



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:29 pm GMT

PDB ID : 4V69  
EMDB ID: : EMD-5036  
Title : Ternary complex-bound E.coli 70S ribosome.  
Authors : Villa, E.; Sengupta, J.; Trabuco, L.G.; LeBarron, J.; Baxter, W.T.; Shaikh, T.R.; Grassucci, R.A.; Nissen, P.; Ehrenberg, M.; Schulten, K.; Frank, J.  
Deposited on : 2008-12-11  
Resolution : 6.70 Å(reported)  
Based on PDB ID : 2i2u, 2i2v, 2j00, 1ob2

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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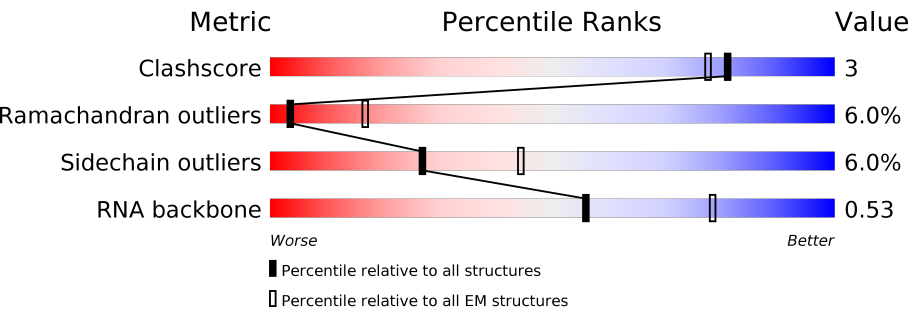
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.70 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	AJ	98	66% 26% 7% .
2	AK	117	69% 26% ..
3	AL	123	67% 26% 7% .
4	AM	113	58% 28% 13%
5	AN	96	58% 28% 13% .
6	AO	88	65% 27% 6% .
7	AP	80	65% 29% 6%
8	AQ	80	74% 18% 9%









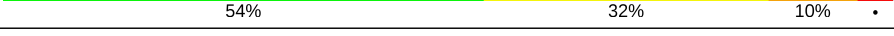


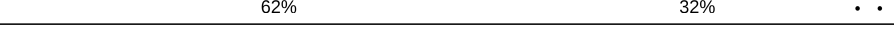

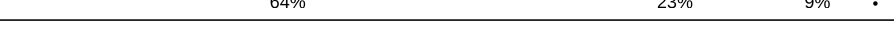


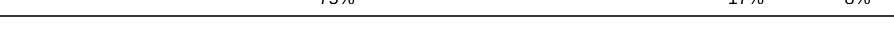

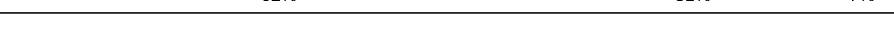
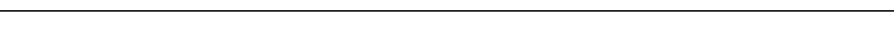

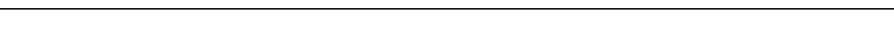



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Mol	Chain	Length	Quality of chain
9	AR	55	
10	AS	79	
11	AT	85	
12	AU	51	
13	AB	218	
14	AC	206	
15	AD	205	
16	AE	150	
17	AF	100	
18	AG	150	
19	AH	129	
20	AI	127	
21	AA	1530	
22	AY	76	
23	AW	76	
24	AX	11	
25	AZ	393	
26	AV	77	
27	B5	234	
28	BI	141	
29	BJ	142	
30	BK	121	
31	BL	143	
32	BM	136	
33	BN	120	

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Mol	Chain	Length	Quality of chain
34	BO	116	
35	BP	114	
36	BQ	117	
37	BR	103	
38	BS	110	
39	BT	93	
40	BU	102	
41	BV	94	
42	BW	79	
43	BX	77	
44	BY	63	
45	BC	271	
46	BZ	58	
47	B0	56	
48	B1	50	
49	B2	46	
50	B3	64	
51	B4	38	
52	BD	209	
53	BE	201	
54	BF	178	
55	BG	176	
56	BH	149	
57	BB	2903	
58	BA	117	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 152250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	113	Total	C	N	O	S	0	0
			877	541	177	156	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	SER	DELETION	UNP P0AG59
AN	?	-	ASP	DELETION	UNP P0AG59
AN	?	-	GLU	DELETION	UNP P0AG59

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Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	ASP	DELETION	UNP P0AG59

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	80	Total	C	N	O	S	0	0
			639	400	126	112	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AR	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 11 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 12 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AU	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 13 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AB	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 15 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	150	Total	C	N	O	S	0	0
			1175	730	226	215	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32832	14642	6024	10636	1530		

- Molecule 22 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AY	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 23 is a RNA chain called P-site tRNA fMet (Unmodified bases except for Thymine 54).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0
			232	106	44	72	10		

- Molecule 25 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AZ	393	Total	C	N	O	S	0	0
			3035	1918	523	581	13		

- Molecule 26 is a RNA chain called E-site tRNA Phe.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	77	Total	C	N	O	P	0	0
			1645	733	297	538	77		

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BK	121	Total	C	N	O	S	0	0
			931	582	179	165	5		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BN	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BT	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BU	102	Total	C	N	O		
			780	492	146	142	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BW	79	Total	C	N	O	S		
			596	367	120	108	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BC	271	Total	C	N	O	S		
			2083	1288	423	365	7	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 53 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

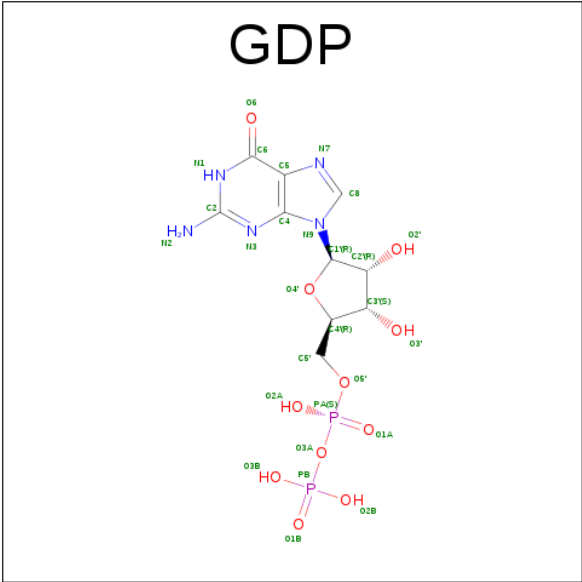
- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BB	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BA	117	Total	C	N	O	P	0	0
			2508	1116	459	816	117		

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

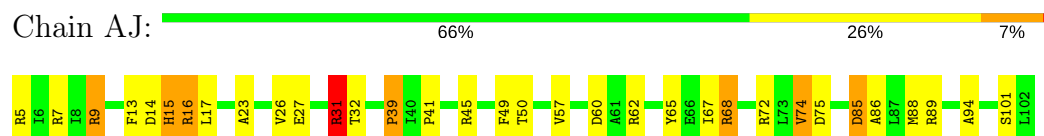


Mol	Chain	Residues	Atoms					AltConf
59	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	

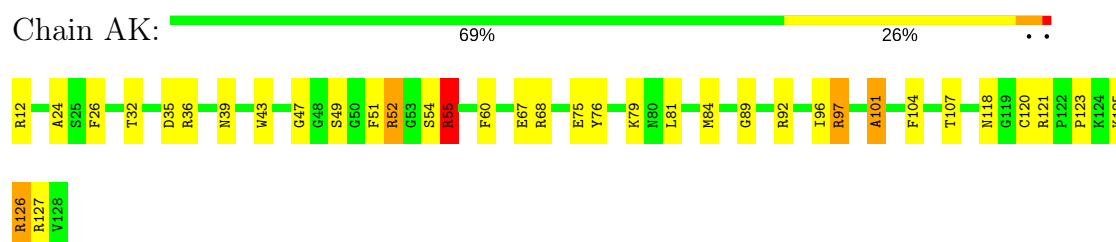
### 3 Residue-property plots

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. 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. 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.

