



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 5, 2016 – 04:49 PM EST

PDB ID : 5LZB
EMDB ID: : EMD-4122
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the initial binding state (IB)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 5.30 Å(reported)

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

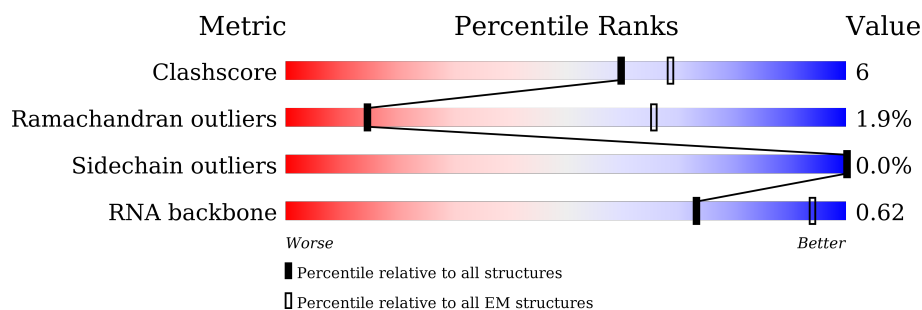
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 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.



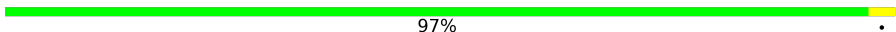

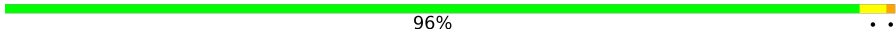
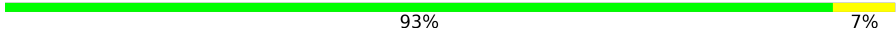
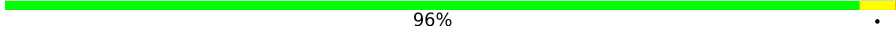
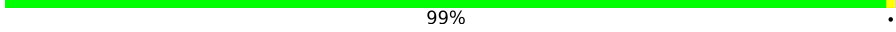
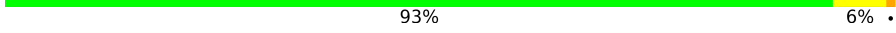
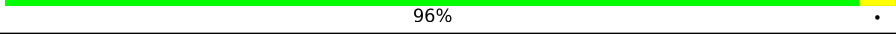
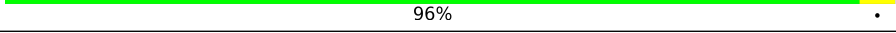
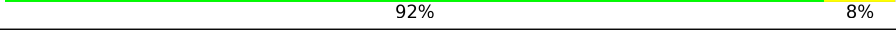
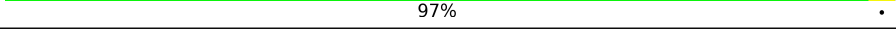
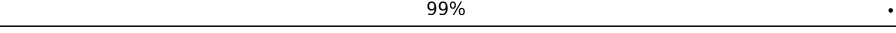
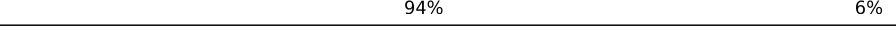
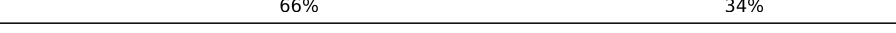
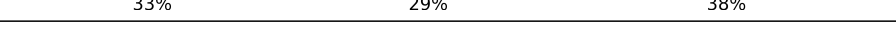

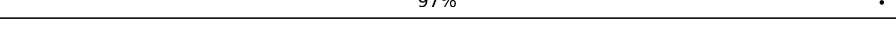
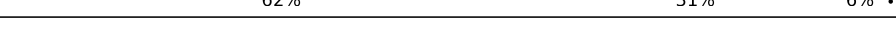


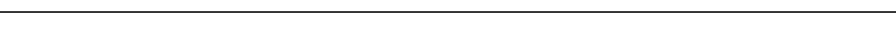




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	1539	75% 22% .
2	b	218	96% .
3	c	206	97% .
4	d	205	97% .
5	e	157	95% 5%
6	f	100	95% 5%
7	g	151	97% .
8	h	129	98% .












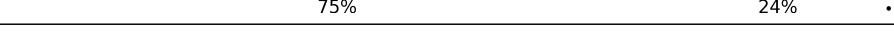







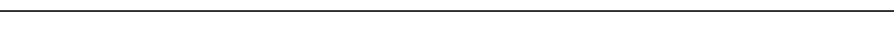

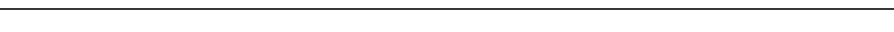
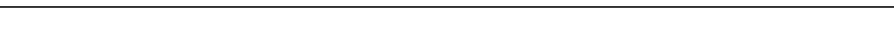


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Mol	Chain	Length	Quality of chain
9	i	127	 97% .
10	j	98	 92% 7% .
11	k	116	 96% ..
12	l	123	 93% 7%
13	m	114	 96% ..
14	n	100	 99% .
15	o	88	 93% 6% .
16	p	82	 96% .
17	q	80	 96% .
18	r	65	 92% 8%
19	s	79	 97% .
20	t	85	 99% .
21	u	65	 94% 6%
22	v	77	 66% 34%
23	x	48	 33% 29% 38%
24	y	95	 44% 39% 17%
25	z	614	 97% .
26	A	2903	 62% 31% 6% .
27	B	120	 64% 29% 5% .
28	C	271	 82% 17%
29	D	209	 78% 22%
30	E	201	 87% 13%
31	F	177	 81% 18% .
32	G	176	 74% 23% .
33	I	141	 78% 21% ..

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Mol	Chain	Length	Quality of chain
34	H	149	 83% 15% .
35	J	142	 82% 17% .
36	K	122	 78% 21% .
37	L	143	 78% 22% .
38	M	136	 81% 18% .
39	N	120	 82% 18%
40	O	116	 83% 17%
41	P	114	 81% 19%
42	Q	117	 85% 15%
43	R	103	 80% 20%
44	S	110	 87% 11% .
45	T	93	 75% 24% .
46	U	102	 67% 31% .
47	V	94	 86% 14%
48	W	75	 83% 17%
49	X	77	 91% 9%
50	Y	63	 83% 16% .
51	Z	58	 76% 24%
52	0	56	 84% 16%
53	1	50	 76% 24%
54	2	46	 87% 13%
55	3	64	 86% 13% .
56	4	38	 82% 16% .
57	6	66	 73% 21% 6%
58	w	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152991 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	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

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

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called Sec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	1	0
			4863	3049	904	893	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

