wwPDB EM Validation Summary Report (i)

Feb 19, 2025 – 12:31 pm GMT

PDB ID	:	8P7Y
EMDB ID	:	EMD-17135
Title	:	Mycoplasma pneumoniae 70S ribosome with second S4 protein on large subunit
Authors	:	Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on	:	2023-05-31
Resolution	:	3.70 Å(reported)
Based on initial models	:	7OOD, 7OOC

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

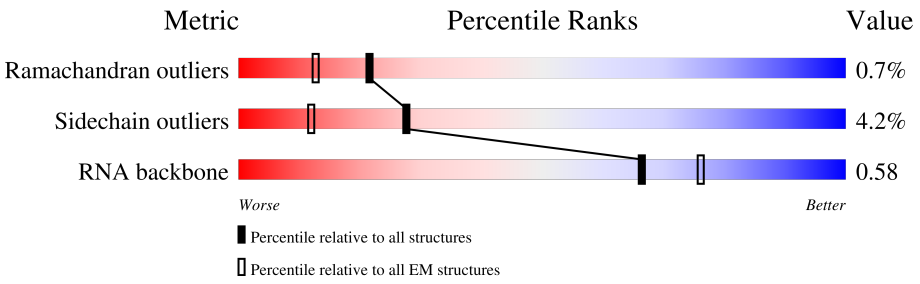
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	0	48	98% .
2	1	59	95% 5%
3	2	37	97% .
4	3	2907	81% 18%
5	4	108	73% 27%
6	5	1520	82% 17% .
7	6	76	57% 39% .
8	7	75	71% 28% .
9	8	76	70% 29% .

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Mol	Chain	Length	Quality of chain
10	A	294	85% 5% 10%
11	B	273	80% • 15%
12	C	205	94% 5%
12	U	205	88% 11%
13	D	219	70% 29%
14	E	215	80% 6% 14%
15	F	155	95% 5% •
16	G	142	89% 10% ••
17	H	132	92% 5% •
18	I	108	91% 5% • •
19	J	121	88% 6% 6%
20	K	139	93% • •
21	L	124	90% 7% ••
22	M	61	95% • •
23	N	86	94% 5% •
24	O	94	86% 6% 7%
25	P	85	94% 6%
26	Q	104	65% •• 32%
27	R	87	94% 5% •
28	S	87	86% 5% 9%
29	T	60	90% 7% ••
30	X	444	6% • 93%
31	Y	21	33% 67%
32	Z	36	100%
33	a	287	98% ••

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Mol	Chain	Length	Quality of chain
34	b	287	76% 5% 20%
35	c	212	94% 6%
36	d	180	95%
37	e	184	91%
38	f	149	95%
39	g	161	75% 22%
40	h	137	93% 7%
41	i	146	95%
42	j	122	97%
43	k	151	98%
44	l	139	94%
45	m	124	90% 6%
46	n	116	94% 6%
47	o	119	96%
48	p	127	91% 7%
49	q	100	91% 8%
50	r	159	86% 11%
51	s	237	39% 60%
52	t	111	95% 5%
53	u	104	82% 15%
54	v	65	92% 6%
55	w	111	95% 5%
56	x	97	91% 8%
57	y	57	88% 11%
58	z	53	92% 6%

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 153255 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	48	392	242	85	63	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	477	300	99	77	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	37	304	189	65	46	4	0	0

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	2893	61995	27704	11293	20105	2893	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	108	2305	1030	415	752	108	0	0

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	1507	32258	14420	5847	10484	1507	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	6	76	1620	723	287	534	76	0	0

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	75	1599	712	279	533	75	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	8	76	1615	722	284	533	76	0	0

- Molecule 10 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	266	2138	1359	376	394	9	0	0

- Molecule 11 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	232	1835	1158	343	329	5	0	0

- Molecule 12 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	204	1669	1057	316	292	4	0	0
12	U	204	1669	1057	316	292	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	155	1191	753	228	207	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	184	1509	950	270	287	2	0	0

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	155	1254	790	240	217	7	0	0

- Molecule 16 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	141	1110	723	193	192	2	0	0

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	129	1040	661	195	183	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	I	104	832	536	147	148	1	0	0

- Molecule 19 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	114	829	514	153	156	6	0	0

- Molecule 20 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	K	135	1071	677	212	180	2	0	0

- Molecule 21 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	L	123	991	618	200	173	0	0

- Molecule 22 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	M	60	474	302	96	72	4	0	0

- Molecule 23 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	N	85	689	436	130	123	0	0

- Molecule 24 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	O	87	705	453	130	118	4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	P	85	693	436	138	118	1	0	0

- Molecule 26 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Q	71	590	378	115	93	4	0	0

- Molecule 27 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	86	700	444	132	122	2	0	0

- Molecule 28 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	S	79	643	391	138	114	0	0

- Molecule 29 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	T	59	519	326	111	80	2	0	0

- Molecule 30 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	30	242	155	43	43	1	0	0

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	Y	21	446	200	80	145	21	0	0

- Molecule 32 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	Z	36	187	112	37	38	0	0

- Molecule 33 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	a	285	2225	1385	437	397	6	0	0

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	b	230	1769	1124	319	319	7	0	0

- Molecule 35 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	c	211	1654	1053	299	299	3	0	0

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	179	1416	910	251	251	4	0	0

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	e	176	1396	899	247	250	0	0

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	149	1210	780	212	215	3	0	0

- Molecule 39 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	125	951	606	165	177	3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	128	959	616	160	177	6	0	0

- Molecule 41 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	144	1164	737	213	209	5	0	0

- Molecule 42 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	122	944	595	178	167	4	0	0

- Molecule 43 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	150	1170	741	228	200	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	136	1079	694	196	182	7	0	0

- Molecule 45 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	119	958	609	175	171	3	0	0

- Molecule 46 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	116	918	573	181	162	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	118	966	609	186	170	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	118	981	624	194	161	2	0	0

- Molecule 49 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	q	99	811	525	148	134	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	142	1091	677	212	195	7	0	0

- Molecule 51 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	95	740	486	125	128	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	t	111	871	550	166	152	3	0	0

- Molecule 53 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	u	88	670	416	132	121	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	v	64	520	320	109	90	1	0	0

- Molecule 55 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	w	110	906	576	168	162	0	0

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	96	761	481	133	143	4	0	0

- Molecule 57 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	56	452	274	98	75	5	0	0

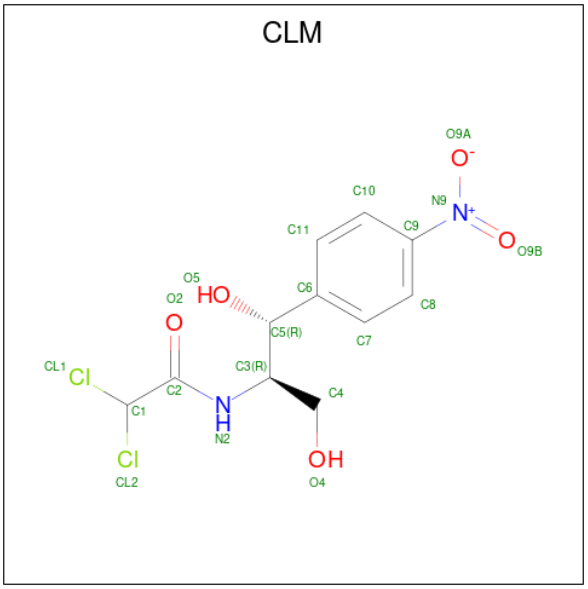
- Molecule 58 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	z	50	408	255	81	68	4	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	2	1	1	1	0
59	M	1	1	1	0
59	Q	1	1	1	0
59	x	1	1	1	0
59	y	1	1	1	0
59	z	1	1	1	0

- Molecule 60 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
60	3	1	20	11	2	2	5	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
61	3	1	1	1	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	3	221	221	221	0
62	4	1	1	1	0
62	5	90	90	90	0
62	6	1	1	1	0
62	7	2	2	2	0
62	8	2	2	2	0