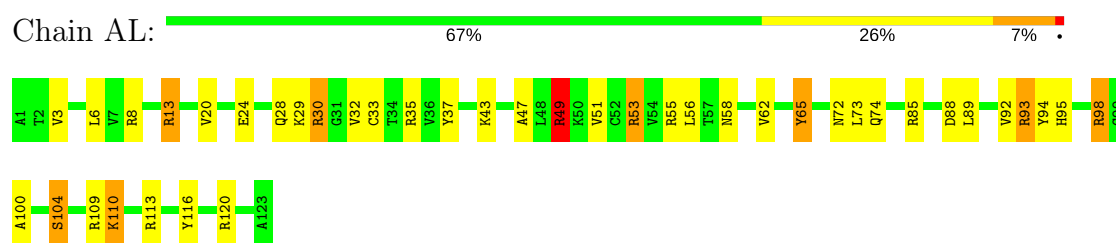
- Molecule 1: 30S ribosomal protein S10



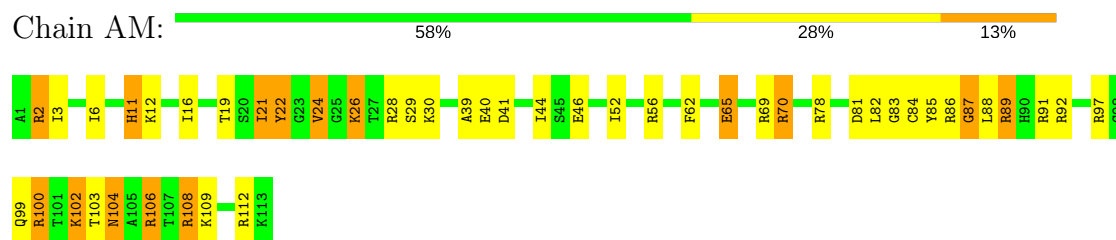
- Molecule 2: 30S ribosomal protein S11



- Molecule 3: 30S ribosomal protein S12

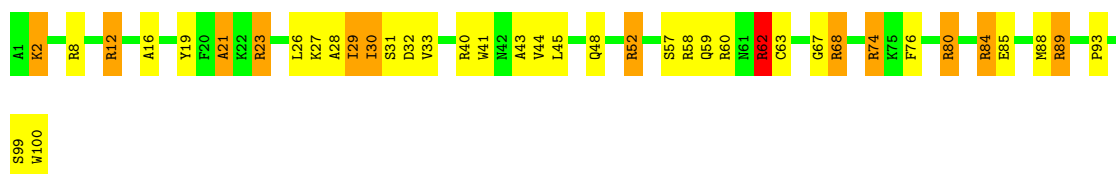


- Molecule 4: 30S ribosomal protein S13



- Molecule 5: 30S ribosomal protein S14





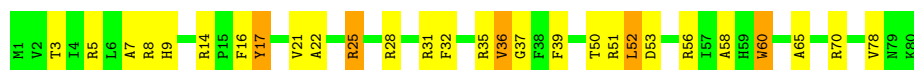
- Molecule 6: 30S ribosomal protein S15

Chain AO: 65% 27% 6%



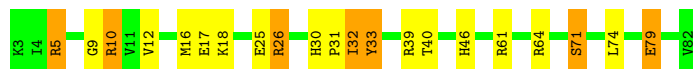
- Molecule 7: 30S ribosomal protein S16

Chain AP: 65% 29% 6%



- Molecule 8: 30S ribosomal protein S17

Chain AQ: 74% 18% 9%



- Molecule 9: 30S ribosomal protein S18

Chain AR: 67% 22% 11%



- Molecule 10: 30S ribosomal protein S19

Chain AS: 65% 27% 9%



- Molecule 11: 30S ribosomal protein S20

Chain AT: 76% 20% 4%



- Molecule 12: 30S ribosomal protein S21

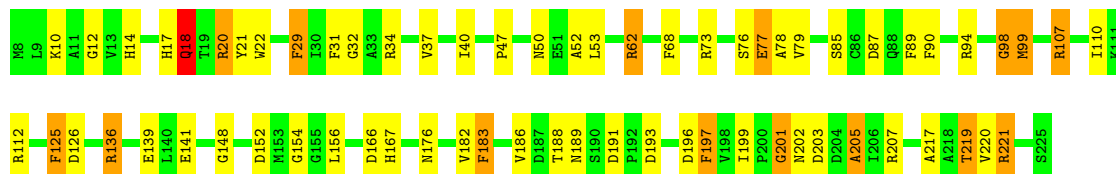
Chain AU: 59% 29% 12%





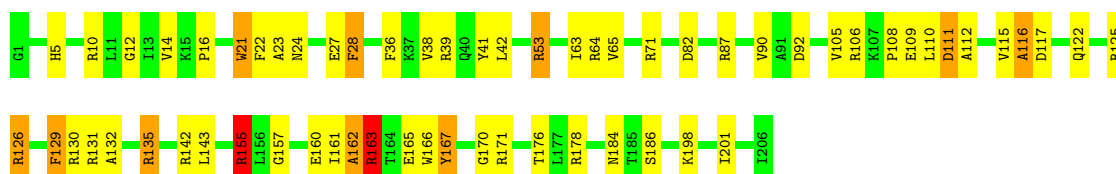
- Molecule 13: 30S ribosomal protein S2

Chain AB: 70% 23% 7%



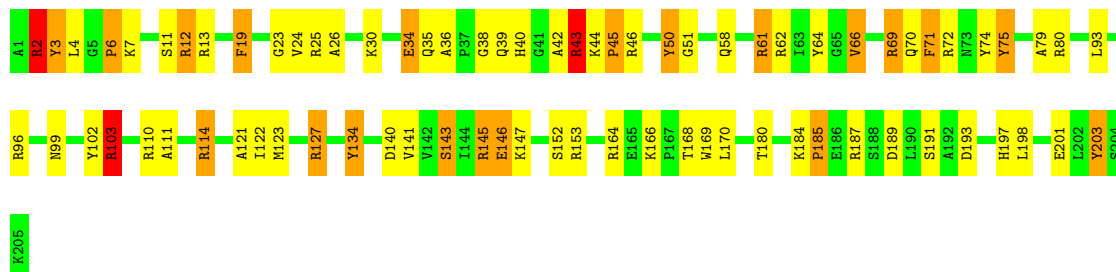
- Molecule 14: 30S ribosomal protein S3

Chain AC: 70% 24% 5%



- Molecule 15: 30S ribosomal protein S4

Chain AD: 62% 26% 10%



- Molecule 16: 30S ribosomal protein S5

Chain AE: 68% 29% 3%



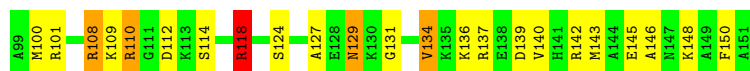
- Molecule 17: 30S ribosomal protein S6

Chain AF: 69% 25% 5%



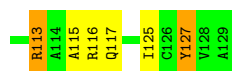
- Molecule 18: 30S ribosomal protein S7

Chain AG: 60% 33% 6%



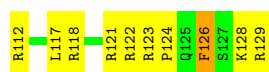
- Molecule 19: 30S ribosomal protein S8

Chain AH: 68% 27% 5%



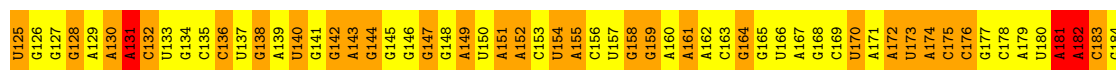
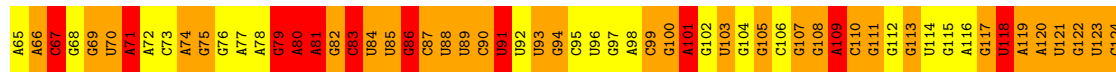
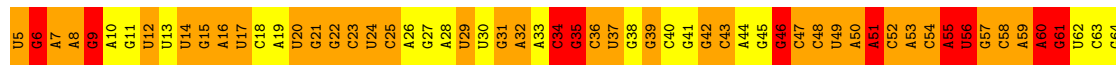
- Molecule 20: 30S ribosomal protein S9

Chain AI: 65% 28% 6%

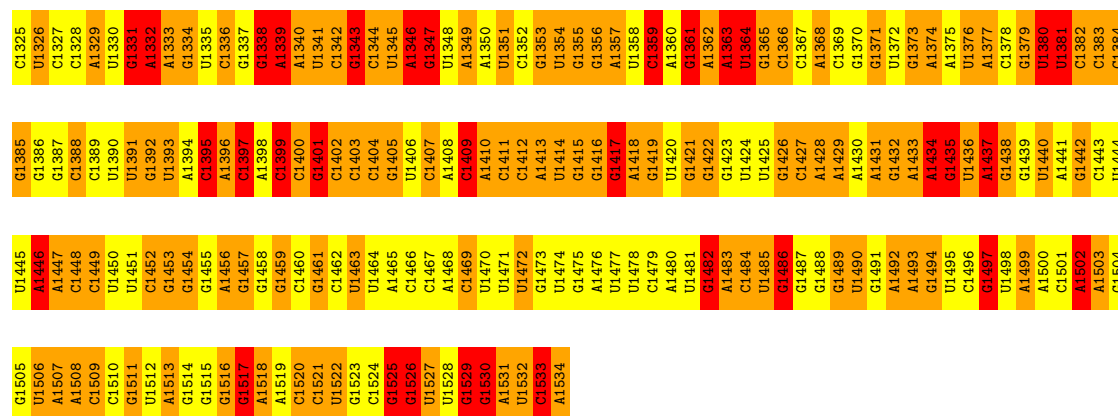


- Molecule 21: 16S rRNA

Chain AA: 36% 47% 16%

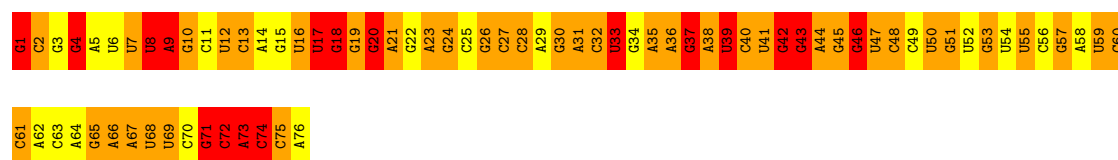


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G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G726	G866	G606	A546	U486	U426	A366	A306
C1267	C1207	U1147	G1087	C1027	G967	A907	G847	G727	G867	A607	A547	U487	U427	U367	C307
G1268	G1208	U1148	G1088	C1028	A968	A908	G848	A728	G868	A608	C548	C488	C428	U368	C308
A1269	A1209	C1149	G1089	U1029	G969	A909	G849	A729	G869	A609	C549	C489	U429	G369	A309
C1210	C1210	C1150	U1090	U1030	C970	C910	U850	G730	G670	U610	C550	C490	A430	C370	G310
A1271	A1211	A1151	U1091	C1031	G971	U911	G851	G731	G871	C611	U551	G491	A431	A371	C311
G1272	U1212	A1152	A1092	G1032	C972	C912	G852	G732	U872	C612	U552	C492	A432	C372	C312
C1213	C1273	G1153	A1093	G1033	G973	A913	C853	G733	U873	C613	A553	G493	A433	A373	A313
A1274	C1214	G1154	G1094	A1034	A974	A914	U854	G734	G874	C614	U554	G494	U434	A374	C314
C1215	G1215	A1155	U1095	A1035	A975	A915	U855	G735	G875	G615	U555	G495	U435	U375	A315
G1216	A1216	C1156	C1096	A1036	G976	U916	C856	G736	G876	G616	C556	A496	C436	G376	G316
C1217	C1217	A1157	C1097	A1037	G977	G917	C857	G737	U877	C617	U557	G497	U437	G377	U317
G1218	C1218	C1158	C1098	C1038	A978	A918	G858	G738	U878	C618	C558	A498	U438	G378	G318
A1279	A1219	U1159	G1099	G1039	C979	A919	G859	G739	C879	U619	A559	A499	U439	C379	G319
C1280	G1220	C1160	C1100	U1040	C980	U920	A860	U740	C880	U620	A560	G500	C440	G380	A320
C1281	G1221	C1161	A1101	U1041	U981	U921	G861	G741	A681	A621	U561	C501	A441	C381	A321
U1263	G1222	C1162	U982	A1042	G982	G922	C862	G742	A682	A622	U562	A502	G442	A382	C322
C1284	U1224	A1163	C1103	G1043	C983	A923	U863	A743	G683	C623	C563	C503	C443	A383	U323
A1285	A1225	G1164	G1104	A1044	C984	C924	A864	G744	U684	C624	C564	C504	G445	C384	G324
U1286	C1226	U1165	A1105	C1045	G985	G925	A865	G745	G685	U625	U565	G505	G445	C385	A325
A1287	A1227	G1166	G1106	A1046	U986	G926	C866	A746	U686	G626	C566	G506	G446	C386	G326
C1288	C1228	A1168	G1108	G1048	G988	G928	G868	A748	G688	G628	C568	U508	A448	U387	A327
A1289	A1229	C1169	C1109	U1049	U989	G929	G869	G749	C889	A629	C569	A509	G449	A389	C328
G1290	C1230	A1170	A1110	G1050	C990	C930	U870	G750	G890	A630	C570	A510	G450	U390	C330
U1291	G1231	C1171	A1111	C1051	U991	C931	U871	G751	G891	C631	U571	C511	A451	G391	G331
C1292	U1232	C1172	C1112	U1052	U992	C932	A872	G752	U892	U632	A572	U512	A452	C392	C332
C1293	G1233	U1173	C1113	G1053	G993	G933	A873	A753	G893	G633	A573	C513	G453	A393	U333
U1294	C1234	A1174	A994	C1174	G994	C934	G874	G754	A694	C634	A574	C514	G454	G394	C334
U1295	U1235	G1175	U1115	A1055	C995	A935	U875	G755	A695	A635	C575	G515	G455	C395	C335
C1296	A1236	A1176	U1116	U1056	A996	C936	C876	G756	A696	C636	C576	U516	A456	C396	A336
G1297	C1237	U1177	A1117	G1057	U997	A937	G877	U757	U897	C637	G577	C517	G457	A397	G337
A1298	A1238	G1178	U1118	G1058	C998	A938	A878	G758	G898	U638	C578	C518	U458	U398	A338
U1299	C1239	A1179	C1119	U1059	C999	G939	C879	A759	G899	A639	A579	C519	G459	A399	C339
G1300	U1240	A1180	C1120	U1060	A1000	C940	C880	G760	G900	A640	C580	A520	A460	C400	U340
U1301	G1241	G1181	U1121	G1061	C1001	G941	G881	G761	U701	U641	G581	G521	A461	C401	C341
C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	U762	A702	A642	C582	C522	G462	G402	C342
G1303	C1243	U1183	U1123	C1063	G1003	U943	C883	G763	G703	C643	A583	A523	U463	C403	U343
C1304	G1244	G1184	G1124	U1064	A1004	G944	U884	G764	A704	U644	G584	G524	U464	G404	A344
G1305	C1245	G1185	U1125	G1065	A1005	G945	G885	G765	G705	G645	C585	C525	A465	U405	C345
A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	A766	A706	G646	C586	C526	A466	G406	G346
U1307	U1247	G1187	G1127	A1067	U1007	G947	G887	A767	U707	C647	G587	C527	U467	U407	G347
U1308	C1248	A1188	C1128	G1068	U1008	C948	G888	A768	C708	A648	G588	C528	A468	A408	G348
G1310	U1250	U1189	C1129	C1069	U1009	A949	A889	G769	U709	A649	U589	G529	C469	U409	A349
A1311	A1251	A1191	A1131	U1071	U1010	U950	G890	C770	G710	G650	U590	G530	C470	A410	G350
G1312	A1252	C1192	C1132	G1072	C1011	G951	U891	G771	G711	C651	U591	U531	U471	A411	G351
U1313	G1253	G1193	G1133	U1073	G1012	U952	A892	U772	A712	U652	C592	A532	U472	G412	C352
C1314	A1254	U1194	G1134	G1074	A1014	G954	G894	G774	G714	G654	U594	U534	G474	A414	A353
U1315	G1255	C1195	U1135	U1075	G1015	U955	G895	G775	A715	A655	A595	A535	C475	A415	C355
A1316	A1256	A1196	C1136	U1076	A1016	U956	C896	G776	A716	G656	A596	A536	C476	A416	A356
C1317	G1257	U1197	C1137	G1077	U1017	U957	C897	A777	U717	U657	C597	G537	C477	G417	C357
A1318	A1258	G1198	G1138	U1078	G1018	A958	G898	G778	A718	C658	U598	G538	C478	A418	U358
U1319	C1259	U1199	C1139	G1079	C899	U959	G899	C779	C599	U659	C599	A539	U479	C419	G359
G1320	G1260	C1200	C1140	A1080	U1020	U960	A900	A780	C720	C660	A600	G540	U480	U420	G360
U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	A781	G721	C661	G501	G541	G481	U421	G361
C1322	C1262	U1202	G1142	A1082	A1022	C962	G902	A782	G722	U662	A602	G542	A482	C422	G362
G1323	U1083	C1203	G1143	U1083	A1023	G963	G903	A783	U723	U663	U603	G543	C483	G423	A363
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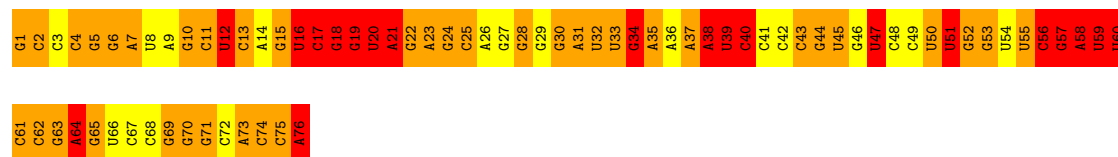
• Molecule 22: A/T-site tRNA Phe

