wwPDB EM Validation Summary Report

Feb 19, 2025 – 12:23 pm GMT

PDB ID	:	8P8B
EMDB ID	:	EMD-17134
Title	:	Mycoplasma pneumoniae large ribosomal subunit in chloramphenicol-treated cells
Authors	:	Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on	:	2023-05-31
Resolution	:	2.90 Å(reported)
Based on initial models	:	7OOC, 7OOD

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:

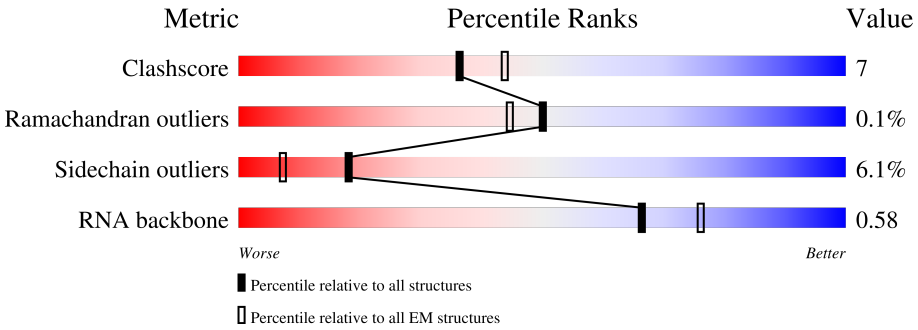
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	210492	15764
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	75% 25%
2	1	59	81% 17% .
3	2	37	89% 11%
4	3	2907	69% 27% .
5	4	108	63% 31% 6%
6	5	1520	.. 98%
7	6	76	. 97%

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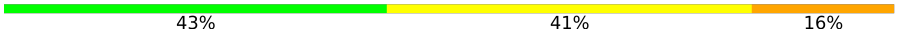
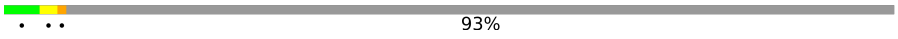
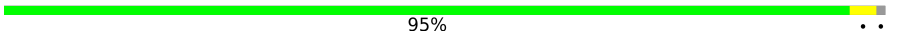
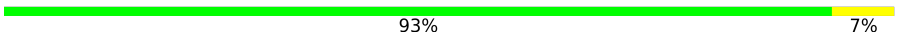
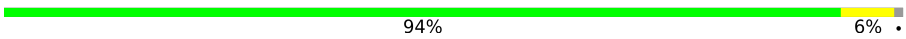
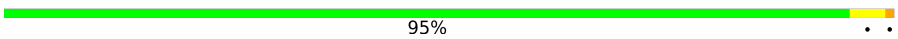
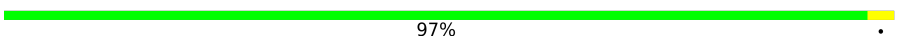
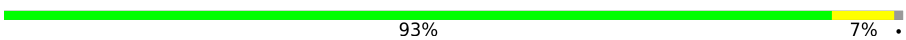
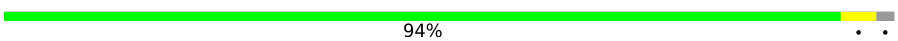
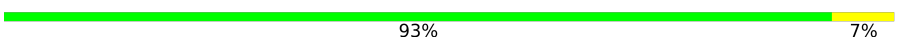
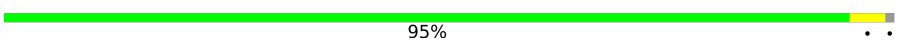
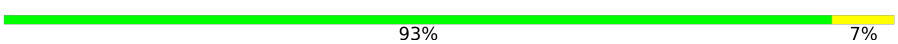
Mol	Chain	Length	Quality of chain
8	7	75	
9	8	76	
10	X	444	
11	Y	9	
12	Z	36	
13	a	287	
14	b	287	
15	c	212	
16	d	180	
17	e	184	
18	f	149	
19	g	161	
20	h	137	
21	i	146	
22	j	122	
23	k	151	
24	l	139	
25	m	124	
26	n	116	
27	o	119	
28	p	127	
29	q	100	
30	r	159	
31	s	237	
32	t	111	

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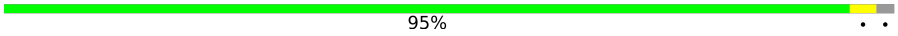
Mol	Chain	Length	Quality of chain
33	u	104	
34	v	65	
35	w	111	
36	x	97	
37	y	57	
38	z	53	

2 Entry composition (i)

There are 47 unique types of molecules in this entry. The entry contains 97182 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	32	683	307	124	220	32	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
7	6	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

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

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

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
9	8	76	Total	C	N	O	P	0	0
			1615	722	284	533	76		

- Molecule 10 is a protein called Trigger factor.

