



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:24 AM UTC

PDB ID : 1N34 / pdb_00001n34
Title : Structure of the Thermus thermophilus 30S ribosomal subunit in the presence of codon and crystallographically disordered near-cognate transfer rna anticodon stem-loop mismatched at the first codon position
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on : 2002-10-25
Resolution : 3.80 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

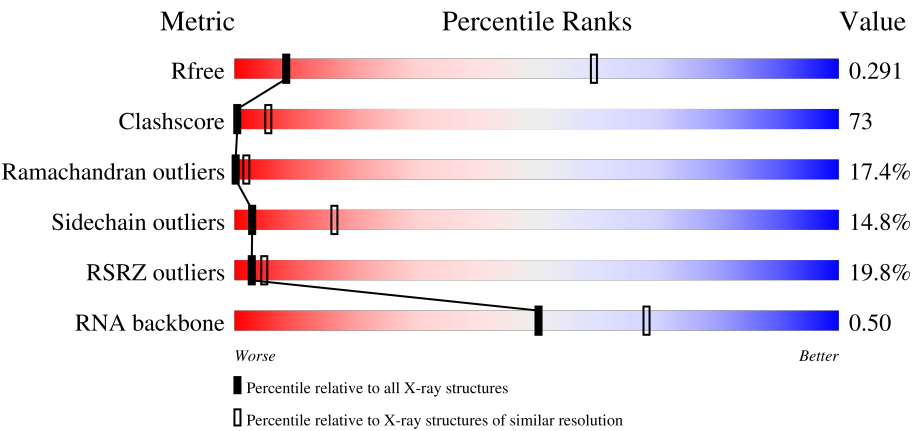
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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	A	1522	28% 10% 71% 15% • •
2	Z	6	50% 17% 50% 33%
3	B	256	9% 8% 53% 28% • 9%
4	C	239	12% 9% 49% 26% • 14%

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Mol	Chain	Length	Quality of chain
5	D	208	
6	E	161	
7	F	101	
8	G	155	
9	H	138	
10	I	128	
11	J	104	
12	K	129	
13	L	135	
14	M	126	
15	N	60	
16	O	88	
17	P	88	
18	Q	104	
19	R	88	
20	S	92	
21	T	106	
22	V	26	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 51757 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	42	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	conflict	UNP Q5SHQ2
H	37	ARG	LYS	conflict	UNP Q5SHQ2
H	52	ASP	GLU	conflict	UNP Q5SHQ2
H	61	VAL	ILE	conflict	UNP Q5SHQ2
H	62	TYR	HIS	conflict	UNP Q5SHQ2
H	81	HIS	LYS	conflict	UNP Q5SHQ2
H	88	LYS	ARG	conflict	UNP Q5SHQ2
H	115	SER	PRO	conflict	UNP Q5SHQ2

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	conflict	UNP Q5SHP7
Q	53	LEU	VAL	conflict	UNP Q5SHP7
Q	62	SER	ALA	conflict	UNP Q5SHP7
Q	79	SER	GLU	conflict	UNP Q5SHP7
Q	82	MET	LEU	conflict	UNP Q5SHP7
Q	90	ILE	VAL	conflict	UNP Q5SHP7
Q	96	GLN	ALA	conflict	UNP Q5SHP7

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

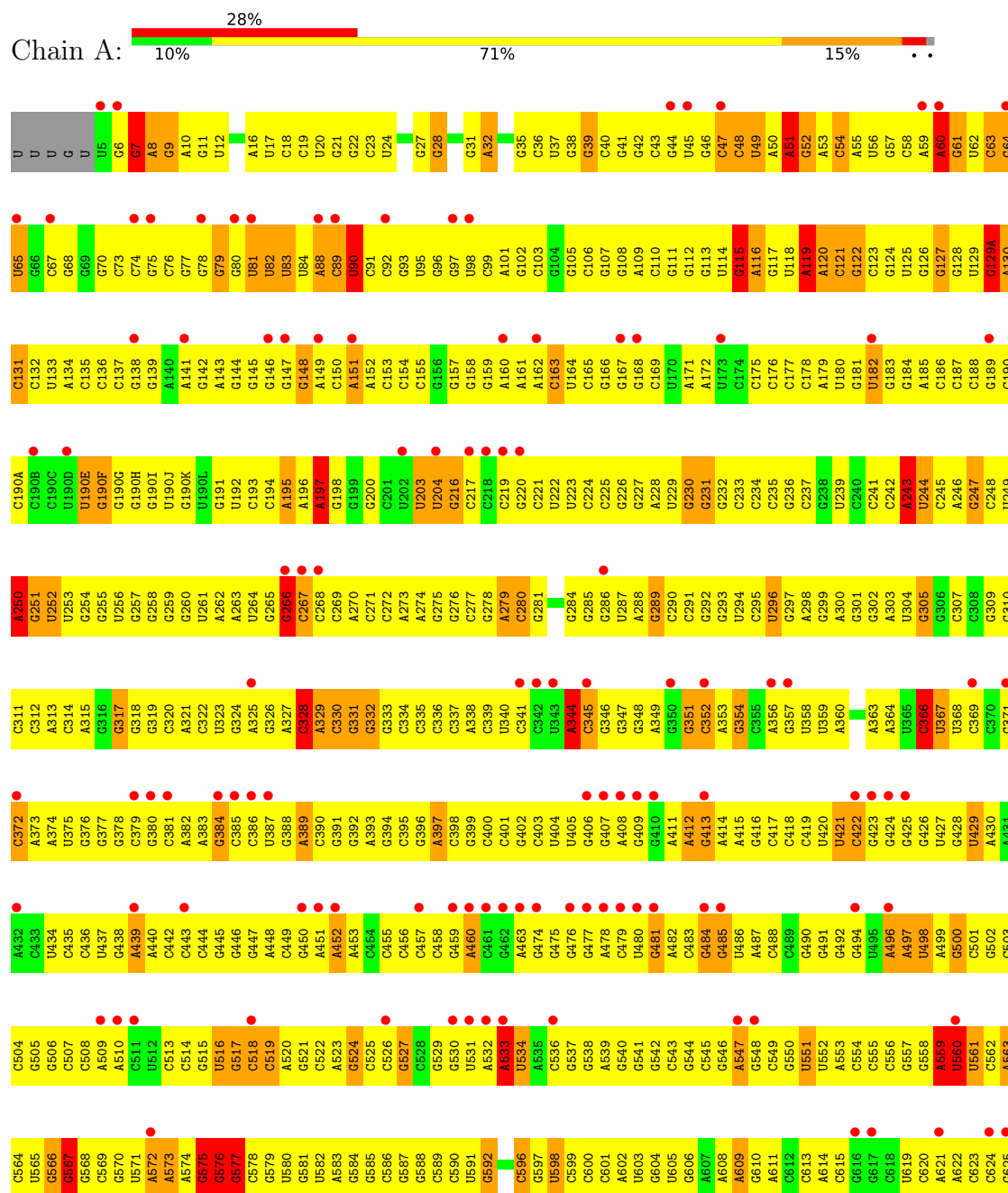
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