Chain AY: 26% 51% 22%



• Molecule 23: P-site tRNA fMet (Unmodified bases except for Thymine 54)

Chain AW: 24% 50% 26%



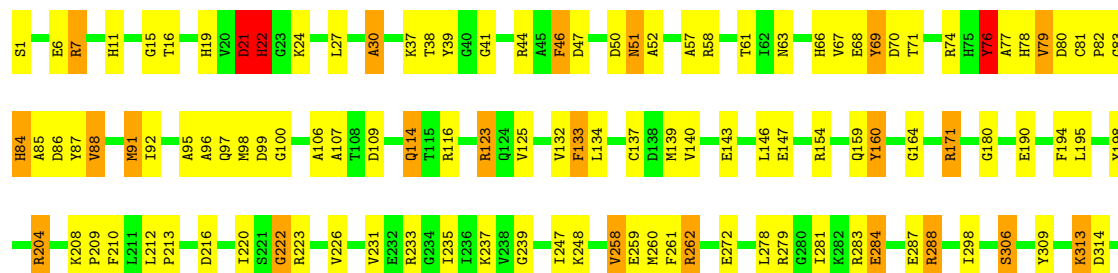
• Molecule 24: mRNA

Chain AX: 55% 27% 18%



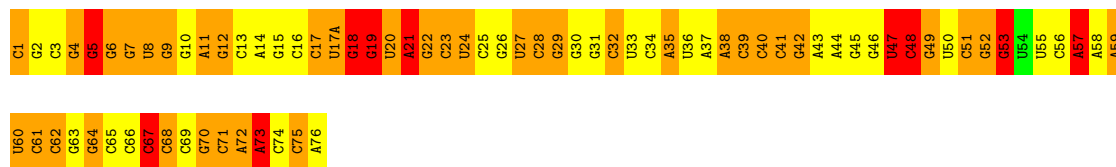
• Molecule 25: Elongation factor Tu

Chain AZ: 64% 28% 7%

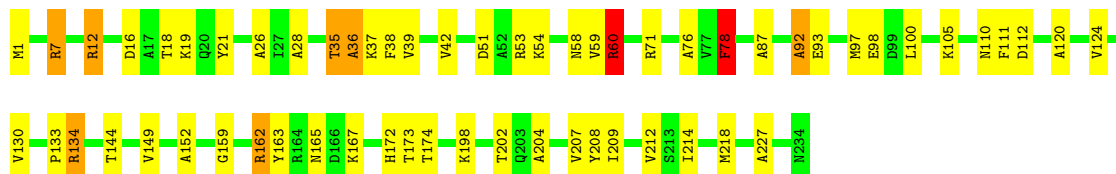




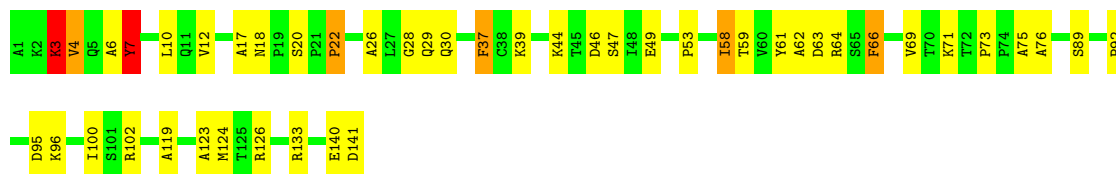
• Molecule 26: E-site tRNA Phe



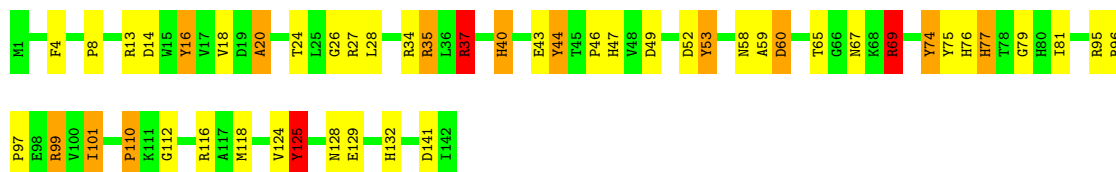
• Molecule 27: 50S ribosomal protein L1



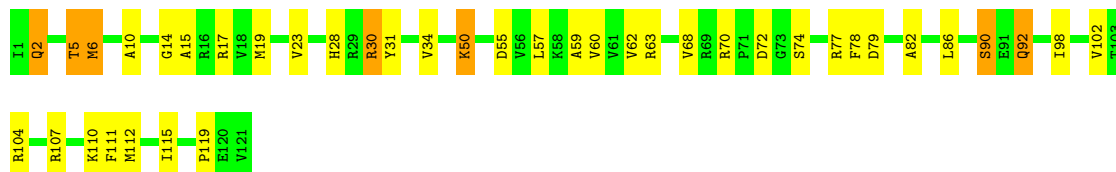
• Molecule 28: 50S ribosomal protein L11



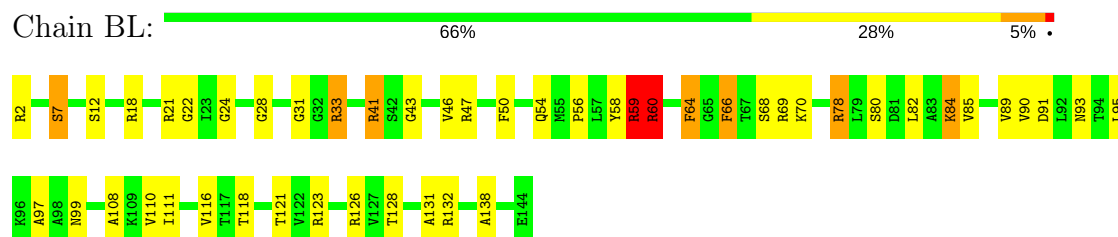
• Molecule 29: 50S ribosomal protein L13



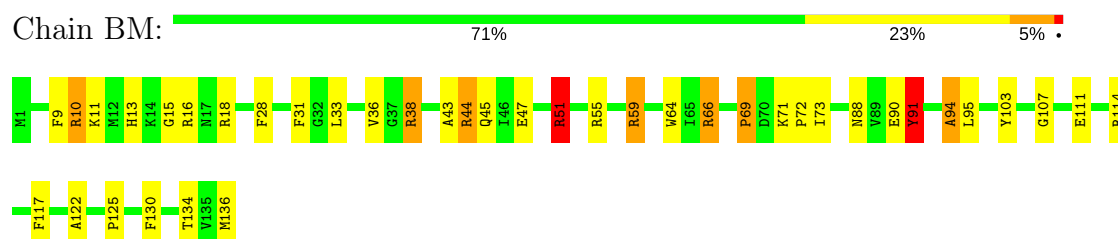
• Molecule 30: 50S ribosomal protein L14



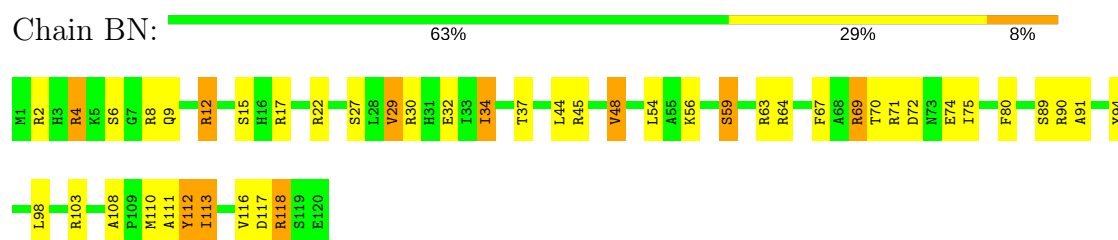
- Molecule 31: 50S ribosomal protein L15



