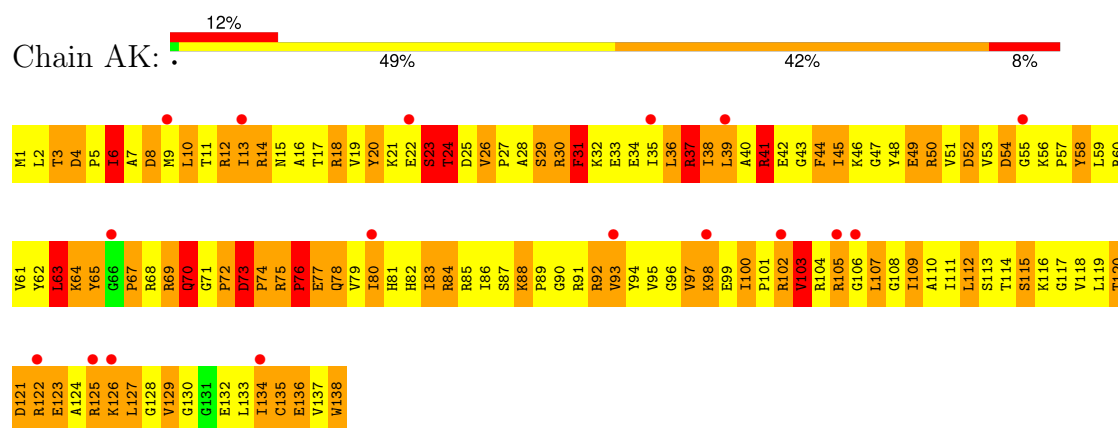
• Molecule 9: 30S ribosomal protein S6



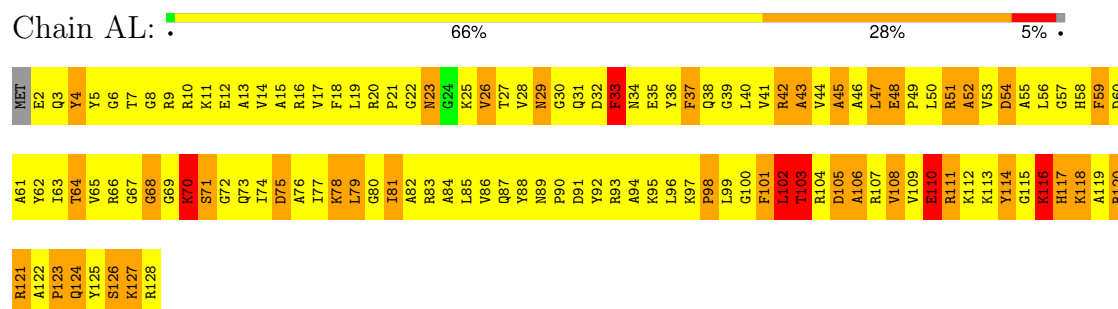
• Molecule 10: 30S ribosomal protein S7



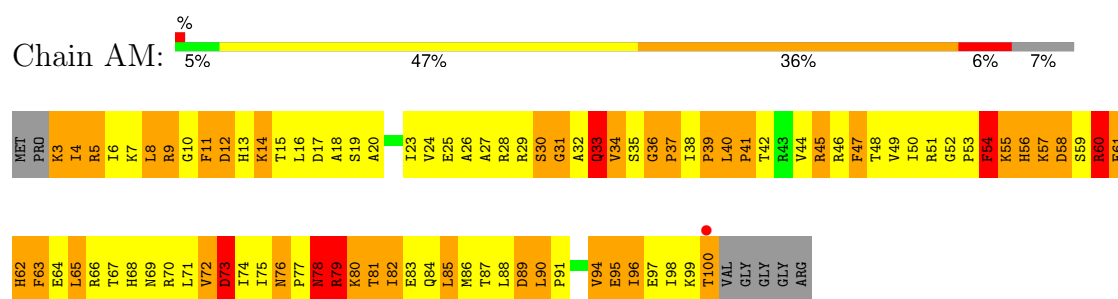
- Molecule 11: 30S ribosomal protein S8



- Molecule 12: 30S ribosomal protein S9

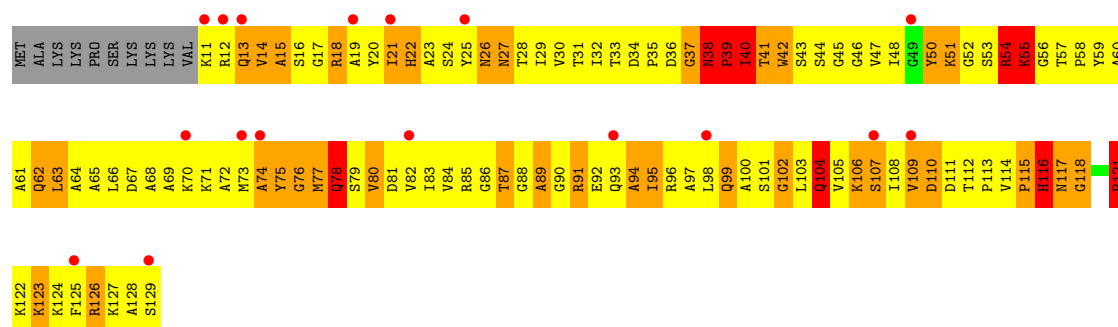


- Molecule 13: 30S ribosomal protein S10



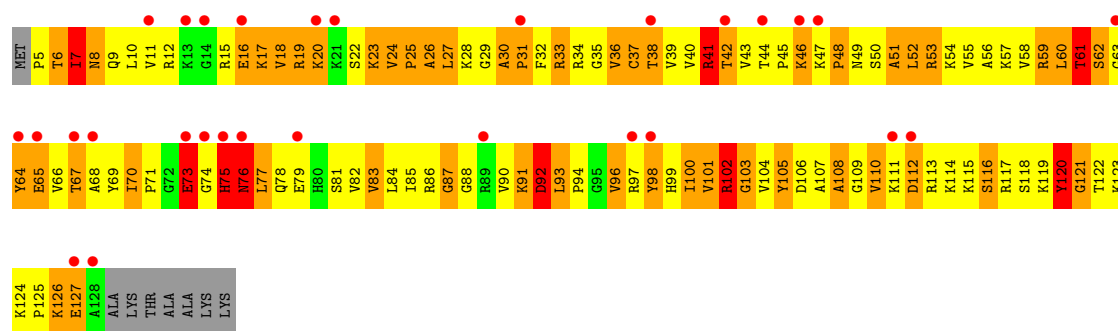
- Molecule 14: 30S ribosomal protein S11

Chain AN: 




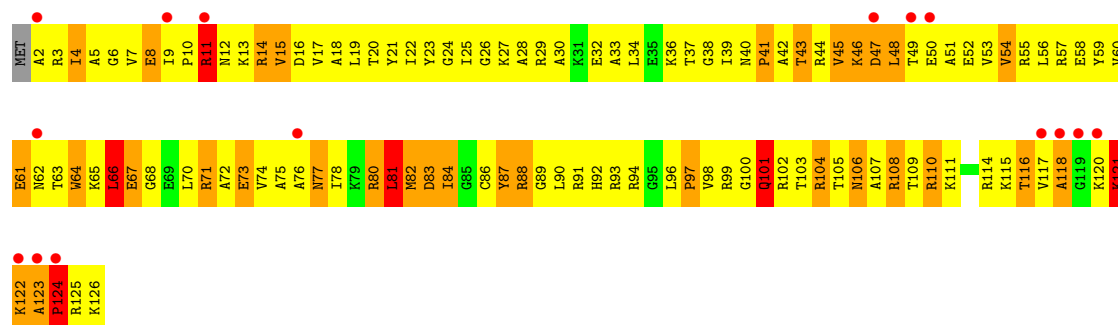
• Molecule 15: 30S ribosomal protein S12

Chain AO: 



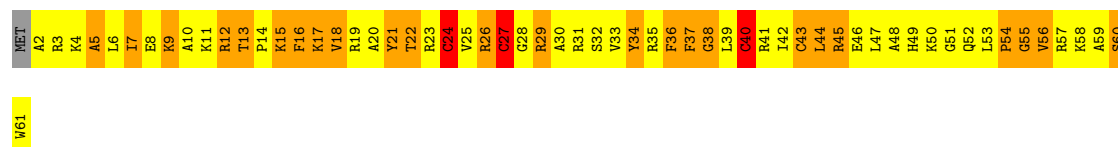
• Molecule 16: 30S ribosomal protein S13

Chain AP: 

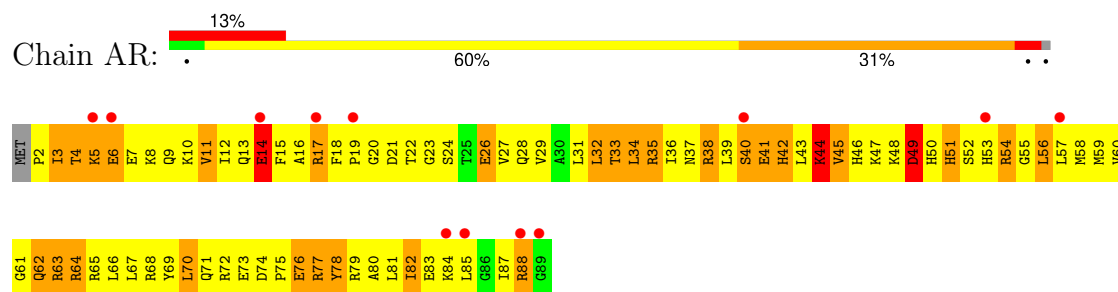


• Molecule 17: 30S ribosomal protein S14

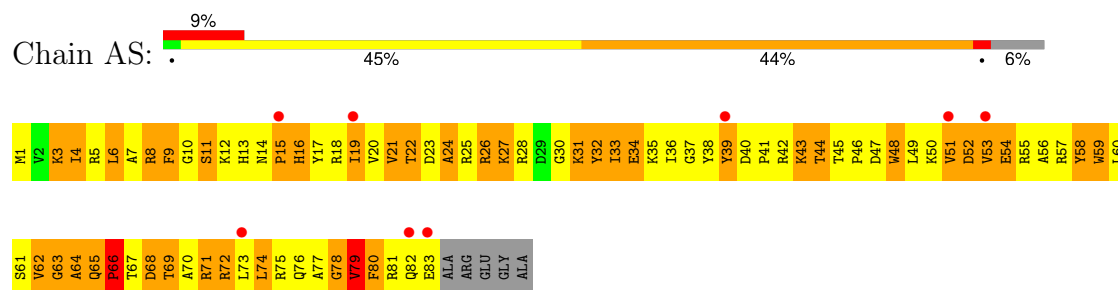
Chain AQ: 