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

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

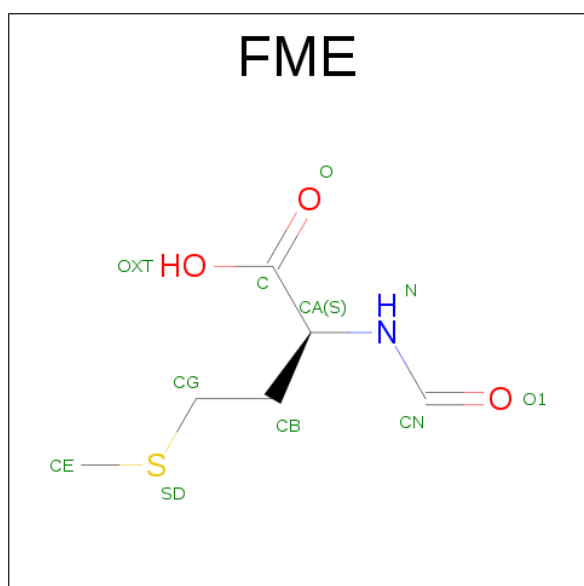
- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

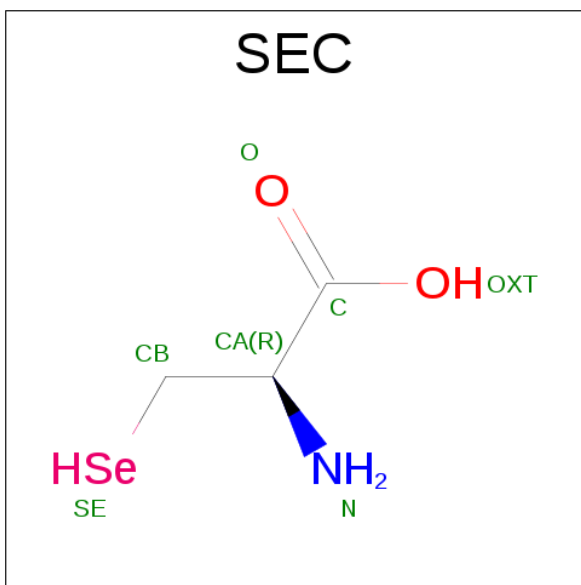
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



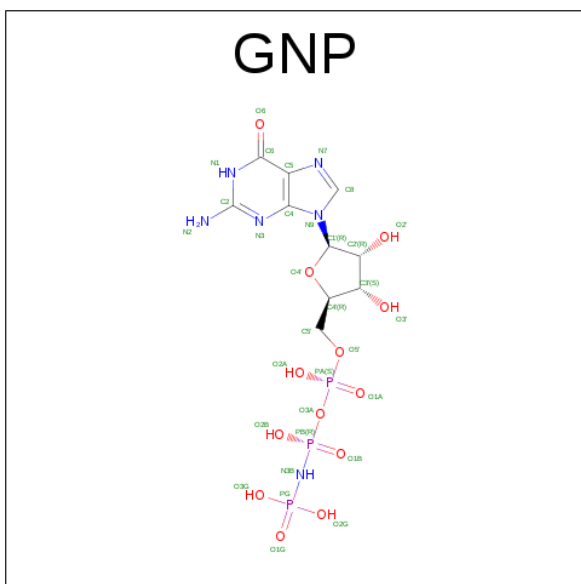
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: C₃H₇NO₂Se).



Mol	Chain	Residues	Atoms					AltConf
60	y	1	Total	C	N	O	Se	0
			6	3	1	1	1	

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	z	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	4	1	Total	Zn	0
			1	1	
63	6	1	Total	Zn	0
			1	1	

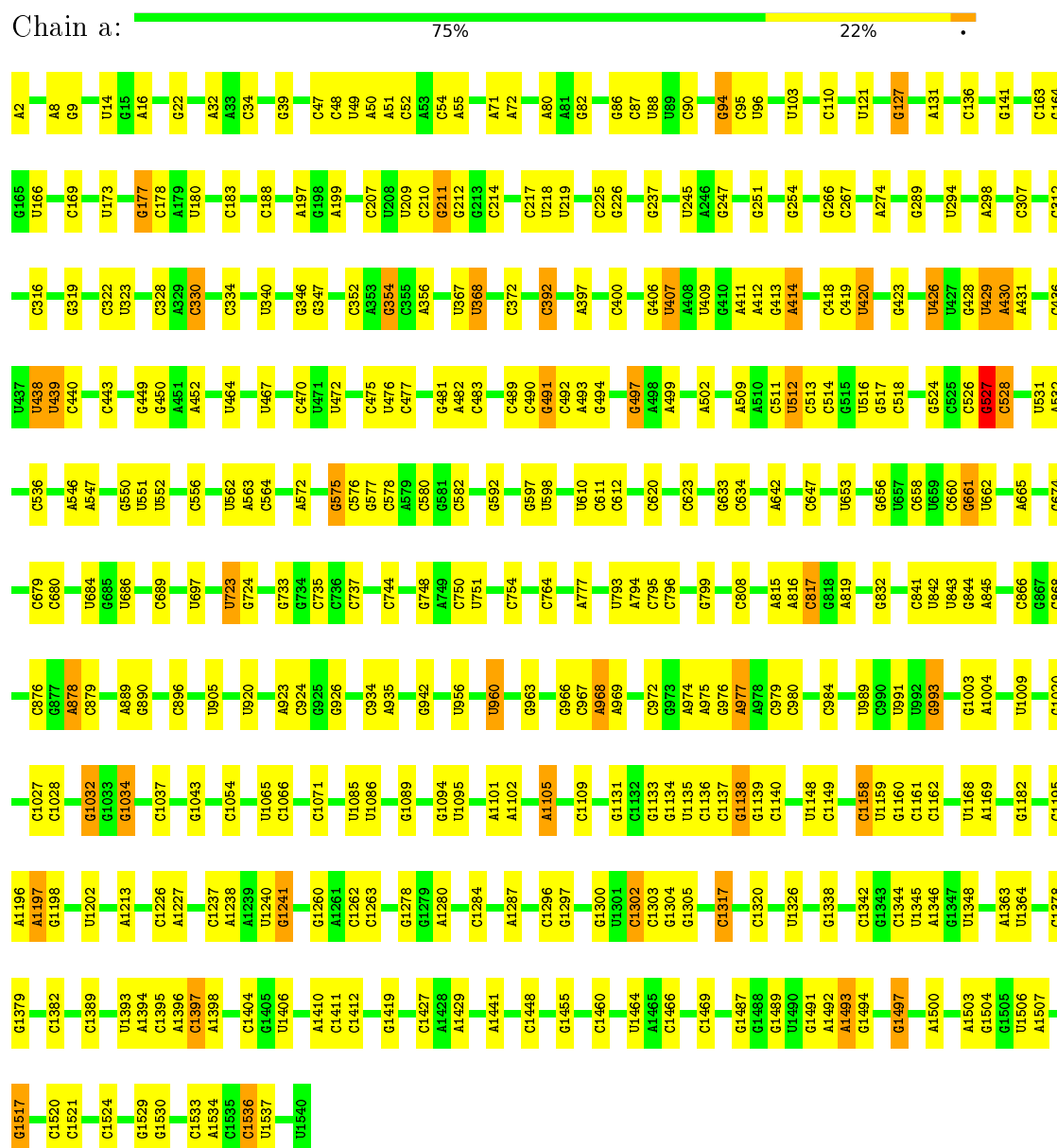
- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	z	2	Total	O	0
			2	2	

3 Residue-property plots [i](#)

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



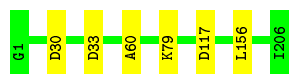
- Molecule 2: 30S ribosomal protein S2

Chain b:  96% .