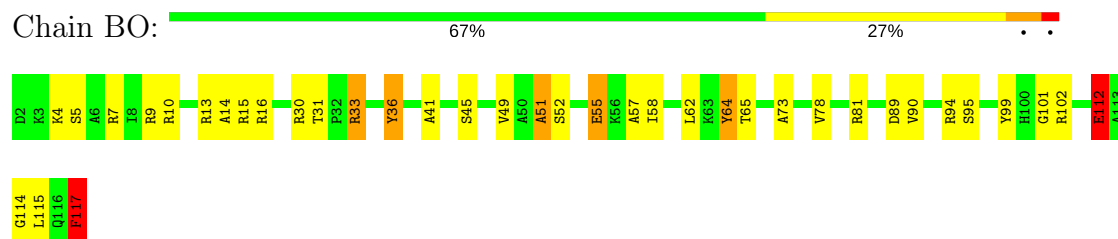
- Molecule 32: 50S ribosomal protein L16



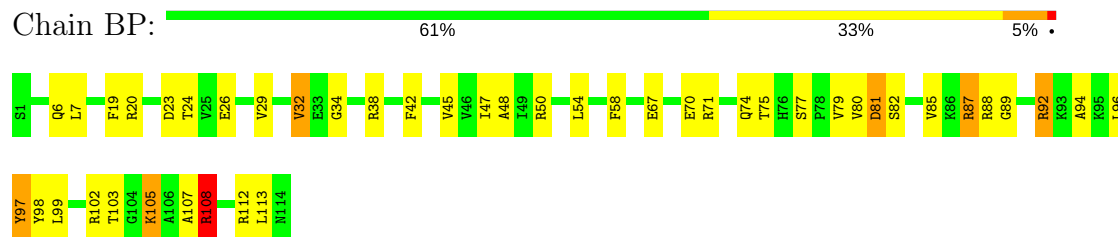
- Molecule 33: 50S ribosomal protein L17



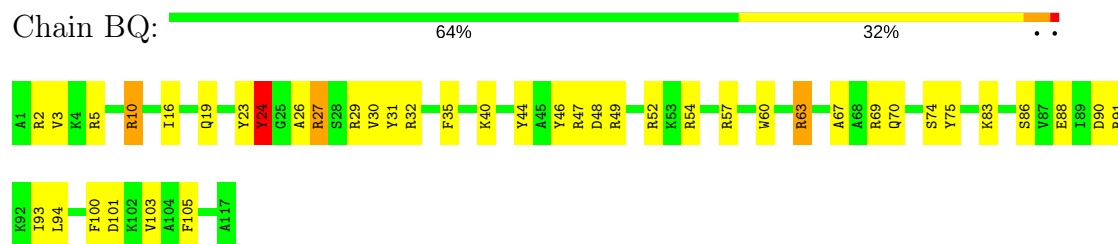
- Molecule 34: 50S ribosomal protein L18



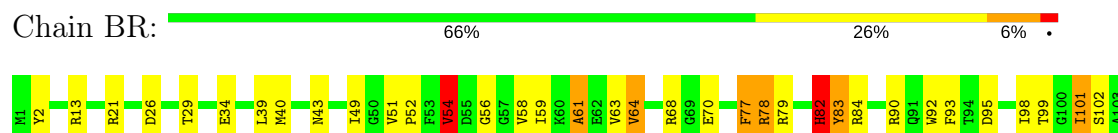
- Molecule 35: 50S ribosomal protein L19



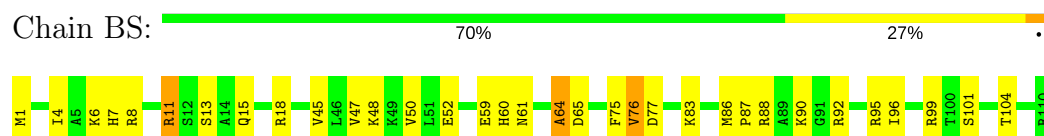
- Molecule 36: 50S ribosomal protein L20



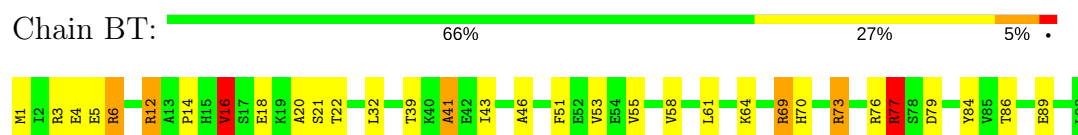
- Molecule 37: 50S ribosomal protein L21



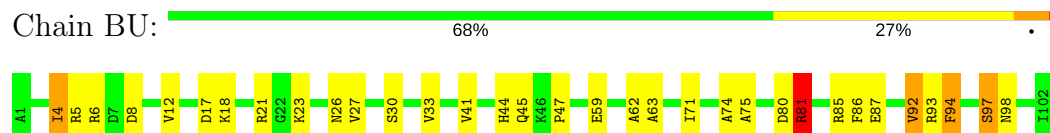
- Molecule 38: 50S ribosomal protein L22



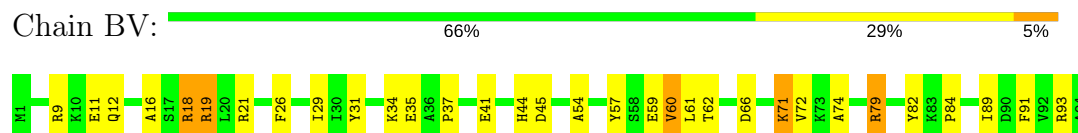
- Molecule 39: 50S ribosomal protein L23



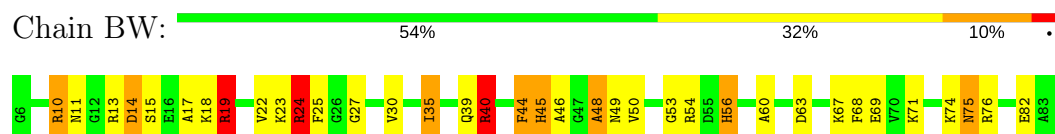
- Molecule 40: 50S ribosomal protein L24



- Molecule 41: 50S ribosomal protein L25

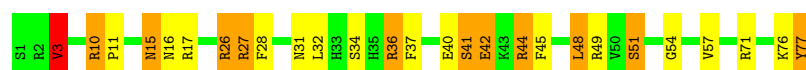


- Molecule 42: 50S ribosomal protein L27



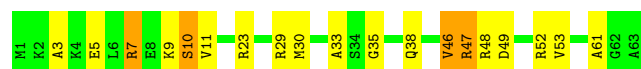
- Molecule 43: 50S ribosomal protein L28

Chain BX: 



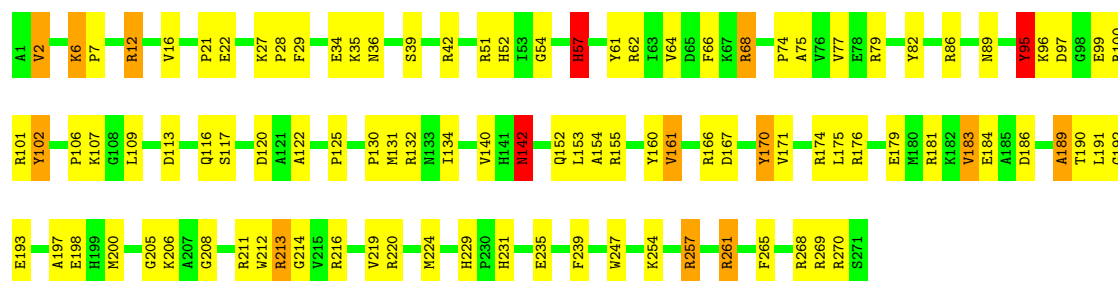
- Molecule 44: 50S ribosomal protein L29

Chain BY: 



- Molecule 45: 50S ribosomal protein L2

Chain BC: 



- Molecule 46: 50S ribosomal protein L30

Chain BZ: 



- Molecule 47: 50S ribosomal protein L32

Chain B0: 



- Molecule 48: 50S ribosomal protein L33

Chain B1: 



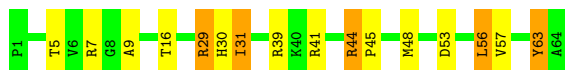
- Molecule 49: 50S ribosomal protein L34

Chain B2: 

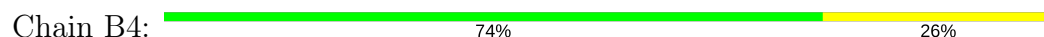




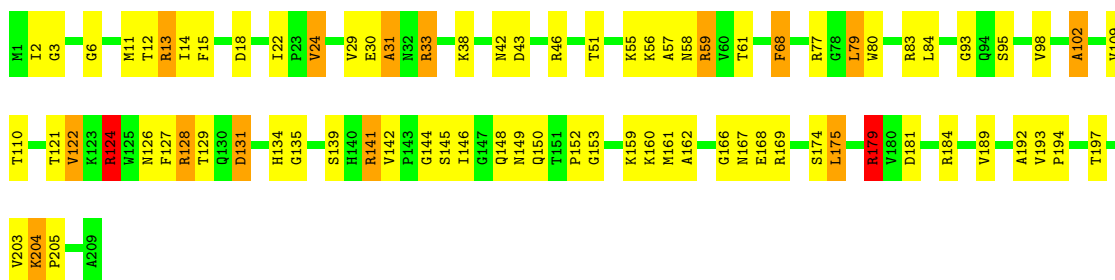
- Molecule 50: 50S ribosomal protein L35



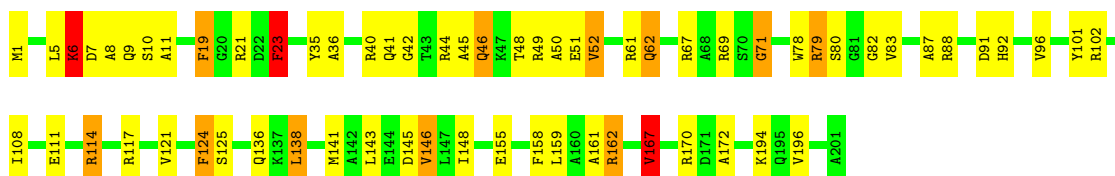
- Molecule 51: 50S ribosomal protein L36