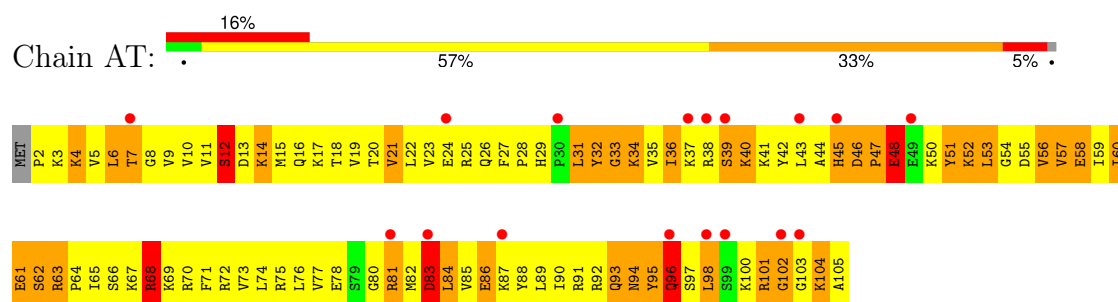
- Molecule 18: 30S ribosomal protein S15



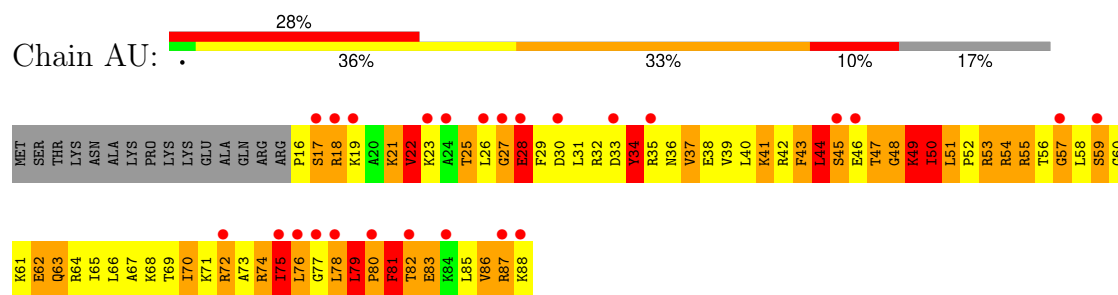
- Molecule 19: 30S ribosomal protein S16



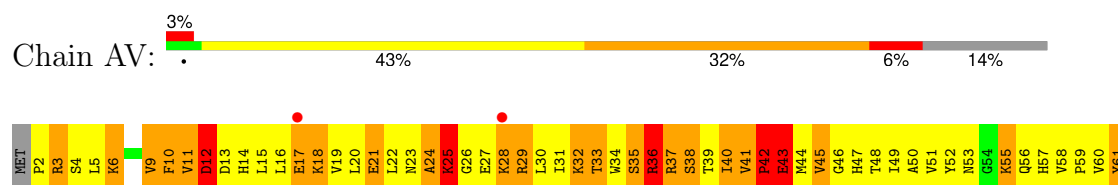
- Molecule 20: 30S ribosomal protein S17



- Molecule 21: 30S ribosomal protein S18

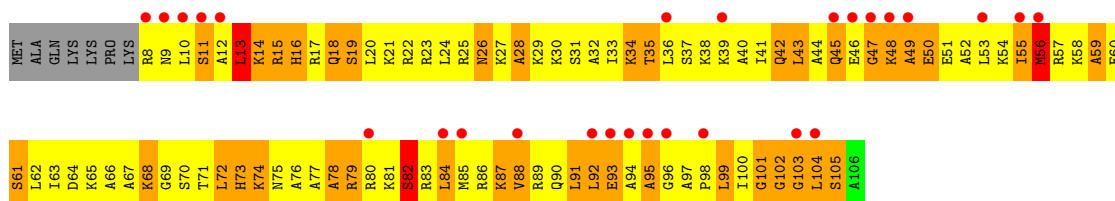


- Molecule 22: 30S ribosomal protein S19





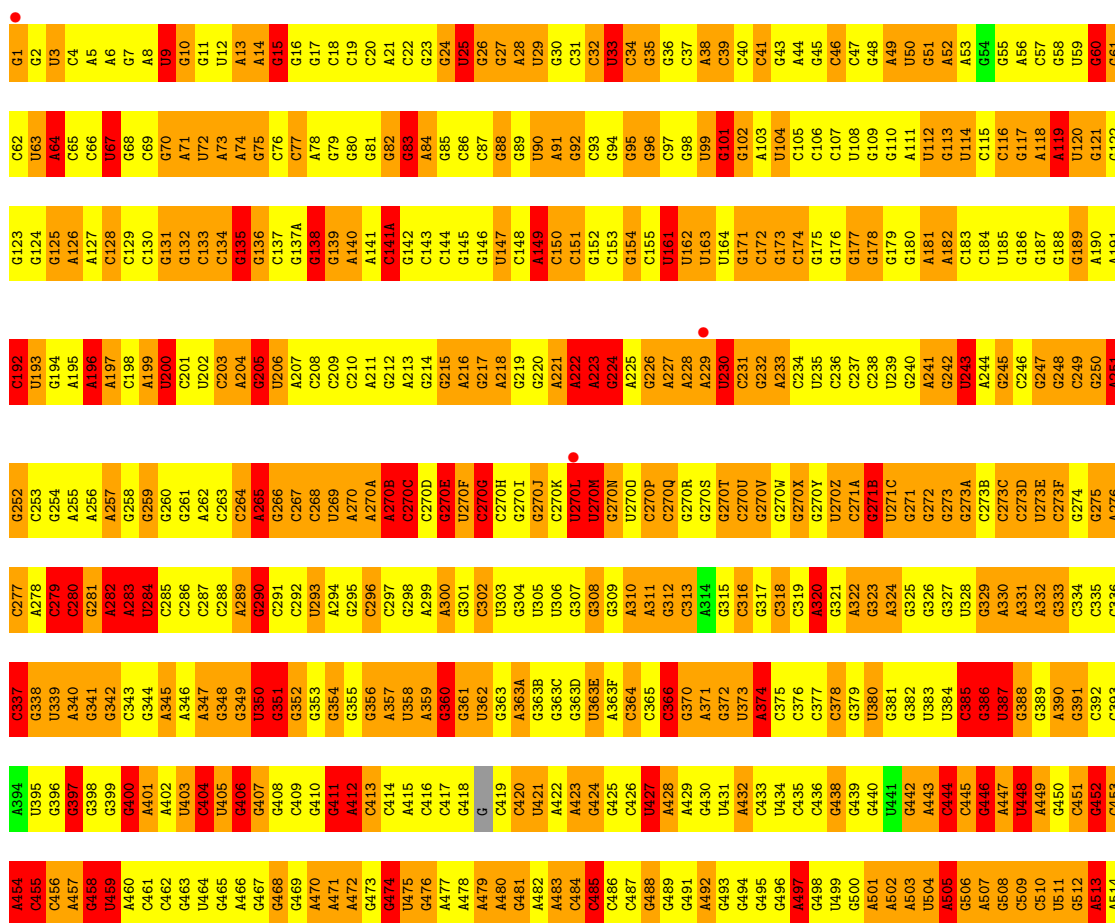
● Molecule 23: 30S ribosomal protein S20



