



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:44 PM BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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

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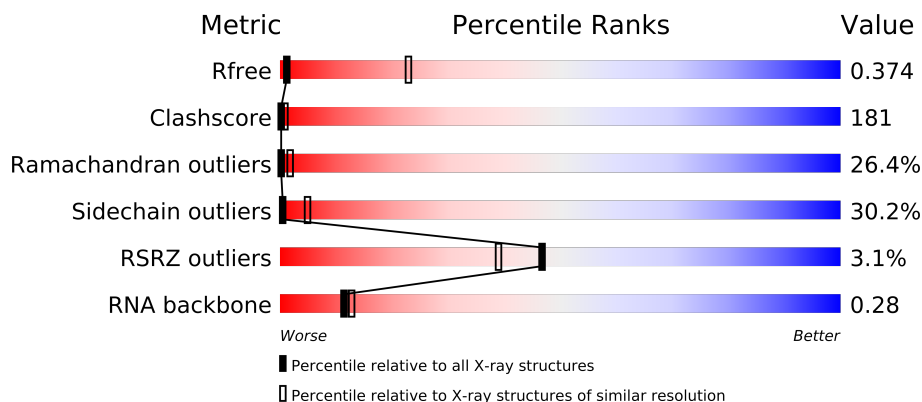
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.51 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	1029 (5.50-3.50)
Clashscore	79885	1300 (5.50-3.50)
Ramachandran outliers	78287	1222 (5.50-3.50)
Sidechain outliers	78261	1203 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)
RNA backbone	1838	1031 (6.22-2.80)

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  $\geq 3$ , 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	AA	1522	
2	AC	76	
3	AD	76	
4	A1	27	
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	
9	AI	101	
10	AJ	156	
11	AK	138	
12	AL	128	

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Mol	Chain	Length	Quality of chain
13	AM	105	
14	AN	129	
15	AO	132	
16	AP	126	
17	AQ	61	
18	AR	89	
19	AS	88	
20	AT	105	
21	AU	88	
22	AV	93	
23	AW	106	
24	AX	27	
25	BA	2916	
26	BB	123	
27	BC	229	
28	BD	276	
29	BE	206	
30	BF	210	
31	BG	182	
32	BH	180	
33	BK	148	
34	BL	147	
35	BM	140	
36	BN	122	
37	BO	150	
38	BP	141	
39	BQ	118	
40	BR	112	
41	BS	146	
42	BT	118	
43	BU	101	
44	BV	113	
45	BW	96	
46	BX	110	
47	BY	206	
48	BZ	85	
49	B1	67	
50	B2	60	
51	B3	71	
52	B4	60	
53	B5	54	
54	B6	49	

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Mol	Chain	Length	Quality of chain
55	B7	65	<div><div></div></div>
56	B8	37	<div><div></div></div>

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 149640 atoms, of which 0 are 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 16S rRNA.

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

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

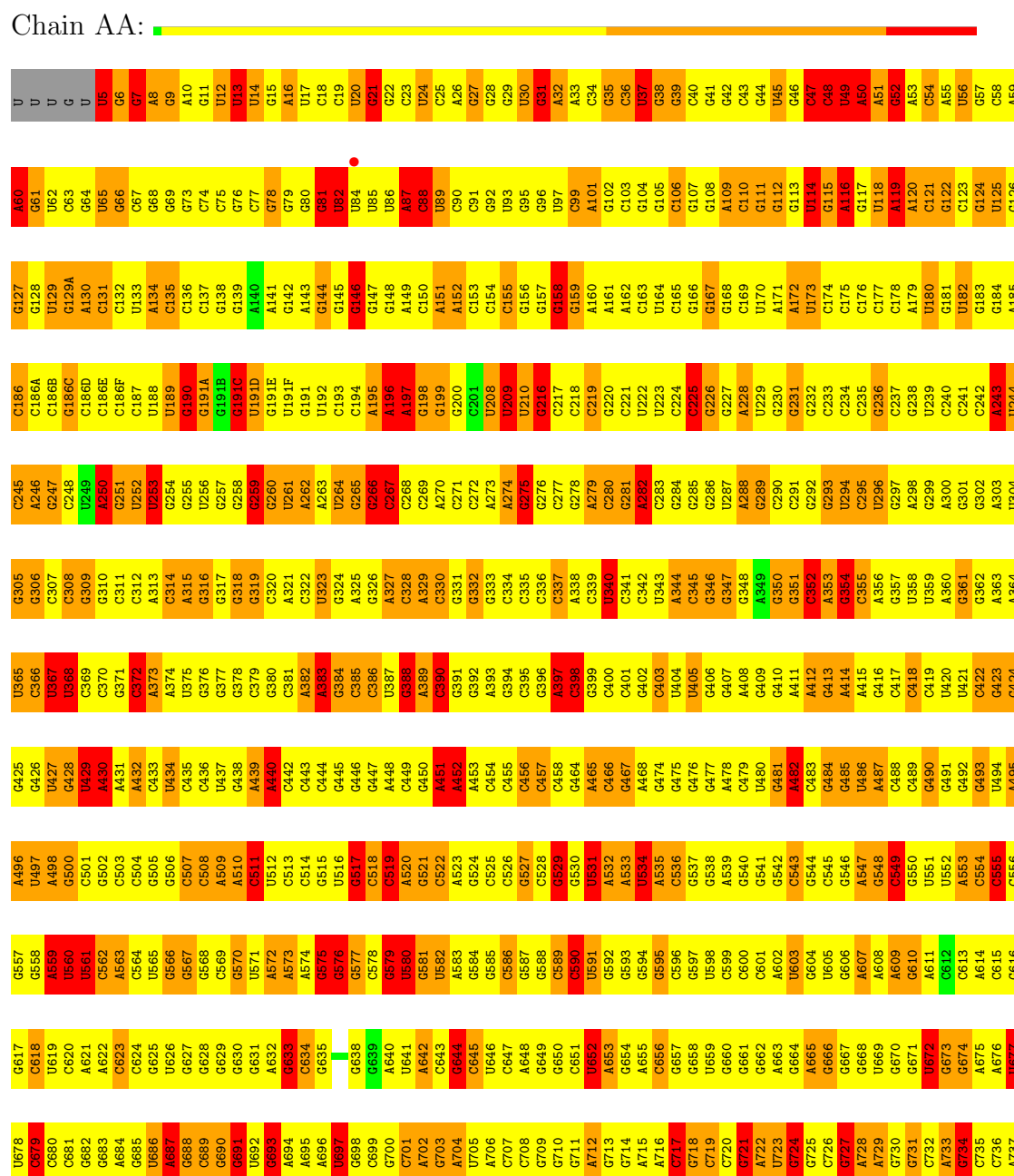
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

### 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: 16S rRNA



C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C29	C30	C31	C32	C33	C34	C35	C36	C37	C38	C39	C40	C41	C42	C43	C44	C45	C46	C47	C48	C49	C50	C51	C52	C53	C54	C55	C56	C57	C58	C59	C60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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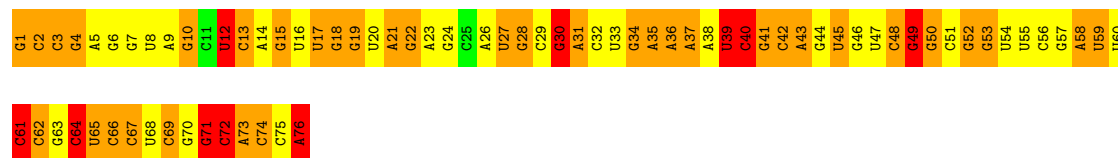
• Molecule 2: tRNA fMET (unmodified bases)

Chain AC:



• Molecule 3: tRNA PHE (unmodified bases)

Chain AD:



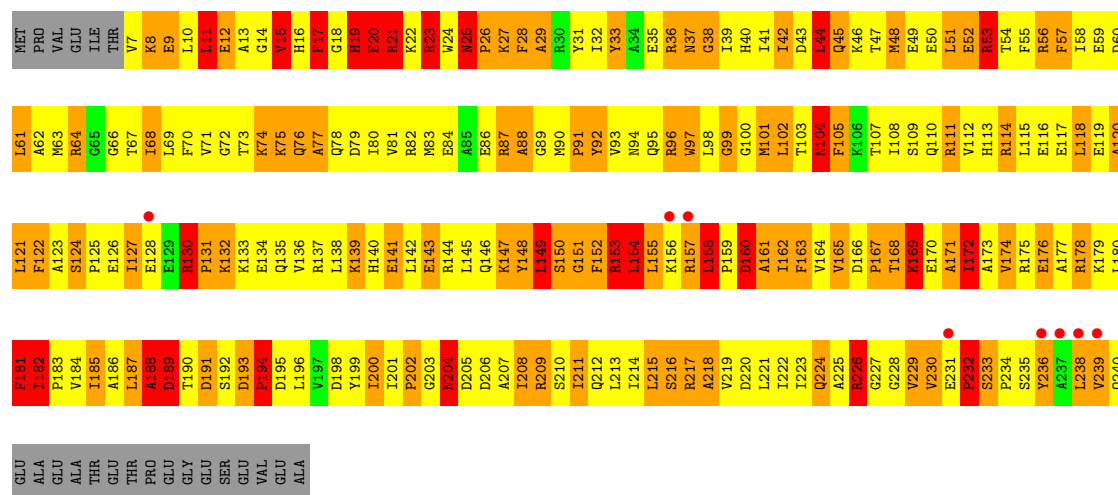
• Molecule 4: mRNA

Chain A1:



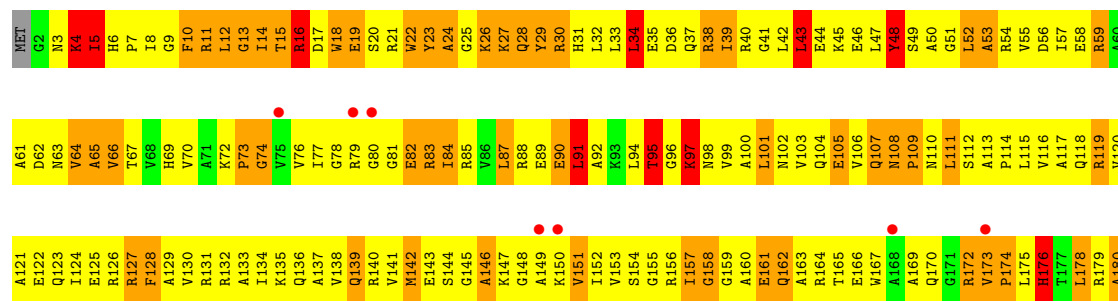
• Molecule 5: 30S ribosomal protein S2

Chain AE:

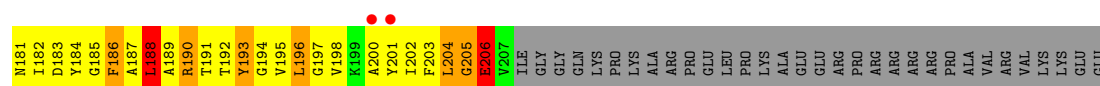


• Molecule 6: 30S ribosomal protein S3

Chain AF:







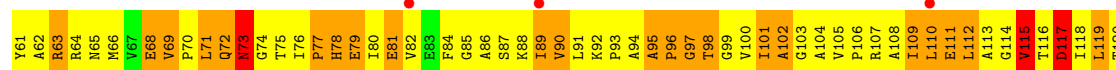
• Molecule 7: 30S ribosomal protein S4

Chain AG:



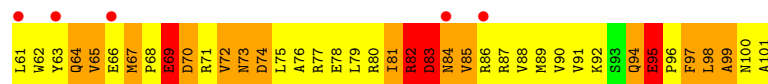
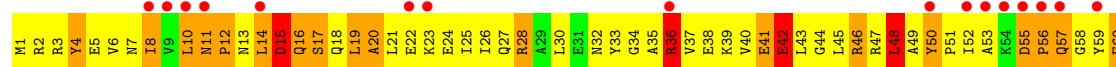
• Molecule 8: 30S ribosomal protein S5

Chain AH:



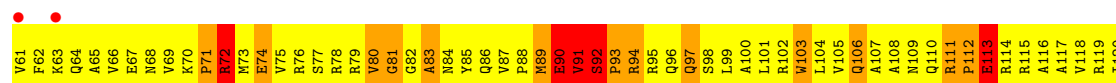
• Molecule 9: 30S ribosomal protein S6

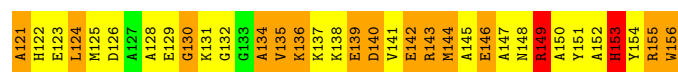
Chain AI:



• Molecule 10: 30S ribosomal protein S7

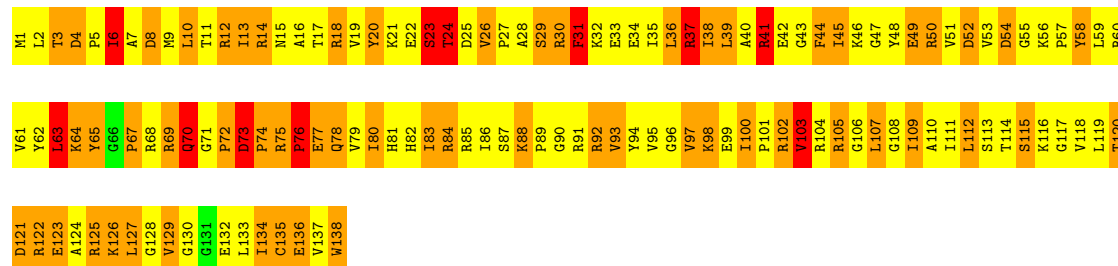
Chain AJ:





• Molecule 11: 30S ribosomal protein S8

Chain AK:



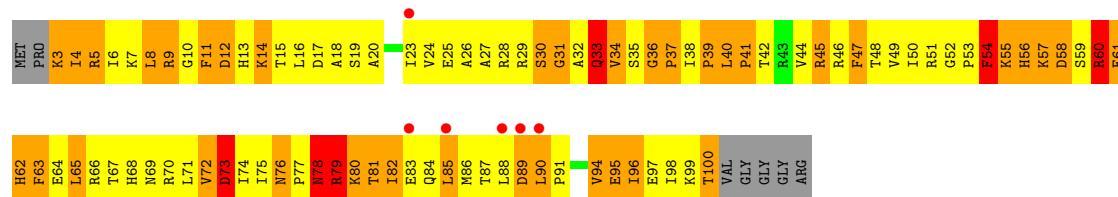
• Molecule 12: 30S ribosomal protein S9

Chain AL:



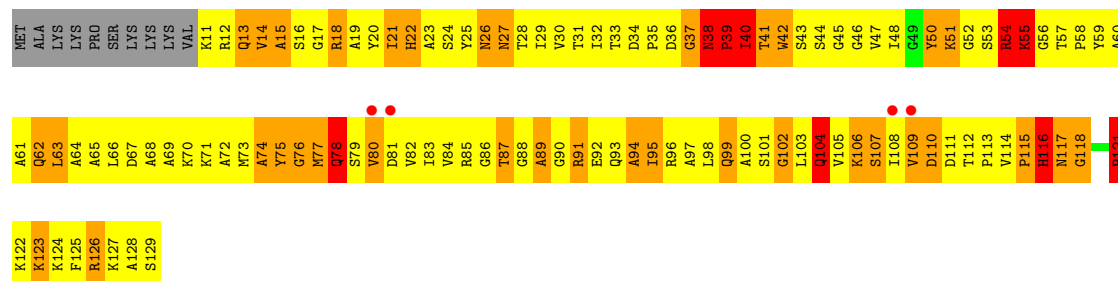
• Molecule 13: 30S ribosomal protein S10

Chain AM:



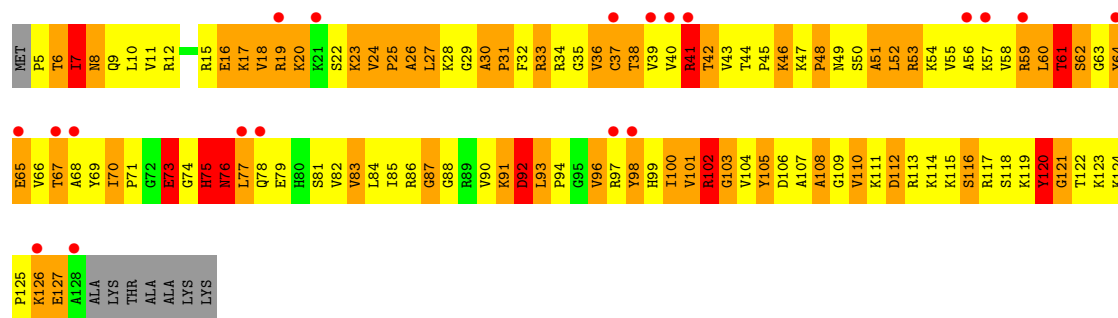
• Molecule 14: 30S ribosomal protein S11

Chain AN:



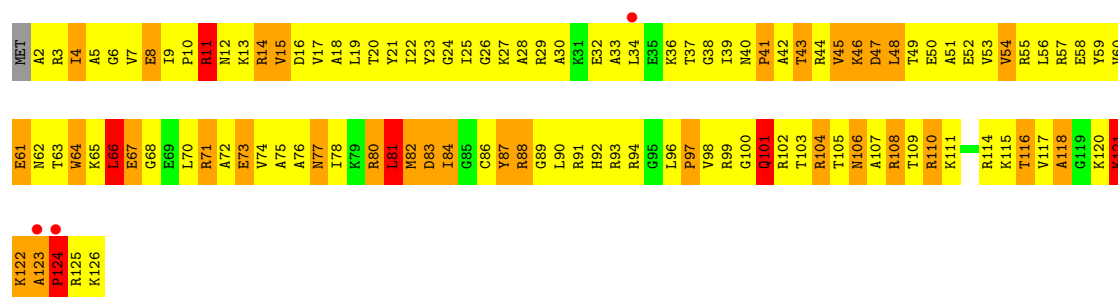
• Molecule 15: 30S ribosomal protein S12

Chain AO:



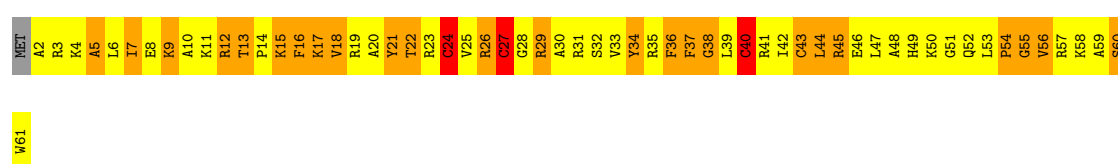
- Molecule 16: 30S ribosomal protein S13

Chain AP:



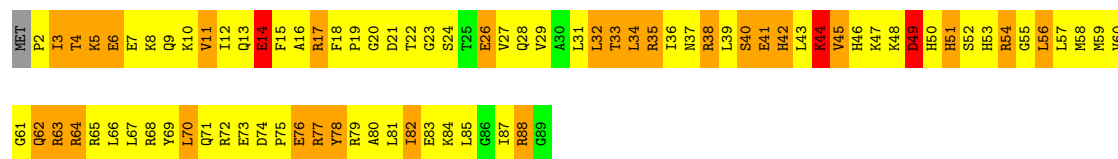
- Molecule 17: 30S ribosomal protein S14

Chain AQ:



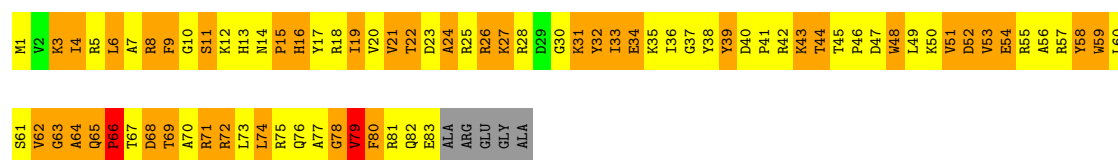
- Molecule 18: 30S ribosomal protein S15

Chain AR:



- Molecule 19: 30S ribosomal protein S16

Chain AS:



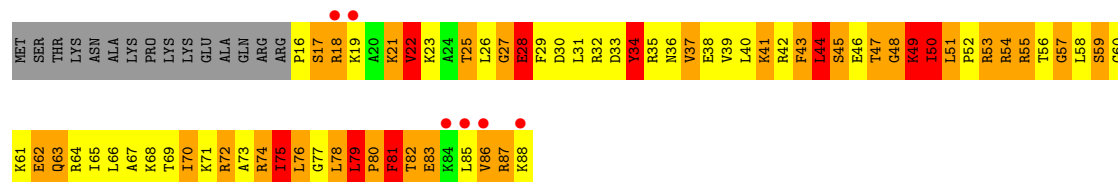
- Molecule 20: 30S ribosomal protein S17

Chain AT:



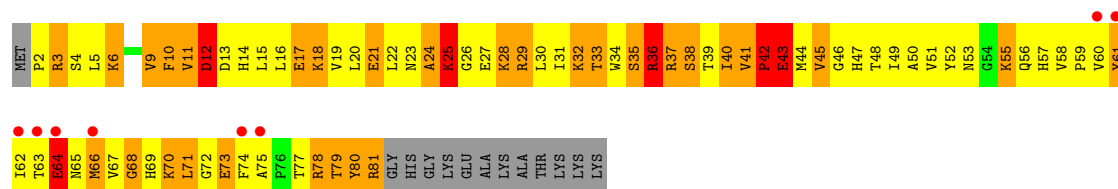
- Molecule 21: 30S ribosomal protein S18

Chain AU:



- Molecule 22: 30S ribosomal protein S19

Chain AV:



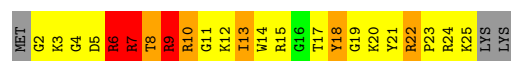
- Molecule 23: 30S ribosomal protein S20

Chain AW:



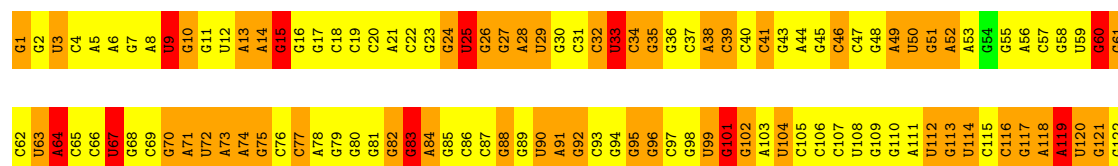
- Molecule 24: 30S ribosomal protein Thx

Chain AX:



- Molecule 25: 23S rRNA

Chain BA:



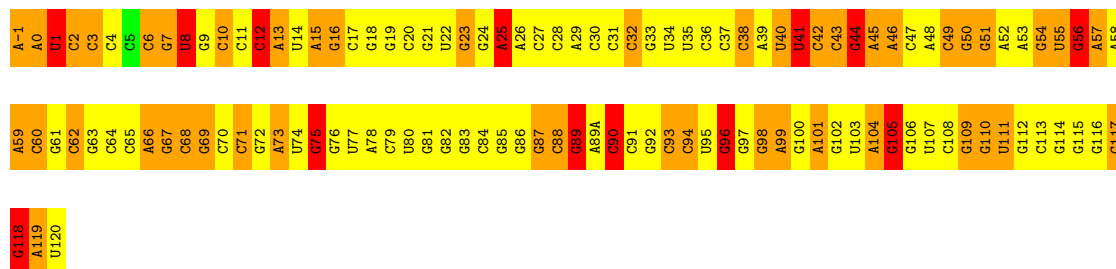
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G975	C915	G854	G794	A734	G674	G636	A578	C516	C455	G395	G338	A278	C253	U193	G124
G976	C916	G855	G795	A735	A675	A637	G579	C517	C456	G396	G339	C279	G254	G194	G125
G977	A917	C856	C796	A736	A676	G638	C580	C518	A457	G397	A340	C280	A255	A195	A126
G978	G918	C857	G797	C737	A677	G639	C581	C519	G458	G398	G341	G281	A256	A196	A127
G979	G919	G858	G798	G738	C678	G640	G582	C520	U459	G399	G342	A282	A257	A197	C128
A980	G920	G859	G799	G739	C679	G641	G583	G521	A460	G400	C343	A283	G258	C198	C129
A981	G921	U860	A800	U740	G680	G642	C584	G522	C461	A401	G344	U284	G259	A199	G130
C982	G922	A861	G801	G741	G681	A643	G585	C523	C462	A402	A345	G285	G260	U200	G131
A983	C923	G862	A802	G742	G682	A644	A586	C524	U463	U403	A346	C286	G261	C201	G132
A984	C924	A863	U803	G743	C683	C645	C587	C525	U464	C404	A347	C287	A262	U202	C133
C985	C925	G864	A804	G744	G684	A646	U588	A526	G465	U405	G348	C288	C263	C203	G134
A986	A926	C865	G805	G745	A685	G647	C589	C527	A466	G406	G349	A289	C264	A204	G135
G987	G928	A866	C806	A746	C686	G648	A590	A528	G467	G407	U350	G290	A265	G205	G136
A988	G929	C867	U807	U747	C687	G649	C591	A529	G468	G408	G351	C291	G266	U206	C137
C989	U930	U868	G808	U748	U688	C	C592	C530	G469	C409	G352	C292	G267	A207	G137A
A990	G931	G869	G809	C749	A689	G	U593	C531	U470	C410	G353	U293	C268	C208	G138
C991	G932	A870	U810	A750	G690	C	U594	A532	A471	G411	G354	A294	U269	C209	G139
C992	A933	U871	C691	A751	C691	A	C595	G533	A472	A412	G355	G295	A270	C210	A140
G993	G934	A872	C692	A752	C692	A	C596	U534	G473	C413	G356	C296	A270A	A211	A141
C994	C935	G873	U813	C753	C693	G	U597	C535	C474	C414	A357	C297	A270B	G212	C141A
C995	C936	G874	C814	C754	U694	C	C598	A536	U475	A415	U358	G298	C270C	A213	G142
A996	U937	G875	C815	C755	G695	C	C599	C537	A476	C416	A359	A299	C270D	G214	C143
G997	G938	C876	C816	C756	G696	G	G600	C539	A477	C417	G360	A300	C270E	G215	C144
C998	G939	U877	C817	U757	C697	G	C601	C540	A478	G418	G361	G301	U270F	A216	G145
U999	G940	A878	G818	C758	C698	C	G602	C541	A479	G	U362	C302	C270G	G217	G146
A1000	A941	G879	A819	G759	A699	C	A603	C542	A480	C419	G363	U303	C270H	A218	U147
A1001	G942	G880	A820	G760	G700	G	G604	C543	G481	C420	A363A	G304	C270I	G219	C148
G1002	U943	G881	A821	A761	C701	C	C605	C544	A482	U421	G363B	U305	G270J	G220	A149
G1003	G944	G882	U822	U762	G702	A	U606	C545	A483	A422	G363C	U306	C270K	A221	C150
A945	A945	G883	G823	G763	U703	C	U607	C546	C484	A423	G363D	G307	U270L	C151	C151
G946	G946	C884	A824	A764	G704	C	A608	A547	C485	G424	U363E	G308	U270M	A223	G152
C1006	G947	C885	C825	G765	A705	C	A609	A548	C486	G425	A363F	G309	G270N	G224	C153
C1007	C948	C886	U826	C766	A706	G	G609A	C549	G488	U427	C364	A310	U270O	A225	G154
C1008	G949	A887	U827	U767	G707	G	C610	C550	G489	U428	C365	A311	C270P	G226	C155
A1009	G950	C888	U828	G768	C708	C	C611	C551	G490	A429	C366	G312	C270Q	A227	U161
C951	C951	C889	A829	G769	U709	C	G612	C552	G491	A429	G370	C313	G270R	A228	U162
G952	G952	G890	G830	G770	G710	G	U613	U553	A492	G430	A371	C314	G270S	A229	U163
A953	C953	G891	G831	G771	G711	G651	U614	U554	G493	U431	G372	G315	G270T	U230	U164
C1012	C1012	C892	G832	C772	G712	C652	C615	C556	G494	A432	U373	C316	C270U	C231	G171
U1014	U1014	C893	U833	U773	G713	A653	A616	U557	G495	C433	A374	G317	G270V	G232	C172
G1015	G1015	U895	C834	A774	U714	A654	G617	C558	G496	U434	C375	C318	G270W	A233	G173
U1019	U1019	A896	A835	G775	G715	A655	G618	C559	A497	C435	C376	C319	G270X	C234	C174
A1020	A1020	C897	G836	C776	A716	G656	C618A	C560	G498	C436	C377	A320	G270Y	U235	G175
A959	A959	C898	C837	A777	G717	U657	G619	C561	U499	G438	C378	G321	U270Z	C236	G176
A1021	A960	A899	C838	G778	A718	C658	G620	U562	G500	G439	G379	A322	C271A	C237	G177
G1022	C961	A900	U839	U779	C719	C659	A621	C563	A501	G440	U380	G323	G271B	C238	G178
U1023	G962	A901	C940	G780	C720	G660	G622	C564	A502	U441	G381	A324	U271C	U239	G179
G1024	U963	C902	A841	A781	G721	C661	G623	C565	A503	G442	G382	G325	G271	G240	G180
U1025	C964	C903	G942	A782	A722	G662	C624	U566	U504	A443	U383	G326	G272	A241	A181
U1026	C965	C904	G943	A783	G723	G663	G625	A567	A505	C444	U384	G327	G273	G242	A182
A1027	G966	U905	A844	A784	U724	C664	U626	U568	G506	C445	C385	U328	G273A	U243	C183
C967	C967	G906	G945	G785	G725	C665	A627	U569	A507	G446	G386	A329	C273B	A244	C184
A1029	G968	U907	C946	C786	G726	C666	G628	C570	G508	A447	U387	A330	C273C	G245	U185
G1030	U969	C908	U847	U787	A727	U667	G629	A571	C509	U448	G388	A331	C273D	C246	G186
G1031	G1031	A909	G948	A788	G728	G668	G630	A572	C510	A449	G389	A332	U273E	G247	G187
A1032	C971	A910	A849	A789	G729	G669	A631	C573	U511	G450	A390	G333	C273F	G248	G188
U1033	G972	A911	C850	C790	C730	A670	A632	C574	G512	C451	G391	C334	G274	C249	A189
G1034	A973	C912	U851	A633	C731	C671	A633	C575	A513	G452	C392	C335	G275	G250	A190
U1035	G974	U913	G852	C792	C732	C672	C634	U576	A514	C453	C393	C336	A276	A251	A191

