



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 13, 2017 – 02:59 PM EST

PDB ID : 3JCE
EMDB ID: : EMD-6550
Title : Structure of Escherichia coli EF4 in pretranslocational ribosomes (Pre EF4)
Authors : Zhang, D.; Yan, K.; Liu, G.; Song, G.; Luo, J.; Shi, Y.; Cheng, E.; Wu, S.;
Jiang, T.; Low, J.; Gao, N.; Qin, Y.
Deposited on : 2015-12-01
Resolution : 3.20 Å(reported)
Based on PDB ID : 4V9O

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : rb-20028442

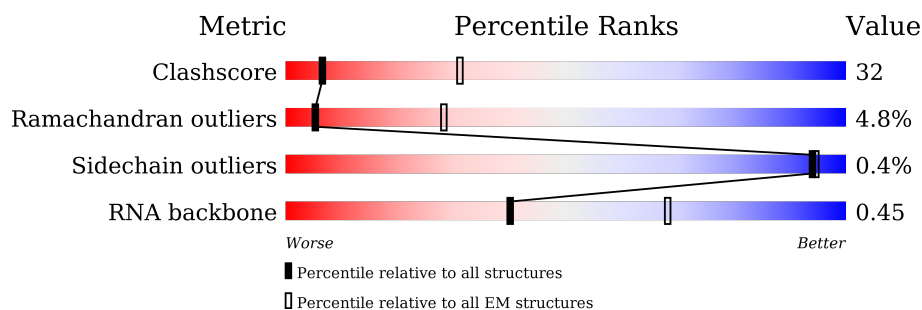
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.





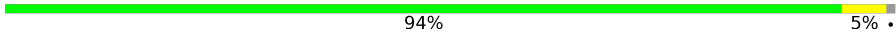
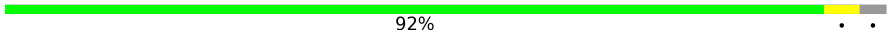

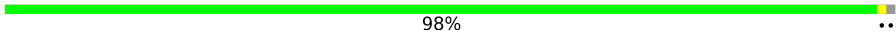
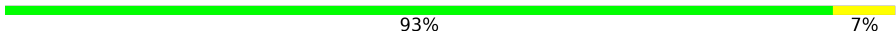
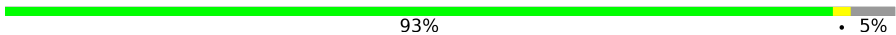


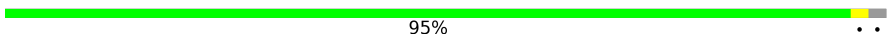














Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	a	1533	80% 20%
2	c	233	86% 12%
3	d	206	96% .
4	e	167	87% 10%
5	f	135	70% 5% 24%
6	g	179	82% . 16%
7	h	130	98% ..
8	i	130	95% ..




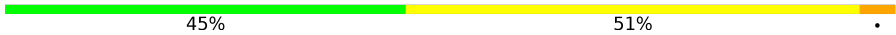
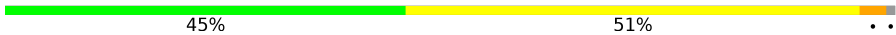
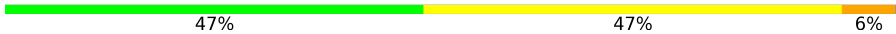
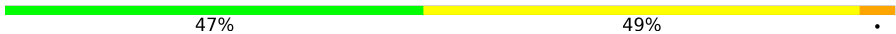

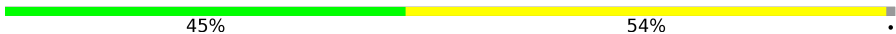


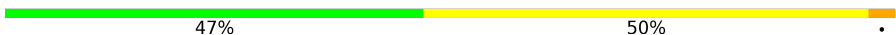
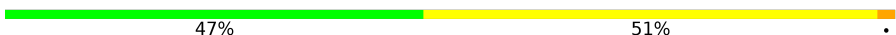
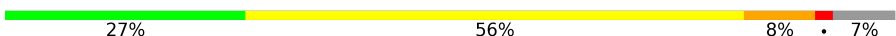


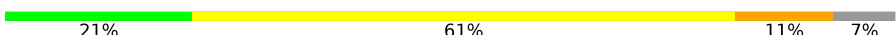








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Mol	Chain	Length	Quality of chain
9	j	103	
10	k	129	
11	l	124	
12	m	118	
13	n	101	
14	o	89	
15	p	82	
16	q	84	
17	r	75	
18	s	92	
19	t	87	
20	u	71	
21	b	241	
22	0	57	
23	1	55	
24	2	46	
25	3	65	
26	4	38	
27	5	234	
28	A	2904	
29	B	120	
30	C	273	
31	D	209	
32	E	201	
33	F	179	

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Mol	Chain	Length	Quality of chain
34	G	177	
35	H	149	
36	I	142	
37	J	142	
38	K	123	
39	L	144	
40	M	136	
41	N	127	
42	O	117	
43	P	115	
44	Q	118	
45	R	103	
46	S	110	
47	T	100	
48	U	104	
49	V	94	
50	W	85	
51	X	78	
52	Y	63	
53	Z	59	
54	6	76	
55	7	15	
56	8	77	
57	x	599	
58	9	76	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 154017 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a protein called 30S ribosomal protein S2.

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

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a RNA chain called 23 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	2903	Total	C	N	O	P	0	0
			62320	27801	11467	20149	2903		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	76	Total	C	N	O	P	0	0
			1633	732	291	534	76		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	15	Total	C	N	O	P	0	0
			320	144	59	102	15		

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

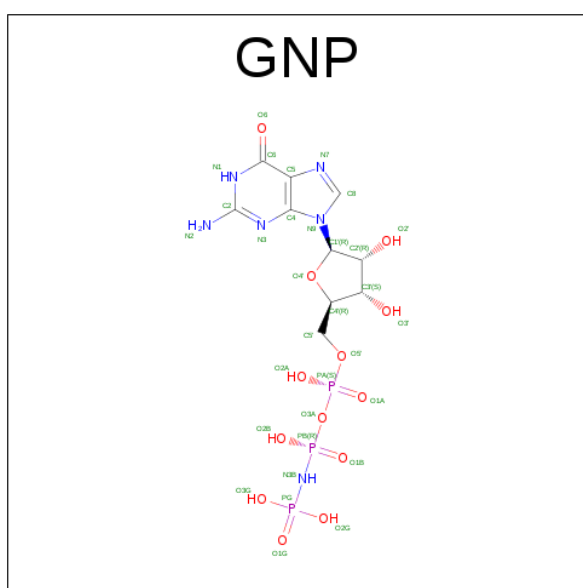
- Molecule 57 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	586	Total	C	N	O	S	0	0
			4573	2885	792	875	21		

- Molecule 58 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	9	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
59	x	1	Total	C	N	O	P	0
			32	10	6	13	3	

