



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:05 PM BST

PDB ID : 4V7D
EMDB ID: : EMD-5800
Title : Structure of the Ribosome with Elongation Factor G Trapped in the Pre-Translocation State (pre-translocation 70S*tRNA*EF-G structure)
Authors : Brilot, A.F.; Korostelev, A.A.; Ermolenko, D.N.; Grigorieff, N.
Deposited on : 2013-11-21
Resolution : 7.60 Å(reported)
Based on PDB ID : 1DD3, 1MMS, 3R8S, 1ZAV, 3U4M

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

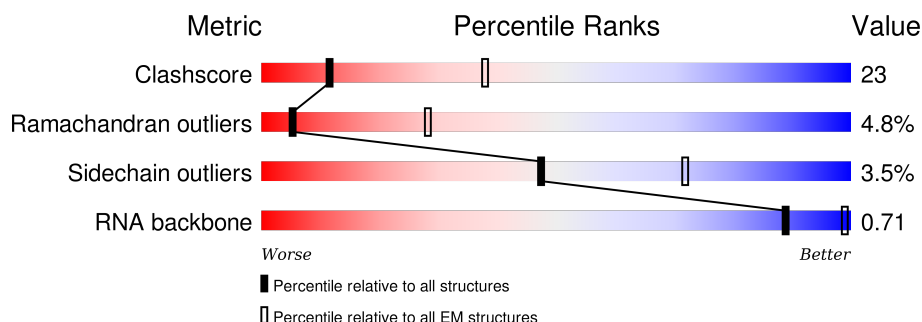
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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.




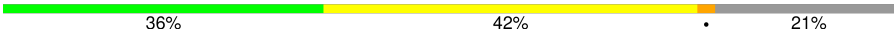




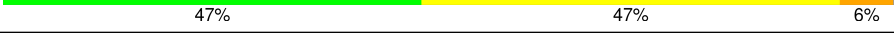

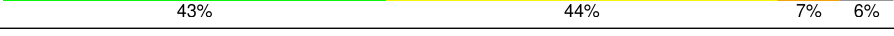

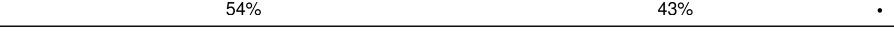
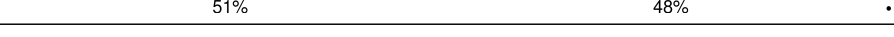

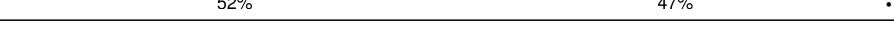


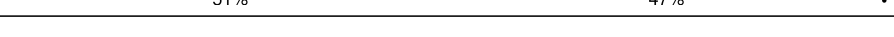

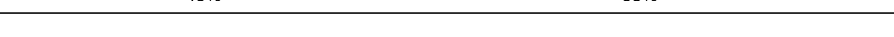




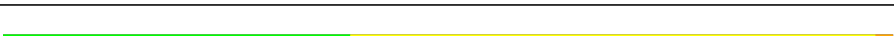

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	2903	52% 43% 6%
2	AB	119	56% 38% 6%
3	AC	233	49% 47% ..
4	AD	272	43% 53% .
5	AE	209	58% 40% .
6	AF	201	55% 43% .
7	AG	178	36% 59% . .
8	AH	176	55% 41% .

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Mol	Chain	Length	Quality of chain
9	AI	149	
10	AJ	165	
11	AK	141	
12	AL	120	
13	AM	142	
14	AN	123	
15	AO	144	
16	AP	136	
17	AQ	127	
18	AR	117	
19	AS	114	
20	AT	117	
21	AU	103	
22	AV	110	
23	AW	100	
24	AX	103	
25	AY	94	
26	AZ	84	
27	A1	77	
28	A2	63	
29	A3	58	
30	A4	56	
31	A5	54	
32	A6	46	
33	A7	64	


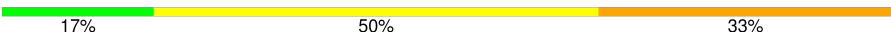
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Mol	Chain	Length	Quality of chain
34	A8	38	
35	BA	1542	
36	BB	240	
37	BC	232	
38	BD	205	
39	BE	166	
40	BF	131	
41	BG	178	
42	BH	129	
43	BI	129	
44	BJ	103	
45	BK	128	
46	BL	123	
47	BM	117	
48	BN	100	
49	BO	88	
50	BP	82	
51	BQ	83	
52	BR	74	
53	BS	91	
54	BT	86	
55	BU	70	
56	BV	76	
56	BW	76	
57	BX	18	

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Mol	Chain	Length	Quality of chain
58	BZ	711	
59	BY	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	5OH	BY	6	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153817 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	2897	Total	C	N	O	P	0	0
			62192	27744	11444	20107	2897		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	225	Total	C	N	O	S	0	0
			1675	1047	305	317	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	53	Total	C	N	O	S	0	0
			409	261	74	73	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

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

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

- Molecule 12 is a protein called 50S ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AL	68	Total	C	N	O	0	0
			487	306	82	99		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A4	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A5	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1538	Total	C	N	O	P	0	0
			32995	14716	6050	10691	1538		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		
56	BW	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BX	18	Total	C	N	O	P	0	0
			386	173	71	124	18		

- Molecule 58 is a protein called Elongation Factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BZ	686	Total	C	N	O	S	0	0
			5301	3341	912	1025	23		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	705	LEU	-	EXPRESSION TAG	UNP P0A6M8
BZ	706	GLU	-	EXPRESSION TAG	UNP P0A6M8
BZ	707	HIS	-	EXPRESSION TAG	UNP P0A6M8
BZ	708	HIS	-	EXPRESSION TAG	UNP P0A6M8
BZ	709	HIS	-	EXPRESSION TAG	UNP P0A6M8
BZ	710	HIS	-	EXPRESSION TAG	UNP P0A6M8
BZ	711	HIS	-	EXPRESSION TAG	UNP P0A6M8
BZ	712	HIS	-	EXPRESSION TAG	UNP P0A6M8

- Molecule 59 is a protein called viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BY	6	Total	C	N	O	0	0
			48	25	13	10		

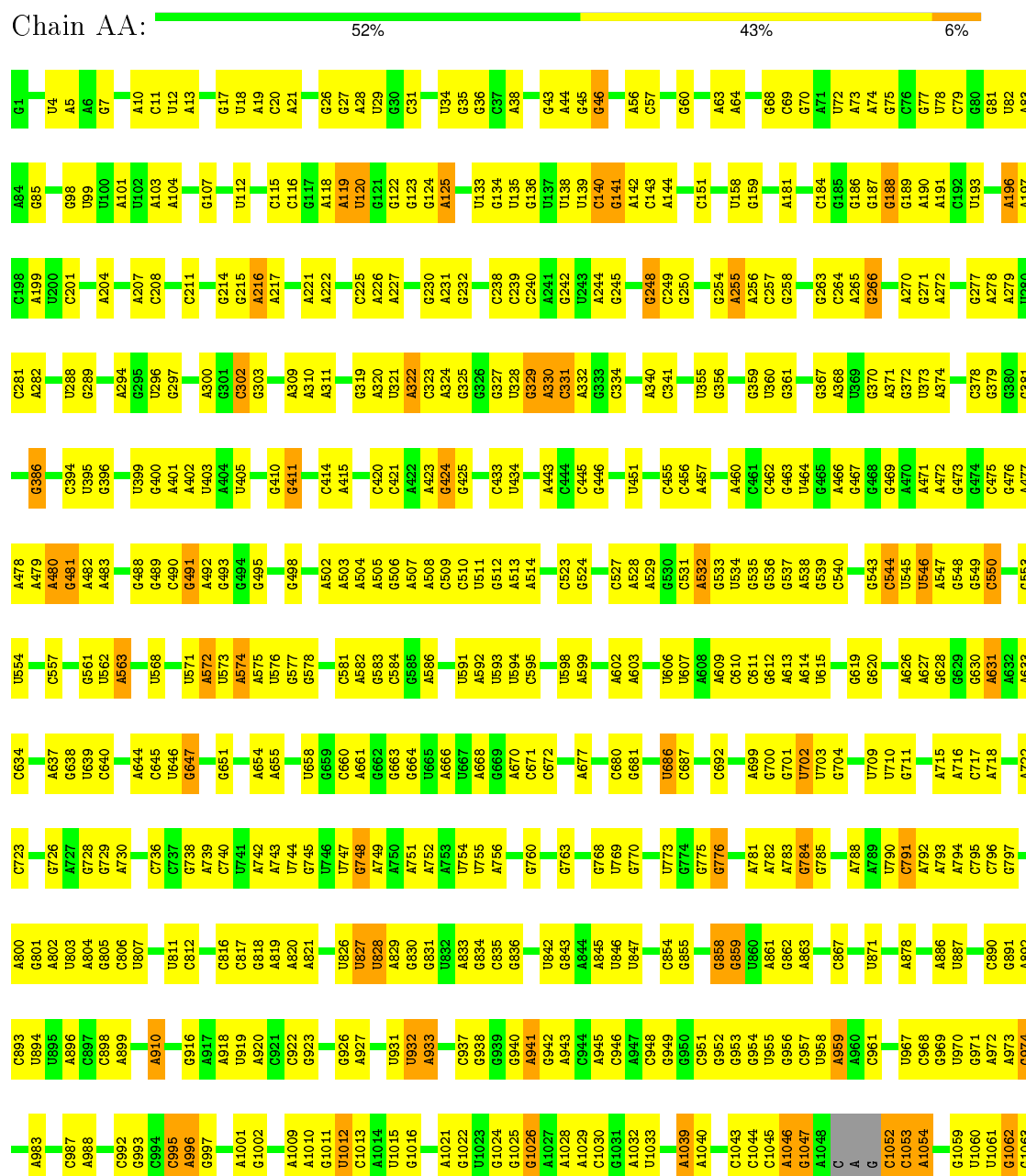
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	A8	1	Total	Zn	0
			1	1	