- Molecule 3: 30S ribosomal protein S3

Chain c:  97% .



- Molecule 4: 30S ribosomal protein S4

Chain d:  97% .



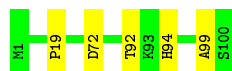
- Molecule 5: 30S ribosomal protein S5

Chain e:  95% 5%



- Molecule 6: 30S ribosomal protein S6

Chain f:  95% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g:  97% .



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  97% .



- Molecule 10: 30S ribosomal protein S10

Chain j: 92% 7% .



- Molecule 11: 30S ribosomal protein S11

Chain k: 96% . .



- Molecule 12: 30S ribosomal protein S12

Chain l: 93% 7%



- Molecule 13: 30S ribosomal protein S13

Chain m: 96% . .



- Molecule 14: 30S ribosomal protein S14

Chain n: 99% .



- Molecule 15: 30S ribosomal protein S15

Chain o: 93% 6% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 96% .



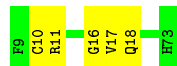
- Molecule 17: 30S ribosomal protein S17

Chain q:  96% .



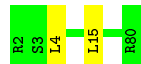
- Molecule 18: 30S ribosomal protein S18

Chain r:  92% 8%



- Molecule 19: 30S ribosomal protein S19

Chain s:  97% .



- Molecule 20: 30S ribosomal protein S20

Chain t:  99% .



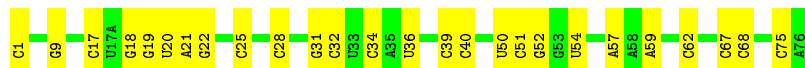
- Molecule 21: 30S ribosomal protein S21

Chain u:  94% 6%

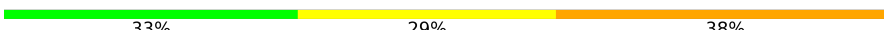


- Molecule 22: fMet-tRNA^{fMet}

Chain v:  66% 34%



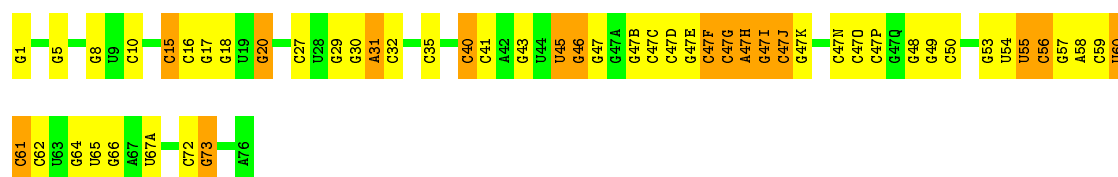
- Molecule 23: SECIS mRNA

Chain x:  33% 29% 38%



- Molecule 24: Sec-tRNA^{Sec}

Chain y:  44% 39% 17%



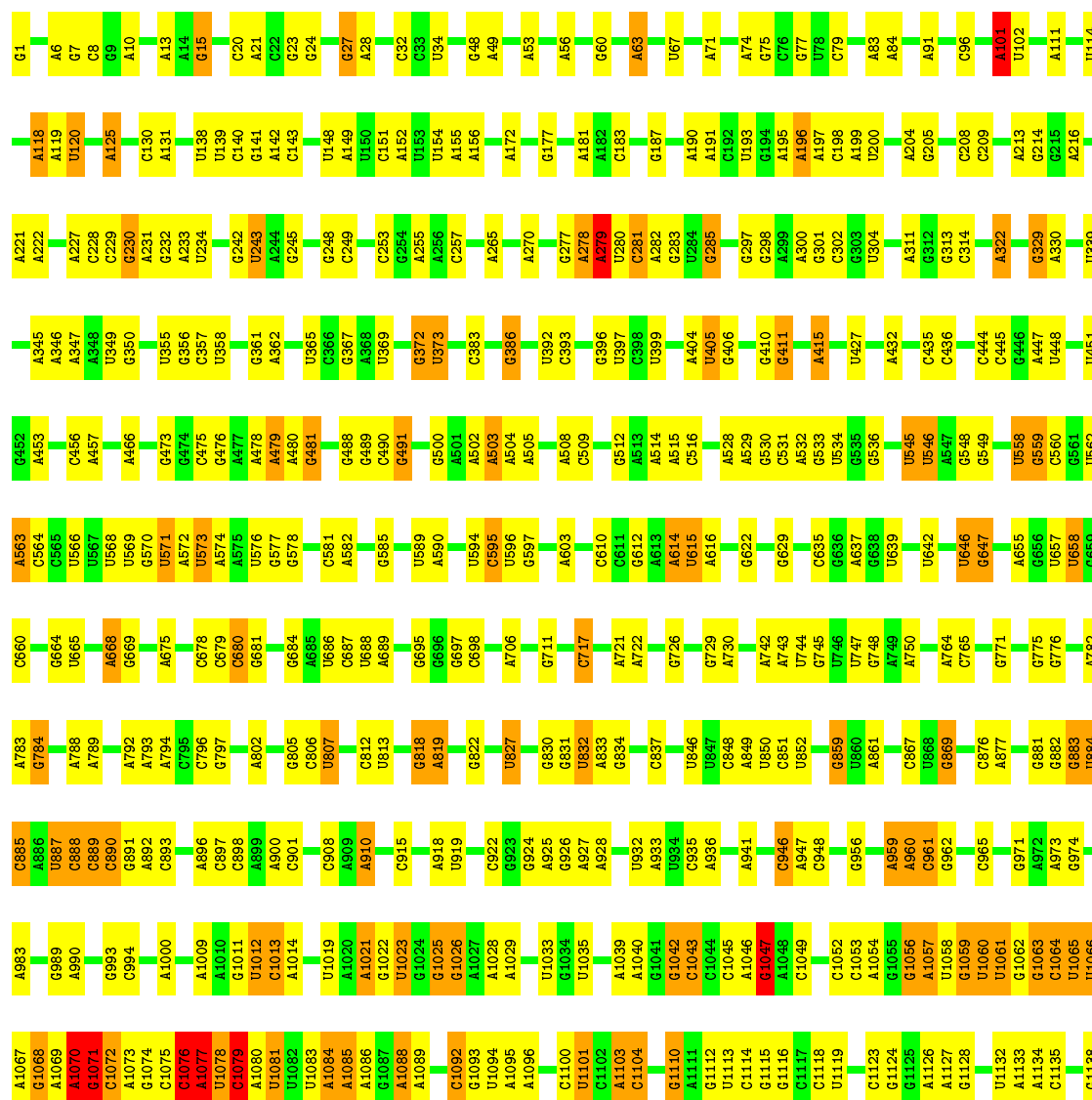
- Molecule 25: Selenocysteine-specific elongation factor

Chain z: 97% .