● Molecule 24: 30S ribosomal protein Thx

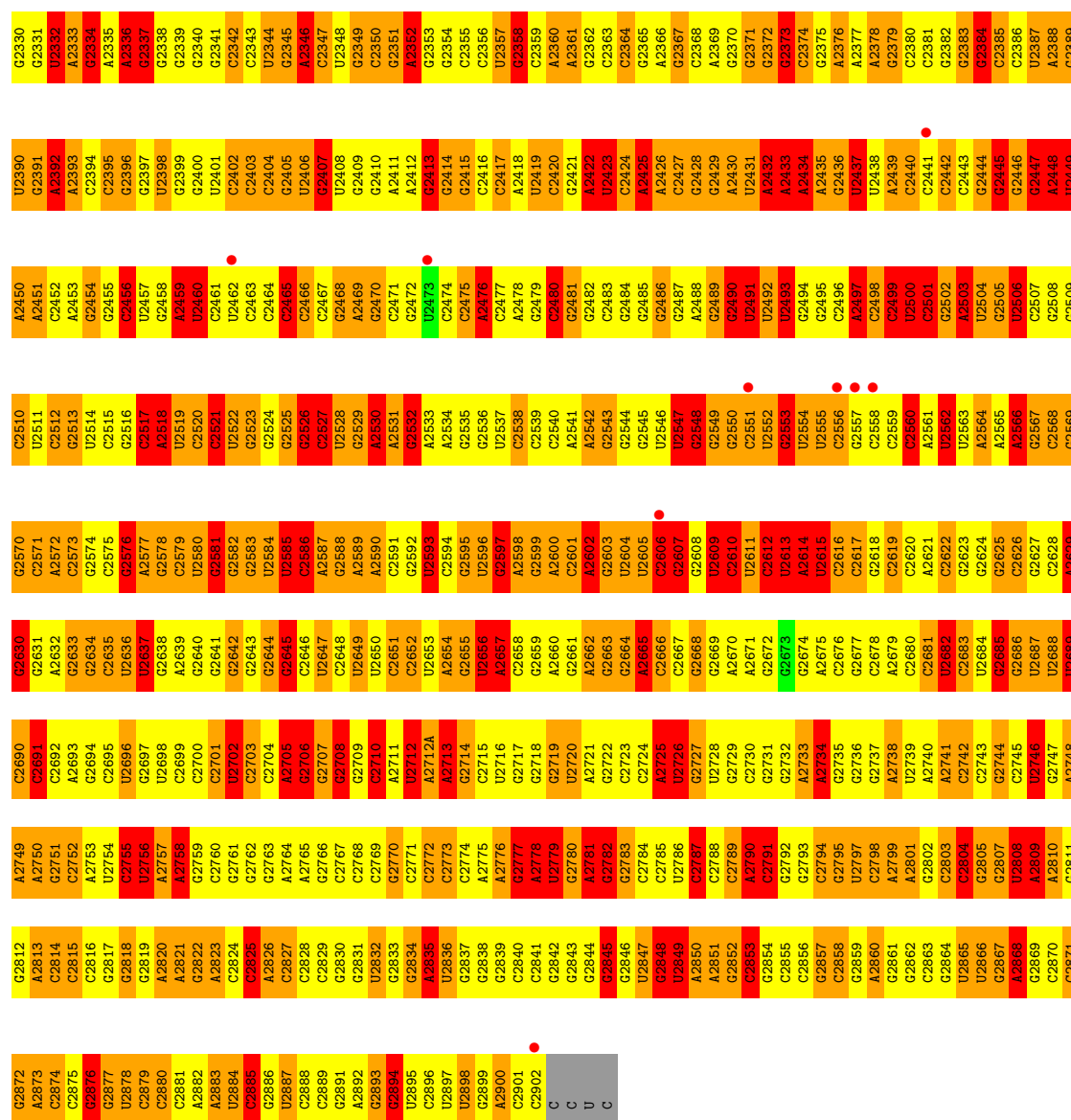


● Molecule 25: 23S rRNA



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U1397	G1337	G1277	C1217	A1156	U1097	G1037	G975	C915	G854	G794	A734	C674	G636	A578	C516
C1398	G1338	A1278	C1218	G1157	A1098	C1038	C976	A917	G855	G795	A735	A676	A637	A579	C517
C1399	G1339	G1279	G1219	C1158	G1099	G1039	G977	A918	G856	G796	C736	A677	G638	C580	G518
G1400	U1340	G1280	A1220	U1159	C1100	C1040	G978	A919	C857	G797	C737	C678	U639	C581	U519
G1401	U1341	G1281	C1221	G1160	U1101	G1041	G979	G920	U858	G798	G738	C679	G640	G582	G520
C1402	A1342	U1282	C1222	C1161	C1102	G1042	A980	G921	G859	G799	G739	C680	C641	G583	G521
C1403	G1343	G1283	C1223	G1162	A1103	C1043	A981	G922	U860	A800	U740	G681	G642	C584	G522
A1284	G1344	A1284	G1224	G1163	C1104	G1044	C982	U922	A861	G801	G741	G682	A643	G585	C523
G1285	G1345	C1225	C1225	G1164	U1105	A1045	A984	C923	G862	A802	G742	G683	A644	A586	U524
A1286	G1346	G1226	G1226	U1165	G1106	A1046	A984	C924	A863	U803	G743	C684	C645	C587	U525
A1287	G1347	A1227	G1227	U1166	G1107	G1047	C985	C925	A864	A804	G744	G684	G646	U588	A526
U1288	G1348	G1228	G1228	U1167	U1108	A1048	C986	A926	G865	G805	G745	C685	G647	C589	C527
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G1290	C1350	C1230	C1230	G1169	G1110	A1050	A988	G929	U867	U807	U747	G687	G649	A529	A529
C1411	C1351	G1231	G1231	G1170	A1111	G1051	G989	G930	U868	G808	G748	U688	C	G592	G530
A1412	U1352	G1232	G1232	G1171	G1112	C1052	A990	G931	U869	G809	C749	A689	G	G593	C531
C1413	A1353	C1233	C1233	G1173	U1113	C1053	C991	G932	A870	U810	A750	G690	C	U594	A532
G1414	A1354	U1234	U1234	A1174	G1114	A1054	C992	A833	U871	U811	A751	C691	A	C595	G533
U1415	G1355	G1235	G1235	U1175	G1115	G1055	G993	G934	A872	C812	A752	C692	A	G596	U534
G1296	G1356	G1236	G1236	G1176	C1116	G1056	C994	C935	U873	U813	A753	C693	G	U597	C535
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G1421	G1361	A1241	A1241	C1181	C1121	U1061	U999	G940	A878	C818	C758	C698	C	G602	C541
G1422	A1362	A1242	A1242	A1182	G1122	G1062	A1000	A941	G879	A819	G759	A699	C	A603	C542
G1423	C1363	G1243	G1243	G1183	C1123	G1063	A1001	G942	G880	A820	G760	G700	C	G604	C543
C1304	G1364	G1244	G1244	G1184	C1124	C1064	G1002	U943	G881	A821	G761	G701	C	C605	C544
G1425	A1365	C1305	G1245	C1185	G1125	U1065	G1003	G944	G882	U822	U762	G702	A	U606	G545
C1306	A1366	U1246	U1246	G1186	A1126	U1066	C1004	A945	G883	G823	G763	U703	C	U607	C546
A1427	A1367	A1247	A1247	G1187	A1127	A1067	C1005	G946	C884	A824	A764	G704	G	A608	C547
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C1310	C1370	G1310	G1250	G1190	U1130	A1070	C1008	C949	A887	U827	G767	G707	G	C610	G550
U1431	G1371	G1311	C1251	G1191	G1131	G1071	A1009	G950	C888	U828	G768	C708	C	C611	G551
C1432	U1372	G1312	G1252	G1192	A1132	C1072	A1010	C951	C889	A829	G769	U709	C	G612	G552
U1433	A1373	A1253	A1253	G1193	U1133	A1073	G1011	G952	A890	G830	G770	G710	C	U613	U553
A1434	G1374	C1314	A1254	A1194	G1134	G1074	U1012	A953	G892	G831	G771	G711	G651	U614	U554
G1435	C1375	U1255	U1255	G1195	C1135	C1075	U1013	G954	C893	G832	C772	G712	C652	G615	G556
G1436	C1376	G1256	G1256	C1196	G1136	C1076	U1014	G955	C894	U833	C773	G713	A653	A616	U557
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G1440	G1380	C1320	G1260	C1200	C1140	C1080	A1020	A959	C898	C837	A777	G717	U657	G619	G561
G1441	G1381	A1321	C1261	C1201	U1141	U1081	A1021	A960	A899	C838	G778	A718	C658	G620	U562
G1442	U1382	C1262	A1262	C1202	U1142	U1082	G1022	C961	A900	U839	U779	C719	C659	A621	G563
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G1444	A1384	G1324	G1264	A1204	A1143	A1084	G1024	U963	C902	A841	A781	C721	C661	G623	C565
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G1445	C1386	G1266	G1266	G1206	C1145	A1086	U1026	G965	C904	G843	A783	G723	G663	G625	A567
C1446	G1387	U1267	U1267	C1207	C1146	G1087	A1027	G966	U905	C844	A784	G724	C664	U626	U568
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G1448	G1389	U1329	A1269	C1209	A1148	G1089	A1029	G968	U907	C846	G786	G726	G666	G628	G570
A1449	U1390	G1330	G1270	U1210	G1149	U1090	G1030	U969	C908	U847	U787	A727	G667	G629	A571
G1449A	U1391	A1331	G1271	U1211	C1150	G1091	G1031	C970	A909	G848	A788	G728	G668	G630	A572
C1450	A1392	G1332	A1272	G1212	G1151	C1092	A1032	C971	A910	A849	A789	G729	G669	A631	C573
C1451	A1393	C1333	U1273	A1213	C1152	G1093	U1033	G972	A911	C850	C790	C730	A670	A632	C574
A1453	U1394	A1274	C1334	A1214	C1153	U1094	G1034	G973	C912	U851	C791	C731	G671	A633	A575
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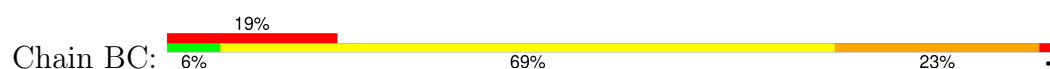
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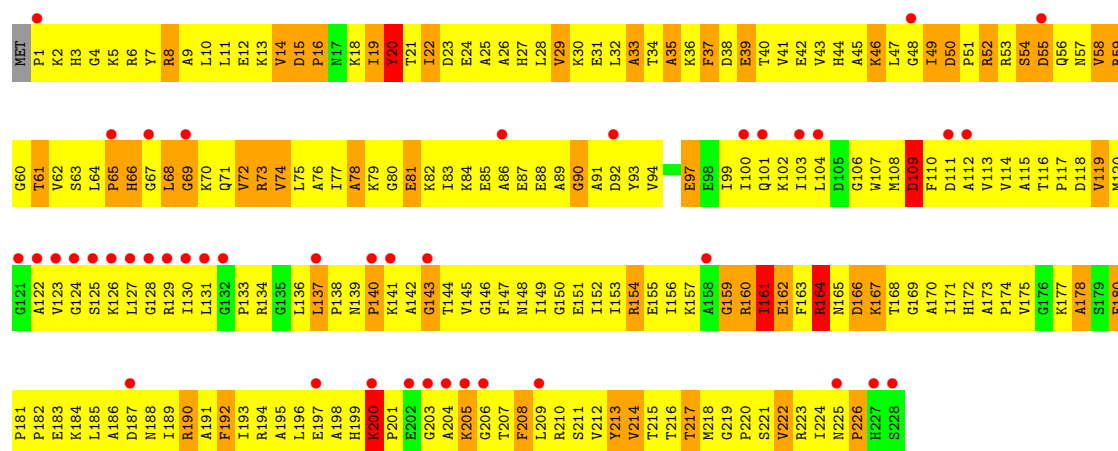