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

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	9	Total	C	N	O	P	0	0
			195	87	38	61	9		

- Molecule 12 is a protein called nascent peptide.

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

- Molecule 13 is a protein called 50S ribosomal protein L2.

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

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	231	Total 1778	C 1129	N 320	O 322	S 7	0	0

- Molecule 15 is a protein called 50S ribosomal protein L4.

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

- Molecule 16 is a protein called 50S ribosomal protein L5.

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

- Molecule 17 is a protein called 50S ribosomal protein L6.

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

- Molecule 18 is a protein called 50S ribosomal protein L9.

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

- Molecule 19 is a protein called 50S ribosomal protein L10.

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

- Molecule 20 is a protein called 50S ribosomal protein L11.

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

- Molecule 21 is a protein called 50S ribosomal protein L13.

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

- Molecule 22 is a protein called 50S ribosomal protein L14.

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

- Molecule 23 is a protein called 50S ribosomal protein L15.

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

- Molecule 24 is a protein called 50S ribosomal protein L16.

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

- Molecule 25 is a protein called 50S ribosomal protein L17.

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

- Molecule 26 is a protein called 50S ribosomal protein L18.

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

- Molecule 27 is a protein called 50S ribosomal protein L19.

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

- Molecule 28 is a protein called 50S ribosomal protein L20.

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

- Molecule 29 is a protein called 50S ribosomal protein L21.

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

- Molecule 30 is a protein called 50S ribosomal protein L22.

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

- Molecule 31 is a protein called 50S ribosomal protein L23.

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

- Molecule 32 is a protein called 50S ribosomal protein L24.

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

- Molecule 33 is a protein called 50S ribosomal protein L27.

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

- Molecule 34 is a protein called 50S ribosomal protein L28.

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

- Molecule 35 is a protein called 50S ribosomal protein L29.

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

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	46	Total	C	N	O	S	0	0
			366	235	59	68	4		

- Molecule 37 is a protein called 50S ribosomal protein L32.

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

- Molecule 38 is a protein called 50S ribosomal protein L33 1.

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

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	2	1	Total	Zn	0
			1	1	
39	x	1	Total	Zn	0
			1	1	
39	y	1	Total	Zn	0
			1	1	

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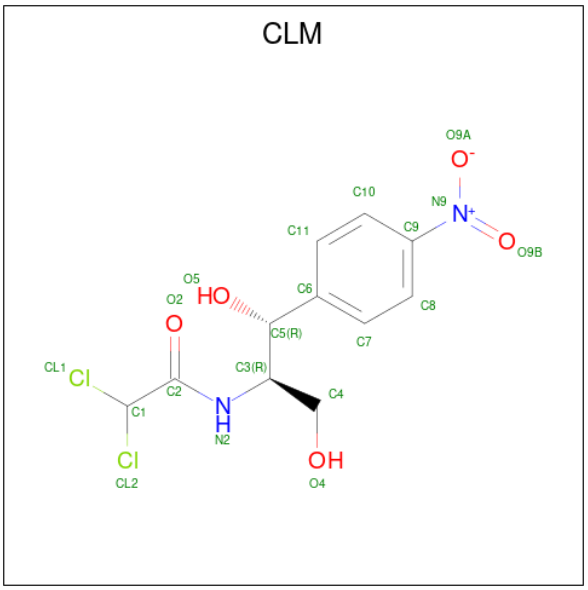
Mol	Chain	Residues	Atoms	AltConf
39	z	1	Total Zn 1 1	0

- Molecule 40 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
40	3	1	Total C Cl N O 20 11 2 2 5	0

- Molecule 41 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
41	3	1	Total K 1 1	0

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
42	3	219	Total Mg 219 219	0
42	4	1	Total Mg 1 1	0
42	6	1	Total Mg 1 1	0