- Molecule 26: 23S ribosomal RNA

Chain A: 62% 31% 6% .

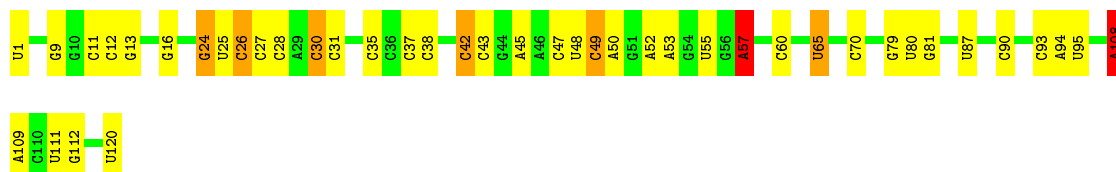


U2656	A2565	C2475	A2358	U2259	A2170	G2100	G2002	C1905	U1775	G1667	U1468	C1350	U1249	A1142
A2657	A2566	A2476	C2359	C2264	A2171	C2103	U2007	G1906	A1783	A1668	A1469	A1350	G1250	A1143
G2663	G2567	A2477	G2375	A2267	A2172	G2104	G2011	G1907	A1784	A1669	A1265	A1353	G1251	
U2684	U2568	U2478	G2378	A2268	C2174	U2105	U2012	A1913	A1787	G1673	G1475	G1358	A1263	G1149
U2689	A2572	G2480	A2378	G2269	C2175	U2106	G2013	C1914	A1791	G1674	U1476	A1359	A1264	C1150
U2690	C2573	A2482	G2383	G2276	A2176	G2107	A2014	71915		C1675	A1477	A1357	U1255	A1151
C2691	C2574	C2483	C2385	G2277	C2177	A2108		71916		U1578	G1478	A1365	G1256	C1152
U2698	C2575	C2484		G2278	C2178	U2109	C2021	C1924	U1796	C1582	U1258	A1378	G1257	G1153
C2699	C2576	G2485	U2390	G2279	C2179	G2110	C2022		U1797	G1482	U1259	A1379	A1260	G1154
A2700	G2579	G2488	U2393	G2282	U2180	G2111	C2023	A1927	U1798	G1483	U1485	G1380	C1261	A1155
G2702	U2580		C2394	C2283	U2181	U2112	G2024	A1928	U1799	G1484	U1486	A1387		A1156
U2707	G2581	G2489	U2402	A2287	U2182	G2113		G1929	G1799	G1485	U1487	A1388		G1157
	U2582	A2497	C2403	U2291	U2183			G1930	C1800	G1687	A1264	A1389	A1265	C1158
C2710	U2583	U2404	U2404	U2292	U2184	G2116	U2028	G1931	A1801		A1266	A1386	A1266	
	C2591	G2405	G2405	C2295	U2185	A2117	G2029	G1932	A1802	U1693	A1267	A1387	U1267	A1169
G2714	G2592	A2407	U2407	U2296	U2186	U2118	N2030	A1933	A1803	U1699	C1392	A1387		C1170
C2716	G2593	U2408	A2411	U2302	U2187	A2119	G2031	U1938		A1700	A1495	A1392	C1270	C1172
G2717	U2594	U2409		G2303	U2188	G2120	G2032	U1939	G1807	A1704	A1496	A1393	G1271	
G2718	U2595			G2304	U2189	G2121		U1940	A1808	A1705	U1497	A1394	U1272	A1175
G2719	U2596			U2305	U2190	G2122	U2041	U1941	A1809	C1708	C1498	U1395	U1273	
U2720	C2597	U2500	C2416	G2306	U2191	U2123	A2042	C1941	A1810	G1715	C1499	U1396	A1274	G1178
A2726	C2598	C2501		U2307	U2192	U2124	C2043	A1936	A1811	U1716	A1499	C1397	A1275	G1179
	G2599	G2502		G2308	U2193	U2125	C2044	U1937	A1812	A1717	A1500	C1398		U1180
C2727	U2599	U2503		U2309	U2194	U2126	C2045	A1938	U1813	A1718	A1501	U1400	C1278	U1181
G2728	C2600	U2504		U2310	U2195	U2127	G2046	U1939	U1814	U1719	U1502	U1401	U1182	
	A2601	G2505		G2311	U2196	G2128	C2047	U1940	U1815	G1723	C1507	U1402	U1288	U1183
A2726	A2602	U2506		U2312	U2197	U2129	G2048	U1941	U1816	C1727	A1508	A1403		
	G2603	U2507		U2313	U2198	U2130		U1955	U1817	C1728	A1509		U1294	G1186
U2733	U2604	C2510		U2314	U2199	U2131	A2051	C1957	U1818	U1728	C1512	G1407	U1300	G1187
	U2605	C2511		U2315	U2200	U2132	A2052	C1958	U1819	G1737	C1513	G1408	A1301	U1188
U2739	C2606	U2512		U2316	U2201	U2133	C2055	U1963	U1820	G1738	G1514	G1410	G1190	
G2742	U2607	U2513		U2317	U2202	U2134	C2056	C1962	U1821	G1743	G1515	G1416		G1197
U2743	U2608	U2514		U2318	U2203	U2135	G2057	U1964	U1822	U1751	G1516	C1417	U1312	
G2744	U2609	U2515		U2319	U2204	U2136	A2058	G1964	U1823	G1752		A1420	U1313	C1200
	C2610	U2516		U2320	U2205		A2059	C1967	U1824	G1753	G1527	A1428	C1315	G1206
	U2613	U2517		U2321	U2206		A2060	C1968	U1825	U1754	A1528		U1316	
U2746	U2614	U2518		U2322	U2207		A2061	C1969	U1826	A1755	C1532	C1428	G1317	G1210
	U2615	U2519		U2323	U2208		C2065	U1971	U1827	A1756	C1533		A1321	C1211
C2752	U2616	U2520		U2324	U2209		C2066	U1972	U1828	G1757	U1534	G1432	A1322	
	U2617	U2521		U2325	U2210		C2067	U1973	U1829	U1758	A1535	A1433	A1323	G1223
	C2626	U2522		U2326	U2211		C2068	U1974	U1830	U1759	G1536	A1434	G1324	
	U2629	U2523		U2327	U2212		C2069	U1975	U1831	C1760	G1537	G1435	G1325	A1226
U2756	U2630	U2524		U2328	U2213		C2070	U1976	U1832	C1761	U1538	C1436	G1227	
A2757	U2631	U2525		U2329	U2214		C2071	U1977	U1833	A1762	U1539	C1437	U1329	G1228
G2759	U2632	U2526		U2330	U2215		C2072	U1978	U1834	G1763	G1543		A1333	C1229
	U2633	U2527		U2331	U2216		C2073	U1979	U1835	C1764	A1544	A1453	G1333	A1230
A2764	U2634	U2528		U2332	U2217		C2074	U1980	U1836	U1769	A1548	C1454	U1340	G1236
U2766	U2635	U2529		U2333	U2218		C2075	U1981	U1837	U1770	U1563	G1455	C1345	
	U2636	U2530		U2334	U2219		C2076	U1982	U1838	C1771	C1564	U1459	C1348	A1244
C2773	U2637	U2531		U2335	U2220		C2077	U1983	U1839	A1772	A1565	U1460		
	U2638	U2532		U2336	U2221		C2078	U1984	U1840	C1773	A1566		C1349	G1248
A2778	U2639	U2533		U2337	U2222		C2079	U1985	U1841	C1774	A1567			
	U2640	U2534		U2338	U2223		C2080	U1986	U1842					
	C2645	U2535		U2339	U2224		C2081	U1987	U1843					
	U2646	U2536		U2340	U2225		C2082	U1988	U1844					
	U2647	U2537		U2341	U2226		C2083	U1989	U1845					
	C2648	U2538		U2342	U2227		C2084	U1990	U1846					
	U2649	U2539		U2343	U2228		C2085	U1991	U1847					
		U2562		U2344	U2229		C2086	U1992	U1848					
				U2345	U2230		C2087	U1993	U1849					
				U2346	U2231		C2088	U1994	U1850					
				U2347	U2232		C2089	U1995	U1851					
				U2348	U2233		C2090	U1996	U1852					
				U2349	U2234		C2091	U1997	U1853					
				U2350	U2235		C2092	U1998	U1854					
				U2351	U2236		C2093	U1999	U1855					
				U2352	U2237		C2094	U2000	U1856					
				U2353	U2238		C2095	U2001	U1857					
				U2354	U2239		C2096	U2002	U1858					
				U2355	U2240		C2097	U2003	U1859					
				U2356	U2241		C2098	U2004	U1860					
				U2357	U2242		C2099	U2005	U1861					
				U2358	U2243		C2100	U2006	U1862					
				U2359	U2244		C2101	U2007	U1863					
				U2360	U2245		C2102	U2008	U1864					
				U2361	U2246		C2103	U2009	U1865					
				U2362	U2247		C2104	U2010	U1866					
				U2363	U2248		C2105	U2011	U1867					
				U2364	U2249		C2106	U2012	U1868					
				U2365	U2250		C2107	U2013	U1869					
				U2366	U2251		C2108	U2014	U1870					
				U2367	U2252		C2109	U2015	U1871					
				U2368	U2253		C2110	U2016	U1872					
				U2369	U2254		C2111	U2017	U1873					
				U2370	U2255		C2112	U2018	U1874					
				U2371	U2256		C2113	U2019	U1875					
				U2372	U2257		C2114	U2020	U1876					
				U2373	U2258		C2115	U2021	U1877					
				U2374	U2259		C2116	U2022	U1878					
				U2375	U2260		C2117	U2023	U1879					
				U2376	U2261		C2118	U2024	U1880					
				U2377	U2262		C2119	U2025	U1881					
				U2378	U2263		C2120	U2026	U1882					
				U2379	U2264		C2121	U2027	U1883					
				U2380	U2265		C2122	U2028	U1884					
				U2381	U2266		C2123	U2029	U1885					
				U2382	U2267		C2124	U2030	U1886					
				U2383	U2268		C2125	U2031	U1887					
				U2384	U2269		C2126	U2032	U1888					
				U2385	U2270		C2127	U2033	U1889					
				U2386	U2271		C2128	U2034	U1890					
				U2387	U2272		C2129	U2035	U1891					
				U2388	U2273		C2130	U2036	U1892					
				U2389	U2274		C2131	U2037	U1893					
				U2390	U2275		C2132	U2038	U1894					
				U2391	U2276		C2133	U2039	U1895					
				U2392	U2277		C2134	U2040	U1896					
				U2393	U2278		C2135	U2041	U1897					
	</													



