



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:48 pm BST

PDB ID : 4V4Y
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

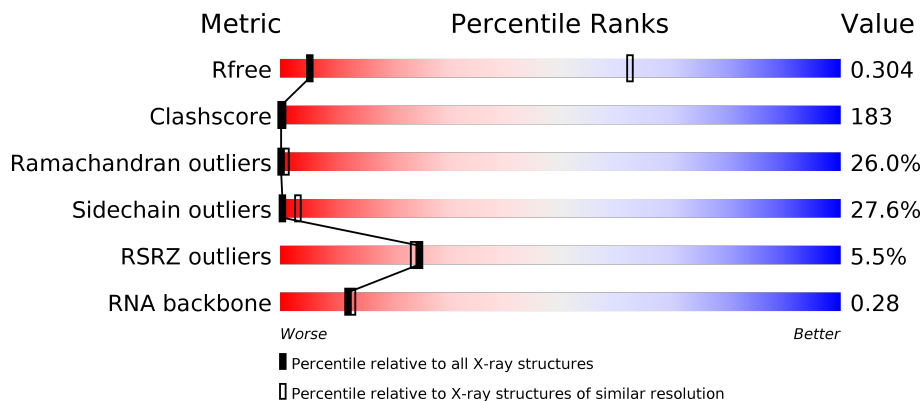
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)
RNA backbone	3102	1074 (7.80-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	A1	50	
3	AB	76	
3	AC	76	



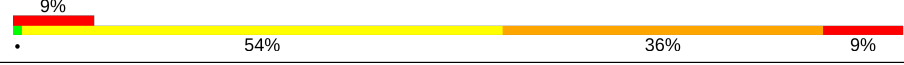
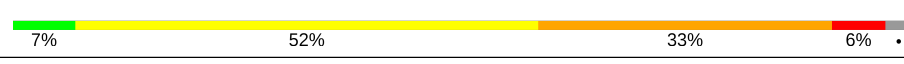
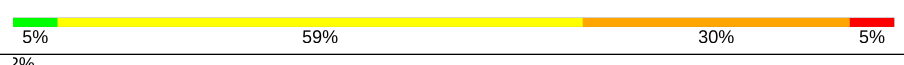
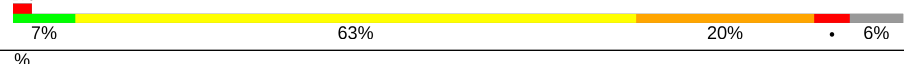






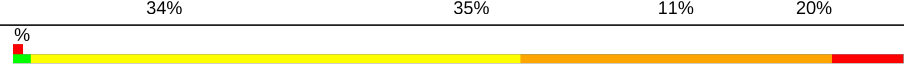

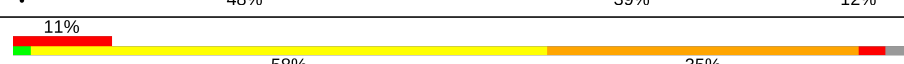
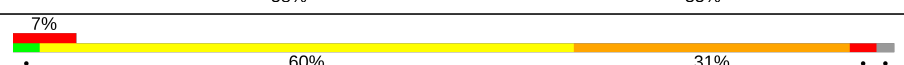
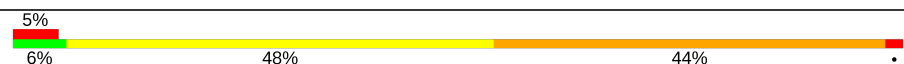

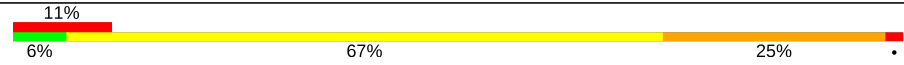




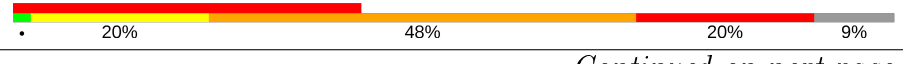

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Mol	Chain	Length	Quality of chain
3	AD	76	
4	AE	256	
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	



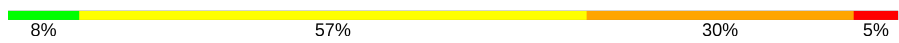
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Mol	Chain	Length	Quality of chain
28	BE	206	
29	BF	210	
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ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

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Mol	Chain	Length	Quality of chain
53	B6	49	
54	B7	65	
55	B8	37	

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 151691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A1	50	1025	459	128	388	50	0	0	0

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

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

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

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

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 26 is a protein called 50S ribosomal protein L1.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called Ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

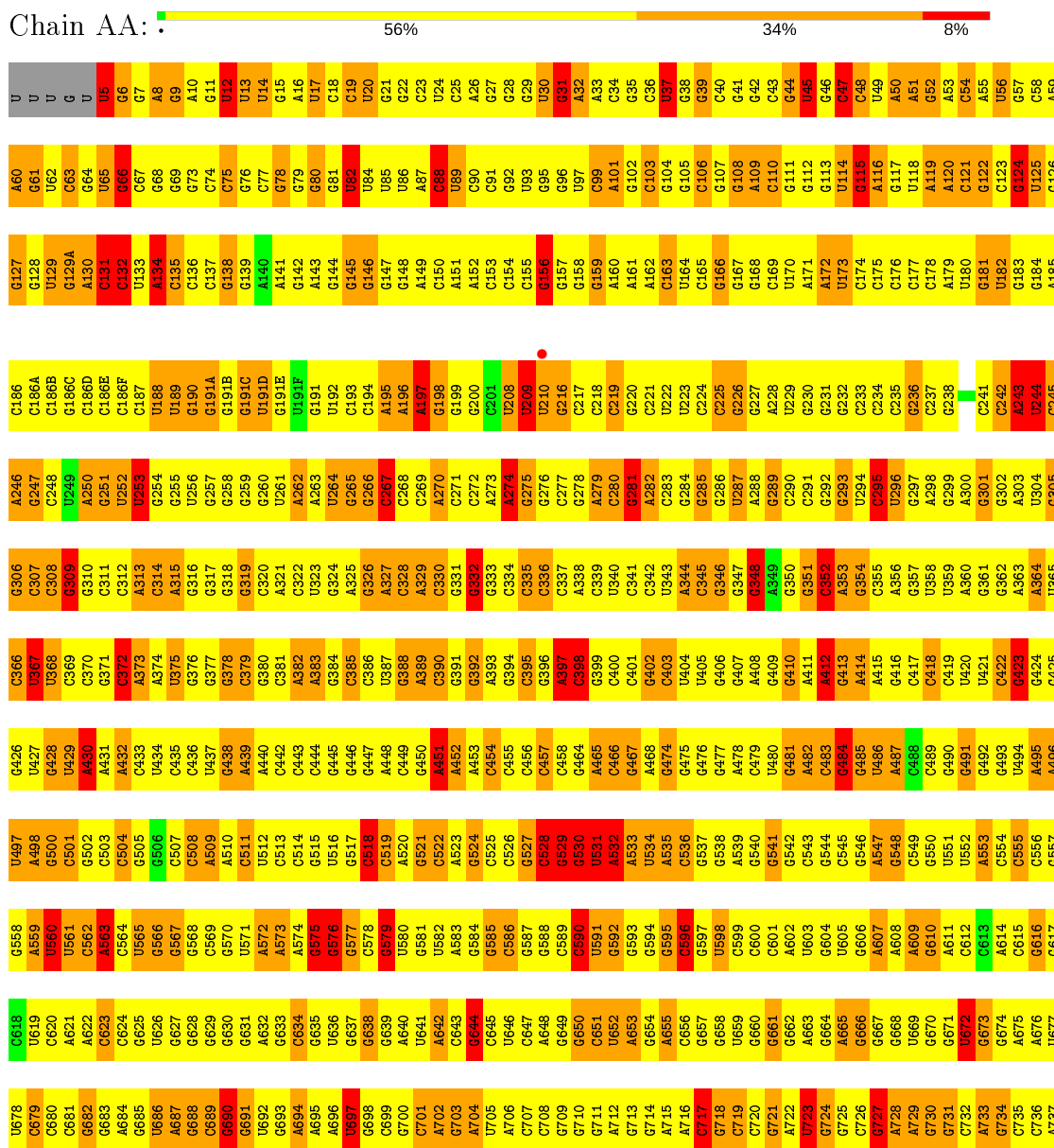
- Molecule 55 is a protein called 50S ribosomal protein L36.

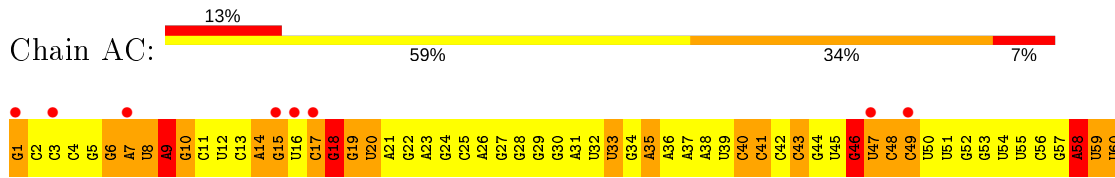
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B8	37	307	188	68	47	4	0	0	0

3 Residue-property plots

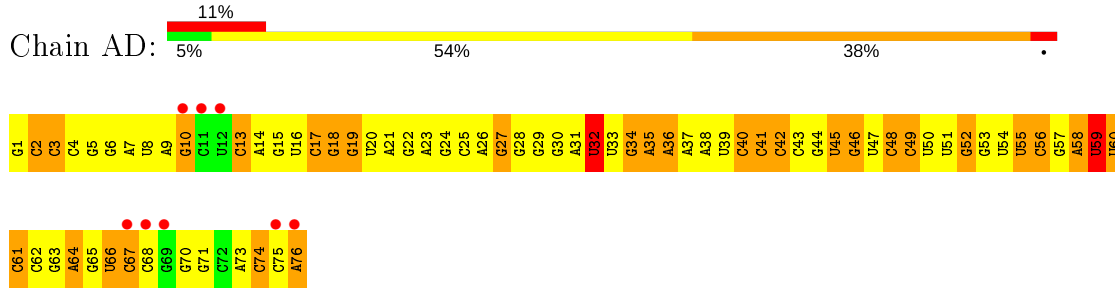
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