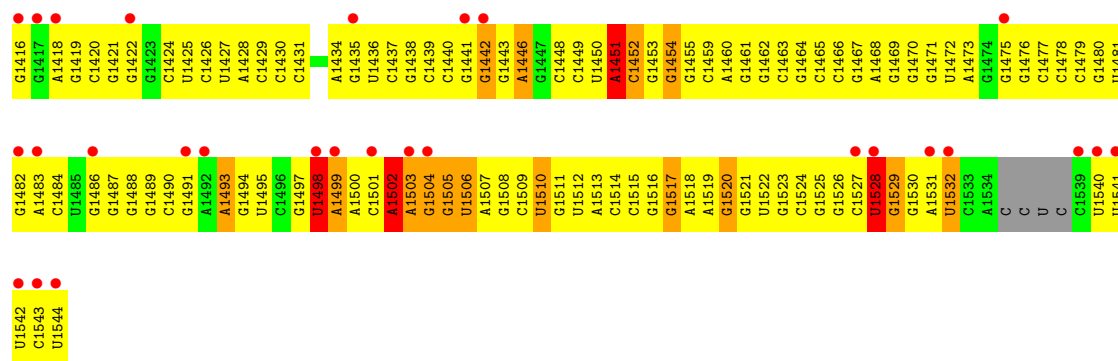
3 Residue-property plots

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.

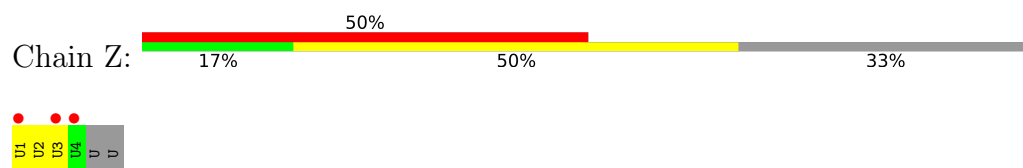
• Molecule 1: 16S RIBOSOMAL RNA



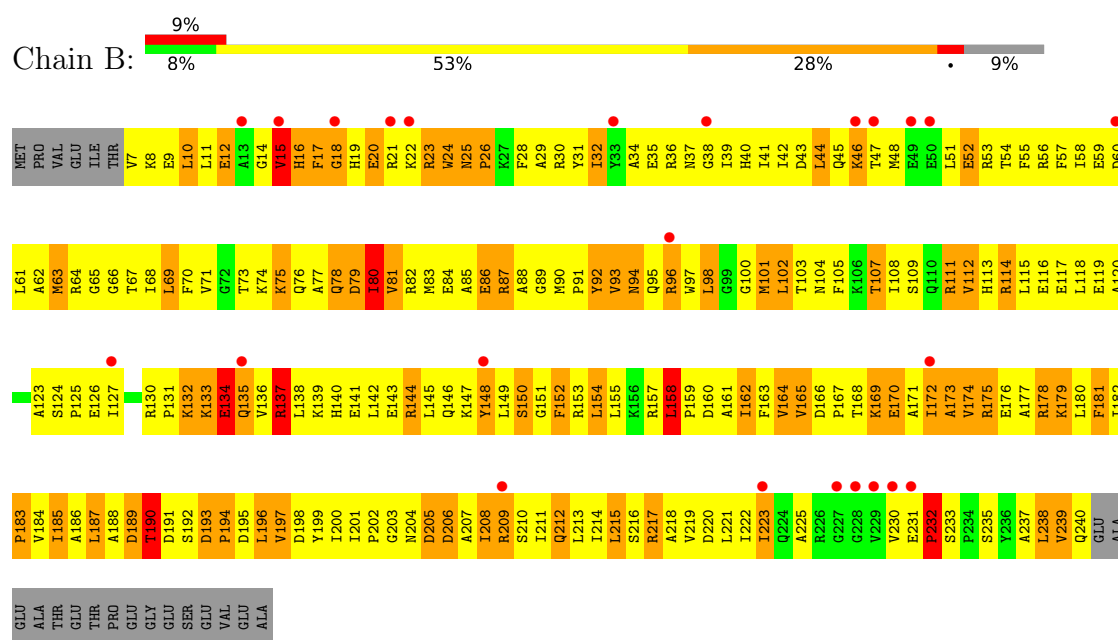
G1356	A1236	C1115	A1055	U1000	A807	A746	U686	U626
A1357	C1237	C1116	U1056	A1001	C808	C747	A687	G627
A1358	A1238	G1117	G1057	G1002	G809	C748	G688	G628
C1359	A1239	C1118	G1058	G1003	G810	C749	C689	G629
A1360	A1240	C1119	C1059	G1003A	C811	C750	G690	G630
G1361	G1241	G1120	C1060	A1004	G811	G751	G691	G631
C1361A	C1242	U1121	G1061	A1005	G812	G752	U692	A632
A1362	C1243	U1122	U1062	C1006	A814	A753	G693	A633
A1363	G1244	A1123	C1063	A1007	A815	C754	A694	G634
U1364	A1245	A1124	G1064	C1008	A816	C755	A695	A635
G1365	G1246	U1125	U1065	G1009	C817	C756	A696	U636
C1366	U1247	U1126	C1066	G1010	A819	G757	G697	G637
C1367	G1248	G1127	A1067	G1011	U820	G758	G698	G638
G1368	A1249	C1128	G1068	U1012	G821	A759	C699	G639
A1369	A1250	C1129	C1069	U1013	C822	G760	G700	A640
G1370	U1251	A1130	U1070	A1014	G823	G761	C701	U641
G1371	C1131	G1131	C1071	A1015	G824	C762	A702	A642
U1372	G1253	C1132	G1072	A1016	G825	G763	G703	G643
G1373	C1254	G1133	U1073	G1017	C826	C764	A704	G644
A1374	G1255	G1134	G1074	C1018	U827	G765	U705	G645
A1375	A1256	U1135	C1075	C1019	A828	A766	A706	U646
U1376	U1257	U1136	C1076	G1021	G829	A767	C707	C647
G1377	G1258	C1137	G1077	U1020	G830	A768	C708	A648
C1378	C1259	G1138	U1078	G1022	U831	G711	G709	G649
G1379	G1260	G1139	U1079	G1023	C832	C712	G710	G650
U1380	A1261	C1140	A1080	G1024	U833	U772	G711	C651
U1381	C1262	C1141	G1081	U1025	U834	G773	A712	U652
C1382	G1263	G1142	G1082	G1026	U835	G774	G713	G653
C1383	C1264	G1143	U1083	C1027	G836	G775	G714	G654
C1384	U1205	G1144	G1084	G1028	G837	G776	A715	G655
G1385	G1265	C1145	U1085	C1029	G838	A777	A716	C656
G1386	C1267	A1146	U1086	C1030	U839	G778	C717	G657
G1387	A1268	C1147	G1087	G1030A	C840	G779	G718	G658
A1388	U1269	U1148	G1088	C1030B	U841	A780	C719	U659
C1389	C1270	C1149	U1089	G1030C	U842	C720	C720	G660
U1390	G1271	U1150	U1090	A1030D	C849	A781	G721	G661
U1391	G1272	A1151	U1091	G1031	U850	G783	A722	G662
G1392	G1273	A1152	A1092	G1032	G851	C784	U723	A663
U1393	G1274	C1153	A1093	G1033	G852	G785	G724	A664
A1394	A1275	G1154	U1094	A1034	G853	G786	G725	A665
C1395	G1276	G1155	U1095	A1035	G854	A787	C726	G666
A1396	C1277	U1156	C1096	G1036	G855	U788	G727	G667
C1397	U1278	G1157	C1097	G1037	G858	U789	A728	G668
A1398	G1279	C1158	U1098	C1038	G859	A790	A729	U669
C1399	A1280	U1159	G1099	C1039	G860	G791	G730	G670
U1400	U1281	G1160	A1101	U1040	A859	A792	C731	U671
G1401	C1282	C1161	C1102	A1041	G861	U793	C732	G672
C1402	G1283	C1162	C1103	G1042	C862	A794	A733	G673
C1403	C1284	C1163	G1104	C1043	U863	C795	G734	G674
A1404	A1285	G1164	A1044	A1044	A864	C796	C735	A675
G1405	C1286	C1165	A1045	C1045	A865	C797	C736	A676
U1406	A1287	U1166	A1046	U1046	C866	G799	C737	U677
C1407	C1288	A1167	G1107	G1047	G867	G799	C738	U678
A1408	A1289	U1168	U1108	U1048	G868	G800	C739	C679
U1409	C1290	A1169	C1109	U1049	U869	U801	G680	C680
G1410	G1291	G1171	A1110	G1050	U870	A802	C681	C681
C1411	U1292	C1172	A1111	C1051	U871	G803	G742	G682
A1412	G1293	G1173	U1112	U1052	A872	U804	U743	G683
U1413	C1294	U1174	C1113	G1053	A873	C805	A874	C684
G1414	G1295	G1175	C1114	C1054	G874	C806	C745	G685