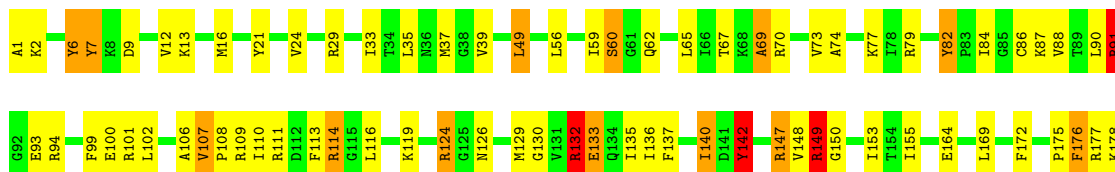
- Molecule 52: 50S ribosomal protein L3

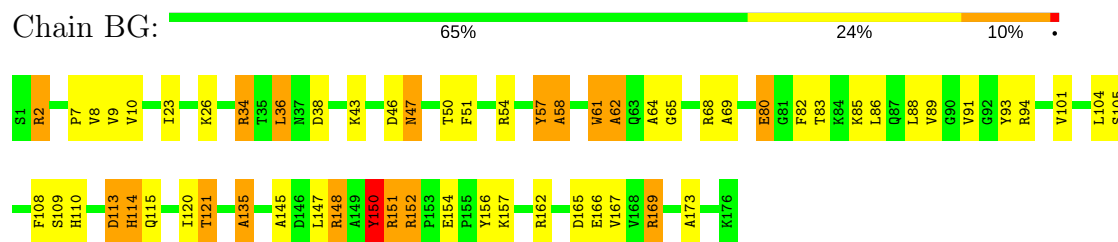


- Molecule 53: 50S ribosomal protein L4

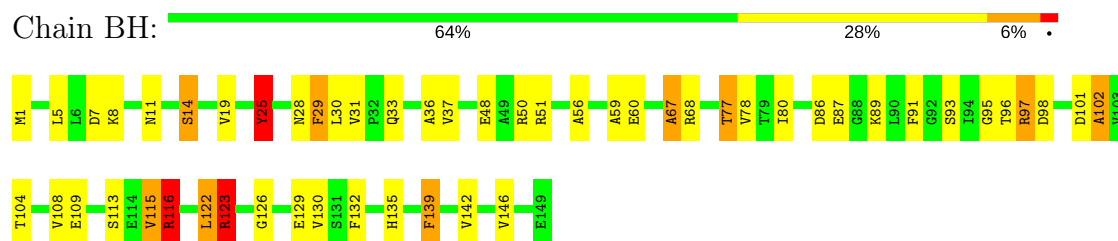


- Molecule 54: 50S ribosomal protein L5

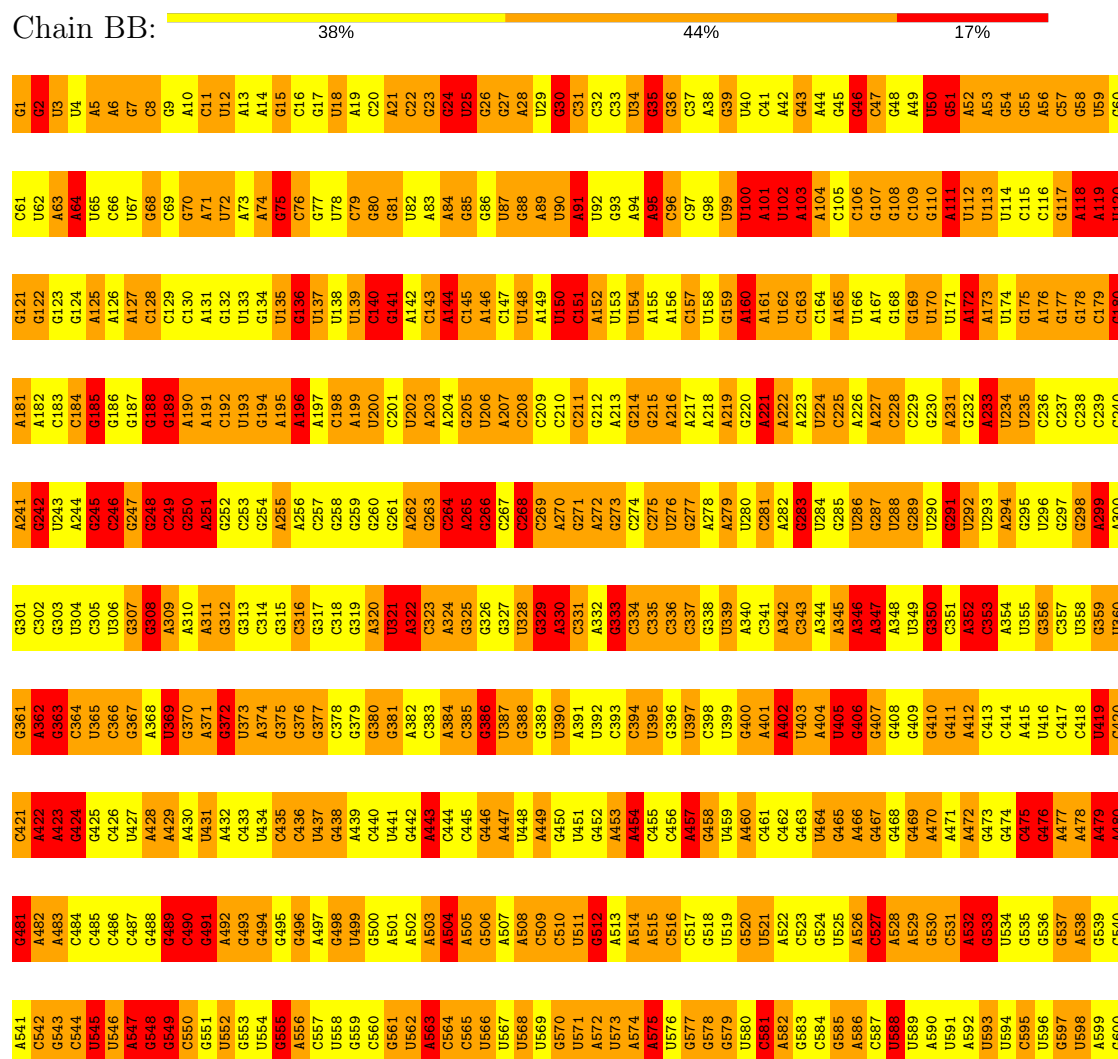




• Molecule 56: 50S ribosomal protein L9



• Molecule 57: 23S ribosomal RNA



A1502	A1503	U1442	G1382	A1322	A1262	G1202	A1142	U1082	A1021	C961	C901	G841	A781	A721	A661	C601
A1504	A1505	G1444	A1383	C1323	U1263	U1203	A1143	U1083	G1022	G962	C902	U842	A782	A722	G662	A602
A1506	U1506	G1445	A1384	G1324	A1264	A1084	A1144	A1085	U1023	U963	C903	G843	A783	C723	G663	A603
C1507	C1507	C1446	A1386	U1326	A1265	A1085	C1145	A1086	G1024	G964	C904	A844	A784	C724	G664	A604
A1508	A1508	C1447	A1387	U1327	U1266	G1087	C1146	A1086	G1025	G965	A905	U845	G785	G725	U665	G605
G1509	G1509	G1448	A1388	A1328	U1268	A1088	U1147	A1088	G1026	G966	U906	U846	G786	G726	A666	U606
G1510	G1510	G1449	A1389	U1329	A1269	A1089	U1148	A1089	A1027	U967	G907	U847	C787	A727	U667	U607
G1511	G1511	G1450	U1390	C1330	C1270	A1090	G1149	A1090	A1028	C968	C908	C848	A788	G728	A668	A608
G1512	G1512	G1451	U1391	G1331	G1271	G1091	A1150	A1091	C1030	G969	A909	A849	A789	G729	G669	A609
U1513	A1453	A1452	A1392	G1332	A1272	C1092	A1151	G1092	G1031	U970	A910	U850	U790	A730	A670	C610
G1514	U1454	U1394	U1393	G1333	U1273	G1093	C1152	C1093	A1032	G971	A911	C851	C791	C731	C611	C611
A1515	A1455	A1395	U1394	G1334	A1274	U1094	G1153	A1094	U1033	A972	C912	U852	A792	C732	C672	G612
G1516	G1456	A1396	A1275	C1335	G1275	A1095	A1154	A1095	G1034	A973	U913	C853	A793	C733	C673	A613
G1517	U1457	A1397	A1276	G1336	U1276	A1096	A1155	A1096	U1035	C974	G914	C854	A794	A734	C674	A614
U1518	U1458	C1398	G1277	G1337	U1277	U1097	A1156	A1097	U1036	A975	C915	G855	C795	A735	A675	U615
G1519	G1519	G1399	G1278	U1338	C1278	A1098	C1157	A1098	G1037	G976	G916	C856	C796	G736	A676	A616
U1520	U1400	U1340	G1280	U1340	U1280	C1100	U1158	G1099	G1038	G977	A917	G857	G797	C737	G617	C617
G1521	G1401	G1341	G1281	C1221	G1221	C1101	G1160	C1101	A1039	G978	U918	G858	G798	G738	C678	G618
A1522	A1462	A1342	U1282	U1222	U1222	U1102	C1161	U1102	A1040	A979	U919	G859	G799	A739	C679	G619
U1523	G1463	A1403	G1283	G1223	G1223	G1103	G1162	A1103	G1041	A980	A920	U860	A800	C740	C680	G620
G1524	G1464	A1344	A1284	C1224	A1284	C1104	G1163	A1104	G1042	A981	C921	A861	A801	U741	G681	A621
A1525	A1465	C1345	A1285	G1225	A1285	U1105	A1164	A1105	C1043	C982	C922	G862	A802	A742	G682	C622
C1526	U1466	U1405	A1286	A1226	A1286	G1106	A1165	A1106	C1044	A984	G924	G864	A804	U744	G684	C624
G1527	U1467	A1347	A1287	G1227	A1287	G1107	C1167	A1107	A1045	C985	A925	C865	G805	G745	A685	G625
A1528	U1468	U1348	G1288	C1228	G1288	U1108	C1168	A1108	U1046	C986	G926	A866	C806	U746	U686	A626
G1529	A1469	C1349	C1289	G1229	C1289	U1109	G1169	A1109	G1047	C987	A927	C867	U807	U747	C687	A627
U1530	G1470	A1410	C1290	A1230	G1290	G1110	C1170	A1110	A1048	A988	U928	U868	G808	G748	U688	G628
C1531	G1471	C1351	C1291	U1231	G1291	G1111	C1171	A1111	C1049	A989	U929	C869	A809	A749	A689	G629
A1532	G1472	U1412	G1292	C1232	G1292	G1112	C1172	A1112	A1050	A990	G930	U870	U810	A750	G690	G630
C1533	G1473	A1353	C1293	C1233	C1293	U1113	C1173	U1113	C1052	C992	U932	U872	C812	A752	C692	A632
U1534	G1474	A1354	U1294	U1234	U1294	C1114	U1174	C1114	C1053	G993	A933	C873	U813	A753	A693	A633
A1535	G1475	G1355	C1295	G1235	G1295	G1115	A1175	G1115	A1054	C994	U934	G874	C814	U754	G694	C634
G1536	U1476	U1416	G1296	G1236	G1296	G1116	U1176	G1116	G1055	C995	C935	G875	C815	U755	G695	C635
G1537	A1477	C1357	C1297	A1237	C1297	G1117	G1177	A996	G1056	A996	A936	C876	C816	A756	G696	G636
G1538	G1478	G1358	G1298	G1238	G1298	C1118	C1178	A997	A1057	C997	C937	A877	C817	G757	G697	A637
U1539	G1479	A1359	G1299	G1239	G1299	U1119	G1179	C998	U1058	C998	G938	A878	C818	C758	C698	G638
G1540	C1480	A1420	G1300	U1240	G1300	G1120	U1180	U999	G1059	U999	G939	G879	A819	G759	A699	U639
U1541	G1481	A1301	A1301	A1241	A1301	C1121	U1181	A1000	U1060	A1000	G940	G880	A820	G760	G700	C640
U1542	G1482	G1422	A1302	U1242	A1302	G1122	U1182	A1001	U1061	A1001	A941	G881	A821	A761	G701	U641
G1543	G1483	C1363	G1303	C1243	G1303	C1123	U1183	G1002	G1062	G1002	G942	G882	G822	U762	U702	U642
A1544	U1484	A1364	A1304	A1244	A1304	G1124	U1184	G1003	G1063	A943	A943	G883	C823	G763	G703	A643
U1545	U1485	A1365	C1305	G1245	G1305	G1125	G1185	U1004	C1064	U1004	C944	U884	U824	A764	G704	A644
G1546	U1486	A1366	C1306	A1246	A1306	A1126	G1186	C1005	A1067	A1067	A945	C885	A825	C765	A705	G645
C1547	U1487	A1367	A1307	A1247	A1307	A1127	G1187	C1006	G1068	C1006	G946	A886	U826	U766	A706	G646
A1548	G1488	A1368	A1308	G1248	A1308	G1128	U1188	C1007	U1069	C1007	A947	U887	U827	U767	G707	G647
A1549	C1489	G1369	G1309	U1249	G1309	A1129	A1189	A1008	A1069	C948	C948	C888	A828	G768	G708	G648
C1550	A1490	G1430	G1310	G1250	G1310	U1130	G1190	A1009	A1070	A1009	G949	C889	A829	U769	U709	A649
A1551	G1491	G1311	G1311	C1251	G1311	G1131	G1191	A1010	G1071	A1010	G950	C890	G830	G770	U710	C650
A1552	G1492	U1372	U1312	G1252	U1312	U1132	G1192	G1011	C1072	G1011	C951	G891	G831	G771	G711	G651
A1553	G1493	A1373	U1313	A1253	U1313	A1133	G1193	U1012	A1073	U1012	C952	A892	U832	G772	G712	U652
U1554	A1494	G1374	C1314	A1254	A1314	G1074	A1194	C953	G1075	C953	G953	C893	A833	G773	G713	U653
G1555	A1495	U1375	C1315	U1255	G1315	C1075	G1195	A1014	C1076	A1014	G954	U894	A834	G774	U714	A654
C1556	U1496	G1376	U1316	G1256	U1316	G1136	C1196	U955	C1077	G1015	U955	U895	C835	G775	A715	A655
C1557	U1497	G1377	G1317	C1257	G1317	C1077	G1197	G1016	A1077	G1016	G956	A896	G836	G776	A716	G656
C1558	C1498	A1378	U1318	U1258	U1318	G1138	U1198	G1017	U1078	G1017	C957	C897	C837	G777	C717	U657
U1559	G1499	U1379	C1319	G1259	C1319	G1139	U1199	U958	C1079	U958	U958	C898	C838	G778	A718	U658
G1560	U1440	C1380	C1320	A1260	C1320	A1080	U1199	U1018	A1080	U1018	A959	C899	C839	U779	A719	G659
G1561	G1501	G1381	A1321	C1261	A1321	U1141	U1201	A1020	U1081	A1020	A960	A900	C840	G780	U720	C660