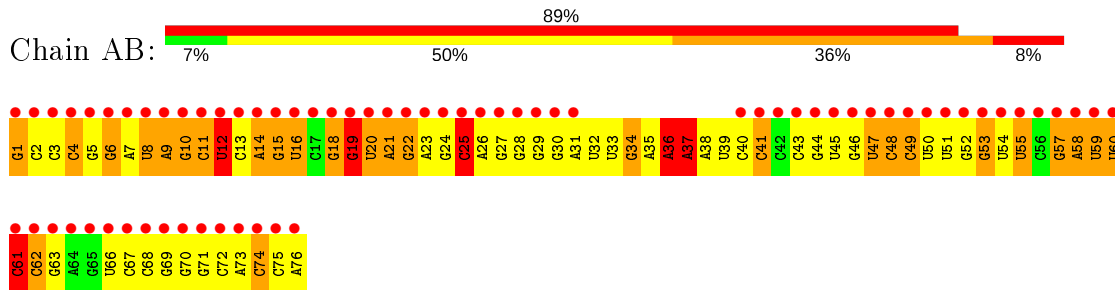




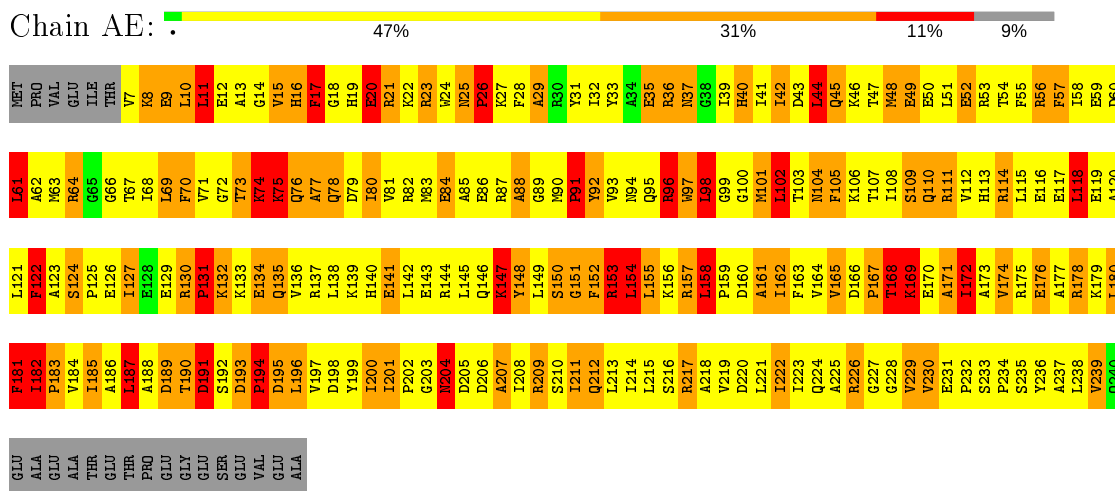
• Molecule 3: tRNA PHE (unmodified bases)



• Molecule 3: tRNA PHE (unmodified bases)

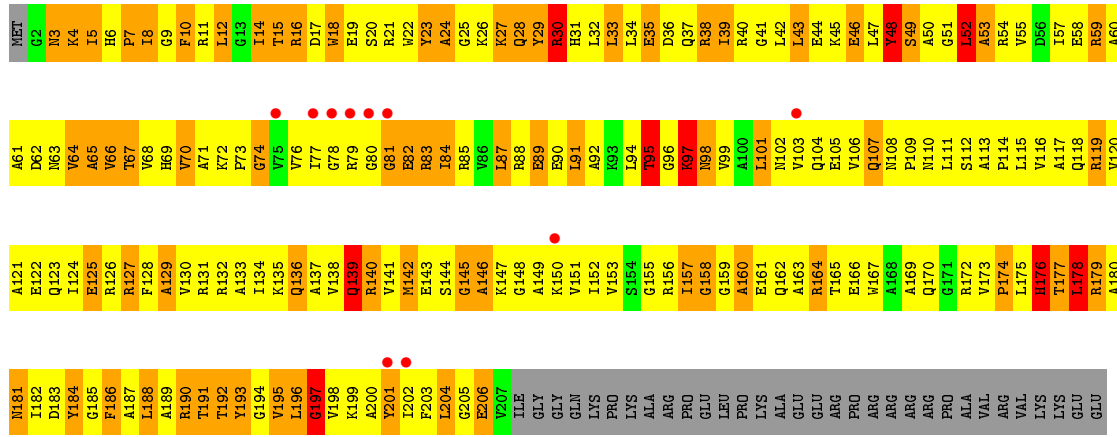


• Molecule 4: 30S ribosomal protein S2

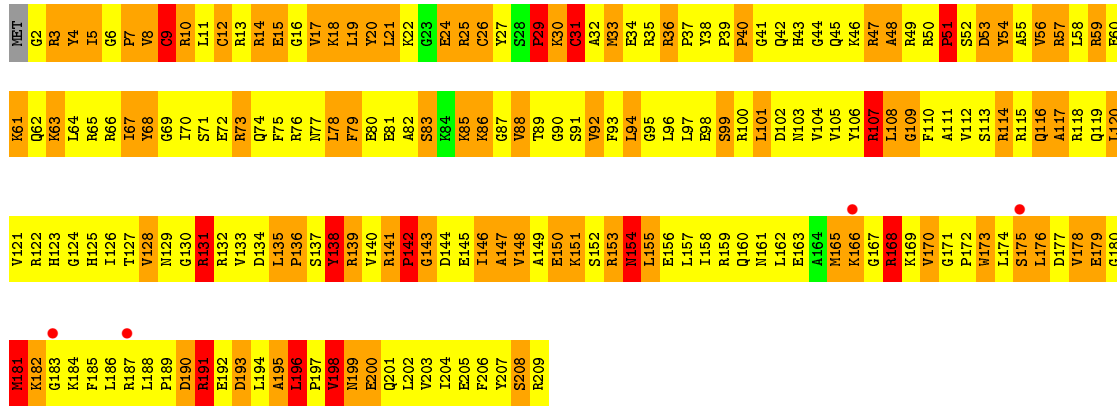


• Molecule 5: 30S ribosomal protein S3

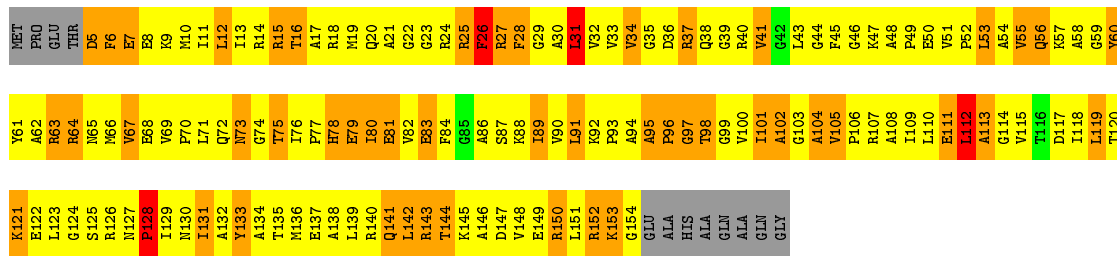




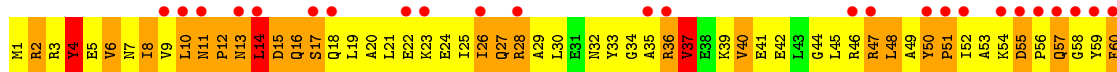
• Molecule 6: 30S ribosomal protein S4

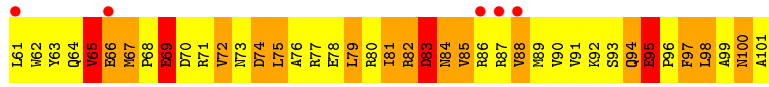


• Molecule 7: 30S ribosomal protein S5

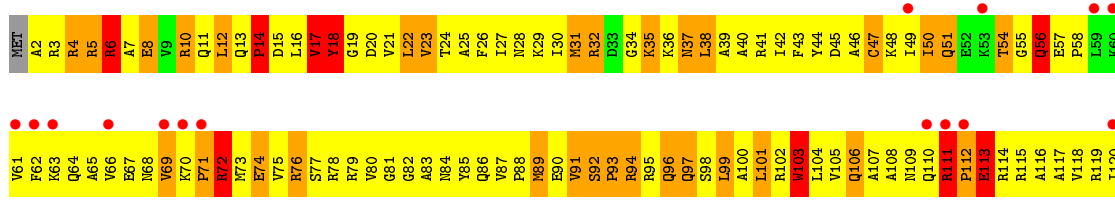


• Molecule 8: 30S ribosomal protein S6

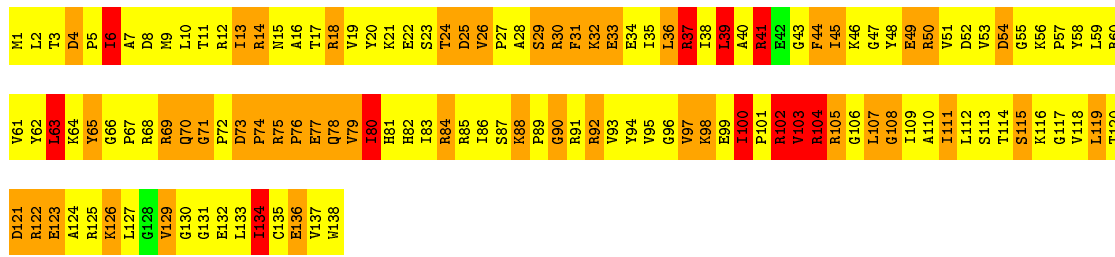




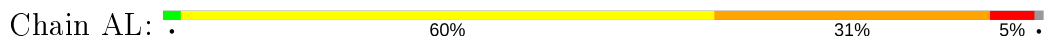
• Molecule 9: 30S ribosomal protein S7



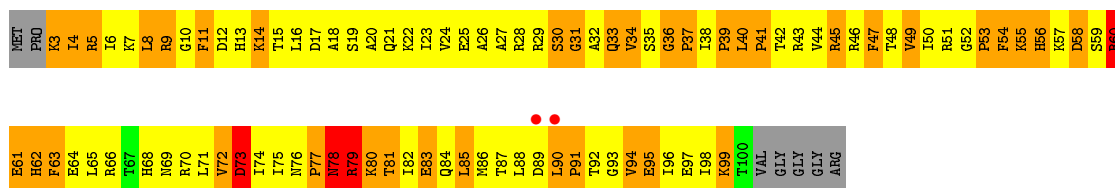
• Molecule 10: 30S ribosomal protein S8



• Molecule 11: 30S ribosomal protein S9



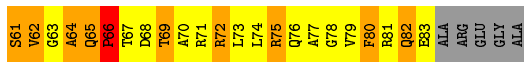
• Molecule 12: 30S ribosomal protein S10