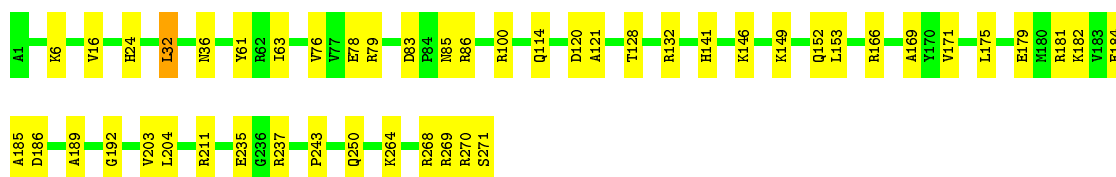
• Molecule 27: 5S ribosomal RNA

Chain B: 64% 29% 5%



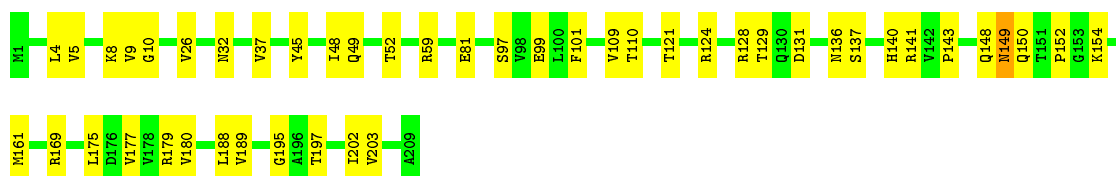
• Molecule 28: 50S ribosomal protein L2

Chain C: 82% 17%



• Molecule 29: 50S ribosomal protein L3

Chain D: 78% 22%



• Molecule 30: 50S ribosomal protein L4

Chain E: 87% 13%



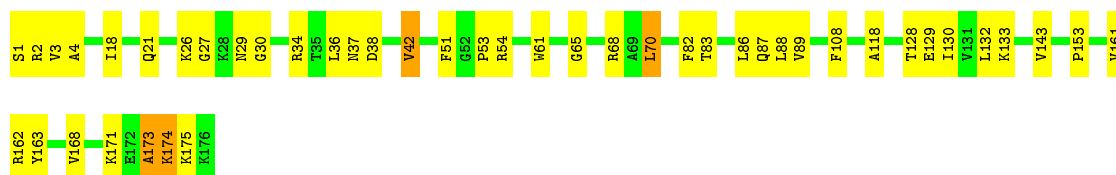
• Molecule 31: 50S ribosomal protein L5

Chain F: 81% 18%



• Molecule 32: 50S ribosomal protein L6

Chain G: 74% 23%



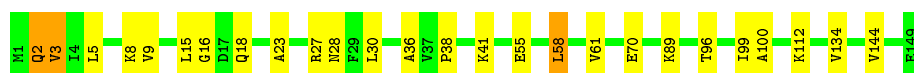
- Molecule 33: 50S ribosomal protein L11

Chain I: 78% 21% ..



- Molecule 34: 50S ribosomal protein L9

Chain H: 83% 15% .



- Molecule 35: 50S ribosomal protein L13

Chain J: 82% 17% .



- Molecule 36: 50S ribosomal protein L14

Chain K: 78% 21% .



- Molecule 37: 50S ribosomal protein L15

Chain L: 78% 22% .



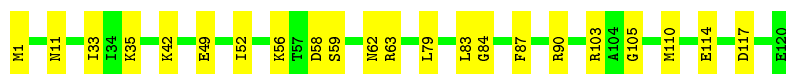
- Molecule 38: 50S ribosomal protein L16

Chain M: 81% 18% .