C2462	C2463	C2464	C2465	C2466	C2467	C2468	A2469	G2470	A2471	A2412	G2413	G2414	G2415	G2416	G2417	A2418	G2419	C2420	G2421	A2482	C2483	G2484	A2485	C2486	G2487	G2488	G2489	A2490	A2491	G2492	A2493	G2494	G2495	G2496	A2497	G2498	G2499	G2500	C2501	G2502	A2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	A2513	G2514	G2515	G2516	G2517	A2518	G2519	G2520	G2521
U2402	C2403	U2404	U2405	A2406	A2407	A2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	G2416	G2417	A2418	G2419	C2420	G2421	A2482	C2483	G2484	A2485	C2486	G2487	G2488	G2489	A2490	A2491	G2492	A2493	G2494	G2495	G2496	A2497	G2498	G2499	G2500	C2501	G2502	A2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	A2513	G2514	G2515	G2516	G2517	A2518	G2519	G2520	G2521
C2222	G2223	G2224	A2225	G2226	A2227	G2228	G2229	G2230	U2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	A2241	G2242	U2243	G2244	U2245	G2246	A2247	G2248	G2249	C2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	A2266	A2267	G2268	G2269	G2270	G2271	G2272	A2273	G2274	G2275	G2276	G2277	G2278	G2279	A2280	A2281
G2282	C2283	C2284	C2285	G2286	A2287	G2288	G2289	G2290	U2291	G2292	G2293	G2294	G2295	G2296	G2297	A2298	G2299	G2300	C2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	C2310	A2311	G2312	G2313	A2314	G2315	G2316	A2317	G2318	G2319	G2320	U2321	A2322	G2323	U2324	G2325	G2326	A2327	A2328	G2329	G2330	G2331	C2332	A2333	U2334	A2335	G2336	G2337	C2338	A2339	G2340	G2341
C2342	U2343	U2344	G2345	A2346	C2347	U2348	G2349	C2350	A2351	G2352	G2353	G2354	G2355	G2356	G2357	A2358	G2359	G2360	G2361	C2362	G2363	G2364	G2365	A2366	G2367	C2368	G2369	A2370	G2371	U2372	G2373	G2374	G2375	A2376	G2377	U2378	A2379	G2380	A2381	G2382	G2383	U2384	G2385	A2386	G2387	A2388	G2389	U2390	G2391	A2392	U2393	G2394	G2395	G2396	G2397	C2398	A2399	G2400	U2401
U2402	C2403	U2404	G2405	A2406	A2407	U2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	G2416	G2417	A2418	G2419	C2420	G2421	A2482	C2483	G2484	A2485	C2486	G2487	G2488	G2489	A2490	A2491	G2492	A2493	G2494	G2495	G2496	A2497	G2498	G2499	G2500	C2501	G2502	A2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	A2513	G2514	G2515	G2516	G2517	A2518	G2519	G2520	G2521
C1622	G1623	U1624	C1625	A1626	G1627	G1628	U1629	A1630	G1631	A1632	G1633	A1634	A1635	U1636	G1637	U1638	A1639	C1640	A1641	G1642	G1643	C1644	G1645	A1646	U1647	G1648	U1649	G1650	A1651	G1652	C1653	A1654	G1655	U1656	U1657	G1658	G1659	C1660	G1661	U1662	G1663	A1664	C1665	G1666	G1667	A1668	A1669	C1670	U1671	A1672	G1673	A1674	C1675	U1676	G1677	A1678	G1679	U1680	G1681
G1682	U1683	C1684	U1685	A1686	G1687	U1688	A1689	A1690	G1691	A1692	G1693	A1694	G1695	U1696	G1697	A1698	G1699	A1700	A1701	G1702	G1703	C1704	A1705	G1706	G1707	C1708	U1709	G1710	A1711	G1712	C1713	A1714	U1715	U1716	A1717	G1718	G1719	U1720	G1721	U1722	G1723	A1724	U1725	C1726	G1727	C1728	U1729	C1730	G1731	C1732	G1733	A1734	U1735	U1736	G1737	G1738	A1739	G1740	A1801
U1742	G1743	C1744	U1745	A1746	G1747	U1748	A1749	G1750	U1751	A1752	G1753	A1754	A1755	U1756	G1757	A1758	A1759	C1760	C1761	G1762	G1763	C1764	U1765	G1766	G1767	C1768	U1769	G1770	A1771	A1772	A1773	C1774	G1775	U1776	U1777	U1778	U1779	A1780	G1781	U1782	A1783	A1784	U1785	A1786	U1787	C1788	U1789	C1790	U1791	C1792	G1793	A1794	U1795	U1796	G1797	U1798	G1799	C1800	A1801
A1802	G1803	C1804	U1805	A1806	G1807	A1808	A1809	A1810	G1811	U1812	G1813	A1814	A1815	U1816	G1817	U1818	A1819	U1820	A1821	G1822	G1823	C1824	A1825	U1826	U1827	G1828	A1829	G1830	G1831	A1832	C1833	U1834	G1835	C1836	C1837	U1838	G1839	G1840	U1841	G1842	C1843	G1844	G1845	G1846	A1847	A1848	G1849	U1850	U1851	U1852	A1853	A1854	U1855	U1856	G1857	A1858	U1859	G1860	G1861
G1862	G1863	U1864	U1865	A1866	G1867	C1868	G1869	C1870	A1871	A1872	G1873	A1874	G1875	A1876	U1877	G1878	A1879	U1880	C1881	G1882	U1883	C1884	A1885	U1886	C1887	G1888	A1889	G1890	G1891	A1892	C1893	U1894	G1895	C1896	U1897	U1898	A1899	A1900	A1901	G1902	G1903	G1904	C1905	G1906	G1907	C1908	C1909	A1910	U1911	A1912	A1913	C1914	G1915	U1916	A1917	A1918	U1919	G1920	G1921
G1922	U1923	C1924	U1925	A1926	G1927	A1928	G1929	G1930	U1931	A1932	G1933	A1934	G1935	A1936	U1937	A1938	U1939	U1940	C1941	G1942	U1943	U1944	G1945	U1946	C1947	G1948	G1949	G1950	U1951	A1952	A1953	U1954	U1955	U1956	C1957	U1958	G1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	U1971	G1972	G1973	U1974	G1975	U1976	A1977	A1978	U1979	G1980	A1981
U1982	G1983	C1984	U1985	A1986	G1987	U1988	G1989	C1990	U1991	G1992	U1993	A1994	U1995	U1996	C1997	A1998	U1999	C2000	C2001	G2002	A2003	G2004	A2005	C2006	U2007	C2008	A2009	G2010	U2011	G2012	A2013	A2014	U2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	U2036	C2037	G2038	U2039	G2040	U2041
A2042	C2043	C2044	C2045	G2046	C2047	G2048	G2049	C2050	A2051	A2052	G2053	A2054	C2055	G2056	G2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	C2073	C2074	U2075	U2076	A2077	C2078	U2079	A2080	U2081	A2082	G2083	C2084	U2085	U2086	A2087	A2088	C2089	A2090	C2091	U2092	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101
G2102	C2103	C2104	U2105	U2106	G2107	A2108	G2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	A2123	G2124	G2125	A2126	G2127	U2128	G2129	U2130	A2131	U2132	G2133	A2134	G2135	U2136	U2137	G2138	U2139	G2140	U2141	C2142	G2143	G2144	C2145	G2146	A2147	G2148	U2149	C2150	U2151	G2152	A2153	C2154	U2155	G2156	U2157	A2158	C2159	G2160	C2161
G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	U2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	G2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	C2196	U2197	A2198	A2199	C2200	G2201	U2202	U2203	G2204	A2205	C2206	C2207	C2208	G2209	U2210	A2211	A2212	U2213	C2214	C2215	G2216	U2217	G2218	U2219	U2220	G2221
C2222	G2223	G2224	A2225	G2226	A2227	G2228	G2229	G2230	U2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	G2248	G2249	C2250	G2251	G2252	G2253	A2254	G2255	G2256	U2257	G2258	G2259	G2260	G2261	U2262	G2263	G2264	A2265	A2266	A2267	G2268	G2269	G2270	G2271	G2272	A2273	G2274	G2275	G2276	G2277	G2278	G2279	A2280	A2281
G2282	C2283	C2284	C2285	G2286	A2287	G2288	G2289	G2290	U2291	G2292	G2293	G2294	G2295	G2296	G2297	A2298	G2299	G2300	C2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	C2310	A2311	G2312	G2313	A2314	G2315	G2316	A2317	G2318	G2319	G2320	U2321	A2322	G2323	U2324	G2325	C2326	A2327	A2328	G2329	G2330	G2331	C2332	A2333	U2334	A2335	G2336	G2337	C2338	A2339	G2340	G2341
C2342	U2343	U2344	G2345	A2346	C2347	U2348	G2349	C2350	A2351	G2352	G2353	G2354	G2355	G2356	G2357	A2358	G2359	G2360	G2361	C2362	G2363	G2364	G2365	A2366	G2367	C2368	G2369	A2370	G2371	U2372	G2373	G2374	G2375	A2376	G2377	U2378	A2379	G2380	A2381	G2382	G2383	U2384	G2385	A2386	G2387	A2388	G2389	U2390	G2391	A2392	U2393	G2394	G2395	G2396	G2397	C2398	A2399	G2400	U2401
U2402	C2403	U2404	G2405	A2406	A2407	U2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	G2416	G2417	A2418	G2419	C2420	G2421	A2482	C2483	G2484	A2485	C2486	G2487	G2488	G2489	A2490	A2491	G2492	A2493	G2494	G2495	G2496	A2497	G2498	G2499	G2500	C2501	G2502	A2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	A2513	G2514	G2515	G2516	G2517	A2518	G2519	G2520	G2521