- Molecule 18: 30S ribosomal protein S16

Chain AS: 56% 33% 6% 6%



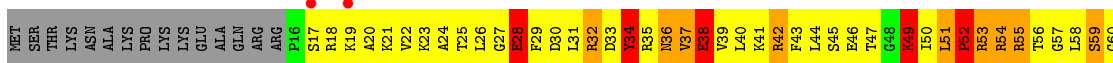
- Molecule 19: 30S ribosomal protein S17

Chain AT: 54% 35% 6%



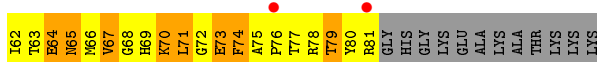
- Molecule 20: 30S ribosomal protein S18

Chain AU: 7% 50% 22% 9% 17%



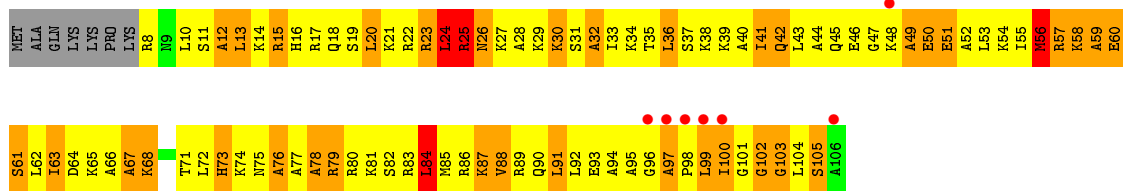
- Molecule 21: 30S ribosomal protein S19

Chain AV: 4% 48% 29% 5% 14%

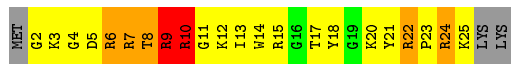


- Molecule 22: 30S ribosomal protein S20

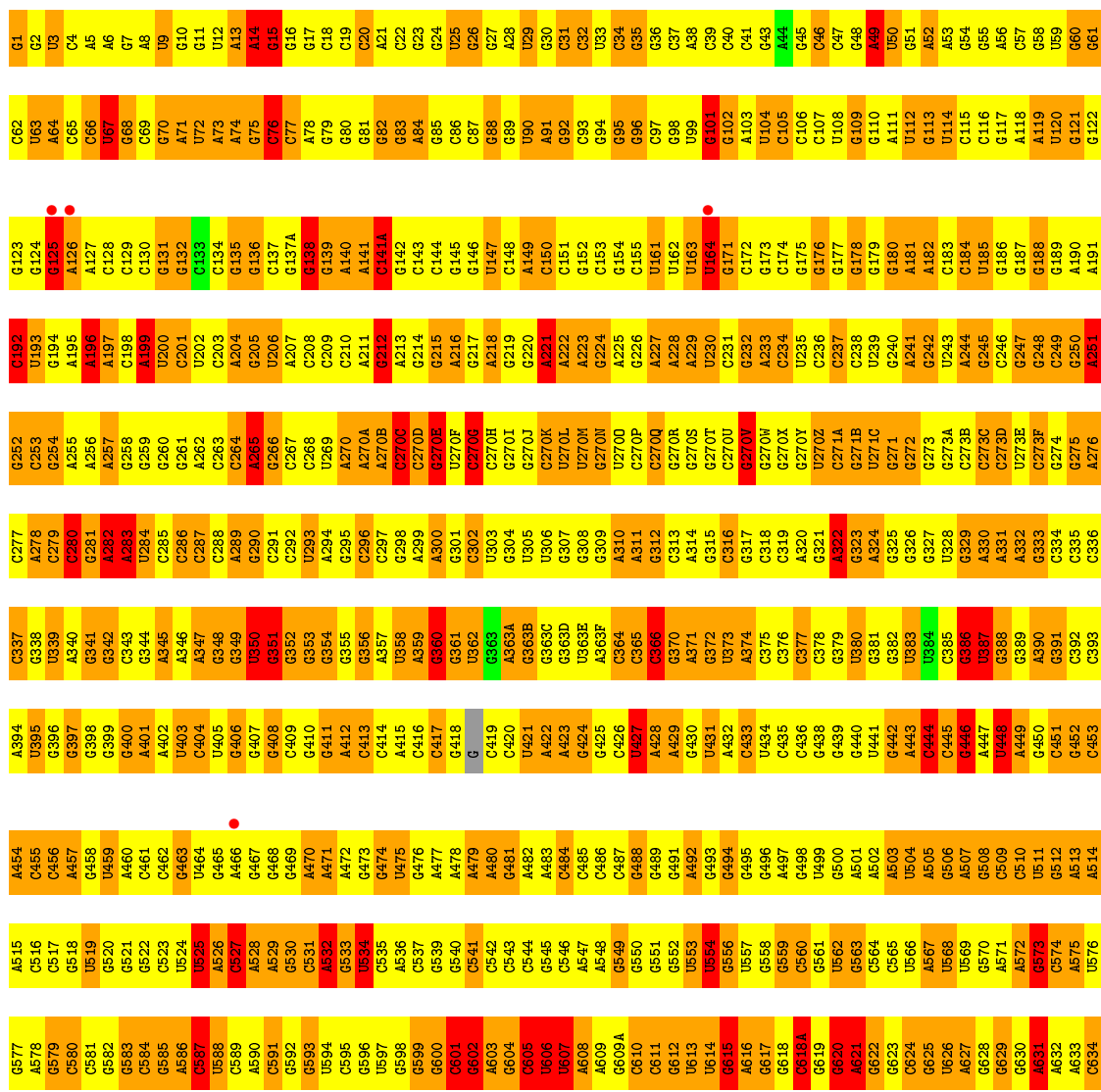
Chain AW: 7% 53% 33% 7% 7%



• Molecule 23: 30S ribosomal protein Thx



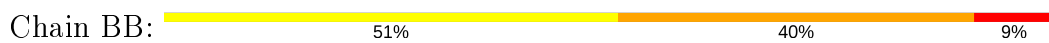
• Molecule 24: 23S ribosomal RNA



U1454	A1395	U1385	A1214	C1153	U1094	G1034	C974A	C914	G853	A793	G733	G635
G1455	U1396	A1336	G1215	G1194	A095	U1035	G975	C915	G854	G794	G674	G636
G1456	U1397	A1337	G1216	A1156	A096	G1036	G976	G916	G855	C795	A674	A637
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G1458	C1399	G1339	G1218	G1158	A098	G1038	G978	A918	C857	C797	A676	C645
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G1460	G1401	U1341	G1221	U1160	C1100	C1040	A980	G920	G859	G799	G678	G641
G1461	G1402	A1342	G1222	G1161	G101	C1041	A981	G921	U860	A800	G679	G642
C1403	C1403	G1343	C1223	G1162	C1102	G1042	C982	U922	A861	G801	G680	A643
C1404	G1404	A1344	G1224	G1163	A103	G1043	A983	C923	A862	A802	G681	A644
C1464	U1405	G1345	G1225	G1164	C1104	C1044	A984	C924	A863	U803	G682	C646
G1465	U1406	G1346	G1226	U1165	U1105	A1045	C985	C925	A864	A804	G683	A647
G1466	G1407	A1347	A1227	U1166	G1106	A1046	C986	A926	G865	G805	G684	G648
G1467	C1408	U1348	G1228	C1166	G1107	G1047	G987	G928	A866	C806	G685	G649
C1468	A1349	C1289	G1229	U1167	U1108	A1048	A988	G929	C867	U807	G687	C
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A1472	G1413	C1293	C1233	G1171	G1112	C1052	C992	A933	U871	U811	C691	A
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G1475	C1416	G1355	G1236	U1175	G1115	G1055	C995	U936	G874	C814	G694	C
C1476	G1417	C1296	A1237	U1176	C1116	G1056	A996	U937	G875	C815	G695	G
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G1421	A1301	A1241	A1241	C1180	A094	U1060	A1000	A941	G879	A819	G699	C
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G1428	G1368	A1308	G1248	U1187	A127	A1067	C1007	G948	C886	U826	A706	G
G1429	G1369	G1309	U1249	U1188	A128	U1068	C1008	C949	A887	U827	G707	G
C1430	G1370	G1310	G1250	A1189	A1129	A1069	A1009	G950	C888	U828	G708	C
U1431	U1371	U1311	G1251	G1190	U1130	A1070	A1010	C951	C889	A829	U709	C
C1432	U1372	U1312	G1252	G1191	G1131	C1071	G1011	C952	A890	G830	G710	G850
U1433	A1373	C1313	A1253	G1192	A132	C1072	U1012	A953	G892	G831	G711	G851
A1434	G1374	C1314	U1254	G1193	U1133	A1073	C1013	G954	C893	G832	G712	G852
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C1501	G1441	A1321	C1261	C1200	C1140	C1080	A1020	C961	A900	U839	C719	C859
C1502	G1442	A1322	A1262	C1201	U1141	U1081	A1021	G962	A901	C940	G720	G660
C1503	G1443	U1323	U1263	C1202	U1142	U1082	G1022	U963	A841	A781	C721	C661
C1504	G1444	G1324	G1264	G1203	A1142A	U1083	U1023	C964	C903	G842	A722	G662
C1505	A1444A	G1325	A1265	A1204	A1143	A1084	G1024	C965	G843	G843	G723	G663
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A1507	G1446	C1327	A1267	G1206	G1145	A1086	U1026	G967	G906	A784	G725	G665
A1508	G1447	G1328	U1268	C1207	C1146	G1087	G1027	G968	U907	C946	G726	G666
C1509	G1448	U1329	A1269	C1208	C1147	A1088	A1028	U969	C908	U847	A727	U667
U1510	A1449	U1330	C1270	G1209	A1148	G1089	A1029	C970	A809	G848	A728	G668
A1511	G1449A	A1331	G1271	A1210	G1149	U1090	A1029	C971	A910	A789	G729	G669
C1512	C1450	C1332	U1272	U1211	G1150	G1091	G1031	G972	A849	C850	C730	A670
C1513	C1451	C1333	U1273	G1212	G1151	C1092	A1032	G973	C912	U851	G731	C671
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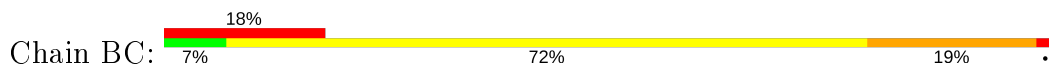
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C2443	A2503	U2563	G2623	U2684	G2743	G2805	U2866	G2927
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G2445	G2505	G2565	G2625	G2686	C2745	U2808	A2868	A2929
G2446	U2506	A2566	C2626	U2687	U2746	A2809	G2869	A2930
G2447	C2507	C2567	G2627	U2688	G2747	U2810	C2870	A2931
A2448	G2508	C2568	C2628	U2689	A2748	G2811	C2871	A2932
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● Molecule 25: 5S ribosomal RNA