• Molecule 26: 5S rRNA

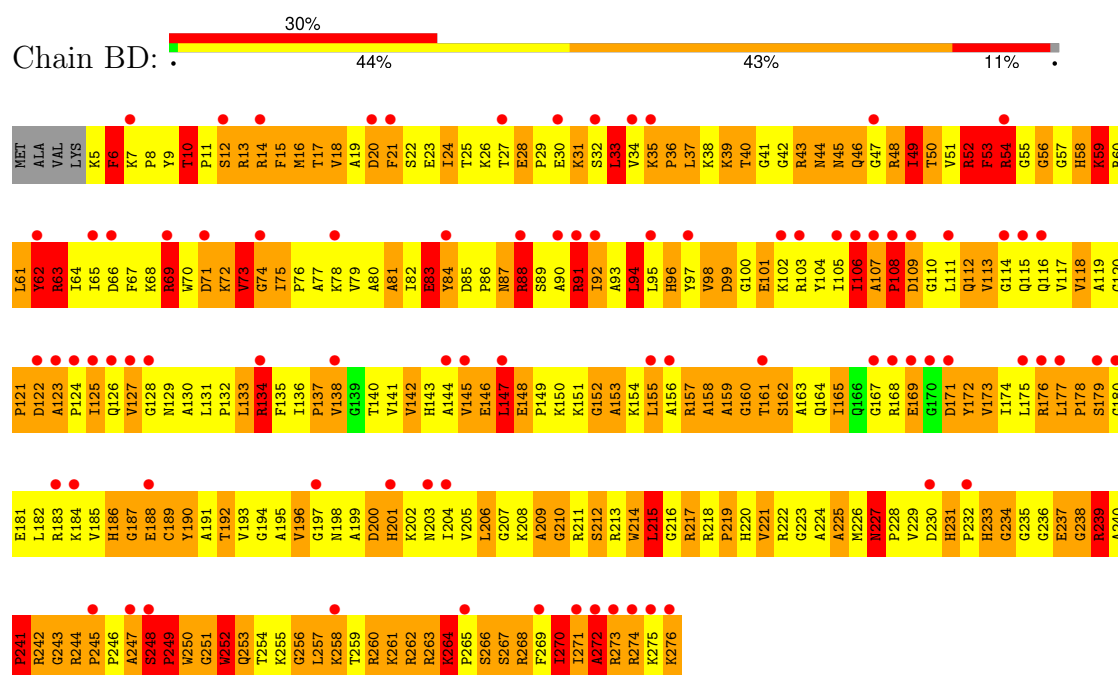


• Molecule 27: 50S RIBOSOMAL PROTEIN L1

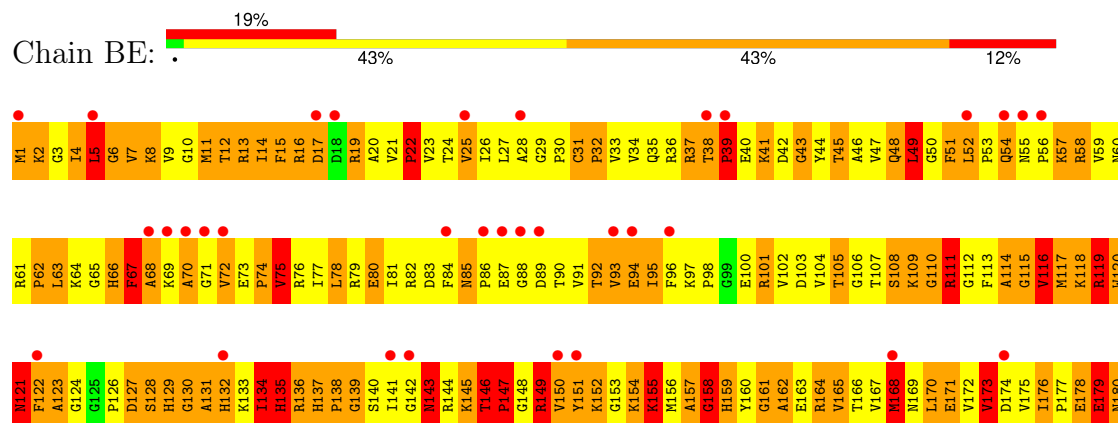


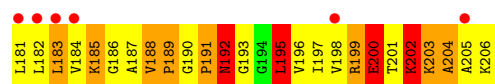


• Molecule 28: 50S RIBOSOMAL PROTEIN L2

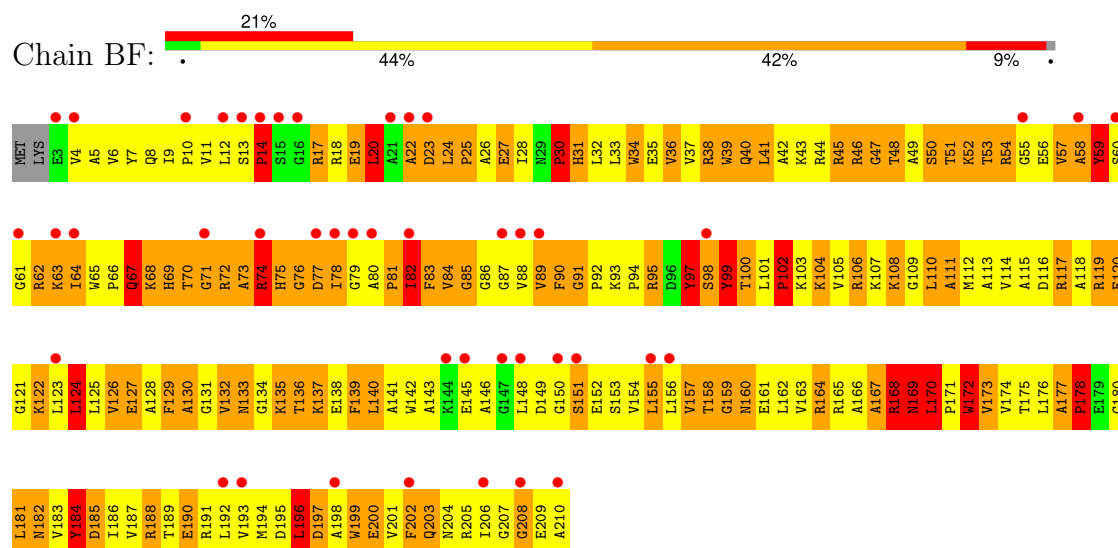


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

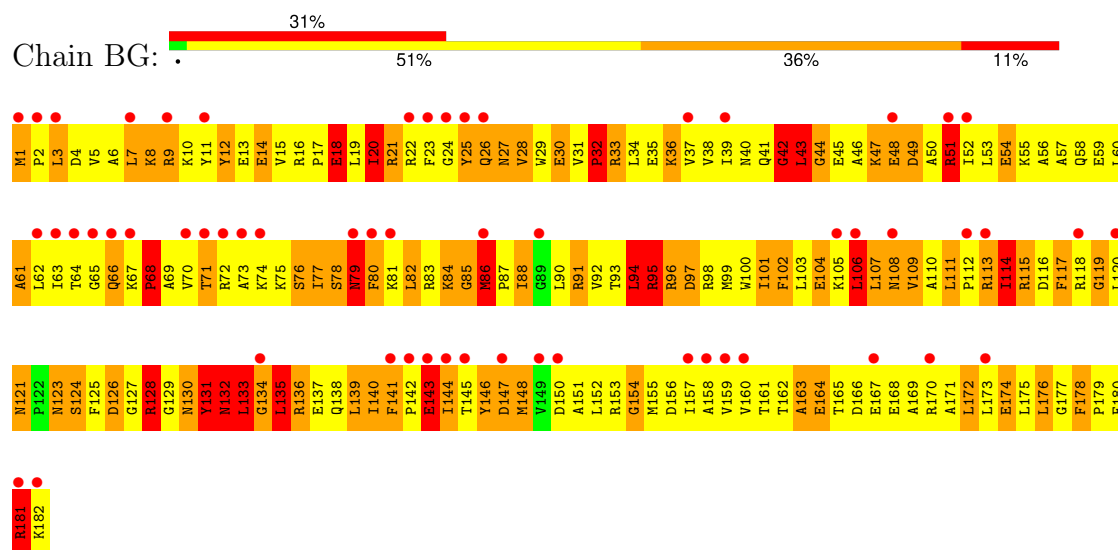




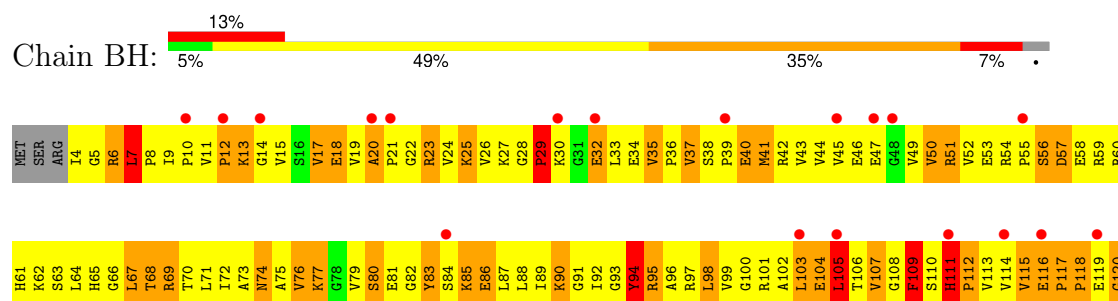
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



• Molecule 31: 50S RIBOSOMAL PROTEIN L5

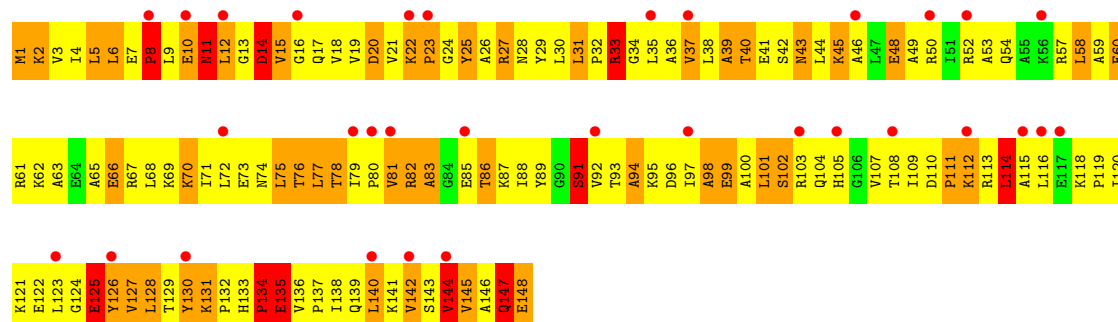


• Molecule 32: 50S RIBOSOMAL PROTEIN L6

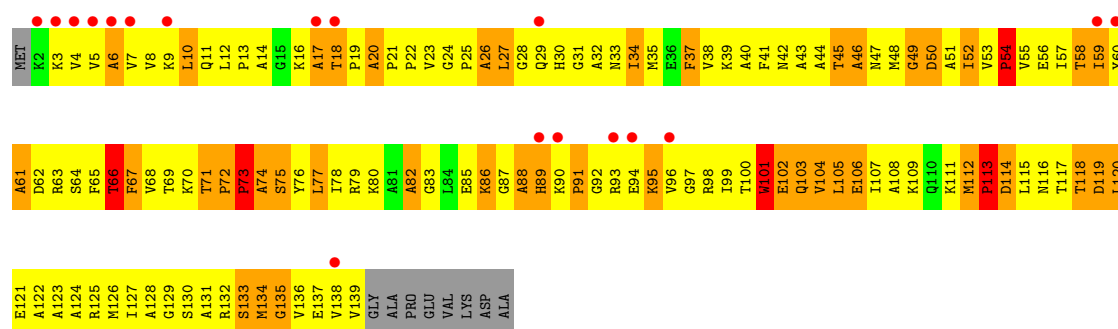




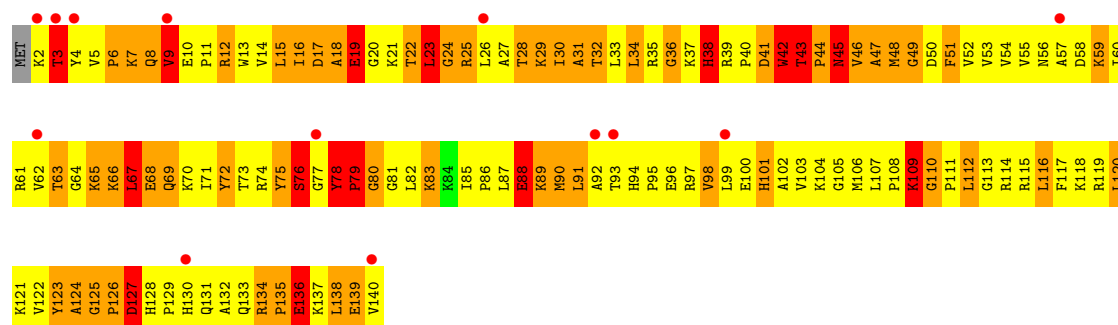
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