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Correction of reconstruction of each defocus group	Depositor
Microscope	FEI Polara 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	4520	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	58279	Depositor
Image detector	Kodak SO163 Film	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AJ	1.80	12/797 (1.5%)	1.89	19/1077 (1.8%)
10	AS	1.77	6/653 (0.9%)	1.98	15/877 (1.7%)
11	AT	1.70	8/671 (1.2%)	1.88	12/888 (1.4%)
12	AU	1.95	8/431 (1.9%)	2.14	13/570 (2.3%)
13	AB	1.69	20/1736 (1.2%)	2.01	42/2338 (1.8%)
14	AC	1.76	18/1652 (1.1%)	1.95	34/2225 (1.5%)
15	AD	1.79	20/1665 (1.2%)	2.02	46/2227 (2.1%)
16	AE	1.75	12/1119 (1.1%)	2.03	28/1504 (1.9%)
17	AF	1.80	5/836 (0.6%)	1.98	19/1128 (1.7%)
18	AG	1.83	15/1188 (1.3%)	2.09	34/1591 (2.1%)
19	AH	1.72	10/989 (1.0%)	2.00	24/1326 (1.8%)
2	AK	1.83	17/893 (1.9%)	2.02	24/1205 (2.0%)
20	AI	1.77	10/1034 (1.0%)	2.01	29/1375 (2.1%)
21	AA	3.42	4975/36763 (13.5%)	3.74	8350/57350 (14.6%)
22	AY	4.00	354/1814 (19.5%)	4.28	526/2827 (18.6%)
23	AW	5.13	269/1809 (14.9%)	3.87	451/2819 (16.0%)
24	AX	3.54	39/260 (15.0%)	3.68	65/403 (16.1%)
25	AZ	1.79	30/3091 (1.0%)	2.04	97/4182 (2.3%)
26	AV	3.50	261/1814 (14.4%)	3.81	416/2825 (14.7%)
27	B5	1.66	6/1748 (0.3%)	2.01	42/2355 (1.8%)
28	BI	1.69	5/1046 (0.5%)	2.02	30/1410 (2.1%)
29	BJ	1.75	9/1152 (0.8%)	1.97	27/1551 (1.7%)
3	AL	1.73	7/969 (0.7%)	1.96	24/1300 (1.8%)
30	BK	1.76	6/940 (0.6%)	2.06	30/1258 (2.4%)
31	BL	1.85	17/1054 (1.6%)	2.05	30/1403 (2.1%)
32	BM	1.83	16/1093 (1.5%)	2.20	29/1460 (2.0%)
33	BN	1.87	16/974 (1.6%)	2.12	35/1301 (2.7%)
34	BO	1.87	15/902 (1.7%)	2.04	26/1209 (2.2%)
35	BP	1.78	6/929 (0.6%)	2.00	27/1242 (2.2%)
36	BQ	1.78	14/960 (1.5%)	2.16	38/1278 (3.0%)
37	BR	1.86	14/829 (1.7%)	2.09	25/1107 (2.3%)
38	BS	1.71	14/864 (1.6%)	1.97	19/1156 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BT	1.61	3/745 (0.4%)	2.03	23/994 (2.3%)
4	AM	1.83	12/885 (1.4%)	2.12	35/1181 (3.0%)
40	BU	1.72	5/788 (0.6%)	1.96	14/1051 (1.3%)
41	BV	1.70	7/766 (0.9%)	1.99	27/1025 (2.6%)
42	BW	1.85	15/603 (2.5%)	2.15	22/797 (2.8%)
43	BX	1.85	11/635 (1.7%)	1.98	18/848 (2.1%)
44	BY	1.67	5/510 (1.0%)	1.93	14/677 (2.1%)
45	BC	1.78	22/2122 (1.0%)	2.01	50/2852 (1.8%)
46	BZ	1.64	4/453 (0.9%)	1.99	11/605 (1.8%)
47	B0	1.78	2/450 (0.4%)	2.04	14/599 (2.3%)
48	B1	1.75	2/417 (0.5%)	1.91	8/554 (1.4%)
49	B2	1.87	7/380 (1.8%)	2.44	22/498 (4.4%)
5	AN	1.84	13/786 (1.7%)	2.19	27/1046 (2.6%)
50	B3	1.63	5/513 (1.0%)	1.85	10/676 (1.5%)
51	B4	1.88	3/303 (1.0%)	1.98	8/397 (2.0%)
52	BD	1.71	15/1586 (0.9%)	2.02	39/2134 (1.8%)
53	BE	1.71	13/1571 (0.8%)	1.99	42/2113 (2.0%)
54	BF	1.75	12/1444 (0.8%)	2.09	40/1937 (2.1%)
55	BG	1.76	21/1343 (1.6%)	2.07	37/1816 (2.0%)
56	BH	1.65	10/1122 (0.9%)	2.01	37/1515 (2.4%)
57	BB	3.38	9332/69800 (13.4%)	3.73	15942/108892 (14.6%)
58	BA	3.35	371/2804 (13.2%)	3.76	649/4371 (14.8%)
6	AO	1.75	9/724 (1.2%)	1.94	16/966 (1.7%)
7	AP	1.90	14/649 (2.2%)	2.07	22/870 (2.5%)
8	AQ	1.80	10/658 (1.5%)	1.95	11/881 (1.2%)
9	AR	1.81	5/463 (1.1%)	2.10	16/621 (2.6%)
All	All	3.03	16162/165195 (9.8%)	3.37	27780/246683 (11.3%)

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	AJ	0	3
10	AS	0	1
11	AT	0	3
12	AU	0	5
13	AB	0	4
14	AC	0	5
15	AD	0	9
16	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	AF	0	2
18	AG	0	4
19	AH	0	4
2	AK	0	4
20	AI	0	6
21	AA	0	713
22	AY	0	40
23	AW	3	39
24	AX	0	3
25	AZ	0	8
26	AV	0	37
27	B5	1	7
28	BI	0	3
29	BJ	0	9
3	AL	0	7
30	BK	0	1
31	BL	0	8
32	BM	0	4
33	BN	0	3
34	BO	0	4
35	BP	0	2
36	BQ	0	4
37	BR	0	6
38	BS	0	1
39	BT	0	2
4	AM	0	5
40	BU	0	2
41	BV	0	4
42	BW	0	3
43	BX	0	3
44	BY	0	2
45	BC	0	9
46	BZ	0	3
47	B0	0	4
48	B1	0	2
49	B2	0	1
5	AN	0	5
50	B3	0	2
51	B4	0	1
52	BD	0	5
53	BE	0	7
54	BF	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BG	0	5
56	BH	0	3
57	BB	0	1349
58	BA	0	56
6	AO	0	5
7	AP	0	3
8	AQ	0	1
9	AR	0	4
All	All	4	2445

The worst 5 of 16162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	63	G	N9-C8	84.56	1.97	1.37
23	AW	63	G	N7-C5	78.06	1.86	1.39
23	AW	63	G	C5-C4	69.51	1.87	1.38
23	AW	63	G	N9-C4	65.35	1.90	1.38
23	AW	63	G	C8-N7	61.20	1.67	1.30

The worst 5 of 27780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	523	A	N1-C6-N6	27.08	134.85	118.60
57	BB	2097	A	N1-C6-N6	26.55	134.53	118.60
57	BB	725	G	N1-C6-O6	26.46	135.78	119.90
57	BB	2274	A	N1-C6-N6	26.21	134.33	118.60
58	BA	9	G	N1-C6-O6	25.88	135.43	119.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	AW	17	C	C1'
23	AW	47	U	C1'
23	AW	70	G	C3'
27	B5	37	LYS	CA

5 of 2445 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AJ	16	ARG	Sidechain
1	AJ	68	ARG	Sidechain
1	AJ	9	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	AK	26	PHE	Sidechain
2	AK	55	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AJ	787	0	828	4	0
2	AK	877	0	887	1	0
3	AL	955	0	1019	9	0
4	AM	877	0	937	8	0
5	AN	774	0	828	9	0
6	AO	716	0	742	8	0
7	AP	639	0	656	2	0
8	AQ	649	0	691	3	0
9	AR	456	0	478	4	0
10	AS	638	0	665	7	0
11	AT	665	0	714	1	0
12	AU	426	0	449	0	0
13	AB	1705	0	1732	9	0
14	AC	1625	0	1699	7	0
15	AD	1643	0	1710	17	0
16	AE	1106	0	1148	6	0
17	AF	818	0	808	6	0
18	AG	1175	0	1230	10	0
19	AH	979	0	1034	4	0
20	AI	1022	0	1070	4	0
21	AA	32832	0	16503	179	0
22	AY	1622	0	812	11	0
23	AW	1619	0	822	22	0
24	AX	232	0	120	2	0
25	AZ	3035	0	3049	17	0
26	AV	1645	0	834	6	0
27	B5	1733	0	1823	10	0
28	BI	1032	0	1088	4	0
29	BJ	1129	0	1162	8	0
30	BK	931	0	1003	5	0
31	BL	1045	0	1117	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BM	1074	0	1157	1	0
33	BN	961	0	1000	5	0
34	BO	892	0	923	2	0
35	BP	917	0	965	5	0
36	BQ	947	0	1022	4	0
37	BR	816	0	839	3	0
38	BS	857	0	922	3	0
39	BT	739	0	807	4	0
40	BU	780	0	834	5	0
41	BV	753	0	780	3	0
42	BW	596	0	610	5	0
43	BX	625	0	655	3	0
44	BY	509	0	543	1	0
45	BC	2083	0	2157	16	0
46	BZ	449	0	491	0	0
47	B0	444	0	461	6	0
48	B1	410	0	440	4	0
49	B2	377	0	418	3	0
50	B3	504	0	574	3	0
51	B4	302	0	343	0	0
52	BD	1565	0	1616	16	0
53	BE	1552	0	1619	7	0
54	BF	1420	0	1460	10	0
55	BG	1323	0	1374	7	0
56	BH	1111	0	1148	4	0
57	BB	62321	0	31298	323	0
58	BA	2508	0	1268	8	0
59	AZ	28	0	12	0	0
All	All	152250	0	103394	772	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 772 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)
23:AW:63:G:C4	23:AW:63:G:C5	1.87	1.59
23:AW:63:G:C8	23:AW:63:G:N7	1.67	1.56
23:AW:63:G:N7	23:AW:63:G:C5	1.86	1.43
23:AW:63:G:C4	23:AW:63:G:N9	1.90	1.40
23:AW:63:G:C8	23:AW:63:G:N9	1.97	1.31

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 PDB entries followed by that with respect to all EM entries.