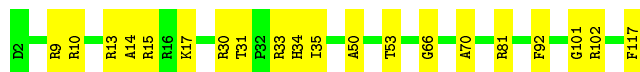
- Molecule 39: 50S ribosomal protein L17

Chain N: 82% 18%



- Molecule 40: 50S ribosomal protein L18

Chain O: 83% 17%



- Molecule 41: 50S ribosomal protein L19

Chain P: 81% 19%



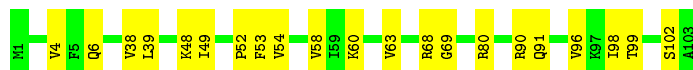
- Molecule 42: 50S ribosomal protein L20

Chain Q: 85% 15%



- Molecule 43: 50S ribosomal protein L21

Chain R: 80% 20%



- Molecule 44: 50S ribosomal protein L22

Chain S: 87% 11%



- Molecule 45: 50S ribosomal protein L23

Chain T: 75% 24%




- Molecule 46: 50S ribosomal protein L24

Chain U: 67% 31%




- Molecule 47: 50S ribosomal protein L25

Chain V:  86% 14%



- Molecule 48: 50S ribosomal protein L27

Chain W:  83% 17%




- Molecule 49: 50S ribosomal protein L28

Chain X:  91% 9%




- Molecule 50: 50S ribosomal protein L29

Chain Y:  83% 16% .




- Molecule 51: 50S ribosomal protein L30

Chain Z:  76% 24%



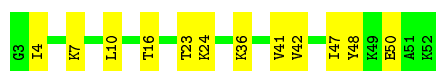
- Molecule 52: 50S ribosomal protein L32

Chain 0:  84% 16%



- Molecule 53: 50S ribosomal protein L33

Chain 1:  76% 24%



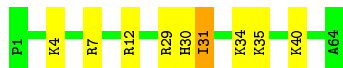
- Molecule 54: 50S ribosomal protein L34

Chain 2:  87% 13%



- Molecule 55: 50S ribosomal protein L35

Chain 3: 86% 13% .



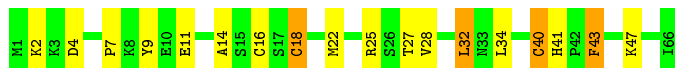
- Molecule 56: 50S ribosomal protein L36

Chain 4: 82% 16% .



- Molecule 57: 50S ribosomal protein L31

Chain 6: 73% 21% 6%



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	8002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	Not provided	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, MA6, 2MA, 2MG, 1MG, 3TD, G7M, SEC, UR3, 5MU, ZN, 6IA, 5MC, 6MZ, FME, OMC, MG, OMG, H2U, OMU, 4OC, 4SU, PSU

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	0.58	3/36701 (0.0%)	1.30	392/57246 (0.7%)
10	j	0.44	0/797	0.87	1/1077 (0.1%)
11	k	0.48	0/886	0.87	3/1195 (0.3%)
12	l	0.43	0/969	0.79	1/1300 (0.1%)
13	m	0.42	0/893	0.90	1/1193 (0.1%)
14	n	0.45	0/806	0.82	1/1074 (0.1%)
15	o	0.42	0/722	0.81	3/964 (0.3%)
16	p	0.55	0/659	0.78	0/884
17	q	0.45	0/658	0.88	0/881
18	r	0.36	0/512	0.67	0/689
19	s	0.37	0/653	0.73	2/877 (0.2%)
2	b	0.45	0/1736	0.85	4/2338 (0.2%)
20	t	0.43	0/671	0.77	0/888
21	u	0.43	0/501	0.85	1/668 (0.1%)
22	v	0.62	2/1745 (0.1%)	1.33	25/2716 (0.9%)
23	x	0.88	1/1145 (0.1%)	1.84	45/1781 (2.5%)
24	y	0.89	2/2168 (0.1%)	1.92	110/3375 (3.3%)
25	z	0.47	0/4963	0.89	12/6727 (0.2%)
26	A	0.57	13/69240 (0.0%)	1.24	539/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.24	27/4478 (0.6%)
28	C	0.42	0/2122	0.77	1/2852 (0.0%)
29	D	0.45	0/1586	0.75	0/2134
3	c	0.41	0/1652	0.76	3/2225 (0.1%)
30	E	0.43	0/1571	0.75	2/2113 (0.1%)
31	F	0.52	1/1435 (0.1%)	0.90	4/1926 (0.2%)
32	G	0.47	0/1343	0.82	3/1816 (0.2%)
33	I	0.49	0/1046	0.97	5/1410 (0.4%)
34	H	0.40	0/1122	0.74	1/1515 (0.1%)
35	J	0.42	0/1152	0.70	2/1551 (0.1%)
36	K	0.47	0/948	0.75	0/1268
37	L	0.42	0/1054	0.75	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	M	0.43	0/1093	0.74	1/1460 (0.1%)
39	N	0.43	0/974	0.68	0/1301
4	d	0.49	0/1665	0.93	3/2227 (0.1%)
40	O	0.43	0/902	0.72	0/1209
41	P	0.43	0/929	0.72	1/1242 (0.1%)
42	Q	0.41	0/960	0.58	1/1278 (0.1%)
43	R	0.42	0/829	0.79	0/1107
44	S	0.39	0/864	0.80	2/1156 (0.2%)
45	T	0.44	0/745	0.77	0/994
46	U	0.43	0/788	0.91	1/1051 (0.1%)
47	V	0.47	0/766	0.72	0/1025
48	W	0.39	0/582	0.69	0/769
49	X	0.35	0/635	0.70	1/848 (0.1%)
5	e	0.45	0/1170	0.88	0/1573
50	Y	0.48	0/510	0.92	2/677 (0.3%)
51	Z	0.40	0/453	0.72	1/605 (0.2%)
52	0	0.44	0/450	0.80	0/599
53	1	0.36	0/417	0.77	0/554
54	2	0.40	0/380	0.69	0/498
55	3	0.40	0/513	0.63	0/676
56	4	0.48	0/303	0.80	1/397 (0.3%)
57	6	0.46	0/532	1.01	5/709 (0.7%)
58	w	0.32	0/68	0.98	0/103
6	f	0.51	0/836	0.85	1/1128 (0.1%)
7	g	0.46	0/1196	0.81	2/1602 (0.1%)
8	h	0.43	0/989	0.78	1/1326 (0.1%)
9	i	0.47	0/1034	0.84	0/1375
All	All	0.55	23/164912 (0.0%)	1.17	1211/246067 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
10	j	0	2
11	k	0	1
12	l	0	2
13	m	0	2
15	o	0	1
18	r	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	2
25	z	0	3
26	A	2	0
28	C	0	1
33	I	0	2
34	H	0	3
36	K	0	1
38	M	0	1
44	S	0	1
46	U	0	2
5	e	0	1
55	3	0	1
All	All	4	28