• Molecule 34: 50S RIBOSOMAL PROTEIN L11

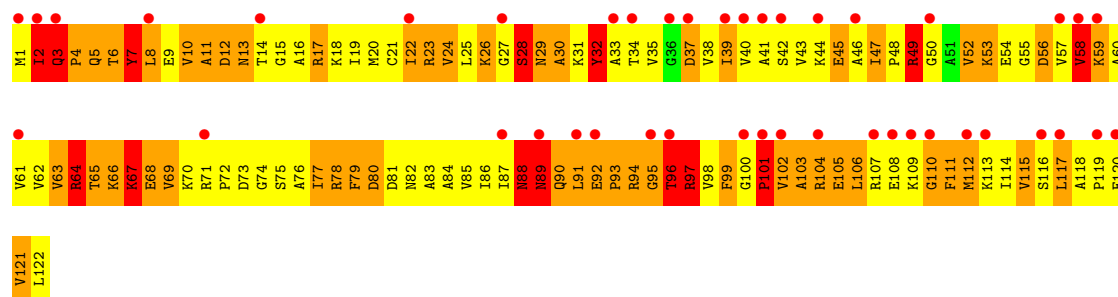


• Molecule 35: 50S RIBOSOMAL PROTEIN L13

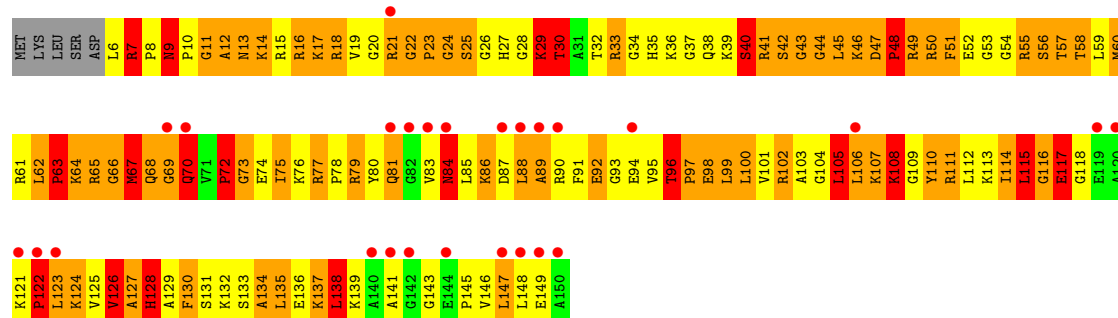


• Molecule 36: 50S RIBOSOMAL PROTEIN L14

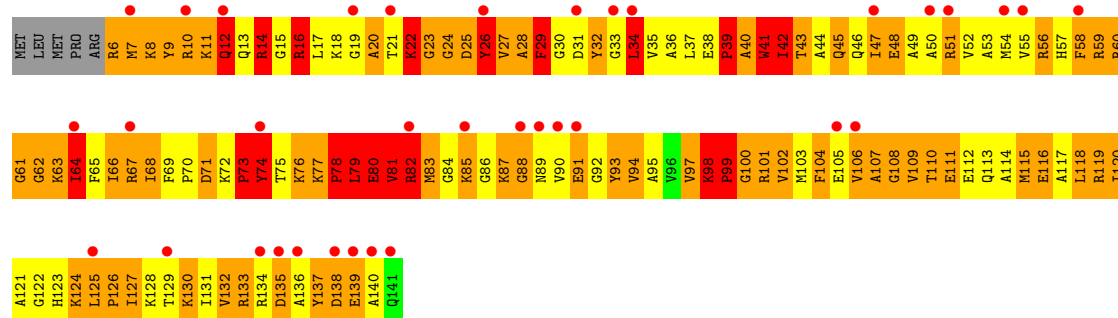




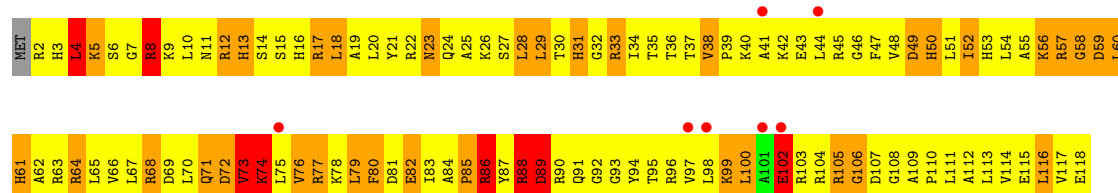
• Molecule 37: 50S RIBOSOMAL PROTEIN L15



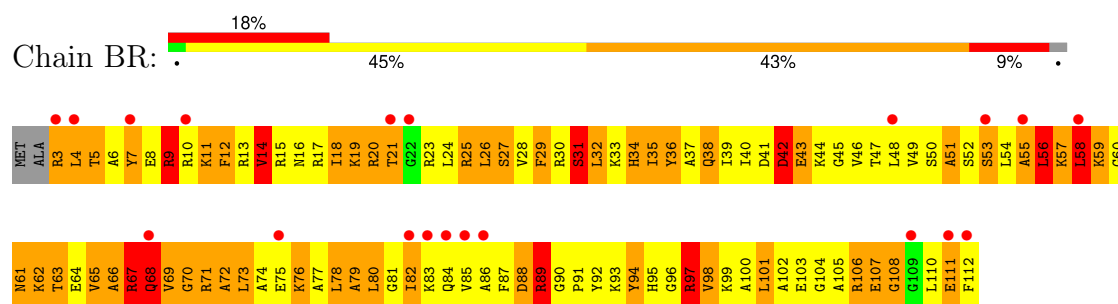
• Molecule 38: 50S RIBOSOMAL PROTEIN L16



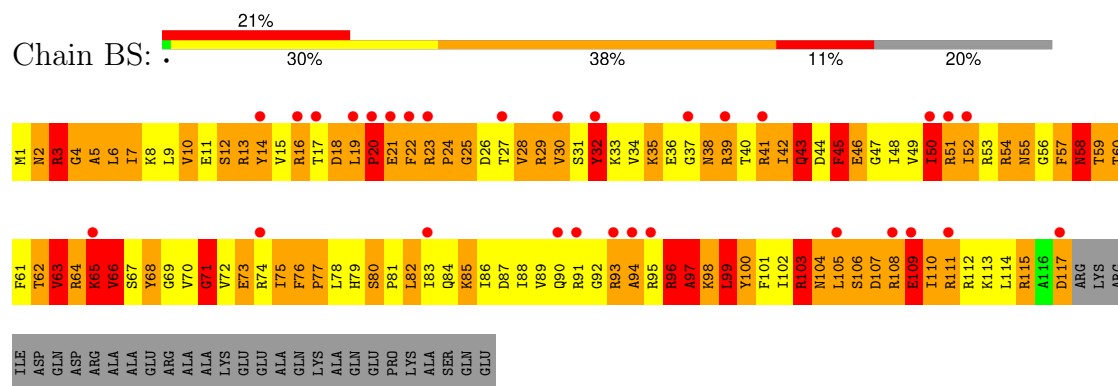
• Molecule 39: 50S RIBOSOMAL PROTEIN L17



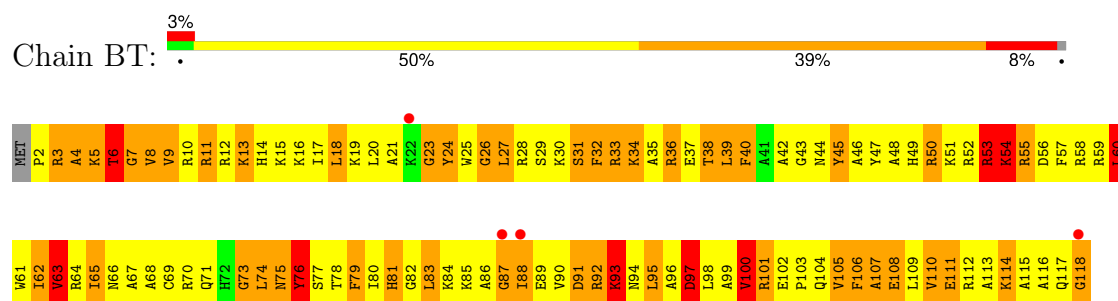
• Molecule 40: 50S RIBOSOMAL PROTEIN L18



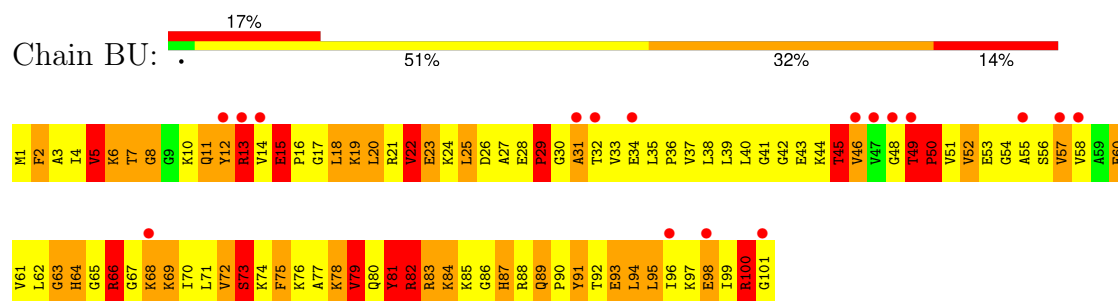
• Molecule 41: 50S RIBOSOMAL PROTEIN L19