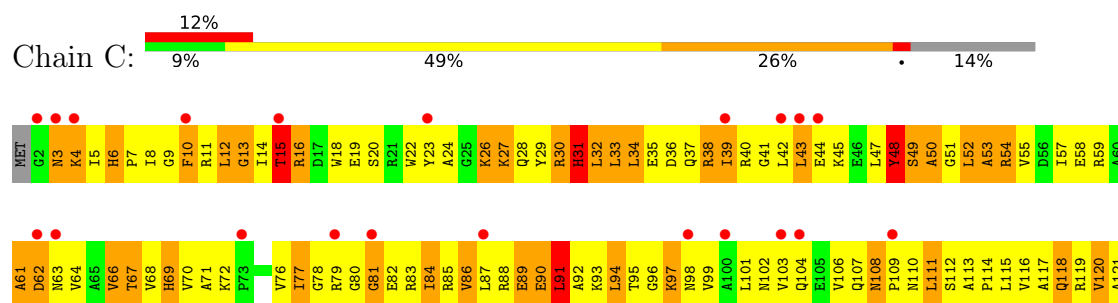
• Molecule 2: A-SITE MESSENGER RNA FRAGMENT

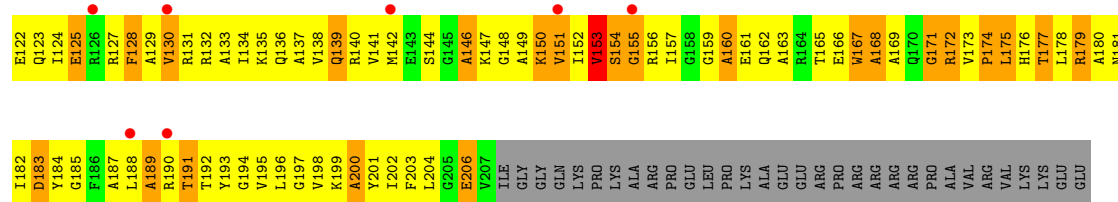


• Molecule 3: 30S RIBOSOMAL PROTEIN S2

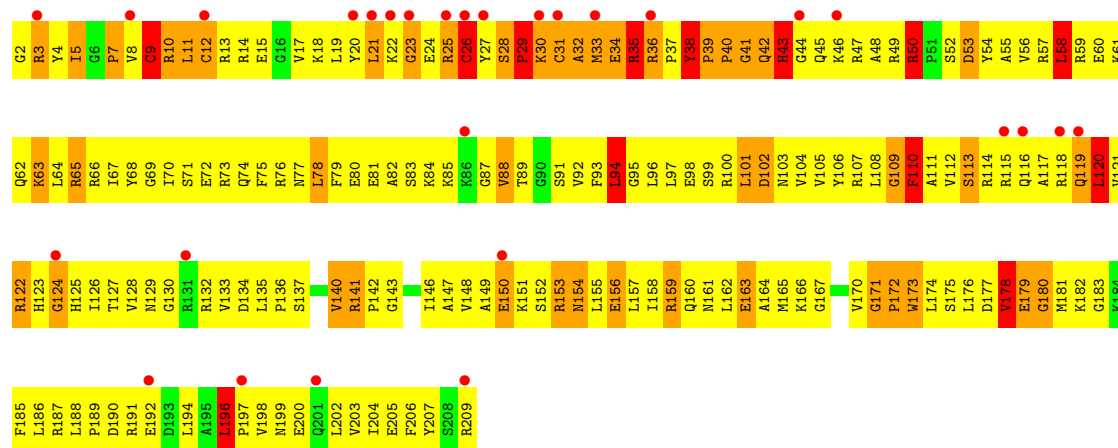
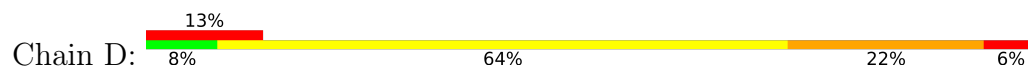