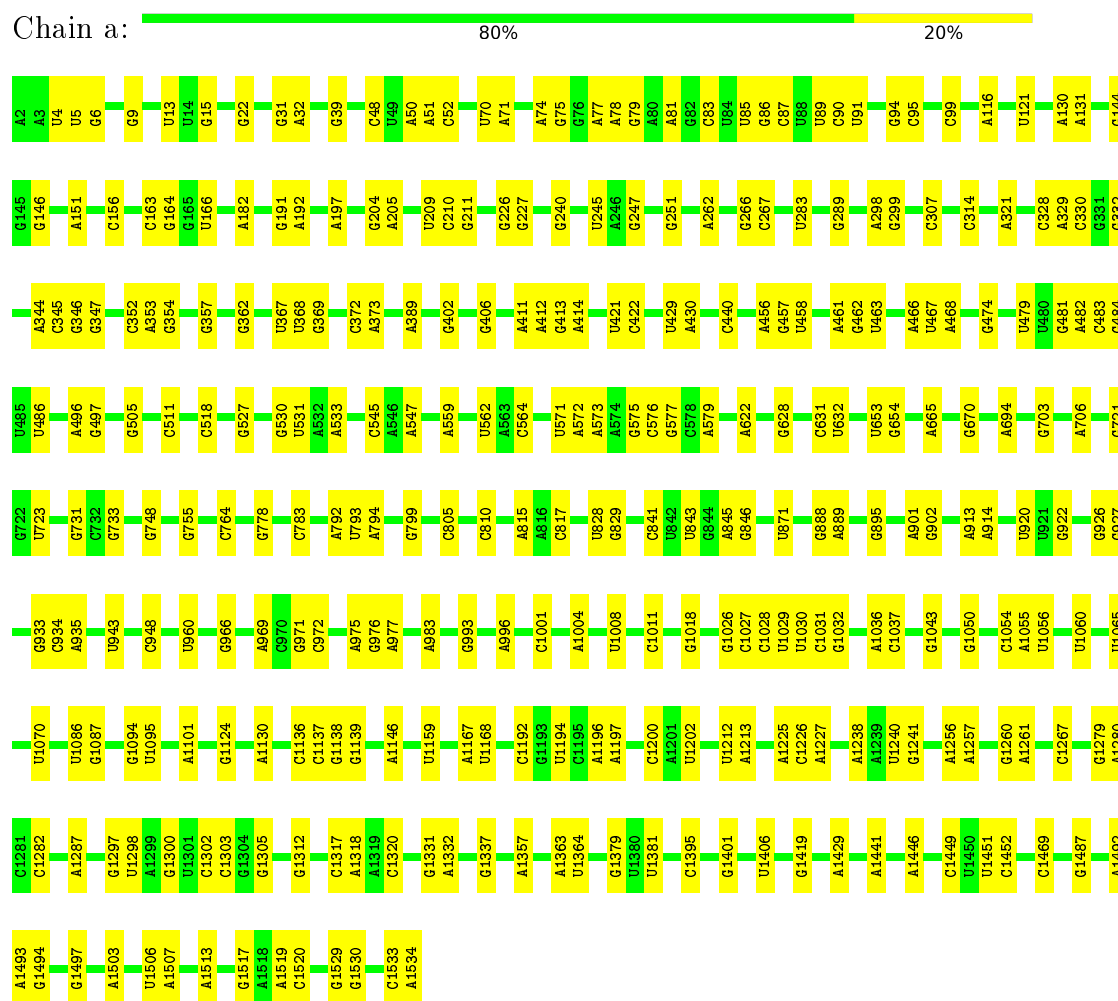
- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	x	1	Total	Mg	0
			1	1	

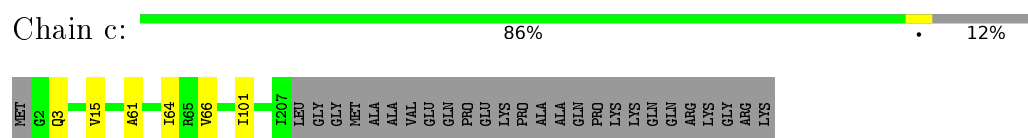
3 Residue-property plots

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: 16S ribosomal RNA



• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

Chain d:  96%



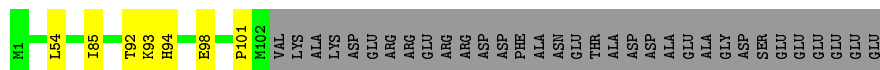
- Molecule 4: 30S ribosomal protein S5

Chain e:  87% 10%




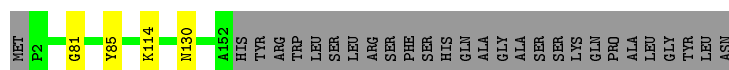
- Molecule 5: 30S ribosomal protein S6

Chain f:  70% 5% 24%



- Molecule 6: 30S ribosomal protein S7

Chain g:  82% 16%



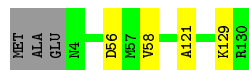
- Molecule 7: 30S ribosomal protein S8

Chain h:  98%




- Molecule 8: 30S ribosomal protein S9

Chain i:  95%



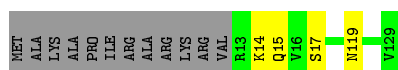
- Molecule 9: 30S ribosomal protein S10

Chain j:  86% 9% 5%



- Molecule 10: 30S ribosomal protein S11

Chain k:  88% 9%



- Molecule 11: 30S ribosomal protein S12

Chain l: 94% 5%



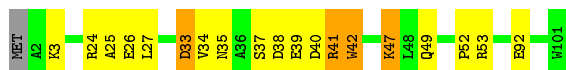
- Molecule 12: 30S ribosomal protein S13

Chain m: 92%



- Molecule 13: 30S ribosomal protein S14

Chain n: 80% 15%



- Molecule 14: 30S ribosomal protein S15

Chain o: 98%



- Molecule 15: 30S ribosomal protein S16

Chain p: 93% 7%



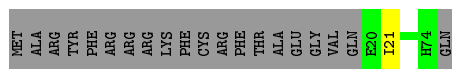
- Molecule 16: 30S ribosomal protein S17

Chain q: 93% 5%




- Molecule 17: 30S ribosomal protein S18

Chain r: 72% 27%



- Molecule 18: 30S ribosomal protein S19

Chain s:  82% 14%



- Molecule 19: 30S ribosomal protein S20

Chain t:  95%




- Molecule 20: 30S ribosomal protein S21

Chain u:  66% 6% 28%



- Molecule 21: 30S ribosomal protein S2

Chain b:  88% 10%

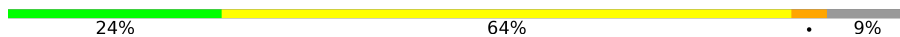


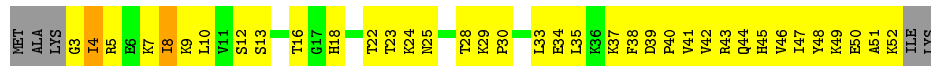
- Molecule 22: 50S ribosomal protein L32

