



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:40 PM BST

PDB ID : 4V4P
Title : Crystal structure of 70S ribosome with thrS operator and tRNAs.
Authors : Jenner, L.; Romby, P.; Rees, B.; Schulze-Bries, C.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.; Yusupova, G.; Yusupov, M.
Deposited on : 2005-01-19
Resolution : 5.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

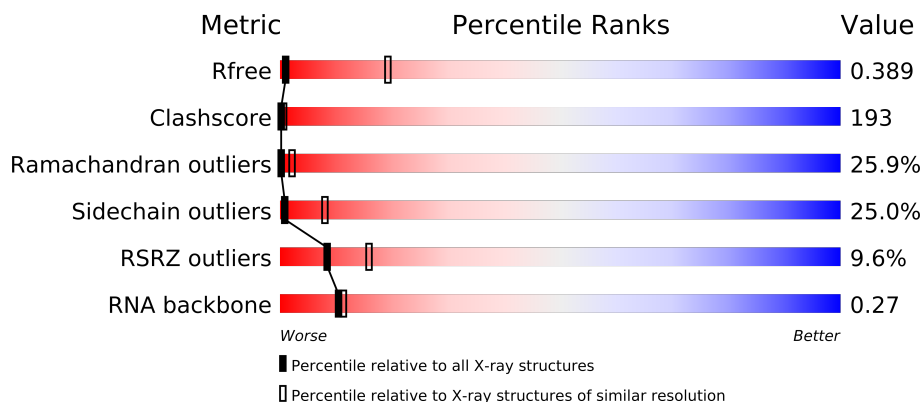
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 5.50 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}	66092	1083 (7.50-3.50)
Clashscore	79885	1008 (7.40-3.52)
Ramachandran outliers	78287	1275 (7.50-3.50)
Sidechain outliers	78261	1251 (7.50-3.50)
RSRZ outliers	66119	1082 (7.50-3.50)
RNA backbone	1838	1040 (7.50-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AB	123	
2	AA	2915	
3	AC	228	
4	AD	178	
5	AE	338	
6	AF	246	
7	AG	176	
8	AH	177	
9	AI	128	
9	AJ	128	
10	AK	149	
11	AL	141	

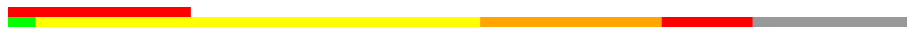
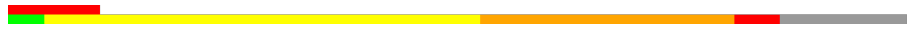


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	AM	145	
13	AN	122	
14	AO	164	
15	AP	138	
16	AQ	186	
17	AR	66	
18	AS	113	
19	AT	84	
20	AU	119	
21	AV	253	
22	AW	70	
23	AX	60	
24	A0	118	
25	A1	118	
26	A2	100	
27	A3	91	
28	A4	73	
29	A5	60	
30	A6	82	
31	A7	47	
32	A8	64	
33	A9	36	
34	BA	1522	
35	BB	76	
35	BC	76	
36	B1	78	
37	BE	256	
38	BF	239	
39	BG	209	
40	BH	162	
41	BI	101	
42	BJ	156	
43	BK	138	
44	BL	128	
45	BM	105	
46	BN	129	
47	BO	135	
48	BP	126	
49	BQ	61	
50	BR	89	
51	BS	88	
52	BT	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BU	88	
54	BV	93	
55	BW	106	
56	BX	27	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148539 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	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
AB	-1	A	-	INSERTION	GB 48271
AB	120	U	-	INSERTION	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	2872	Total	C	N	O	P	0	0	0
			61847	27526	11556	19893	2872			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	494	G	-	INSERTION	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	221	Total	C	N	O	S	0	0	0
			1687	1066	306	312	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 9 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			
9	AJ	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	84	Total	C	N	O	S	0	0	0
			639	391	109	139				

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	108	Total	C	N	O	S	0	0	0
			860	542	169	149				

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	110	Total	C	N	O	S	0	0	0
			879	531	166	182				

- Molecule 21 is a protein called 50S general stress protein CTC (L25).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	105	Total	C	N	O	S	0	0	0
			855	536	174	145				

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

- Molecule 34 is a RNA chain called 16S rRNA.

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

- Molecule 35 is a RNA chain called tRNA Phe (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			
35	BC	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			

- Molecule 36 is a RNA chain called thrS mRNA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B1	66	Total	C	N	O	P	0	0	0
			1405	629	247	463	66			

- Molecule 37 is a protein called 30S ribosomal protein S2.

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

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	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
BK	25	ASP	GLU	CONFLICT	UNP Q5SHQ2
BK	37	ARG	LYS	CONFLICT	UNP Q5SHQ2
BK	52	ASP	GLU	CONFLICT	UNP Q5SHQ2
BK	61	VAL	ILE	CONFLICT	UNP Q5SHQ2
BK	62	TYR	HIS	CONFLICT	UNP Q5SHQ2
BK	81	HIS	LYS	CONFLICT	UNP Q5SHQ2
BK	88	LYS	ARG	CONFLICT	UNP Q5SHQ2
BK	115	SER	PRO	CONFLICT	UNP Q5SHQ2

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	41	VAL	ILE	CONFLICT	UNP Q5SIH2

- Molecule 56 is a protein called 30S ribosomal protein Thx.

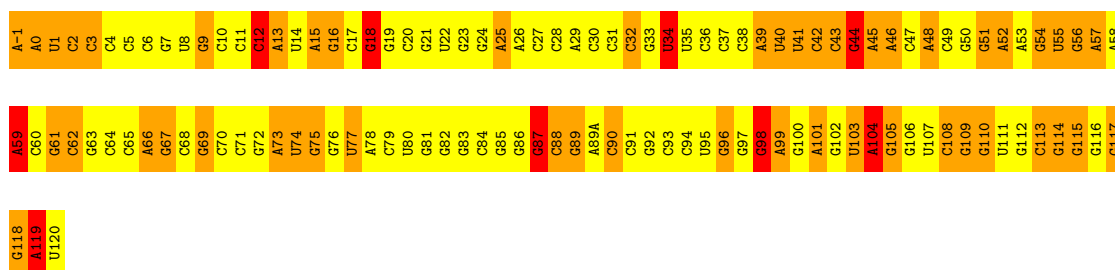
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	24	Total	C	N	O	0	0	0
			208	128	50	30			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

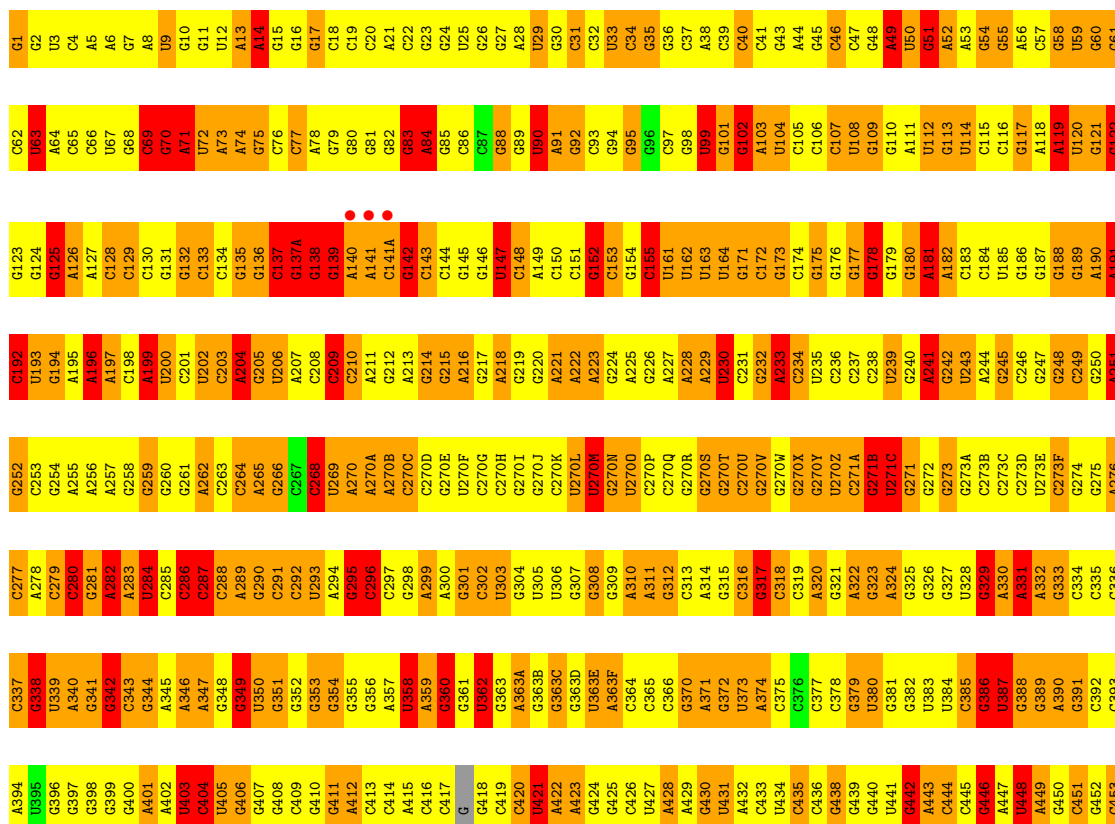
• Molecule 1: 5S ribosomal RNA

Chain AB:



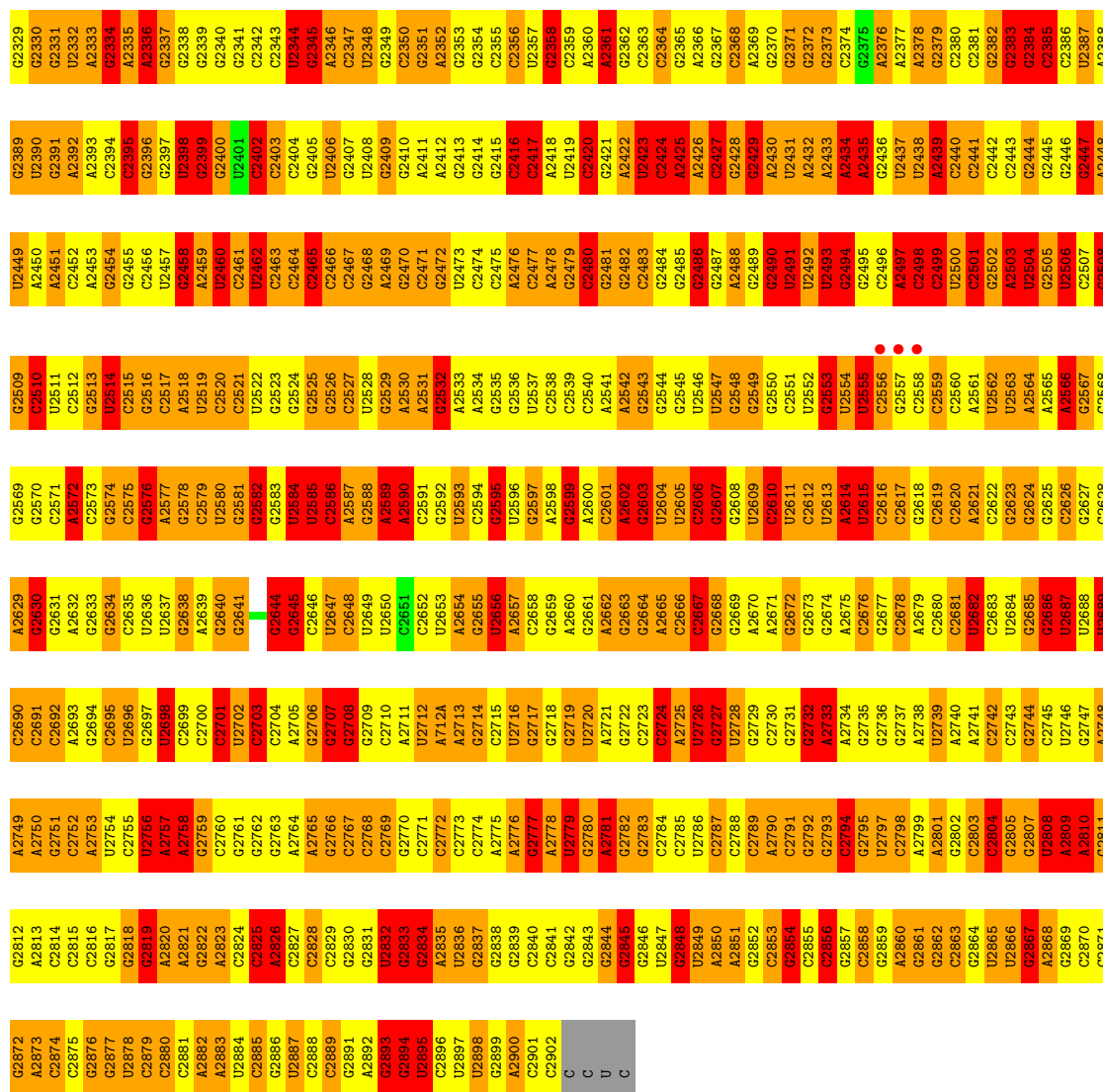
• Molecule 2: 23S ribosomal RNA

Chain AA:



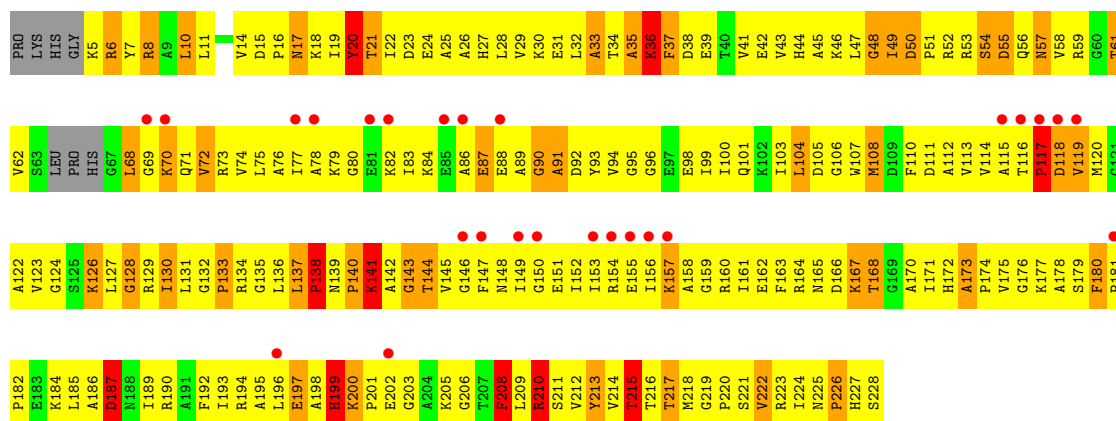
U1335	A1275	G1215	G1154	A1095	U1035	G975	C915	G854	G794	A734	G674	C635	G577	A515	A454
A1336	A1276	G1216	A1155	A1096	G1036	C976	G916	G855	C795	A735	A675	G636	A578	C516	C454
G1337	G1277	G1217	A1156	U1097	G1037	G977	A917	C856	C796	A736	A676	A637	G579	C517	C456
G1338	A1278	C1218	G1157	A1098	C1038	G978	A918	C857	C797	C737	A677	G638	C580	G518	A457
G1339	G1279	G1219	U1158	G1099	G1039	G979	G919	U858	G798	G738	C678	U639	C581	U519	G458
U1340	G1280	C1220	U1159	C1100	C1040	A980	G920	G859	G799	G739	C679	G640	G582	G520	U459
U1341	G1281	C1221	G1160	U1101	U1041	A981	G921	U860	A800	U740	G680	C641	G583	G521	U460
A1342	U1282	C1222	C1161	C1102	G1042	C982	U922	A861	A801	G741	G681	G642	C584	G522	C461
G1343	G1283	C1223	A1162	A1103	C1043	A983	C923	G862	A802	G742	G682	G643	C585	G523	C462
G1344	A1284	G1224	G1163	G1104	G1044	A984	C924	A863	U803	G743	C683	A644	A586	U524	C463
C1345	G1285	C1225	G1164	U1105	A1045	C985	C925	G864	A804	G744	G684	C645	C587	U525	U464
G1346	A1286	G1226	U1165	G1106	A1046	C986	A926	C865	G805	G745	A685	A646	U588	A526	C465
G1347	A1287	G1227	C1166	G1107	G1047	G987	G928	A866	C806	A746	G686	G647	C589	C527	A466
G1348	U1288	G1228	U1167	U1108	A1048	A988	G929	C867	U807	U747	C687	G648	A590	A528	G467
A1349	C1289	G1229	G1168	C1109	C1049	G989	U930	U868	G808	G748	U688	G649	C591	A529	G468
C1350	C1290	G1230	G1169	G1110	A1050	A990	G931	G869	G809	C749	A689	C	G592	G530	C469
C1351	C1291	G1231	G1170	A1111	G1051	C991	G932	A870	U810	A750	G690	G	G593	C531	A470
U1352	U1292	G1232	G1171	G1112	C1052	C992	A933	U871	U811	A751	C691	C	U594	A532	A471
A1353	C1293	C1233	G1173	U1113	C1053	G993	G934	A872	C812	A752	C692	A	C595	G533	A472
A1354	U1294	U1234	A1174	G1114	A1054	C994	C935	G873	U813	C753	C693	A	G596	U534	G473
G1355	G1295	G1235	U1175	G1115	G1055	C995	C936	G874	C814	C754	G694	G	U597	C535	G474
G1356	G1296	G1236	G1176	C1116	A1056	A996	U937	G875	C815	C755	G695	C	G598	A536	U475
U1357	C1297	A1237	A1177	G1117	A1057	G997	G938	C876	C816	C756	G696	G	G599	C537	G476
G1358	C1298	G1238	C1178	C1118	G1058	C998	G939	U877	C817	U757	G697	G	G600	G539	A477
A1359	G1299	G1239	U1179	C1119	U1059	U999	G940	A878	C818	C758	C698	G	C601	G540	A478
A1360	U1300	U1240	C1180	G1120	U1060	A1000	A941	C885	A819	G759	A699	C	G602	C541	A479
G1361	A1301	A1241	C1181	C1121	G1061	U1001	G942	G886	U826	G760	G700	C	A603	C542	A480
C1362	A1302	A1242	A1182	G1122	U1062	G1002	U943	G887	U827	A761	G701	G	G604	C543	G481
G1363	C1303	G1243	G1183	C1123	G1063	G1003	G944	G888	U828	U762	G702	C	C605	C544	A482
G1364	C1304	G1244	G1184	C1124	C1064	G1004	A945	G889	A829	G763	U703	A	U606	G545	A483
A1365	C1305	G1245	C1185	G1125	U1065	C1005	G946	C884	A824	A764	G704	C	U607	C546	C484
A1366	C1306	A1246	G1186	A1126	U1066	C1006	G947	C885	C825	G765	A705	G	A608	A547	C485
A1367	A1307	A1247	G1187	A1127	A1067	C1007	G948	C886	U826	C766	A706	C	A609	A548	C486
G1368	G1308	G1248	U1188	A1128	G1068	U1008	C949	A887	U827	G767	G707	G	G609A	G549	C487
G1369	G1309	U1249	A1189	A1129	A1069	A1009	G950	C888	U828	G768	C708	G	C610	G550	G488
C1370	G1310	G1250	G1190	U1130	A1070	A1010	C951	C889	A829	G769	U709	C	C611	G551	G489
G1371	G1311	G1251	G1191	G1131	G1071	U1011	G952	A890	G830	G770	G710	G650	G612	G552	G491
U1372	U1312	G1252	G1192	A1132	C1072	U1012	A953	G892	G831	G771	G711	G651	U613	U553	A492
A1373	U1313	A1253	G1193	U1133	A1073	C1013	G954	C893	G832	C772	G712	C852	U614	U554	G493
G1374	C1314	A1254	A1194	G1134	G1074	U1014	C955	C894	U833	U773	G713	G653	G615	G556	G494
C1375	C1315	U1255	G1195	C1135	C1075	G1015	G956	U895	C834	A774	U714	A654	A616	U557	G495
C1376	U1316	G1256	C1196	G1136	C1076	G1016	A957	A896	A835	G775	G715	G655	G617	G558	G496
G1377	A1317	C1257	G1197	U1137	A1077	G1017	U958	C897	G836	G776	A716	G656	G618	G559	A497
U1378	C1318	C1258	U1198	G1138	U1078	C1018	A959	C898	C837	A777	G717	U657	C618A	C560	G498
A1379	G1319	G1259	U1199	G1139	C1079	U1019	A960	A899	C838	G778	A718	C858	G619	G561	U499
G1380	C1320	G1260	C1200	C1140	C1080	A1020	C961	A900	U839	U779	C719	C859	G620	U562	G500
G1381	A1321	C1261	C1201	U1141	U1081	A1021	G962	A901	C840	G780	C720	G660	A621	G563	A501
C1382	A1322	A1262	C1202	U1142	U1082	G1022	U963	C902	A841	A781	C721	C861	G622	C564	A502
C1383	U1323	G1263	G1203	A142A	U1083	U1023	C964	C903	C842	A782	A722	G662	G623	C565	A503
A1384	G1324	G1264	A1204	A1143	A1084	G1024	C965	C904	G843	A783	G723	G663	C624	U566	U504
G1385	G1325	A1265	U1205	G1144	A1085	U1025	G966	U905	C844	A784	U724	C864	G625	A567	A505
C1386	U1326	G1266	G1206	C1145	A1086	U1026	C967	G906	G845	G785	G725	C865	U626	U568	G506
C1387	C1327	U1267	C1207	C1146	G1087	A1027	G968	U907	C846	C786	G726	G666	A627	U569	A507
G1388	G1328	A1268	C1208	C1147	A1088	A1028	U969	C908	U847	U787	A727	U667	G628	G570	G508
G1389	U1329	A1269	G1209	A1148	G1089	A1029	C970	A909	A848	A788	G728	G668	G629	A571	C509
C1390	C1330	C1270	A1210	G1149	U1090	G1030	C971	A910	G849	A789	G729	G669	G630	A572	C510
U1391	A1331	G1271	U1211	C1150	G1091	G1031	G972	A911	C850	C790	C730	A870	A631	C573	U511
A1392	A1272	U1272	G1212	G1151	C1092	A1032	A973	C912	U851	C791	C731	C871	A632	C574	G512
A1393	C1332	U1273	A1213	G1093	G1093	U1033	G974	U913	G852	G792	A633	C575	A634	A513	A514
U1394	G1334	A1274	A1214	C1153	U1094	G1034	C974A	C914	G853	A793	G733	C673	C634	U576	A514

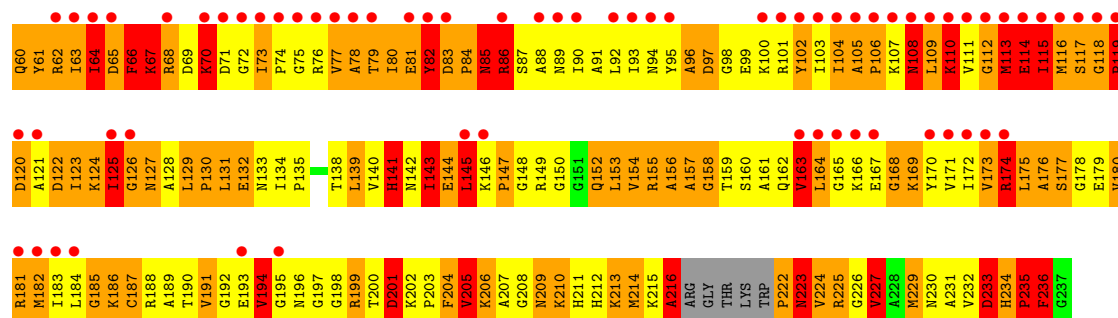
A2269	A2199	C2139	U2079	A2019	G1959	G1830	G1770	C1694	A1634	C1574	C1515	U1454	A1395
G2270	C2205	C2140	G2080	A2020	A1960	G1831	C1771	G1695	G1635	C1575	U1516	G1485	U1396
G2271	C2206	C2141	C2081	C2021	C1961	G1832	C1772	G1696	C1636	U1576	G1517	G1456	U1397
A2272	C2207	C2142	A2082	U2022	C1962	U1833	A1773	G1697	A1637	C1577	C1518	A1457	C1398
A2273	U2208	C2143	G2083	G2023	U1963	U1834	C1774	A1698	U1638	U1578	G1519	C1458	C1399
A2274	C2209	U2144	C2084	G2024	G1904	G1835	U1775	G1699	U1639	U1579	U1520	G1459	G1400
C2275	G2210	C2145	C2085	C2025	C1905	C1836	G1776	A1700	C1640	A1580	G1521	A1460	G1401
G2276	G2211	C2146	U2086	C2026	G1906	C1837	U1777	A1701	A1641	G1581	G1522	G1461	C1402
G2277	A2212	G2147	G2087	G2027	C1907	G1838	U1778	G1702	G1642	G1582	U1523	G1462	C1403
A2278	U2213	G2148	U2088	U2028	C1908	G1839	A1779	G1703	C1643	A1583	G1524	C1463	C1404
G2279	G2215	G2149	U2089	G2029	A1969	A1840	U1780	G1704	G1644	C1585	G1525	C1464	C1405
G2280	U2150	U2150	G2090	A2030	A1970	U1841	C1781	G1705	G1645	A1586	G1526	G1465	U1406
C2281	G2216	A2031	A1971	G2031	A1971	G1842	C1782	U1706	G1646	A1587	G1527	G1466	C1407
G2282	G2218	G2152	U2092	G2032	A1972	C1843	A1783	G1707	G1647	C1588	A1528	C1467	C1408
C2283	G2219	G2153	G2093	A2033	A1973	C1844	A1784	C1708	G1648	C1589	A1529	C1468	C1409
A2284	U2224	G2154	U2094	U2034	C1974	G1845	A1785	U1709	G1649	U1590	G1530	A1469	G1410
A2285	A2225	G2155	C2095	G2035	U1975	G1846	A1786	C1710	G1650	G1591	C1531	G1470	C1411
C2286	G2226	G2156	U2096	G2036	U1976	A1847	A1787	C1711	G1651	C1592	C1532	A1471	C1412
A2287	A2227	G	C2097	G2037	A1977	A1848	C1788	C1712	A1652	G1593	C1533	A1472	G1413
A2288	G2228	A	U2098	G2038	A1978	G1849	A1789	U1716	G1653	G1594	G1534	G1473	G1414
G2289	C2229	G	U2099	G2039	C1979	G1850	C1790	U1717	G1654	G1595	U1535	C1474	U1415
G2290	G2230	G	G2100	C2040	A1980	G1851	A1791	G1718	A1655	A1596	A1536	G1475	G1416
U2291	C2231	C	G2101	U2041	G1981	U1852	G1792	G1725	C1656	A1597	C1537	C1476	C1417
C2292	U2232	G	C2102	A2042	C1982	A1853	C1793	G1726	C1657	C1598	G1538	A1477	G1418
C2293	U2233	C	U2103	C2043	C1983	G1854	U1794	U1727	G1658	C1599	G1539	G1478	A1419
C2294	G2234	C	G2104	C2044	G1984	G1855	C1795	G1728	U1659	C1600	G1540	G1479	U1420
G2295	G2235	G	G2105	G2045	G1985	G1856	U1796	A1729	C1660	G1601	U1541	G1480	G1421
U2296	G2236	G	G2106	G2046	A1986	G1857	C1797	U1730	G1661	U1602	C1542	U1482	G1422
G2297	G2237	U	C2107	U2047	G1987	G1858	U1798	G1731	C1662	A1603	A1543	G1483	G1423
G2298	G2238	G	C2108	G2048	C1988	A1859	U1799	A1732	C1663	C1604	C1544	G1484	G1424
G2299	G2239	A	U2109	G2049	G1989	G1860	G1800	G1733	A1664	C1605	A1545	G1485	G1425
G2300	C2240	A	G2110	C2050	C1990	G1861	G1801	G1734	A1665	G1606	A1546	A1486	G1426
A2301	A2241	A	C2111	A2051	U1991	G1862	A1802	C1735	G1666	C1607	C1546	G1487	G1427
G2302	G2242	U	G2112	G2052	C1992	G1863	A1803	C1741	G1667	A1608	C1547	U1488	C1428
G2303	U2243	A	U2113	G2053	G1993	U1864	C1804	G1742	A1668	A1609	C1548	G1489	G1429
G2304	U2244	A2054	A2114	A2054	C1994	G1869	U1805	G1743	A1669	A1610	C1549	A1490	C1430
A2305	U2245	C2175	G2115	C2055	U1995	C1870	C1806	G1746	G1670	C1611	C1550	G1491	U1431
C2306	G2246	A2176	G2116	G2056	C1996	A1871	G1807	G1747	U1671	C1612	C1551	G1492	C1432
G2307	A2247	C2177	A2117	A2057	G1997	A1872	U1808	G1748	C1672	G1613	G1552	C1493	U1433
G2308	C2248	C2178	U2118	A2058	A1998	G1878	A1809	A1749	U1673	A1614	A1553	A1494	A1434
A2309	U2249	C2179	A2119	A2059	C1999	C1879	A1810	G1750	G1674	C1615	A1554	A1495	G1435
A2310	G2250	U2180	G2120	A2060	G2000	C1880	G1811	C1751	C1675	A1616	G1555	A1496	G1436
A2311	G2251	G2181	G2121	G2061	A2001	C1881	A1812	C1752	A1676	C1617	C1556	U1497	C1437
G2312	G2252	G2182	U2122	A2062	G2002	C1882	G1813	G1753	A1677	A1618	C1557	C1498	U1438
C2313	G2253	C2183	G2123	C2063	G2003	G1883	G1814	C1754	G1678	G1619	A1558	C1499	A1439
C2314	C2254	G2184	G2124	C2064	G2004	A1884	A1815	A1755	U1679	G1620	G1559	G1500	G1440
G2315	G2255	C2185	G2125	C2065	A2005	A1885	G1816	G1756	U1680	U1621	G1560	C1501	G1441
C2316	G2256	G2186	A2126	C2066	C2006	C1886	G1817	U1757	G1681	G1622	G1561	C1502	G1442
C2317	U2257	G2187	G2127	G2067	C2007	C1887	U1818	G1758	G1682	G1623	A1562	U1503	G1443
G2318	C2258	C2188	C2128	U2068	C2008	G1888	A1819	A1759	C1683	G1624	C1563	C1504	G1444
G2319	G2259	U2189	C2129	G2069	G2009	A1889	U1820	A1760	C1684	G1625	C1564	C1505	A4444
A2320	C2260	G2190	U2130	G2070	G1950	A1890	A1821	A1761	C1685	G1626	C1565	C1506	A4445
G2321	G2261	C2191	U2131	A2071	U1951	G1891	A1762	U1762	C1686	G1627	A1566	A1507	C1446
A2322	U2262	G2192	U2132	G2072	A1952	C1892	G1823	G1763	C1687	G1628	A1567	A1508	G1447
G2323	C2263	G2193	G2133	C2073	A1953	C1893	G1824	G1764	U1688	U1629	G1568	C1509	G1448
C2324	C2264	G2194	A2134	U2074	G1954	C1894	A1825	G1765	A1689	G1630	A1510	A1449	A1449
G2325	U2265	C2195	A2135	U2075	U1955	G1895	G1826	U1766	A1690	C630A	A1570	A1511	G449A
A2326	A2266	C2196	U2016	U2076	U1956	G1896	G1827	U1767	C1691	A1571	A1572	G1512	C1450
C2327	U2267	A2197	U2017	A2077	C1957	G1897	G1828	C1768	U1692	A1572	C1513	G1513	C1451
A2328	A2268	A2198	C2138	C2078	G2018	U1898	A1829	G1769	U1693	G1633	G1573	U1514	A1453



