



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:35 pm GMT

PDB ID : 7PJZ  
EMDB ID : EMD-13465  
Title : Structure of the 70S-EF-G-GDP ribosome complex with tRNAs in chimeric state 2 (CHI2-EF-G-GDP)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 6.00 Å (reported)  
Based on initial models : 4AQY, 5LZD, 5J9Z, 6YSS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

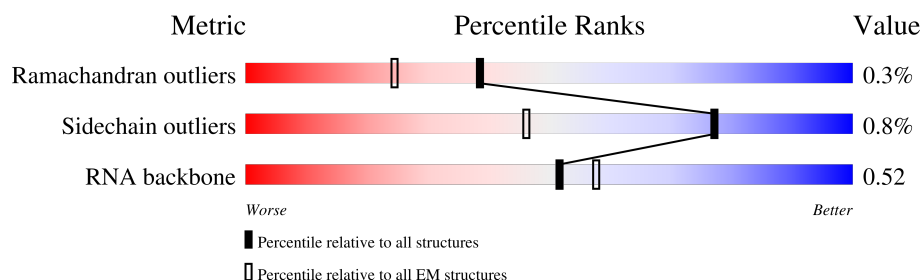
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 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.



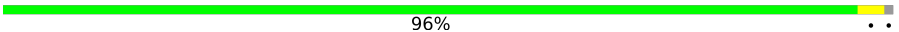
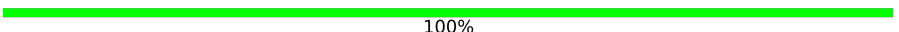
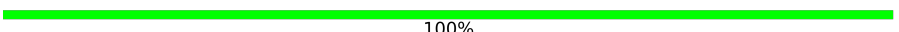
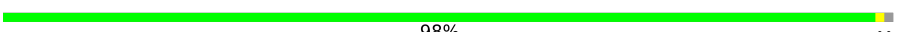
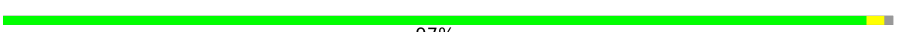
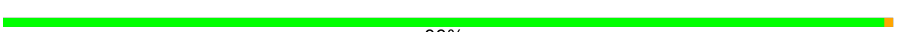






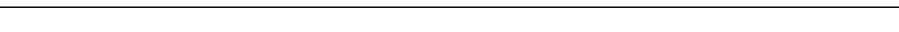

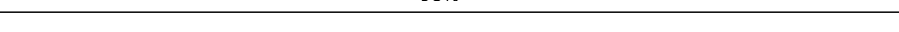
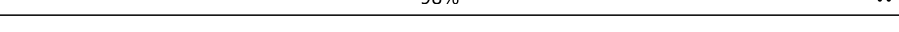
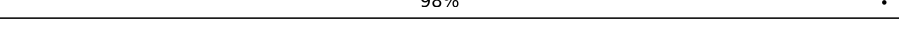
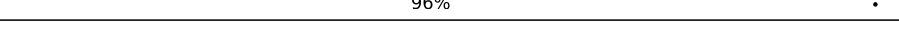

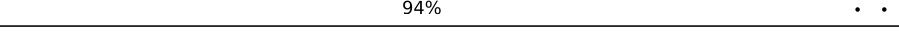
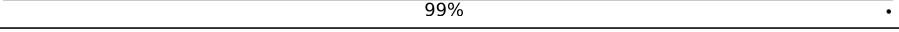

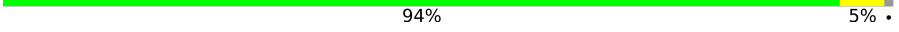
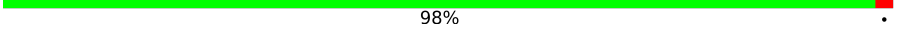
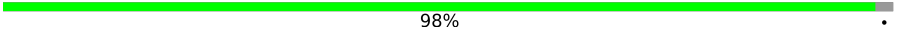
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	



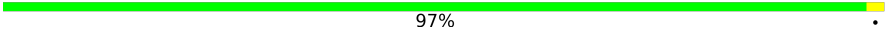



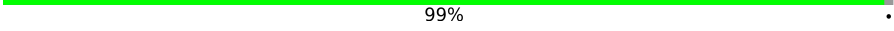
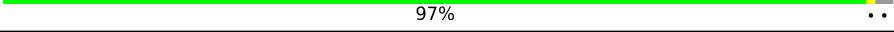
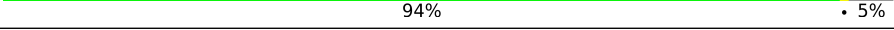

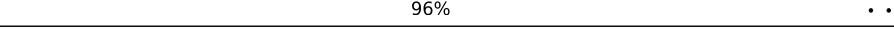
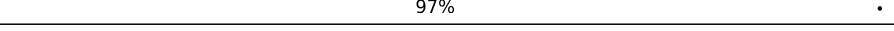
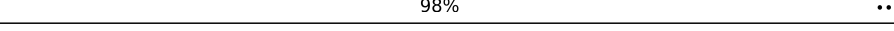
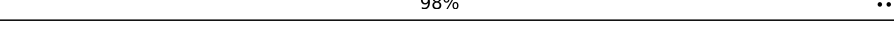
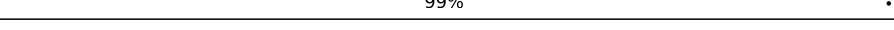
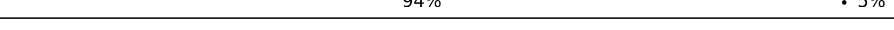


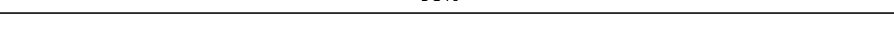
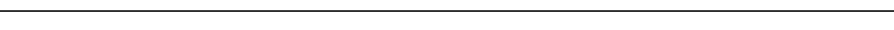

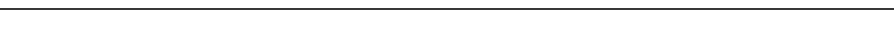
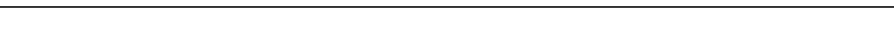