Chain 0:  51% 46%



- Molecule 23: 50S ribosomal protein L33

Chain 1:  24% 64% 9%



- Molecule 24: 50S ribosomal protein L34

Chain 2:  70% 30%

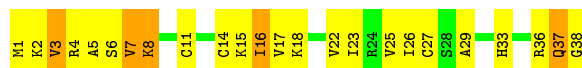


- Molecule 25: 50S ribosomal protein L35

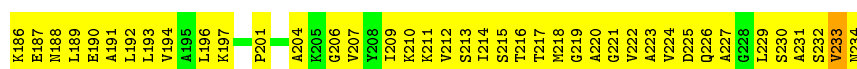
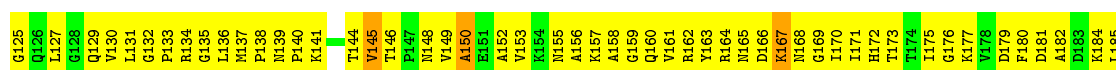
Chain 3:  51% 45%



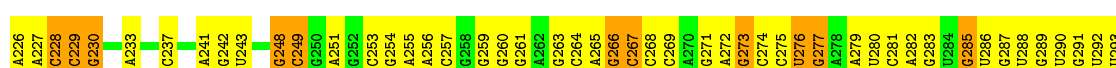
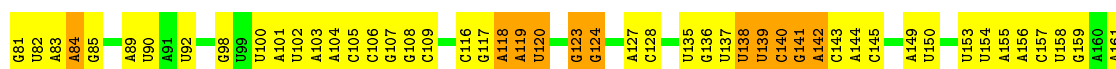
- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L1



- Molecule 28: 23 ribosomal RNA



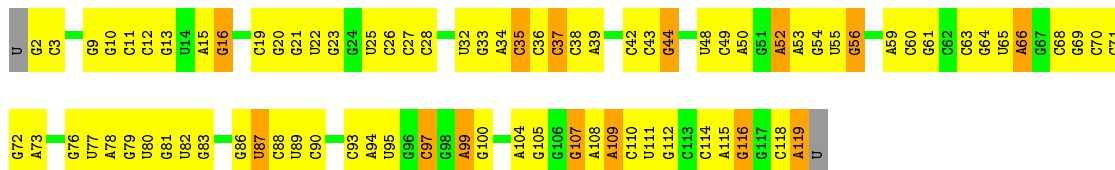
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G1622	A1551	G1491	U1409	C1319	G1236	G1160	A1094	A1028	C888	C889	A819	G745	U591	A527
A1626	A1553	G1492	U1411	C1320	A1095	G1162	A1096	C1030	C890	C891	A821	U746	U594	A528
G1627	G1554	C1493	U1412	A1322	G1238	G1163	U1097	G1031	G966	G891	U824	U747	C595	G530
G1628	G1555	A1494	A1413	C1323	U1242	C1167	A1098	A1032	U967	A892	A825	C748	C596	C531
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A1630	G1560	A1496	U1415	G1325	A1244	C1169	U1101	G1036	A973	U894	U827	A750	U598	A533
G1631	C1561	U1497	G1416	U1326	G1245	C1170	A1102	G1037	G974	A896	U828	A751	A599	U534
A1634	U1562	C1498	G1418	A1328	G1248	G1171	A1103	G1041	A975	C897	A829	G757	C601	G535
U1635	A1419	A1500	A1418	A1328	U1249	G1172	C1104	C830	G976	C898	G830	C758	A602	G536
C1636	A1420	G1421	A1420	G1331	U1250	U1173	U1105	G831	G977	A899	G831	G759	A603	A537
C1638	A1502	G1421	G1421	G1332	U1258	U1181	G1106	G1042	C978	A900	U832	G760	G604	A538
C1639	A1503	G1431	A1431	A1347	U1263	G1182	G1107	C1043	C987	A910	U833	A761	C540	G539
A1640	A1504	G1432	A1432	C1348	U1265	U1183	U1108	A844	A988	C912	U845	G762	A610	A541
A1641	A1505	G1433	A1433	C1349	A1263	G1184	C1121	U913	A990	U913	U846	G775	C619	C542
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G1645	A1509	G1432	A1432	A1348	U1268	G1188	G1125	G1062	C996	A920	C854	G781	A627	G554
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U1648	A1511	A1434	A1434	A1353	A1270	U1190	G1127	C1064	C998	C922	G856	G783	A621	G548
G1649	A1512	A1435	A1435	A1365	A1271	U1191	G1128	U1065	C999	G923	G857	G784	G622	G549
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G1653	U1514	G1437	A1437	A1367	A1273	G1193	G1130	U1067	A1001	A925	C859	G786	A633	C560
A1654	A1515	A1438	A1438	A1367	A1274	U1194	U1131	A1069	A1002	G926	U860	C787	C634	U562
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C1658	G1459	G1458	G1458	A1378	G1291	A1205	C1135	A1073	C1006	U933	C869	A794	U640	G570
A1661	U1466	U1466	U1466	G1379	G1292	G1206	G1138	G1074	C1007	U934	U870	C795	U641	U571
G1662	A1469	A1469	A1469	G1380	U1293	C1207	U1139	C1075	A1008	U934	U871	C796	U642	A572
G1663	C1456	U1467	U1467	A1383	C1295	C1208	G1140	C1076	A1009	C935	U872	C796	A643	U573
A1668	A1472	U1468	U1468	A1384	G1296	C1211	U1141	A1077	G1010	G940	C873	A800	U643	G574
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G1681	G1482	G1482	G1482	U1401	G1309	C1229	U1153	A1086	A1021	G954	U882	G809	G656	C587
A1699	C1483	C1483	C1483	U1402	G1309	C1230	G1154	A1087	G1022	U955	U883	U840	U658	U588
A1610	A1403	A1403	A1403	A1403	U1313	C1231	G1155	A1088	G1023	U956	U884	C812	G738	
G1694	U1484	U1484	U1484	A1403	C1314	G1232	A1156	A1089	G1024	G956	C885			
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G1696	U1486	U1486	U1486	U1405	C1315	G1233	G1157	G1091						
A1700	U1487	U1487	U1487	U1406	C1315	G1233								

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A2800	A2564	U2564	A2418	A2418	U2493	A2418	G2346	A2285	G2205	A2142	C2072	C2006	C1914	U1812	A1745
G2801	U2565	U2565	U2419	U2419	U2493	U2419	A2347	G2286	U2210	G2143	C2073	C2006	C1915	U1813	A1746
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C2815	G2576	U2576	U2431	U2431	U2506	U2431	A2358	U2297	G2225	U2155	A2094	C2023	A1928	A1829	A1762
G2816	U2577	U2577	A2432	A2432	C2507	A2432	G2359	U2298	G2226	G2156	C2095	C2024	G1929	G1763	G1763
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U2818	U2511	U2511	U2434	U2434	C2512	U2434	G2361	C2301	G2230	A2158	U2098	C2026	U1931	G1765	U1765
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A2821	U2514	U2514	U2436	U2436	U2515	U2436	G2365	U2304	G2233	C2161	A2101	U2028	C1934	C1771	C1771
U2822	U2515	U2515	U2437	U2437	A2516	U2437	A2366	U2305	U2234	G2162	G2102	G2029	G1935	U1856	A1772
A2823	A2587	U2587	U2441	U2441	U2516	U2441	G2367	U2306	U2235	A2163	C2103	A2030	A1936	G1857	A1772