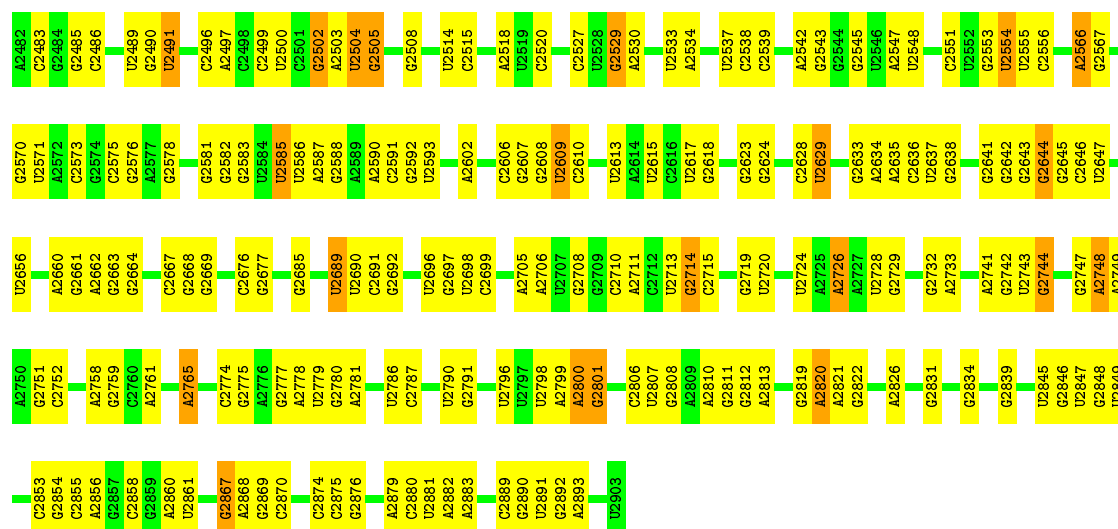
3 Residue-property plots

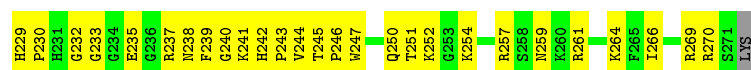
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 23S ribosomal RNA