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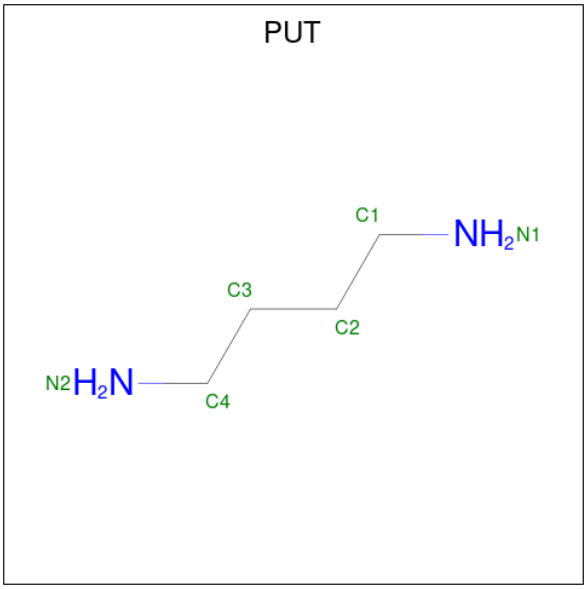
Mol	Chain	Residues	Atoms	AltConf
42	7	1	Total Mg 1 1	0
42	8	2	Total Mg 2 2	0
42	b	2	Total Mg 2 2	0
42	i	1	Total Mg 1 1	0
42	y	2	Total Mg 2 2	0

- Molecule 43 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0
43	3	1	Total C N 6 4 2	0

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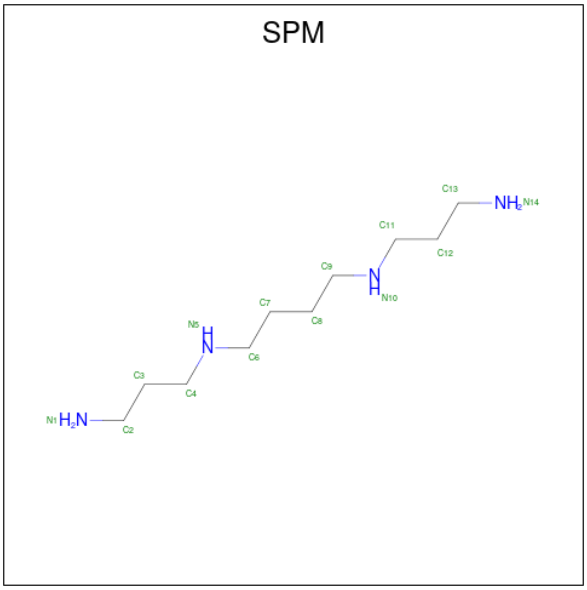
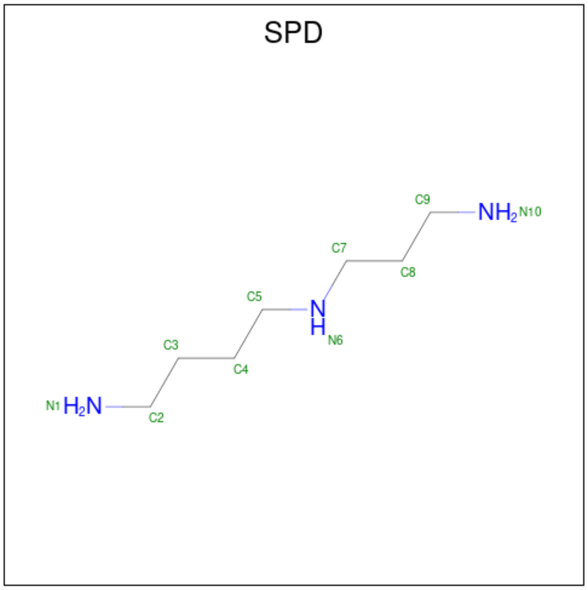
Mol	Chain	Residues	Atoms	AltConf
43	3	1	Total C N 6 4 2	0

- Molecule 44 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
44	3	1	Total C N 14 10 4	0
44	3	1	Total C N 14 10 4	0
44	3	1	Total C N 14 10 4	0
44	b	1	Total C N 14 10 4	0