• Molecule 4: 30S RIBOSOMAL PROTEIN S3

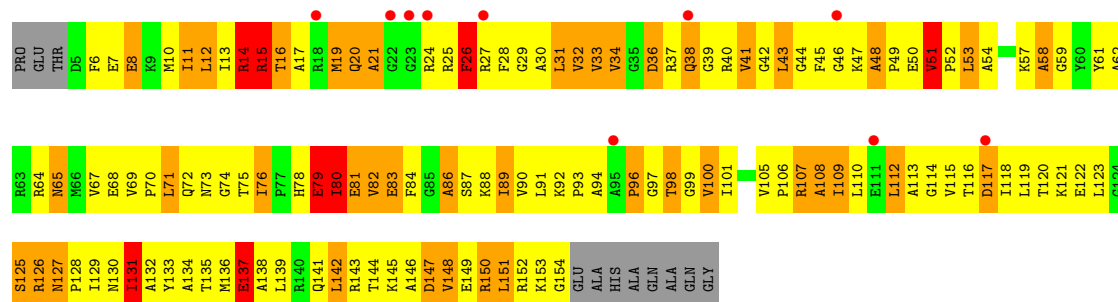
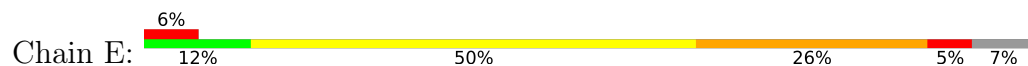




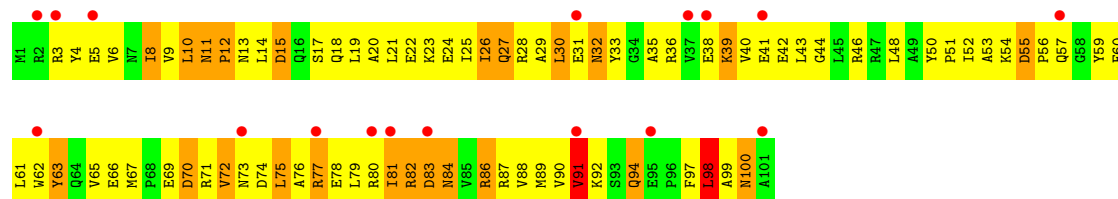
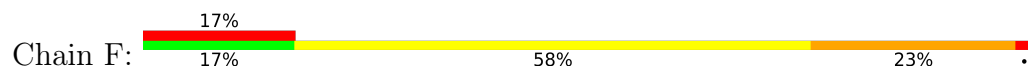
● Molecule 5: 30S RIBOSOMAL PROTEIN S4