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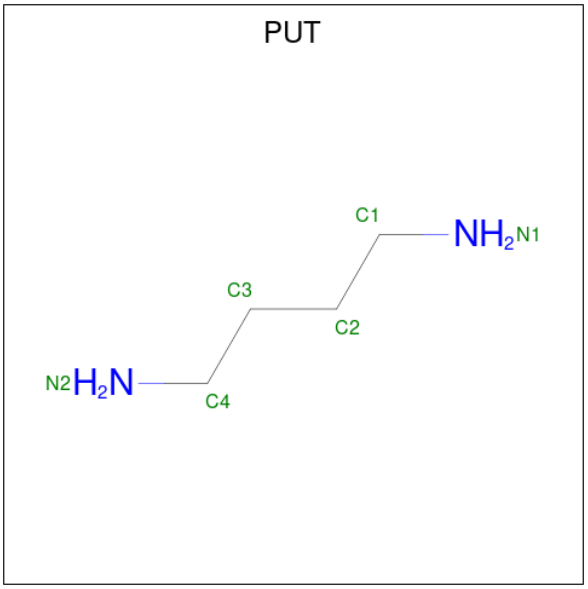
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	K	1	1	1	0
62	P	1	1	1	0
62	Y	2	2	2	0
62	b	2	2	2	0
62	i	1	1	1	0
62	y	2	2	2	0

- Molecule 63 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	3	1	6	4	2	0
63	3	1	6	4	2	0
63	3	1	6	4	2	0
63	3	1	6	4	2	0
63	3	1	6	4	2	0

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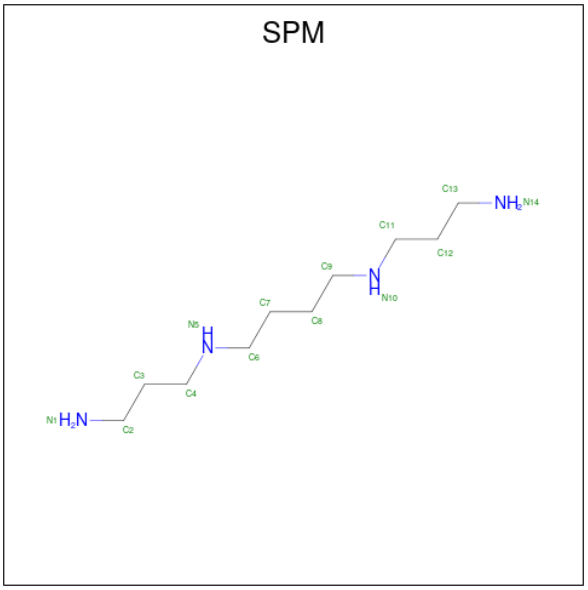
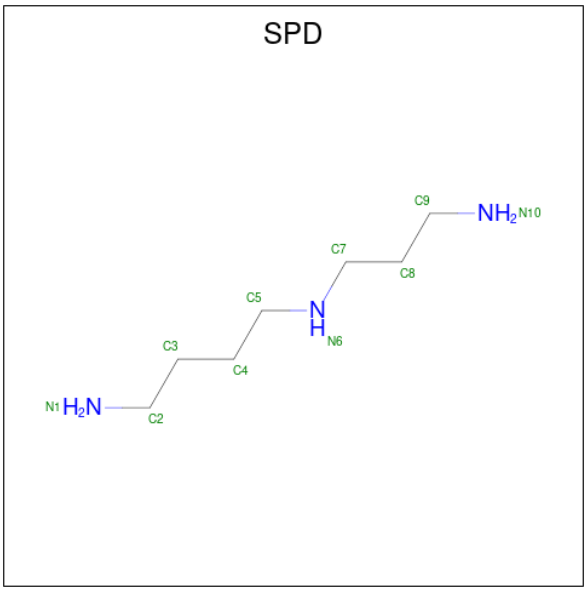
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	3	1	6	4	2	0
			Total	C	N	
63	3	1	6	4	2	0
			Total	C	N	
63	5	1	6	4	2	0

- Molecule 64 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
64	3	1	14	10	4	0
			Total	C	N	
64	3	1	14	10	4	0
			Total	C	N	
64	3	1	14	10	4	0
			Total	C	N	
64	b	1	14	10	4	0

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		
65	3	1	Total	C	N		0
			10	7	3		

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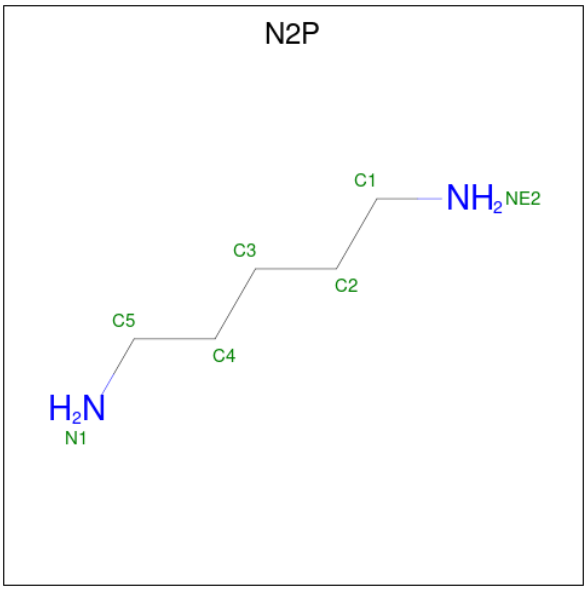
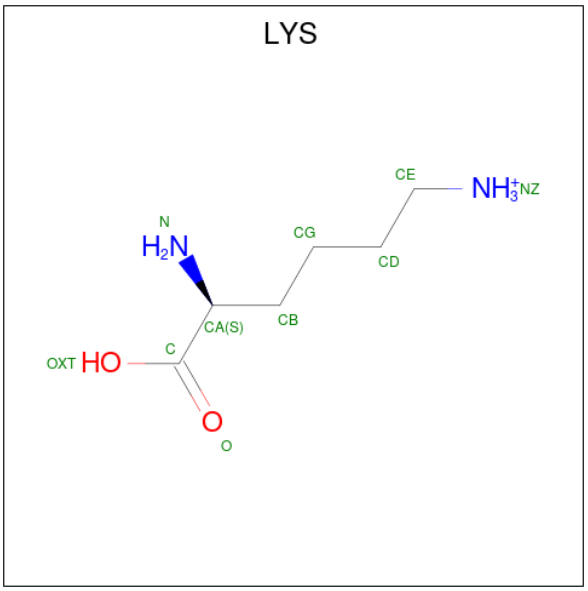
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
65	3	1	10	7	3	0
65	3	1	10	7	3	0
65	5	1	10	7	3	0
65	5	1	10	7	3	0

- Molecule 66 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
66	3	1	7	5	2	0
66	3	1	7	5	2	0
66	3	1	7	5	2	0
66	5	1	7	5	2	0

- Molecule 67 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



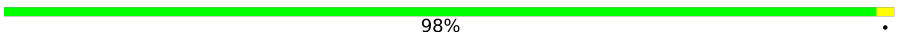
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	8	1	9	6	2	1	0

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.

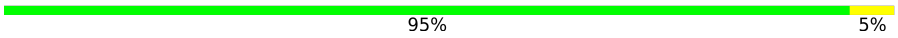
- Molecule 1: 50S ribosomal protein L34

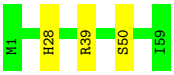
Chain 0:



- Molecule 2: 50S ribosomal protein L35

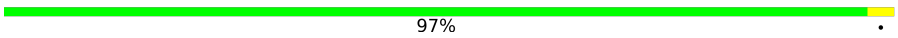
Chain 1:





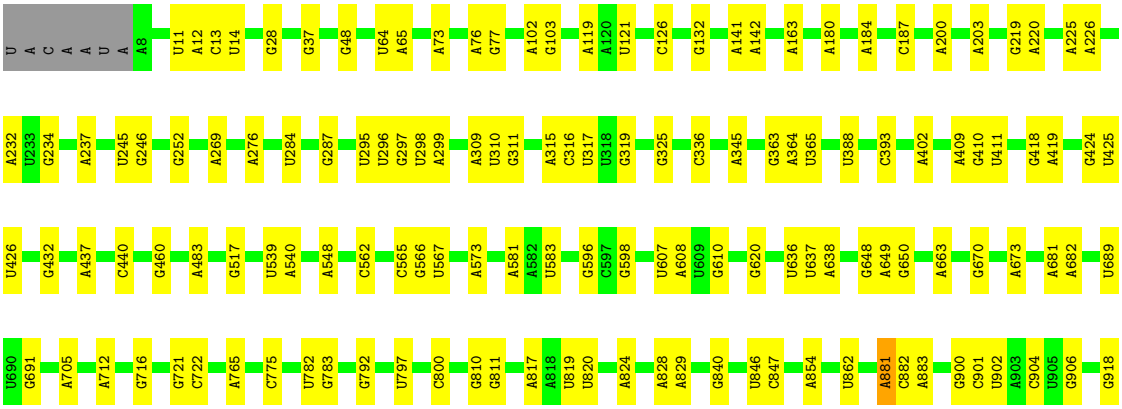
- Molecule 3: 50S ribosomal protein L36

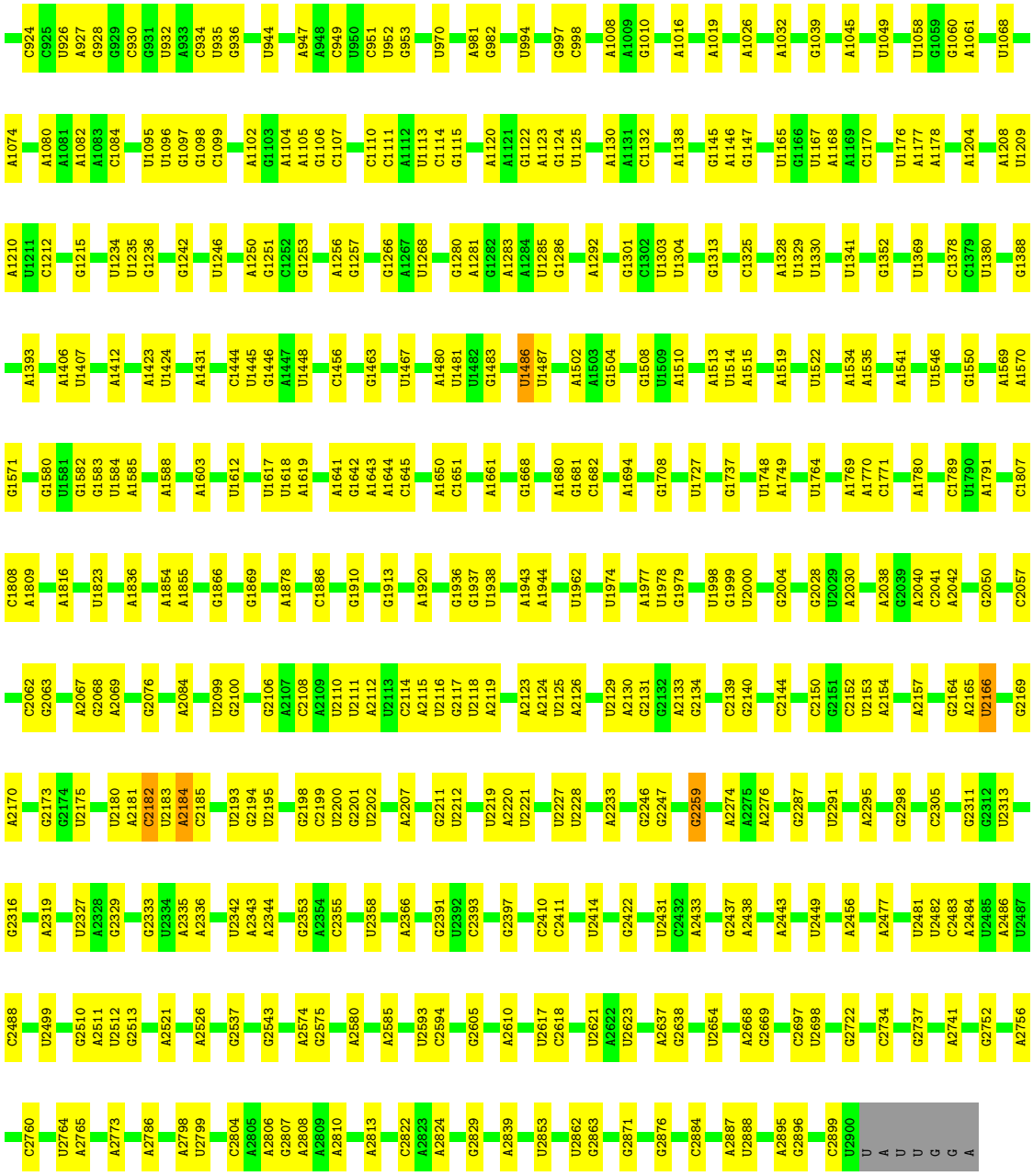
Chain 2:



- Molecule 4: 23S ribosomal RNA

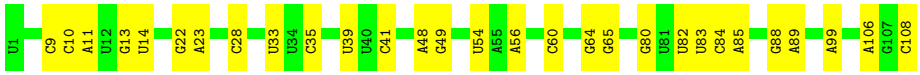
Chain 3:





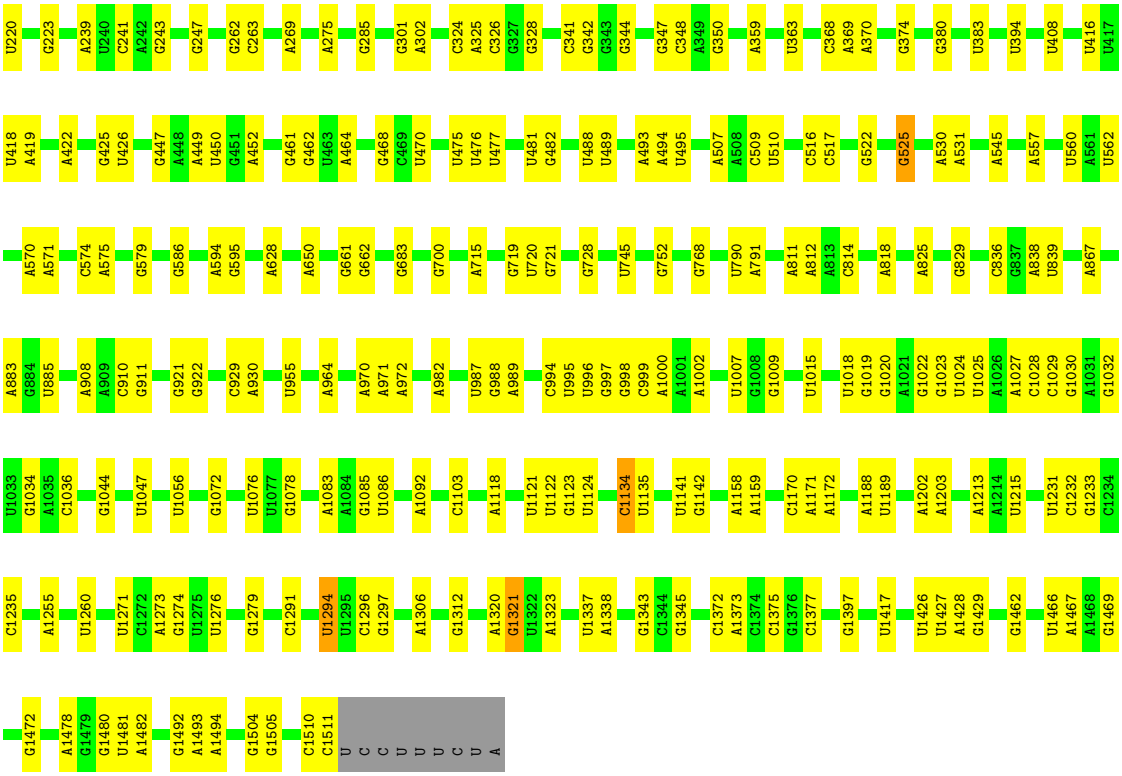
- Molecule 5: 5S ribosomal RNA

Chain 4:



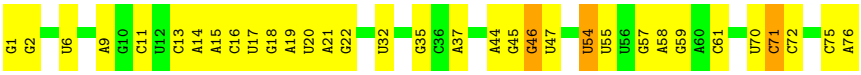
- Molecule 6: 16S ribosomal RNA

Chain 5:



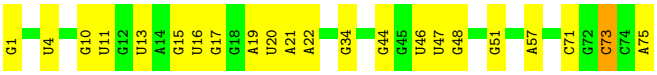
- Molecule 7: tRNA-Ala (E-site)