• Molecule 3: 50S ribosomal protein L1

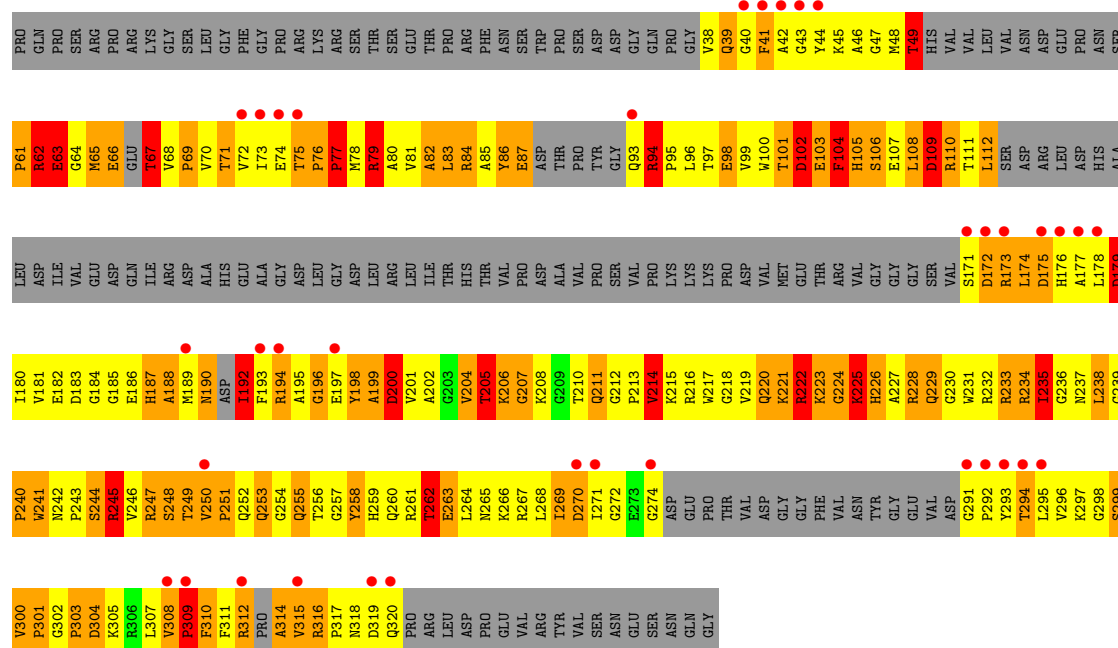
Chain AC:





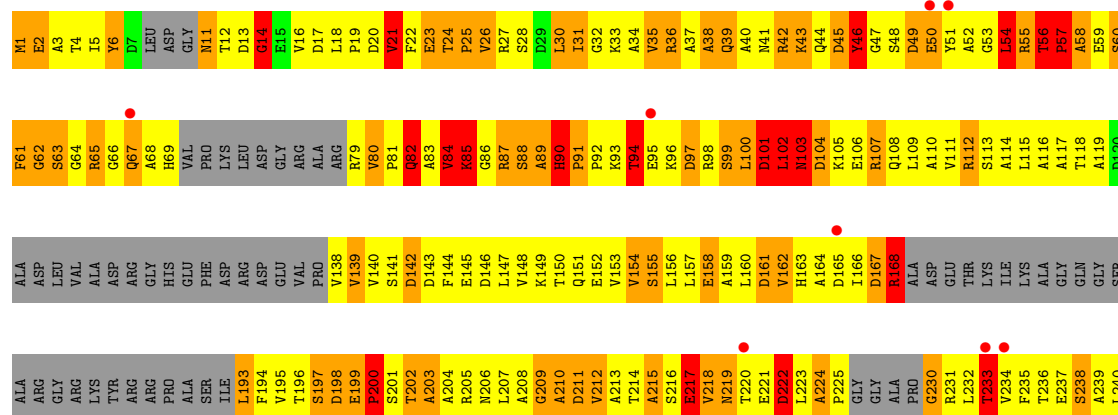
• Molecule 5: 50S ribosomal protein L3

Chain AE:



• Molecule 6: 50S ribosomal protein L4

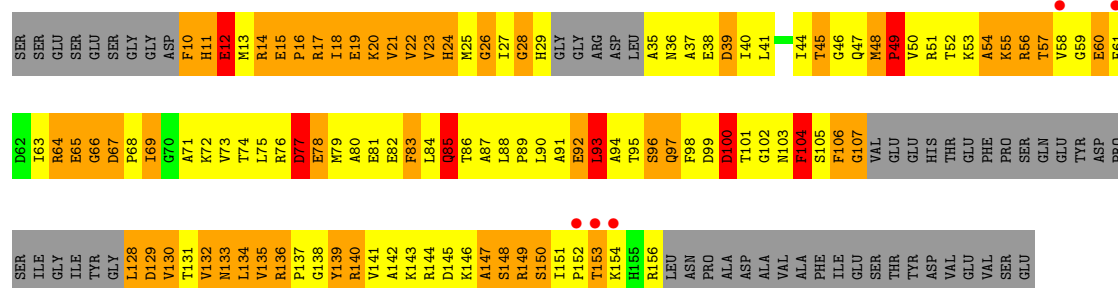
Chain AF:





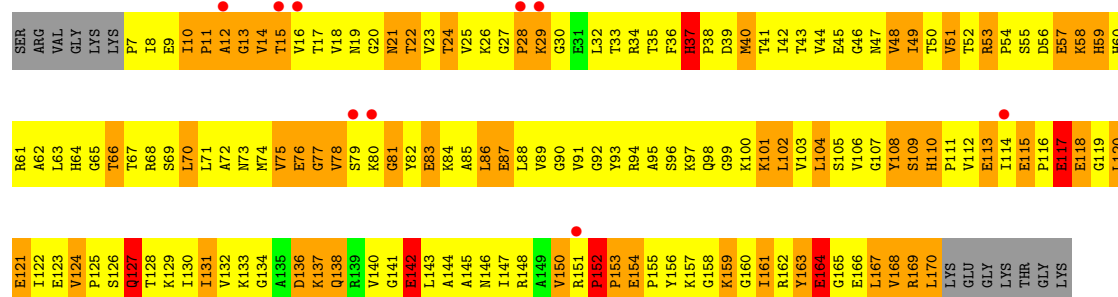
• Molecule 7: 50S ribosomal protein L5

Chain AG:



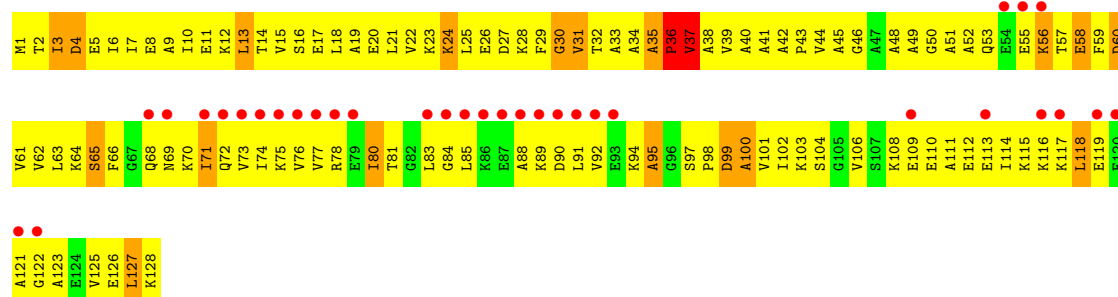
• Molecule 8: 50S ribosomal protein L6

Chain AH:



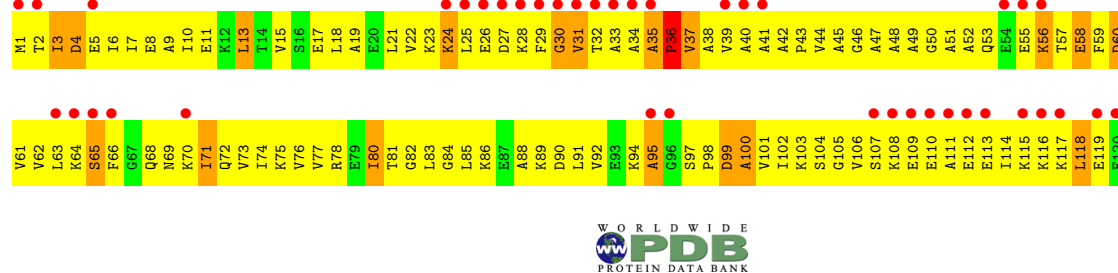
• Molecule 9: 50S ribosomal protein L7/L12

Chain AI:



• Molecule 9: 50S ribosomal protein L7/L12

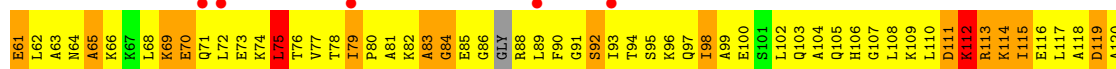
Chain AJ:





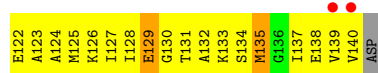
- Molecule 10: 50S ribosomal protein L9

Chain AK:



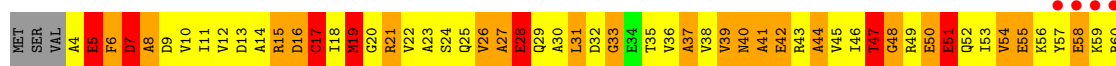
- Molecule 11: 50S ribosomal protein L11

Chain AL:



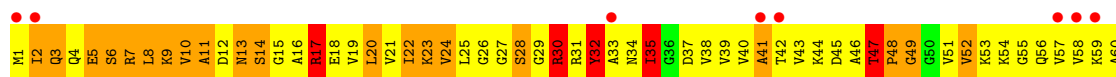
- Molecule 12: 50S ribosomal protein L13

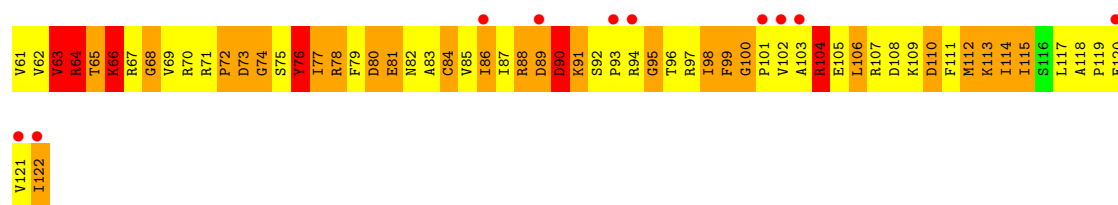
Chain AM:



- Molecule 13: 50S ribosomal protein L14

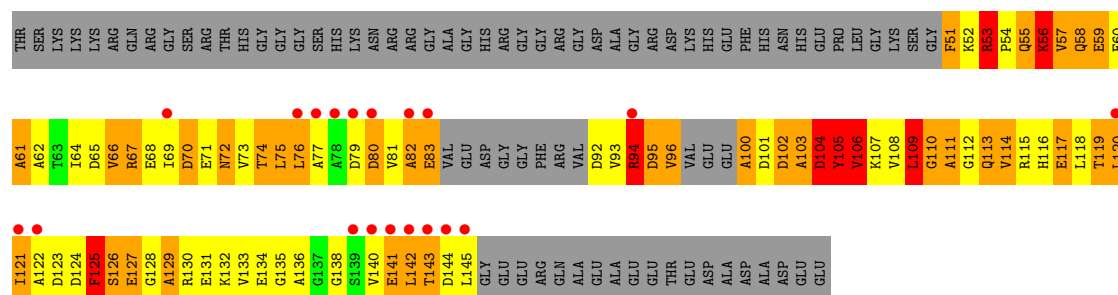
Chain AN:





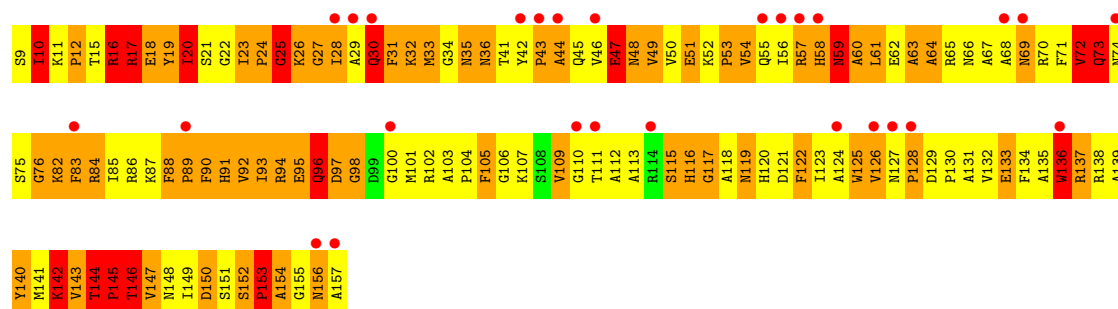
• Molecule 14: 50S ribosomal protein L15

Chain AO:



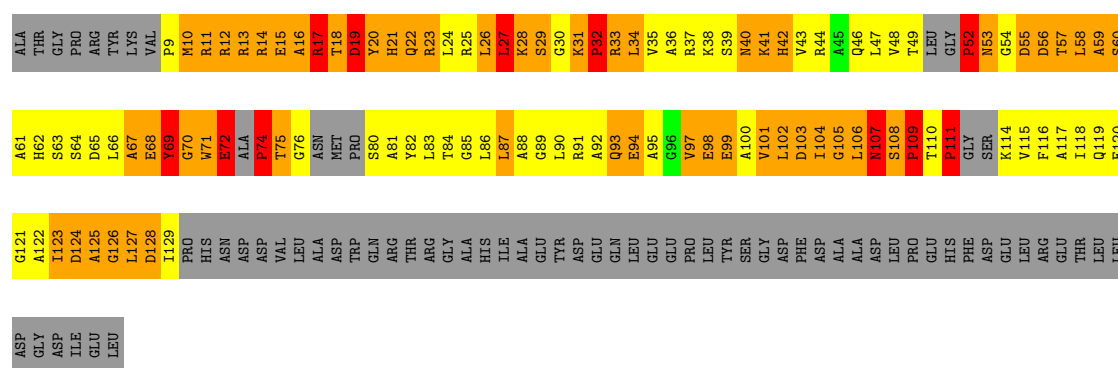
• Molecule 15: 50S ribosomal protein L16

Chain AP:



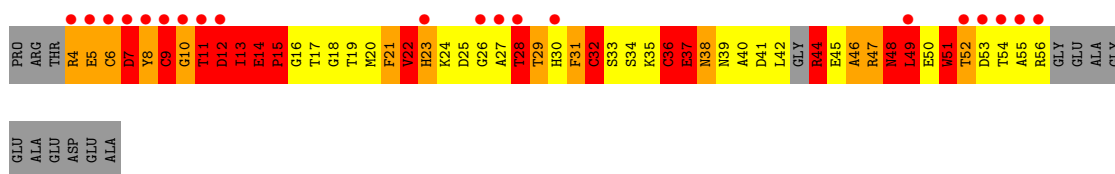
• Molecule 16: 50S ribosomal protein L18

Chain AQ:



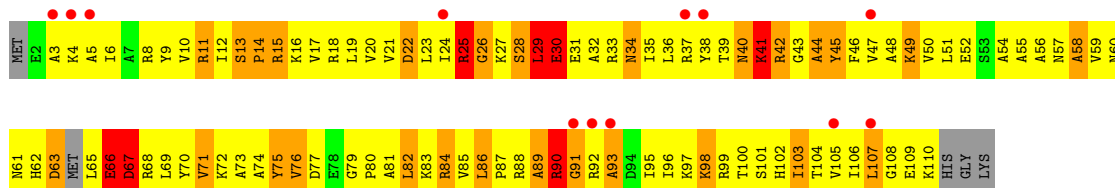
• Molecule 17: 50S ribosomal protein L19

Chain AR:



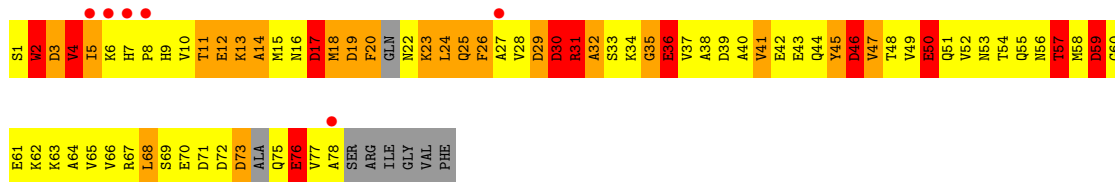
• Molecule 18: 50S ribosomal protein L22

Chain AS:



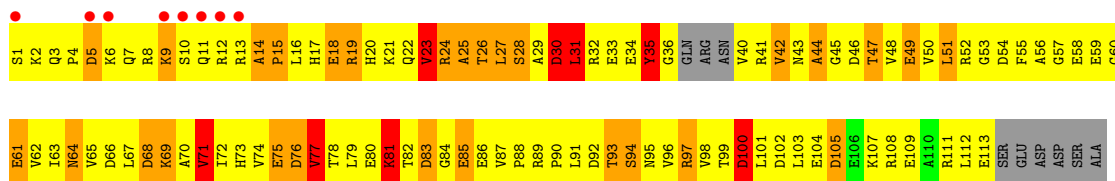
• Molecule 19: 50S ribosomal protein L23

Chain AT:



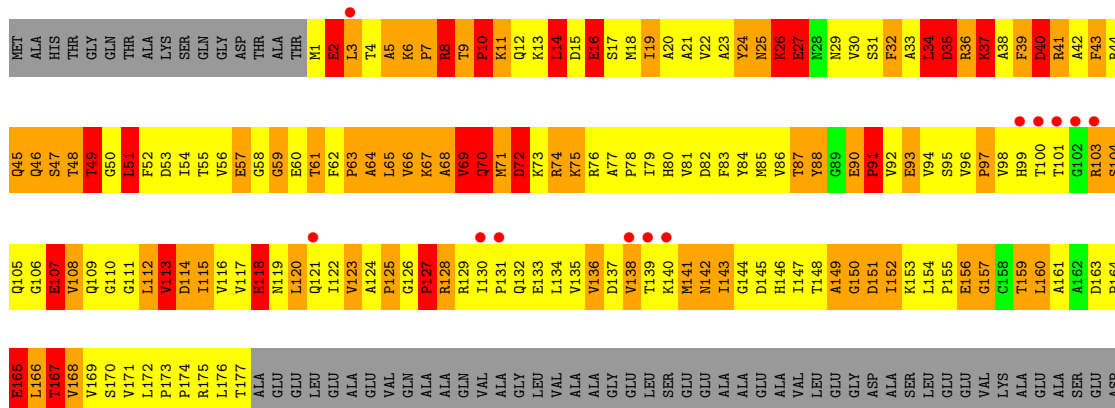
• Molecule 20: 50S ribosomal protein L24

Chain AU:



• Molecule 21: 50S general stress protein CTC (L25)

Chain AV:



ASN
ALA
GLY
THR
ASP
SER
GLU
ASP
ASN
SER
ASP
ALA
GLN

- Molecule 22: 50S ribosomal protein L29

Chain AW:

T1 V2 L3 H4 V5 Q6 E7 I8 R9 D10 M11 T12 P13 A14 E15 E16 E17 A18 E19 L20 D21 D22 L23 K24 T25 E26 L27 L28 R29 A30 R31 ALA V33 Q34 A35 GLU A36 L37 G38 A39 P40 E41 N42 P43 G44 R45 K46 K47 E48 L49 R50 K51 A52 I53 A54 R55 I56 K57 T58 I59 Q60

G61 E62 E63 G64 D65 LEU GLN ASN GLU

- Molecule 23: 50S ribosomal protein L30

Chain AX:

M1 P2 R3 L4 K5 V6 K7 L8 V9 K10 S11 P12 P13 G14 Y15 P16 K17 L18 L19 K20 A21 A22 N23 K24 K25 A26 L26 G27 L28 R29 R30 R31 G32 Q33 Q34 E34 R35 V36 L37 E38 D39 T40 P41 A42 I43 R44 G45 N46 V47 E48 K49 V50 A51 H52 L53 V54 R55 V56 E57 V58 V59 E60

- Molecule 24: 50S ribosomal protein L17

Chain A0:

MET ARG HIS LEU SER GLY ARG LYS LEU ASN ARG HIS S14 S15 H16 R17 L18 L19 A19 L20 Y21 N22 N23 Q24 A25 A26 S27 R28 L29 R30 T30 H31 G32 Q33 R34 T35 T36 T37 V38 P39 K40 K41 A42 K43 E44 R45 G46 F47 V48 D49 H50 L51 L52 L53 A54 A55 R56 R57 G58 D59 L60

H61 A62 R63 R64 L65 V66 L67 R68 D69 L70 Q71 D72 V73 K74 R75 R76 R77 K78 L79 F80 D81 E82 I83 A84 P85 A86 R87 Y87 R88 D89 R90 Q91 G92 G93 Y94 T95 R96 V97 L98 K99 L100 L101 A101 E102 R103 R104 R105 G106 D107 A108 A109 P110 L111 L112 L113 V114 E115 L116 V117 E118

- Molecule 25: 50S ribosomal protein L20

Chain A1:

MET P2 R3 A4 T5 K6 T7 I8 V9 R10 R11 R12 R13 R14 H14 K15 K16 K17 V17 L18 R19 R20 A21 K22 K23 G23 F24 F25 G26 S27 R28 S29 K30 K31 Q31 Y32 R33 R34 A35 A36 F36 Q37 T38 L39 L40 N41 N42 A43 T44 Y45 E46 Y47 A48 D49 R50 R51 N52 N53 K54 K55 R56 D57 R58 R59 L60

W61 I62 Q63 R64 I65 N66 A67 G68 A69 R70 L71 H72 G73 M74 N75 N76 S77 T78 F79 L80 N81 G82 L83 K84 R85 A86 R87 R88 D89 L90 L91 N91 R92 R93 V94 L95 A96 D97 T98 A99 A100 R101 E102 P103 A104 A105 F106 K107 A108 L109 V110 D111 A112 S113 R114 K115 N115 A116 R117 Q118