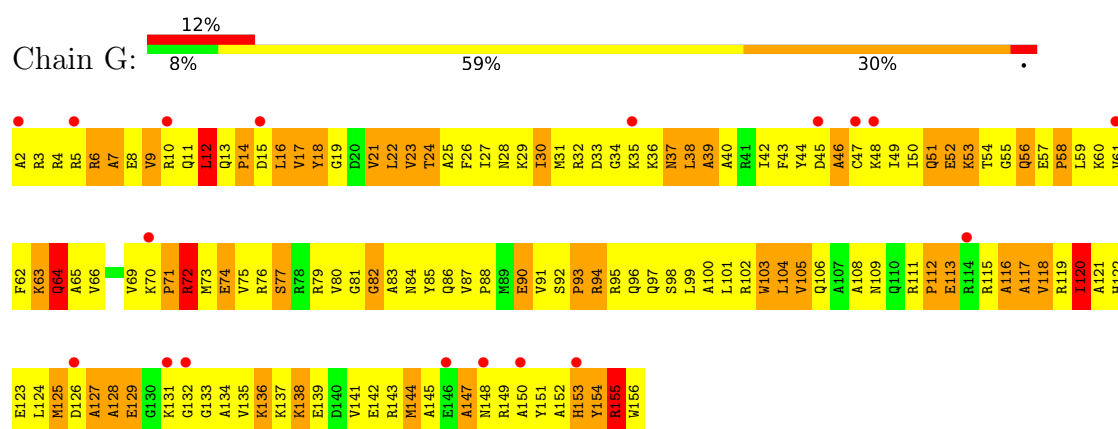
● Molecule 6: 30S RIBOSOMAL PROTEIN S5



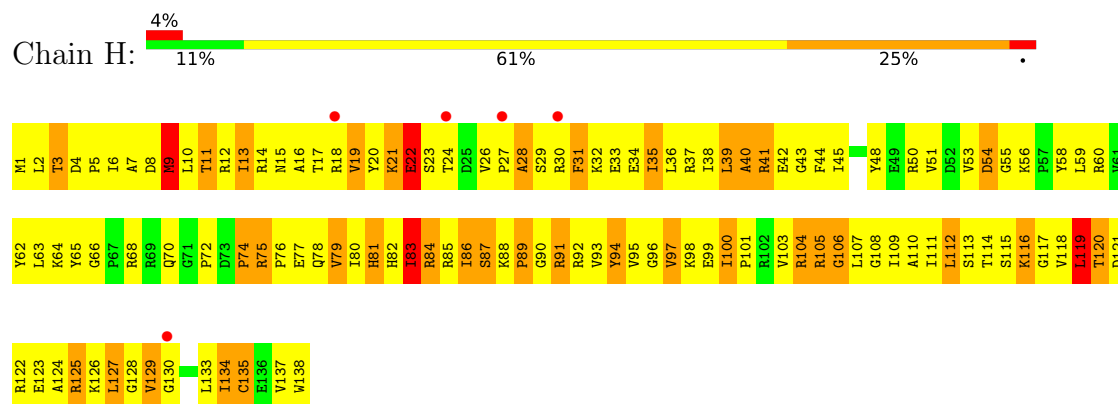
● Molecule 7: 30S RIBOSOMAL PROTEIN S6



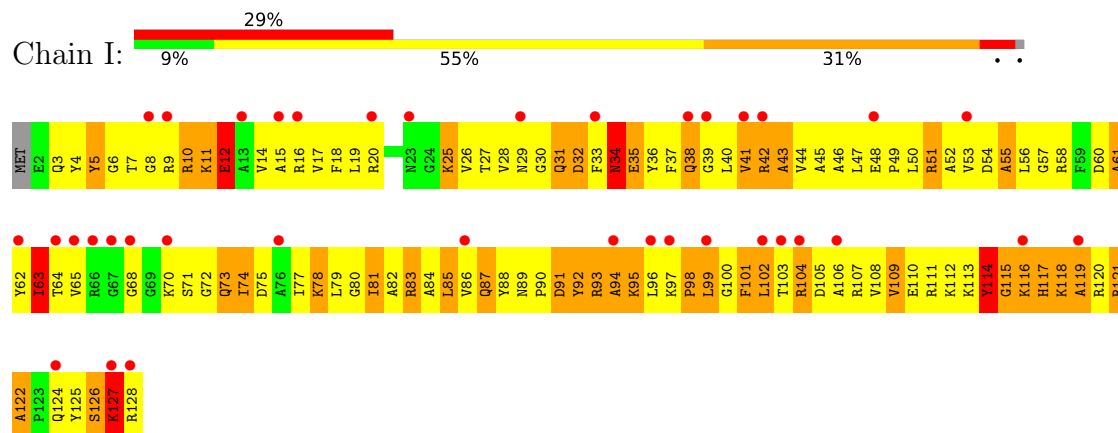
● Molecule 8: 30S RIBOSOMAL PROTEIN S7



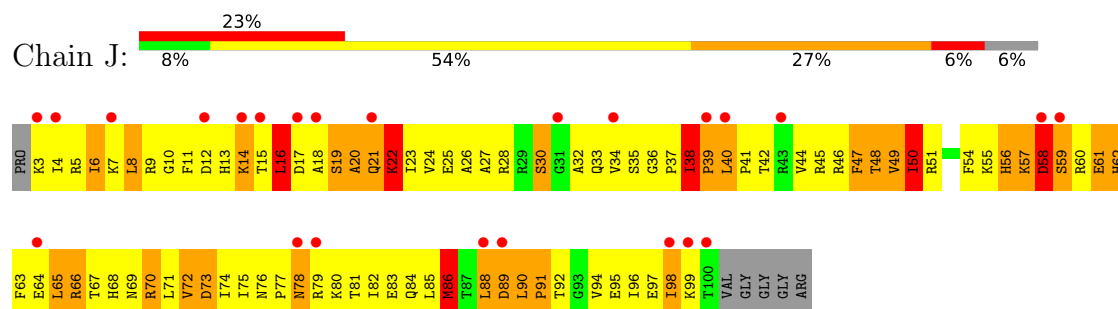
• Molecule 9: 30S RIBOSOMAL PROTEIN S8



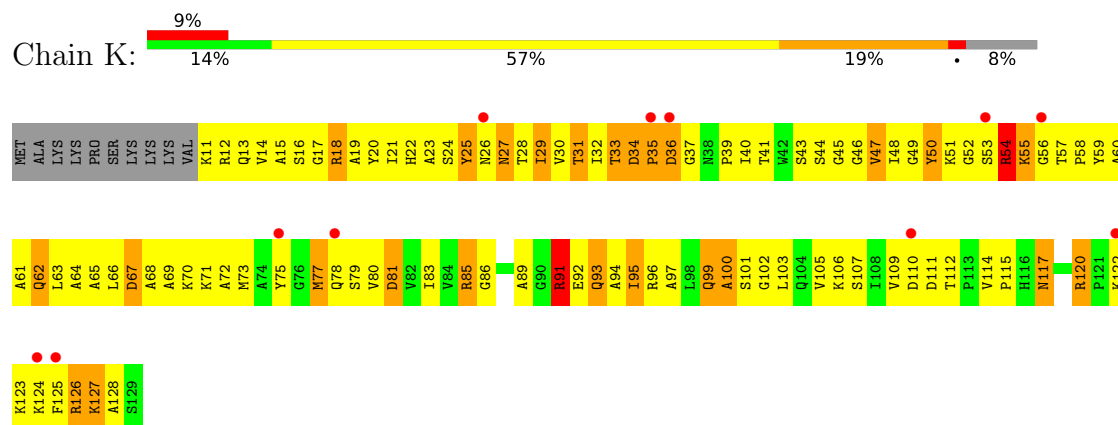
• Molecule 10: 30S RIBOSOMAL PROTEIN S9



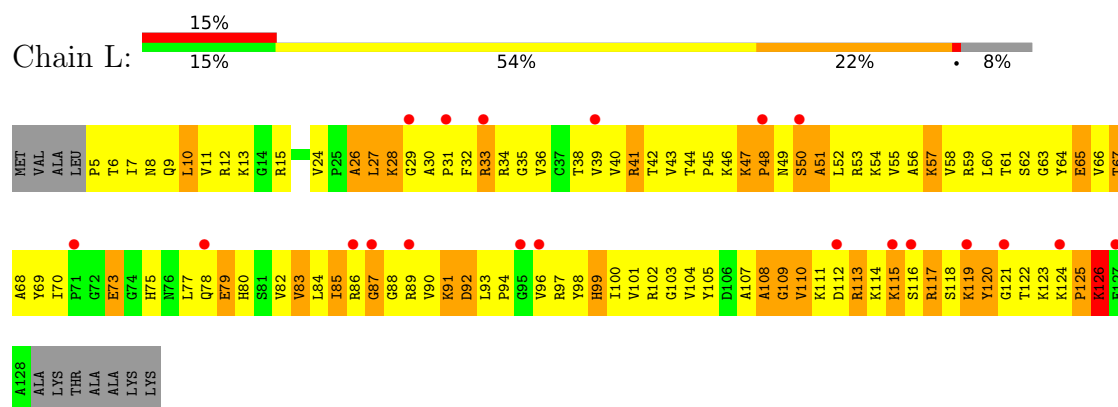
• Molecule 11: 30S RIBOSOMAL PROTEIN S10