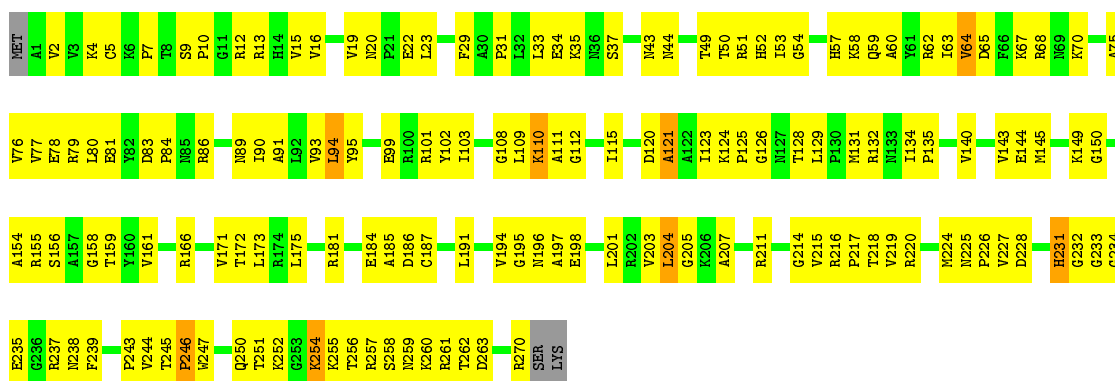
• Molecule 29: 5S ribosomal RNA

Chain B: 30% 57% 12%



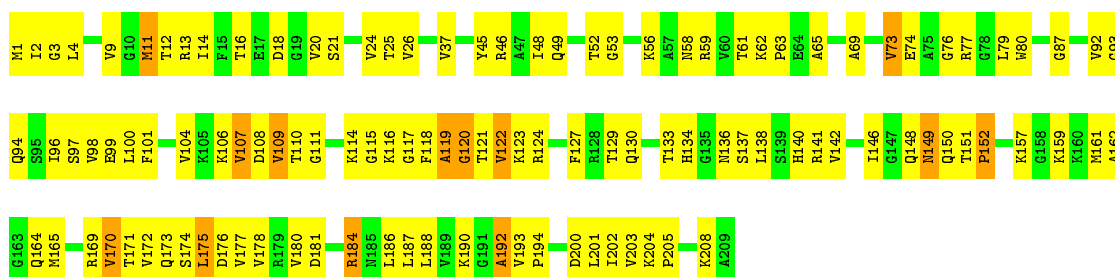
• Molecule 30: 50S ribosomal protein L2

Chain C: 44% 52%



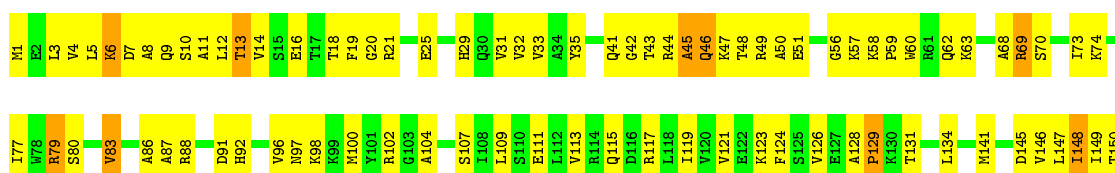
• Molecule 31: 50S ribosomal protein L3

Chain D: 45% 49% 6%



• Molecule 32: 50S ribosomal protein L4

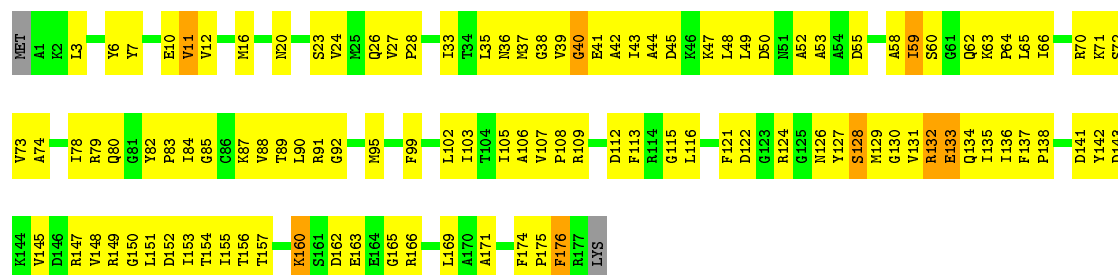
Chain E: 43% 52% 5%





• Molecule 33: 50S ribosomal protein L5

Chain F: 36% 58%



• Molecule 34: 50S ribosomal protein L6

Chain G: 35% 60%



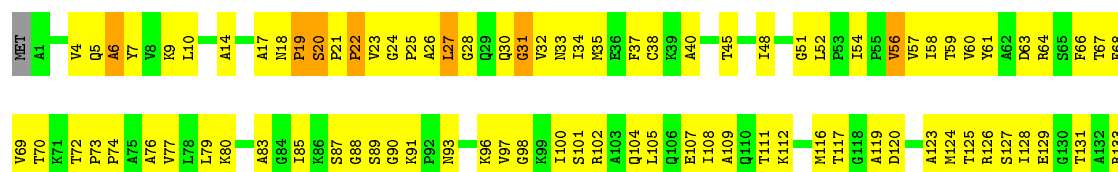
• Molecule 35: 50S ribosomal protein L9

Chain H: 24% 69% 7%



• Molecule 36: 50S ribosomal protein L11

Chain I: 33% 61% 5%



S134
M135
G136
L137
V138
V139
E140
D141

• Molecule 37: 50S ribosomal protein L13

Chain J: 45% 51%

H1 H2 T3 F4 K7 T10 V11 K12 R13 D14 H15 Y16 V17 V18 G26 A29 T30 E31 L32 R35 K36 L36 R37 G38 K39 R40 R41 R42 R43 R44 T45 P46 R47 V48 D49 T50 G51 D52 Y53 I54 I55 V56 L57 M58 A59 V64 T65 K68 R69 T70 D71 R72 V73 T74

Y75 H80 I81 G82 G83 I84 T88 F89 E90 E91 R96 P97 E98 R99 I103 A104 V105 P110 K111 G112 P113 L114 G115 R116 A117 M118 F119 K120 K121 L122 K123 V124 Y125 A126 E129 H132 Q135 Q136 P137 L140 D141 I142

• Molecule 38: 50S ribosomal protein L14

Chain K: 45% 51%

H1 I2 Q3 E4 Q5 T6 M7 L8 N9 V10 A11 D12 H13 S14 G15 A16 R17 R18 R19 M20 C21 I22 R23 V24 L25 V35 G36 I39 K40 K41 I41 T42 I43 K44 E45 A46 I47 P48 R49 G50 K51 D56 V61 V62 V63 R64 T65 G68 V69 R70 R71 P72 D73 V76 I77