Chain 6: 57% 39% •



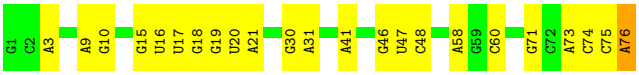
- Molecule 8: tRNA-Asp (P-site)

Chain 7: 71% 28% •



- Molecule 9: tRNA-Lys (A-site)

Chain 8: 70% 29% •

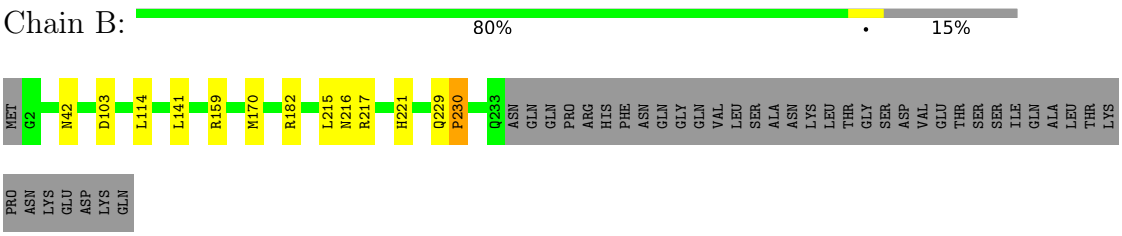


- Molecule 10: 30S ribosomal protein S2

Chain A: 85% 5% 10%

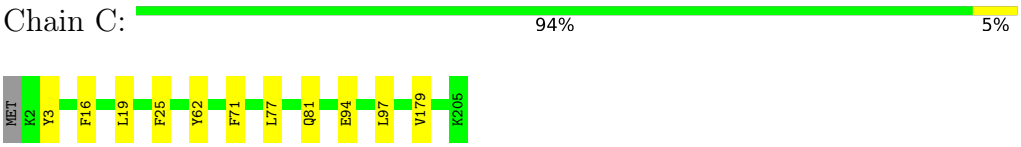
- Molecule 11: 30S ribosomal protein S3

Chain B:



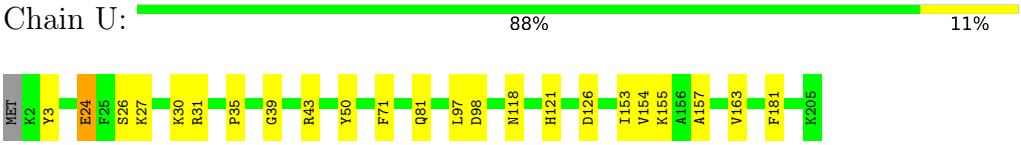
- Molecule 12: 30S ribosomal protein S4

Chain C:



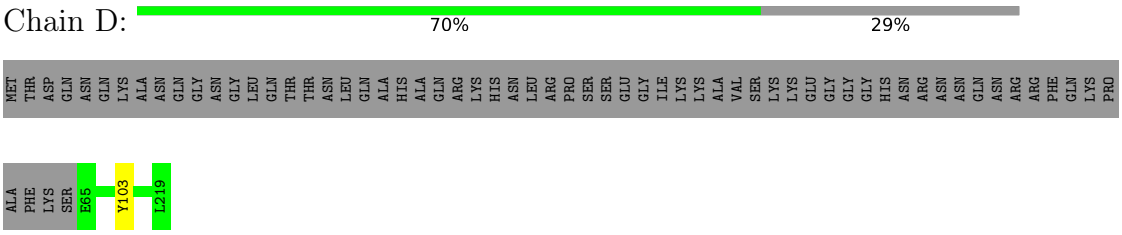
- Molecule 12: 30S ribosomal protein S4

Chain U:



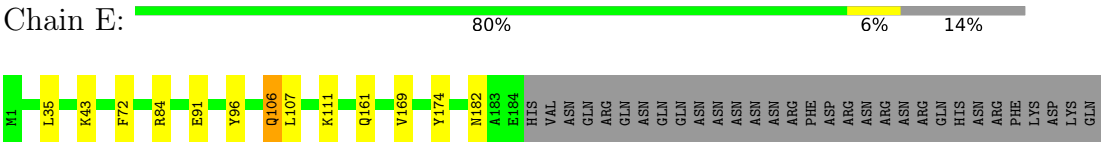
- Molecule 13: 30S ribosomal protein S5

Chain D:



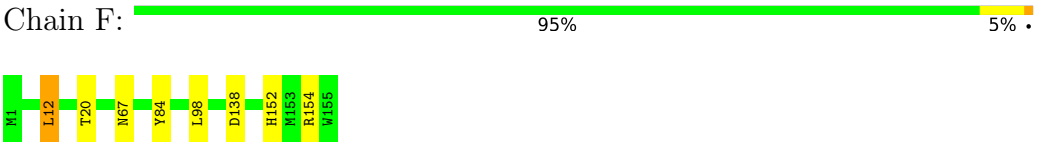
- Molecule 14: 30S ribosomal protein S6

Chain E:



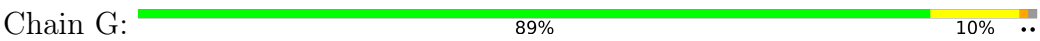
- Molecule 15: 30S ribosomal protein S7

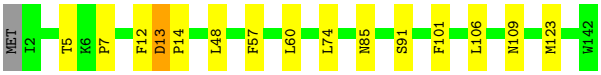
Chain F:



- Molecule 16: 30S ribosomal protein S8

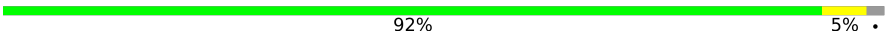
Chain G:





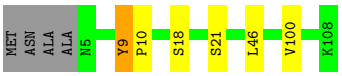
• Molecule 17: 30S ribosomal protein S9

Chain H:



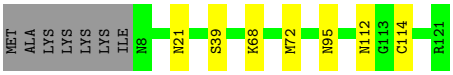
• Molecule 18: 30S ribosomal protein S10

Chain I:



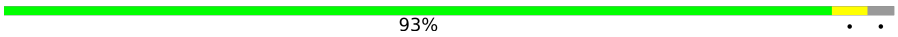
• Molecule 19: 30S ribosomal protein S11

Chain J:



• Molecule 20: 30S ribosomal protein S12

Chain K:

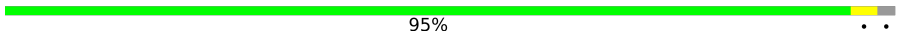


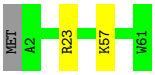
• Molecule 21: 30S ribosomal protein S13

Chain L:

• Molecule 22: 30S ribosomal protein S14 type Z

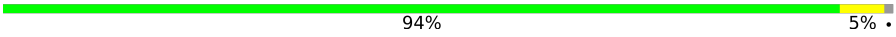
Chain M:

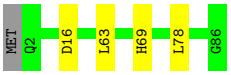




• Molecule 23: 30S ribosomal protein S15

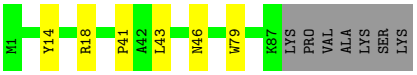
Chain N:





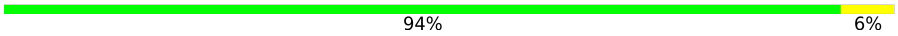
• Molecule 24: 30S ribosomal protein S16

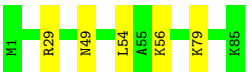
Chain O:



• Molecule 25: 30S ribosomal protein S17

Chain P:



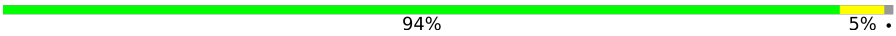


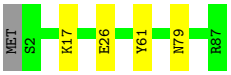
• Molecule 26: 30S ribosomal protein S18

Chain Q:

• Molecule 27: 30S ribosomal protein S19

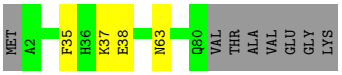
Chain R:





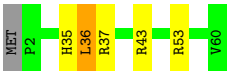
• Molecule 28: 30S ribosomal protein S20

Chain S:



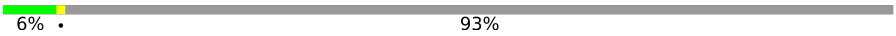
• Molecule 29: 30S ribosomal protein S21