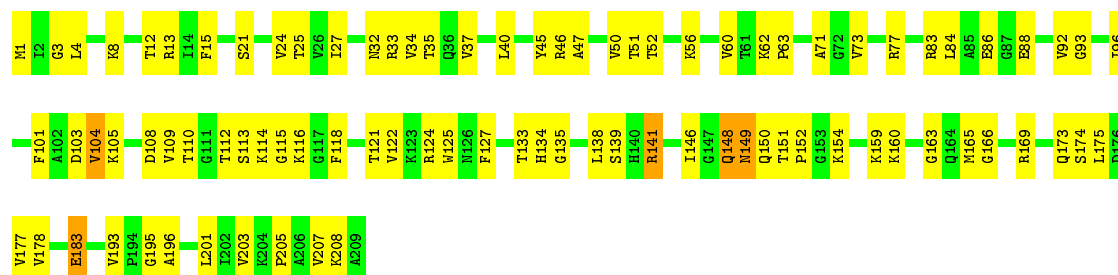




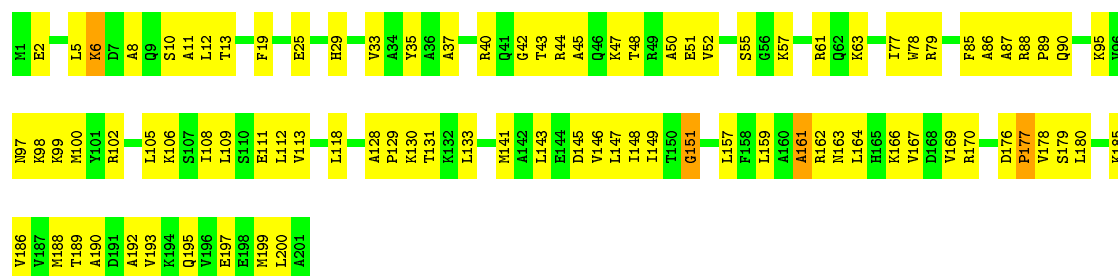
• Molecule 5: 50S ribosomal protein L3

Chain AE: 58% 40%



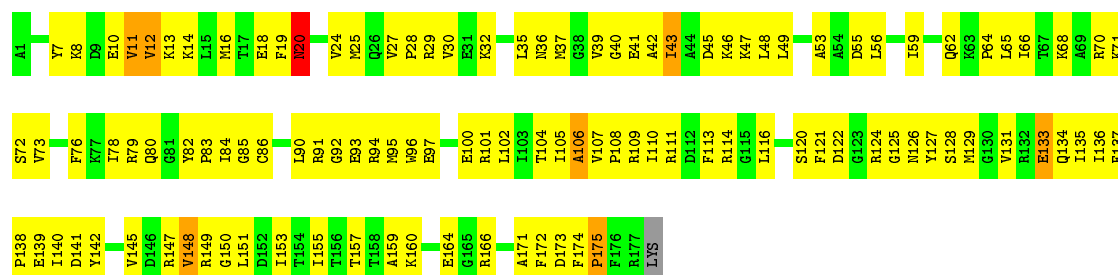
• Molecule 6: 50S ribosomal protein L4

Chain AF: 55% 43%



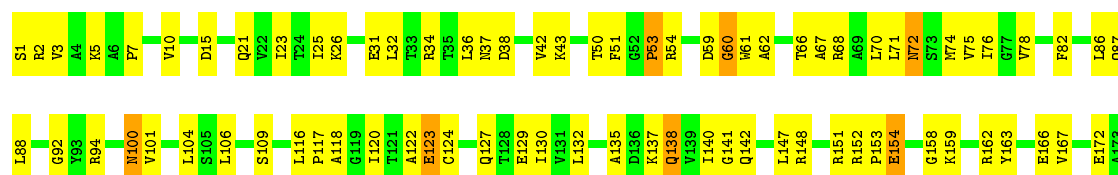
• Molecule 7: 50S ribosomal protein L5

Chain AG: 36% 59%



• Molecule 8: 50S ribosomal protein L6

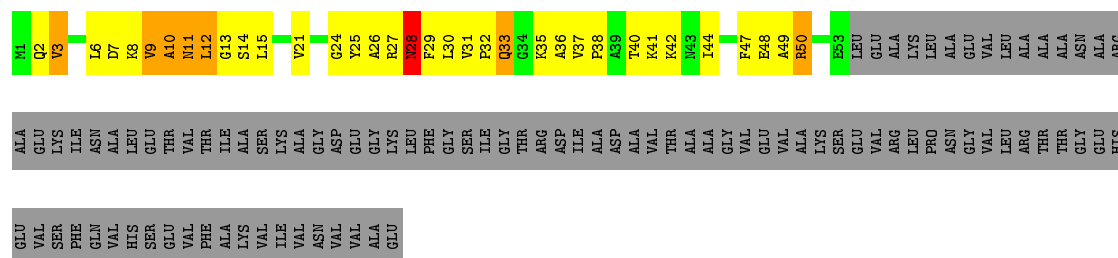
Chain AH: 55% 41%



K174
K175
K176

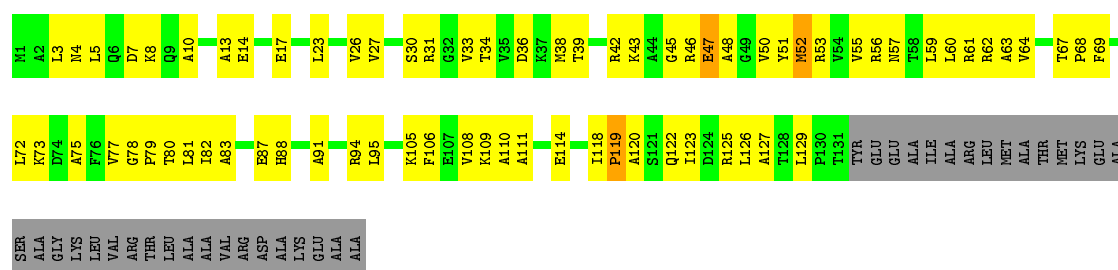
- Molecule 9: 50S ribosomal protein L9

Chain AI: 12% 18% 5% 64%



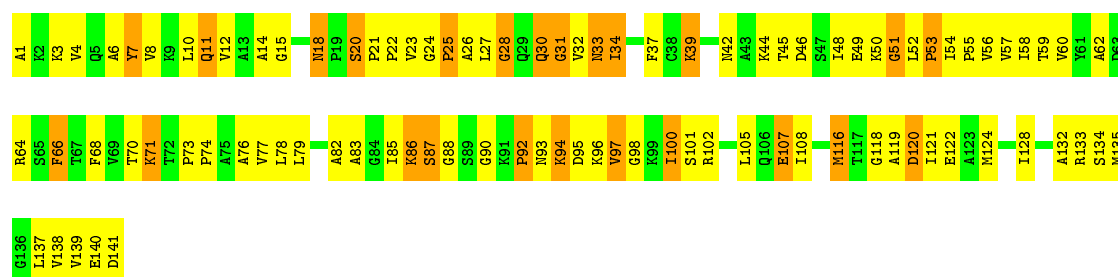
- Molecule 10: 50S ribosomal protein L10

Chain AJ:  36% 42% 0% 21%



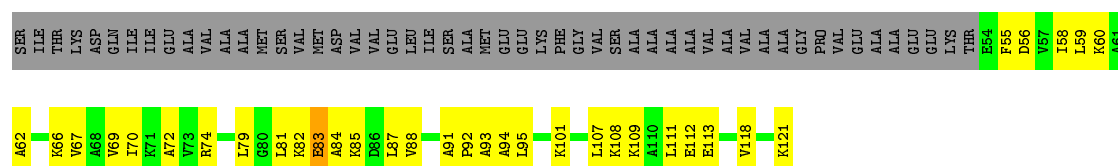
- Molecule 11: 50S ribosomal protein L11

Chain AK: 

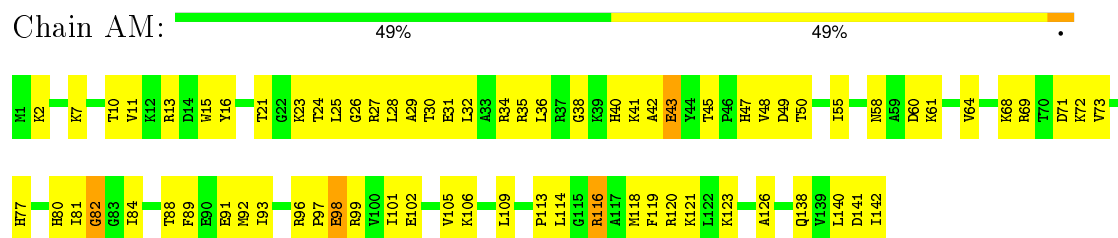


- Molecule 12: 50S ribosomal protein L12

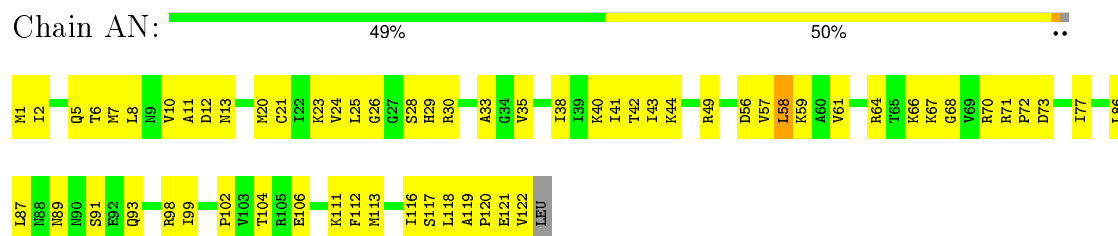
Chain AL: 28% 28% • 43%



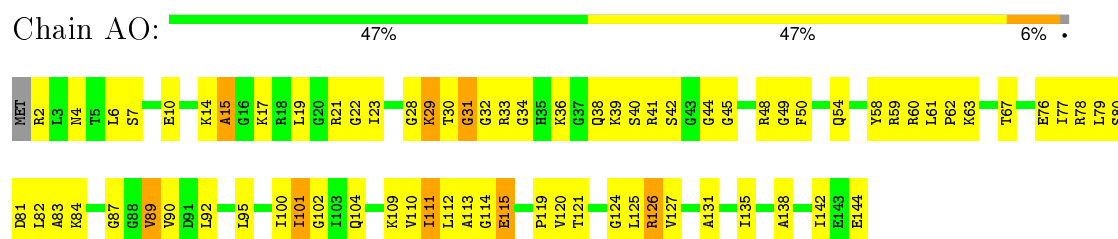
- Molecule 13: 50S ribosomal protein L13



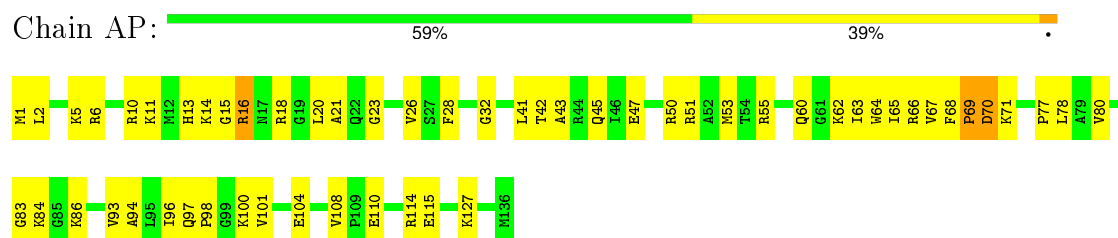
- Molecule 14: 50S ribosomal protein L14



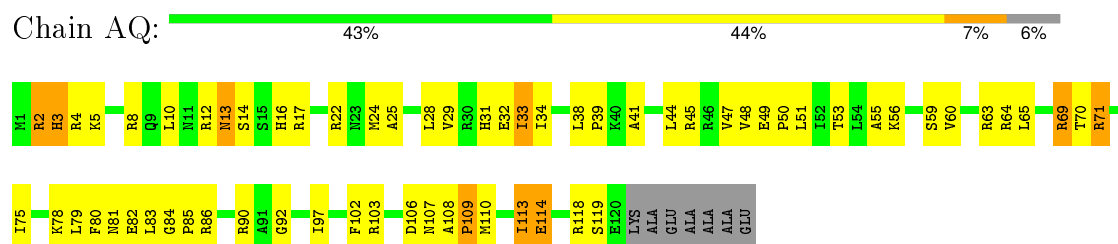
- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16

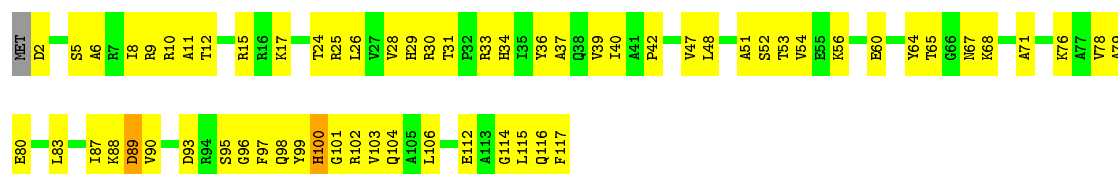


- Molecule 17: 50S ribosomal protein L17



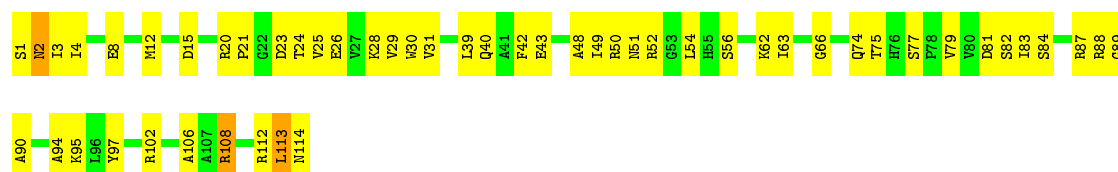
- Molecule 18: 50S ribosomal protein L18





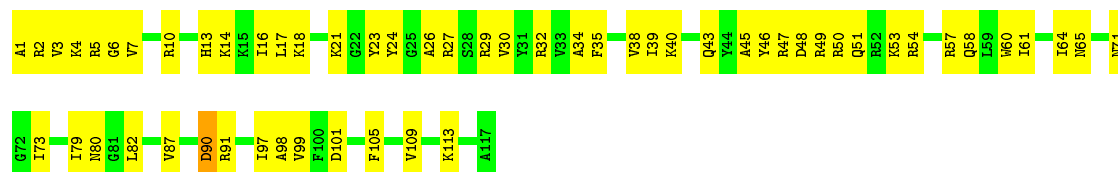
- Molecule 19: 50S ribosomal protein L19

Chain AS: 54% 43% .