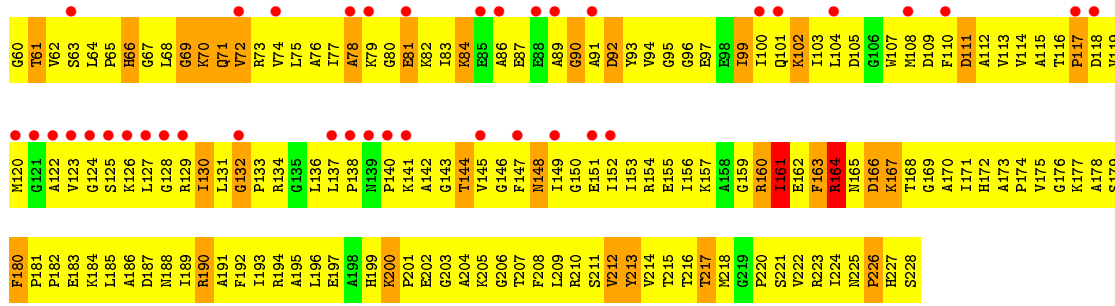


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C4	C64	
C5	C65	
C6	A66	
C7	G67	
U8	C68	
G9	A69	
C10	C70	
C11	G71	
C12	G72	
A13	U73	
U14	G74	
A15	G75	
G16	C76	
C17	U77	
G18	A78	
G19	C79	
C20	U80	
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C22	G82	
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G24	C84	
A25	G85	
A26	G86	
G27	G87	
L28	C88	
V29	C89	
K30	G89	
E31	A89A	
L32	C90	
C33	C91	
G34	G92	
A35	C93	
K36	U94	
F37	U95	
D38	G96	
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T40	G98	
V41	A99	
E42	G100	
H43	A101	
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A45	U103	
K46	A104	
L47	G105	
G48	G106	
I49	U107	
D50	C108	
P51	G109	
R52	G110	
R53	U111	
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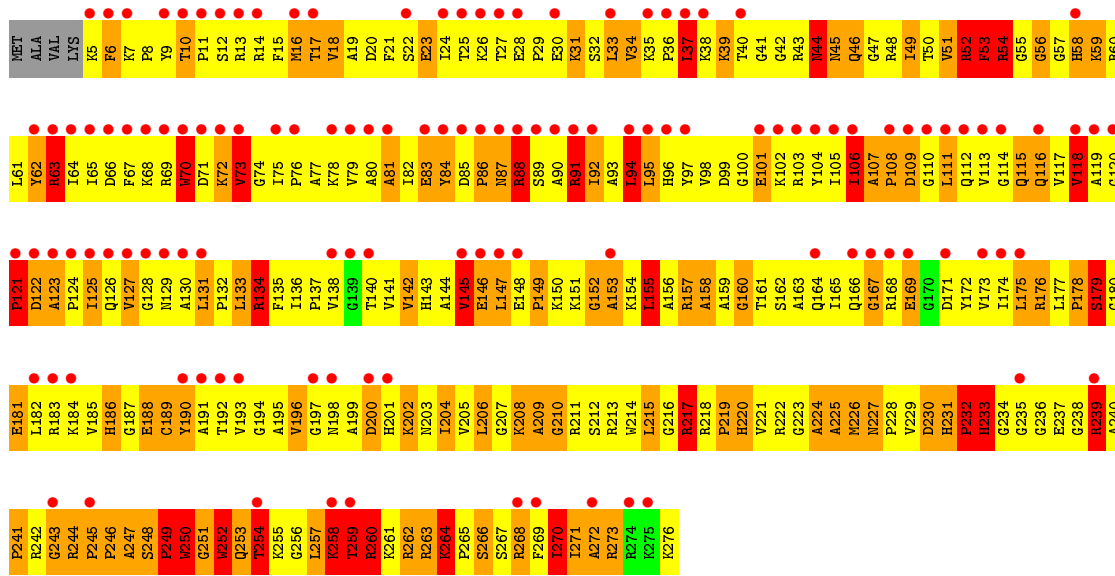
● Molecule 26: 50S ribosomal protein L1



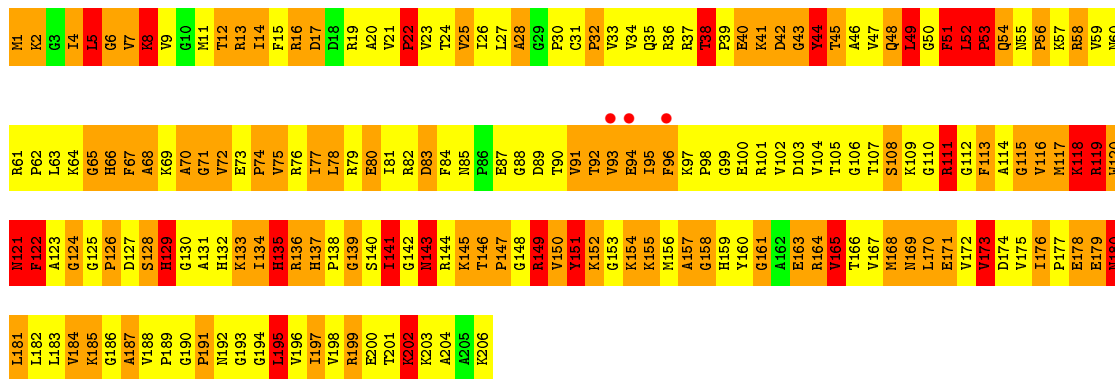
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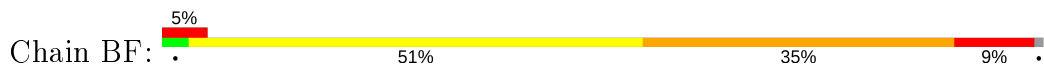
• Molecule 27: 50S ribosomal protein L2

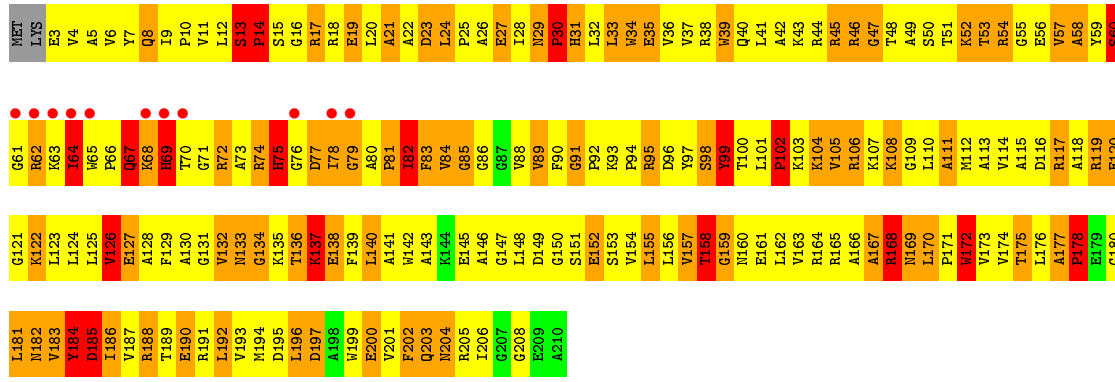


• Molecule 28: 50S ribosomal protein L3

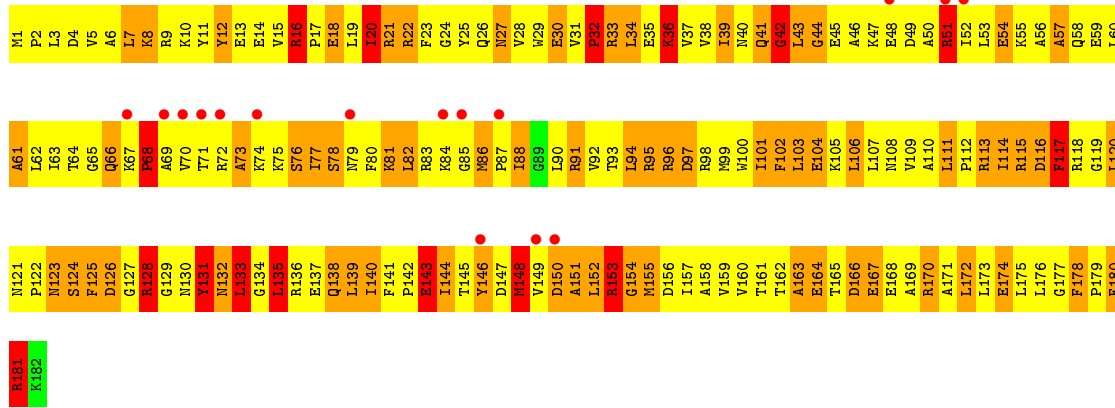


• Molecule 29: 50S ribosomal protein L4

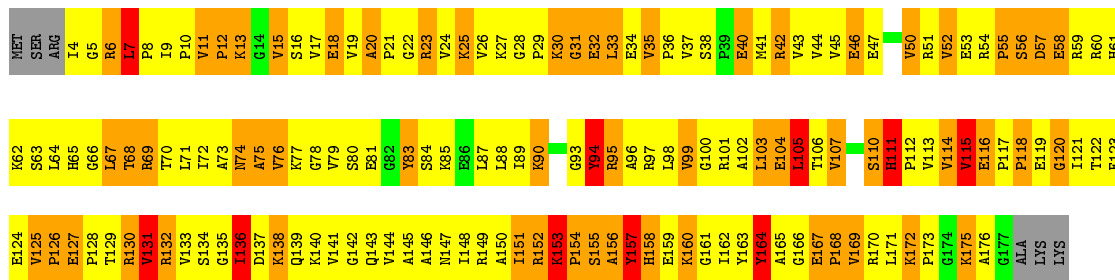
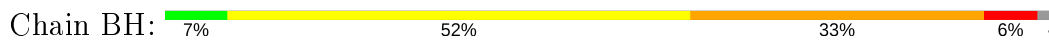