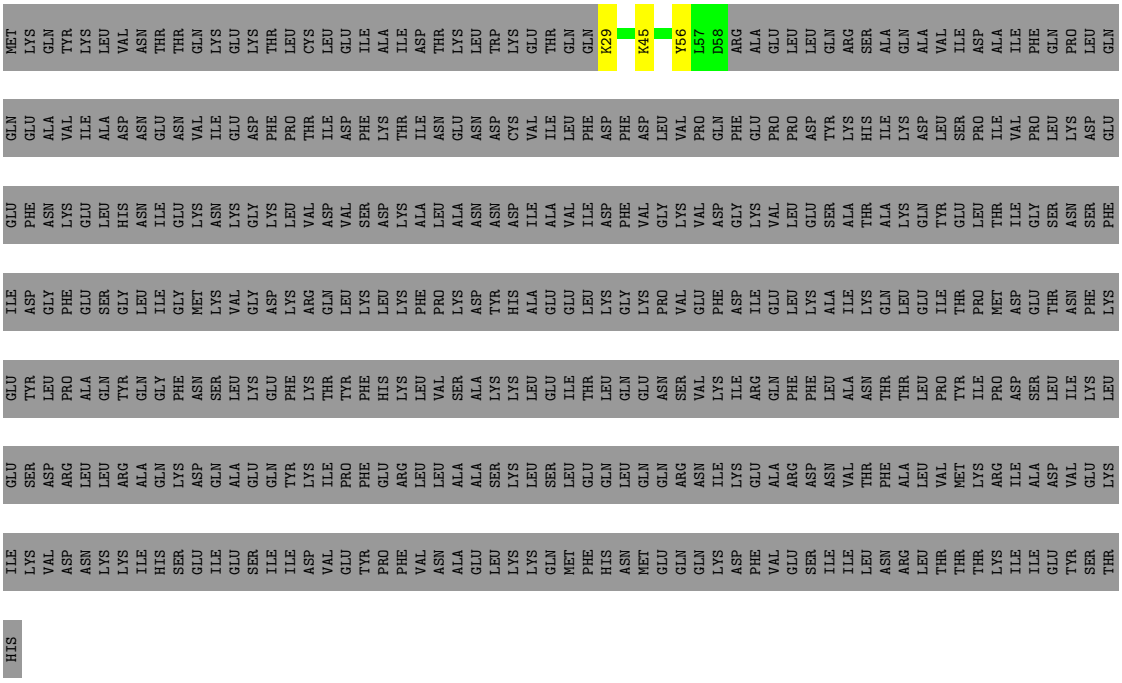
Chain T:



• Molecule 30: Trigger factor

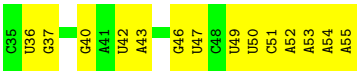
Chain X:





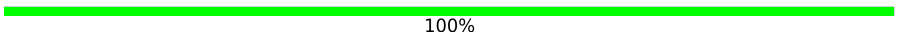
- Molecule 31: mRNA

Chain Y:



- Molecule 32: Nascent chain

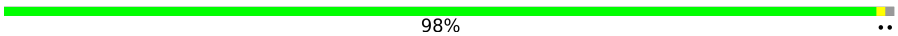
Chain Z:



There are no outlier residues recorded for this chain.

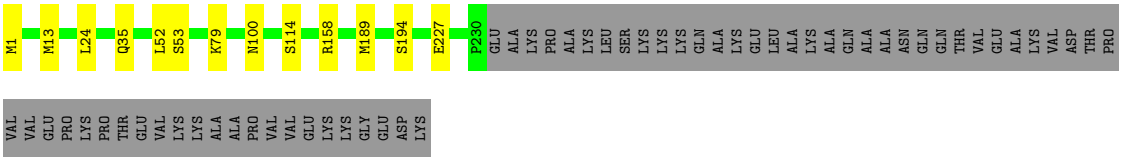
- Molecule 33: 50S ribosomal protein L2

Chain a:



- Molecule 34: 50S ribosomal protein L3

Chain b:

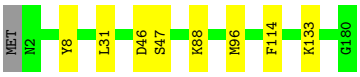


- Molecule 35: 50S ribosomal protein L4

Chain c: 94% 6%

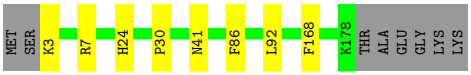
• Molecule 36: 50S ribosomal protein L5

Chain d: 95%



• Molecule 37: 50S ribosomal protein L6

Chain e: 91%

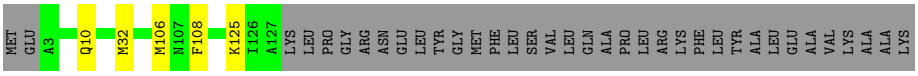


• Molecule 38: 50S ribosomal protein L9

Chain f: 95%

• Molecule 39: 50S ribosomal protein L10

Chain g: 75% 22%

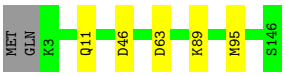


• Molecule 40: 50S ribosomal protein L11

Chain h: 93% 7%

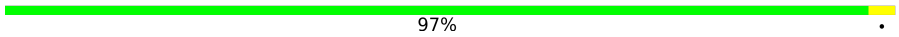
• Molecule 41: 50S ribosomal protein L13

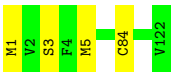
Chain i: 95%



• Molecule 42: 50S ribosomal protein L14

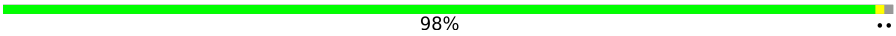
Chain j:





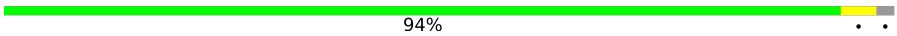
• Molecule 43: 50S ribosomal protein L15

Chain k:



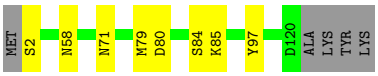
• Molecule 44: 50S ribosomal protein L16

Chain l:



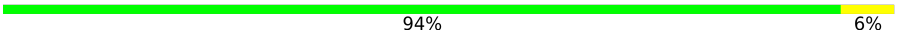
• Molecule 45: 50S ribosomal protein L17

Chain m:



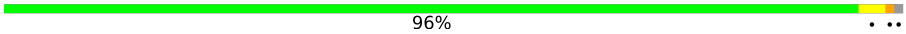
• Molecule 46: 50S ribosomal protein L18

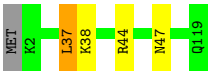
Chain n:



• Molecule 47: 50S ribosomal protein L19

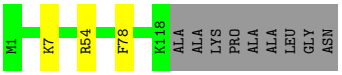
Chain o:





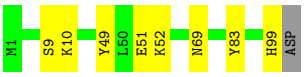
• Molecule 48: 50S ribosomal protein L20

Chain p:



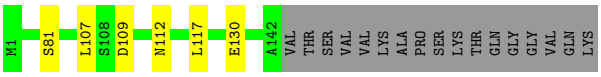
• Molecule 49: 50S ribosomal protein L21

Chain q: 91% 8%



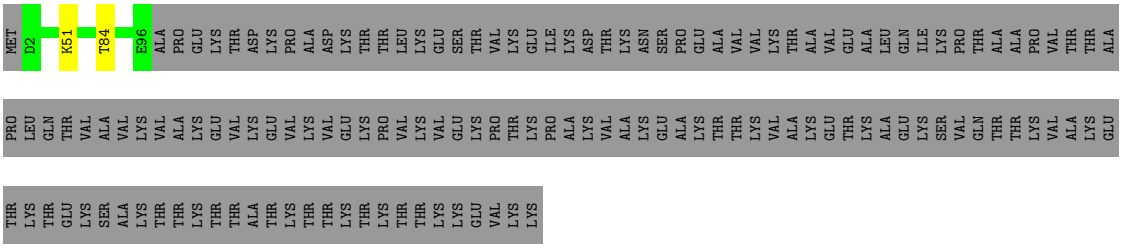
• Molecule 50: 50S ribosomal protein L22

Chain r: 86% 11%



• Molecule 51: 50S ribosomal protein L23

Chain s: 39% 60%

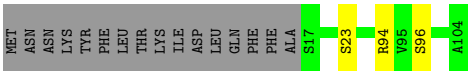


• Molecule 52: 50S ribosomal protein L24

Chain t: 95% 5%

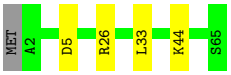
• Molecule 53: 50S ribosomal protein L27