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Mol	Chain	Length	Quality of chain
10	C	273	 96% ..
11	D	209	 100%
12	E	201	 100%
13	F	179	 98% ..
14	G	177	 97% ..
15	H	149	 99% .
16	I	142	 99% ..
17	J	142	 99% .
18	K	123	 96% ..
19	L	144	 97% ..
20	M	136	 97% .
21	N	127	 93% . 6%
22	O	117	 97% ..
23	P	115	 98% ..
24	Q	118	 98% ..
25	R	103	 98% .
26	S	110	 96% .
27	T	100	 90% . 7%
28	U	104	 94% ..
29	V	94	 99% .
30	W	85	 87% . 12%
31	X	78	 94% 5% .
32	Y	63	 98% .
33	Z	59	 98% .
34	a	1542	 39% 49% 11%

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Mol	Chain	Length	Quality of chain
35	b	240	 88% 9%
36	c	233	 88% 12%
37	d	206	 97%
38	e	167	 92% 6%
39	f	135	 74% 26%
40	g	179	 83% 16%
41	h	130	 99%
42	i	130	 97%
43	j	103	 94% 5%
44	k	129	 89% 10%
45	l	124	 96%
46	m	118	 97%
47	n	102	 98%
48	o	89	 98%
49	p	82	 99%
50	q	84	 94% 5%
51	r	75	 84% 13%
52	s	92	 86% 11%
53	t	87	 98%
54	u	71	 90% 8%
55	v	77	 43% 47% 10%
56	w	76	 46% 42% 12%
57	x	704	 92% 5%
58	y	2	 50% 50%
59	z	33	 21% 9% 70%

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.



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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	x	669	Total	C	N	O	S		1	0
			5192	3275	900	994	23			

- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	10	Total	C	N	O	P	0	0
			208	93	29	76	10		

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

Mol	Chain	Residues	Atoms		AltConf
60	6	1	Total	Zn	0
			1	1	

- Molecule 61 is APRAMYCIN (three-letter code: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				AltConf
61	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



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

### 3 Residue-property plots [i](#)


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

- Molecule 1: 50S ribosomal protein L32

Chain 0:  98% .



- Molecule 2: 50S ribosomal protein L33

Chain 1:  91% 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  96% .



- Molecule 4: 50S ribosomal protein L35

Chain 3:  95% . .




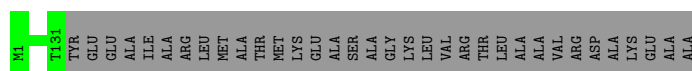
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

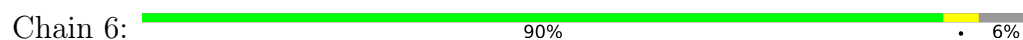
There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L10