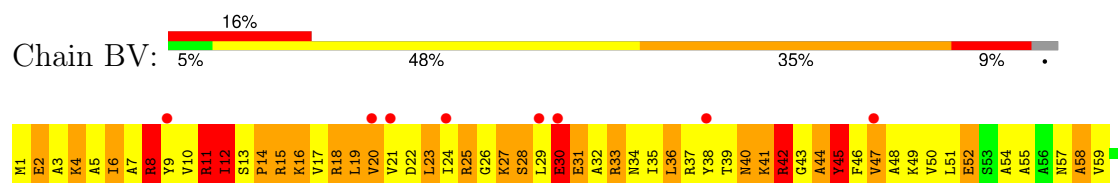
• Molecule 42: 50S RIBOSOMAL PROTEIN L20

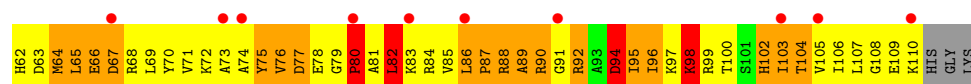


• Molecule 43: 50S RIBOSOMAL PROTEIN L21

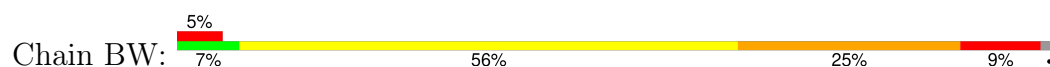


• Molecule 44: 50S RIBOSOMAL PROTEIN L22

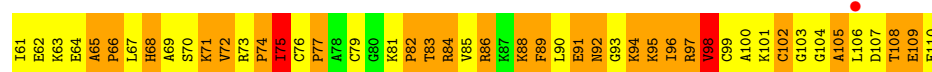




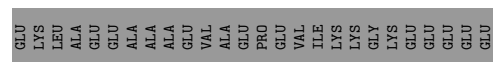
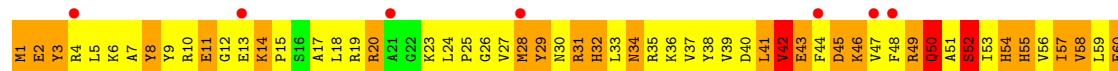
• Molecule 45: 50S RIBOSOMAL PROTEIN L23



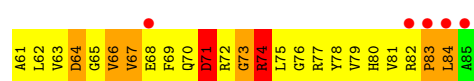
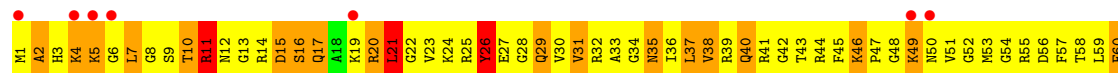
• Molecule 46: 50S RIBOSOMAL PROTEIN L24



• Molecule 47: 50S RIBOSOMAL PROTEIN L25



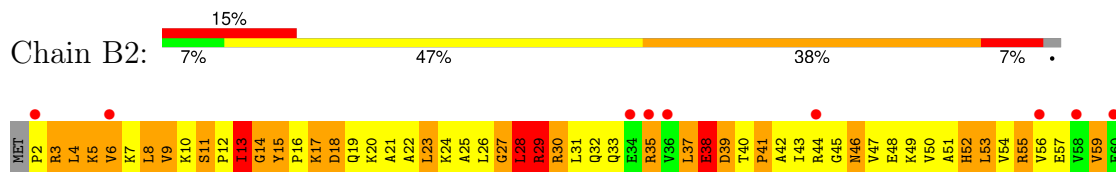
• Molecule 48: 50S RIBOSOMAL PROTEIN L27



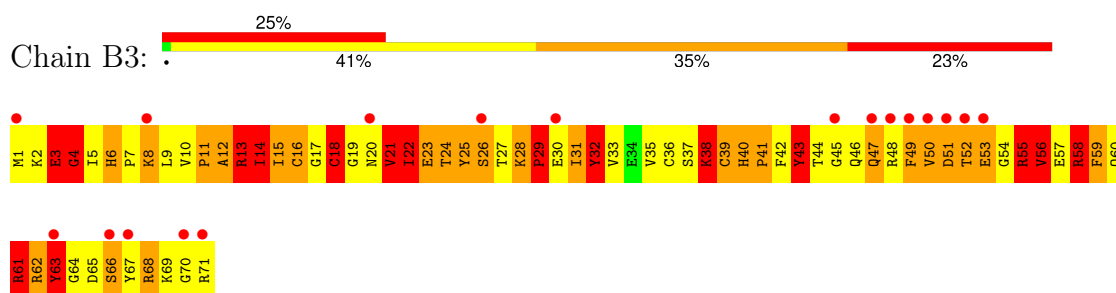
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



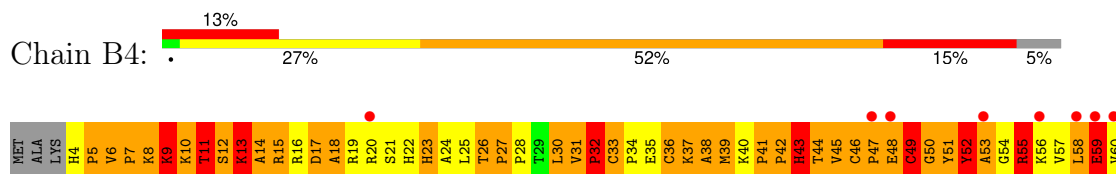
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



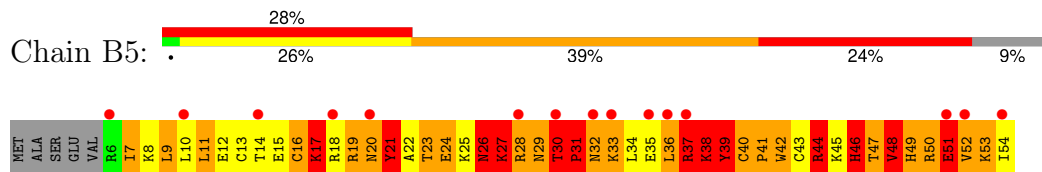
• Molecule 51: 50S RIBOSOMAL PROTEIN L31



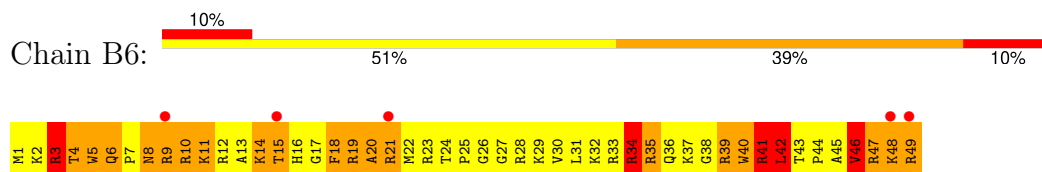
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



• Molecule 53: 50S RIBOSOMAL PROTEIN L33

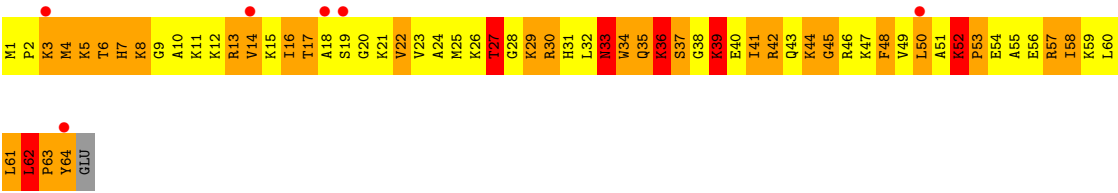


• Molecule 54: 50S RIBOSOMAL PROTEIN L34



• Molecule 55: 50S RIBOSOMAL PROTEIN L35





● Molecule 56: 50S RIBOSOMAL PROTEIN L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51 300.00 – 4.51	Depositor EDS
% Data completeness (in resolution range)	90.3 (300.00-4.51) 95.0 (300.00-4.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.298 , 0.345 0.264 , 0.306	Depositor DCC
R_{free} test set	14716 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	198.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	149640	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.93	38/36438 (0.1%)	1.05	172/56869 (0.3%)
2	AC	0.93	2/1814 (0.1%)	1.01	4/2825 (0.1%)
3	AD	1.47	34/1813 (1.9%)	1.27	21/2823 (0.7%)
4	A1	0.81	1/673 (0.1%)	1.07	3/1048 (0.3%)
5	AE	0.63	0/1935	1.01	4/2609 (0.2%)
6	AF	0.53	0/1636	0.93	4/2205 (0.2%)
7	AG	0.67	1/1733 (0.1%)	1.10	7/2318 (0.3%)
8	AH	0.70	0/1162	1.08	4/1564 (0.3%)
9	AI	0.69	0/856	1.03	3/1154 (0.3%)
10	AJ	0.54	0/1276	0.87	0/1709
11	AK	0.73	0/1136	1.08	3/1527 (0.2%)
12	AL	0.51	0/1029	0.84	1/1379 (0.1%)
13	AM	0.50	0/807	0.85	0/1085
14	AN	0.67	0/900	1.06	0/1213
15	AO	0.67	0/986	1.09	3/1320 (0.2%)
16	AP	0.51	0/1008	0.91	2/1347 (0.1%)
17	AQ	0.53	0/501	1.02	3/664 (0.5%)
18	AR	0.67	0/745	0.98	0/992
19	AS	0.72	0/716	1.04	4/963 (0.4%)
20	AT	0.67	0/870	1.05	2/1159 (0.2%)
21	AU	0.65	0/603	1.12	3/799 (0.4%)
22	AV	0.49	0/661	0.91	1/890 (0.1%)
23	AW	0.66	0/765	1.05	1/1007 (0.1%)
24	AX	0.47	0/212	0.82	0/277
25	BA	1.06	139/69685 (0.2%)	1.19	514/108786 (0.5%)
26	BB	0.80	2/2954 (0.1%)	1.00	4/4606 (0.1%)
27	BC	0.50	0/1775	0.89	2/2393 (0.1%)
28	BD	0.88	2/2174 (0.1%)	1.35	22/2927 (0.8%)
29	BE	0.87	0/1611	1.36	19/2171 (0.9%)
30	BF	0.74	0/1660	1.26	11/2247 (0.5%)
31	BG	0.60	0/1507	1.07	5/2027 (0.2%)
32	BH	0.64	0/1354	1.08	5/1831 (0.3%)
33	BK	0.68	0/1170	1.10	8/1581 (0.5%)
34	BL	0.50	0/1044	0.92	1/1415 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	BM	0.85	1/1140 (0.1%)	1.19	7/1537 (0.5%)
36	BN	1.07	4/942 (0.4%)	1.42	7/1268 (0.6%)
37	BO	0.75	0/1123	1.24	9/1493 (0.6%)
38	BP	0.86	1/1100 (0.1%)	1.23	9/1470 (0.6%)
39	BQ	0.70	0/974	1.07	2/1302 (0.2%)
40	BR	0.73	0/887	1.14	5/1180 (0.4%)
41	BS	0.98	0/990	1.52	16/1325 (1.2%)
42	BT	0.81	0/982	1.19	7/1306 (0.5%)
43	BU	0.94	1/790 (0.1%)	1.40	10/1057 (0.9%)
44	BV	0.73	0/886	1.21	7/1189 (0.6%)
45	BW	0.60	0/756	0.97	5/1015 (0.5%)
46	BX	0.61	0/857	1.10	3/1142 (0.3%)
47	BY	0.66	0/1467	1.11	5/1992 (0.3%)
48	BZ	0.67	0/679	1.02	1/902 (0.1%)
49	B1	0.60	0/569	0.89	1/751 (0.1%)
50	B2	0.71	1/474 (0.2%)	1.10	4/635 (0.6%)
51	B3	1.05	0/594	1.44	10/795 (1.3%)
52	B4	0.79	0/459	1.22	2/621 (0.3%)
53	B5	0.98	1/433 (0.2%)	1.49	6/576 (1.0%)
54	B6	0.84	1/438 (0.2%)	1.08	1/575 (0.2%)
55	B7	0.69	0/523	1.22	5/690 (0.7%)
56	B8	0.73	0/310	1.13	1/407 (0.2%)
All	All	0.94	229/162582 (0.1%)	1.13	959/242958 (0.4%)