Chain u: 82% 15%



• Molecule 54: 50S ribosomal protein L28

Chain v: 92% 6%

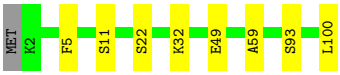


• Molecule 55: 50S ribosomal protein L29

Chain w: 95% 5%

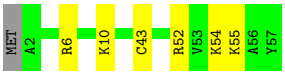
• Molecule 56: 50S ribosomal protein L31

Chain x:



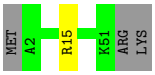
• Molecule 57: 50S ribosomal protein L32

Chain y:



• Molecule 58: 50S ribosomal protein L33 1

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	10154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, B8T, 1MG, SPM, 5MC, PUT, SPD, MA6, ZN, 2MA, N2P, 7MG, CLM, MG, 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	0.29	0/395	0.69	0/518
2	1	0.27	0/484	0.60	0/637
3	2	0.26	0/306	0.65	0/401
4	3	0.17	0/69363	0.71	19/108161 (0.0%)
5	4	0.16	0/2578	0.72	0/4016
6	5	0.16	0/35992	0.71	8/56111 (0.0%)
7	6	0.40	1/1810 (0.1%)	0.91	5/2817 (0.2%)
8	7	0.30	1/1785 (0.1%)	0.81	1/2779 (0.0%)
9	8	0.49	3/1804 (0.2%)	1.04	8/2807 (0.3%)
10	A	0.34	0/2172	0.75	5/2934 (0.2%)
11	B	0.31	0/1863	0.76	4/2516 (0.2%)
12	C	0.32	0/1700	0.70	1/2278 (0.0%)
12	U	0.40	1/1700 (0.1%)	0.85	1/2278 (0.0%)
13	D	0.31	0/1206	0.68	0/1616
14	E	0.35	0/1536	0.77	4/2072 (0.2%)
15	F	0.31	0/1274	0.76	2/1710 (0.1%)
16	G	0.36	0/1126	0.94	12/1517 (0.8%)
17	H	0.37	0/1056	0.76	2/1409 (0.1%)
18	I	0.30	0/843	0.76	3/1132 (0.3%)
19	J	0.35	0/844	0.70	0/1136
20	K	0.30	0/1089	0.70	0/1461
21	L	0.31	0/1002	0.87	4/1340 (0.3%)
22	M	0.36	0/483	0.75	1/643 (0.2%)
23	N	0.25	0/695	0.71	2/926 (0.2%)
24	O	0.34	0/718	0.81	2/962 (0.2%)
25	P	0.28	0/702	0.69	0/934
26	Q	0.42	0/601	0.95	2/801 (0.2%)
27	R	0.35	0/716	0.68	0/958
28	S	0.32	0/645	0.71	0/857
29	T	0.46	0/524	0.85	1/685 (0.1%)
30	X	0.28	0/245	0.64	0/325
31	Y	0.28	0/498	0.88	0/773

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.75	0/26	1.33	0/33
33	a	0.29	0/2267	0.65	1/3044 (0.0%)
34	b	0.29	0/1803	0.59	1/2424 (0.0%)
35	c	0.29	0/1681	0.58	1/2257 (0.0%)
36	d	0.30	0/1437	0.67	0/1931
37	e	0.30	0/1420	0.64	2/1912 (0.1%)
38	f	0.32	0/1233	0.64	0/1653
39	g	0.27	0/960	0.64	0/1284
40	h	0.28	0/968	0.66	3/1298 (0.2%)
41	i	0.31	0/1186	0.70	2/1592 (0.1%)
42	j	0.33	0/953	0.73	1/1275 (0.1%)
43	k	0.31	0/1187	0.64	0/1581
44	l	0.39	0/1104	0.73	1/1481 (0.1%)
45	m	0.28	0/973	0.65	1/1309 (0.1%)
46	n	0.30	0/927	0.74	0/1239
47	o	0.29	0/976	0.68	1/1296 (0.1%)
48	p	0.27	0/996	0.63	0/1325
49	q	0.29	0/828	0.64	0/1111
50	r	0.32	0/1100	0.69	2/1471 (0.1%)
51	s	0.29	0/752	0.61	0/1015
52	t	0.29	0/878	0.70	3/1165 (0.3%)
53	u	0.29	0/678	0.64	0/902
54	v	0.39	0/526	0.82	2/703 (0.3%)
55	w	0.26	0/916	0.60	1/1222 (0.1%)
56	x	0.28	0/776	0.67	1/1033 (0.1%)
57	y	0.26	0/457	0.70	0/601
58	z	0.32	0/412	0.63	0/547
All	All	0.23	6/165175 (0.0%)	0.72	110/246214 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	U	0	2
22	M	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	76	A	C6-N6	15.02	1.46	1.33
8	7	1	G	OP3-P	-7.62	1.52	1.61
7	6	1	G	OP3-P	-7.59	1.52	1.61
9	8	76	A	N7-C5	-6.67	1.35	1.39
9	8	76	A	N9-C8	-6.22	1.32	1.37

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	8	76	A	C2-N3-C4	22.02	121.61	110.60
9	8	76	A	N1-C2-N3	-15.22	121.69	129.30
9	8	76	A	N3-C4-C5	-12.67	117.93	126.80
10	A	173	PRO	CA-N-CD	-11.43	95.50	111.50
4	3	2166	U	O5'-P-OP1	-10.79	95.99	105.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	M	23	ARG	Sidechain
12	U	121	HIS	Peptide
12	U	153	ILE	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 (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	
1	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	A	262/294 (89%)	236 (90%)	24 (9%)	2 (1%)	16	49
11	B	230/273 (84%)	203 (88%)	23 (10%)	4 (2%)	7	36
12	C	202/205 (98%)	167 (83%)	33 (16%)	2 (1%)	13	44
12	U	202/205 (98%)	147 (73%)	39 (19%)	16 (8%)	1	10
13	D	153/219 (70%)	143 (94%)	10 (6%)	0	100	100
14	E	182/215 (85%)	156 (86%)	25 (14%)	1 (0%)	25	57
15	F	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	10	40
16	G	139/142 (98%)	133 (96%)	6 (4%)	0	100	100
17	H	127/132 (96%)	113 (89%)	14 (11%)	0	100	100
18	I	102/108 (94%)	89 (87%)	12 (12%)	1 (1%)	13	44
19	J	112/121 (93%)	106 (95%)	5 (4%)	1 (1%)	14	47
20	K	133/139 (96%)	116 (87%)	14 (10%)	3 (2%)	5	31
21	L	121/124 (98%)	109 (90%)	10 (8%)	2 (2%)	7	36
22	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
23	N	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
24	O	85/94 (90%)	79 (93%)	6 (7%)	0	100	100
25	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	11	41
26	Q	69/104 (66%)	64 (93%)	5 (7%)	0	100	100
27	R	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
28	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	10	40
29	T	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	X	28/444 (6%)	25 (89%)	3 (11%)	0	100	100
32	Z	3/36 (8%)	3 (100%)	0	0	100	100
33	a	283/287 (99%)	269 (95%)	13 (5%)	1 (0%)	30	62
34	b	228/287 (79%)	219 (96%)	9 (4%)	0	100	100
35	c	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
36	d	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
37	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
38	f	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	9	39
39	g	123/161 (76%)	119 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
41	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
42	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
43	k	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
44	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
45	m	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
46	n	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
47	o	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
48	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
49	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
50	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
51	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
52	t	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
53	u	86/104 (83%)	83 (96%)	3 (4%)	0	100	100
54	v	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	w	108/111 (97%)	104 (96%)	4 (4%)	0	100	100
56	x	94/97 (97%)	70 (74%)	22 (23%)	2 (2%)	5	33
57	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
58	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6248/7355 (85%)	5762 (92%)	445 (7%)	41 (1%)	21	51

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	B	229	GLN
11	B	230	PRO
20	K	56	LYS
25	P	54	LEU
12	U	39	GLY