R78 F79 N82 A83 G84 V85 L86 L87 E92 Q93 P94 R98 V103 T104 R105 E106 L107 R108 S109 E110 M113 L118 A119 V122 L120

• Molecule 39: 50S ribosomal protein L15

Chain L: 47% 47% 6%

MET R2 L3 N4 T5 L6 S7 P8 K14 L19 G20 R21 G22 G26 L27 G28 K29 T30 G31 G32 R33 K36 G37 R38 R39 R40 R41 R47 Q54 P55 P56 L57 R60 L61 P62 P66 P67 S68 R69 R70 A71 T74 I77 R78 L79 S80 D81 L82 A83 R84

V85 E86 V89 V90 N93 T94 L95 K96 I100 I101 I105 E106 F107 A108 K109 V110 I111 L112 A113 T117 T118 P119 V120 R121 V122 R123 G124 L125 R126 V127 G130 I135 A138 K141 I142 E143 E144

• Molecule 40: 50S ribosomal protein L16

Chain M: 47% 49%

M1 L2 P3 K8 F9 R10 H13 K14 L20 A21 G22 G23 T24 D25 V26 S27 F28 G29 S30 F31 G32 A35 V36 G37 R40 L41 T42 A43 R44 Q45 I46 E47 R50 M53 A56 R59 K62 I63 W64 I65 R66 V67 V68 P69 D70 K71 P72 I73 T74

P77 M82 K86 G87 V93 A94 L95 I96 O97 P98 L102 Y103 E104 M105 D106 G107 V108 P109 E110 F111 L112 A113 R114 F117 A120 K123 L124 P125 I126 K127 T128 V131 T132 K133 T134 V135 M136

• Molecule 41: 50S ribosomal protein L17

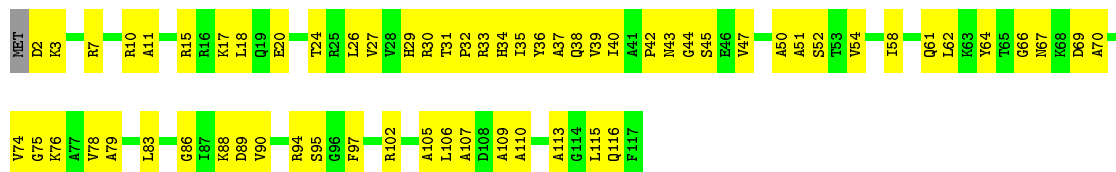
Chain N: 49% 44% 6%

H1 R2 R12 R17 N20 F21 N24 A25 G26 S27 L28 V29 R31 E32 I33 T36 T37 L38 P39 R40 A41 R42 E43 E44 V48 E49 F50 L51 A55 V56 D57 D58 S59 N62 R63 F67 A68 R69 T70 T71 D72 I73 E74 I75 V76 A77 K78 L79 F80 N81



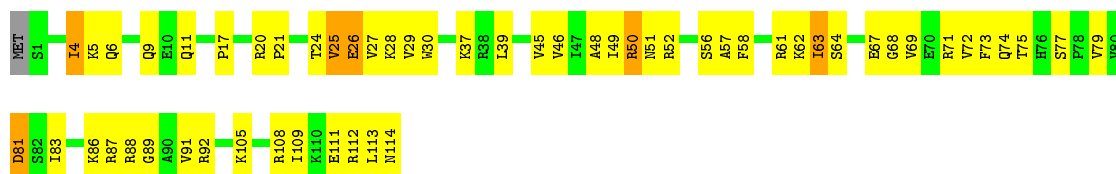
• Molecule 42: 50S ribosomal protein L18

Chain O: 45% 54%



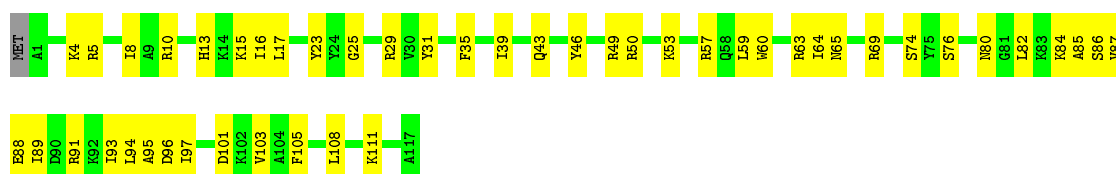
• Molecule 43: 50S ribosomal protein L19

Chain P: 50% 43% 5%



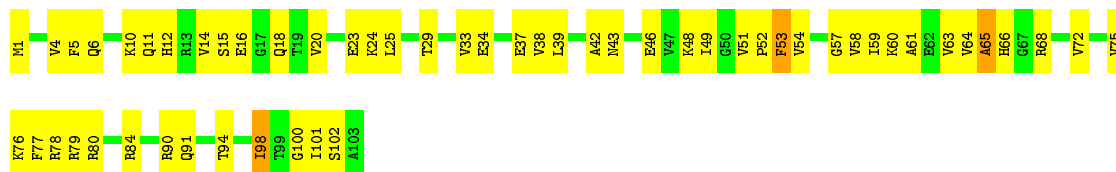
• Molecule 44: 50S ribosomal protein L20

Chain Q: 59% 40%



• Molecule 45: 50S ribosomal protein L21

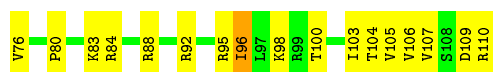
Chain R: 47% 50%



• Molecule 46: 50S ribosomal protein L22

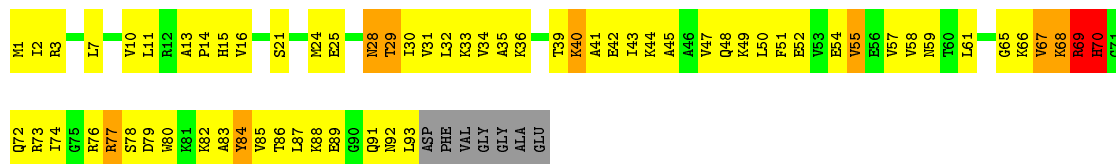
Chain S: 47% 51%





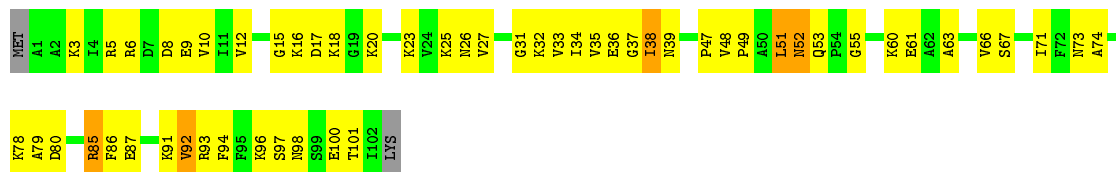
• Molecule 47: 50S ribosomal protein L23

Chain T: 27% 56% 8% 7%



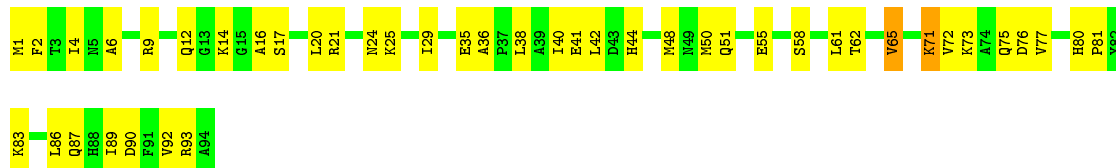
• Molecule 48: 50S ribosomal protein L24