- Molecule 26: 50S ribosomal protein L21

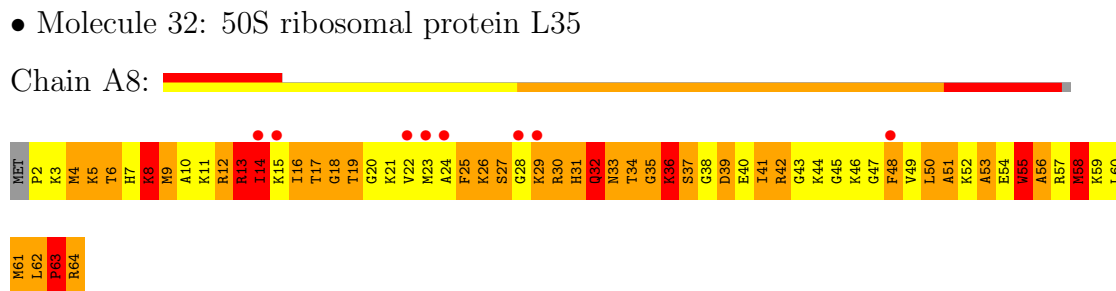
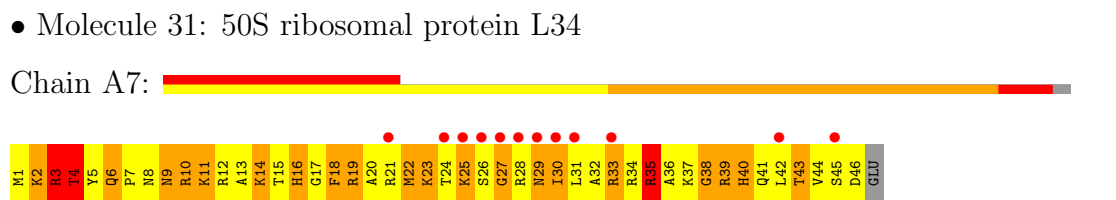
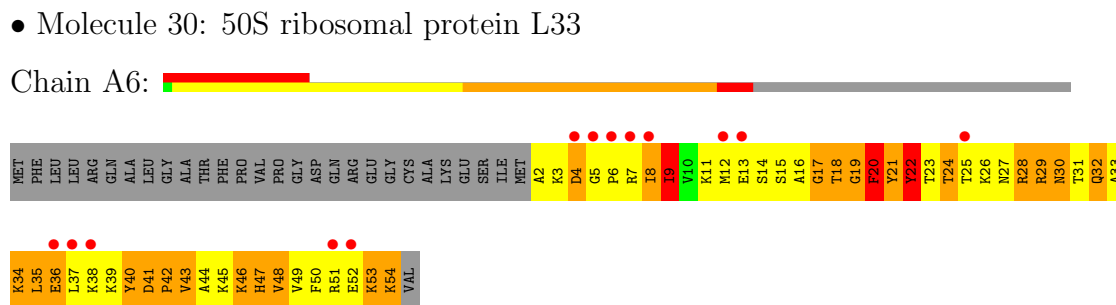
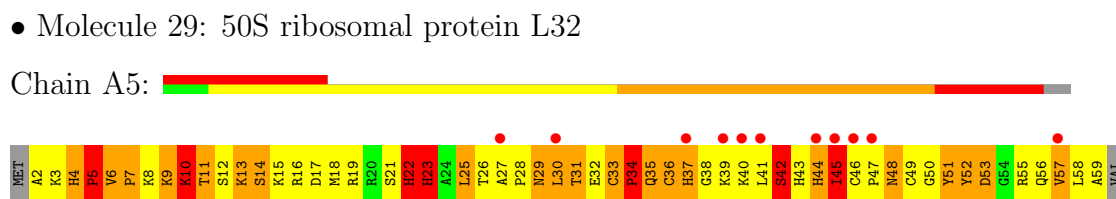
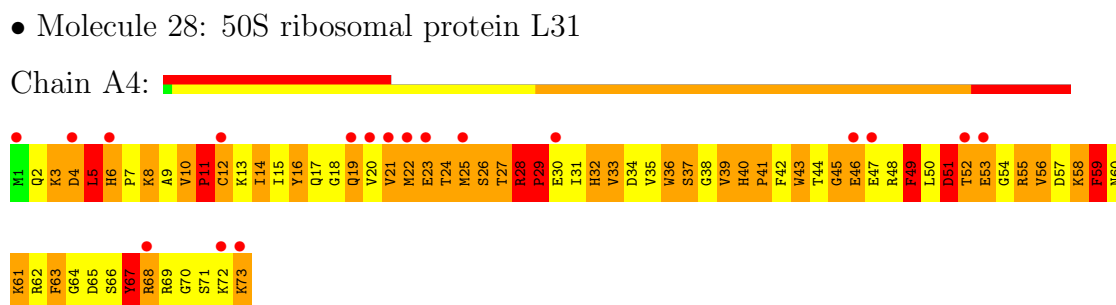
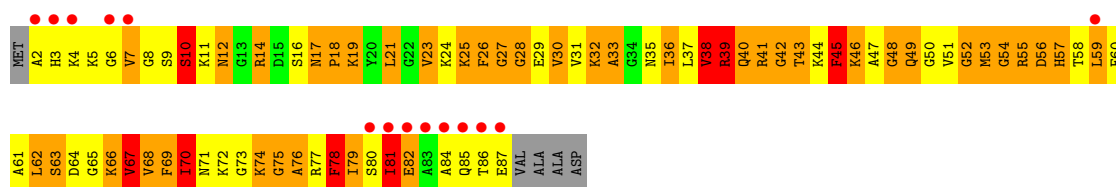
Chain A2:

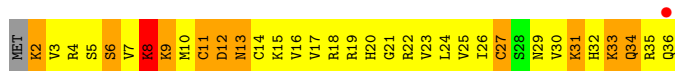
M1 F2 A3 I4 I5 Q6 T7 G8 G9 R10 Q11 Q12 R13 R14 V14 S15 E16 E17 D18 V19 R20 A21 E22 E23 S24 S25 Q26 G27 R28 R29 A30 G30 D31 D32 K33 V33 E34 L35 K36 A37 L38 F39 V40 G41 G42 E43 Q44 T45 V46 F47 G48 E49 D50 A51 G52 K53 Y54 T55 N56 Q57 A58 E59 V60

V61 E62 H63 G64 R65 G66 K67 K68 I69 I70 I71 I72 K73 R74 R75 S76 S77 G78 V79 R80 R81 R82 R83 T84 G85 G86 R87 Q88 R89 F90 T91 A92 I93 R94 I95 L96 L97 G98 Q99 G100

- Molecule 27: 50S ribosomal protein L27

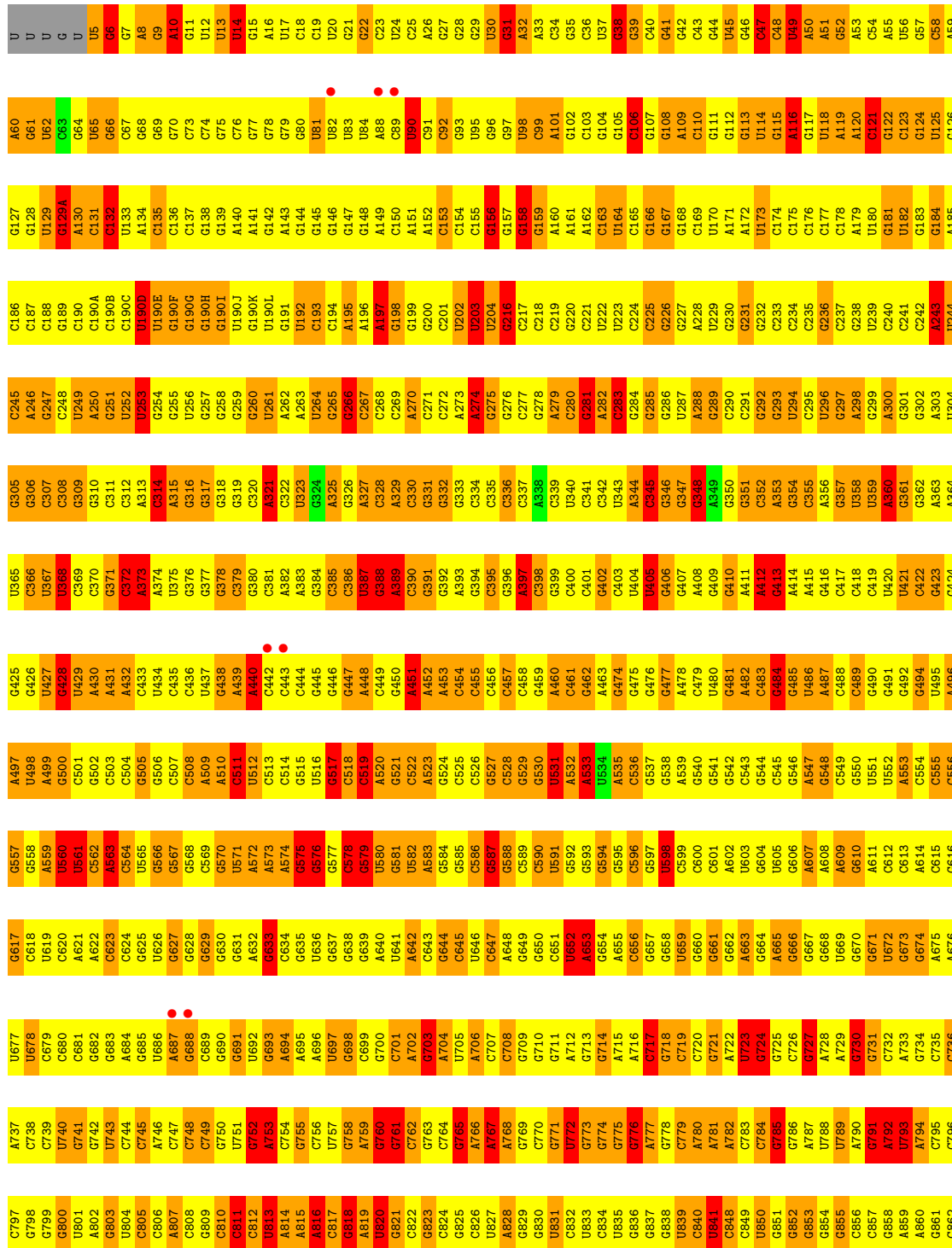
Chain A3:

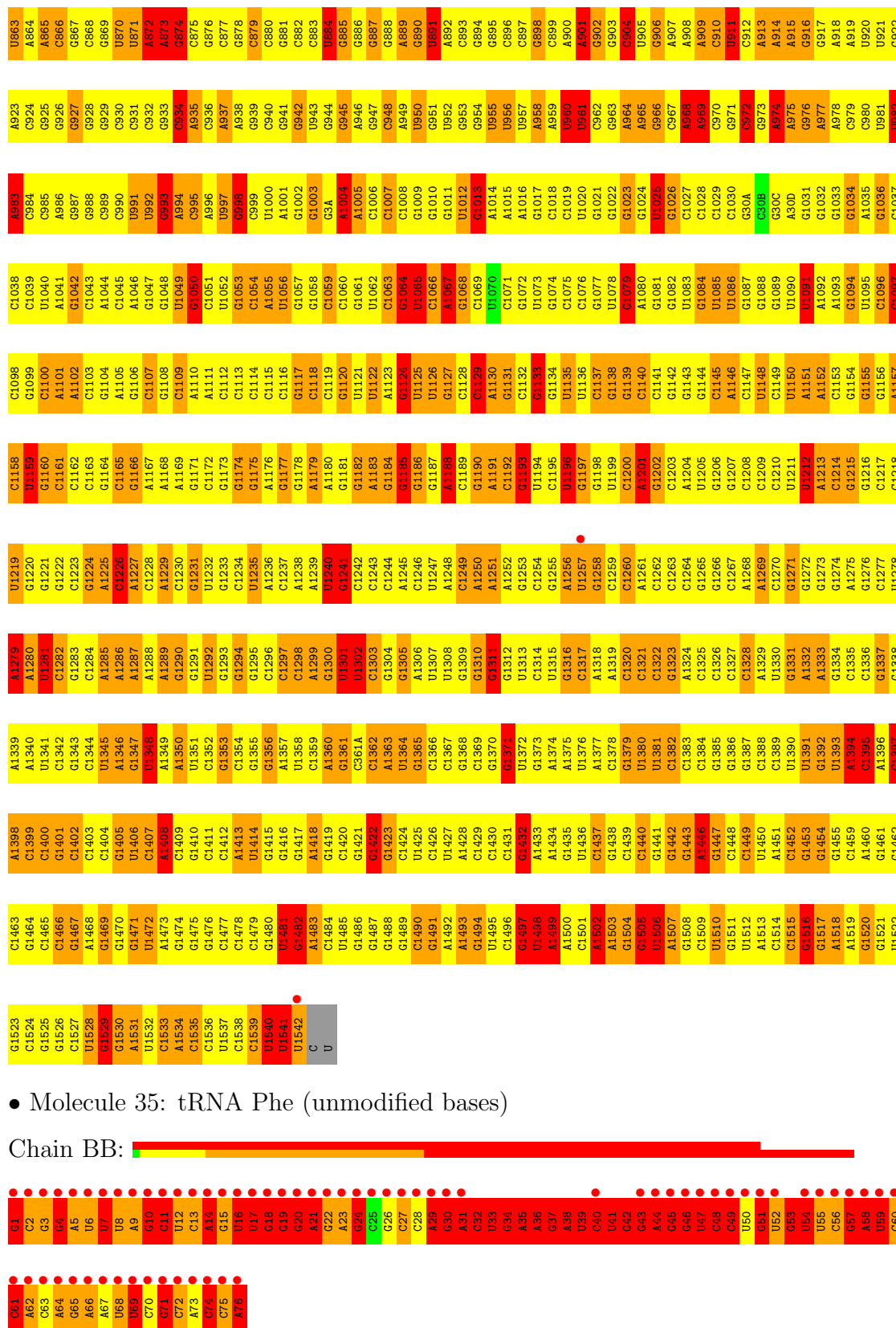




Molecule 34: 16S rRNA

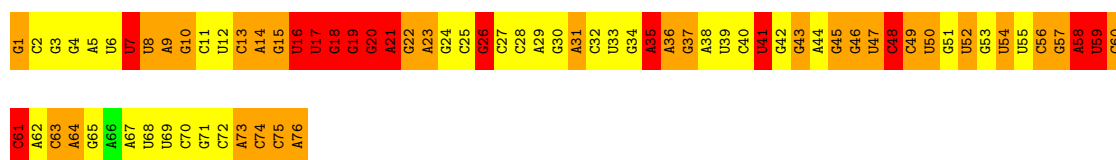
Chain BA:





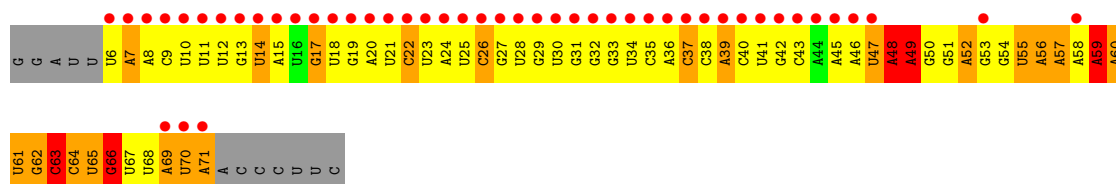
● Molecule 35: tRNA Phe (unmodified bases)

Chain BC:



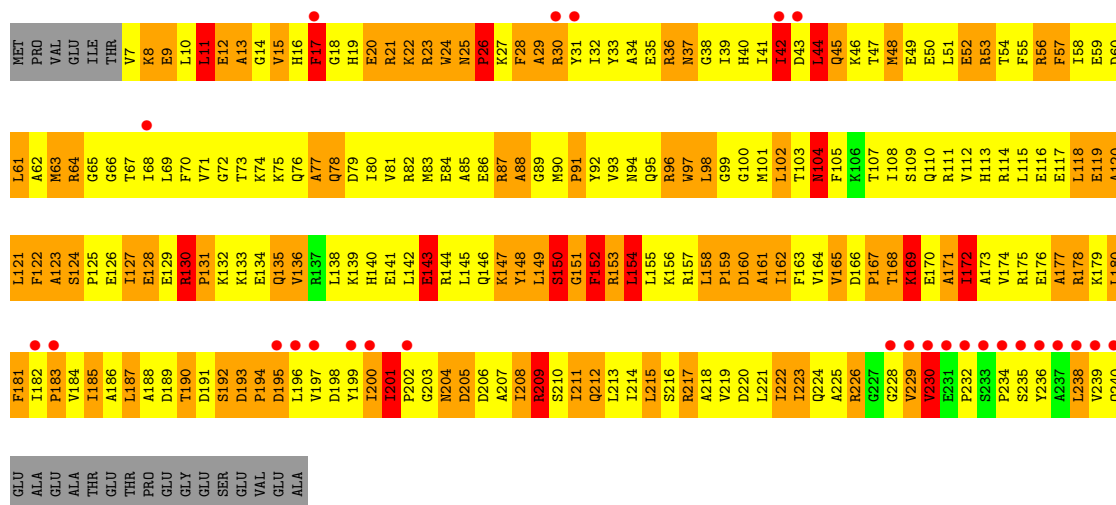
• Molecule 36: thrS mRNA operator

Chain B1:



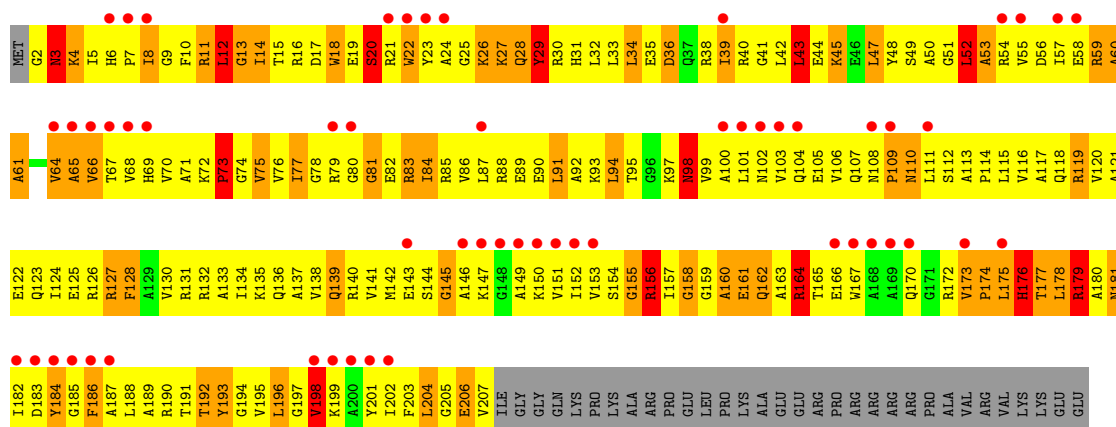
• Molecule 37: 30S ribosomal protein S2

Chain BE:



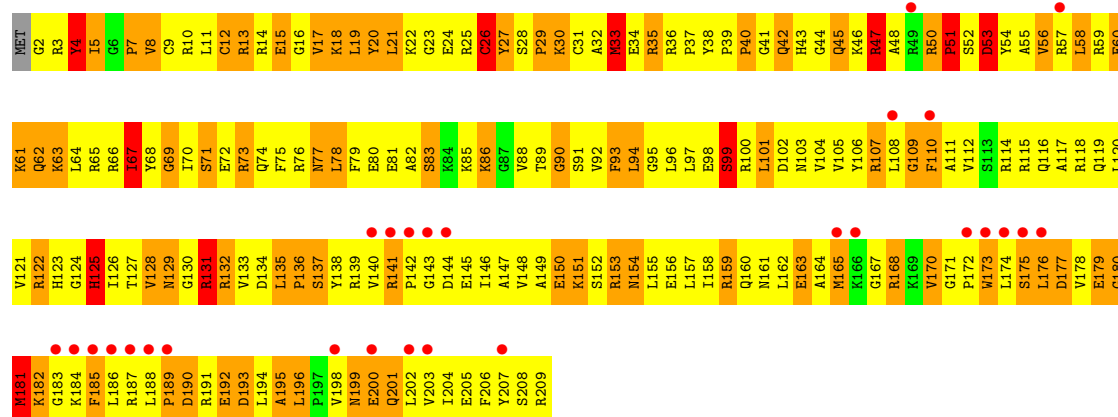
• Molecule 38: 30S ribosomal protein S3

Chain BF:



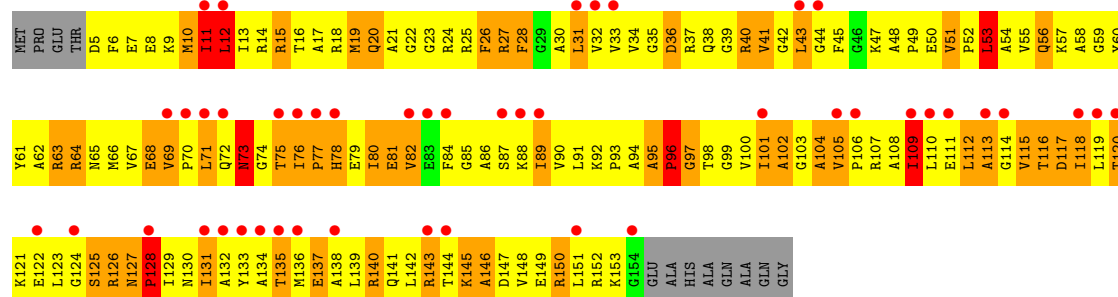
• Molecule 39: 30S ribosomal protein S4

Chain BG:



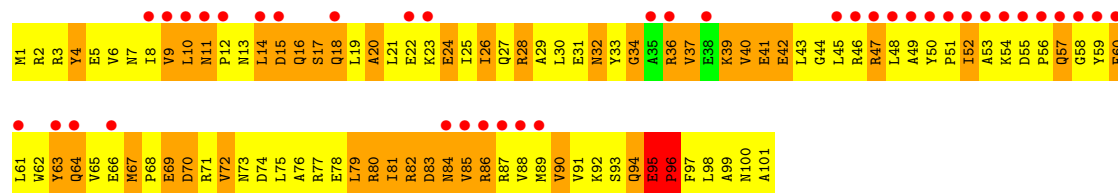
- Molecule 40: 30S ribosomal protein S5

Chain BH:



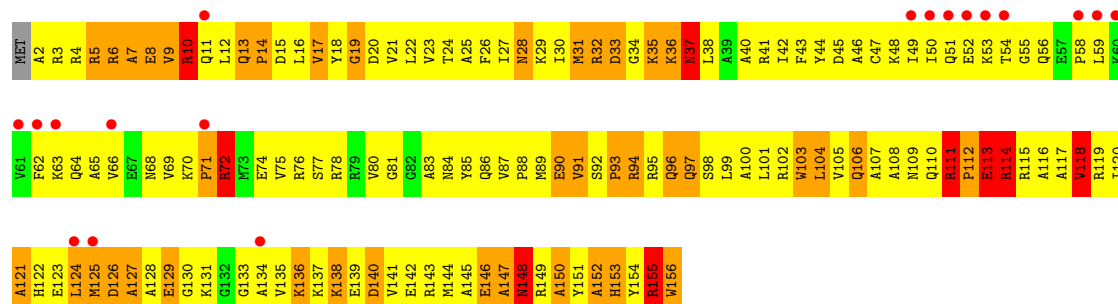
- Molecule 41: 30S ribosomal protein S6

Chain BI:



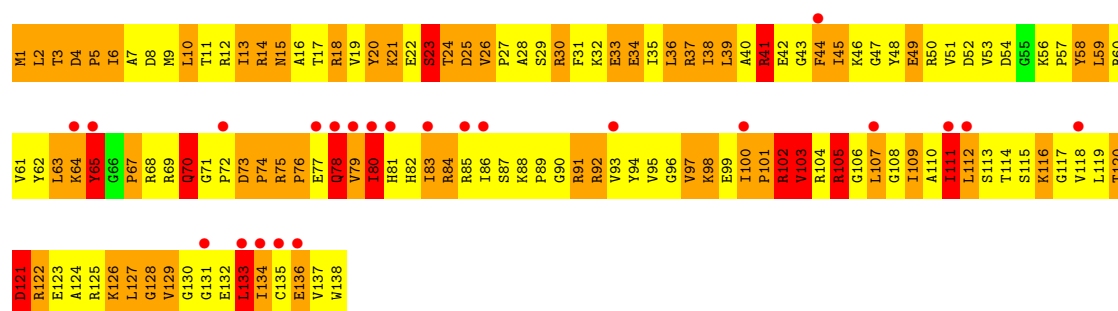
- Molecule 42: 30S ribosomal protein S7

Chain BJ:



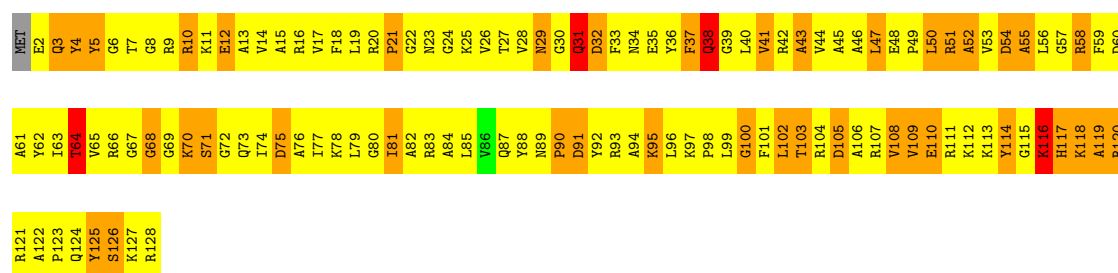
- Molecule 43: 30S ribosomal protein S8

Chain BK:



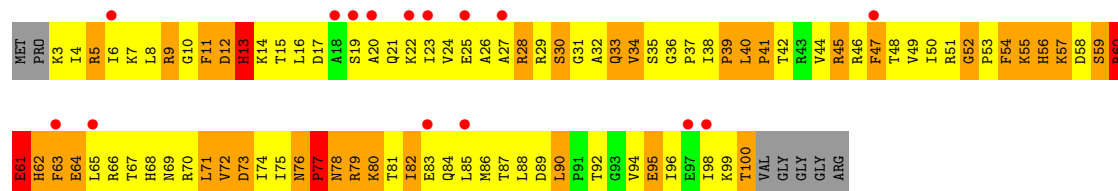
- Molecule 44: 30S ribosomal protein S9

Chain BL:



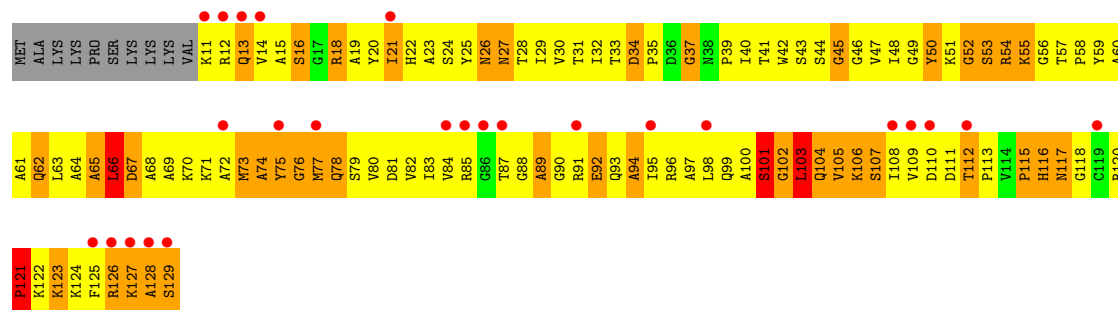
- Molecule 45: 30S ribosomal protein S10

Chain BM:



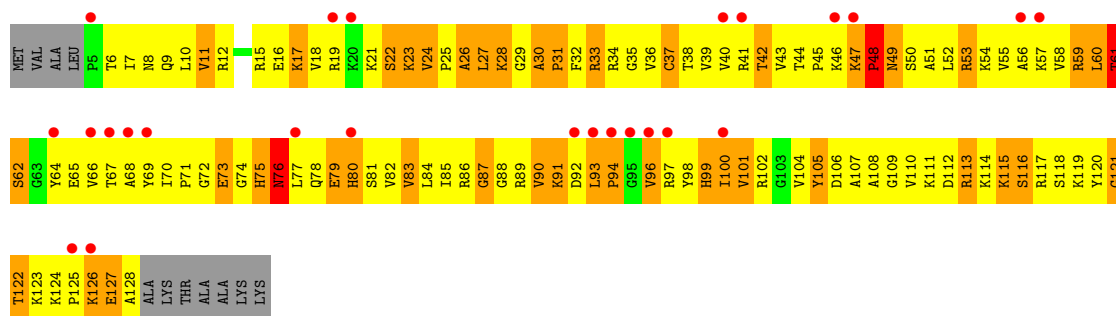
- Molecule 46: 30S ribosomal protein S11

Chain BN:



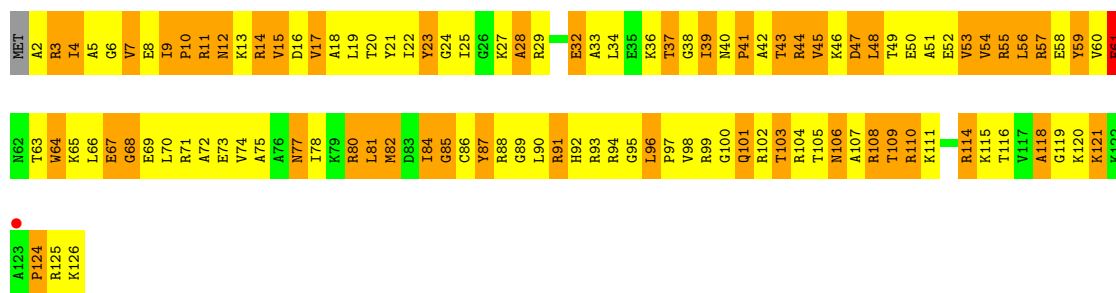
- Molecule 47: 30S ribosomal protein S12