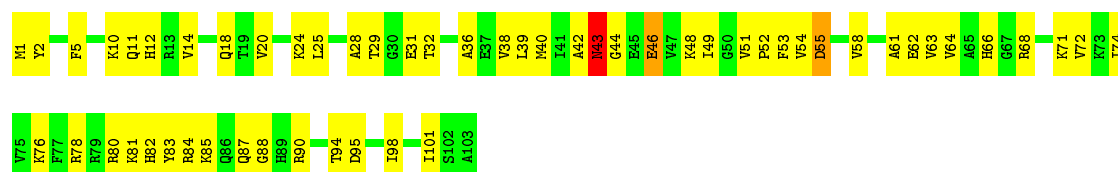
- Molecule 20: 50S ribosomal protein L20

Chain AT: 51% 48% .



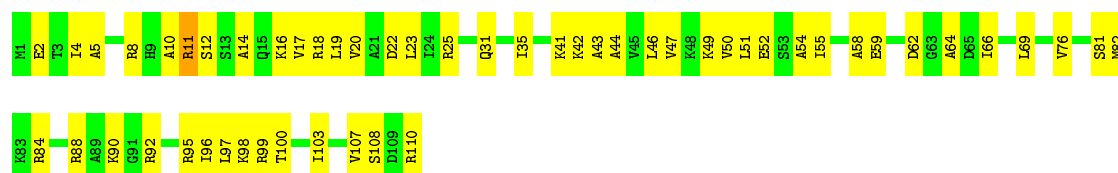
- Molecule 21: 50S ribosomal protein L21

Chain AU: 47% 50% ..



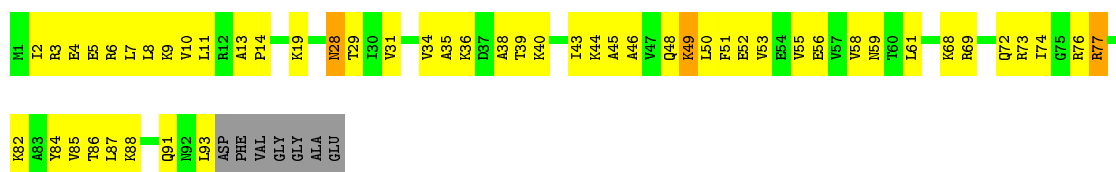
- Molecule 22: 50S ribosomal protein L22

Chain AV: 52% 47% .



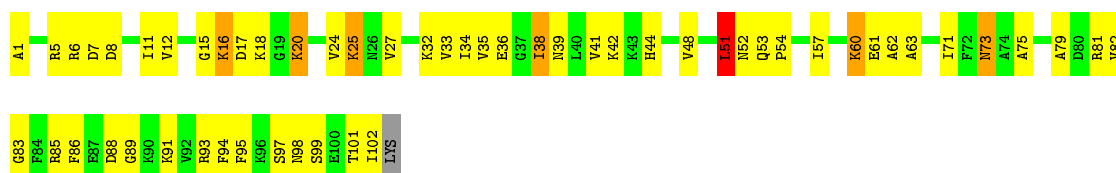
- Molecule 23: 50S ribosomal protein L23

Chain AW: 41% 49% 7% .



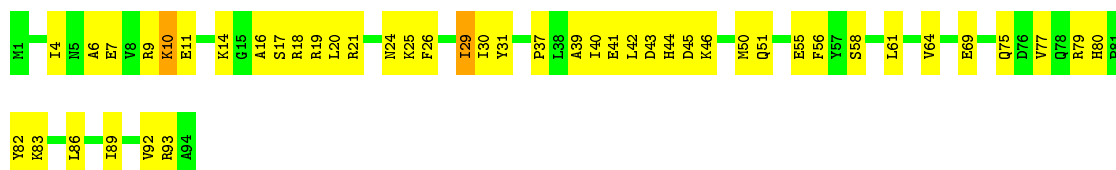
- Molecule 24: 50S ribosomal protein L24

Chain AX: 46% 47% 6% ..



- Molecule 25: 50S ribosomal protein L25

Chain AY: 51% 47% .



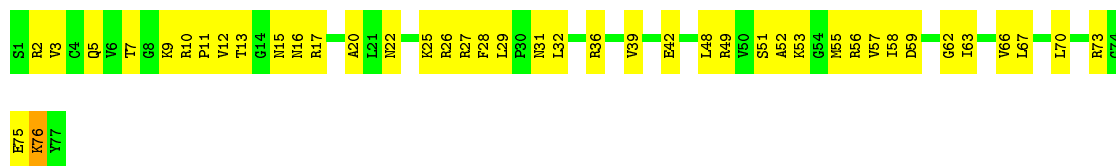
- Molecule 26: 50S ribosomal protein L27

Chain AZ: 58% 30% 10% .



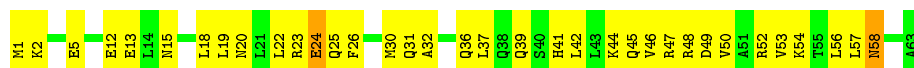
- Molecule 27: 50S ribosomal protein L28

Chain A1: 45% 53% .



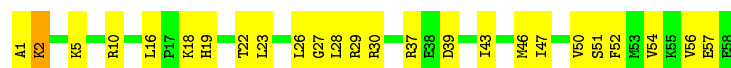
- Molecule 28: 50S ribosomal protein L29

Chain A2: 44% 52% .



- Molecule 29: 50S ribosomal protein L30

Chain A3: 



- Molecule 30: 50S ribosomal protein L32

Chain A4: 



- Molecule 31: 50S ribosomal protein L33

Chain A5: 



- Molecule 32: 50S ribosomal protein L34

Chain A6: 



- Molecule 33: 50S ribosomal protein L35

Chain A7: 



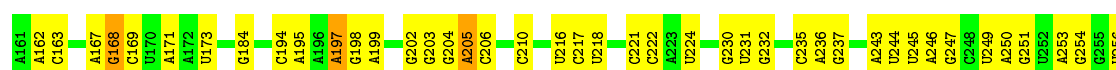
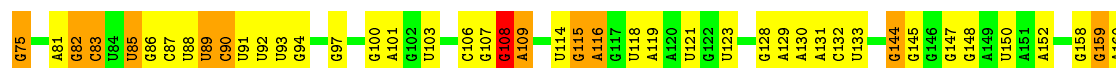
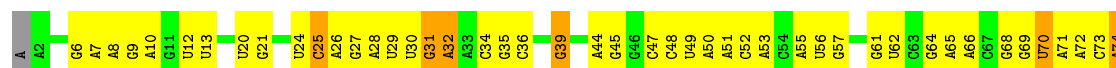
- Molecule 34: 50S ribosomal protein L36

Chain A8: 



- Molecule 35: 16S ribosomal RNA

Chain BA: 