Chain U: 45% 48% 5%



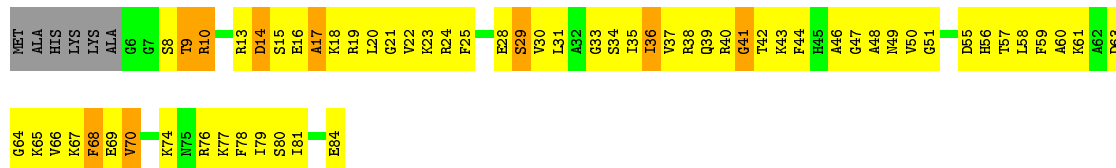
• Molecule 49: 50S ribosomal protein L25

Chain V: 53% 45%



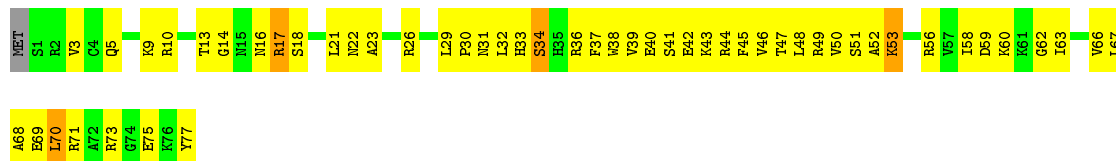
• Molecule 50: 50S ribosomal protein L27

Chain W: 21% 61% 11% 7%



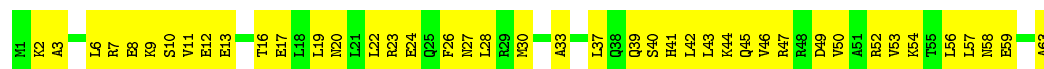
• Molecule 51: 50S ribosomal protein L28

Chain X: 32% 62% 5%



- Molecule 52: 50S ribosomal protein L29

Chain Y: 33% 67%



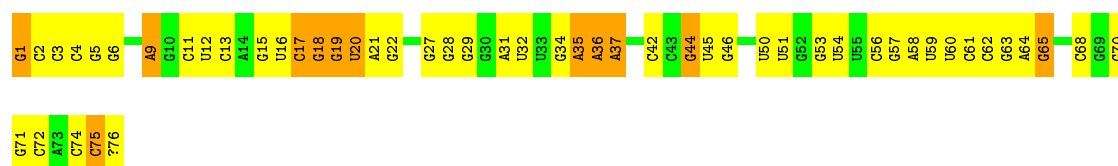
- Molecule 53: 50S ribosomal protein L30

Chain Z: 54% 41% ..



- Molecule 54: tRNA

Chain 6: 32% 53% 16%



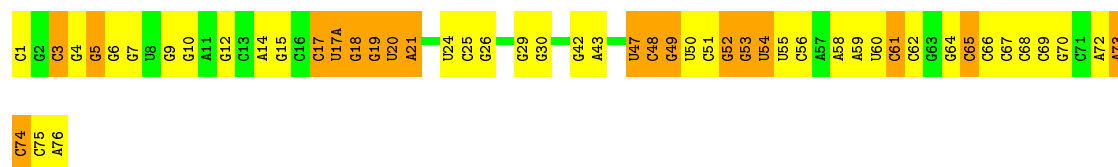
- Molecule 55: mRNA

Chain 7:  7% 47% 40% 7%



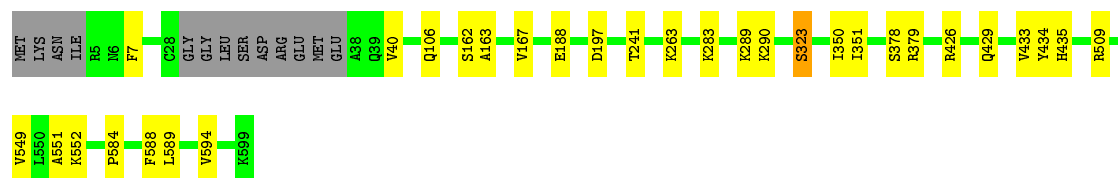
- Molecule 56: tRNA

Chain 8:  34% 43% 23%



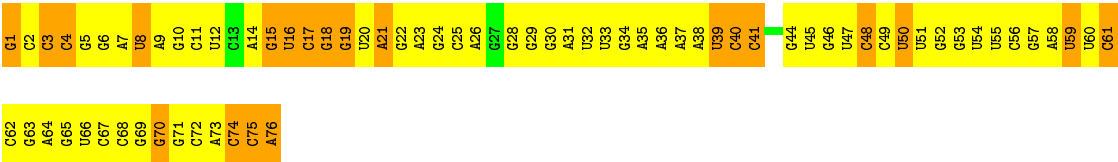
- Molecule 57: Elongation factor 4

Chain x:  93% 5% •



- Molecule 58: tRNA

Chain 9: 5% 67% 28%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	107706	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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: GNP, MG, F3O