Chain BO:



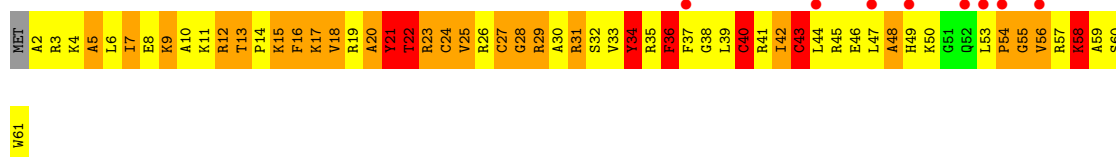
- Molecule 48: 30S ribosomal protein S13

Chain BP:



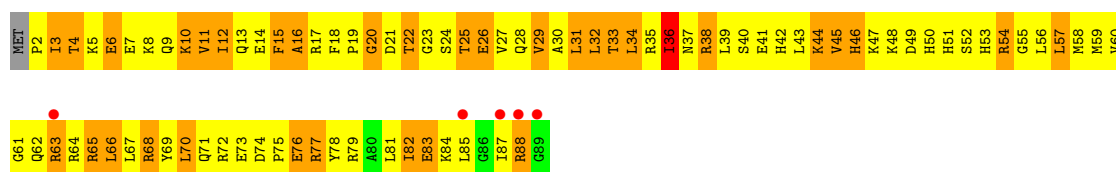
- Molecule 49: 30S ribosomal protein S14

Chain BQ:



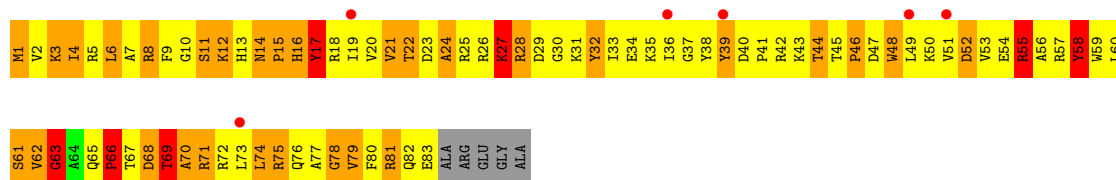
- Molecule 50: 30S ribosomal protein S15

Chain BR:



- Molecule 51: 30S ribosomal protein S16

Chain BS:



- Molecule 52: 30S ribosomal protein S17

- Molecule 53: 30S ribosomal protein S18

- Molecule 54: 30S ribosomal protein S19

- Molecule 55: 30S ribosomal protein S20

- Molecule 56: 30S ribosomal protein Thx

MET	G2	K3	G4	D5	R6	R7	T8	R9	R10	G11	K12	I13	W14	R15	G16	T17	Y18	G19	K20	Y21	R22	P23	R24	K25	LYS	LYS
-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.64Å 508.64Å 806.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 268.38 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (300.00-5.50) 97.5 (268.38-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 5.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.307 , 0.356 0.356 , 0.389	Depositor DCC
R_{free} test set	7724 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	206.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 161.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 169564 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	148539	wwPDB-VP
Average B, all atoms (Å ²)	338.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	AB	0.95	1/2954 (0.0%)	1.06	7/4606 (0.2%)
2	AA	1.16	181/69267 (0.3%)	1.22	549/108130 (0.5%)
3	AC	0.62	0/1715	0.94	2/2310 (0.1%)
4	AD	1.11	6/1329 (0.5%)	1.52	22/1787 (1.2%)
5	AE	1.04	3/1542 (0.2%)	1.41	21/2084 (1.0%)
6	AF	0.82	0/1446	1.26	14/1960 (0.7%)
7	AG	0.83	0/972	1.20	6/1307 (0.5%)
8	AH	0.76	0/1272	1.13	1/1721 (0.1%)
9	AI	0.48	0/950	0.72	0/1275
9	AJ	0.43	0/950	0.68	0/1275
10	AK	0.73	0/1157	1.17	8/1547 (0.5%)
11	AL	0.48	0/1015	0.91	4/1366 (0.3%)
12	AM	1.04	2/928 (0.2%)	1.23	2/1248 (0.2%)
13	AN	1.06	2/946 (0.2%)	1.43	14/1269 (1.1%)
14	AO	0.67	0/643	1.30	9/870 (1.0%)
15	AP	1.04	1/1109 (0.1%)	1.43	16/1499 (1.1%)
16	AQ	0.71	0/880	1.23	5/1189 (0.4%)
17	AR	1.37	4/413 (1.0%)	2.01	18/557 (3.2%)
18	AS	0.81	0/869	1.19	3/1166 (0.3%)
19	AT	0.76	0/609	1.05	0/823
20	AU	0.46	0/887	0.89	0/1195
21	AV	0.71	0/1385	1.10	7/1883 (0.4%)
22	AW	0.73	0/497	1.05	1/668 (0.1%)
23	AX	0.81	0/482	1.18	2/646 (0.3%)
24	A0	0.86	0/867	1.24	3/1162 (0.3%)
25	A1	1.03	0/994	1.33	6/1323 (0.5%)
26	A2	0.71	0/797	1.14	4/1061 (0.4%)
27	A3	0.72	0/649	1.14	3/860 (0.3%)
28	A4	0.97	1/620 (0.2%)	1.18	4/831 (0.5%)
29	A5	0.79	0/469	1.41	5/629 (0.8%)
30	A6	0.93	0/438	1.25	4/583 (0.7%)
31	A7	0.78	0/387	1.05	0/509
32	A8	0.98	2/503 (0.4%)	1.48	8/657 (1.2%)
33	A9	1.36	1/286 (0.3%)	1.44	4/375 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BA	1.03	30/36438 (0.1%)	1.17	167/56869 (0.3%)
35	BB	2.33	76/1818 (4.2%)	2.48	157/2831 (5.5%)
35	BC	1.09	5/1818 (0.3%)	1.11	7/2831 (0.2%)
36	B1	1.14	7/1571 (0.4%)	0.96	7/2445 (0.3%)
37	BE	0.75	0/1935	1.06	3/2609 (0.1%)
38	BF	0.62	0/1636	0.99	5/2205 (0.2%)
39	BG	0.86	2/1733 (0.1%)	1.16	4/2318 (0.2%)
40	BH	0.85	0/1162	1.12	1/1564 (0.1%)
41	BI	0.78	0/856	1.06	1/1154 (0.1%)
42	BJ	0.70	1/1276 (0.1%)	1.00	6/1709 (0.4%)
43	BK	0.81	0/1136	1.18	5/1527 (0.3%)
44	BL	0.52	0/1029	0.86	1/1378 (0.1%)
45	BM	0.58	0/807	0.94	2/1085 (0.2%)
46	BN	0.75	0/900	1.04	0/1213
47	BO	0.78	0/986	1.22	3/1320 (0.2%)
48	BP	0.59	0/1008	0.98	0/1347
49	BQ	0.83	1/501 (0.2%)	1.09	2/664 (0.3%)
50	BR	0.74	0/745	1.05	2/992 (0.2%)
51	BS	0.81	0/716	1.10	3/963 (0.3%)
52	BT	0.82	0/870	1.11	2/1159 (0.2%)
53	BU	0.72	0/603	1.18	2/799 (0.3%)
54	BV	0.59	0/661	0.98	1/890 (0.1%)
55	BW	0.84	0/764	1.12	2/1006 (0.2%)
56	BX	0.45	0/212	0.81	0/277
All	All	1.05	326/161408 (0.2%)	1.21	1135/241526 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	14
2	AA	0	527
4	AD	0	1
5	AE	0	1
6	AF	0	1
7	AG	0	2
12	AM	0	2
13	AN	0	2
14	AO	0	2
16	AQ	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
23	AX	0	1
25	A1	0	3
26	A2	0	1
28	A4	0	1
30	A6	0	1
34	BA	0	220
35	BB	0	35
35	BC	0	12
36	B1	0	4
38	BF	0	1
39	BG	0	1
41	BI	0	1
43	BK	0	1
48	BP	0	1
51	BS	0	2
All	All	0	838

The worst 5 of 326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	142	G	C5-C6	27.73	1.70	1.42
36	B1	48	A	C5-C6	27.45	1.65	1.41
35	BB	37	G	C2-N2	18.34	1.52	1.34
34	BA	1541	U	C4-C5	17.23	1.59	1.43
2	AA	142	G	C2-N3	16.69	1.46	1.32

The worst 5 of 1135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1064	G	N1-C2-N2	-65.61	57.15	116.20
34	BA	1064	G	N3-C2-N2	63.69	164.48	119.90
34	BA	1064	G	N1-C2-N3	-27.38	107.47	123.90
2	AA	1084	A	O5'-P-OP2	-26.59	78.79	110.70
35	BB	36	A	OP1-P-O3'	-18.47	64.57	105.20

There are no chirality outliers.

5 of 838 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	12	C	Sidechain
1	AB	18	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	AB	34	U	Sidechain
1	AB	39	A	Sidechain
1	AB	44	G	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2641	0	1337	635	1
2	AA	61847	0	31165	17729	1
3	AC	1687	0	1737	723	0
4	AD	1308	0	1355	898	0
5	AE	1507	0	1494	986	0
6	AF	1430	0	1386	832	0
7	AG	957	0	959	519	0
8	AH	1251	0	1298	612	0
9	AI	945	0	999	497	0
9	AJ	945	0	999	362	0
10	AK	1145	0	1227	630	0
11	AL	999	0	1071	497	0
12	AM	917	0	904	616	0
13	AN	937	0	1000	549	0
14	AO	639	0	615	373	0
15	AP	1081	0	1062	743	0
16	AQ	866	0	875	512	0
17	AR	406	0	361	160	0
18	AS	860	0	919	442	0
19	AT	602	0	563	332	0
20	AU	879	0	868	477	0
21	AV	1360	0	1390	788	0
22	AW	494	0	506	240	0
23	AX	477	0	529	309	0
24	A0	855	0	906	492	0
25	A1	978	0	1020	685	0
26	A2	787	0	804	571	0
27	A3	641	0	668	421	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A4	604	0	595	365	0
29	A5	457	0	462	294	0
30	A6	431	0	456	224	0
31	A7	383	0	414	260	0
32	A8	496	0	549	296	0
33	A9	285	0	312	125	0
34	BA	32554	0	16429	7563	1
35	BB	1626	0	817	629	0
35	BC	1626	0	820	429	0
36	B1	1405	0	706	258	1
37	BE	1900	0	1951	930	0
38	BF	1612	0	1677	662	0
39	BG	1703	0	1763	719	0
40	BH	1146	0	1207	489	1
41	BI	843	0	857	398	0
42	BJ	1257	0	1296	527	0
43	BK	1116	0	1177	677	0
44	BL	1011	0	1043	442	0
45	BM	794	0	840	332	0
46	BN	885	0	904	409	0
47	BO	970	0	1057	459	0
48	BP	997	0	1072	493	0
49	BQ	492	0	529	258	0
50	BR	734	0	771	330	0
51	BS	700	0	720	318	0
52	BT	857	0	930	423	0
53	BU	597	0	668	334	0
54	BV	647	0	673	254	0
55	BW	762	0	859	366	0
56	BX	208	0	221	103	0
All	All	148539	0	99792	47710	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 193.

The worst 5 of 47710 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AA:2515:C:N4	2:AA:2569:G:H1	1.08	1.45
34:BA:292:G:H1	34:BA:308:C:N4	1.08	1.45
34:BA:144:G:H1	34:BA:178:C:N4	1.13	1.45
2:AA:447:A:H1'	2:AA:449:A:N6	1.28	1.44
33:A9:11:CYS:SG	33:A9:11:CYS:CB	2.06	1.44