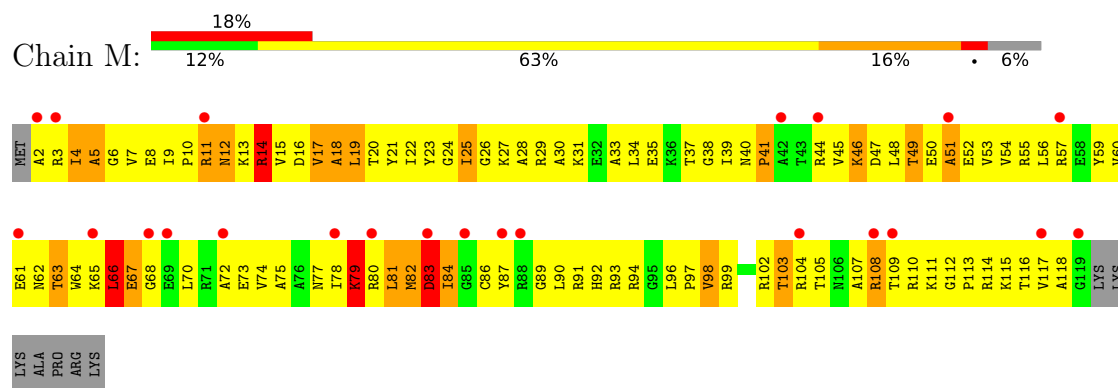
- Molecule 12: 30S RIBOSOMAL PROTEIN S11



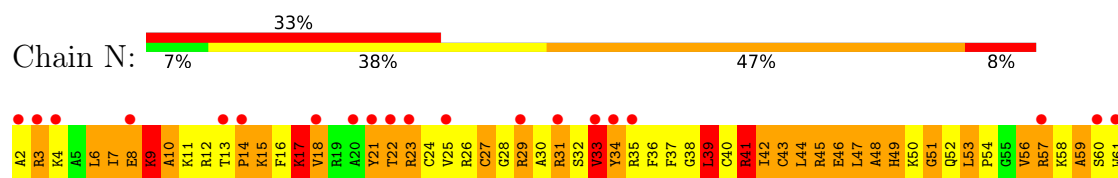
- Molecule 13: 30S RIBOSOMAL PROTEIN S12



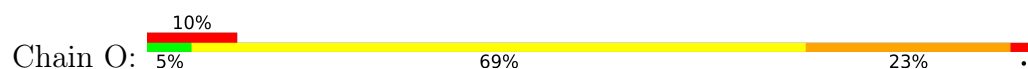
- Molecule 14: 30S RIBOSOMAL PROTEIN S13

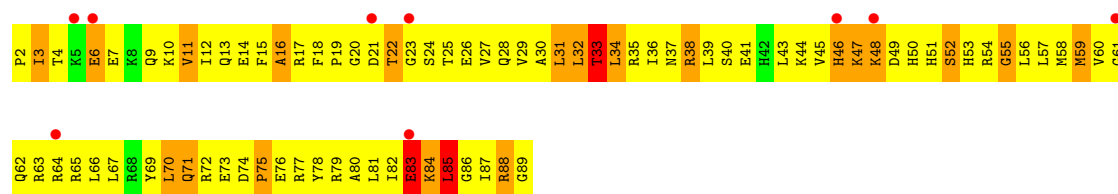


- Molecule 15: 30S RIBOSOMAL PROTEIN S14

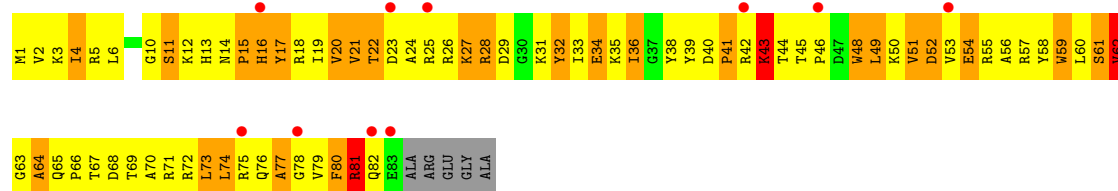


- Molecule 16: 30S RIBOSOMAL PROTEIN S15

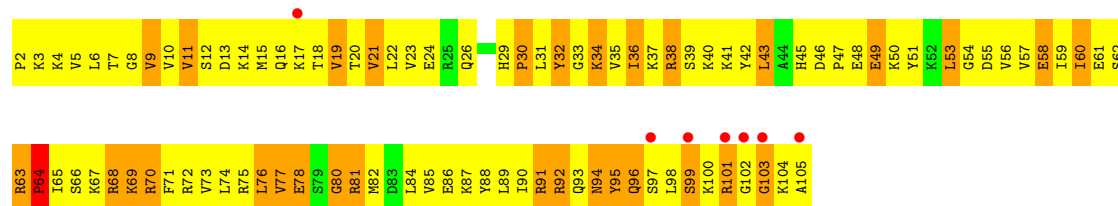
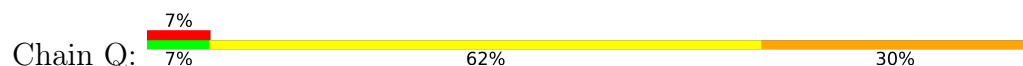




• Molecule 17: 30S RIBOSOMAL PROTEIN S16



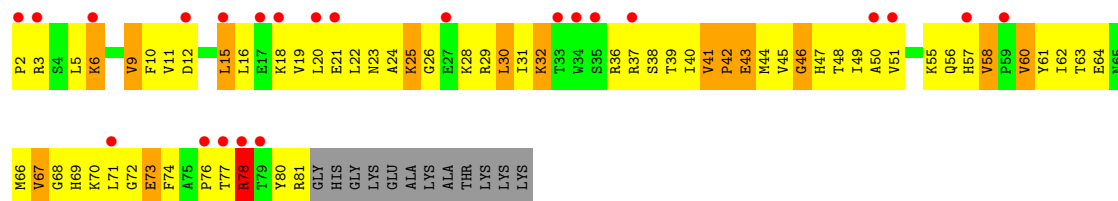
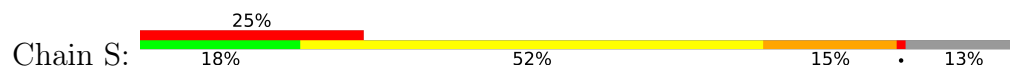
• Molecule 18: 30S RIBOSOMAL PROTEIN S17