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	a	0.73	0/36834	0.79	0/57462
10	k	0.43	0/893	0.54	0/1205
11	l	0.46	0/969	0.55	0/1300
12	m	0.38	0/892	0.55	0/1193
13	n	0.37	0/817	0.52	0/1088
14	o	0.43	0/722	0.50	0/964
15	p	0.36	0/659	0.47	0/884
16	q	0.42	0/657	0.54	0/881
17	r	0.43	0/462	0.49	0/621
18	s	0.36	0/652	0.50	0/877
19	t	0.37	0/671	0.46	0/888
2	c	0.42	0/1651	0.52	0/2225
20	u	0.38	0/430	0.53	0/570
21	b	0.35	0/1735	0.51	0/2338
22	0	0.48	0/450	0.54	0/599
23	1	0.44	0/416	0.52	0/554
24	2	0.52	0/380	0.57	0/498
25	3	0.45	0/513	0.58	0/676
26	4	0.45	0/303	0.58	0/397
27	5	0.24	0/1748	0.53	0/2355
28	A	0.84	0/69799	0.81	2/108892 (0.0%)
29	B	0.63	0/2828	0.74	0/4410
3	d	0.38	0/1665	0.50	0/2227
30	C	0.52	0/2115	0.58	0/2844
31	D	0.48	0/1586	0.56	0/2134
32	E	0.43	0/1571	0.54	0/2113
33	F	0.37	0/1434	0.47	0/1926
34	G	0.37	0/1343	0.51	0/1816
35	H	0.30	0/1122	0.57	0/1515
36	I	0.28	0/1046	0.50	0/1410
37	J	0.50	0/1152	0.58	0/1551
38	K	0.49	0/947	0.58	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	L	0.45	0/1054	0.57	0/1403
4	e	0.46	0/1118	0.56	0/1504
40	M	0.49	0/1093	0.61	0/1460
41	N	0.48	0/973	0.56	0/1301
42	O	0.38	0/902	0.48	0/1209
43	P	0.45	0/929	0.56	0/1242
44	Q	0.57	0/960	0.55	0/1278
45	R	0.48	0/829	0.54	0/1107
46	S	0.48	0/864	0.57	0/1156
47	T	0.40	0/744	0.57	0/994
48	U	0.37	0/787	0.54	0/1051
49	V	0.40	0/766	0.49	0/1025
5	f	0.37	0/851	0.53	0/1150
50	W	0.47	0/603	0.64	0/797
51	X	0.47	0/635	0.56	0/848
52	Y	0.41	0/510	0.51	0/677
53	Z	0.41	0/453	0.58	0/605
54	6	0.63	1/1788 (0.1%)	0.78	0/2784
55	7	0.64	0/358	0.92	2/555 (0.4%)
56	8	0.64	0/1832	0.76	0/2855
57	x	0.39	0/4646	0.52	0/6285
58	9	0.40	1/1813 (0.1%)	0.79	0/2823
6	g	0.37	0/1195	0.49	0/1602
7	h	0.43	0/989	0.52	0/1326
8	i	0.39	0/1034	0.56	0/1375
9	j	0.37	0/796	0.51	0/1077
All	All	0.70	2/166984 (0.0%)	0.74	4/249170 (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
11	l	0	1
20	u	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	9	1	G	OP3-P	-10.74	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	1	G	OP3-P	-10.67	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	323	C	N1-C2-O2	5.44	122.17	118.90
55	7	21	C	C2-N1-C1'	5.24	124.56	118.80
55	7	21	C	N1-C2-O2	5.22	122.03	118.90
28	A	2689	U	C2-N1-C1'	-5.05	111.64	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	l	23	ALA	Peptide
20	u	37	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32895	0	16553	0	0
2	c	1624	0	1696	0	0
3	d	1643	0	1707	0	0
4	e	1105	0	1148	0	0
5	f	832	0	824	0	0
6	g	1181	0	1238	0	0
7	h	979	0	1031	0	0
8	i	1022	0	1070	0	0
9	j	786	0	828	0	0
10	k	877	0	887	0	0
11	l	955	0	1016	0	0
12	m	883	0	941	0	0
13	n	805	0	843	0	0
14	o	714	0	734	0	0
15	p	649	0	666	0	0
16	q	648	0	691	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	r	455	0	478	0	0
18	s	637	0	665	0	0
19	t	665	0	714	0	0
20	u	425	0	449	0	0
21	b	1704	0	1732	0	0
22	0	444	0	461	39	0
23	1	409	0	440	53	0
24	2	377	0	418	16	0
25	3	504	0	574	34	0
26	4	302	0	340	40	0
27	5	1733	0	1824	393	0
28	A	62320	0	31344	2129	0
29	B	2529	0	1281	94	0
30	C	2076	0	2152	168	0
31	D	1565	0	1616	144	0
32	E	1552	0	1619	134	0
33	F	1410	0	1447	127	0
34	G	1323	0	1374	155	0
35	H	1111	0	1148	235	0
36	I	1032	0	1088	163	0
37	J	1129	0	1162	114	0
38	K	938	0	1012	76	0
39	L	1045	0	1117	97	0
40	M	1074	0	1157	81	0
41	N	960	0	1000	59	0
42	O	892	0	923	83	0
43	P	917	0	965	86	0
44	Q	947	0	1022	100	0
45	R	816	0	839	93	0
46	S	857	0	922	61	0
47	T	738	0	807	100	0
48	U	779	0	834	53	0
49	V	753	0	780	47	0
50	W	596	0	610	121	0
51	X	625	0	655	63	0
52	Y	509	0	543	45	0
53	Z	449	0	491	33	0
54	6	1633	0	830	51	0
55	7	320	0	162	18	0
56	8	1640	0	837	50	0
57	x	4573	0	4619	0	0
58	9	1623	0	821	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	x	32	0	13	0	0
60	x	1	0	0	0	0
All	All	154017	0	105158	4944	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 32.

The worst 5 of 4944 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)
50:W:37:VAL:HG12	50:W:38:ARG:HG3	1.19	1.17
35:H:90:LEU:HD11	35:H:146:VAL:HG23	1.27	1.15
42:O:51:ALA:HB3	42:O:78:VAL:HG12	1.25	1.14
31:D:119:ALA:HB1	31:D:124:ARG:HB2	1.24	1.13
31:D:184:ARG:HG2	31:D:186:LEU:HD13	1.26	1.13

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	
2	c	204/233 (88%)	182 (89%)	16 (8%)	6 (3%)	6	36
3	d	203/206 (98%)	180 (89%)	16 (8%)	7 (3%)	5	31
4	e	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	6	39
5	f	100/135 (74%)	84 (84%)	9 (9%)	7 (7%)	1	10
6	g	149/179 (83%)	134 (90%)	11 (7%)	4 (3%)	6	39
7	h	127/130 (98%)	114 (90%)	11 (9%)	2 (2%)	12	54
8	i	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	5	33
9	j	96/103 (93%)	76 (79%)	11 (12%)	9 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	115/129 (89%)	102 (89%)	9 (8%)	4 (4%)	4	31
11	l	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	27
12	m	112/118 (95%)	101 (90%)	6 (5%)	5 (4%)	3	24
13	n	98/101 (97%)	70 (71%)	15 (15%)	13 (13%)	0	1
14	o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	60
15	p	80/82 (98%)	66 (82%)	8 (10%)	6 (8%)	1	9
16	q	78/84 (93%)	62 (80%)	14 (18%)	2 (3%)	7	40
17	r	53/75 (71%)	50 (94%)	2 (4%)	1 (2%)	10	50
18	s	77/92 (84%)	68 (88%)	5 (6%)	4 (5%)	2	19
19	t	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	7	43
20	u	49/71 (69%)	39 (80%)	7 (14%)	3 (6%)	2	15
21	b	216/241 (90%)	189 (88%)	20 (9%)	7 (3%)	5	33
22	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	10	50
23	1	48/55 (87%)	41 (85%)	6 (12%)	1 (2%)	9	46
24	2	44/46 (96%)	43 (98%)	0	1 (2%)	8	44
25	3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	5	33
26	4	36/38 (95%)	25 (69%)	5 (14%)	6 (17%)	0	1
27	5	232/234 (99%)	190 (82%)	34 (15%)	8 (3%)	5	31
30	C	268/273 (98%)	228 (85%)	28 (10%)	12 (4%)	3	24
31	D	207/209 (99%)	169 (82%)	23 (11%)	15 (7%)	1	10
32	E	199/201 (99%)	171 (86%)	14 (7%)	14 (7%)	1	10
33	F	175/179 (98%)	146 (83%)	21 (12%)	8 (5%)	3	23
34	G	174/177 (98%)	140 (80%)	21 (12%)	13 (8%)	1	9
35	H	147/149 (99%)	114 (78%)	22 (15%)	11 (8%)	1	9
36	I	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	1	13
37	J	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	3	25
38	K	120/123 (98%)	100 (83%)	14 (12%)	6 (5%)	3	21
39	L	141/144 (98%)	115 (82%)	17 (12%)	9 (6%)	2	13
40	M	134/136 (98%)	112 (84%)	15 (11%)	7 (5%)	2	19
41	N	118/127 (93%)	104 (88%)	10 (8%)	4 (3%)	5	31
42	O	114/117 (97%)	104 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	P	112/115 (97%)	93 (83%)	13 (12%)	6 (5%)	2	19
44	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
45	R	101/103 (98%)	81 (80%)	15 (15%)	5 (5%)	3	21
46	S	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	6	37
47	T	91/100 (91%)	61 (67%)	18 (20%)	12 (13%)	0	1
48	U	100/104 (96%)	81 (81%)	11 (11%)	8 (8%)	1	7
49	V	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	8	45
50	W	77/85 (91%)	49 (64%)	17 (22%)	11 (14%)	0	1
51	X	75/78 (96%)	64 (85%)	7 (9%)	4 (5%)	2	19
52	Y	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
53	Z	56/59 (95%)	51 (91%)	3 (5%)	2 (4%)	4	30
57	x	582/599 (97%)	496 (85%)	58 (10%)	28 (5%)	3	22
All	All	6442/6818 (94%)	5465 (85%)	667 (10%)	310 (5%)	5	22