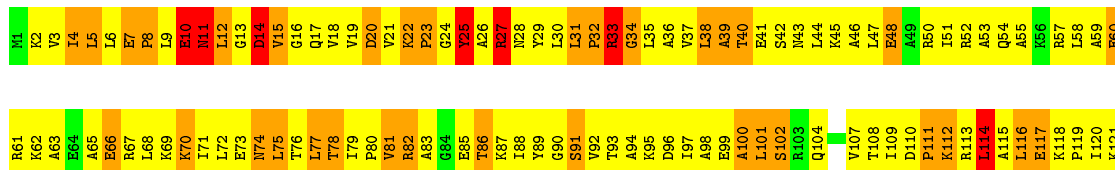
• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

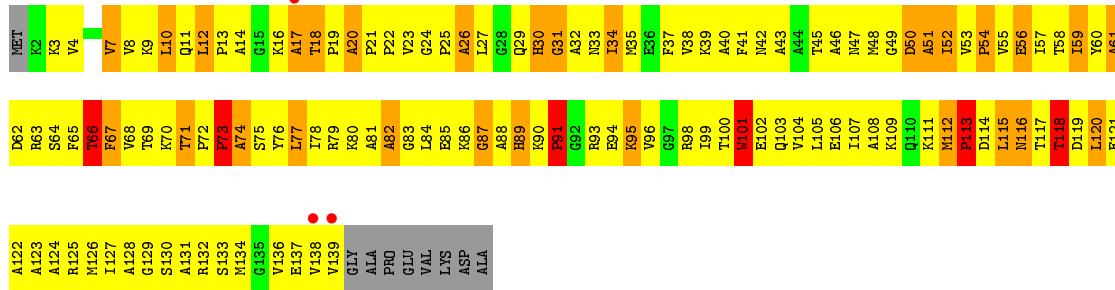
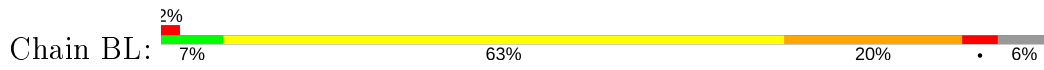


• Molecule 32: 50S ribosomal protein L9

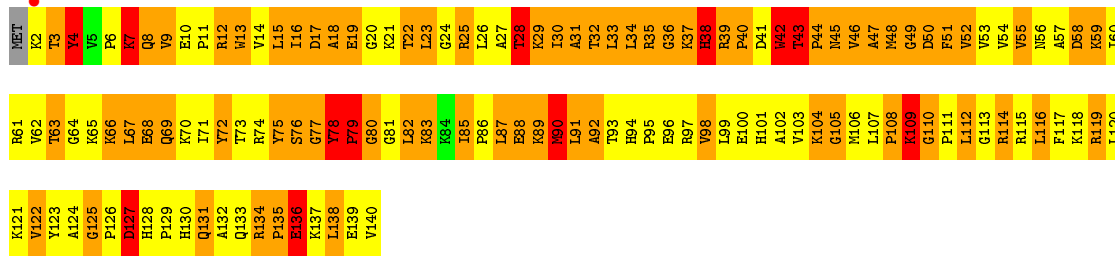




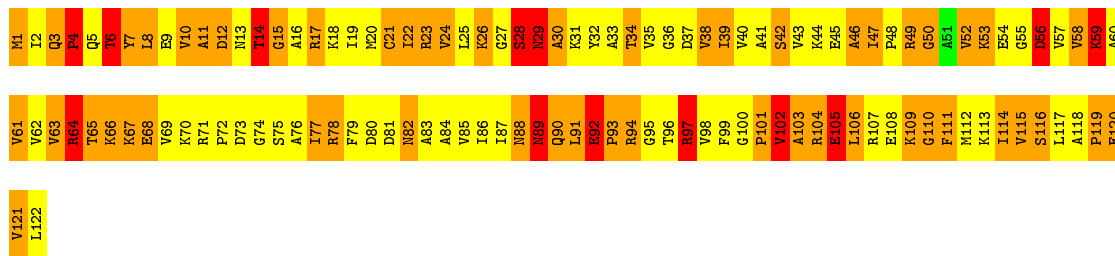
• Molecule 33: 50S ribosomal protein L11



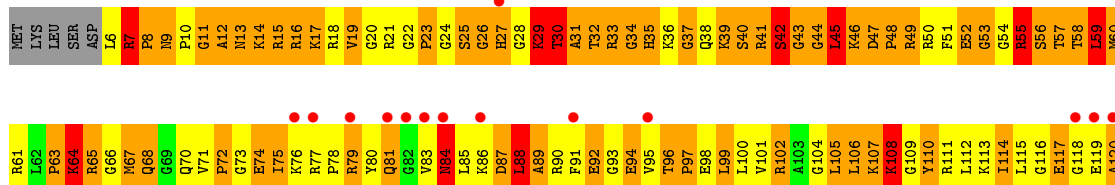
• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14

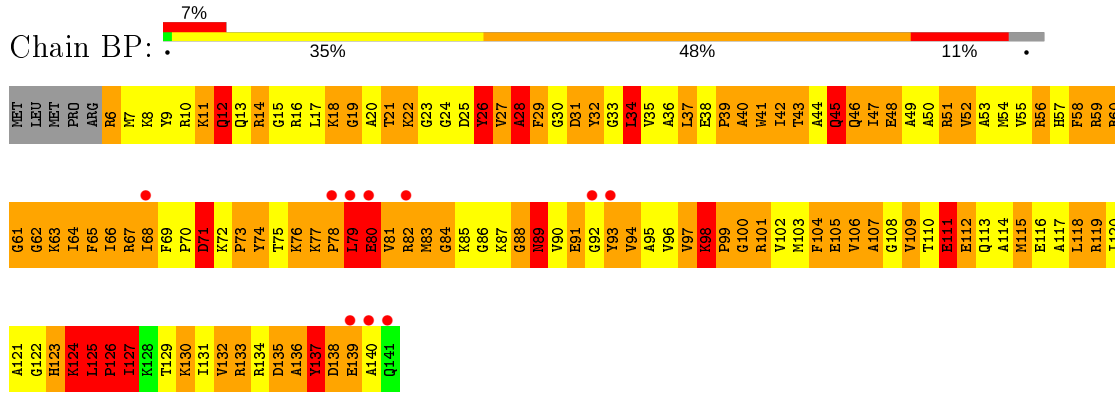


• Molecule 36: 50S ribosomal protein L15

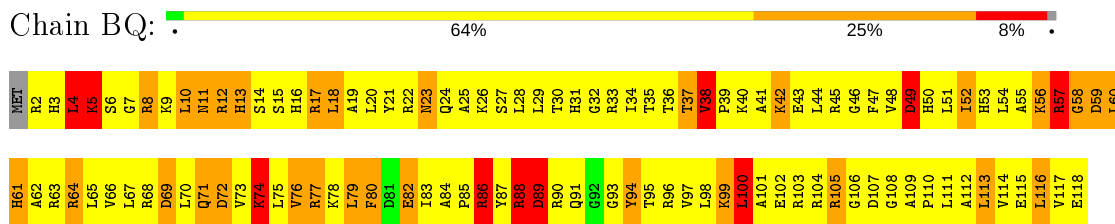




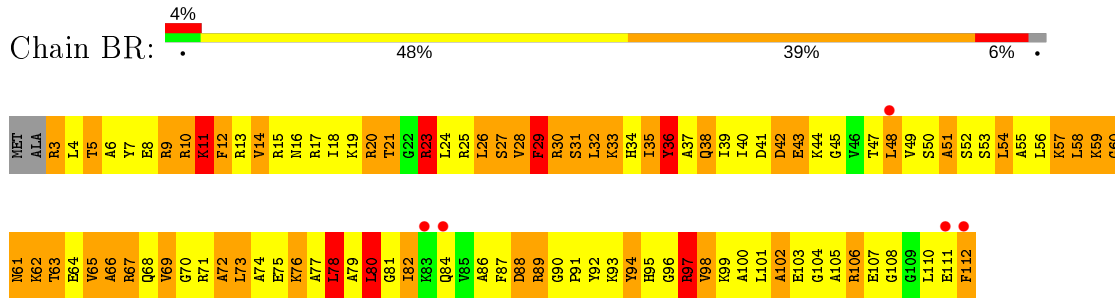
• Molecule 37: 50S ribosomal protein L16



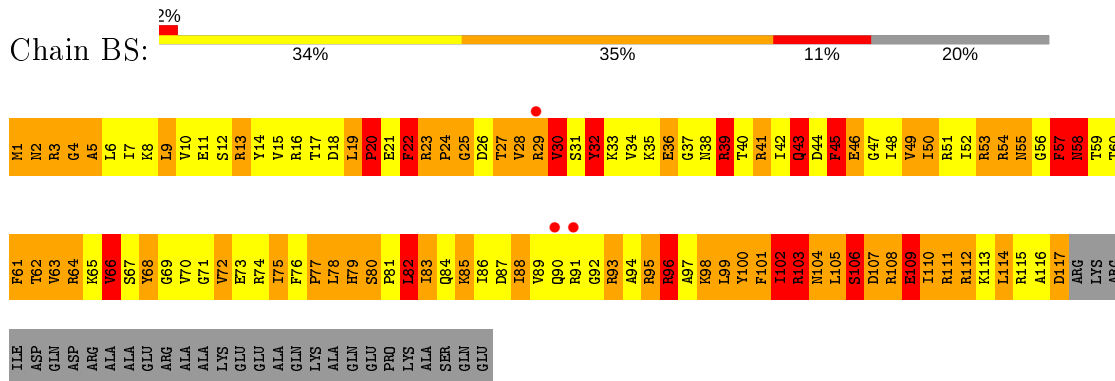
• Molecule 38: 50S ribosomal protein L17



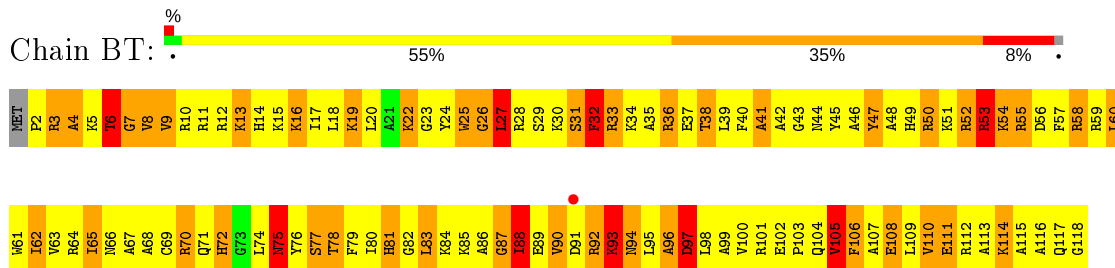
• Molecule 39: 50S ribosomal protein L18