5.3.2 Protein sidechains (i)

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	41/41 (100%)	40 (98%)	1 (2%)	44	63
2	1	51/51 (100%)	48 (94%)	3 (6%)	16	44
3	2	35/35 (100%)	34 (97%)	1 (3%)	37	59
10	A	238/262 (91%)	229 (96%)	9 (4%)	28	53
11	B	195/232 (84%)	189 (97%)	6 (3%)	35	57
12	C	182/183 (100%)	174 (96%)	8 (4%)	24	50
12	U	182/183 (100%)	177 (97%)	5 (3%)	40	61
13	D	125/178 (70%)	124 (99%)	1 (1%)	79	85
14	E	165/196 (84%)	155 (94%)	10 (6%)	15	43
15	F	132/132 (100%)	127 (96%)	5 (4%)	28	53
16	G	123/124 (99%)	115 (94%)	8 (6%)	14	41
17	H	112/115 (97%)	107 (96%)	5 (4%)	23	50
18	I	97/99 (98%)	94 (97%)	3 (3%)	35	57
19	J	91/97 (94%)	85 (93%)	6 (7%)	14	41
20	K	117/120 (98%)	114 (97%)	3 (3%)	41	61
21	L	104/105 (99%)	97 (93%)	7 (7%)	13	40
22	M	47/48 (98%)	47 (100%)	0	100	100
23	N	77/78 (99%)	75 (97%)	2 (3%)	41	61
24	O	76/82 (93%)	72 (95%)	4 (5%)	19	46
25	P	75/75 (100%)	71 (95%)	4 (5%)	19	46
26	Q	62/94 (66%)	60 (97%)	2 (3%)	34	57
27	R	76/77 (99%)	72 (95%)	4 (5%)	19	46
28	S	71/77 (92%)	68 (96%)	3 (4%)	25	51
29	T	55/56 (98%)	50 (91%)	5 (9%)	7	30
30	X	27/406 (7%)	24 (89%)	3 (11%)	5	24
32	Z	2/2 (100%)	2 (100%)	0	100	100
33	a	241/243 (99%)	238 (99%)	3 (1%)	67	79
34	b	187/233 (80%)	175 (94%)	12 (6%)	14	42
35	c	183/184 (100%)	172 (94%)	11 (6%)	16	43
36	d	153/154 (99%)	145 (95%)	8 (5%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	e	153/159 (96%)	147 (96%)	6 (4%)	27	53
38	f	134/134 (100%)	128 (96%)	6 (4%)	23	50
39	g	100/129 (78%)	95 (95%)	5 (5%)	20	47
40	h	102/110 (93%)	102 (100%)	0	100	100
41	i	126/128 (98%)	123 (98%)	3 (2%)	44	63
42	j	103/103 (100%)	100 (97%)	3 (3%)	37	59
43	k	125/126 (99%)	123 (98%)	2 (2%)	58	74
44	l	113/115 (98%)	108 (96%)	5 (4%)	24	50
45	m	105/109 (96%)	98 (93%)	7 (7%)	13	40
46	n	99/99 (100%)	92 (93%)	7 (7%)	12	39
47	o	104/105 (99%)	100 (96%)	4 (4%)	28	53
48	p	104/108 (96%)	101 (97%)	3 (3%)	37	59
49	q	90/91 (99%)	82 (91%)	8 (9%)	8	31
50	r	118/132 (89%)	114 (97%)	4 (3%)	32	56
51	s	84/208 (40%)	82 (98%)	2 (2%)	44	63
52	t	96/96 (100%)	93 (97%)	3 (3%)	35	57
53	u	70/85 (82%)	67 (96%)	3 (4%)	25	50
54	v	59/60 (98%)	57 (97%)	2 (3%)	32	56
55	w	97/98 (99%)	93 (96%)	4 (4%)	26	52
56	x	85/86 (99%)	80 (94%)	5 (6%)	16	44
57	y	48/49 (98%)	42 (88%)	6 (12%)	3	19
58	z	47/50 (94%)	46 (98%)	1 (2%)	48	67
All	All	5484/6342 (86%)	5253 (96%)	231 (4%)	27	51

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	b	53	SER
56	x	22	SER
37	e	7	ARG
56	x	5	PHE
49	q	83	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
12	U	171	ASN
53	u	43	GLN
35	c	76	GLN
41	i	80	HIS
34	b	225	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	Y	20/21 (95%)	14 (70%)	4 (20%)
4	3	2891/2907 (99%)	520 (17%)	21 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1503/1520 (98%)	253 (16%)	7 (0%)
7	6	75/76 (98%)	29 (38%)	6 (8%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	4745/4783 (99%)	888 (18%)	40 (0%)

5 of 888 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	6	17	U
8	7	46	U
7	6	18	G
7	6	58	A
31	Y	49	U

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

8 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	$\#\|Z\| > 2$
6	B8T	5	1377	6	19,22,23	3.30	8 (42%)	26,31,34	0.83	1 (3%)
6	5MC	5	1375	6	18,22,23	4.07	7 (38%)	26,32,35	1.02	2 (7%)
6	MA6	5	1493	6	18,26,27	1.07	2 (11%)	19,38,41	3.38	3 (15%)
4	2MA	3	2511	4,62	17,25,26	2.64	5 (29%)	17,37,40	1.32	3 (17%)
4	1MG	3	783	4	18,26,27	2.75	6 (33%)	19,39,42	1.47	3 (15%)
6	MA6	5	1494	6	18,26,27	1.06	2 (11%)	19,38,41	3.39	3 (15%)
4	OMG	3	2259	8,4,62	18,26,27	2.88	8 (44%)	19,38,41	1.60	4 (21%)
6	7MG	5	525	6	22,26,27	3.88	10 (45%)	29,39,42	2.03	9 (31%)

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
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
6	MA6	5	1493	6	-	0/7/29/30	0/3/3/3
4	2MA	3	2511	4,62	-	2/3/25/26	0/3/3/3
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
6	MA6	5	1494	6	-	3/7/29/30	0/3/3/3
4	OMG	3	2259	8,4,62	-	3/5/27/28	0/3/3/3
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C6-C5	10.02	1.51	1.34
6	5	525	7MG	C8-N9	9.81	1.51	1.46
6	5	525	7MG	C5-N7	8.01	1.44	1.35
4	3	2511	2MA	C2-N3	7.90	1.48	1.31
6	5	1375	5MC	C4-N3	7.54	1.46	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N1-C6-N6	-12.26	104.16	117.06
6	5	1493	MA6	N1-C6-N6	-12.20	104.22	117.06
6	5	1493	MA6	C1'-N9-C4	5.62	136.51	126.64
6	5	1494	MA6	C1'-N9-C4	5.54	136.38	126.64
6	5	1494	MA6	N3-C2-N1	-5.53	120.03	128.68

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	525	7MG	O4'-C4'-C5'-O5'
6	5	525	7MG	C3'-C4'-C5'-O5'

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 369 ligands modelled in this entry, 333 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
67	LYS	8	103	9	7,8,9	0.84	0	3,8,10	0.35	0
64	SPM	3	3251	-	13,13,13	0.36	0	12,12,12	0.90	0
65	SPD	3	3235	-	9,9,9	0.32	0	8,8,8	0.87	0
65	SPD	3	3240	-	9,9,9	0.33	0	8,8,8	0.86	0
64	SPM	3	3229	-	13,13,13	0.36	0	12,12,12	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
65	SPD	3	3234	-	9,9,9	0.35	0	8,8,8	0.79	0
65	SPD	3	3252	-	9,9,9	0.18	0	8,8,8	0.19	0
65	SPD	3	3242	-	9,9,9	0.32	0	8,8,8	0.86	0
63	PUT	3	3244	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.87	0
65	SPD	3	3232	-	9,9,9	0.33	0	8,8,8	0.83	0
63	PUT	5	1604	-	5,5,5	0.25	0	4,4,4	0.54	0
66	N2P	3	3246	-	6,6,6	0.25	0	5,5,5	0.65	0
64	SPM	3	3243	-	13,13,13	0.34	0	12,12,12	0.91	0
63	PUT	3	3225	-	5,5,5	0.24	0	4,4,4	0.54	0
66	N2P	3	3249	-	6,6,6	0.25	0	5,5,5	0.65	0
63	PUT	3	3233	-	5,5,5	0.25	0	4,4,4	0.53	0
65	SPD	3	3241	-	9,9,9	0.32	0	8,8,8	0.85	0
66	N2P	3	3245	-	6,6,6	0.25	0	5,5,5	0.65	0
65	SPD	5	1601	-	9,9,9	0.41	0	8,8,8	1.41	2 (25%)
63	PUT	3	3227	-	5,5,5	0.25	0	4,4,4	0.53	0
65	SPD	3	3247	-	9,9,9	0.33	0	8,8,8	0.89	0
64	SPM	b	303	-	13,13,13	0.16	0	12,12,12	0.32	0
65	SPD	3	3250	-	9,9,9	0.33	0	8,8,8	0.86	0
65	SPD	5	1603	-	9,9,9	0.32	0	8,8,8	0.74	0
65	SPD	3	3238	-	9,9,9	0.33	0	8,8,8	0.90	0
60	CLM	3	3001	-	19,20,20	2.06	2 (10%)	23,27,27	0.86	1 (4%)
66	N2P	5	1602	-	6,6,6	0.25	0	5,5,5	0.65	0
65	SPD	3	3231	-	9,9,9	0.32	0	8,8,8	0.90	0
65	SPD	3	3248	-	9,9,9	0.32	0	8,8,8	0.87	0
63	PUT	3	3224	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3237	-	9,9,9	0.33	0	8,8,8	0.87	0
63	PUT	3	3226	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3239	-	9,9,9	0.33	0	8,8,8	0.91	0
65	SPD	3	3236	-	9,9,9	0.32	0	8,8,8	0.78	0
63	PUT	3	3228	-	5,5,5	0.26	0	4,4,4	0.54	0