- Molecule 45 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0

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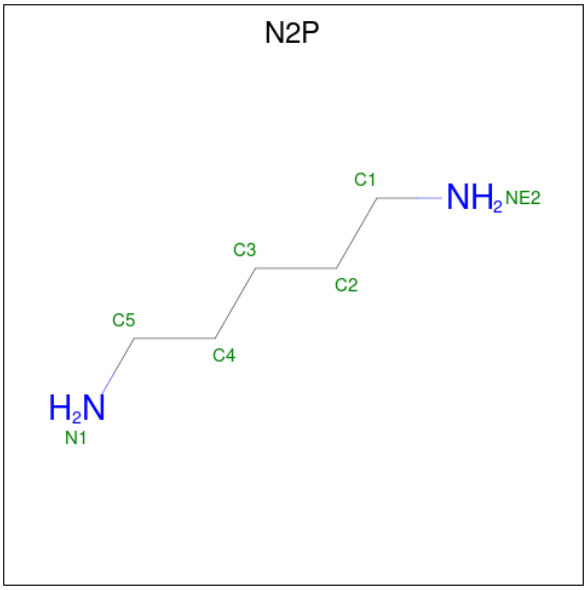
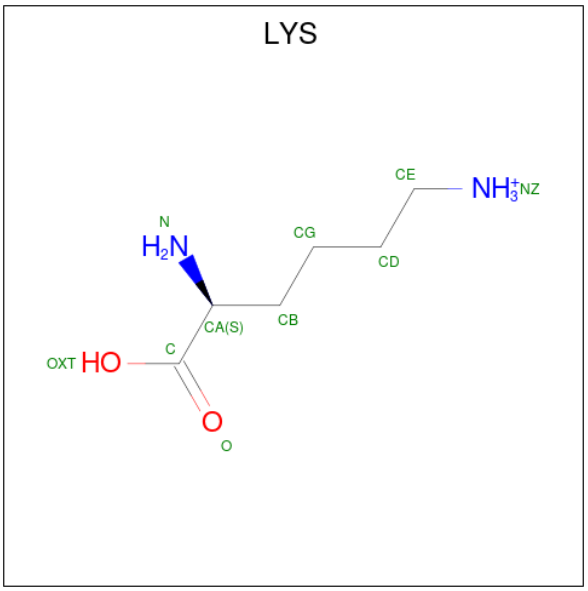
Mol	Chain	Residues	Atoms	AltConf
45	3	1	Total C N 10 7 3	0
45	3	1	Total C N 10 7 3	0

- Molecule 46 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms	AltConf
46	3	1	Total C N 7 5 2	0
46	3	1	Total C N 7 5 2	0
46	3	1	Total C N 7 5 2	0

- Molecule 47 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
47	8	1	9	6	2	1	0

3 Residue-property plots (i)

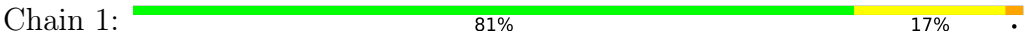
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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:

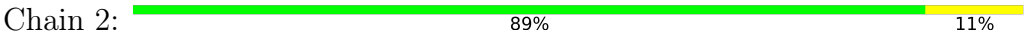
- Molecule 2: 50S ribosomal protein L35

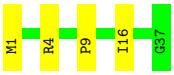
Chain 1:



- Molecule 3: 50S ribosomal protein L36

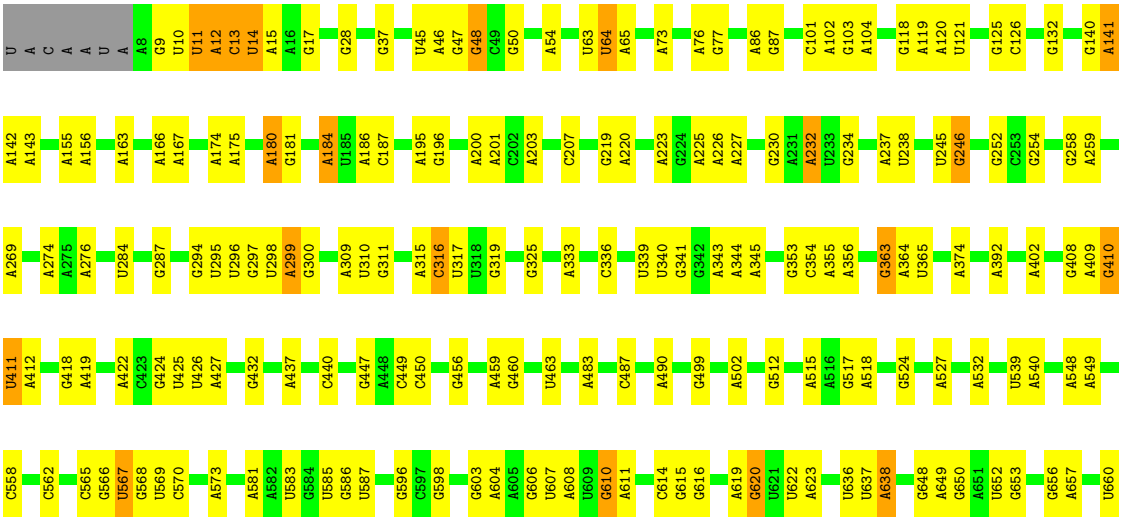
Chain 2:





- Molecule 4: 23S ribosomal RNA

Chain 3:



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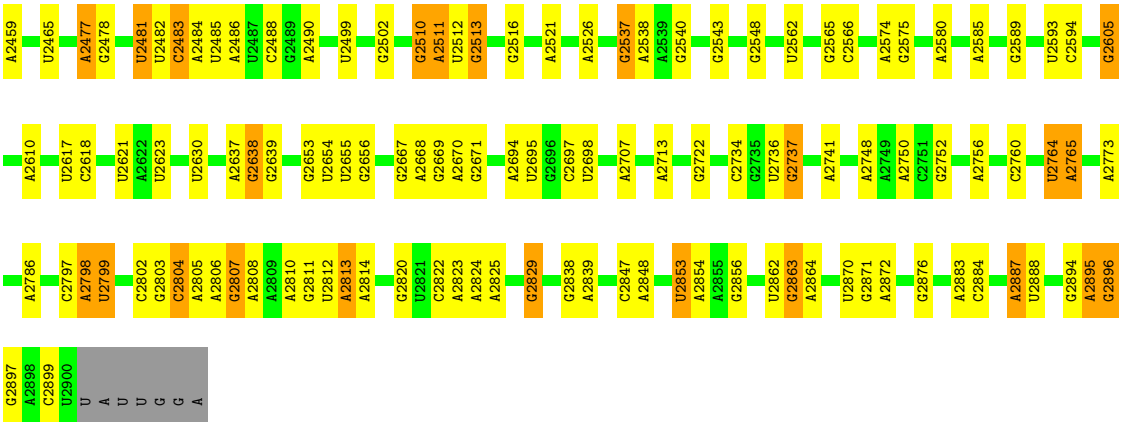
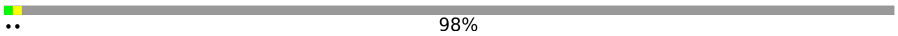