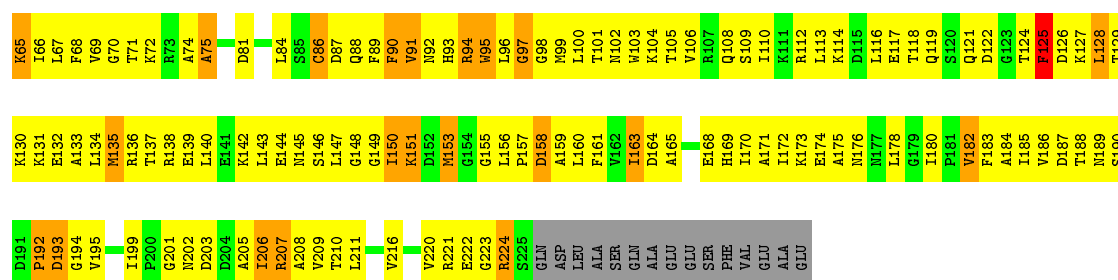


A1480	A1377	G1209	U1126	U1025	A935	C941	C732	A353	G257
U1481	C1378	C1210	C1129	U1030	C940	U842	G733	G354	G258
G1482	U1379	U1211	A1130	U1031	C941	U843	C734	C355	G259
G1486	U1381	U1212	G1299	G1030	G942	G844	C735	A356	G260
G1487	G1300	A1213	G942	G1033	G943	A845	C736	G357	U261
G1488	U1301	A1214	U943	G1032	U943	G846	C737	U358	A262
G1489	C1302	G1214	U943	G1034	U943	G846	C737	G359	A263
G1490	C1303	C1217	A946	G1045	A946	U855	G741	A451	G266
G1491	G1304	C1218	G947	C1046	C948	C956	G742	A452	C267
A1492	G1386	A1219	C948	A1047	A949	G858	A747	A460	U268
G1493	G1387	A1219	A949	G1047	A949	G858	G748	A461	C269
G1494	C1388	U1223	U950	U1048	U950	G859	G749	U467	A270
U1495	U1390	A1225	G951	U1049	G951	A860	A749	A468	C271
C1496	U1391	A1226	G952	G1050	U952	G861	C750	A374	C272
G1497	G1316	A1227	G953	G1053	G953	A864	G751	U375	A279
U1498	C1317	A1227	G954	C1054	U955	A865	G752	G376	
A1503	A1318	G1230	U955	G1054	U955	C866	G755	G377	
G1504	A1319	G1231	U960	G1058	U960	G867	C756	U476	U287
G1506	C1322	U1232	G966	C1059	G966	C868	U757	C477	A288
A1507	G1323	C1234	G966	U1060	G966	A871	G759	A382	G289
G1401	A1324	G1237	A969	G1061	A969	U872	G760	C385	G301
G1402	U1325	U1238	G971	C1063	C970	A873	G761	C386	A302
C1403	U1326	C1237	G971	G1064	G971	A873	U762	U387	G303
C1404	C1327	G1242	C972	U1065	C972	C880	G763	U390	U304
G1405	G1328	C1243	G973	C1066	G973	G881	G764	U391	G305
G1516	A1329	G1244	A974	C1067	A974	G885	G765	C392	A309
G1517	U1330	G1244	A975	A1067	A975	G886	G766	C393	G310
A1518	G1331	A1254	G976	U1073	G976	G886	G769	G394	C311
A1519	A1332	A1254	A977	G1074	A977	A900	A777	C395	C312
C1411	G1334	A1257	A978	U1075	A978	A901	G778	C396	A313
C1412	U1335	G1288	U981	U1078	U981	A906	A779	A397	C314
A1413	C1336	C1259	U982	U1078	U982	A907	A790	G403	A315
U1414	G1337	G1260	A983	A1082	A983	A908	U793	U404	C316
G1415	G1337	A1261	A983	A1082	A983	A909	A794	U405	U317
A1418	G1343	G1268	C990	U1086	C990	A909	U794	G500	A320
G1423	A1346	A1269	U991	G1087	U991	C910	C808	C501	A321
G1435	U1347	G1270	U992	A1092	U992	C912	G809	A502	
U1436	U1348	A1271	G993	A1093	G993	A913	C817	C504	G324
A1437	A1349	G1272	G1001	G1094	G1001	A914	G818	G505	
G1438	C1359	A1274	G1002	U1095	G1002	G917	A819	U508	C328
U1439	A1362	C1277	G1003	G1099	G1003	A918	U820	C506	A329
A1441	A1363	G1278	A1004	C1100	A1004	A919	G821	G507	C330
G1442	U1364	G1279	G1005	A1101	G1005	A920	A715	U512	G331
A1446	G1365	A1280	U1007	A1102	G1006	U921	A825	C513	G332
U1446	C1366	U1283	U1008	C1103	U1007	U922	C826	C514	G335
G1456	C1367	C1284	U1009	G1104	U1008	A923	U827	G515	A336
G1457	A1368	A1285	A1014	A1105	U1009	A923	U828	U516	U427
G1458	C1369	U1286	G1015	G1106	A1014	G926	G829	C599	G428
G1461	G1370	A1287	A1196	C1107	G927	U927	G830	A600	U429
G1478	G1373	A1288	A1197	G1108	A1016	G928	A831	C519	G346
U1478	A1374	C1289	A1201	A1117	G1020	G929	U834	U603	G347
C1479	U1376	U1291	U1202	G1124	A1021	G932	U835	G604	G350
			C1208	G125	G1024	C934	G836	U619	G351
								C620	C352

• Molecule 36: 30S ribosomal protein S2

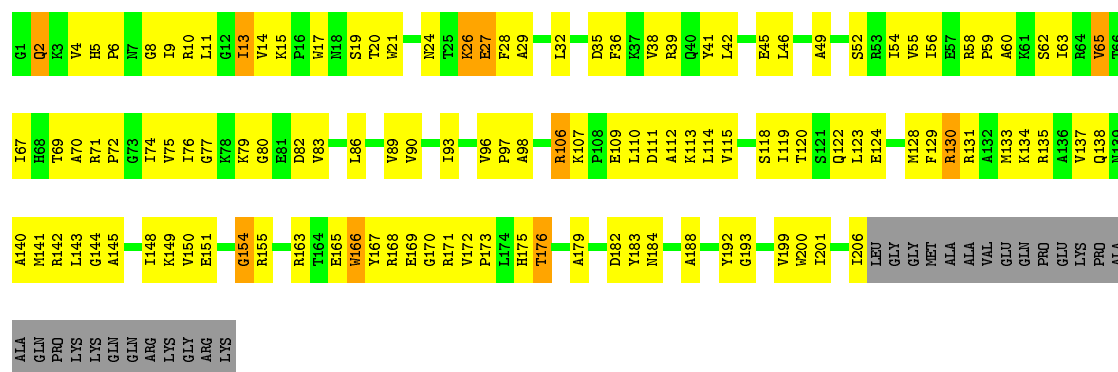
Chain BB: 21% 58% 12% 9%

ALA	P24	R25	P26	K27	P28	F29	L30	F31	G32	A33	R34	R35	K36	V37	R38	U39	L40	P41	E43	K44	T45	T46	P47	P48	P49	N50	P51	A52	L53	L56	N57	K58	L59	A60	K63	P64
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