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	
1	AJ	96/98 (98%)	77 (80%)	11 (12%)	8 (8%)	1	16
2	AK	115/117 (98%)	90 (78%)	18 (16%)	7 (6%)	2	22
3	AL	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	6	41
4	AM	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	15
5	AN	94/96 (98%)	67 (71%)	18 (19%)	9 (10%)	1	13
6	AO	86/88 (98%)	73 (85%)	8 (9%)	5 (6%)	2	24
7	AP	78/80 (98%)	61 (78%)	14 (18%)	3 (4%)	4	32
8	AQ	78/80 (98%)	62 (80%)	13 (17%)	3 (4%)	4	32
9	AR	53/55 (96%)	43 (81%)	10 (19%)	0	100	100
10	AS	77/79 (98%)	55 (71%)	17 (22%)	5 (6%)	1	22
11	AT	83/85 (98%)	73 (88%)	8 (10%)	2 (2%)	7	42
12	AU	49/51 (96%)	35 (71%)	10 (20%)	4 (8%)	1	16
13	AB	216/218 (99%)	166 (77%)	37 (17%)	13 (6%)	2	23
14	AC	204/206 (99%)	168 (82%)	26 (13%)	10 (5%)	2	27
15	AD	203/205 (99%)	161 (79%)	28 (14%)	14 (7%)	1	20
16	AE	148/150 (99%)	118 (80%)	21 (14%)	9 (6%)	2	22
17	AF	98/100 (98%)	79 (81%)	15 (15%)	4 (4%)	3	30
18	AG	148/150 (99%)	122 (82%)	18 (12%)	8 (5%)	2	25
19	AH	127/129 (98%)	96 (76%)	26 (20%)	5 (4%)	3	31
20	AI	125/127 (98%)	102 (82%)	21 (17%)	2 (2%)	11	51
25	AZ	391/393 (100%)	319 (82%)	52 (13%)	20 (5%)	2	26
27	B5	232/234 (99%)	195 (84%)	31 (13%)	6 (3%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BI	139/141 (99%)	121 (87%)	11 (8%)	7 (5%)	2	27
29	BJ	140/142 (99%)	116 (83%)	11 (8%)	13 (9%)	1	14
30	BK	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	3	30
31	BL	141/143 (99%)	118 (84%)	16 (11%)	7 (5%)	2	27
32	BM	134/136 (98%)	101 (75%)	26 (19%)	7 (5%)	2	26
33	BN	118/120 (98%)	97 (82%)	17 (14%)	4 (3%)	4	35
34	BO	114/116 (98%)	100 (88%)	8 (7%)	6 (5%)	2	26
35	BP	112/114 (98%)	87 (78%)	15 (13%)	10 (9%)	1	15
36	BQ	115/117 (98%)	99 (86%)	14 (12%)	2 (2%)	11	50
37	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	27
38	BS	108/110 (98%)	85 (79%)	15 (14%)	8 (7%)	1	18
39	BT	91/93 (98%)	64 (70%)	19 (21%)	8 (9%)	1	15
40	BU	100/102 (98%)	79 (79%)	13 (13%)	8 (8%)	1	17
41	BV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	8	44
42	BW	77/79 (98%)	56 (73%)	10 (13%)	11 (14%)	0	5
43	BX	75/77 (97%)	60 (80%)	10 (13%)	5 (7%)	1	21
44	BY	61/63 (97%)	47 (77%)	11 (18%)	3 (5%)	2	27
45	BC	269/271 (99%)	201 (75%)	43 (16%)	25 (9%)	1	14
46	BZ	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
47	B0	54/56 (96%)	43 (80%)	9 (17%)	2 (4%)	4	33
48	B1	48/50 (96%)	44 (92%)	2 (4%)	2 (4%)	3	30
49	B2	44/46 (96%)	32 (73%)	11 (25%)	1 (2%)	7	43
50	B3	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	2	28
51	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	39
52	BD	207/209 (99%)	152 (73%)	39 (19%)	16 (8%)	1	18
53	BE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	22
54	BF	176/178 (99%)	129 (73%)	28 (16%)	19 (11%)	0	10
55	BG	174/176 (99%)	137 (79%)	23 (13%)	14 (8%)	1	17
56	BH	147/149 (99%)	107 (73%)	23 (16%)	17 (12%)	0	8
All	All	6242/6344 (98%)	4971 (80%)	897 (14%)	374 (6%)	3	23

5 of 374 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AJ	67	ILE
3	AL	24	GLU
4	AM	3	ILE
4	AM	29	SER
4	AM	99	GLN

### 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 PDB entries followed by that with respect to all EM entries.

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	
1	AJ	86/86 (100%)	82 (95%)	4 (5%)	30	62
2	AK	90/90 (100%)	87 (97%)	3 (3%)	43	70
3	AL	103/103 (100%)	98 (95%)	5 (5%)	29	61
4	AM	91/91 (100%)	85 (93%)	6 (7%)	19	52
5	AN	79/79 (100%)	78 (99%)	1 (1%)	73	87
6	AO	76/76 (100%)	74 (97%)	2 (3%)	51	75
7	AP	65/65 (100%)	63 (97%)	2 (3%)	45	71
8	AQ	74/74 (100%)	67 (90%)	7 (10%)	10	36
9	AR	48/48 (100%)	47 (98%)	1 (2%)	59	80
10	AS	70/70 (100%)	67 (96%)	3 (4%)	33	64
11	AT	65/65 (100%)	65 (100%)	0	100	100
12	AU	44/44 (100%)	42 (96%)	2 (4%)	32	63
13	AB	180/180 (100%)	172 (96%)	8 (4%)	33	63
14	AC	170/170 (100%)	158 (93%)	12 (7%)	17	49
15	AD	172/172 (100%)	163 (95%)	9 (5%)	27	59
16	AE	113/113 (100%)	106 (94%)	7 (6%)	21	54
17	AF	87/87 (100%)	81 (93%)	6 (7%)	18	51
18	AG	123/123 (100%)	115 (94%)	8 (6%)	20	52
19	AH	104/104 (100%)	95 (91%)	9 (9%)	12	40
20	AI	105/105 (100%)	97 (92%)	8 (8%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AZ	325/326 (100%)	303 (93%)	22 (7%)	18	51
27	B5	181/181 (100%)	170 (94%)	11 (6%)	22	55
28	BI	109/109 (100%)	100 (92%)	9 (8%)	13	43
29	BJ	116/116 (100%)	107 (92%)	9 (8%)	15	46
30	BK	102/102 (100%)	94 (92%)	8 (8%)	15	46
31	BL	102/102 (100%)	100 (98%)	2 (2%)	60	82
32	BM	109/109 (100%)	100 (92%)	9 (8%)	13	43
33	BN	100/100 (100%)	97 (97%)	3 (3%)	46	72
34	BO	86/86 (100%)	83 (96%)	3 (4%)	41	69
35	BP	99/99 (100%)	92 (93%)	7 (7%)	17	49
36	BQ	89/89 (100%)	86 (97%)	3 (3%)	42	69
37	BR	84/84 (100%)	78 (93%)	6 (7%)	17	49
38	BS	93/93 (100%)	89 (96%)	4 (4%)	33	64
39	BT	80/80 (100%)	72 (90%)	8 (10%)	9	33
40	BU	83/83 (100%)	72 (87%)	11 (13%)	4	24
41	BV	78/78 (100%)	75 (96%)	3 (4%)	38	67
42	BW	59/59 (100%)	53 (90%)	6 (10%)	8	33
43	BX	67/67 (100%)	60 (90%)	7 (10%)	8	32
44	BY	55/55 (100%)	53 (96%)	2 (4%)	40	68
45	BC	216/216 (100%)	205 (95%)	11 (5%)	28	60
46	BZ	48/48 (100%)	44 (92%)	4 (8%)	13	43
47	B0	47/47 (100%)	42 (89%)	5 (11%)	8	31
48	B1	45/45 (100%)	42 (93%)	3 (7%)	19	51
49	B2	38/38 (100%)	37 (97%)	1 (3%)	51	75
50	B3	51/51 (100%)	49 (96%)	2 (4%)	37	66
51	B4	34/34 (100%)	34 (100%)	0	100	100
52	BD	164/164 (100%)	150 (92%)	14 (8%)	12	42
53	BE	165/165 (100%)	157 (95%)	8 (5%)	30	61
54	BF	149/149 (100%)	139 (93%)	10 (7%)	19	51
55	BG	137/137 (100%)	126 (92%)	11 (8%)	14	45
56	BH	114/114 (100%)	107 (94%)	7 (6%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5170/5171 (100%)	4858 (94%)	312 (6%)	27 55

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BI	73	PRO
33	BN	29	VAL
54	BF	91	ARG
29	BJ	18	VAL
30	BK	68	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
25	AZ	11	HIS
25	AZ	329	GLN
52	BD	148	GLN
25	AZ	19	HIS
25	AZ	78	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1530 (99%)	281 (18%)	0
22	AY	75/76 (98%)	20 (26%)	0
23	AW	75/76 (98%)	24 (32%)	0
24	AX	10/11 (90%)	3 (30%)	0
26	AV	76/77 (98%)	14 (18%)	0
57	BB	2902/2903 (99%)	491 (16%)	0
58	BA	116/117 (99%)	19 (16%)	0
All	All	4783/4790 (99%)	852 (17%)	0

5 of 852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	14	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
26	5MU	AV	54	26	14,22,23	2.08	4 (28%)	16,32,35	4.23	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	5MU	AV	54	26	-	0/3/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AV	54	5MU	O2'-C2'	-2.50	1.37	1.43
26	AV	54	5MU	C2'-C1'	-2.14	1.50	1.53
26	AV	54	5MU	O4'-C1'	4.46	1.47	1.41
26	AV	54	5MU	C4-N3	4.47	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AV	54	5MU	C5-C4-N3	-9.12	115.18	125.24
26	AV	54	5MU	O4'-C1'-N1	3.31	114.70	108.08
26	AV	54	5MU	C4-N3-C2	13.53	127.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	GDP	AZ	401	-	25,30,30	2.60	7 (28%)	26,47,47	2.60	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	AZ	401	-	-	0/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AZ	401	GDP	O3'-C3'	-2.19	1.37	1.43
59	AZ	401	GDP	C2'-C1'	-2.01	1.50	1.53
59	AZ	401	GDP	C4-N3	2.24	1.39	1.35
59	AZ	401	GDP	C2-N1	2.67	1.40	1.35
59	AZ	401	GDP	C6-N1	3.63	1.39	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AZ	401	GDP	C5-C6-N1	-8.34	111.61	123.48
59	AZ	401	GDP	N3-C2-N1	-5.04	120.10	127.46
59	AZ	401	GDP	O3'-C3'-C2'	2.27	119.11	111.83
59	AZ	401	GDP	C4-C5-N7	2.49	111.81	109.41
59	AZ	401	GDP	C1'-N9-C4	3.07	131.94	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.