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
67	LYS	8	103	9	-	3/6/7/9	-
64	SPM	3	3251	-	-	2/11/11/11	-
65	SPD	3	3235	-	-	0/7/7/7	-
65	SPD	3	3240	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	SPM	3	3229	-	-	4/11/11/11	-
65	SPD	3	3234	-	-	1/7/7/7	-
65	SPD	3	3252	-	-	0/7/7/7	-
65	SPD	3	3242	-	-	0/7/7/7	-
63	PUT	3	3244	-	-	0/3/3/3	-
65	SPD	3	3230	-	-	0/7/7/7	-
65	SPD	3	3232	-	-	0/7/7/7	-
63	PUT	5	1604	-	-	0/3/3/3	-
66	N2P	3	3246	-	-	2/4/4/4	-
64	SPM	3	3243	-	-	2/11/11/11	-
63	PUT	3	3225	-	-	0/3/3/3	-
66	N2P	3	3249	-	-	1/4/4/4	-
63	PUT	3	3233	-	-	0/3/3/3	-
65	SPD	3	3241	-	-	2/7/7/7	-
66	N2P	3	3245	-	-	1/4/4/4	-
65	SPD	5	1601	-	-	1/7/7/7	-
63	PUT	3	3227	-	-	1/3/3/3	-
65	SPD	3	3247	-	-	0/7/7/7	-
64	SPM	b	303	-	-	2/11/11/11	-
65	SPD	3	3250	-	-	0/7/7/7	-
65	SPD	5	1603	-	-	1/7/7/7	-
65	SPD	3	3238	-	-	0/7/7/7	-
60	CLM	3	3001	-	-	3/20/22/22	0/1/1/1
66	N2P	5	1602	-	-	3/4/4/4	-
65	SPD	3	3231	-	-	1/7/7/7	-
65	SPD	3	3248	-	-	0/7/7/7	-
63	PUT	3	3224	-	-	0/3/3/3	-
65	SPD	3	3237	-	-	0/7/7/7	-
63	PUT	3	3226	-	-	0/3/3/3	-
65	SPD	3	3239	-	-	1/7/7/7	-
65	SPD	3	3236	-	-	1/7/7/7	-
63	PUT	3	3228	-	-	0/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3	3001	CLM	C2-N2	7.20	1.49	1.34
60	3	3001	CLM	O9B-N9	-2.68	1.18	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	5	1601	SPD	C4-C3-C2	-2.25	97.82	113.77
65	5	1601	SPD	C4-C5-N6	-2.07	106.56	112.14
60	3	3001	CLM	C3-N2-C2	-2.06	119.42	123.07

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

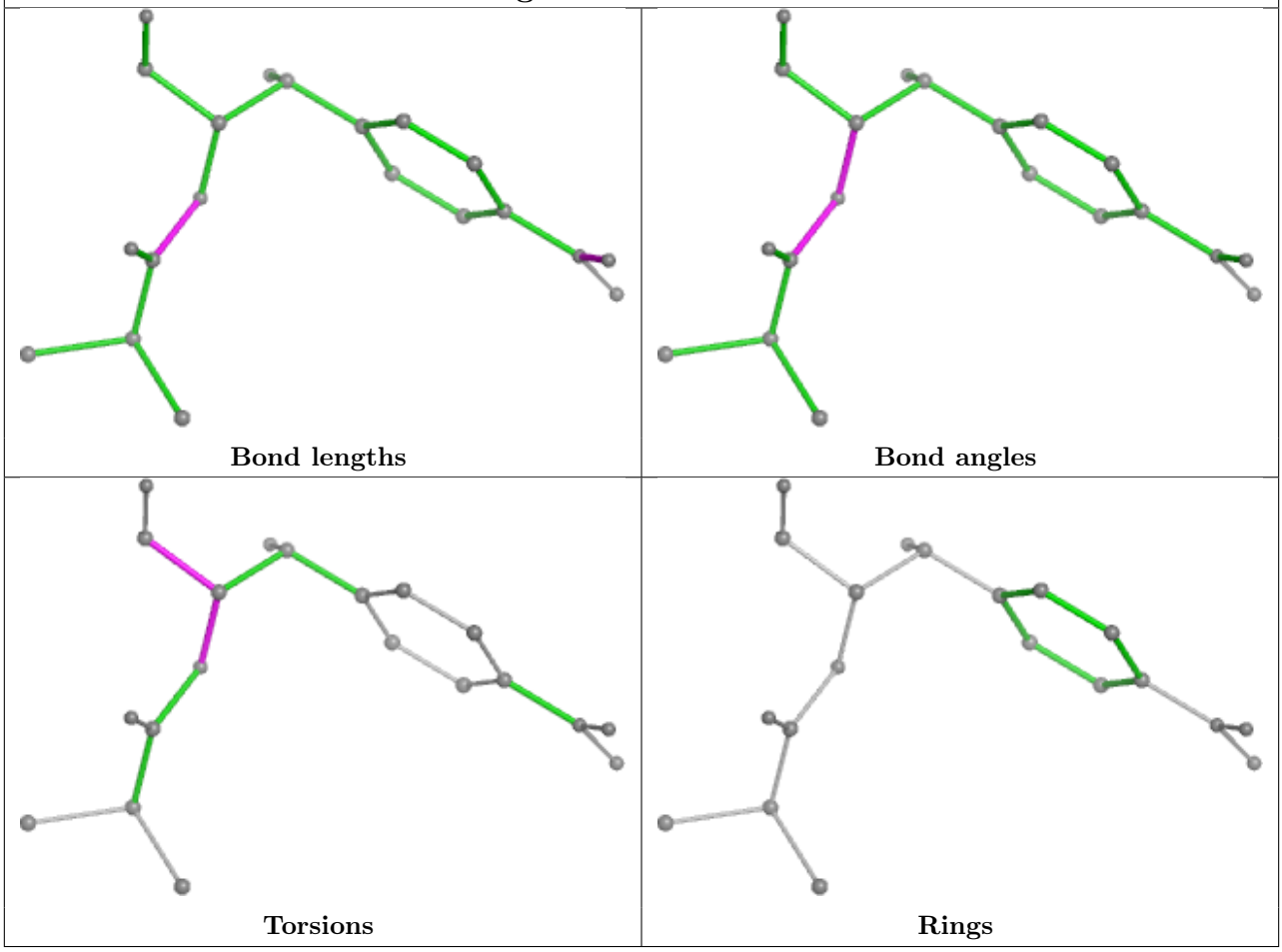
Mol	Chain	Res	Type	Atoms
67	8	103	LYS	O-C-CA-CB
67	8	103	LYS	N-CA-CB-CG
67	8	103	LYS	C-CA-CB-CG
65	5	1603	SPD	C8-C7-N6-C5
66	3	3245	N2P	C2-C3-C4-C5

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 then 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.

Ligand CLM 3 3001



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.