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AB:-1:A:O2'	1:AB:-1:A:O2'[15_545]	1.59	0.61
2:AA:2153:G:O2'	34:BA:423:G:OP2[3_655]	2.16	0.04
36:B1:29:G:O3'	40:BH:5:ASP:OD2[3_655]	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	AC	217/228 (95%)	143 (66%)	36 (17%)	38 (18%)	0	6
4	AD	171/178 (96%)	71 (42%)	38 (22%)	62 (36%)	0	0
5	AE	187/338 (55%)	89 (48%)	41 (22%)	57 (30%)	0	1
6	AF	183/246 (74%)	83 (45%)	40 (22%)	60 (33%)	0	0
7	AG	118/176 (67%)	57 (48%)	29 (25%)	32 (27%)	0	1
8	AH	162/177 (92%)	89 (55%)	39 (24%)	34 (21%)	0	4
9	AI	126/128 (98%)	87 (69%)	24 (19%)	15 (12%)	1	14
9	AJ	126/128 (98%)	86 (68%)	25 (20%)	15 (12%)	1	14
10	AK	146/149 (98%)	83 (57%)	34 (23%)	29 (20%)	0	4
11	AL	131/141 (93%)	66 (50%)	33 (25%)	32 (24%)	0	2
12	AM	113/145 (78%)	48 (42%)	26 (23%)	39 (34%)	0	0
13	AN	120/122 (98%)	60 (50%)	33 (28%)	27 (22%)	0	3
14	AO	82/164 (50%)	40 (49%)	17 (21%)	25 (30%)	0	1
15	AP	136/138 (99%)	50 (37%)	43 (32%)	43 (32%)	0	1
16	AQ	111/186 (60%)	41 (37%)	32 (29%)	38 (34%)	0	0
17	AR	50/66 (76%)	19 (38%)	17 (34%)	14 (28%)	0	1
18	AS	104/113 (92%)	70 (67%)	18 (17%)	16 (15%)	0	8
19	AT	74/84 (88%)	33 (45%)	17 (23%)	24 (32%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AU	108/119 (91%)	60 (56%)	25 (23%)	23 (21%)	0	4
21	AV	175/253 (69%)	69 (39%)	46 (26%)	60 (34%)	0	0
22	AW	62/70 (89%)	21 (34%)	25 (40%)	16 (26%)	0	2
23	AX	58/60 (97%)	29 (50%)	13 (22%)	16 (28%)	0	1
24	A0	103/118 (87%)	50 (48%)	33 (32%)	20 (19%)	0	5
25	A1	115/118 (98%)	48 (42%)	40 (35%)	27 (24%)	0	3
26	A2	98/100 (98%)	54 (55%)	18 (18%)	26 (26%)	0	2
27	A3	84/91 (92%)	32 (38%)	16 (19%)	36 (43%)	0	0
28	A4	71/73 (97%)	21 (30%)	19 (27%)	31 (44%)	0	0
29	A5	56/60 (93%)	25 (45%)	11 (20%)	20 (36%)	0	0
30	A6	51/82 (62%)	26 (51%)	8 (16%)	17 (33%)	0	0
31	A7	44/47 (94%)	14 (32%)	12 (27%)	18 (41%)	0	0
32	A8	61/64 (95%)	24 (39%)	16 (26%)	21 (34%)	0	0
33	A9	33/36 (92%)	19 (58%)	8 (24%)	6 (18%)	0	5
37	BE	232/256 (91%)	107 (46%)	58 (25%)	67 (29%)	0	1
38	BF	204/239 (85%)	113 (55%)	46 (22%)	45 (22%)	0	3
39	BG	206/209 (99%)	97 (47%)	63 (31%)	46 (22%)	0	3
40	BH	148/162 (91%)	90 (61%)	38 (26%)	20 (14%)	0	11
41	BI	99/101 (98%)	55 (56%)	24 (24%)	20 (20%)	0	4
42	BJ	153/156 (98%)	63 (41%)	49 (32%)	41 (27%)	0	2
43	BK	136/138 (99%)	67 (49%)	39 (29%)	30 (22%)	0	3
44	BL	125/128 (98%)	64 (51%)	27 (22%)	34 (27%)	0	1
45	BM	96/105 (91%)	54 (56%)	19 (20%)	23 (24%)	0	3
46	BN	117/129 (91%)	54 (46%)	33 (28%)	30 (26%)	0	2
47	BO	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	3
48	BP	123/126 (98%)	59 (48%)	30 (24%)	34 (28%)	0	1
49	BQ	58/61 (95%)	22 (38%)	10 (17%)	26 (45%)	0	0
50	BR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	6
51	BS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	5
52	BT	102/105 (97%)	62 (61%)	20 (20%)	20 (20%)	0	5
53	BU	71/88 (81%)	29 (41%)	24 (34%)	18 (25%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BV	78/93 (84%)	35 (45%)	17 (22%)	26 (33%)	0	0
55	BW	97/106 (92%)	27 (28%)	46 (47%)	24 (25%)	0	2
56	BX	22/27 (82%)	9 (41%)	5 (23%)	8 (36%)	0	0
All	All	5832/6739 (86%)	2857 (49%)	1467 (25%)	1508 (26%)	0	2

5 of 1508 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	ASN
3	AC	35	ALA
3	AC	54	SER
3	AC	68	LEU
3	AC	87	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	174/180 (97%)	144 (83%)	30 (17%)	3	21
4	AD	135/139 (97%)	90 (67%)	45 (33%)	0	3
5	AE	156/284 (55%)	114 (73%)	42 (27%)	1	6
6	AF	152/193 (79%)	121 (80%)	31 (20%)	2	13
7	AG	102/147 (69%)	74 (72%)	28 (28%)	0	6
8	AH	137/147 (93%)	99 (72%)	38 (28%)	0	6
9	AI	98/98 (100%)	89 (91%)	9 (9%)	13	54
9	AJ	98/98 (100%)	89 (91%)	9 (9%)	13	54
10	AK	119/119 (100%)	96 (81%)	23 (19%)	2	15
11	AL	108/113 (96%)	91 (84%)	17 (16%)	4	27
12	AM	95/121 (78%)	71 (75%)	24 (25%)	1	8
13	AN	101/101 (100%)	74 (73%)	27 (27%)	1	6
14	AO	67/126 (53%)	51 (76%)	16 (24%)	1	9
15	AP	110/110 (100%)	73 (66%)	37 (34%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AQ	89/149 (60%)	58 (65%)	31 (35%)	0	2
17	AR	44/52 (85%)	24 (54%)	20 (46%)	0	0
18	AS	88/92 (96%)	65 (74%)	23 (26%)	1	7
19	AT	67/73 (92%)	48 (72%)	19 (28%)	0	5
20	AU	97/105 (92%)	75 (77%)	22 (23%)	1	10
21	AV	151/203 (74%)	109 (72%)	42 (28%)	0	6
22	AW	51/56 (91%)	36 (71%)	15 (29%)	0	5
23	AX	52/52 (100%)	34 (65%)	18 (35%)	0	3
24	A0	89/101 (88%)	59 (66%)	30 (34%)	0	3
25	A1	96/97 (99%)	67 (70%)	29 (30%)	0	5
26	A2	79/79 (100%)	60 (76%)	19 (24%)	1	8
27	A3	64/67 (96%)	46 (72%)	18 (28%)	0	5
28	A4	66/66 (100%)	50 (76%)	16 (24%)	1	8
29	A5	51/53 (96%)	38 (74%)	13 (26%)	1	8
30	A6	46/69 (67%)	35 (76%)	11 (24%)	1	9
31	A7	39/40 (98%)	30 (77%)	9 (23%)	1	9
32	A8	50/51 (98%)	33 (66%)	17 (34%)	0	3
33	A9	34/35 (97%)	30 (88%)	4 (12%)	8	41
37	BE	202/220 (92%)	152 (75%)	50 (25%)	1	8
38	BF	160/188 (85%)	127 (79%)	33 (21%)	2	13
39	BG	180/181 (99%)	136 (76%)	44 (24%)	1	8
40	BH	115/123 (94%)	66 (57%)	49 (43%)	0	1
41	BI	90/90 (100%)	64 (71%)	26 (29%)	0	5
42	BJ	126/127 (99%)	106 (84%)	20 (16%)	4	26
43	BK	119/119 (100%)	73 (61%)	46 (39%)	0	1
44	BL	98/99 (99%)	81 (83%)	17 (17%)	3	21
45	BM	88/92 (96%)	70 (80%)	18 (20%)	2	13
46	BN	90/99 (91%)	70 (78%)	20 (22%)	1	11
47	BO	104/111 (94%)	85 (82%)	19 (18%)	2	18
48	BP	100/101 (99%)	80 (80%)	20 (20%)	2	14
49	BQ	49/50 (98%)	41 (84%)	8 (16%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	BR	79/80 (99%)	59 (75%)	20 (25%)	1	8
51	BS	72/74 (97%)	44 (61%)	28 (39%)	0	1
52	BT	96/97 (99%)	74 (77%)	22 (23%)	1	10
53	BU	64/77 (83%)	47 (73%)	17 (27%)	1	7
54	BV	71/80 (89%)	59 (83%)	12 (17%)	3	23
55	BW	76/82 (93%)	53 (70%)	23 (30%)	0	5
56	BX	19/22 (86%)	17 (90%)	2 (10%)	10	47
All	All	4903/5528 (89%)	3677 (75%)	1226 (25%)	1	8

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	AX	23	LEU
29	A5	31	THR
51	BS	27	LYS
24	A0	27	SER
25	A1	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
26	A2	79	GLN
31	A7	29	ASN
50	BR	62	GLN
27	A3	17	ASN
28	A4	32	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	122/123 (99%)	47 (38%)	5 (4%)
2	AA	2870/2915 (98%)	1226 (42%)	290 (10%)
34	BA	1515/1522 (99%)	452 (29%)	161 (10%)
35	BB	76/76 (100%)	34 (44%)	16 (21%)
35	BC	75/76 (98%)	31 (41%)	9 (12%)
36	B1	65/78 (83%)	24 (36%)	4 (6%)
All	All	4723/4790 (98%)	1814 (38%)	485 (10%)

5 of 1814 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	0	A
1	AB	1	U
1	AB	2	C
1	AB	3	C
1	AB	9	G

5 of 485 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	1992	G
2	AA	2542	A
34	BA	1498	U
2	AA	2035	G
2	AA	2320	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	AB	123/123 (100%)	-0.51	0 100 100	308, 357, 402, 412	0
2	AA	2872/2915 (98%)	-0.54	22 (0%) 83 72	232, 307, 404, 474	0
3	AC	221/228 (96%)	0.62	26 (11%) 5 12	384, 428, 464, 467	0
4	AD	173/178 (97%)	1.52	68 (39%) 1 3	243, 279, 292, 298	0
5	AE	191/338 (56%)	0.89	36 (18%) 2 6	258, 311, 397, 403	0
6	AF	189/246 (76%)	0.30	8 (4%) 35 33	233, 399, 427, 434	0
7	AG	122/176 (69%)	0.35	5 (4%) 35 34	350, 366, 443, 447	0
8	AH	164/177 (92%)	0.10	9 (5%) 24 27	320, 351, 366, 370	0
9	AI	128/128 (100%)	1.39	33 (25%) 1 4	580, 591, 602, 603	0
9	AJ	128/128 (100%)	1.97	45 (35%) 1 3	569, 582, 594, 596	0
10	AK	148/149 (99%)	0.60	11 (7%) 14 21	305, 329, 353, 361	0
11	AL	133/141 (94%)	0.58	19 (14%) 3 9	455, 504, 541, 543	0
12	AM	117/145 (80%)	0.74	15 (12%) 4 11	286, 310, 364, 368	0
13	AN	122/122 (100%)	0.98	18 (14%) 3 8	245, 262, 277, 293	0
14	AO	84/164 (51%)	1.04	19 (22%) 1 5	330, 452, 471, 473	0
15	AP	138/138 (100%)	1.15	27 (19%) 2 5	283, 324, 364, 379	0
16	AQ	113/186 (60%)	-0.26	0 100 100	317, 367, 386, 390	0
17	AR	52/66 (78%)	1.78	20 (38%) 1 3	251, 267, 285, 288	0
18	AS	108/113 (95%)	0.84	12 (11%) 6 13	280, 311, 324, 332	0
19	AT	76/84 (90%)	0.31	6 (7%) 13 19	329, 344, 360, 363	0
20	AU	110/119 (92%)	0.15	8 (7%) 15 21	647, 661, 722, 724	0
21	AV	177/253 (69%)	0.45	12 (6%) 17 23	295, 365, 416, 424	0
22	AW	64/70 (91%)	1.11	16 (25%) 1 4	346, 364, 373, 375	0
23	AX	60/60 (100%)	0.32	3 (5%) 28 29	291, 306, 315, 316	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
24	A0	105/118 (88%)	0.44	8 (7%)	14 20	263, 281, 304, 308	0
25	A1	117/118 (99%)	0.01	2 (1%)	67 56	267, 297, 311, 317	0
26	A2	100/100 (100%)	1.29	29 (29%)	1 4	416, 430, 462, 470	0
27	A3	86/91 (94%)	1.23	14 (16%)	2 7	359, 389, 475, 486	0
28	A4	73/73 (100%)	1.19	18 (24%)	1 4	319, 354, 373, 378	0
29	A5	58/60 (96%)	0.73	11 (18%)	2 5	259, 314, 361, 373	0
30	A6	53/82 (64%)	0.97	13 (24%)	1 4	287, 316, 332, 340	0
31	A7	46/47 (97%)	1.02	12 (26%)	1 4	316, 339, 352, 357	0
32	A8	63/64 (98%)	0.62	8 (12%)	4 11	262, 282, 294, 306	0
33	A9	35/36 (97%)	0.03	1 (2%)	49 43	281, 303, 316, 319	0
34	BA	1515/1522 (99%)	-0.54	9 (0%)	86 77	251, 312, 419, 609	0
35	BB	76/76 (100%)	10.13	65 (85%)	0 2	631, 651, 667, 669	0
35	BC	76/76 (100%)	-0.82	0 100	100	273, 310, 328, 337	0
36	B1	66/78 (84%)	8.26	47 (71%)	0 2	337, 829, 918, 922	0
37	BE	234/256 (91%)	0.66	27 (11%)	5 12	293, 321, 364, 385	0
38	BF	206/239 (86%)	1.39	56 (27%)	1 4	301, 349, 377, 382	0
39	BG	208/209 (99%)	0.76	28 (13%)	4 10	276, 299, 318, 329	0
40	BH	150/162 (92%)	1.37	46 (30%)	1 4	277, 295, 315, 324	0
41	BI	101/101 (100%)	1.99	39 (38%)	1 3	299, 318, 330, 336	0
42	BJ	155/156 (99%)	0.68	18 (11%)	5 12	326, 357, 370, 373	0
43	BK	138/138 (100%)	0.96	23 (16%)	2 7	266, 284, 297, 306	0
44	BL	127/128 (99%)	0.00	0 100	100	385, 487, 499, 500	0
45	BM	98/105 (93%)	1.03	15 (15%)	3 8	337, 394, 423, 424	0
46	BN	119/129 (92%)	1.14	25 (21%)	1 5	288, 307, 330, 334	0
47	BO	124/135 (91%)	1.00	25 (20%)	2 5	265, 282, 319, 328	0
48	BP	125/126 (99%)	-0.20	1 (0%)	83 72	350, 370, 412, 415	0
49	BQ	60/61 (98%)	0.49	8 (13%)	4 10	322, 352, 360, 365	0
50	BR	88/89 (98%)	0.30	5 (5%)	23 26	277, 288, 315, 318	0
51	BS	83/88 (94%)	0.30	6 (7%)	15 21	271, 284, 303, 316	0
52	BT	104/105 (99%)	0.24	2 (1%)	64 53	249, 268, 323, 344	0
53	BU	73/88 (82%)	1.07	18 (24%)	1 4	259, 296, 323, 348	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	BV	80/93 (86%)	0.48	9 (11%) 6 13	353, 369, 395, 399	0
55	BW	99/106 (93%)	-0.04	4 (4%) 36 35	264, 281, 292, 300	0
56	BX	24/27 (88%)	-0.63	0 100 100	475, 489, 493, 496	0
All	All	10678/11529 (92%)	0.30	1030 (9%) 8 16	232, 322, 533, 922	0

The worst 5 of 1030 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BB	4	G	29.8
35	BB	71	G	27.2
36	B1	32	G	26.9
36	B1	22	C	26.7
35	BB	3	G	26.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.