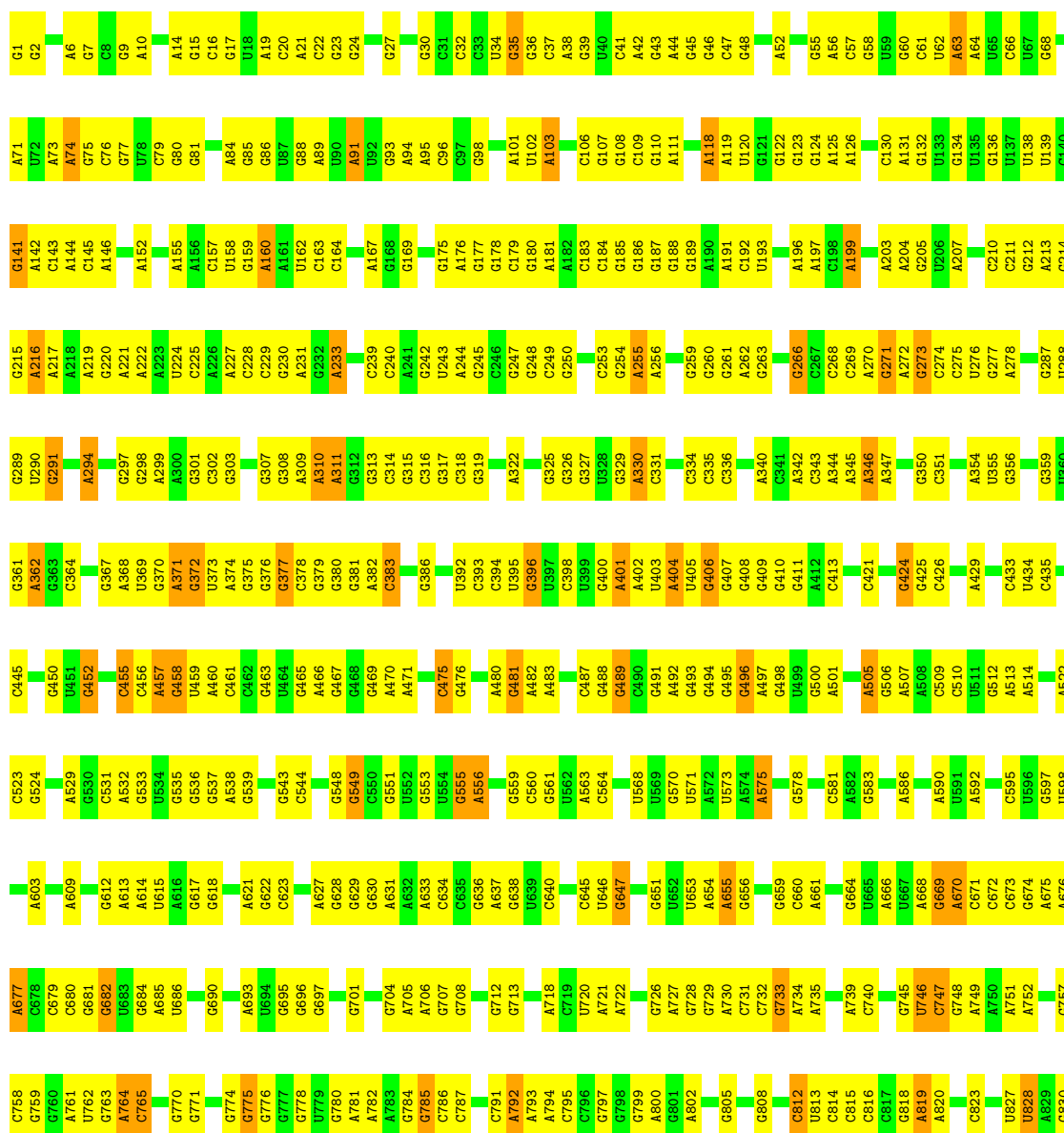
Chain 5:  79% 21%



• Molecule 7: 50S ribosomal protein L31



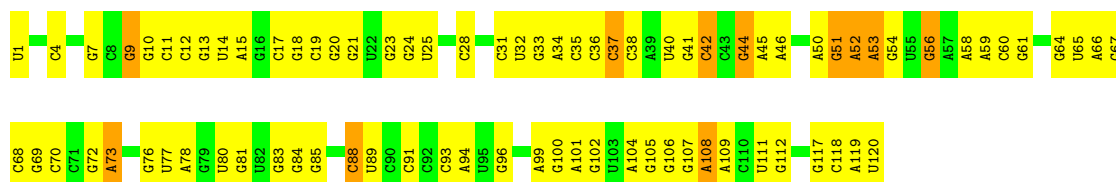
• Molecule 8: 23S ribosomal RNA





G1850	G1774	G1707	G1628	C1550	C1472	G1395	U1312	G1227	C1161	A1098	G1037	U963	A896	G831
G1857	U1775	C1708	G1631	A1551	G1473	A1395	U1313	G1228	G1162	G1099	G1038	C964	C897	U852
G1858	U1781	A1711	G1634	A1552	U1474	C1398	G1317	C1229	G1163	C1100	A1039	C965	C898	A833
G1861	U1782	U1712	A1634	A1553	G1475	C1399	G1317	U1230	C1164	U1101	A1040	C966	A900	G834
G1862	A1783	U1713	G1638	C1556	U1476	U1400	C1320	U1231	G1165	C1102	G1041	G971	G903	G836
G1863	A1784	U1714	C1639	C1557	G1478	G1401	G1323	C1233	G1166	A1103	G1042	A972	G904	C837
U1864	A1785	G1715	G1639	C1558	G1479	U1402	C1323	C1233	C1167	C1104	C1043	A973	C903	G835
U1865	A1786	U1716	G1643	C1561	G1482	A1403	G1332	A1237	G1168	U1106	C1044	A974	G904	G836
U1866	A1787	G1717	G1643	C1561	G1482	C1404	G1332	G1238	A1169	G1107	C1045	G974	G907	G841
U1867	A1788	G1718	G1643	C1561	G1482	C1404	G1333	G1239	G1170	A975	A1046	A975	C908	U842
U1868	A1789	U1719	G1643	C1561	G1482	C1404	G1333	G1240	G1171	G976	G1047	A976	G909	G843
G1869	C1790	G1720	G1643	C1561	G1482	C1404	G1333	U1241	C1172	G977	A1048	G977	A910	A844
G1873	C1793	U1721	G1643	C1561	G1482	C1404	G1333	A1241	U1173	A1111	C1049	G978	A845	A845
G1874	C1797	U1725	G1643	C1561	G1482	C1404	G1333	A1244	U1174	G1112	C1052	A979	U846	U846
G1875	C1797	U1725	G1643	C1561	G1482	C1404	G1333	A1247	U1175	G1113	C1052	A979	U847	U847
G1884	C1800	U1726	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1885	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1886	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1887	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1888	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
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G1892	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1893	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1894	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1895	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1896	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1897	A1801	C1727	G1643	C1561	G1482	C1404	G1333	A1247	U1176	U1113	C1053	C982	C912	C912
G1900	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1901	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1902	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1903	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1904	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1905	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
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G1908	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1909	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1910	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
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G1914	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1915	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1916	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1917	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1918	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
G1919	A1820	G1743	G1670	U1589	A1521	A1433	G1361	A1274	G1197	G1131	A1070	C1005	U931	A866
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A1928	G2002	C2143	G2209	A2288	G2361	A2426	G2496	U2568	G2642	G2718	G2798	U2866
G1929	A2003	G2144	U2210	G2289	G2362	C2427	C2496	G2569	G2643	G2719	U2799	G2867
G1930	A2004	G2145	A2211	G2293	C2363	G2428	A2497	G2570	G2644	U2720	A2800	G2868
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G1936	U2012	A2088	C2222	G2304	A2369	A2435	U2504	A2576	G2653	U2726	G2809	C2875
A1937	A2013	C2091	G2223	G2305	G2370	A2436	G2505	A2577	A2654	U2727	A2810	G2876
A1938	A2014	A2154	G2224	U2305	G2371	G2437	U2506	G2578	G2655	U2728	G2811	G2877
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A1940	A2016	G2093	C2226	G2309	G2373	U2441	G2508	U2580	A2657	G2730	A2813	A2879
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		A2096	U2229	A2312	G2376	U2444	U2511	A2590	A2660	U2733	A2816	A2882
		A2097	G2230	G2313	G2377	G2444	G2512	G2591	G2661	G2734	U2817	U2883
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					G2407			C2625				
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					G2411			U2629		A2776		
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					G2414			G2632		U2779		
					G2415			U2633		G2780		
					G2416			A2634		A2781		
					G2417							
					G2418							
					G2419							
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								G2745				



- Molecule 10: 50S ribosomal protein L2

Chain C:  96%



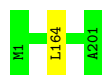
- Molecule 11: 50S ribosomal protein L3

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L4

Chain E:  100%



- Molecule 13: 50S ribosomal protein L5

Chain F:  98%



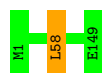
- Molecule 14: 50S ribosomal protein L6

Chain G:  97%



- Molecule 15: 50S ribosomal protein L9

Chain H:  99%



- Molecule 16: 50S ribosomal protein L11

Chain I:  99%



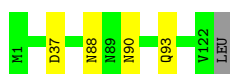
- Molecule 17: 50S ribosomal protein L13

Chain J: 99% .