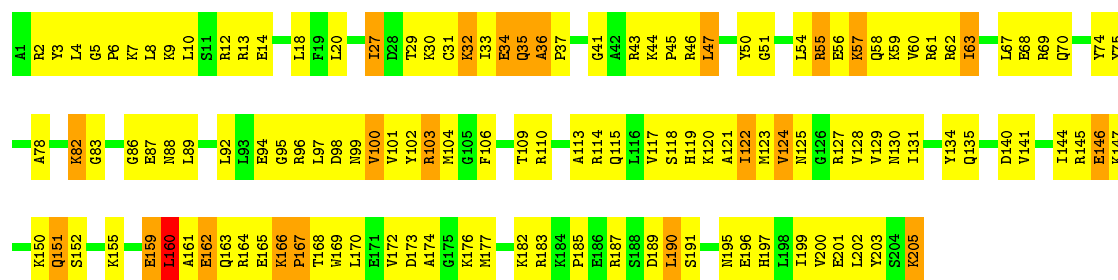
• Molecule 37: 30S ribosomal protein S3

Chain BC: 38% 47% 11%



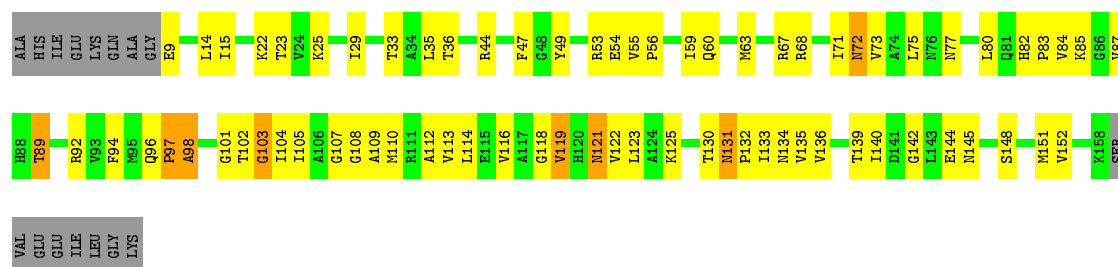
• Molecule 38: 30S ribosomal protein S4

Chain BD: 36% 53% 11%



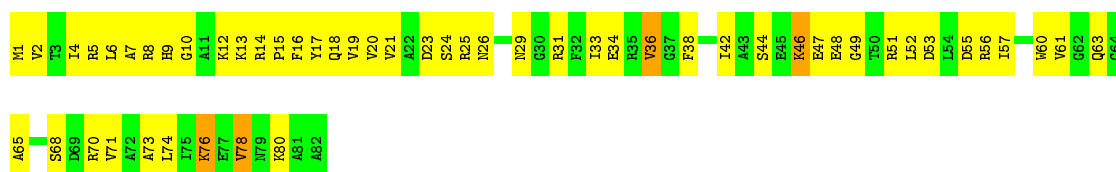
• Molecule 39: 30S ribosomal protein S5

Chain BE: 46% 39% 5% 10%



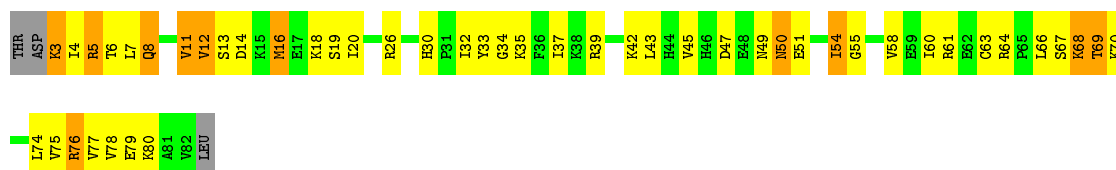
• Molecule 40: 30S ribosomal protein S6





- Molecule 51: 30S ribosomal protein S17

Chain BQ: 39% 45% 13%



- Molecule 52: 30S ribosomal protein S18

Chain BR: 36% 36% 26%



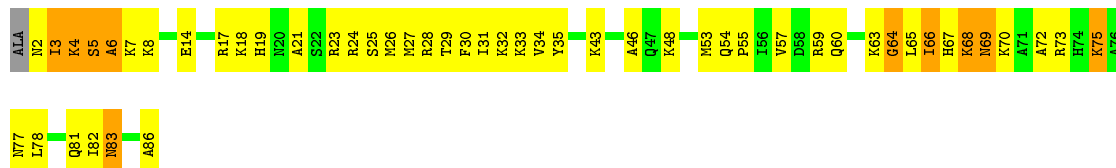
- Molecule 53: 30S ribosomal protein S19

Chain BS: 42% 38% 13%



- Molecule 54: 30S ribosomal protein S20

Chain BT: 40% 48% 12%

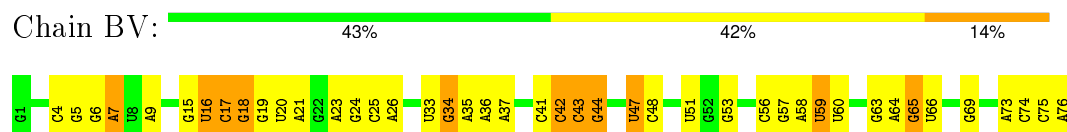


- Molecule 55: 30S ribosomal protein S21

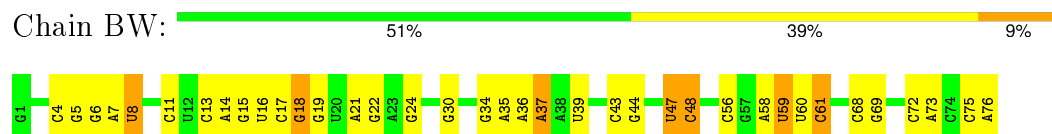
Chain BU: 33% 26% 14% 27%



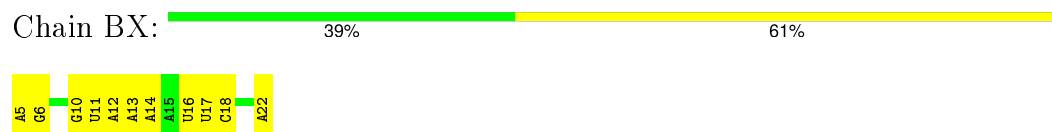
- Molecule 56: tRNA



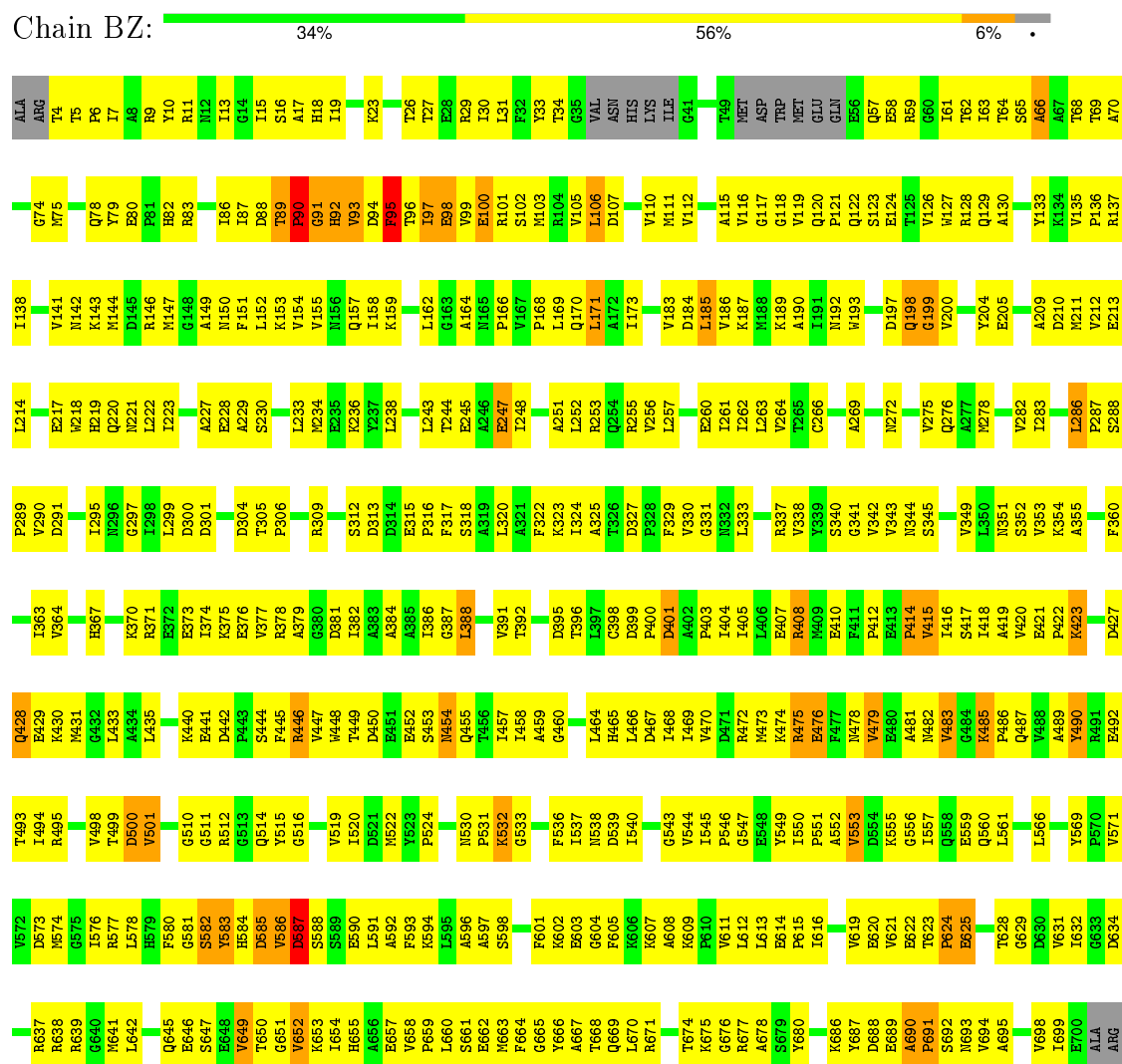
- Molecule 56: tRNA



- Molecule 57: mRNA

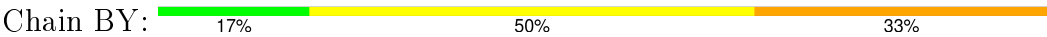


- Molecule 58: Elongation Factor G



GLY
LYS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

● Molecule 59: viomycin



?1
A2
S3
S4
?5
?6

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	85115	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND3, FREALIGN per micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1150	Depositor
Maximum defocus (nm)	6950	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5OH, DPP, UAL, KBE