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.71	1.48	1.61
22	v	1	C	OP3-P	-10.67	1.48	1.61
23	x	87	A	OP3-P	-10.65	1.48	1.61
1	a	2	A	OP3-P	-10.60	1.48	1.61
27	B	1	U	OP3-P	-10.57	1.48	1.61

The worst 5 of 1211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	452	A	O5'-P-OP1	-19.89	86.83	110.70
1	a	450	G	O5'-P-OP1	16.99	131.09	110.70
26	A	1026	G	O5'-P-OP1	-15.92	91.37	105.70
26	A	2169	A	C5-N7-C8	15.84	111.82	103.90
26	A	1178	C	N1-C2-O2	15.82	128.39	118.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
26	A	2069	G7M	C4',C3'

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	b	17	HIS	Mainchain
5	e	92	ARG	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	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	33029	0	16643	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1642	0	839	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1039	0	0
25	z	4863	0	4837	0	0
26	A	62335	0	31375	421	0
27	B	2570	0	1301	20	0
28	C	2083	0	2157	30	0
29	D	1565	0	1616	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	E	1552	0	1619	16	0
31	F	1411	0	1447	20	0
32	G	1323	0	1374	29	0
33	I	1032	0	1088	15	0
34	H	1111	0	1148	13	0
35	J	1129	0	1162	14	0
36	K	939	0	1012	16	0
37	L	1045	0	1117	21	0
38	M	1074	0	1157	17	0
39	N	961	0	1000	14	0
40	O	892	0	923	14	0
41	P	917	0	965	13	0
42	Q	947	0	1022	14	0
43	R	816	0	839	12	0
44	S	857	0	922	9	0
45	T	739	0	807	16	0
46	U	780	0	834	16	0
47	V	753	0	780	10	0
48	W	575	0	592	9	0
49	X	625	0	655	6	0
50	Y	509	0	543	8	0
51	Z	449	0	491	10	0
52	0	444	0	461	6	0
53	1	410	0	440	7	0
54	2	377	0	418	4	0
55	3	504	0	574	7	0
56	4	302	0	340	6	0
57	6	523	0	521	10	0
58	w	62	0	34	0	0
59	v	10	0	10	0	0
60	y	6	0	3	0	0
61	z	32	0	13	0	0
62	z	1	0	0	0	0
63	4	1	0	0	0	0
63	6	1	0	0	0	0
64	z	2	0	0	0	0
All	All	152991	0	104094	728	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 6.

The worst 5 of 728 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)
26:A:279:A:N6	26:A:361:G:N3	2.04	1.05
26:A:2166:U:O2	26:A:2170:A:N6	2.08	0.85
36:K:35:VAL:HG21	36:K:69:VAL:HG12	1.69	0.74
26:A:1072:C:OP1	26:A:1077:A:N6	2.23	0.72
26:A:410:G:N3	26:A:432:A:N6	41.67	0.72

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	b	216/218 (99%)	188 (87%)	24 (11%)	4 (2%)	10	51
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	13	57
4	d	203/205 (99%)	190 (94%)	8 (4%)	5 (2%)	7	45
5	e	155/157 (99%)	142 (92%)	6 (4%)	7 (4%)	3	33
6	f	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	3	34
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	9	51
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	24	69
9	i	125/127 (98%)	108 (86%)	13 (10%)	4 (3%)	5	41
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	2	25
11	k	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	11	53
12	l	121/123 (98%)	110 (91%)	7 (6%)	4 (3%)	5	40
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	6	44
14	n	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	4	39
16	p	80/82 (98%)	72 (90%)	5 (6%)	3 (4%)	4	37
17	q	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	4	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	63/65 (97%)	57 (90%)	3 (5%)	3 (5%)	3	31
19	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
20	t	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	61
21	u	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	3	31
25	z	613/614 (100%)	587 (96%)	20 (3%)	6 (1%)	19	64
28	C	269/271 (99%)	254 (94%)	13 (5%)	2 (1%)	26	71
29	D	207/209 (99%)	197 (95%)	8 (4%)	2 (1%)	19	64
30	E	199/201 (99%)	189 (95%)	8 (4%)	2 (1%)	19	64
31	F	175/177 (99%)	163 (93%)	9 (5%)	3 (2%)	11	54
32	G	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	6	43
33	I	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	6	43
34	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	5	40
35	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26	71
36	K	120/122 (98%)	116 (97%)	2 (2%)	2 (2%)	11	54
37	L	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	14	57
38	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	13	57
39	N	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	24	69
40	O	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	21	66
41	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	9	51
44	S	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	10	51
45	T	91/93 (98%)	79 (87%)	11 (12%)	1 (1%)	17	63
46	U	100/102 (98%)	89 (89%)	5 (5%)	6 (6%)	2	26
47	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	55
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	10	51
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	9	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	48
55	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12	55
56	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
57	6	64/66 (97%)	57 (89%)	5 (8%)	2 (3%)	5	41
All	All	6330/6431 (98%)	5844 (92%)	368 (6%)	118 (2%)	14	51

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	151	LYS
5	e	89	THR
6	f	94	HIS
9	i	57	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	82	92
13	m	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	z	502/501 (100%)	502 (100%)	0	100	100
28	C	216/216 (100%)	216 (100%)	0	100	100
29	D	164/164 (100%)	164 (100%)	0	100	100
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	148 (100%)	0	100	100
32	G	137/137 (100%)	137 (100%)	0	100	100
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	103 (100%)	0	100	100
37	L	102/102 (100%)	102 (100%)	0	100	100
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	100 (100%)	0	100	100
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	80 (100%)	0	100	100
46	U	83/83 (100%)	83 (100%)	0	100	100
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100
49	X	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Y	55/55 (100%)	55 (100%)	0	100	100
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5230/5252 (100%)	5229 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
25	z	529	GLN
29	D	150	GLN
50	Y	58	ASN
28	C	89	ASN
30	E	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	197 (12%)	0
22	v	76/77 (98%)	10 (13%)	0
23	x	47/48 (97%)	29 (61%)	0
24	y	93/95 (97%)	23 (24%)	0
26	A	2898/2903 (99%)	414 (14%)	5 (0%)
27	B	119/120 (99%)	11 (9%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	684 (14%)	5 (0%)

5 of 684 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	818	G
26	A	960	A
26	A	1042	G
26	A	1358	G
26	A	1875	G