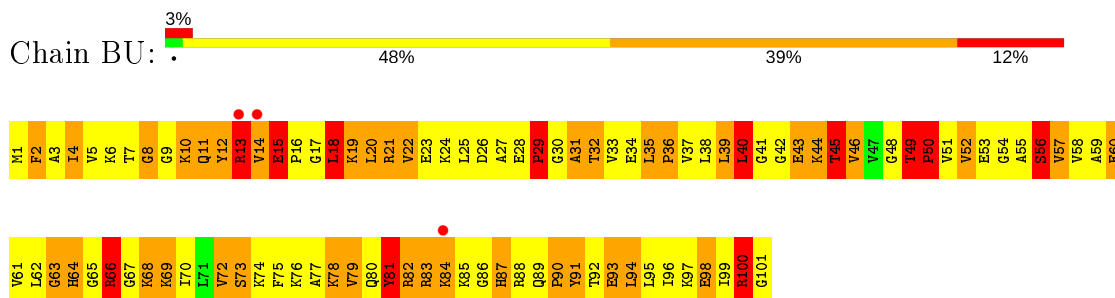
• Molecule 40: 50S ribosomal protein L19



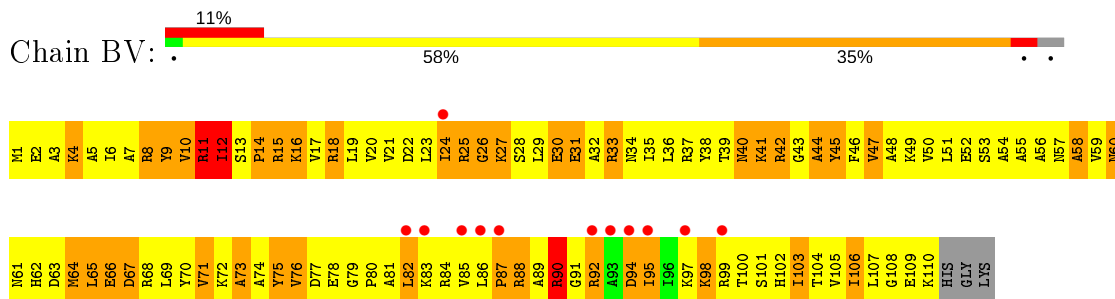
• Molecule 41: 50S ribosomal protein L20



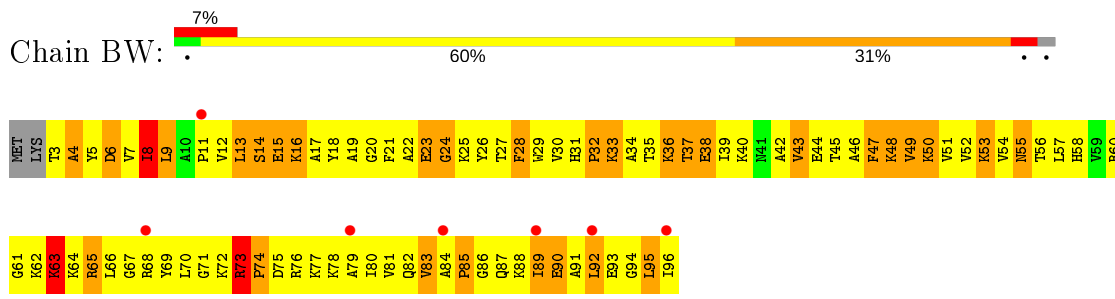
• Molecule 42: 50S ribosomal protein L21



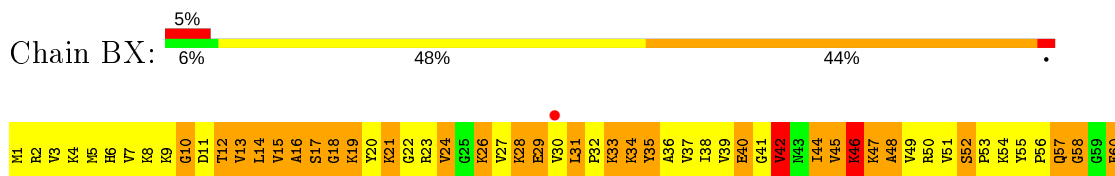
• Molecule 43: 50S ribosomal protein L22



• Molecule 44: 50S ribosomal protein L23

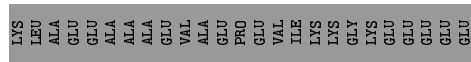
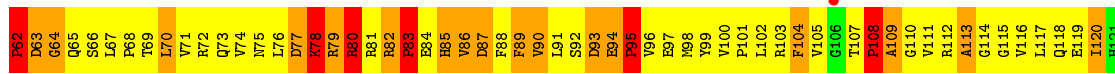
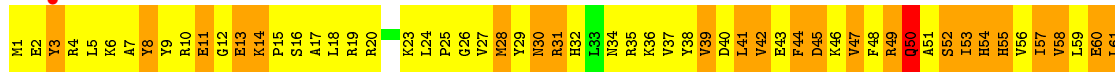


• Molecule 45: 50S ribosomal protein L24

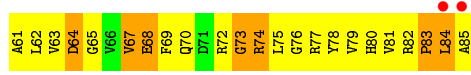
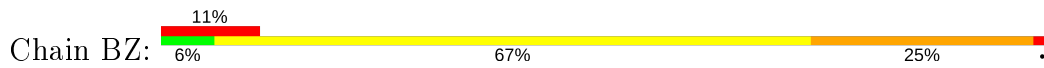




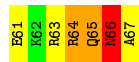
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: Ribosomal protein L27



• Molecule 48: 50S ribosomal protein L29

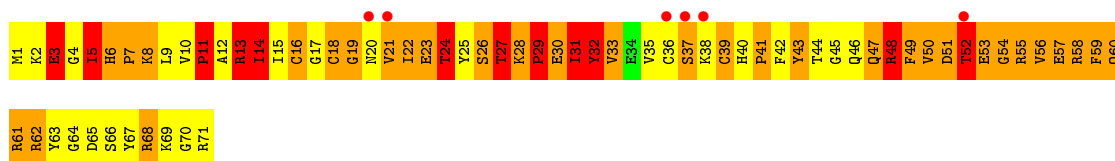


• Molecule 49: 50S ribosomal protein L30



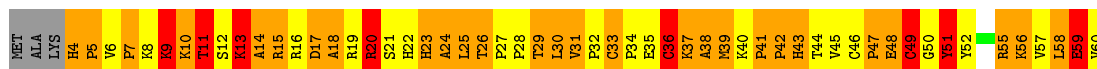
• Molecule 50: 50S ribosomal protein L31





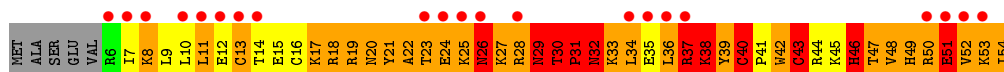
- Molecule 51: 50S ribosomal protein L32

Chain B4: 33% 45% 13% 5%



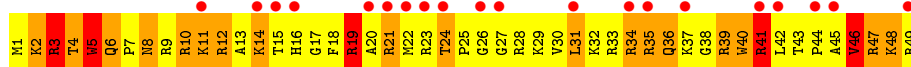
- Molecule 52: 50S ribosomal protein L33

Chain B5: 20% 39% 48% 20% 9%



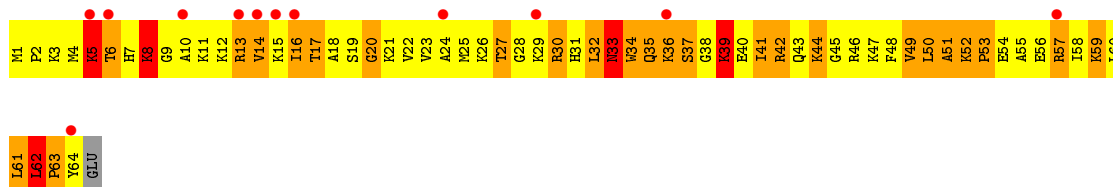
- Molecule 53: 50S ribosomal protein L34

Chain B6: 41% 53% 37% 10%



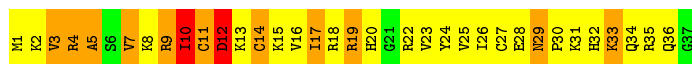
- Molecule 54: 50S ribosomal protein L35