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	AA	0.33	11/69653 (0.0%)	0.64	18/108657 (0.0%)
10	AJ	0.25	0/1001	0.42	0/1350
11	AK	0.24	0/1046	0.44	0/1410
12	AL	0.23	0/488	0.40	0/652
13	AM	0.23	0/1152	0.40	0/1551
14	AN	0.23	0/947	0.42	0/1268
15	AO	0.24	0/1054	0.42	0/1403
16	AP	0.25	0/1093	0.41	0/1460
17	AQ	0.25	0/973	0.39	0/1301
18	AR	0.23	0/902	0.38	0/1209
19	AS	0.24	0/929	0.41	0/1242
2	AB	0.23	0/2847	0.62	0/4440
20	AT	0.25	0/960	0.37	0/1278
21	AU	0.25	0/829	0.43	0/1107
22	AV	0.21	0/864	0.41	0/1156
23	AW	0.22	0/744	0.41	0/994
24	AX	0.25	0/787	0.41	0/1051
25	AY	0.25	0/766	0.39	0/1025
26	AZ	0.26	0/582	0.37	0/769
27	A1	0.25	0/635	0.39	0/848
28	A2	0.24	0/510	0.42	0/677
29	A3	0.23	0/453	0.42	0/605
3	AC	0.22	0/1690	0.41	0/2278
30	A4	0.23	0/450	0.40	0/599
31	A5	0.27	0/416	0.41	0/554
32	A6	0.25	0/380	0.39	0/498
33	A7	0.25	0/513	0.40	0/676
34	A8	0.24	0/303	0.40	0/397
35	BA	0.28	4/36944 (0.0%)	0.65	4/57632 (0.0%)
36	BB	0.25	0/1735	0.43	0/2338
37	BC	0.24	0/1651	0.41	0/2225
38	BD	0.23	0/1665	0.40	0/2227

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BE	0.24	0/1118	0.43	0/1504
4	AD	0.22	0/2121	0.41	0/2852
40	BF	0.24	0/835	0.43	0/1128
41	BG	0.23	0/1195	0.42	0/1602
42	BH	0.24	0/989	0.41	0/1326
43	BI	0.24	0/1034	0.42	0/1375
44	BJ	0.22	0/796	0.45	0/1077
45	BK	0.24	0/893	0.41	0/1205
46	BL	0.22	0/969	0.42	0/1300
47	BM	0.21	0/892	0.42	0/1193
48	BN	0.24	0/785	0.39	0/1043
49	BO	0.23	0/722	0.41	0/964
5	AE	0.24	0/1586	0.41	0/2134
50	BP	0.25	0/659	0.39	0/884
51	BQ	0.24	0/657	0.43	0/881
52	BR	0.23	0/462	0.40	0/621
53	BS	0.25	0/652	0.43	0/877
54	BT	0.24	0/671	0.41	0/888
55	BU	0.26	0/430	0.43	0/570
56	BV	0.33	2/1809 (0.1%)	0.73	6/2819 (0.2%)
56	BW	0.33	1/1812 (0.1%)	0.65	0/2823
57	BX	0.37	0/432	0.67	0/671
58	BZ	0.29	0/5398	0.59	1/7304 (0.0%)
59	BY	2.44	2/11 (18.2%)	0.76	0/13
6	AF	0.23	0/1571	0.40	0/2113
7	AG	0.26	0/1434	0.40	0/1926
8	AH	0.23	0/1343	0.41	0/1816
9	AI	0.27	0/414	0.43	0/556
All	All	0.29	20/166652 (0.0%)	0.59	29/248342 (0.0%)

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	2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1911	U	O3'-P	-49.96	1.01	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	867	G	O3'-P	15.84	1.80	1.61
1	AA	867	C	O3'-P	12.49	1.76	1.61
35	BA	906	A	O3'-P	10.44	1.73	1.61
1	AA	1425	G	O3'-P	7.22	1.69	1.61

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	906	A	P-O3'-C3'	-25.65	88.92	119.70
35	BA	906	A	O3'-P-O5'	18.08	138.35	104.00
1	AA	1911	U	P-O3'-C3'	-15.29	101.35	119.70
35	BA	906	A	OP1-P-O3'	-12.39	77.94	105.20
1	AA	1911	U	OP2-P-O3'	10.59	128.49	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1913	A	Sidechain
1	AA	1915	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62192	0	31283	1405	0
2	AB	2548	0	1292	51	0
3	AC	1675	0	1763	103	0
4	AD	2082	0	2157	180	0
5	AE	1565	0	1616	93	0
6	AF	1552	0	1619	117	0
7	AG	1410	0	1447	129	0
8	AH	1323	0	1374	82	0
9	AI	409	0	429	37	0
10	AJ	988	0	1025	87	0
11	AK	1032	0	1088	123	0
12	AL	487	0	515	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	1129	0	1162	72	0
14	AN	938	0	1012	64	0
15	AO	1045	0	1117	115	0
16	AP	1074	0	1157	65	0
17	AQ	960	0	1000	69	0
18	AR	892	0	923	59	0
19	AS	917	0	965	62	0
20	AT	947	0	1022	76	0
21	AU	816	0	839	67	0
22	AV	857	0	922	56	0
23	AW	738	0	807	73	0
24	AX	779	0	834	54	0
25	AY	753	0	780	42	0
26	AZ	575	0	589	39	0
27	A1	625	0	655	43	0
28	A2	509	0	543	42	0
29	A3	449	0	491	30	0
30	A4	444	0	461	42	0
31	A5	409	0	440	19	0
32	A6	377	0	418	41	0
33	A7	504	0	574	59	0
34	A8	302	0	343	32	0
35	BA	32995	0	16607	686	0
36	BB	1704	0	1732	194	0
37	BC	1624	0	1699	120	0
38	BD	1643	0	1710	171	0
39	BE	1105	0	1148	79	0
40	BF	817	0	808	70	0
41	BG	1181	0	1240	98	0
42	BH	979	0	1034	85	0
43	BI	1022	0	1070	118	0
44	BJ	786	0	828	81	0
45	BK	877	0	887	76	0
46	BL	955	0	1019	99	0
47	BM	883	0	944	82	0
48	BN	774	0	827	92	0
49	BO	714	0	737	56	0
50	BP	649	0	666	63	0
51	BQ	648	0	691	59	0
52	BR	455	0	478	37	0
53	BS	637	0	665	38	0
54	BT	665	0	714	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BU	425	0	449	33	0
56	BV	1619	0	822	56	0
56	BW	1622	0	821	47	0
57	BX	386	0	194	11	0
58	BZ	5301	0	5269	667	0
59	BY	48	0	40	13	0
60	A8	1	0	0	0	0
All	All	153817	0	105761	5995	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 23.

The worst 5 of 5995 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1912:A:C2	1:AA:1919:A:C5	2.13	1.37
1:AA:1052:C:OP1	1:AA:2752:C:H5'	1.10	1.21
1:AA:2876:G:H5''	19:AS:2:ASN:HB2	1.19	1.19
1:AA:1916:A:H2	35:BA:1409:C:OP1	1.21	1.19
1:AA:250:G:H4'	15:AO:59:ARG:HD3	1.18	1.17

There are no symmetry-related clashes.

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 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	
3	AC	223/233 (96%)	203 (91%)	18 (8%)	2 (1%)	21	67
4	AD	269/272 (99%)	222 (82%)	39 (14%)	8 (3%)	5	42
5	AE	207/209 (99%)	179 (86%)	22 (11%)	6 (3%)	6	43
6	AF	199/201 (99%)	170 (85%)	24 (12%)	5 (2%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	175/178 (98%)	145 (83%)	21 (12%)	9 (5%)	2	30
8	AH	174/176 (99%)	144 (83%)	24 (14%)	6 (3%)	5	40
9	AI	51/149 (34%)	28 (55%)	15 (29%)	8 (16%)	0	5
10	AJ	129/165 (78%)	108 (84%)	16 (12%)	5 (4%)	4	36
11	AK	139/141 (99%)	77 (55%)	39 (28%)	23 (16%)	0	5
12	AL	66/120 (55%)	55 (83%)	10 (15%)	1 (2%)	13	57
13	AM	140/142 (99%)	118 (84%)	21 (15%)	1 (1%)	26	71
14	AN	120/123 (98%)	102 (85%)	13 (11%)	5 (4%)	3	34
15	AO	141/144 (98%)	110 (78%)	21 (15%)	10 (7%)	1	22
16	AP	134/136 (98%)	115 (86%)	15 (11%)	4 (3%)	5	42
17	AQ	118/127 (93%)	98 (83%)	14 (12%)	6 (5%)	2	30
18	AR	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	4	39
19	AS	112/114 (98%)	94 (84%)	14 (12%)	4 (4%)	4	38
20	AT	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	21	67
21	AU	101/103 (98%)	81 (80%)	16 (16%)	4 (4%)	4	35
22	AV	108/110 (98%)	88 (82%)	18 (17%)	2 (2%)	10	52
23	AW	91/100 (91%)	79 (87%)	11 (12%)	1 (1%)	17	63
24	AX	100/103 (97%)	76 (76%)	17 (17%)	7 (7%)	1	22
25	AY	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
26	AZ	74/84 (88%)	63 (85%)	10 (14%)	1 (1%)	14	58
27	A1	75/77 (97%)	65 (87%)	10 (13%)	0	100	100
28	A2	61/63 (97%)	51 (84%)	8 (13%)	2 (3%)	5	40
29	A3	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	A4	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
31	A5	48/54 (89%)	38 (79%)	8 (17%)	2 (4%)	3	34
32	A6	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
33	A7	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	12	56
34	A8	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	6	44
36	BB	216/240 (90%)	140 (65%)	51 (24%)	25 (12%)	0	9
37	BC	204/232 (88%)	169 (83%)	28 (14%)	7 (3%)	5	40
38	BD	203/205 (99%)	161 (79%)	26 (13%)	16 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BE	148/166 (89%)	111 (75%)	27 (18%)	10 (7%)	1	23
40	BF	98/131 (75%)	71 (72%)	20 (20%)	7 (7%)	1	22
41	BG	149/178 (84%)	123 (83%)	21 (14%)	5 (3%)	5	40
42	BH	127/129 (98%)	112 (88%)	11 (9%)	4 (3%)	5	42
43	BI	125/129 (97%)	95 (76%)	25 (20%)	5 (4%)	4	35
44	BJ	96/103 (93%)	65 (68%)	19 (20%)	12 (12%)	0	8
45	BK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	3	34
46	BL	121/123 (98%)	95 (78%)	18 (15%)	8 (7%)	1	24
47	BM	112/117 (96%)	94 (84%)	12 (11%)	6 (5%)	2	29
48	BN	92/100 (92%)	67 (73%)	19 (21%)	6 (6%)	1	25
49	BO	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	8	48
50	BP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	2	25
51	BQ	78/83 (94%)	56 (72%)	14 (18%)	8 (10%)	1	12
52	BR	53/74 (72%)	49 (92%)	4 (8%)	0	100	100
53	BS	77/91 (85%)	56 (73%)	14 (18%)	7 (9%)	1	17
54	BT	83/86 (96%)	69 (83%)	7 (8%)	7 (8%)	1	18
55	BU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	8
58	BZ	680/711 (96%)	565 (83%)	76 (11%)	39 (6%)	2	28
59	BY	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	6622/7186 (92%)	5360 (81%)	943 (14%)	319 (5%)	5	32