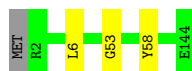
- Molecule 18: 50S ribosomal protein L14

Chain K: 96% ..



- Molecule 19: 50S ribosomal protein L15

Chain L: 97% ..



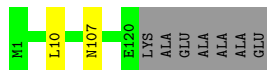
- Molecule 20: 50S ribosomal protein L16

Chain M: 97% .



- Molecule 21: 50S ribosomal protein L17

Chain N: 93% . 6%



- Molecule 22: 50S ribosomal protein L18

Chain O: 97% ..



- Molecule 23: 50S ribosomal protein L19

Chain P: 98% ..



- Molecule 24: 50S ribosomal protein L20

Chain Q: 98%



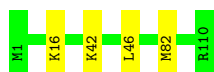
- Molecule 25: 50S ribosomal protein L21

Chain R: 98%



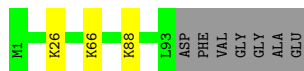
- Molecule 26: 50S ribosomal protein L22

Chain S: 96%



- Molecule 27: 50S ribosomal protein L23

Chain T: 90% 7%



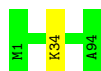
- Molecule 28: 50S ribosomal protein L24

Chain U: 94%



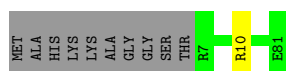
- Molecule 29: 50S ribosomal protein L25

Chain V: 99%



- Molecule 30: 50S ribosomal protein L27

Chain W: 87% 12%



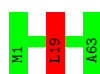
- Molecule 31: 50S ribosomal protein L28

Chain X: 94% 5%



- Molecule 32: 50S ribosomal protein L29

Chain Y: 98%



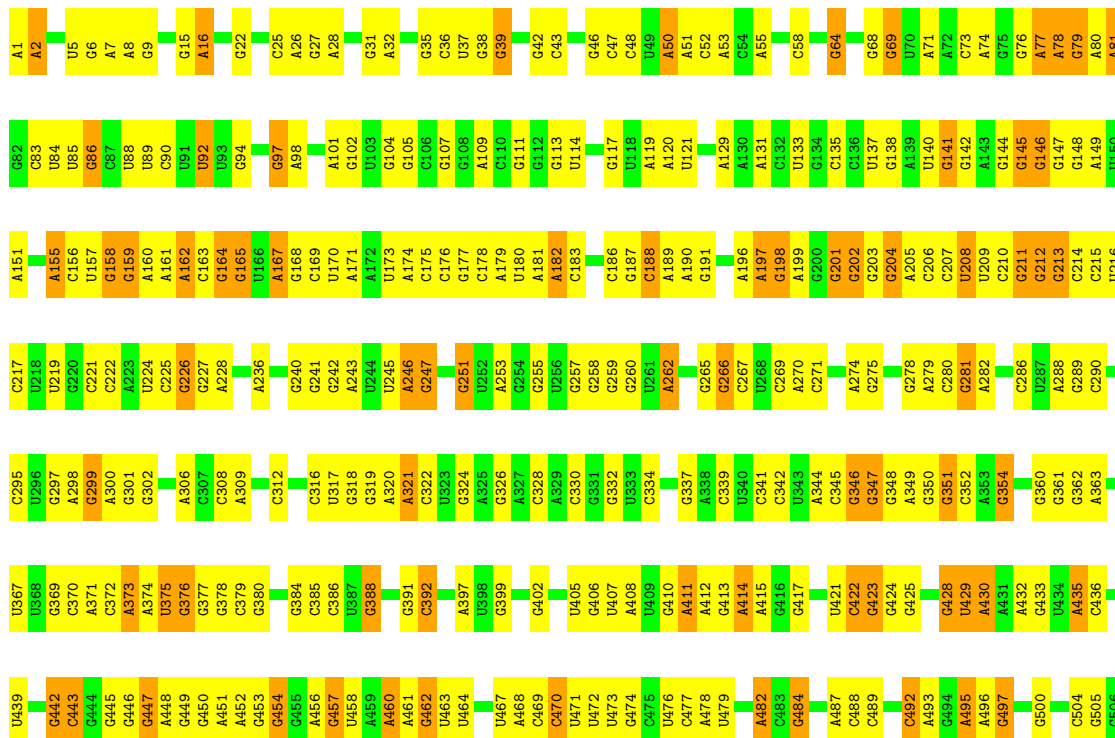
- Molecule 33: 50S ribosomal protein L30

Chain Z: 98%




- Molecule 34: 16S ribosomal RNA

Chain a: 39% 49% 11%




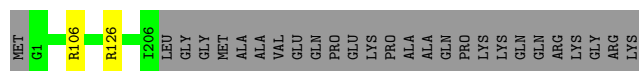
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4	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762
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Chain b:  88% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c:  88% 12%



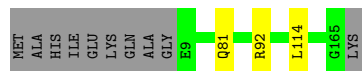
- Molecule 37: 30S ribosomal protein S4

Chain d:  97%



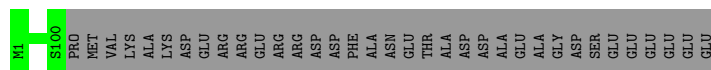
- Molecule 38: 30S ribosomal protein S5

Chain e:  92% 6%




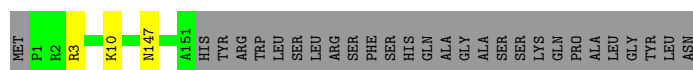
- Molecule 39: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  83% 16%



- Molecule 41: 30S ribosomal protein S8

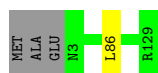
Chain h:  99%



- Molecule 42: 30S ribosomal protein S9



Chain i:  97% ..



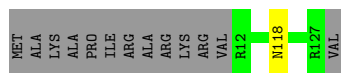
- Molecule 43: 30S ribosomal protein S10

Chain j:  94% • 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  89% • 10%



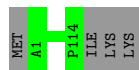
- Molecule 45: 30S ribosomal protein S12

Chain l:  96% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  97% •



- Molecule 47: 30S ribosomal protein S14

Chain n:  98% ..