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	AA	0	241
2	AC	0	9
3	AD	0	12
4	A1	0	5
7	AG	0	1
8	AH	0	1
11	AK	0	2
14	AN	0	1
15	AO	0	1
20	AT	0	1
24	AX	0	1
25	BA	0	610

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BB	0	20
28	BD	0	1
30	BF	0	1
32	BH	0	3
36	BN	0	2
38	BP	0	3
41	BS	0	2
42	BT	0	1
43	BU	0	2
44	BV	0	1
51	B3	0	2
52	B4	0	1
53	B5	0	1
56	B8	0	1
All	All	0	926

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1203	G	O3'-P	-34.71	1.19	1.61
25	BA	1202	C	O3'-P	29.90	1.97	1.61
25	BA	2447	G	O3'-P	-21.30	1.35	1.61
25	BA	2601	C	O3'-P	19.66	1.84	1.61
25	BA	2756	U	O3'-P	19.18	1.84	1.61

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	412	A	O5'-P-OP2	-28.87	76.06	110.70
25	BA	1203	G	P-O3'-C3'	27.73	152.97	119.70
25	BA	2448	A	C5'-C4'-O4'	-27.33	76.31	109.10
30	BF	20	LEU	O-C-N	-25.54	81.83	122.70
1	AA	37	U	N3-C4-O4	-25.04	101.87	119.40

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	16	A	Sidechain
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	24	U	Sidechain
1	AA	7	G	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	AA	32554	0	16429	6699	0
2	AC	1624	0	826	331	0
3	AD	1623	0	809	304	0
4	A1	596	0	296	65	0
5	AE	1900	0	1951	928	0
6	AF	1612	0	1677	661	0
7	AG	1703	0	1763	807	0
8	AH	1146	0	1207	482	0
9	AI	843	0	857	397	0
10	AJ	1257	0	1296	519	0
11	AK	1116	0	1177	666	0
12	AL	1010	0	1037	457	0
13	AM	794	0	840	327	0
14	AN	885	0	904	410	0
15	AO	970	0	1057	413	0
16	AP	997	0	1072	469	0
17	AQ	492	0	529	264	0
18	AR	734	0	771	353	0
19	AS	700	0	720	348	0
20	AT	857	0	930	385	0
21	AU	597	0	668	357	0
22	AV	647	0	673	241	0
23	AW	763	0	861	330	0
24	AX	208	0	221	87	0
25	BA	62218	0	31354	15682	0
26	BB	2641	0	1337	598	0
27	BC	1742	0	1796	761	0
28	BD	2124	0	2207	1434	0
29	BE	1578	0	1647	1120	0
30	BF	1625	0	1666	862	0
31	BG	1482	0	1546	838	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BH	1328	0	1408	664	0
33	BK	1155	0	1244	574	0
34	BL	1025	0	1074	414	0
35	BM	1113	0	1183	722	0
36	BN	932	0	994	703	0
37	BO	1106	0	1183	801	0
38	BP	1080	0	1127	691	0
39	BQ	960	0	1021	505	0
40	BR	877	0	938	472	0
41	BS	976	0	1033	699	0
42	BT	964	0	1022	709	0
43	BU	779	0	852	626	0
44	BV	876	0	941	423	0
45	BW	742	0	800	336	0
46	BX	844	0	930	493	0
47	BY	1435	0	1463	683	0
48	BZ	670	0	700	365	0
49	B1	567	0	621	303	0
50	B2	469	0	518	302	0
51	B3	581	0	577	375	0
52	B4	445	0	459	271	0
53	B5	426	0	452	306	0
54	B6	430	0	480	275	0
55	B7	515	0	587	415	0
56	B8	307	0	335	126	0
All	All	149640	0	102066	45475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 181.

The worst 5 of 45475 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)
25:BA:1204:A:C2	30:BF:188:ARG:HA	1.17	1.61
25:BA:2459:A:N3	25:BA:2460:U:H1'	1.22	1.46
25:BA:1204:A:C2	30:BF:188:ARG:CA	1.98	1.45
25:BA:2745:C:N4	25:BA:2756:U:C5	1.85	1.45
25:BA:1475:G:H1	25:BA:1477:A:N6	1.11	1.44

There are no symmetry-related clashes.

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	
5	AE	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	AF	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	1
7	AG	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	1
8	AH	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	3
9	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
10	AJ	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	1
11	AK	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	1
12	AL	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	1
13	AM	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	0
14	AN	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	1
15	AO	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	AP	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	2
17	AQ	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	0
18	AR	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	3
19	AS	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	2
20	AT	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	3
21	AU	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	AV	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	AW	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	0
24	AX	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	1
27	BC	226/229 (99%)	137 (61%)	52 (23%)	37 (16%)	0	3
28	BD	270/276 (98%)	129 (48%)	49 (18%)	92 (34%)	0	0
29	BE	204/206 (99%)	106 (52%)	39 (19%)	59 (29%)	0	0
30	BF	206/210 (98%)	100 (48%)	47 (23%)	59 (29%)	0	0
31	BG	180/182 (99%)	79 (44%)	42 (23%)	59 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	172/180 (96%)	89 (52%)	41 (24%)	42 (24%)	0	1
33	BK	146/148 (99%)	88 (60%)	32 (22%)	26 (18%)	0	2
34	BL	136/147 (92%)	66 (48%)	32 (24%)	38 (28%)	0	0
35	BM	137/140 (98%)	66 (48%)	31 (23%)	40 (29%)	0	0
36	BN	120/122 (98%)	63 (52%)	21 (18%)	36 (30%)	0	0
37	BO	143/150 (95%)	60 (42%)	31 (22%)	52 (36%)	0	0
38	BP	134/141 (95%)	51 (38%)	35 (26%)	48 (36%)	0	0
39	BQ	115/118 (98%)	64 (56%)	33 (29%)	18 (16%)	0	3
40	BR	108/112 (96%)	45 (42%)	30 (28%)	33 (31%)	0	0
41	BS	115/146 (79%)	53 (46%)	26 (23%)	36 (31%)	0	0
42	BT	115/118 (98%)	49 (43%)	39 (34%)	27 (24%)	0	1
43	BU	99/101 (98%)	51 (52%)	22 (22%)	26 (26%)	0	1
44	BV	108/113 (96%)	69 (64%)	15 (14%)	24 (22%)	0	1
45	BW	92/96 (96%)	59 (64%)	14 (15%)	19 (21%)	0	1
46	BX	108/110 (98%)	41 (38%)	27 (25%)	40 (37%)	0	0
47	BY	178/206 (86%)	93 (52%)	48 (27%)	37 (21%)	0	1
48	BZ	83/85 (98%)	50 (60%)	14 (17%)	19 (23%)	0	1
49	B1	65/67 (97%)	27 (42%)	26 (40%)	12 (18%)	0	2
50	B2	57/60 (95%)	32 (56%)	16 (28%)	9 (16%)	0	3
51	B3	69/71 (97%)	26 (38%)	19 (28%)	24 (35%)	0	0
52	B4	55/60 (92%)	16 (29%)	12 (22%)	27 (49%)	0	0
53	B5	47/54 (87%)	13 (28%)	7 (15%)	27 (57%)	0	0
54	B6	47/49 (96%)	16 (34%)	16 (34%)	15 (32%)	0	0
55	B7	62/65 (95%)	29 (47%)	11 (18%)	22 (36%)	0	0
56	B8	35/37 (95%)	20 (57%)	4 (11%)	11 (31%)	0	0
All	All	5988/6337 (94%)	2997 (50%)	1412 (24%)	1579 (26%)	0	1

5 of 1579 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	13	ALA
5	AE	15	VAL
5	AE	17	PHE