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

43 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
26	6MZ	A	1618	26	17,25,26	1.05	1 (5%)	15,36,39	2.63	2 (13%)
26	2MG	A	1835	26	18,26,27	1.20	2 (11%)	21,38,41	2.53	7 (33%)
26	PSU	A	1911	26	15,21,22	1.22	2 (13%)	16,30,33	2.03	3 (18%)
26	3TD	A	1915	26	15,22,23	3.21	6 (40%)	17,32,35	2.05	5 (29%)
26	PSU	A	1917	26	15,21,22	1.11	2 (13%)	16,30,33	2.39	4 (25%)
26	5MU	A	1939	26	13,22,23	0.61	0	16,32,35	2.47	2 (12%)
26	5MC	A	1962	26	14,22,23	1.20	1 (7%)	17,32,35	1.50	1 (5%)
26	6MZ	A	2030	26	17,25,26	1.09	1 (5%)	15,36,39	1.76	3 (20%)
26	G7M	A	2069	26	18,26,27	1.25	3 (16%)	21,39,42	2.63	9 (42%)
26	OMG	A	2251	26,22	18,26,27	1.22	2 (11%)	21,38,41	1.95	4 (19%)
26	2MG	A	2445	26	18,26,27	1.21	2 (11%)	21,38,41	2.25	5 (23%)
26	H2U	A	2449	26	17,21,22	1.17	3 (17%)	23,30,33	1.99	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PSU	A	2457	26	15,21,22	1.40	1 (6%)	16,30,33	2.19	4 (25%)
26	OMC	A	2498	26	15,22,23	0.59	0	20,31,34	1.36	2 (10%)
26	2MA	A	2503	26	17,25,26	1.75	3 (17%)	18,37,40	2.93	1 (5%)
26	PSU	A	2504	26	15,21,22	1.11	2 (13%)	16,30,33	2.27	4 (25%)
26	OMU	A	2552	26	14,22,23	0.67	0	19,31,34	1.78	1 (5%)
26	PSU	A	2580	26	15,21,22	1.40	1 (6%)	16,30,33	2.21	3 (18%)
26	PSU	A	2604	26	15,21,22	1.14	1 (6%)	16,30,33	2.12	3 (18%)
26	PSU	A	2605	26	15,21,22	1.40	2 (13%)	16,30,33	2.18	4 (25%)
26	1MG	A	745	26	17,26,27	1.58	3 (17%)	19,39,42	2.01	3 (15%)
26	PSU	A	746	26	15,21,22	1.62	1 (6%)	16,30,33	2.23	3 (18%)
26	5MU	A	747	26	13,22,23	0.57	0	16,32,35	2.75	2 (12%)
26	PSU	A	955	26	15,21,22	1.24	2 (13%)	16,30,33	2.29	4 (25%)
1	2MG	a	1207	1	18,26,27	1.17	2 (11%)	21,38,41	2.24	6 (28%)
1	4OC	a	1402	1	15,23,24	0.56	0	21,32,35	1.93	3 (14%)
1	5MC	a	1407	1	14,22,23	1.35	1 (7%)	17,32,35	0.85	1 (5%)
1	UR3	a	1498	1	13,22,23	0.70	0	18,32,35	0.91	1 (5%)
1	2MG	a	1516	1	18,26,27	1.24	2 (11%)	21,38,41	2.20	6 (28%)
1	MA6	a	1518	1	18,26,27	0.93	1 (5%)	15,38,41	2.58	3 (20%)
1	MA6	a	1519	1	18,26,27	0.99	1 (5%)	15,38,41	2.65	3 (20%)
1	PSU	a	516	1	15,21,22	1.11	1 (6%)	16,30,33	2.16	3 (18%)
1	G7M	a	527	1	18,26,27	1.25	2 (11%)	21,39,42	2.99	10 (47%)
1	2MG	a	966	1	18,26,27	1.15	2 (11%)	21,38,41	2.26	7 (33%)
1	5MC	a	967	1	14,22,23	1.36	1 (7%)	17,32,35	0.95	1 (5%)
22	H2U	v	20	22	17,21,22	1.05	2 (11%)	23,30,33	1.73	5 (21%)
22	5MU	v	54	22	13,22,23	0.61	0	16,32,35	2.72	2 (12%)
22	PSU	v	55	22	15,21,22	1.21	2 (13%)	16,30,33	2.26	4 (25%)
22	4SU	v	8	22	12,21,22	0.63	0	15,30,33	1.07	1 (6%)
24	H2U	y	19	24	17,21,22	1.29	3 (17%)	23,30,33	3.00	6 (26%)
24	6IA	y	37	24	20,29,30	0.92	1 (5%)	22,41,44	2.83	4 (18%)
24	5MU	y	54	24	13,22,23	0.60	0	16,32,35	2.66	3 (18%)
24	PSU	y	55	24	15,21,22	1.62	3 (20%)	16,30,33	2.16	4 (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
26	6MZ	A	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	1/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	A	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	A	2030	26	-	0/5/27/28	0/3/3/3
26	G7M	A	2069	26	2/2/5/5	0/3/25/26	0/3/3/3
26	OMG	A	2251	26,22	-	0/5/27/28	0/3/3/3
26	2MG	A	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	A	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	A	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	0/5/27/28	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
26	PSU	A	746	26	-	0/7/25/26	0/2/2/2
26	5MU	A	747	26	-	0/3/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
24	H2U	y	19	24	-	0/7/38/39	0/2/2/2
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
24	5MU	y	54	24	-	0/3/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	746	PSU	C5-C1'	-5.28	1.47	1.52
26	A	2457	PSU	C5-C1'	-4.34	1.48	1.52
26	A	2580	PSU	C5-C1'	-4.25	1.48	1.52
26	A	2605	PSU	C5-C1'	-4.25	1.48	1.52
24	y	55	PSU	C5-C1'	-3.64	1.49	1.52

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	37	6IA	N3-C2-N1	-8.03	122.56	128.87
26	A	747	5MU	C5-C4-N3	-7.87	118.74	125.35
24	y	19	H2U	C4-N3-C2	-7.87	118.63	125.77
1	a	1519	MA6	N3-C2-N1	-7.76	122.78	128.87
1	a	1518	MA6	N3-C2-N1	-7.49	122.99	128.87

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
26	A	2069	G7M	C4'
26	A	2069	G7M	C3'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	1915	3TD	O4'-C1'-C5-C4

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1915	3TD	1	0
26	A	1939	5MU	1	0
26	A	1962	5MC	1	0
26	A	2030	6MZ	1	0
26	A	2457	PSU	1	0
26	A	2504	PSU	1	0
26	A	2604	PSU	1	0
26	A	745	1MG	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	FME	v	101	22	8,9,10	0.94	0	5,9,11	1.16	0
60	SEC	y	701	24	1,5,6	0.71	0	1,5,7	1.58	0
61	GNP	z	701	62	29,34,34	2.64	7 (24%)	28,54,54	1.42	6 (21%)

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	FME	v	101	22	-	1/6/9/11	0/0/0/0
60	SEC	y	701	24	-	0/0/4/6	0/0/0/0
61	GNP	z	701	62	-	0/16/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	C4-N9	-10.50	1.33	1.47
61	z	701	GNP	C8-N9	-3.95	1.34	1.47
61	z	701	GNP	C5-C6	-3.34	1.47	1.53
61	z	701	GNP	C2-N1	-2.29	1.34	1.44
61	z	701	GNP	C1'-N9	3.10	1.48	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
61	z	701	GNP	O3G-PG-O1G	-2.75	106.34	113.58
61	z	701	GNP	C2'-C1'-N9	-2.13	107.72	113.44
61	z	701	GNP	PA-O3A-PB	-2.11	125.07	132.71
61	z	701	GNP	C3'-C2'-C1'	2.05	105.56	101.44
61	z	701	GNP	C4-C5-N7	3.44	108.04	102.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	101	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.