- Molecule 48: 30S ribosomal protein S15

Chain o:  98% ..



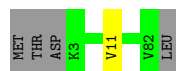
- Molecule 49: 30S ribosomal protein S16

Chain p:  99%




- Molecule 50: 30S ribosomal protein S17

Chain q:  94% 5%




- Molecule 51: 30S ribosomal protein S18

Chain r:  84% 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  86% 11%




- Molecule 53: 30S ribosomal protein S20

Chain t:  98%



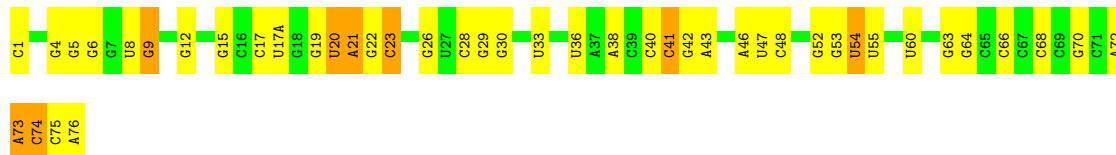
- Molecule 54: 30S ribosomal protein S21

Chain u:  90% 8%



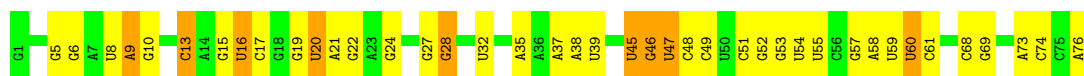
- Molecule 55: P-site tRNA(fMet)

Chain v:  43% 47% 10%



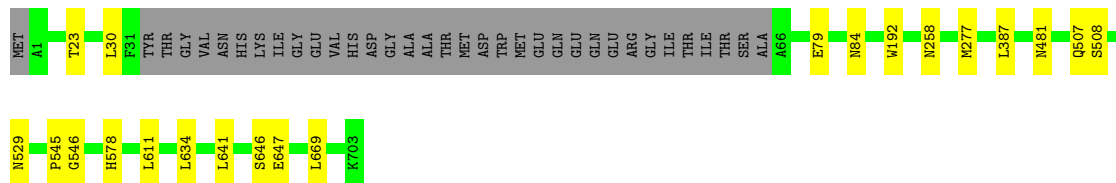
- Molecule 56: P-site fMet-Phe-tRNA(Phe)

Chain w:  46% 42% 12%



- Molecule 57: Elongation factor G

Chain x:  92% 5%



- Molecule 58: Dipeptide (FME-PHE)

Chain y:  50% 50%



- Molecule 59: mRNA

Chain z:  21% 9% 70%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6168	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (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: MA6, MIA, 6MZ, 3TD, H2U, GDP, PSU, 1MG, 5MU, 4SU, ZN, 2MA, 5MC, G7M, 2MG, OMU, UR3, AM2, FME, OMC, 4OC, OMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.81	0/450	1.06	0/599
2	1	0.71	0/416	1.15	0/554
3	2	0.82	0/380	1.08	1/498 (0.2%)
4	3	0.81	0/513	1.07	0/676
5	4	0.77	0/303	1.17	0/397
6	5	0.31	0/646	0.62	0/898
7	6	0.76	0/531	1.04	0/709
8	A	1.65	635/69266 (0.9%)	1.90	2790/108055 (2.6%)
9	B	1.68	28/2873 (1.0%)	2.02	154/4478 (3.4%)
10	C	0.78	1/2121 (0.0%)	1.05	4/2852 (0.1%)
11	D	0.76	0/1586	0.99	0/2134
12	E	0.74	0/1571	0.99	1/2113 (0.0%)
13	F	0.79	0/1434	0.99	1/1926 (0.1%)
14	G	0.76	0/1343	0.98	2/1816 (0.1%)
15	H	0.62	0/1122	0.87	1/1515 (0.1%)
16	I	0.37	0/692	0.66	0/960
17	J	0.82	0/1152	1.03	1/1551 (0.1%)
18	K	0.73	0/947	1.01	0/1268
19	L	0.72	0/1054	1.17	2/1403 (0.1%)
20	M	0.83	0/1093	1.08	3/1460 (0.2%)
21	N	0.77	1/973 (0.1%)	1.14	1/1301 (0.1%)
22	O	0.73	0/902	0.94	2/1209 (0.2%)
23	P	0.81	0/929	1.02	1/1242 (0.1%)
24	Q	0.82	0/960	1.04	1/1278 (0.1%)
25	R	0.81	0/829	1.04	0/1107
26	S	0.79	0/864	1.10	4/1156 (0.3%)
27	T	0.82	0/744	1.10	1/994 (0.1%)
28	U	0.93	1/787 (0.1%)	1.12	1/1051 (0.1%)
29	V	0.93	0/766	0.99	0/1025
30	W	0.76	0/582	1.02	0/769
31	X	0.87	2/635 (0.3%)	1.17	2/848 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.77	0/510	1.08	1/677 (0.1%)
33	Z	0.78	0/453	1.12	0/605
34	a	1.52	254/36725 (0.7%)	1.85	1350/57285 (2.4%)
35	b	0.62	0/1735	0.86	2/2338 (0.1%)
36	c	0.73	0/1651	0.93	1/2225 (0.0%)
37	d	0.70	0/1665	0.96	1/2227 (0.0%)
38	e	0.73	0/1154	1.00	1/1554 (0.1%)
39	f	0.71	0/835	0.89	0/1128
40	g	0.63	0/1195	0.86	1/1602 (0.1%)
41	h	0.66	0/989	0.86	0/1326
42	i	0.65	0/1034	0.93	1/1375 (0.1%)
43	j	0.66	0/796	0.94	1/1077 (0.1%)
44	k	0.65	0/885	0.94	0/1195
45	l	0.75	0/969	1.09	1/1300 (0.1%)
46	m	0.65	0/892	0.95	0/1193
47	n	0.68	0/811	0.97	0/1081
48	o	0.66	0/722	0.97	0/964
49	p	0.70	0/659	0.96	1/884 (0.1%)
50	q	0.81	0/657	1.00	1/881 (0.1%)
51	r	0.73	1/544 (0.2%)	0.98	1/731 (0.1%)
52	s	0.66	0/675	1.02	2/908 (0.2%)
53	t	0.79	0/671	0.90	0/888
54	u	0.59	0/512	0.91	0/683
55	v	1.45	16/1745 (0.9%)	1.88	65/2716 (2.4%)
56	w	1.09	2/1650 (0.1%)	1.48	27/2569 (1.1%)
57	x	0.72	1/5288 (0.0%)	0.95	6/7152 (0.1%)
58	y	0.29	0/11	0.79	0/13
59	z	0.89	0/230	1.17	0/355
All	All	1.39	942/164127 (0.6%)	1.68	4436/244774 (1.8%)