A1900	G1831	G1771	G1685	G1635	U1516	G1455	U1396	A1336	A1276	G1216	A1155	A1096	G1036
A1901	C1832	G1772	G1696	C1636	G1517	G1456	U1397	G1337	G1277	C1217	A1156	U1097	G1037
G1902	U1833	A1773	G1697	U1637	C1518	A1457	C1398	G1338	A1278	C1218	A1157	A1098	C1038
G1903	U1834	G1774	A1698	C1638	G1519	A1458	C1399	G1339	G1279	G1219	C1158	G1099	G1039
G1904	G1835	U1775	G1699	U1639	U1520	G1459	G1400	U1340	G1280	A1220	U1100	C1100	C1040
G1905	C1836	G1776	A1700	C1640	G1521	A1460	G1401	U1341	G1281	C1221	G1160	U1101	C1041
G1906	C1837	U1777	A1701	G1581	G1522	G1461	G1402	A1342	U1282	C1222	C1161	C1102	G1042
G1907	C1838	U1778	G1702	C1582	U1523	G1462	C1403	G1343	G1283	C1223	G1162	A1103	G1043
G1908	G1839	G1779	G1703	A1583	G1524	G1463	C1404	G1344	A1284	G1224	G1163	C1104	G1044
G1909	A1780	G1704	G1705	C1585	G1525	G1464	U1405	C1345	G1285	C1225	G1164	U1105	A1045
G1910	G1781	G1705	G1706	A1586	G1526	G1465	U1406	G1346	A1286	G1226	U1165	A1046	A1046
U1911	G1842	C1782	U1708	C1646	G1527	G1466	G1407	G1347	A1287	G1227	G1166	G1107	G1047
A1912	C1843	G1783	G1707	G1647	A1528	G1467	U1408	G1348	U1288	G1228	U1167	U1108	A1048
A1913	C1844	A1783	C1708	C1648	A1529	C1468	C1409	A1349	C1289	G1229	G1168	C1109	C1049
G1914	G1845	U1785	U1709	G1649	A1530	A1469	G1410	C1350	C1290	G1230	G1169	G1110	A1050
U1915	G1846	G1786	G1710	G1650	C1531	G1470	G1411	C1351	C1291	G1231	G1170	A1111	G1051
A1916	A1847	A1787	C1711	C1651	C1532	A1471	A1412	U1352	U1292	G1232	G1171	U1112	C1052
U1917	G1848	G1788	C1712	G1652	C1533	A1472	G1413	A1353	C1293	C1233	G1173	U1113	C1053
A1918	G1849	U1789	U1716	G1653	G1534	G1473	G1414	A1354	U1294	U1234	A1174	A1114	A1054
U1919	G1850	C1790	G1717	U1654	U1535	C1474	U1415	G1355	C1295	G1235	U1175	G1115	G1055
C1920	U1851	A1791	A1655	A1596	U1536	G1475	G1416	G1356	C1296	G1236	G1176	C1116	G1056
G1921	C1852	G1792	G1725	A1597	C1537	G1476	G1417	U1357	C1297	G1237	A1177	G1117	A1057
G1922	A1853	C1793	G1726	C1657	G1538	A1477	G1418	G1358	C1298	G1238	C1178	C1118	G1058
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C1924	G1855	G1795	U1728	C1659	G1540	G1479	U1420	A1360	U1300	U1240	C1180	G1120	U1060
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A1927	G1858	U1798	G1731	C1662	A1543	G1483	G1423	C1363	G1303	G1243	C1183	C1123	G1063
A1928	A1859	G1799	A1732	C1663	C1544	G1484	G1424	G1364	C1304	G1244	A1184	C1124	C1064
G1929	G1860	G1733	A1733	A1664	A1545	G1485	G1425	A1365	C1305	G1245	C1185	G1125	U1065
G1930	G1861	G1801	C1734	A1665	A1545A	A1486	G1426	A1366	C1306	U1246	G1186	A1126	U1066
A1931	G1862	A1802	G1735	G1666	C1546	G1487	A1427	A1367	A1307	A1247	G1187	A1127	U1067
A1932	G1863	A1803	C1741	G1667	C1547	G1488	G1428	G1368	A1308	G1248	U1188	A1128	G1068
G1933	U1864	C1804	G1742	A1668	C1548	U1489	G1429	G1369	A1189	U1249	A1190	A1129	A1069
C1934	G1869	U1805	G1743	A1669	C1549	A1490	G1430	C1370	G1310	G1250	U1190	U1130	A1070
G1935	C1870	C1806	G1746	C1670	C1550	G1491	U1431	G1371	G1311	C1251	G1191	G1131	G1071
A1936	A1871	G1807	G1747	U1671	C1551	G1492	G1432	U1372	U1312	G1252	G1192	A1132	C1072
A1937	A1872	U1808	G1748	C1672	G1552	G1493	U1433	A1373	U1313	A1253	G1193	U1133	A1073
A1938	G1878	A1809	A1749	G1673	A1553	A1494	A1434	G1374	C1314	U1254	G1194	C1134	G1074
U1939	C1879	G1810	G1750	U1674	A1554	A1495	G1435	C1375	C1315	U1255	G1195	C1135	C1075
U1940	C1880	G1811	C1751	C1675	G1555	A1496	G1436	C1376	U1316	G1256	G1196	G1136	C1076
C1941	C1881	A1812	A1676	A1676	C1556	U1497	G1437	G1377	A1317	C1257	G1197	G1137	A1077
U1942	C1882	G1813	G1753	G1677	A1558	G1498	U1438	A1378	C1198	G1258	U1198	G1138	U1078
U1943	G1883	G1814	C1754	G1678	A1559	C1499	U1439	A1379	U1199	G1259	U1199	C1139	C1079
U1944	A1884	A1815	U1755	U1679	G1559	G1500	G1440	G1380	C1320	G1260	C1200	C1140	C1080
G1945	A1885	G1816	G1756	G1680	U1560	C1501	G1441	G1381	A1321	C1261	C1201	U1141	U1081
U1946	C1886	G1817	U1757	G1681	G1561	C1502	G1442	C1382	A1322	A1262	C1202	U1142	U1082
C1947	C1887	G1818	G1758	G1682	A1562	U1503	G1443	C1383	G1323	U1263	G1203	A1142A	U1083
G1948	G1888	A1819	C1683	G1683	G1563	C1504	G1444	A1384	G1324	G1264	A1204	A1143	A1084
U1949	A1889	U1820	C1684	C1625	C1564	C1505	G1445	G1385	U1325	G1265	U1205	G1144	A1085
G1950	A1890	A1821	C1685	G1626	C1565	C1506	C1446	C1386	U1326	G1266	G1206	C1145	A1086
U1951	G1891	G1822	C1686	G1627	A1566	A1507	G1447	C1387	C1327	U1267	C1207	C1146	G1087
A1952	C1892	G1823	G1763	G1628	A1567	C1508	G1448	G1388	U1328	A1268	C1208	G1147	A1088
A1953	C1893	G1824	U1688	U1629	G1568	C1509	G1449	G1389	U1329	A1269	G1209	A1148	G1089
G1954	C1894	A1825	G1765	G1630	A1569	A1510	A1449	U1390	G1330	G1270	A1210	U1090	U1090
U1955	C1895	G1826	U1766	C1630A	A1570	A1511	G1449A	U1391	U1331	C1271	U1211	C1150	G1091
U1956	G1896	C1827	C1767	A1631	A1571	G1512	C1450	A1392	G1332	A1272	G1212	G1151	C1092
C1957	G1897	G1828	U1768	A1632	A1572	C1513	C1451	A1393	C1333	U1273	A1213	C1152	G1093
G1958	U1898	A1829	G1769	G1633	G1573	U1514	A1453	U1394	G1334	A1274	A1214	C1153	U1094
G1959	C1899	C1830	G1770	C1694	C1574	C1515	U1454	A1395	U1335	A1275	G1215	G1154	A1095



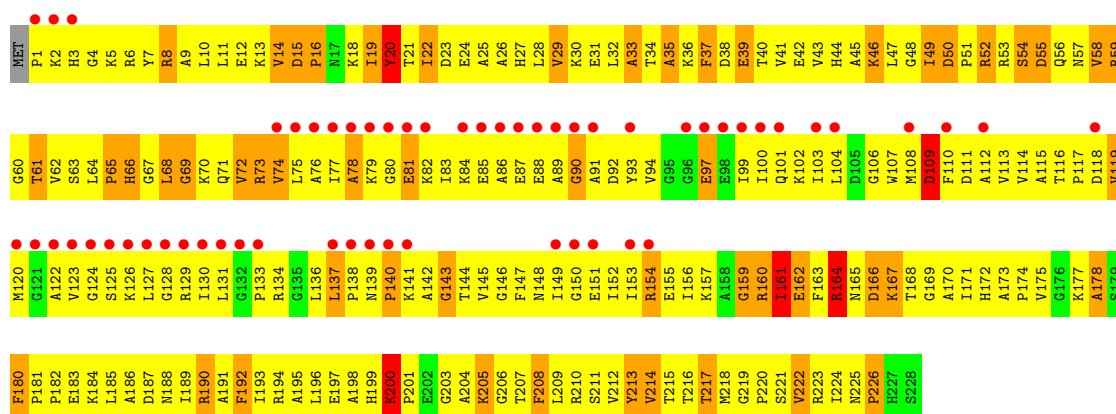
- Molecule 26: 5S rRNA

Chain BB:



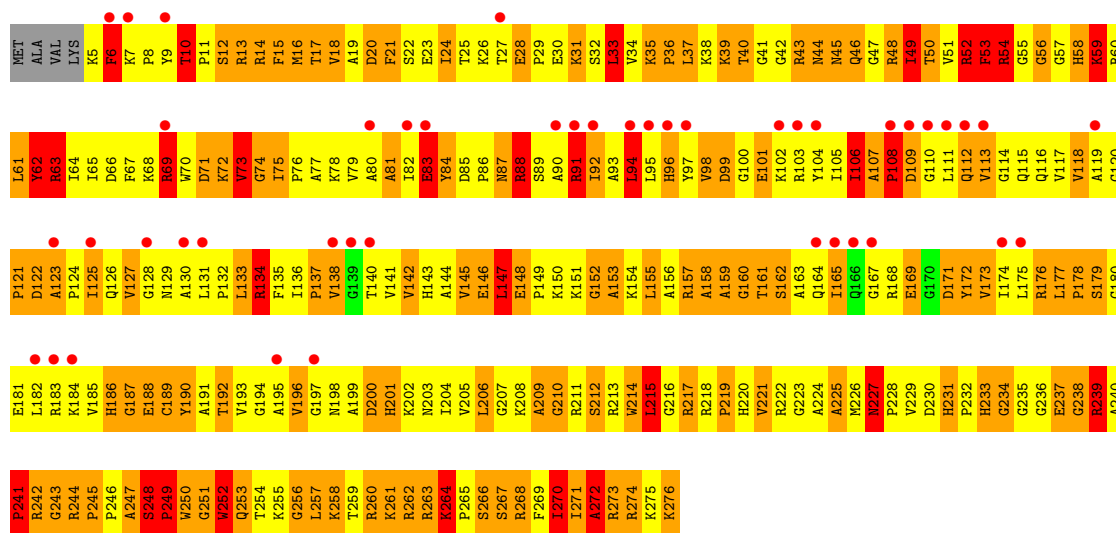
- Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain BC:



- Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD:

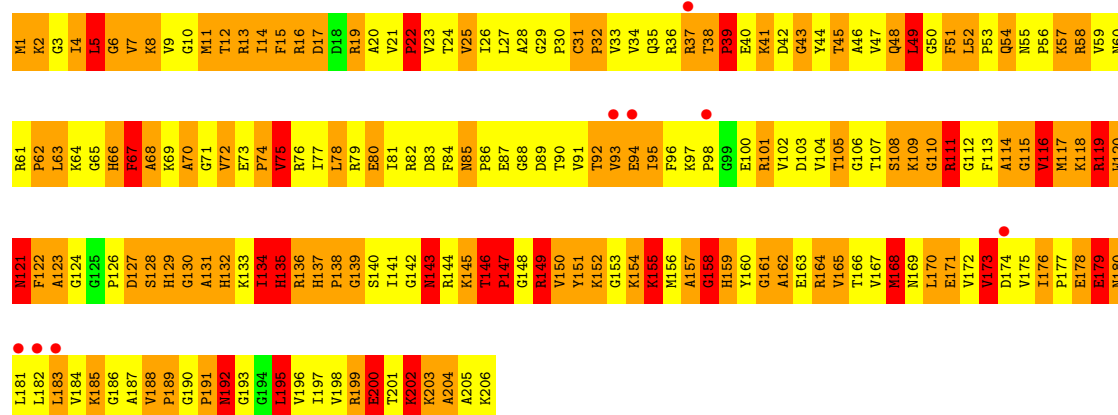


- Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE:

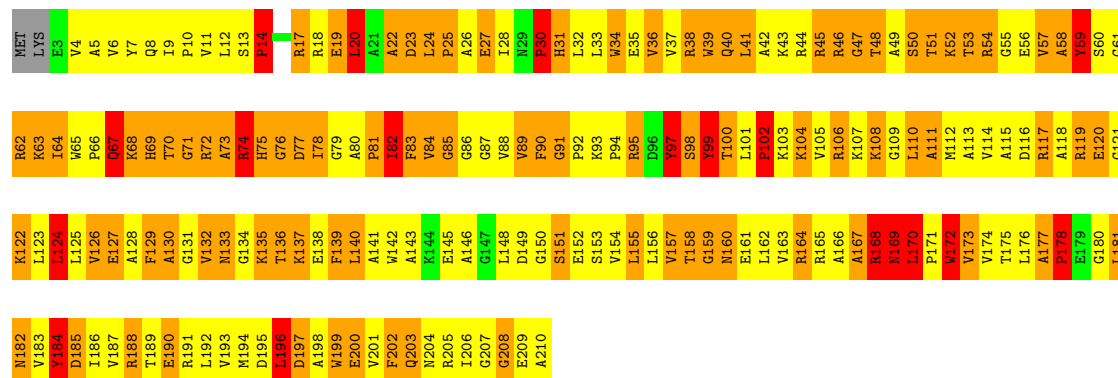






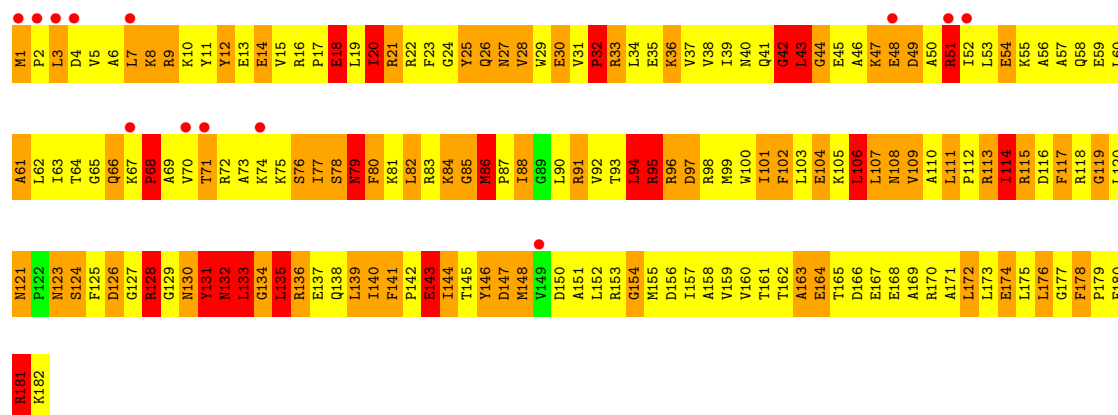
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF:



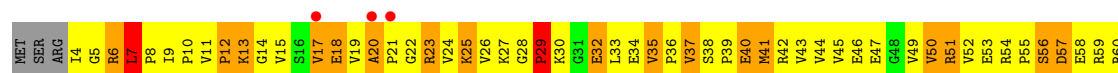
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

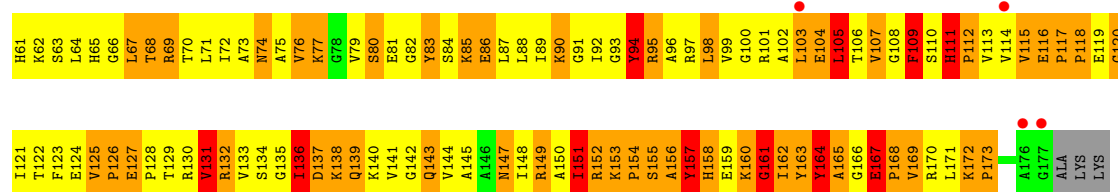
Chain BG:



• Molecule 32: 50S RIBOSOMAL PROTEIN L6

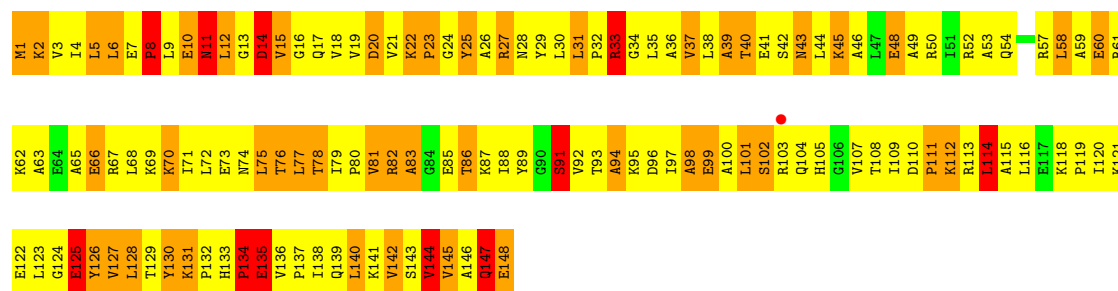
Chain BH:





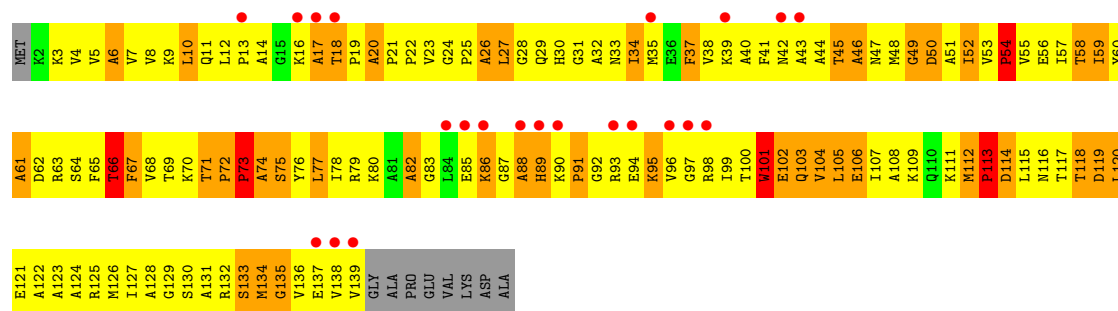
• Molecule 33: 50S RIBOSOMAL PROTEIN L9

Chain BK:



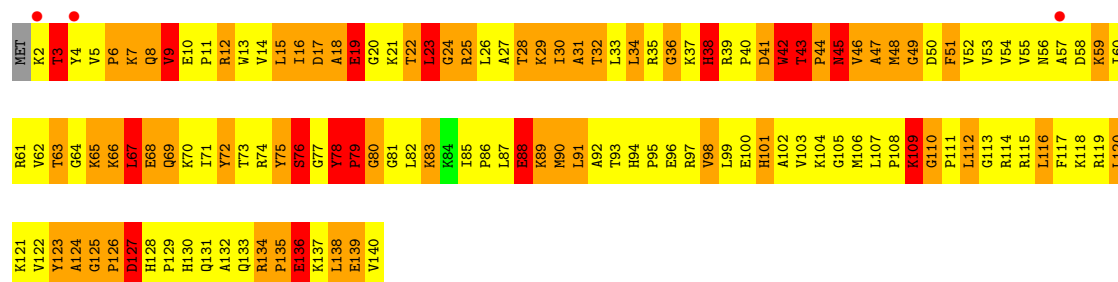
• Molecule 34: 50S RIBOSOMAL PROTEIN L11

Chain BL:



• Molecule 35: 50S RIBOSOMAL PROTEIN L13

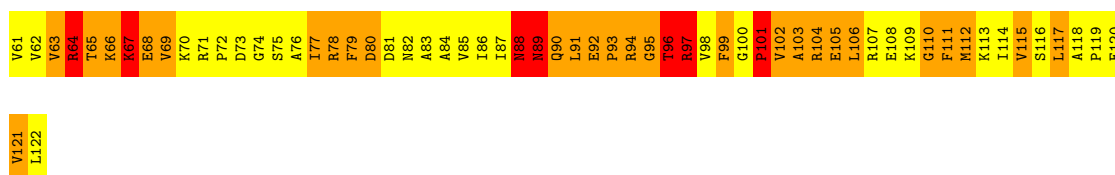
Chain BM:



• Molecule 36: 50S RIBOSOMAL PROTEIN L14

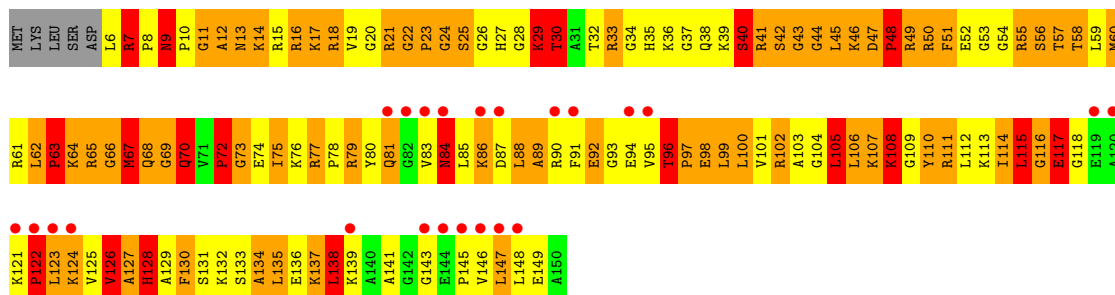
Chain BN:





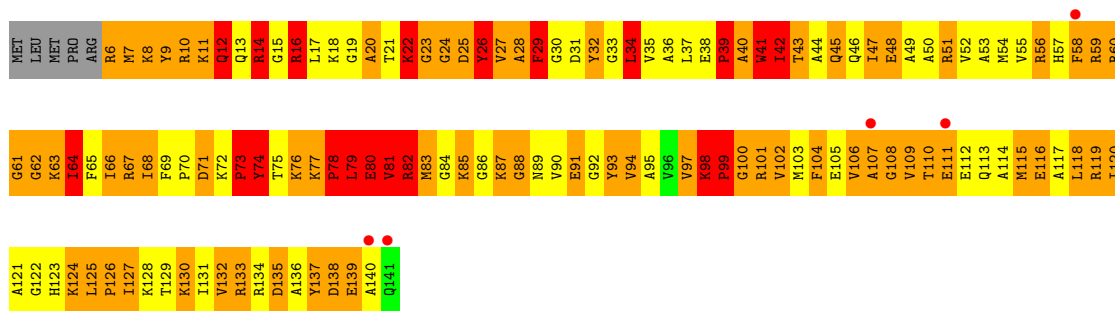
- Molecule 37: 50S RIBOSOMAL PROTEIN L15

Chain BO:



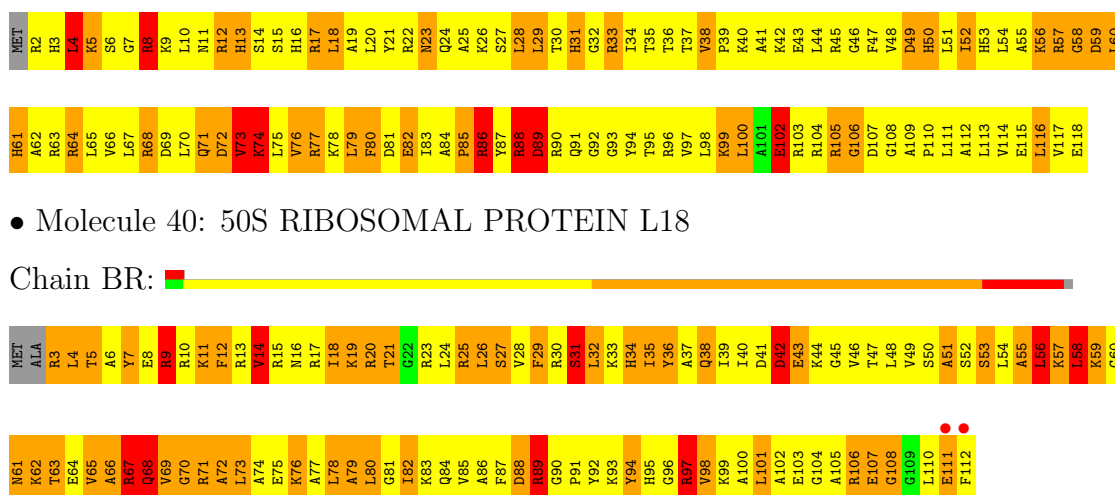
- Molecule 38: 50S RIBOSOMAL PROTEIN L16

Chain BP:



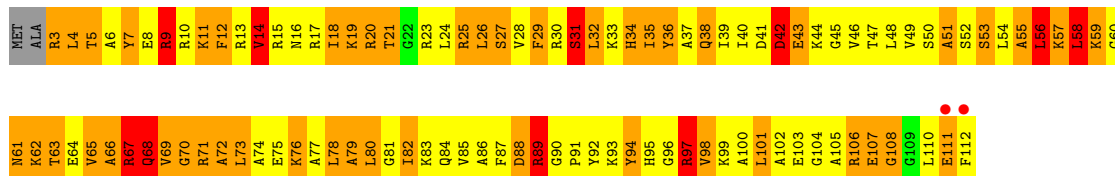
- Molecule 39: 50S RIBOSOMAL PROTEIN L17

Chain BQ:



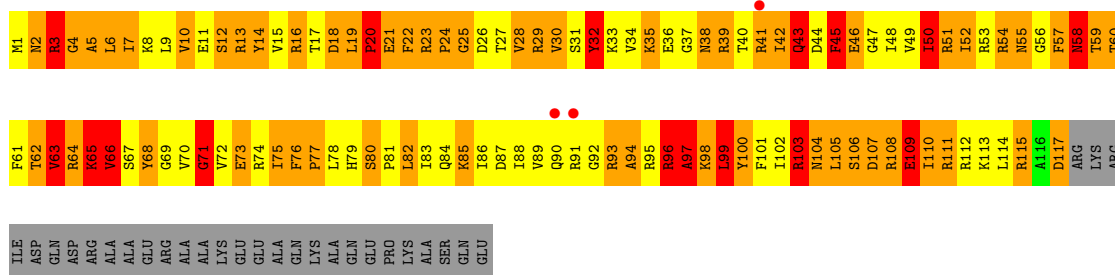
- Molecule 40: 50S RIBOSOMAL PROTEIN L18

Chain BR:



- Molecule 41: 50S RIBOSOMAL PROTEIN L19

Chain BS:



- Molecule 42: 50S RIBOSOMAL PROTEIN L20

Chain BT:



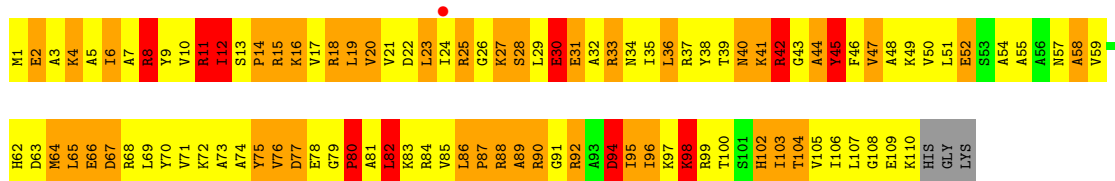
- Molecule 43: 50S RIBOSOMAL PROTEIN L21

Chain BU:



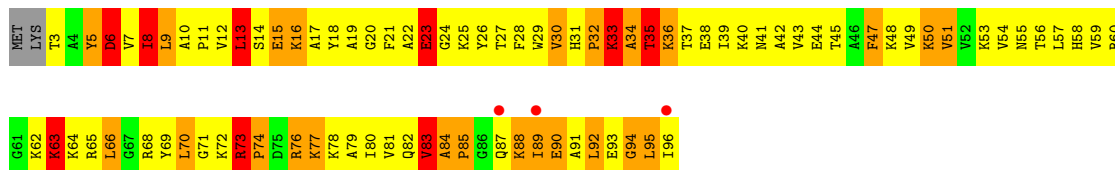
- Molecule 44: 50S RIBOSOMAL PROTEIN L22

Chain BV:



- Molecule 45: 50S RIBOSOMAL PROTEIN L23

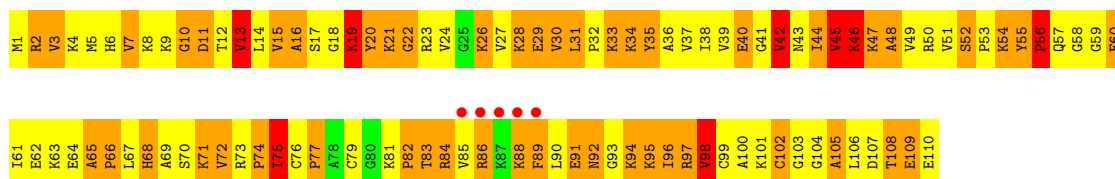
Chain BW:



- Molecule 46: 50S RIBOSOMAL PROTEIN L24

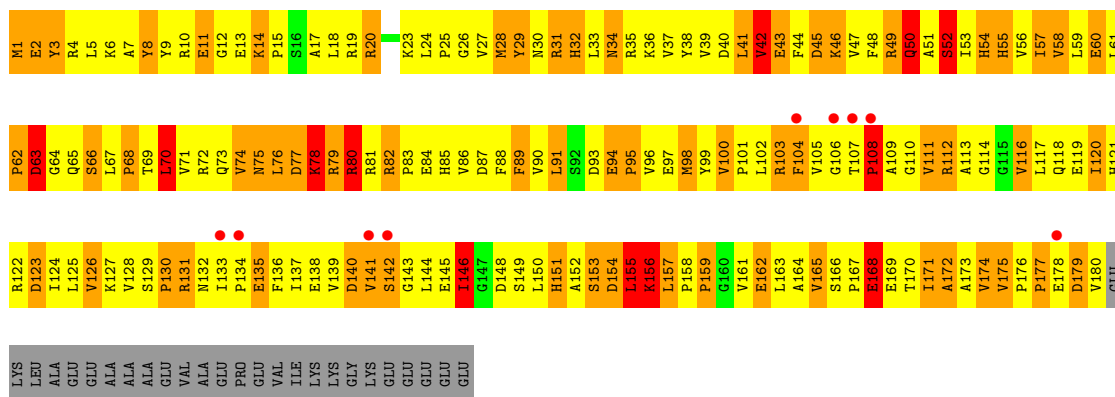
Chain BX:





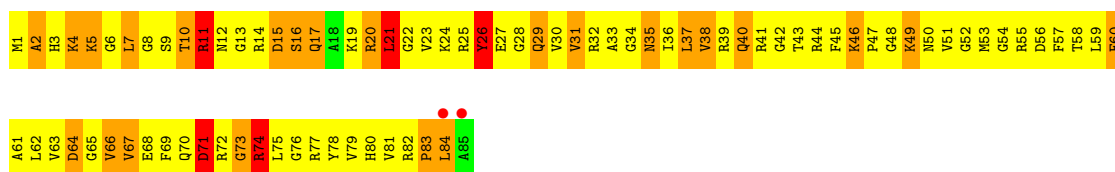
• Molecule 47: 50S RIBOSOMAL PROTEIN L25

Chain BY:



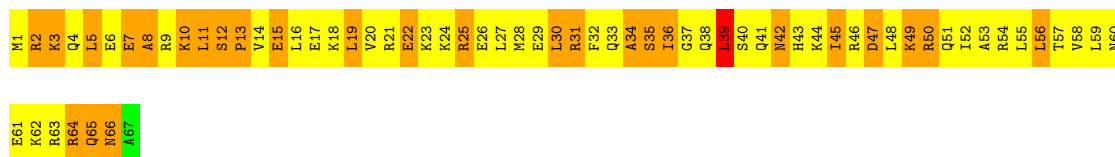
• Molecule 48: 50S RIBOSOMAL PROTEIN L27

Chain BZ:



• Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain B1:



• Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B2:



• Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B3:





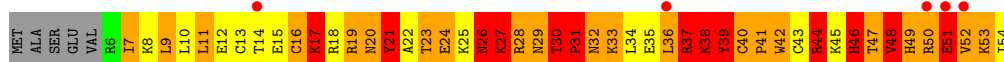
• Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain B4:



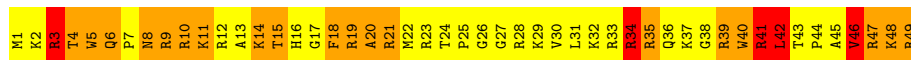
• Molecule 53: 50S RIBOSOMAL PROTEIN L33

Chain B5:



• Molecule 54: 50S RIBOSOMAL PROTEIN L34

Chain B6:



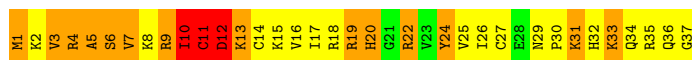
• Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain B7:



• Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain B8:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51 429.82 – 3.98	Depositor EDS
% Data completeness (in resolution range)	90.3 (300.00-4.51) 94.9 (429.82-3.98)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.298 , 0.345 0.341 , 0.374	Depositor DCC
$R_{free}$ test set	14214 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	198.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.08 , 105.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 441813 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	149640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	252.0	wwPDB-VP

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

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



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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	AA	24	U	Sidechain
1	AA	7	G	Sidechain

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	BF	1625	0	1666	862	0
31	BG	1482	0	1546	838	0
32	BH	1328	0	1408	664	0
33	BK	1155	0	1244	574	0
34	BL	1025	0	1074	414	0
35	BM	1113	0	1183	722	0
36	BN	932	0	994	703	0
37	BO	1106	0	1183	801	0
38	BP	1080	0	1127	691	0
39	BQ	960	0	1021	505	0
40	BR	877	0	938	472	0
41	BS	976	0	1033	699	0
42	BT	964	0	1022	709	0
43	BU	779	0	852	626	0
44	BV	876	0	941	423	0
45	BW	742	0	800	336	0
46	BX	844	0	930	493	0
47	BY	1435	0	1463	683	0
48	BZ	670	0	700	365	0
49	B1	567	0	621	303	0
50	B2	469	0	518	302	0
51	B3	581	0	577	375	0
52	B4	445	0	459	271	0
53	B5	426	0	452	306	0
54	B6	430	0	480	275	0
55	B7	515	0	587	415	0
56	B8	307	0	335	126	0
All	All	149640	0	102066	45475	0

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 181.

The worst 5 of 45475 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:BA:1204:A:C2	30:BF:188:ARG:HA	1.17	1.61
25:BA:2459:A:N3	25:BA:2460:U:H1'	1.22	1.46
25:BA:1204:A:C2	30:BF:188:ARG:CA	1.98	1.45
25:BA:2745:C:N4	25:BA:2756:U:C5	1.85	1.45
25:BA:1475:G:H1	25:BA:1477:A:N6	1.11	1.44

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	AF	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	3
7	AG	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	4
8	AH	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	9
9	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	3
10	AJ	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	2
11	AK	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	2
12	AL	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	3
13	AM	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	1
14	AN	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	4
15	AO	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	AP	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	5
17	AQ	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	1
18	AR	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	9
19	AS	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	5
20	AT	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	7
21	AU	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	AV	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	AW	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	1
24	AX	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	3
27	BC	226/229 (99%)	137 (61%)	52 (23%)	37 (16%)	0	7
28	BD	270/276 (98%)	129 (48%)	49 (18%)	92 (34%)	0	0
29	BE	204/206 (99%)	106 (52%)	39 (19%)	59 (29%)	0	1
30	BF	206/210 (98%)	100 (48%)	47 (23%)	59 (29%)	0	1
31	BG	180/182 (99%)	79 (44%)	42 (23%)	59 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	172/180 (96%)	89 (52%)	41 (24%)	42 (24%)	0	2
33	BK	146/148 (99%)	88 (60%)	32 (22%)	26 (18%)	0	6
34	BL	136/147 (92%)	66 (48%)	32 (24%)	38 (28%)	0	1
35	BM	137/140 (98%)	66 (48%)	31 (23%)	40 (29%)	0	1
36	BN	120/122 (98%)	63 (52%)	21 (18%)	36 (30%)	0	1
37	BO	143/150 (95%)	60 (42%)	31 (22%)	52 (36%)	0	0
38	BP	134/141 (95%)	51 (38%)	35 (26%)	48 (36%)	0	0
39	BQ	115/118 (98%)	64 (56%)	33 (29%)	18 (16%)	0	8
40	BR	108/112 (96%)	45 (42%)	30 (28%)	33 (31%)	0	1
41	BS	115/146 (79%)	53 (46%)	26 (23%)	36 (31%)	0	0
42	BT	115/118 (98%)	49 (43%)	39 (34%)	27 (24%)	0	3
43	BU	99/101 (98%)	51 (52%)	22 (22%)	26 (26%)	0	2
44	BV	108/113 (96%)	69 (64%)	15 (14%)	24 (22%)	0	3
45	BW	92/96 (96%)	59 (64%)	14 (15%)	19 (21%)	0	4
46	BX	108/110 (98%)	41 (38%)	27 (25%)	40 (37%)	0	0
47	BY	178/206 (86%)	93 (52%)	48 (27%)	37 (21%)	0	4
48	BZ	83/85 (98%)	50 (60%)	14 (17%)	19 (23%)	0	3
49	B1	65/67 (97%)	27 (42%)	26 (40%)	12 (18%)	0	5
50	B2	57/60 (95%)	32 (56%)	16 (28%)	9 (16%)	0	8
51	B3	69/71 (97%)	26 (38%)	19 (28%)	24 (35%)	0	0
52	B4	55/60 (92%)	16 (29%)	12 (22%)	27 (49%)	0	0
53	B5	47/54 (87%)	13 (28%)	7 (15%)	27 (57%)	0	0
54	B6	47/49 (96%)	16 (34%)	16 (34%)	15 (32%)	0	0
55	B7	62/65 (95%)	29 (47%)	11 (18%)	22 (36%)	0	0
56	B8	35/37 (95%)	20 (57%)	4 (11%)	11 (31%)	0	0
All	All	5988/6337 (94%)	2997 (50%)	1412 (24%)	1579 (26%)	0	2

5 of 1579 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
5	AE	19	HIS
5	AE	20	GLU