Chain B7: 18% 52% 38% 8%



- Molecule 55: 50S ribosomal protein L36

Chain B8: 8% 57% 30% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.54Å 508.54Å 806.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 430.13 – 4.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-5.50) 99.1 (430.13-4.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.88Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.326 0.254 , 0.304	Depositor DCC
R_{free} test set	10840 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	151691	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.87	32/36438 (0.1%)	1.08	147/56869 (0.3%)
2	A1	0.67	1/1133 (0.1%)	0.93	2/1753 (0.1%)
3	AB	0.70	1/1813 (0.1%)	1.02	9/2823 (0.3%)
3	AC	0.98	2/1813 (0.1%)	0.93	2/2823 (0.1%)
3	AD	0.69	1/1813 (0.1%)	0.92	2/2823 (0.1%)
4	AE	0.64	0/1935	1.00	4/2609 (0.2%)
5	AF	0.55	0/1636	0.92	4/2205 (0.2%)
6	AG	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
7	AH	0.63	0/1162	1.01	3/1564 (0.2%)
8	AI	0.60	0/856	0.95	0/1154
9	AJ	0.57	0/1276	0.90	3/1709 (0.2%)
10	AK	0.62	0/1136	1.01	3/1527 (0.2%)
11	AL	0.54	0/1029	0.83	0/1379
12	AM	0.48	0/807	0.89	1/1085 (0.1%)
13	AN	0.62	0/900	0.98	0/1213
14	AO	0.60	0/986	1.00	3/1320 (0.2%)
15	AP	0.50	0/1008	0.91	2/1347 (0.1%)
16	AQ	0.55	0/501	0.96	1/664 (0.2%)
17	AR	0.62	0/745	0.95	0/992
18	AS	0.62	0/716	0.95	1/963 (0.1%)
19	AT	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
20	AU	0.59	0/603	1.01	1/799 (0.1%)
21	AV	0.51	0/661	0.92	0/890
22	AW	0.65	0/765	1.00	2/1007 (0.2%)
23	AX	0.45	0/212	0.80	0/277
24	BA	0.98	108/69685 (0.2%)	1.10	361/108786 (0.3%)
25	BB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
26	BC	0.54	0/1775	0.86	0/2393
27	BD	0.72	2/2174 (0.1%)	1.19	12/2927 (0.4%)
28	BE	0.75	0/1611	1.16	13/2171 (0.6%)
29	BF	0.64	0/1660	1.03	4/2247 (0.2%)
30	BG	0.62	0/1507	1.06	4/2027 (0.2%)
31	BH	0.59	0/1354	0.99	4/1831 (0.2%)
32	BK	0.60	0/1170	1.02	4/1581 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BL	0.61	0/1044	0.94	1/1415 (0.1%)
34	BM	0.77	1/1140 (0.1%)	1.16	8/1537 (0.5%)
35	BN	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
36	BO	0.71	0/1123	1.12	5/1493 (0.3%)
37	BP	0.72	0/1100	1.19	8/1470 (0.5%)
38	BQ	0.70	0/974	1.06	2/1302 (0.2%)
39	BR	0.72	0/887	1.06	4/1180 (0.3%)
40	BS	0.85	0/990	1.31	9/1325 (0.7%)
41	BT	0.76	0/982	1.08	0/1306
42	BU	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
43	BV	0.66	0/886	1.04	1/1189 (0.1%)
44	BW	0.57	0/756	0.93	0/1015
45	BX	0.54	0/857	1.04	2/1142 (0.2%)
46	BY	0.66	0/1467	1.11	7/1992 (0.4%)
47	BZ	0.65	0/679	1.04	1/902 (0.1%)
48	B1	0.59	0/569	0.88	0/751
49	B2	0.59	0/474	1.09	2/635 (0.3%)
50	B3	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
51	B4	0.71	0/459	1.16	3/621 (0.5%)
52	B5	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
53	B6	0.73	0/438	1.01	0/575
54	B7	0.60	0/523	1.14	5/690 (0.7%)
55	B8	0.59	0/310	1.08	1/407 (0.2%)
All	All	0.86	158/164854 (0.1%)	1.07	695/246484 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	175
2	A1	0	3
3	AB	0	6
3	AC	0	8
3	AD	0	8
6	AG	0	1
8	AI	0	1
13	AN	0	1
15	AP	0	1
16	AQ	0	1
24	BA	0	463

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BB	0	18
26	BC	0	1
28	BE	0	1
34	BM	0	1
37	BP	0	1
40	BS	0	1
42	BU	0	1
50	B3	0	1
51	B4	0	1
All	All	0	694

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-34.70	1.19	1.61
24	BA	2500	U	C4-O4	18.52	1.38	1.23
24	BA	2500	U	O3'-P	-15.17	1.43	1.61
24	BA	607	U	N3-C4	-14.53	1.25	1.38
24	BA	2448	A	O3'-P	-14.42	1.43	1.61

The worst 5 of 695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1064	G	N1-C2-N2	-71.65	51.71	116.20
1	AA	1064	G	N3-C2-N2	57.72	160.30	119.90
24	BA	1203	G	P-O3'-C3'	27.70	152.94	119.70
24	BA	2448	A	C5'-C4'-O4'	-27.31	76.33	109.10
1	AA	1064	G	N1-C2-N3	-25.51	108.59	123.90

There are no chirality outliers.

5 of 694 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	31	G	Sidechain
1	AA	37	U	Sidechain
1	AA	45	U	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32554	0	16431	6724	0
2	A1	1025	0	511	175	0
3	AB	1623	0	821	225	0
3	AC	1623	0	821	322	0
3	AD	1623	0	821	288	0
4	AE	1900	0	1951	1040	0
5	AF	1612	0	1677	721	0
6	AG	1703	0	1763	869	0
7	AH	1146	0	1207	588	0
8	AI	843	0	857	384	0
9	AJ	1257	0	1296	577	0
10	AK	1116	0	1177	735	0
11	AL	1010	0	1037	470	0
12	AM	794	0	840	358	0
13	AN	885	0	904	471	0
14	AO	970	0	1057	512	0
15	AP	997	0	1072	521	0
16	AQ	492	0	529	278	0
17	AR	734	0	771	332	0
18	AS	700	0	720	353	0
19	AT	857	0	930	450	0
20	AU	597	0	668	369	0
21	AV	647	0	673	312	0
22	AW	763	0	861	374	0
23	AX	208	0	221	83	0
24	BA	62218	0	31356	15296	0
25	BB	2641	0	1337	605	1
26	BC	1742	0	1796	739	0
27	BD	2124	0	2207	1491	0
28	BE	1578	0	1647	1084	0
29	BF	1625	0	1666	822	0
30	BG	1482	0	1546	898	0
31	BH	1328	0	1408	697	0
32	BK	1155	0	1244	502	0
33	BL	1025	0	1074	441	0
34	BM	1113	0	1183	782	0
35	BN	932	0	994	712	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BO	1106	0	1183	795	0
37	BP	1080	0	1127	752	0
38	BQ	960	0	1021	603	0
39	BR	877	0	938	517	0
40	BS	976	0	1033	636	0
41	BT	964	0	1022	742	0
42	BU	779	0	852	574	0
43	BV	876	0	941	459	0
44	BW	742	0	800	360	0
45	BX	844	0	930	421	0
46	BY	1435	0	1463	720	0
47	BZ	670	0	700	354	0
48	B1	567	0	621	312	0
49	B2	469	0	518	320	0
50	B3	581	0	577	397	0
51	B4	445	0	459	277	0
52	B5	426	0	452	279	0
53	B6	430	0	480	273	0
54	B7	515	0	587	396	0
55	B8	307	0	335	150	0
All	All	151691	0	103113	46416	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 183.

The worst 5 of 46416 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BA:2447:G:C8	24:BA:2500:U:H3'	1.23	1.61
24:BA:1202:C:C5	24:BA:1203:G:H1'	1.39	1.55
24:BA:1203:G:O6	24:BA:1240:U:C2	1.66	1.48
24:BA:2459:A:N3	24:BA:2460:U:H1'	1.38	1.38
24:BA:2596:U:H2'	27:BD:242:ARG:CZ	1.55	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BB:0:A:OP1	25:BB:0:A:OP1[15_545]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
4	AE	232/256 (91%)	114 (49%)	42 (18%)	76 (33%)	0	0
5	AF	204/239 (85%)	107 (52%)	46 (22%)	51 (25%)	0	1
6	AG	206/209 (99%)	96 (47%)	57 (28%)	53 (26%)	0	1
7	AH	148/162 (91%)	93 (63%)	38 (26%)	17 (12%)	0	6
8	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
9	AJ	153/156 (98%)	73 (48%)	45 (29%)	35 (23%)	0	1
10	AK	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	1
11	AL	125/128 (98%)	62 (50%)	33 (26%)	30 (24%)	0	1
12	AM	96/105 (91%)	52 (54%)	20 (21%)	24 (25%)	0	1
13	AN	117/129 (91%)	65 (56%)	29 (25%)	23 (20%)	0	2
14	AO	122/132 (92%)	50 (41%)	30 (25%)	42 (34%)	0	0
15	AP	123/126 (98%)	56 (46%)	34 (28%)	33 (27%)	0	0
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	3
18	AS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	2
19	AT	102/105 (97%)	62 (61%)	23 (22%)	17 (17%)	0	3
20	AU	71/88 (81%)	26 (37%)	26 (37%)	19 (27%)	0	0
21	AV	78/93 (84%)	32 (41%)	23 (30%)	23 (30%)	0	0
22	AW	97/106 (92%)	38 (39%)	32 (33%)	27 (28%)	0	0
23	AX	22/27 (82%)	9 (41%)	6 (27%)	7 (32%)	0	0
26	BC	226/229 (99%)	155 (69%)	41 (18%)	30 (13%)	0	4
27	BD	270/276 (98%)	125 (46%)	59 (22%)	86 (32%)	0	0
28	BE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
29	BF	206/210 (98%)	109 (53%)	46 (22%)	51 (25%)	0	1
30	BG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	172/180 (96%)	80 (46%)	46 (27%)	46 (27%)	0	0
32	BK	146/148 (99%)	91 (62%)	30 (20%)	25 (17%)	0	3
33	BL	136/147 (92%)	69 (51%)	38 (28%)	29 (21%)	0	2
34	BM	137/140 (98%)	64 (47%)	28 (20%)	45 (33%)	0	0
35	BN	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
36	BO	143/150 (95%)	57 (40%)	36 (25%)	50 (35%)	0	0
37	BP	134/141 (95%)	49 (37%)	33 (25%)	52 (39%)	0	0
38	BQ	115/118 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
39	BR	108/112 (96%)	48 (44%)	29 (27%)	31 (29%)	0	0
40	BS	115/146 (79%)	52 (45%)	26 (23%)	37 (32%)	0	0
41	BT	115/118 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
42	BU	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
43	BV	108/113 (96%)	63 (58%)	24 (22%)	21 (19%)	0	2
44	BW	92/96 (96%)	57 (62%)	16 (17%)	19 (21%)	0	2
45	BX	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
46	BY	178/206 (86%)	95 (53%)	44 (25%)	39 (22%)	0	1
47	BZ	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	6
48	B1	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	4
49	B2	57/60 (95%)	34 (60%)	8 (14%)	15 (26%)	0	1
50	B3	69/71 (97%)	23 (33%)	16 (23%)	30 (44%)	0	0
51	B4	55/60 (92%)	14 (26%)	19 (34%)	22 (40%)	0	0
52	B5	47/54 (87%)	14 (30%)	7 (15%)	26 (55%)	0	0
53	B6	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
All	All	5988/6337 (94%)	2955 (49%)	1476 (25%)	1557 (26%)	0	1

5 of 1557 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	8	LYS
4	AE	11	LEU
4	AE	13	ALA

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Mol	Chain	Res	Type
4	AE	15	VAL
4	AE	16	HIS