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
4	3	0	1
25	R	0	1
28	U	0	1
32	Y	0	1
35	b	0	1
37	d	0	3

*Continued on next page...*

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	u	0	1
57	x	0	1
All	All	0	10

The worst 5 of 942 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1	G	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.72	1.48	1.61
55	v	1	C	OP3-P	-10.66	1.48	1.61
8	A	1055	G	N9-C4	-10.60	1.29	1.38
34	a	640	A	N9-C4	-9.66	1.32	1.37

The worst 5 of 4436 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1055	G	N3-C4-C5	16.27	136.74	128.60
34	a	921	U	C6-N1-C2	-14.36	112.39	121.00
8	A	1055	G	N3-C4-N9	-14.11	117.53	126.00
34	a	201	G	N3-C4-C5	12.85	135.03	128.60
34	a	604	G	N3-C4-C5	12.82	135.01	128.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	30	HIS	Peptide
25	R	51	VAL	Peptide
28	U	97	SER	Peptide
32	Y	19	LEU	Peptide
35	b	87	ASP	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	38
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	107 (83%)	22 (17%)	0	100	100
7	6	64/70 (91%)	57 (89%)	5 (8%)	2 (3%)	3	22
10	C	269/273 (98%)	245 (91%)	24 (9%)	0	100	100
11	D	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
12	E	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
13	F	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
14	G	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
15	H	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
16	I	139/142 (98%)	124 (89%)	14 (10%)	1 (1%)	19	57
17	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
18	K	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
19	L	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
20	M	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
21	N	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
22	O	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
23	P	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	13	49
26	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
27	T	91/100 (91%)	81 (89%)	9 (10%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	U	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	13	49
29	V	92/94 (98%)	92 (100%)	0	0	100	100
30	W	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	38
33	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
35	b	216/240 (90%)	180 (83%)	35 (16%)	1 (0%)	25	65
36	c	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
37	d	203/206 (98%)	172 (85%)	30 (15%)	1 (0%)	25	65
38	e	155/167 (93%)	140 (90%)	15 (10%)	0	100	100
39	f	98/135 (73%)	89 (91%)	9 (9%)	0	100	100
40	g	149/179 (83%)	134 (90%)	15 (10%)	0	100	100
41	h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/130 (96%)	106 (85%)	19 (15%)	0	100	100
43	j	96/103 (93%)	78 (81%)	18 (19%)	0	100	100
44	k	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
45	l	121/124 (98%)	104 (86%)	16 (13%)	1 (1%)	16	55
46	m	112/118 (95%)	100 (89%)	12 (11%)	0	100	100
47	n	99/102 (97%)	90 (91%)	9 (9%)	0	100	100
48	o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
49	p	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
50	q	78/84 (93%)	65 (83%)	13 (17%)	0	100	100
51	r	63/75 (84%)	54 (86%)	9 (14%)	0	100	100
52	s	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
53	t	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
54	u	63/71 (89%)	51 (81%)	12 (19%)	0	100	100
57	x	666/704 (95%)	588 (88%)	71 (11%)	7 (1%)	12	47
All	All	6516/6924 (94%)	5877 (90%)	621 (10%)	18 (0%)	38	73

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	6	64	PHE

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Mol	Chain	Res	Type
57	x	387	LEU
57	x	545	PRO
57	x	546	GLY
4	3	31	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	59
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	58 (98%)	1 (2%)	56	72
10	C	216/218 (99%)	213 (99%)	3 (1%)	62	75
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	135 (98%)	2 (2%)	60	75
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	83
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	99 (96%)	4 (4%)	27	48
19	L	102/103 (99%)	101 (99%)	1 (1%)	73	82
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	84/84 (100%)	84 (100%)	0	100	100
26	S	93/93 (100%)	92 (99%)	1 (1%)	70	80
27	T	80/84 (95%)	79 (99%)	1 (1%)	65	77
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	77 (99%)	1 (1%)	65	77
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	71
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	177 (98%)	3 (2%)	56	72
36	c	170/190 (90%)	169 (99%)	1 (1%)	84	88
37	d	172/173 (99%)	170 (99%)	2 (1%)	67	79
38	e	114/126 (90%)	112 (98%)	2 (2%)	54	71
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	122 (98%)	2 (2%)	58	74
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	105 (100%)	0	100	100
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	88 (99%)	1 (1%)	70	80
45	l	103/104 (99%)	101 (98%)	2 (2%)	52	69
46	m	92/96 (96%)	92 (100%)	0	100	100
47	n	79/84 (94%)	78 (99%)	1 (1%)	65	77
48	o	76/77 (99%)	75 (99%)	1 (1%)	65	77
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	74 (100%)	0	100	100
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	71 (99%)	1 (1%)	62	75
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	x	551/578 (95%)	545 (99%)	6 (1%)	70	80
58	y	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5178/5408 (96%)	5138 (99%)	40 (1%)	77 85

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	k	118	ASN
57	x	84	ASN
45	l	4	ASN
48	o	16	ARG
57	x	481	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	l	44	GLN
38	e	81	GLN
44	k	21	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	447 (29%)	0
55	v	76/77 (98%)	20 (26%)	0
56	w	74/76 (97%)	23 (31%)	0
59	z	9/33 (27%)	3 (33%)	0
8	A	2898/2903 (99%)	593 (20%)	39 (1%)
9	B	119/120 (99%)	21 (17%)	3 (2%)
All	All	4712/4751 (99%)	1107 (23%)	42 (0%)