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	202/220 (92%)	135 (67%)	67 (33%)	0	3
6	AF	160/188 (85%)	123 (77%)	37 (23%)	1	10
7	AG	180/181 (99%)	127 (71%)	53 (29%)	0	5
8	AH	115/123 (94%)	75 (65%)	40 (35%)	0	3
9	AI	90/90 (100%)	64 (71%)	26 (29%)	0	5
10	AJ	126/127 (99%)	95 (75%)	31 (25%)	1	9
11	AK	119/119 (100%)	76 (64%)	43 (36%)	0	2
12	AL	98/99 (99%)	76 (78%)	22 (22%)	1	11
13	AM	88/92 (96%)	65 (74%)	23 (26%)	1	7
14	AN	90/99 (91%)	62 (69%)	28 (31%)	0	4
15	AO	104/109 (95%)	77 (74%)	27 (26%)	1	7
16	AP	100/101 (99%)	79 (79%)	21 (21%)	1	12
17	AQ	49/50 (98%)	37 (76%)	12 (24%)	1	9
18	AR	79/80 (99%)	56 (71%)	23 (29%)	0	5
19	AS	72/74 (97%)	48 (67%)	24 (33%)	0	3
20	AT	96/97 (99%)	71 (74%)	25 (26%)	1	7
21	AU	64/77 (83%)	41 (64%)	23 (36%)	0	2
22	AV	71/80 (89%)	57 (80%)	14 (20%)	2	15
23	AW	76/82 (93%)	56 (74%)	20 (26%)	1	7
24	AX	19/22 (86%)	13 (68%)	6 (32%)	0	4
27	BC	180/181 (99%)	151 (84%)	29 (16%)	3	26
28	BD	215/218 (99%)	151 (70%)	64 (30%)	0	5
29	BE	166/166 (100%)	102 (61%)	64 (39%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BF	164/166 (99%)	104 (63%)	60 (37%)	0	2
31	BG	156/156 (100%)	112 (72%)	44 (28%)	0	5
32	BH	143/148 (97%)	97 (68%)	46 (32%)	0	4
33	BK	124/124 (100%)	87 (70%)	37 (30%)	0	5
34	BL	105/111 (95%)	85 (81%)	20 (19%)	2	17
35	BM	118/119 (99%)	80 (68%)	38 (32%)	0	4
36	BN	100/100 (100%)	65 (65%)	35 (35%)	0	2
37	BO	111/116 (96%)	64 (58%)	47 (42%)	0	1
38	BP	106/111 (96%)	55 (52%)	51 (48%)	0	0
39	BQ	100/101 (99%)	69 (69%)	31 (31%)	0	5
40	BR	87/88 (99%)	55 (63%)	32 (37%)	0	1
41	BS	105/127 (83%)	69 (66%)	36 (34%)	0	3
42	BT	93/94 (99%)	64 (69%)	29 (31%)	0	4
43	BU	82/82 (100%)	59 (72%)	23 (28%)	0	6
44	BV	90/92 (98%)	56 (62%)	34 (38%)	0	1
45	BW	76/78 (97%)	55 (72%)	21 (28%)	0	6
46	BX	91/91 (100%)	66 (72%)	25 (28%)	0	6
47	BY	159/179 (89%)	110 (69%)	49 (31%)	0	5
48	BZ	67/67 (100%)	52 (78%)	15 (22%)	1	11
49	B1	62/62 (100%)	46 (74%)	16 (26%)	1	8
50	B2	51/52 (98%)	34 (67%)	17 (33%)	0	3
51	B3	63/63 (100%)	42 (67%)	21 (33%)	0	3
52	B4	50/52 (96%)	30 (60%)	20 (40%)	0	1
53	B5	48/52 (92%)	32 (67%)	16 (33%)	0	3
54	B6	42/42 (100%)	30 (71%)	12 (29%)	0	5
55	B7	54/55 (98%)	40 (74%)	14 (26%)	1	7
56	B8	34/34 (100%)	25 (74%)	9 (26%)	1	7
All	All	5040/5237 (96%)	3520 (70%)	1520 (30%)	0	5

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

Mol	Chain	Res	Type
29	BE	101	ARG

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Mol	Chain	Res	Type
32	BH	103	LEU
49	B1	45	ILE
29	BE	155	LYS
30	BF	175	THR

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

Mol	Chain	Res	Type
22	AV	23	ASN
29	BE	129	HIS
51	B3	46	GLN
23	AW	45	GLN
28	BD	87	ASN

### 5.3.3 RNA ⓘ

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

5 of 1834 RNA backbone outliers are listed below:

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

5 of 480 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	562	U
25	BA	974(A)	C
25	BA	2610	C

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Mol	Chain	Res	Type
25	BA	616	A
25	BA	783	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1202:C	O3'	1203:G	P	1.97
1	BA	1203:G	O3'	1204:A	P	1.19

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1515/1522 (99%)	-0.99	3 (0%) 93 89	188, 245, 349, 445	0
2	AC	76/76 (100%)	-1.14	1 (1%) 74 60	213, 249, 283, 294	0
3	AD	76/76 (100%)	-0.95	0 100 100	301, 334, 358, 368	0
4	A1	27/27 (100%)	1.47	9 (33%) 1 2	225, 347, 415, 416	0
5	AE	234/256 (91%)	-0.12	8 (3%) 43 36	218, 248, 286, 307	0
6	AF	206/239 (86%)	0.31	9 (4%) 33 30	246, 269, 288, 296	0
7	AG	208/209 (99%)	-0.14	4 (1%) 64 51	202, 233, 251, 265	0
8	AH	150/162 (92%)	0.12	5 (3%) 44 37	202, 220, 245, 262	0
9	AI	101/101 (100%)	1.12	21 (20%) 1 4	219, 237, 254, 271	0
10	AJ	155/156 (99%)	0.29	5 (3%) 45 38	250, 273, 285, 301	0
11	AK	138/138 (100%)	-0.31	0 100 100	203, 222, 236, 246	0
12	AL	127/128 (99%)	-0.26	1 (0%) 83 71	247, 317, 349, 353	0
13	AM	98/105 (93%)	0.29	6 (6%) 21 22	256, 296, 311, 317	0
14	AN	119/129 (92%)	0.45	4 (3%) 43 36	214, 234, 252, 279	0
15	AO	124/132 (93%)	0.69	19 (15%) 3 6	189, 217, 243, 263	0
16	AP	125/126 (99%)	-0.13	3 (2%) 56 45	253, 281, 302, 306	0
17	AQ	60/61 (98%)	-0.10	0 100 100	243, 273, 286, 290	0
18	AR	88/89 (98%)	-0.50	0 100 100	199, 222, 244, 251	0
19	AS	83/88 (94%)	-0.37	0 100 100	192, 212, 232, 267	0
20	AT	104/105 (99%)	-0.48	0 100 100	192, 218, 252, 296	0
21	AU	73/88 (82%)	0.05	6 (8%) 12 16	192, 228, 255, 277	0
22	AV	80/93 (86%)	0.43	8 (10%) 8 12	251, 287, 306, 310	0
23	AW	99/106 (93%)	-0.32	0 100 100	200, 228, 250, 254	0
24	AX	24/27 (88%)	-0.51	0 100 100	268, 289, 303, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BA	2889/2916 (99%)	-0.96	2 (0%) 93 91	168, 241, 340, 398	0
26	BB	123/123 (100%)	-0.79	0 100 100	236, 293, 329, 343	0
27	BC	228/229 (99%)	1.36	57 (25%) 1 3	299, 326, 342, 347	0
28	BD	272/276 (98%)	0.71	44 (16%) 2 5	184, 216, 235, 256	0
29	BE	206/206 (100%)	-0.05	8 (3%) 37 33	155, 205, 250, 276	0
30	BF	208/210 (99%)	-0.29	0 100 100	186, 255, 283, 288	0
31	BG	182/182 (100%)	0.10	13 (7%) 16 18	247, 283, 306, 311	0
32	BH	174/180 (96%)	0.00	7 (4%) 36 32	230, 260, 278, 284	0
33	BK	148/148 (100%)	-0.05	1 (0%) 84 73	212, 241, 261, 265	0
34	BL	138/147 (93%)	0.62	22 (15%) 3 5	305, 358, 399, 403	0
35	BM	139/140 (99%)	0.05	3 (2%) 59 47	187, 217, 245, 270	0
36	BN	122/122 (100%)	0.07	0 100 100	172, 201, 228, 240	0
37	BO	145/150 (96%)	0.58	23 (15%) 3 5	189, 271, 304, 346	0
38	BP	136/141 (96%)	0.05	5 (3%) 39 34	199, 234, 257, 266	0
39	BQ	117/118 (99%)	-0.42	0 100 100	195, 214, 246, 256	0
40	BR	110/112 (98%)	-0.33	2 (1%) 65 53	232, 266, 293, 300	0
41	BS	117/146 (80%)	0.14	3 (2%) 53 43	182, 205, 238, 244	0
42	BT	117/118 (99%)	-0.22	1 (0%) 81 69	191, 221, 241, 250	0
43	BU	101/101 (100%)	0.33	4 (3%) 36 32	190, 244, 272, 277	0
44	BV	110/113 (97%)	-0.06	1 (0%) 81 69	203, 226, 250, 260	0
45	BW	94/96 (97%)	-0.17	3 (3%) 45 38	237, 253, 304, 309	0
46	BX	110/110 (100%)	-0.10	5 (4%) 32 29	244, 282, 303, 312	0
47	BY	180/206 (87%)	0.22	9 (5%) 28 26	235, 267, 281, 287	0
48	BZ	85/85 (100%)	-0.29	2 (2%) 56 45	236, 259, 272, 289	0
49	B1	67/67 (100%)	-0.22	0 100 100	251, 264, 276, 281	0
50	B2	59/60 (98%)	-0.24	0 100 100	208, 244, 261, 268	0
51	B3	71/71 (100%)	-0.29	0 100 100	212, 239, 259, 276	0
52	B4	57/60 (95%)	-0.13	1 (1%) 65 53	200, 227, 276, 299	0
53	B5	49/54 (90%)	0.45	5 (10%) 7 12	211, 247, 269, 277	0
54	B6	49/49 (100%)	-0.21	0 100 100	189, 228, 244, 250	0
55	B7	64/65 (98%)	-0.37	0 100 100	201, 220, 235, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
56	B8	37/37 (100%)	-0.65	0	100	100	212, 230, 240, 244	0
All	All	10794/11077 (97%)	-0.36	333 (3%)	47	39	155, 245, 336, 445	0

The worst 5 of 333 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BO	123	LEU	15.2
27	BC	126	LYS	11.3
4	A1	1	G	10.8
1	AA	1542	U	10.0
34	BL	85	GLU	8.3

## 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.