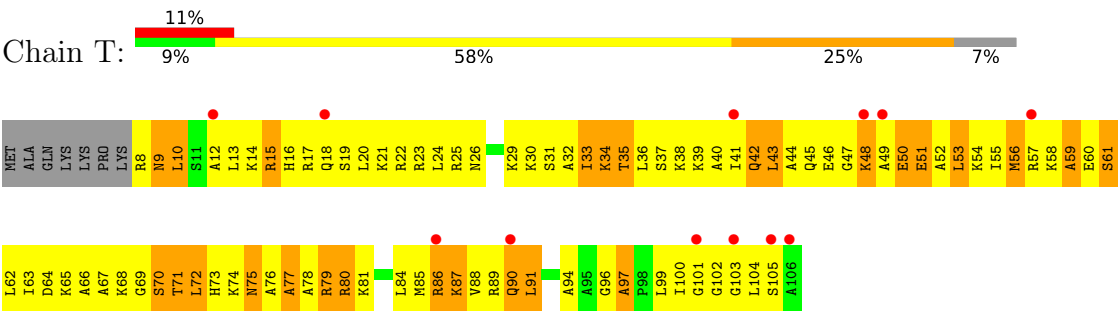
• Molecule 19: 30S RIBOSOMAL PROTEIN S18



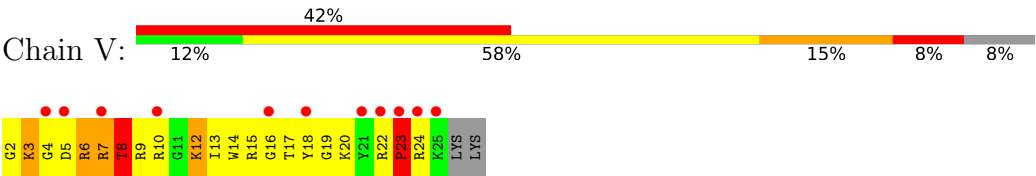
• Molecule 20: 30S RIBOSOMAL PROTEIN S19



• Molecule 21: 30S RIBOSOMAL PROTEIN S20



● Molecule 22: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.84Å 401.84Å 173.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.80 141.42 – 3.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (141.42-3.80) 92.6 (141.42-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.312 0.225 , 0.291	Depositor DCC
R_{free} test set	6465 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 827.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: ZN

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	A	0.50	0/36387	0.76	52/56789 (0.1%)
2	Z	0.55	0/84	0.83	0/128
3	B	0.50	0/1935	1.12	20/2609 (0.8%)
4	C	0.45	0/1636	1.09	18/2205 (0.8%)
5	D	0.51	0/1733	1.13	22/2318 (0.9%)
6	E	0.68	0/1162	1.26	18/1564 (1.2%)
7	F	0.42	0/856	1.02	6/1154 (0.5%)
8	G	0.42	0/1276	1.02	10/1709 (0.6%)
9	H	0.73	0/1136	1.35	15/1527 (1.0%)
10	I	0.44	0/1029	1.07	9/1378 (0.7%)
11	J	0.46	0/805	1.13	7/1082 (0.6%)
12	K	0.57	0/900	1.08	9/1213 (0.7%)
13	L	0.51	0/986	1.14	7/1320 (0.5%)
14	M	0.50	0/947	1.12	10/1270 (0.8%)
15	N	0.44	0/501	1.04	4/664 (0.6%)
16	O	0.56	0/745	0.96	3/992 (0.3%)
17	P	0.56	0/716	1.00	2/963 (0.2%)
18	Q	0.69	0/870	1.24	11/1159 (0.9%)
19	R	0.51	0/603	1.11	7/799 (0.9%)
20	S	0.44	0/661	1.08	6/890 (0.7%)
21	T	0.44	0/765	1.02	1/1007 (0.1%)
22	V	0.49	0/212	1.05	1/277 (0.4%)
All	All	0.51	0/55945	0.89	238/83017 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	42

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	P	0	1
All	All	2	43

There are no bond length outliers.

The worst 5 of 238 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	100	ILE	CA-C-N	15.18	135.42	119.78
9	H	100	ILE	C-N-CA	15.18	135.42	119.78
1	A	51	A	C2'-C3'-O3'	14.37	131.06	109.50
1	A	266	G	C2'-C3'-O3'	13.61	129.91	109.50
1	A	1498	U	C2'-C3'-O3'	13.27	129.41	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	51	A	C3'
1	A	1498	U	C3'

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	G	Sidechain
1	A	148	G	Sidechain
1	A	197	A	Sidechain
1	A	28	G	Sidechain
1	A	90	U	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	A	32508	0	16414	2482	0
2	Z	77	0	42	5	0
3	B	1900	0	1951	450	0
4	C	1612	0	1677	412	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1703	0	1765	399	0
6	E	1146	0	1207	261	0
7	F	843	0	857	163	0
8	G	1257	0	1296	270	0
9	H	1116	0	1177	246	0
10	I	1011	0	1043	253	0
11	J	792	0	835	255	0
12	K	885	0	904	151	0
13	L	970	0	1057	193	0
14	M	937	0	995	178	0
15	N	492	0	533	149	0
16	O	734	0	771	159	0
17	P	700	0	720	186	0
18	Q	857	0	930	191	0
19	R	597	0	668	154	0
20	S	647	0	673	121	0
21	T	763	0	861	187	0
22	V	208	0	221	55	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51757	0	36597	6455	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 73.

The worst 5 of 6455 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:A:818:G:O2'	1:A:819:A:H5''	1.44	1.17
1:A:1064:G:H4'	1:A:1065:U:H5'	1.28	1.15
1:A:1443:G:H5''	1:A:1446:A:H5'	1.21	1.14
19:R:53:ARG:HH21	19:R:60:GLY:N	1.46	1.14
6:E:13:ILE:HG22	6:E:30:ALA:HA	1.22	1.13