5 of 1107 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	34	U
8	A	35	G
8	A	46	G
8	A	62	U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	2287	A
8	A	2406	A
8	A	2308	G
8	A	2346	A
8	A	2750	A

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

46 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$
8	1MG	A	745	8	18,26,27	2.35	6 (33%)	19,39,42	1.58	5 (26%)
55	4SU	v	8	55	18,21,22	3.41	8 (44%)	26,30,33	2.15	4 (15%)
8	2MG	A	1835	8	18,26,27	2.08	7 (38%)	16,38,41	2.13	4 (25%)
8	5MU	A	1939	8	19,22,23	4.63	7 (36%)	28,32,35	3.83	9 (32%)
8	6MZ	A	2030	8	18,25,26	1.80	6 (33%)	16,36,39	2.37	5 (31%)
8	PSU	A	2604	8	18,21,22	3.51	8 (44%)	22,30,33	2.41	6 (27%)
34	2MG	a	966	34	18,26,27	0.99	1 (5%)	16,38,41	1.40	3 (18%)
55	PSU	v	55	55	18,21,22	3.82	6 (33%)	22,30,33	1.89	5 (22%)
56	G7M	w	46	56	20,26,27	4.39	14 (70%)	17,39,42	2.21	3 (17%)
8	PSU	A	1911	8	18,21,22	3.58	7 (38%)	22,30,33	1.96	5 (22%)
8	PSU	A	2605	8	18,21,22	3.48	7 (38%)	22,30,33	2.27	6 (27%)
8	5MC	A	747	8	18,22,23	3.41	7 (38%)	26,32,35	1.39	2 (7%)
8	OMU	A	2552	8	19,22,23	2.66	5 (26%)	26,31,34	2.07	6 (23%)
8	PSU	A	2457	8	18,21,22	3.52	8 (44%)	22,30,33	2.16	4 (18%)
34	PSU	a	516	34	18,21,22	3.65	7 (38%)	22,30,33	1.90	5 (22%)
8	OMC	A	2498	8	19,22,23	3.08	8 (42%)	26,31,34	0.84	0
8	PSU	A	2504	8	18,21,22	3.85	7 (38%)	22,30,33	1.84	4 (18%)
8	PSU	A	2580	8	18,21,22	3.28	7 (38%)	22,30,33	2.54	6 (27%)
58	FME	y	101	58	8,9,10	1.03	1 (12%)	7,9,11	1.05	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	MA6	a	1518	34	18,26,27	1.53	3 (16%)	19,38,41	3.38	3 (15%)
8	OMG	A	2251	56,8	18,26,27	2.49	8 (44%)	19,38,41	1.52	5 (26%)
8	5MC	A	1962	8	18,22,23	2.96	7 (38%)	26,32,35	1.34	2 (7%)
34	2MG	a	1516	34	18,26,27	2.32	7 (38%)	16,38,41	1.40	3 (18%)
56	5MU	w	54	56	19,22,23	1.38	6 (31%)	28,32,35	2.21	9 (32%)
8	3TD	A	1915	8	18,22,23	7.27	11 (61%)	22,32,35	1.73	2 (9%)
34	MA6	a	1519	34	18,26,27	1.53	3 (16%)	19,38,41	3.54	5 (26%)
8	PSU	A	955	8	18,21,22	3.55	7 (38%)	22,30,33	1.98	4 (18%)
55	5MU	v	54	55	19,22,23	4.60	7 (36%)	28,32,35	3.73	10 (35%)
8	G7M	A	2069	8	20,26,27	1.78	6 (30%)	17,39,42	1.85	4 (23%)
8	2MG	A	2445	8	18,26,27	1.89	5 (27%)	16,38,41	1.36	2 (12%)
56	PSU	w	32	56	18,21,22	3.91	6 (33%)	22,30,33	1.85	6 (27%)
34	2MG	a	1207	34	18,26,27	2.13	7 (38%)	16,38,41	1.50	4 (25%)
34	5MC	a	967	34	18,22,23	3.28	7 (38%)	26,32,35	1.29	4 (15%)
34	UR3	a	1498	34	19,22,23	2.46	6 (31%)	26,32,35	1.12	2 (7%)
55	H2U	v	20	55	18,21,22	3.58	3 (16%)	21,30,33	2.03	5 (23%)
8	PSU	A	746	8	18,21,22	3.74	6 (33%)	22,30,33	1.68	5 (22%)
56	PSU	w	55	56	18,21,22	1.43	3 (16%)	22,30,33	1.91	5 (22%)
8	6MZ	A	1618	8	18,25,26	1.72	6 (33%)	16,36,39	2.94	4 (25%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	2.74	10 (38%)
34	4OC	a	1402	34	20,23,24	3.16	8 (40%)	26,32,35	1.13	3 (11%)
56	4SU	w	8	56	18,21,22	1.89	5 (27%)	26,30,33	2.11	6 (23%)
34	5MC	a	1407	34	18,22,23	3.16	7 (38%)	26,32,35	1.09	2 (7%)
56	PSU	w	39	56	18,21,22	3.75	6 (33%)	22,30,33	2.22	5 (22%)
34	G7M	a	527	34	20,26,27	2.07	4 (20%)	17,39,42	1.44	3 (17%)
8	PSU	A	1917	8	18,21,22	3.68	6 (33%)	22,30,33	1.92	5 (22%)
8	2MA	A	2503	8	19,25,26	3.11	7 (36%)	21,37,40	1.95	5 (23%)

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
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	3/5/27/28	0/3/3/3
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	OMC	A	2498	8	-	2/9/27/28	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
58	FME	y	101	58	-	4/7/9/11	-
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	OMG	A	2251	56,8	-	0/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	3/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	5MC	a	967	34	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	1/7/38/39	0/2/2/2
8	PSU	A	746	8	-	1/7/25/26	0/2/2/2
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
8	2MA	A	2503	8	-	2/3/25/26	0/3/3/3