5 of 319 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	104	VAL
8	AH	37	ASN
8	AH	118	ALA
9	AI	3	VAL
9	AI	9	VAL

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	
3	AC	175/180 (97%)	173 (99%)	2 (1%)	80	91
4	AD	216/217 (100%)	213 (99%)	3 (1%)	74	89
5	AE	164/164 (100%)	162 (99%)	2 (1%)	78	90
6	AF	165/165 (100%)	165 (100%)	0	100	100
7	AG	148/149 (99%)	145 (98%)	3 (2%)	63	85
8	AH	137/137 (100%)	132 (96%)	5 (4%)	42	74
9	AI	42/114 (37%)	39 (93%)	3 (7%)	18	55
10	AJ	100/123 (81%)	99 (99%)	1 (1%)	82	92
11	AK	109/109 (100%)	98 (90%)	11 (10%)	9	38
12	AL	47/84 (56%)	46 (98%)	1 (2%)	61	84
13	AM	116/116 (100%)	113 (97%)	3 (3%)	54	80
14	AN	103/104 (99%)	102 (99%)	1 (1%)	82	92
15	AO	102/103 (99%)	100 (98%)	2 (2%)	63	85
16	AP	109/109 (100%)	106 (97%)	3 (3%)	51	78
17	AQ	100/103 (97%)	96 (96%)	4 (4%)	38	71
18	AR	86/87 (99%)	85 (99%)	1 (1%)	78	90
19	AS	99/99 (100%)	97 (98%)	2 (2%)	63	85
20	AT	89/89 (100%)	89 (100%)	0	100	100
21	AU	84/84 (100%)	82 (98%)	2 (2%)	57	82
22	AV	93/93 (100%)	93 (100%)	0	100	100
23	AW	80/84 (95%)	77 (96%)	3 (4%)	40	73
24	AX	83/84 (99%)	78 (94%)	5 (6%)	24	60
25	AY	78/78 (100%)	76 (97%)	2 (3%)	54	80
26	AZ	56/62 (90%)	55 (98%)	1 (2%)	66	87
27	A1	67/67 (100%)	66 (98%)	1 (2%)	72	88
28	A2	55/55 (100%)	54 (98%)	1 (2%)	66	87
29	A3	48/48 (100%)	47 (98%)	1 (2%)	61	84
30	A4	47/47 (100%)	45 (96%)	2 (4%)	35	70
31	A5	45/48 (94%)	45 (100%)	0	100	100
32	A6	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	A7	51/51 (100%)	50 (98%)	1 (2%)	63	85
34	A8	34/34 (100%)	34 (100%)	0	100	100
36	BB	180/198 (91%)	168 (93%)	12 (7%)	20	57
37	BC	170/189 (90%)	162 (95%)	8 (5%)	32	68
38	BD	172/172 (100%)	159 (92%)	13 (8%)	16	53
39	BE	113/125 (90%)	109 (96%)	4 (4%)	43	74
40	BF	87/112 (78%)	84 (97%)	3 (3%)	44	75
41	BG	124/146 (85%)	119 (96%)	5 (4%)	38	71
42	BH	104/104 (100%)	101 (97%)	3 (3%)	50	78
43	BI	105/106 (99%)	96 (91%)	9 (9%)	13	47
44	BJ	86/90 (96%)	83 (96%)	3 (4%)	43	74
45	BK	90/98 (92%)	84 (93%)	6 (7%)	20	57
46	BL	103/103 (100%)	101 (98%)	2 (2%)	65	86
47	BM	92/95 (97%)	89 (97%)	3 (3%)	45	76
48	BN	79/83 (95%)	73 (92%)	6 (8%)	16	53
49	BO	76/76 (100%)	73 (96%)	3 (4%)	39	72
50	BP	65/65 (100%)	62 (95%)	3 (5%)	33	68
51	BQ	74/77 (96%)	69 (93%)	5 (7%)	20	57
52	BR	48/64 (75%)	47 (98%)	1 (2%)	61	84
53	BS	70/78 (90%)	66 (94%)	4 (6%)	25	62
54	BT	65/65 (100%)	62 (95%)	3 (5%)	33	68
55	BU	44/60 (73%)	40 (91%)	4 (9%)	12	43
58	BZ	563/585 (96%)	539 (96%)	24 (4%)	35	70
59	BY	2/2 (100%)	2 (100%)	0	100	100
All	All	5478/5818 (94%)	5288 (96%)	190 (4%)	47	74

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BC	167	TYR
41	BG	3	ARG
58	BZ	171	LEU
38	BD	55	ARG
38	BD	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
28	A2	15	ASN
37	BC	5	HIS
58	BZ	157	GLN
28	A2	27	ASN
30	A4	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2894/2903 (99%)	291 (10%)	4 (0%)
2	AB	118/119 (99%)	11 (9%)	0
35	BA	1537/1542 (99%)	164 (10%)	4 (0%)
56	BV	75/76 (98%)	15 (20%)	1 (1%)
56	BW	75/76 (98%)	11 (14%)	0
57	BX	17/18 (94%)	3 (17%)	0
All	All	4716/4734 (99%)	495 (10%)	9 (0%)

5 of 495 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	34	U
1	AA	35	G
1	AA	46	G
1	AA	74	A

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	74	A
56	BV	15	G
35	BA	1101	A
1	AA	2157	G
35	BA	115	G

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

4 non-standard protein/DNA/RNA residues are 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	KBE	BY	1	59	8,8,9	0.52	0	7,8,10	0.99	1 (14%)
59	DPP	BY	2	59	2,5,6	0.60	0	1,5,7	1.86	0
59	UAL	BY	5	59	7,8,9	2.19	3 (42%)	4,9,11	1.52	1 (25%)
59	5OH	BY	6	59	8,12,13	0.53	0	6,16,18	1.68	1 (16%)

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	KBE	BY	1	59	-	0/7/7/8	0/0/0/0
59	DPP	BY	2	59	-	0/2/4/6	0/0/0/0
59	UAL	BY	5	59	-	0/3/7/9	0/0/0/0
59	5OH	BY	6	59	-	0/1/18/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BY	5	UAL	C1-N1	-3.73	1.34	1.40
59	BY	5	UAL	C-CA	-3.68	1.39	1.45
59	BY	5	UAL	CA-N	2.29	1.40	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BY	6	5OH	CR-CB-CA	-3.48	109.22	112.77
59	BY	5	UAL	O-C-CA	-2.65	121.90	125.59
59	BY	1	KBE	CD-CG-CB	-2.15	108.72	115.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	BY	1	KBE	2	0
59	BY	5	UAL	3	0
59	BY	6	5OH	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1916:A	O3'	1917:U	P	2.39
1	AA	1911:U	O3'	1912:A	P	1.01