5.3.2 Protein sidechains [i](#)

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
4	AE	202/220 (92%)	138 (68%)	64 (32%)	0 2
5	AF	160/188 (85%)	123 (77%)	37 (23%)	1 5
6	AG	180/181 (99%)	131 (73%)	49 (27%)	0 3
7	AH	115/123 (94%)	78 (68%)	37 (32%)	0 2
8	AI	90/90 (100%)	61 (68%)	29 (32%)	0 2
9	AJ	126/127 (99%)	93 (74%)	33 (26%)	0 3
10	AK	119/119 (100%)	86 (72%)	33 (28%)	0 3
11	AL	98/99 (99%)	73 (74%)	25 (26%)	0 4
12	AM	88/92 (96%)	67 (76%)	21 (24%)	0 4
13	AN	90/99 (91%)	74 (82%)	16 (18%)	2 11
14	AO	104/109 (95%)	81 (78%)	23 (22%)	1 6
15	AP	100/101 (99%)	75 (75%)	25 (25%)	0 4
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0 3
17	AR	79/80 (99%)	64 (81%)	15 (19%)	1 9
18	AS	72/74 (97%)	49 (68%)	23 (32%)	0 2
19	AT	96/97 (99%)	67 (70%)	29 (30%)	0 2
20	AU	64/77 (83%)	48 (75%)	16 (25%)	0 4
21	AV	71/80 (89%)	55 (78%)	16 (22%)	1 6
22	AW	76/82 (93%)	59 (78%)	17 (22%)	1 6
23	AX	19/22 (86%)	17 (90%)	2 (10%)	7 26
26	BC	180/181 (99%)	151 (84%)	29 (16%)	2 14
27	BD	215/218 (99%)	153 (71%)	62 (29%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
29	BF	164/166 (99%)	105 (64%)	59 (36%)	0	1
30	BG	156/156 (100%)	112 (72%)	44 (28%)	0	3
31	BH	143/148 (97%)	109 (76%)	34 (24%)	0	4
32	BK	124/124 (100%)	92 (74%)	32 (26%)	0	4
33	BL	105/111 (95%)	89 (85%)	16 (15%)	3	15
34	BM	118/119 (99%)	79 (67%)	39 (33%)	0	2
35	BN	100/100 (100%)	69 (69%)	31 (31%)	0	2
36	BO	111/116 (96%)	71 (64%)	40 (36%)	0	1
37	BP	106/111 (96%)	65 (61%)	41 (39%)	0	0
38	BQ	100/101 (99%)	71 (71%)	29 (29%)	0	2
39	BR	87/88 (99%)	63 (72%)	24 (28%)	0	3
40	BS	105/127 (83%)	68 (65%)	37 (35%)	0	1
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
42	BU	82/82 (100%)	57 (70%)	25 (30%)	0	2
43	BV	90/92 (98%)	64 (71%)	26 (29%)	0	2
44	BW	76/78 (97%)	57 (75%)	19 (25%)	0	4
45	BX	91/91 (100%)	72 (79%)	19 (21%)	1	7
46	BY	159/179 (89%)	120 (76%)	39 (24%)	0	4
47	BZ	67/67 (100%)	51 (76%)	16 (24%)	0	4
48	B1	62/62 (100%)	44 (71%)	18 (29%)	0	2
49	B2	51/52 (98%)	36 (71%)	15 (29%)	0	2
50	B3	63/63 (100%)	45 (71%)	18 (29%)	0	2
51	B4	50/52 (96%)	31 (62%)	19 (38%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	44 (82%)	10 (18%)	1	10
55	B8	34/34 (100%)	29 (85%)	5 (15%)	3	16
All	All	5040/5237 (96%)	3649 (72%)	1391 (28%)	0	3

5 of 1391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BE	45	THR
30	BG	174	GLU
48	B1	32	PHE
28	BE	119	ARG
29	BF	106	ARG

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

Mol	Chain	Res	Type
26	BC	148	ASN
30	BG	40	ASN
52	B5	20	ASN
26	BC	188	ASN
28	BE	55	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	463 (30%)	137 (9%)
2	A1	49/50 (98%)	21 (42%)	4 (8%)
24	BA	2888/2916 (99%)	1204 (41%)	253 (8%)
25	BB	122/123 (99%)	46 (37%)	3 (2%)
3	AB	75/76 (98%)	32 (42%)	1 (1%)
3	AC	75/76 (98%)	23 (30%)	4 (5%)
3	AD	75/76 (98%)	23 (30%)	1 (1%)
All	All	4799/4839 (99%)	1812 (37%)	403 (8%)

5 of 1812 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	19	C

5 of 403 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	503	A
24	BA	944	G

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Mol	Chain	Res	Type
24	BA	2571	C
24	BA	530	G
24	BA	745	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2756:U	O3'	2757:A	P	1.77
1	BA	1203:G	O3'	1204:A	P	1.19

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1515/1522 (99%)	-0.35	2 (0%) 95 94	145, 221, 302, 356	0
2	A1	50/50 (100%)	-0.06	1 (2%) 65 57	200, 320, 348, 357	0
3	AB	76/76 (100%)	14.11	68 (89%) 0 0	288, 351, 370, 374	0
3	AC	76/76 (100%)	0.58	10 (13%) 3 6	167, 214, 260, 284	0
3	AD	76/76 (100%)	0.07	8 (10%) 6 8	222, 271, 293, 316	0
4	AE	234/256 (91%)	-1.03	0 100 100	189, 226, 271, 304	0
5	AF	206/239 (86%)	-0.23	10 (4%) 29 27	222, 244, 266, 277	0
6	AG	208/209 (99%)	-0.42	4 (1%) 66 58	168, 215, 233, 242	0
7	AH	150/162 (92%)	-0.73	0 100 100	174, 210, 235, 257	0
8	AI	101/101 (100%)	1.25	30 (29%) 0 1	191, 223, 236, 261	0
9	AJ	155/156 (99%)	0.62	20 (12%) 3 6	210, 240, 256, 275	0
10	AK	138/138 (100%)	-1.14	0 100 100	186, 208, 225, 232	0
11	AL	127/128 (99%)	-0.98	0 100 100	222, 261, 276, 287	0
12	AM	98/105 (93%)	-0.53	2 (2%) 65 57	230, 260, 274, 282	0
13	AN	119/129 (92%)	0.77	17 (14%) 2 5	193, 212, 245, 267	0
14	AO	124/132 (93%)	0.41	11 (8%) 9 11	179, 199, 233, 267	0
15	AP	125/126 (99%)	-0.78	0 100 100	223, 243, 272, 278	0
16	AQ	60/61 (98%)	-0.92	0 100 100	215, 248, 259, 263	0
17	AR	88/89 (98%)	-0.57	1 (1%) 80 73	186, 207, 231, 238	0
18	AS	83/88 (94%)	-0.98	0 100 100	180, 201, 226, 249	0
19	AT	104/105 (99%)	-0.52	1 (0%) 82 75	164, 193, 244, 277	0
20	AU	73/88 (82%)	-0.42	6 (8%) 11 12	184, 209, 258, 287	0
21	AV	80/93 (86%)	-0.05	4 (5%) 28 26	226, 252, 266, 270	0
22	AW	99/106 (93%)	-0.22	7 (7%) 16 15	167, 195, 225, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	AX	24/27 (88%)	-1.10	0 100 100	230, 249, 280, 288	0
24	BA	2889/2916 (99%)	-0.28	57 (1%) 65 57	129, 215, 297, 342	0
25	BB	123/123 (100%)	-0.51	0 100 100	199, 259, 293, 316	0
26	BC	228/229 (99%)	0.60	42 (18%) 1 3	250, 281, 300, 313	0
27	BD	272/276 (98%)	2.05	125 (45%) 0 0	130, 199, 221, 259	0
28	BE	206/206 (100%)	-0.56	3 (1%) 73 64	148, 186, 232, 269	0
29	BF	208/210 (99%)	-0.15	11 (5%) 26 25	164, 238, 263, 276	0
30	BG	182/182 (100%)	0.29	16 (8%) 10 11	212, 246, 268, 276	0
31	BH	174/180 (96%)	-0.91	0 100 100	196, 241, 260, 271	0
32	BK	148/148 (100%)	-0.88	0 100 100	202, 227, 249, 257	0
33	BL	138/147 (93%)	-0.40	3 (2%) 62 53	271, 298, 312, 327	0
34	BM	139/140 (99%)	-0.73	1 (0%) 87 82	167, 198, 224, 235	0
35	BN	122/122 (100%)	-0.27	0 100 100	148, 177, 209, 221	0
36	BO	145/150 (96%)	0.80	20 (13%) 2 5	166, 247, 276, 315	0
37	BP	136/141 (96%)	0.33	10 (7%) 14 14	166, 208, 234, 241	0
38	BQ	117/118 (99%)	-0.49	0 100 100	168, 192, 219, 226	0
39	BR	110/112 (98%)	-0.50	5 (4%) 33 29	186, 235, 263, 289	0
40	BS	117/146 (80%)	-0.12	3 (2%) 56 47	164, 194, 227, 242	0
41	BT	117/118 (99%)	-0.46	1 (0%) 84 77	183, 202, 220, 232	0
42	BU	101/101 (100%)	-0.28	3 (2%) 50 41	168, 225, 246, 257	0
43	BV	110/113 (97%)	0.28	12 (10%) 5 8	180, 209, 237, 248	0
44	BW	94/96 (97%)	0.26	7 (7%) 14 14	212, 232, 280, 288	0
45	BX	110/110 (100%)	-0.24	6 (5%) 25 24	221, 255, 287, 305	0
46	BY	180/206 (87%)	0.04	5 (2%) 53 44	208, 246, 268, 279	0
47	BZ	85/85 (100%)	0.48	9 (10%) 6 8	211, 229, 242, 271	0
48	B1	67/67 (100%)	-0.37	0 100 100	218, 243, 263, 268	0
49	B2	59/60 (98%)	0.05	2 (3%) 45 38	204, 224, 249, 259	0
50	B3	71/71 (100%)	0.37	6 (8%) 10 11	199, 223, 238, 246	0
51	B4	57/60 (95%)	-0.46	0 100 100	164, 209, 264, 289	0
52	B5	49/54 (90%)	1.78	21 (42%) 0 0	206, 232, 242, 252	0
53	B6	49/49 (100%)	1.69	20 (40%) 0 0	162, 209, 221, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	B7	64/65 (98%)	0.97	12 (18%) 1 3	164, 195, 225, 242	0
55	B8	37/37 (100%)	-1.02	0 100 100	205, 215, 224, 226	0
All	All	10893/11176 (97%)	-0.08	602 (5%) 25 24	129, 223, 295, 374	0

The worst 5 of 602 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AB	69	G	37.6
3	AB	67	C	32.7
3	AB	70	G	30.8
3	AB	68	C	30.1
3	AB	19	G	29.9

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.