5 of 310 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	125	VAL
5	f	98	GLU
5	f	101	PRO
9	j	57	VAL
9	j	61	ALA

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	
2	c	170/190 (90%)	170 (100%)	0	100	100
3	d	172/173 (99%)	172 (100%)	0	100	100
4	e	113/126 (90%)	113 (100%)	0	100	100
5	f	89/116 (77%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	g	124/147 (84%)	124 (100%)	0	100	100
7	h	104/105 (99%)	104 (100%)	0	100	100
8	i	105/107 (98%)	105 (100%)	0	100	100
9	j	86/90 (96%)	86 (100%)	0	100	100
10	k	90/99 (91%)	90 (100%)	0	100	100
11	l	103/104 (99%)	103 (100%)	0	100	100
12	m	92/96 (96%)	92 (100%)	0	100	100
13	n	83/84 (99%)	73 (88%)	10 (12%)	6	28
14	o	76/77 (99%)	76 (100%)	0	100	100
15	p	65/65 (100%)	65 (100%)	0	100	100
16	q	74/78 (95%)	74 (100%)	0	100	100
17	r	48/65 (74%)	48 (100%)	0	100	100
18	s	70/79 (89%)	70 (100%)	0	100	100
19	t	65/66 (98%)	65 (100%)	0	100	100
20	u	44/61 (72%)	44 (100%)	0	100	100
21	b	180/199 (90%)	180 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	44 (98%)	1 (2%)	60	87
24	2	38/38 (100%)	38 (100%)	0	100	100
25	3	51/52 (98%)	51 (100%)	0	100	100
26	4	34/34 (100%)	34 (100%)	0	100	100
27	5	181/181 (100%)	181 (100%)	0	100	100
30	C	215/218 (99%)	215 (100%)	0	100	100
31	D	164/164 (100%)	164 (100%)	0	100	100
32	E	165/165 (100%)	165 (100%)	0	100	100
33	F	148/150 (99%)	148 (100%)	0	100	100
34	G	137/138 (99%)	137 (100%)	0	100	100
35	H	114/114 (100%)	114 (100%)	0	100	100
36	I	109/110 (99%)	109 (100%)	0	100	100
37	J	116/116 (100%)	116 (100%)	0	100	100
38	K	103/104 (99%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	L	102/103 (99%)	102 (100%)	0	100	100
40	M	109/109 (100%)	109 (100%)	0	100	100
41	N	100/103 (97%)	100 (100%)	0	100	100
42	O	86/87 (99%)	86 (100%)	0	100	100
43	P	99/100 (99%)	99 (100%)	0	100	100
44	Q	89/90 (99%)	89 (100%)	0	100	100
45	R	84/84 (100%)	84 (100%)	0	100	100
46	S	93/93 (100%)	93 (100%)	0	100	100
47	T	80/84 (95%)	74 (92%)	6 (8%)	17	55
48	U	83/85 (98%)	83 (100%)	0	100	100
49	V	78/78 (100%)	78 (100%)	0	100	100
50	W	59/63 (94%)	59 (100%)	0	100	100
51	X	67/68 (98%)	67 (100%)	0	100	100
52	Y	55/55 (100%)	55 (100%)	0	100	100
53	Z	48/49 (98%)	48 (100%)	0	100	100
57	x	500/511 (98%)	496 (99%)	4 (1%)	86	96
All	All	5352/5570 (96%)	5331 (100%)	21 (0%)	94	98

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	n	47	LYS
47	T	66	LYS
57	x	106	GLN
13	n	42	TRP
57	x	323	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
32	E	165	HIS
37	J	40	HIS
57	x	407	HIS
34	G	21	GLN
34	G	110	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1532/1533 (99%)	302 (19%)	0
28	A	2902/2904 (99%)	566 (19%)	24 (0%)
29	B	117/120 (97%)	18 (15%)	0
54	6	74/76 (97%)	15 (20%)	3 (4%)
55	7	14/15 (93%)	7 (50%)	1 (7%)
56	8	76/77 (98%)	20 (26%)	0
58	9	75/76 (98%)	24 (32%)	2 (2%)
All	All	4790/4801 (99%)	952 (19%)	30 (0%)

5 of 952 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	13	U

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1020	A
28	A	1847	A
55	7	20	U
28	A	1584	U
28	A	1905	C

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
54	F3O	6	76	54	29,35,37	1.11	1 (3%)	31,49,54	2.15	6 (19%)

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
54	F3O	6	76	54	-	0/14/36/38	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	76	F3O	O3'-C	4.84	1.45	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	6	76	F3O	N3-C2-N1	-9.62	121.31	128.87
54	6	76	F3O	C3'-O3'-C	-3.35	112.54	118.06
54	6	76	F3O	O3'-C-O	-2.46	119.12	123.88
54	6	76	F3O	C4'-O4'-C1'	2.32	112.10	109.64
54	6	76	F3O	C3'-C2'-C1'	2.65	105.82	100.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	6	76	F3O	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GNP	x	701	60	29,34,34	2.80	10 (34%)	28,54,54	1.95	7 (25%)

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	GNP	x	701	60	-	0/16/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	701	GNP	C4-N9	-7.78	1.37	1.47
59	x	701	GNP	C5-C6	-6.26	1.41	1.53
59	x	701	GNP	PB-O3A	-5.91	1.51	1.59
59	x	701	GNP	PB-O2B	-3.23	1.48	1.56
59	x	701	GNP	C8-N9	-3.04	1.37	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	701	GNP	PA-O3A-PB	-3.63	119.55	132.71
59	x	701	GNP	O3G-PG-O1G	-2.99	105.70	113.58
59	x	701	GNP	O6-C6-N1	-2.45	119.58	122.80
59	x	701	GNP	O3G-PG-O2G	2.39	114.62	107.67
59	x	701	GNP	O2B-PB-O1B	4.42	118.72	110.02

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.