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	
3	B	232/256 (91%)	134 (58%)	71 (31%)	27 (12%)	0	4
4	C	204/239 (85%)	95 (47%)	64 (31%)	45 (22%)	0	1
5	D	206/208 (99%)	109 (53%)	63 (31%)	34 (16%)	0	2
6	E	148/161 (92%)	98 (66%)	30 (20%)	20 (14%)	0	3
7	F	99/101 (98%)	56 (57%)	30 (30%)	13 (13%)	0	3
8	G	153/155 (99%)	68 (44%)	47 (31%)	38 (25%)	0	0
9	H	136/138 (99%)	91 (67%)	28 (21%)	17 (12%)	0	4
10	I	125/128 (98%)	70 (56%)	27 (22%)	28 (22%)	0	1
11	J	96/104 (92%)	51 (53%)	26 (27%)	19 (20%)	0	1
12	K	117/129 (91%)	72 (62%)	31 (26%)	14 (12%)	0	4
13	L	122/135 (90%)	81 (66%)	22 (18%)	19 (16%)	0	2
14	M	116/126 (92%)	66 (57%)	33 (28%)	17 (15%)	0	2
15	N	58/60 (97%)	25 (43%)	8 (14%)	25 (43%)	0	0
16	O	86/88 (98%)	42 (49%)	30 (35%)	14 (16%)	0	2
17	P	81/88 (92%)	44 (54%)	20 (25%)	17 (21%)	0	1
18	Q	102/104 (98%)	60 (59%)	27 (26%)	15 (15%)	0	2
19	R	71/88 (81%)	36 (51%)	24 (34%)	11 (16%)	0	2
20	S	78/92 (85%)	45 (58%)	24 (31%)	9 (12%)	0	4
21	T	97/106 (92%)	34 (35%)	42 (43%)	21 (22%)	0	1
22	V	22/26 (85%)	10 (46%)	7 (32%)	5 (23%)	0	0
All	All	2349/2532 (93%)	1287 (55%)	654 (28%)	408 (17%)	0	2

5 of 408 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	20	GLU

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Mol	Chain	Res	Type
3	B	158	LEU
3	B	232	PRO
3	B	239	VAL
4	C	4	LYS

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	B	202/220 (92%)	157 (78%)	45 (22%)	1	5
4	C	160/188 (85%)	145 (91%)	15 (9%)	8	30
5	D	180/180 (100%)	156 (87%)	24 (13%)	4	19
6	E	115/122 (94%)	89 (77%)	26 (23%)	1	5
7	F	90/90 (100%)	80 (89%)	10 (11%)	6	24
8	G	126/126 (100%)	111 (88%)	15 (12%)	5	22
9	H	119/119 (100%)	103 (87%)	16 (13%)	4	19
10	I	98/99 (99%)	78 (80%)	20 (20%)	1	7
11	J	87/91 (96%)	71 (82%)	16 (18%)	1	11
12	K	90/99 (91%)	76 (84%)	14 (16%)	2	15
13	L	104/111 (94%)	94 (90%)	10 (10%)	8	29
14	M	94/101 (93%)	85 (90%)	9 (10%)	8	29
15	N	49/49 (100%)	35 (71%)	14 (29%)	0	2
16	O	79/79 (100%)	67 (85%)	12 (15%)	3	16
17	P	72/74 (97%)	58 (81%)	14 (19%)	1	9
18	Q	96/96 (100%)	81 (84%)	15 (16%)	2	15
19	R	64/77 (83%)	60 (94%)	4 (6%)	16	42
20	S	71/79 (90%)	66 (93%)	5 (7%)	14	40
21	T	76/82 (93%)	68 (90%)	8 (10%)	6	26
22	V	19/21 (90%)	17 (90%)	2 (10%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1991/2103 (95%)	1697 (85%)	294 (15%)	3 16

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	N	53	LEU
21	T	42	GLN
16	O	32	LEU
18	Q	11	VAL
6	E	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	37	ASN
17	P	65	GLN
20	S	53	ASN
5	D	160	GLN
5	D	154	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	236 (15%)	51 (3%)
2	Z	3/6 (50%)	0	0
All	All	1514/1528 (99%)	236 (15%)	51 (3%)

5 of 236 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	960	U

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Mol	Chain	Res	Type
1	A	1085	U
1	A	1498	U
1	A	976	G
1	A	1049	U

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1511/1522 (99%)	1.44	421 (27%) 1 2	15, 88, 187, 199	0
2	Z	4/6 (66%)	2.30	3 (75%) 0 0	168, 184, 185, 199	0
3	B	234/256 (91%)	0.72	24 (10%) 12 14	23, 99, 178, 199	0
4	C	206/239 (86%)	1.05	28 (13%) 7 10	46, 134, 198, 199	0
5	D	208/208 (100%)	0.79	28 (13%) 7 10	14, 86, 165, 189	0
6	E	150/161 (93%)	0.35	10 (6%) 24 20	6, 56, 120, 160	0
7	F	101/101 (100%)	0.93	17 (16%) 4 7	44, 111, 171, 185	0
8	G	155/155 (100%)	0.91	18 (11%) 9 12	43, 141, 195, 199	0
9	H	138/138 (100%)	0.20	5 (3%) 46 32	3, 46, 115, 127	0
10	I	127/128 (99%)	1.43	37 (29%) 1 2	40, 146, 195, 199	0
11	J	98/104 (94%)	1.58	24 (24%) 2 3	63, 154, 199, 199	0
12	K	119/129 (92%)	0.55	11 (9%) 14 16	16, 93, 164, 199	0
13	L	124/135 (91%)	0.83	20 (16%) 4 8	19, 96, 159, 196	0
14	M	118/126 (93%)	1.04	23 (19%) 3 5	61, 125, 173, 199	0
15	N	60/60 (100%)	1.66	20 (33%) 1 2	42, 134, 185, 199	0
16	O	88/88 (100%)	0.40	9 (10%) 12 14	25, 70, 145, 189	0
17	P	83/88 (94%)	0.66	10 (12%) 9 12	12, 69, 141, 188	0
18	Q	104/104 (100%)	0.73	7 (6%) 24 20	2, 69, 140, 199	0
19	R	73/88 (82%)	0.71	13 (17%) 4 6	27, 87, 168, 194	0
20	S	80/92 (86%)	1.55	23 (28%) 1 2	55, 152, 198, 199	0
21	T	99/106 (93%)	0.69	12 (12%) 8 12	24, 82, 169, 199	0
22	V	24/26 (92%)	1.81	11 (45%) 0 1	39, 125, 181, 195	0
All	All	3904/4060 (96%)	1.08	774 (19%) 3 5	2, 98, 186, 199	0

The worst 5 of 774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Q	102	GLY	12.0
11	J	89	ASP	8.3
15	N	20	ALA	7.8
8	G	2	ALA	7.7
1	A	1117	G	7.4

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 oligosaccharides in this entry.

6.4 Ligands [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
23	ZN	D	306	1/1	0.94	0.34	78,78,78,78	0
23	ZN	N	307	1/1	0.99	0.07	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.