The worst 5 of 288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	O4'-C1'	17.31	1.67	1.43
8	A	1915	3TD	C2'-C1'	-15.67	1.33	1.53
8	A	1915	3TD	C6-C5	13.05	1.50	1.35
55	v	20	H2U	C2-N1	12.16	1.53	1.35
8	A	1939	5MU	C2-N1	10.72	1.55	1.38

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	13.01	126.41	115.31
34	a	1519	MA6	N1-C6-N6	-12.93	103.44	117.06
34	a	1518	MA6	N1-C6-N6	-12.58	103.82	117.06
55	v	54	5MU	C5-C4-N3	12.04	125.59	115.31
8	A	1939	5MU	C5-C6-N1	-10.62	112.41	123.34

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1519	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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$
61	AM2	a	2001	-	40,40,40	0.24	0	53,60,60	0.60	2 (3%)
62	GDP	x	801	-	24,30,30	5.24	12 (50%)	30,47,47	1.86	11 (36%)

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
61	AM2	a	2001	-	-	4/12/84/84	0/4/4/4
62	GDP	x	801	-	-	7/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	x	801	GDP	C2'-C1'	-17.38	1.27	1.53
62	x	801	GDP	O4'-C1'	10.27	1.55	1.41
62	x	801	GDP	C3'-C4'	-10.01	1.27	1.53
62	x	801	GDP	C2-N2	4.96	1.46	1.34
62	x	801	GDP	O4'-C4'	4.81	1.55	1.45

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	N2-C2-N1	4.60	126.50	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	C3'-C2'-C1'	3.21	105.81	100.98
62	x	801	GDP	N2-C2-N3	-3.20	113.50	119.74
62	x	801	GDP	C2'-C3'-C4'	2.63	107.75	102.64
62	x	801	GDP	PA-O3A-PB	-2.62	123.84	132.83

There are no chirality outliers.

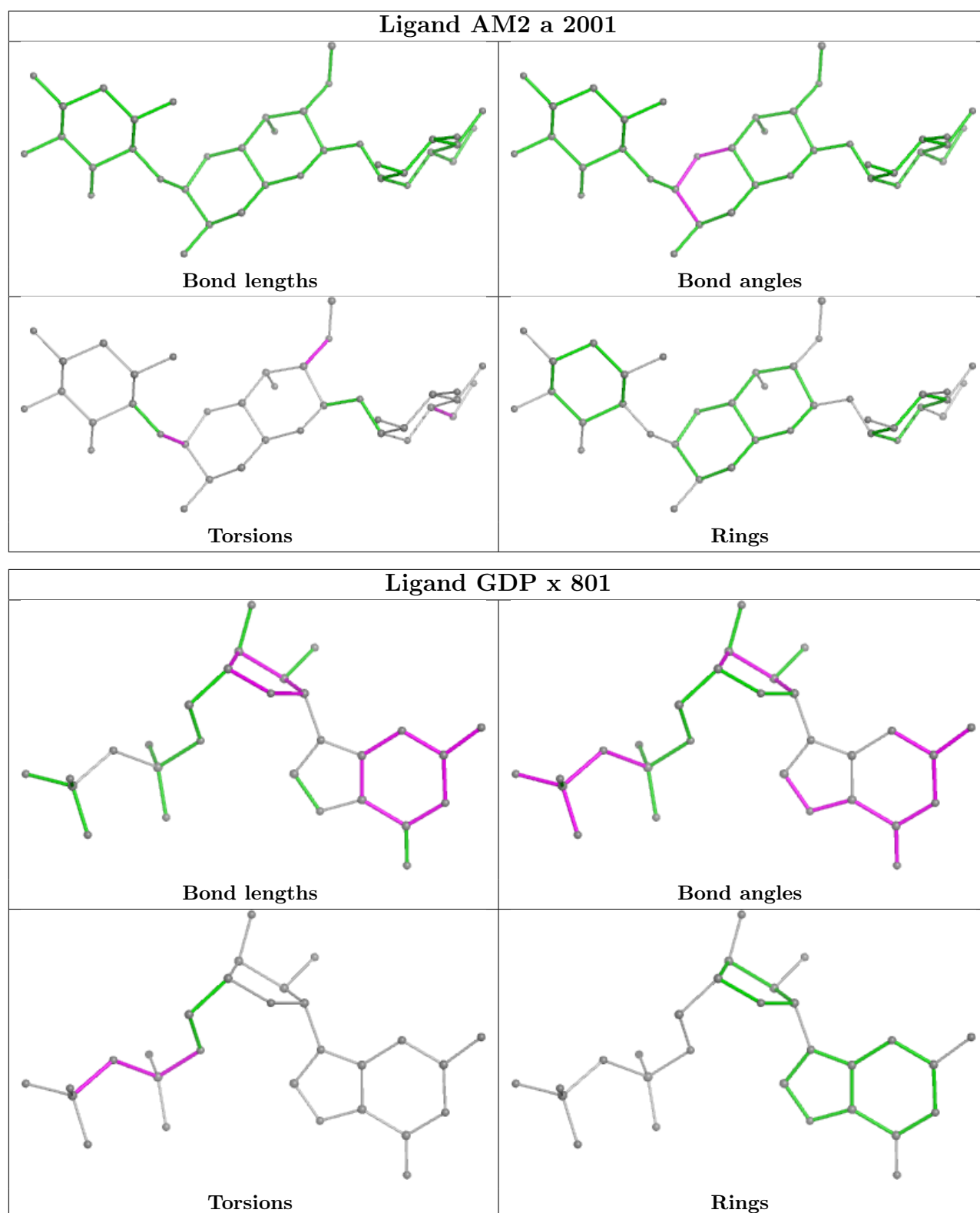
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	a	2001	AM2	CA8-CA7-NA7-CA9
62	x	801	GDP	C5'-O5'-PA-O3A
61	a	2001	AM2	OB1-CB5-CB6-OB6
62	x	801	GDP	PA-O3A-PB-O3B
61	a	2001	AM2	OA4-CA1-OA1-CC1

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.