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Mol	Chain	Res	Type
5	AE	19	HIS
5	AE	20	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	
5	AE	202/220 (92%)	135 (67%)	67 (33%)	0	2
6	AF	160/188 (85%)	123 (77%)	37 (23%)	0	4
7	AG	180/181 (99%)	127 (71%)	53 (29%)	0	2
8	AH	115/123 (94%)	75 (65%)	40 (35%)	0	1
9	AI	90/90 (100%)	64 (71%)	26 (29%)	0	2
10	AJ	126/127 (99%)	95 (75%)	31 (25%)	0	3
11	AK	119/119 (100%)	76 (64%)	43 (36%)	0	1
12	AL	98/99 (99%)	76 (78%)	22 (22%)	1	5
13	AM	88/92 (96%)	65 (74%)	23 (26%)	0	3
14	AN	90/99 (91%)	62 (69%)	28 (31%)	0	2
15	AO	104/109 (95%)	77 (74%)	27 (26%)	0	3
16	AP	100/101 (99%)	79 (79%)	21 (21%)	1	5
17	AQ	49/50 (98%)	37 (76%)	12 (24%)	0	3
18	AR	79/80 (99%)	56 (71%)	23 (29%)	0	2
19	AS	72/74 (97%)	48 (67%)	24 (33%)	0	2
20	AT	96/97 (99%)	71 (74%)	25 (26%)	0	3
21	AU	64/77 (83%)	41 (64%)	23 (36%)	0	1
22	AV	71/80 (89%)	57 (80%)	14 (20%)	1	7
23	AW	76/82 (93%)	56 (74%)	20 (26%)	0	3
24	AX	19/22 (86%)	13 (68%)	6 (32%)	0	2
27	BC	180/181 (99%)	151 (84%)	29 (16%)	2	11
28	BD	215/218 (99%)	151 (70%)	64 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
30	BF	164/166 (99%)	104 (63%)	60 (37%)	0	1
31	BG	156/156 (100%)	112 (72%)	44 (28%)	0	2
32	BH	143/148 (97%)	97 (68%)	46 (32%)	0	2
33	BK	124/124 (100%)	87 (70%)	37 (30%)	0	2
34	BL	105/111 (95%)	85 (81%)	20 (19%)	1	7
35	BM	118/119 (99%)	80 (68%)	38 (32%)	0	2
36	BN	100/100 (100%)	65 (65%)	35 (35%)	0	1
37	BO	111/116 (96%)	64 (58%)	47 (42%)	0	0
38	BP	106/111 (96%)	55 (52%)	51 (48%)	0	0
39	BQ	100/101 (99%)	69 (69%)	31 (31%)	0	2
40	BR	87/88 (99%)	55 (63%)	32 (37%)	0	0
41	BS	105/127 (83%)	69 (66%)	36 (34%)	0	1
42	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
43	BU	82/82 (100%)	59 (72%)	23 (28%)	0	3
44	BV	90/92 (98%)	56 (62%)	34 (38%)	0	0
45	BW	76/78 (97%)	55 (72%)	21 (28%)	0	3
46	BX	91/91 (100%)	66 (72%)	25 (28%)	0	3
47	BY	159/179 (89%)	110 (69%)	49 (31%)	0	2
48	BZ	67/67 (100%)	52 (78%)	15 (22%)	1	5
49	B1	62/62 (100%)	46 (74%)	16 (26%)	0	3
50	B2	51/52 (98%)	34 (67%)	17 (33%)	0	2
51	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
52	B4	50/52 (96%)	30 (60%)	20 (40%)	0	0
53	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
54	B6	42/42 (100%)	30 (71%)	12 (29%)	0	2
55	B7	54/55 (98%)	40 (74%)	14 (26%)	0	3
56	B8	34/34 (100%)	25 (74%)	9 (26%)	0	3
All	All	5040/5237 (96%)	3520 (70%)	1520 (30%)	0	2

5 of 1520 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BL	120	LEU
40	BR	56	LEU
35	BM	88	GLU
34	BL	119	ASP
37	BO	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
33	BK	74	ASN
42	BT	66	ASN
34	BL	47	ASN
38	BP	13	GLN
45	BW	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	479 (31%)	151 (9%)
2	AC	75/76 (98%)	30 (40%)	7 (9%)
25	BA	2888/2916 (99%)	1241 (42%)	313 (10%)
26	BB	122/123 (99%)	46 (37%)	5 (4%)
3	AD	75/76 (98%)	27 (36%)	3 (4%)
4	A1	26/27 (96%)	11 (42%)	1 (3%)
All	All	4701/4740 (99%)	1834 (39%)	480 (10%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 480 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	687	C
25	BA	2610	C
25	BA	1197	G

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Mol	Chain	Res	Type
25	BA	2566	A
25	BA	2879	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	6
1	AA	2

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1202:C	O3'	1203:G	P	1.97
1	AA	173:U	O3'	174:C	P	1.84
1	BA	2601:C	O3'	2602:A	P	1.84
1	BA	2756:U	O3'	2757:A	P	1.84
1	BA	2755:C	O3'	2756:U	P	1.75

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	AA	1515/1522 (99%)	-0.30	8 (0%) 87 76	188, 245, 349, 445	0
2	AC	76/76 (100%)	0.06	3 (3%) 44 34	213, 249, 283, 294	0
3	AD	76/76 (100%)	0.19	4 (5%) 33 27	301, 334, 358, 368	0
4	A1	27/27 (100%)	1.10	5 (18%) 4 6	225, 347, 415, 416	0
5	AE	234/256 (91%)	0.05	8 (3%) 48 36	218, 248, 286, 307	0
6	AF	206/239 (86%)	0.41	20 (9%) 15 15	246, 269, 288, 296	0
7	AG	208/209 (99%)	0.98	39 (18%) 4 6	202, 233, 251, 265	0
8	AH	150/162 (92%)	0.94	21 (14%) 7 10	202, 220, 245, 262	0
9	AI	101/101 (100%)	2.48	56 (55%) 0 1	219, 237, 254, 271	0
10	AJ	155/156 (99%)	0.18	2 (1%) 74 60	250, 273, 285, 301	0
11	AK	138/138 (100%)	0.70	17 (12%) 9 11	203, 222, 236, 246	0
12	AL	127/128 (99%)	-0.30	0 100 100	247, 317, 349, 353	0
13	AM	98/105 (93%)	-0.21	1 (1%) 79 64	256, 296, 311, 317	0
14	AN	119/129 (92%)	0.67	17 (14%) 7 9	214, 234, 252, 279	0
15	AO	124/132 (93%)	1.20	29 (23%) 2 5	189, 217, 243, 263	0
16	AP	125/126 (99%)	0.65	15 (12%) 10 12	253, 281, 302, 306	0
17	AQ	60/61 (98%)	-0.37	0 100 100	243, 273, 286, 290	0
18	AR	88/89 (98%)	0.89	12 (13%) 8 10	199, 222, 244, 251	0
19	AS	83/88 (94%)	0.77	8 (9%) 15 15	192, 212, 232, 267	0
20	AT	104/105 (99%)	0.88	17 (16%) 5 8	192, 218, 252, 296	0
21	AU	73/88 (82%)	1.36	25 (34%) 1 3	192, 228, 254, 276	0
22	AV	80/93 (86%)	0.19	3 (3%) 44 34	251, 287, 306, 310	0
23	AW	99/106 (93%)	1.29	27 (27%) 2 4	200, 228, 250, 254	0
24	AX	24/27 (88%)	-0.67	0 100 100	268, 289, 303, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BA	2889/2916 (99%)	-0.10	54 (1%) 66 50	168, 241, 340, 398	0
26	BB	123/123 (100%)	-0.24	1 (0%) 82 69	236, 293, 329, 343	0
27	BC	228/229 (99%)	1.15	43 (18%) 4 6	299, 326, 342, 347	0
28	BD	272/276 (98%)	1.65	83 (30%) 1 3	184, 216, 235, 256	0
29	BE	206/206 (100%)	0.95	39 (18%) 4 6	155, 205, 250, 276	0
30	BF	208/210 (99%)	0.91	44 (21%) 3 5	186, 255, 283, 288	0
31	BG	182/182 (100%)	1.48	57 (31%) 1 3	247, 283, 306, 311	0
32	BH	174/180 (96%)	0.58	23 (13%) 8 10	230, 260, 278, 284	0
33	BK	148/148 (100%)	1.22	32 (21%) 3 5	212, 241, 261, 265	0
34	BL	138/147 (93%)	0.72	18 (13%) 9 10	305, 358, 399, 403	0
35	BM	139/140 (99%)	0.57	13 (9%) 15 15	187, 217, 245, 270	0
36	BN	122/122 (100%)	1.65	43 (35%) 1 3	172, 201, 228, 240	0
37	BO	145/150 (96%)	0.83	26 (17%) 4 6	189, 271, 304, 346	0
38	BP	136/141 (96%)	1.15	35 (25%) 2 4	199, 234, 257, 266	0
39	BQ	117/118 (99%)	0.27	7 (5%) 29 24	195, 214, 246, 256	0
40	BR	110/112 (98%)	0.92	20 (18%) 4 6	232, 266, 293, 300	0
41	BS	117/146 (80%)	1.38	30 (25%) 2 4	182, 205, 238, 244	0
42	BT	117/118 (99%)	0.20	4 (3%) 48 36	191, 221, 241, 250	0
43	BU	101/101 (100%)	0.76	17 (16%) 5 7	190, 244, 272, 277	0
44	BV	110/113 (97%)	0.95	18 (16%) 5 8	203, 226, 250, 260	0
45	BW	94/96 (97%)	0.12	5 (5%) 33 27	237, 253, 304, 309	0
46	BX	110/110 (100%)	0.06	1 (0%) 81 67	244, 282, 303, 312	0
47	BY	180/206 (87%)	0.86	28 (15%) 6 8	235, 267, 281, 287	0
48	BZ	85/85 (100%)	0.97	12 (14%) 7 10	236, 258, 272, 289	0
49	B1	67/67 (100%)	-0.22	0 100 100	251, 264, 276, 281	0
50	B2	59/60 (98%)	0.90	9 (15%) 6 9	208, 244, 261, 268	0
51	B3	71/71 (100%)	1.36	18 (25%) 2 4	212, 239, 259, 276	0
52	B4	57/60 (95%)	0.86	8 (14%) 7 10	200, 227, 276, 299	0
53	B5	49/54 (90%)	1.61	15 (30%) 1 3	211, 247, 269, 277	0
54	B6	49/49 (100%)	0.43	5 (10%) 13 14	189, 228, 244, 250	0
55	B7	64/65 (98%)	0.48	6 (9%) 15 15	201, 220, 235, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	B8	37/37 (100%)	0.04	2 (5%) 32 26	212, 230, 240, 244	0
All	All	10794/11077 (97%)	0.38	1053 (9%) 14 15	155, 245, 336, 445	0

The worst 5 of 1053 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	BC	125	SER	13.8
40	BR	85	VAL	10.2
16	AP	124	PRO	9.9
27	BC	126	LYS	9.9
28	BD	170	GLY	9.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.