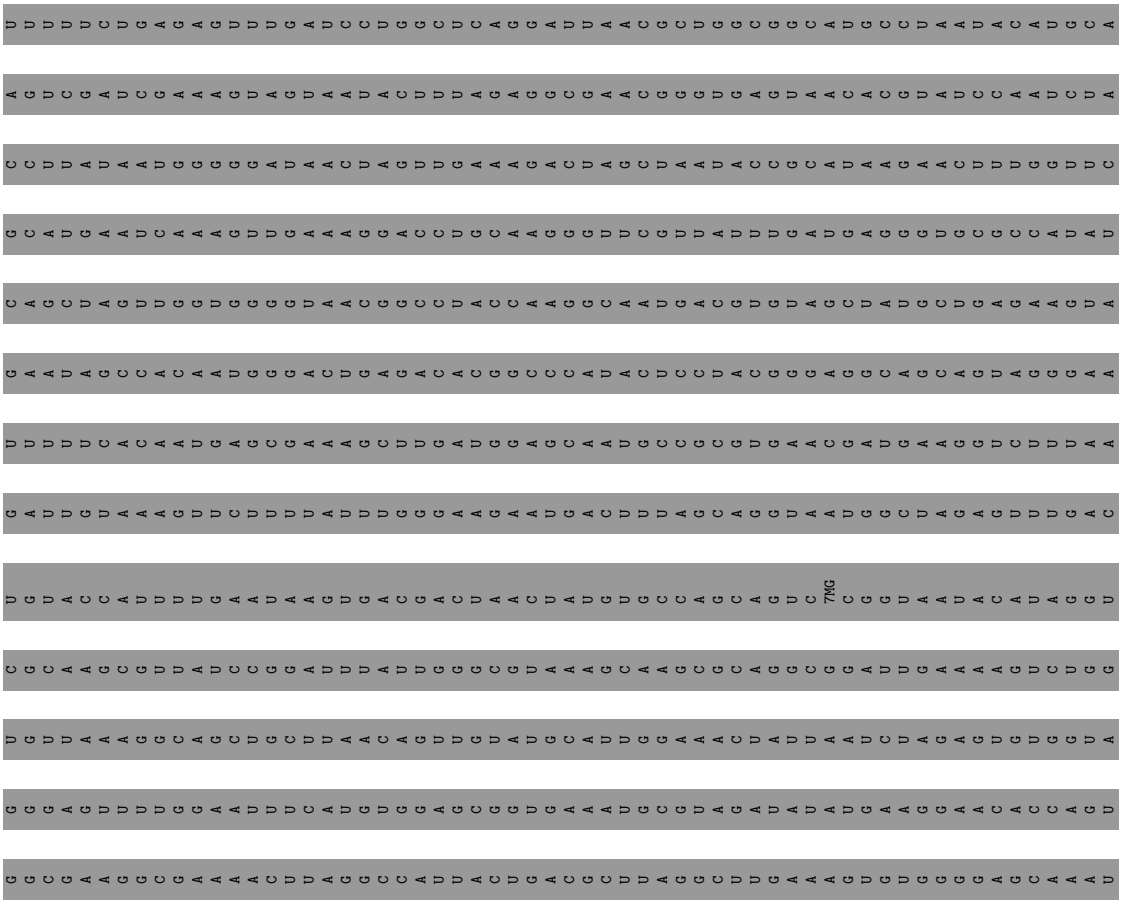
• Molecule 5: 5S ribosomal RNA

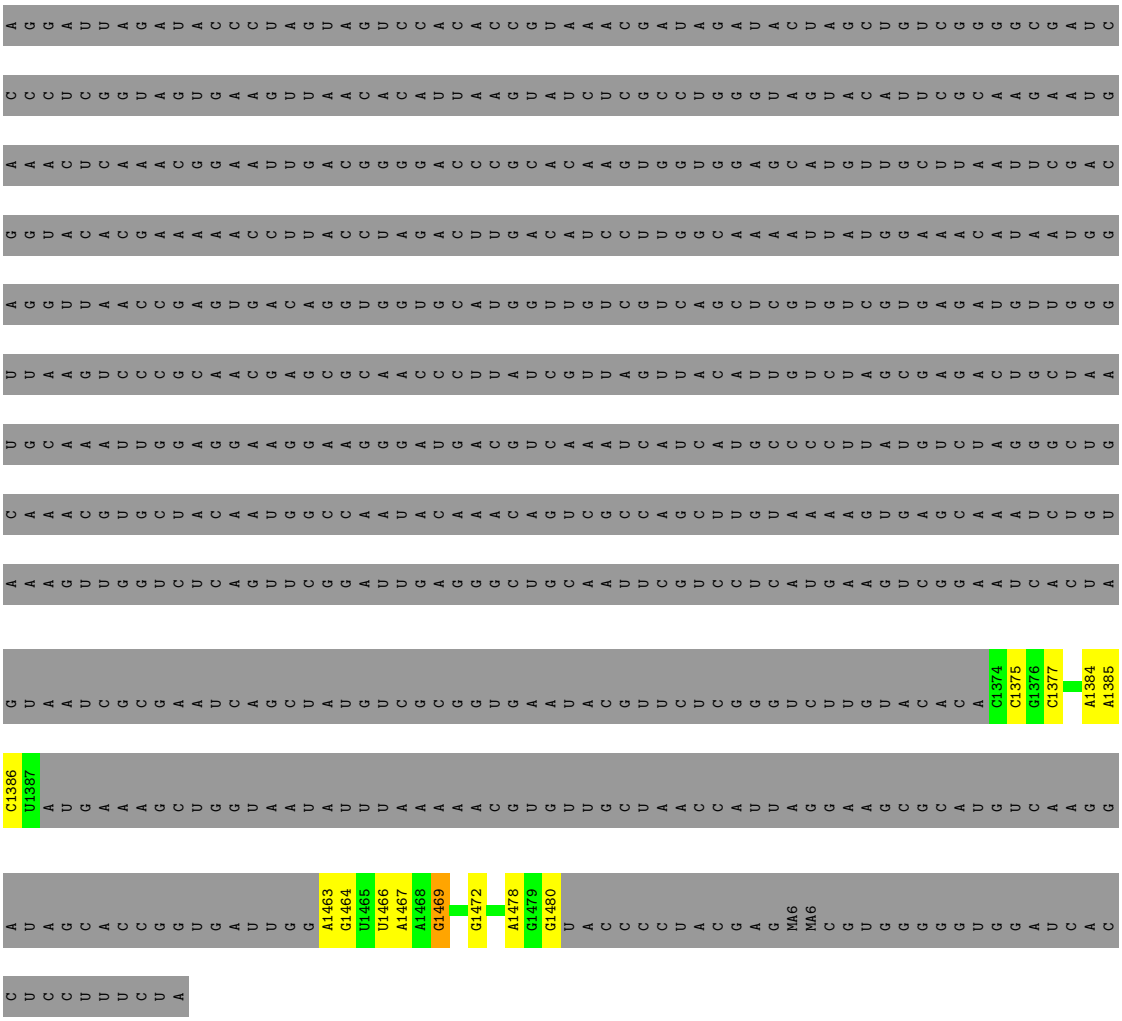
Chain 4:

• Molecule 6: 16S ribosomal RNA

Chain 5:

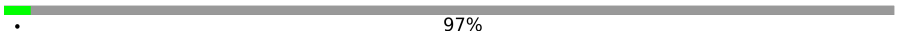


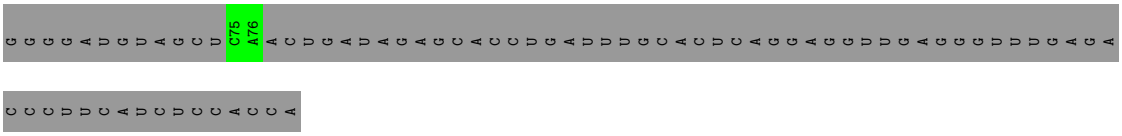




• Molecule 7: tRNA-Ala (E-site)

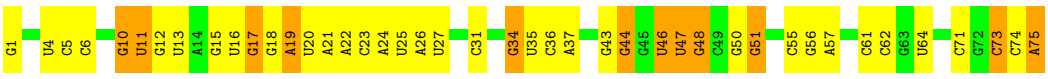
Chain 6:





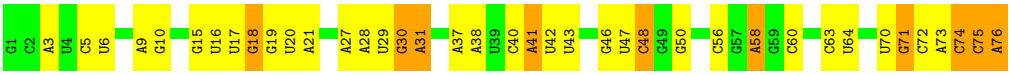
• Molecule 8: tRNA-Asp (P-site)

Chain 7:



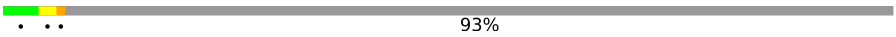
• Molecule 9: tRNA-Lys (A-site)

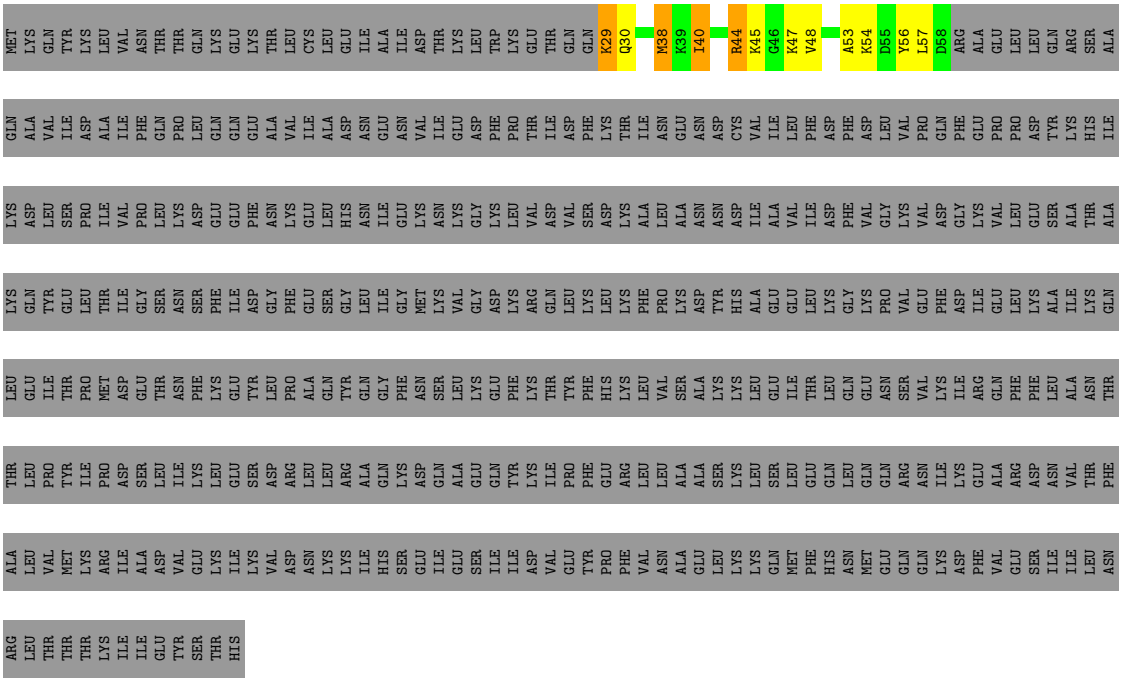
Chain 8:



• Molecule 10: Trigger factor

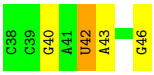
Chain X:





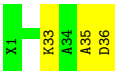
• Molecule 11: mRNA

Chain Y:



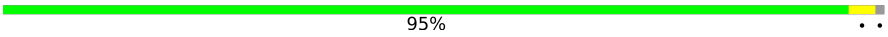
• Molecule 12: nascent peptide

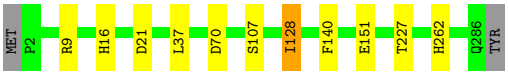
Chain Z:



• Molecule 13: 50S ribosomal protein L2

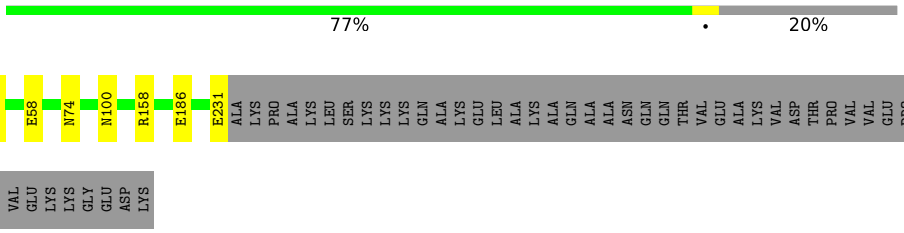
Chain a:





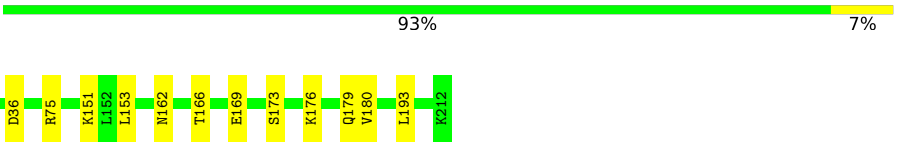
• Molecule 14: 50S ribosomal protein L3

Chain b:



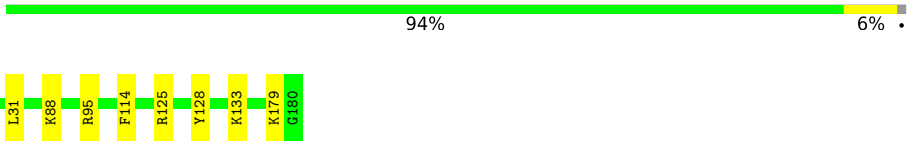
• Molecule 15: 50S ribosomal protein L4

Chain c:



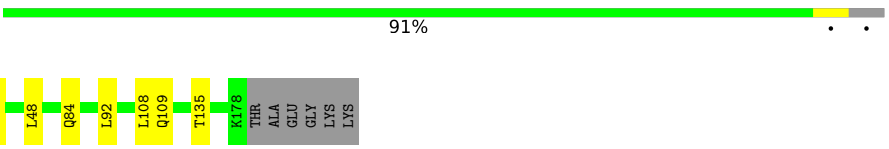
• Molecule 16: 50S ribosomal protein L5

Chain d:



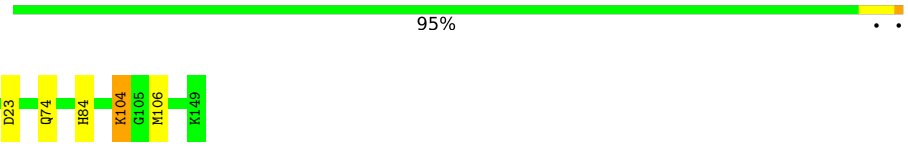
• Molecule 17: 50S ribosomal protein L6

Chain e:



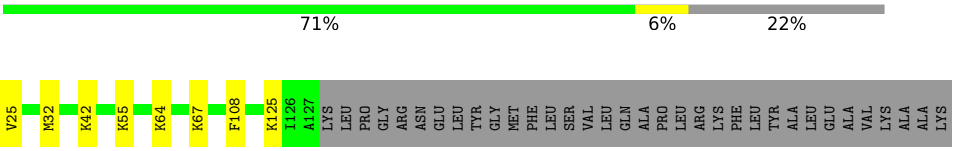
• Molecule 18: 50S ribosomal protein L9

Chain f:



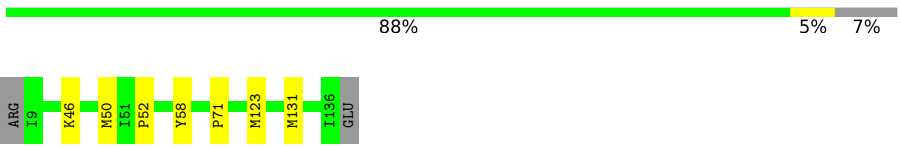
• Molecule 19: 50S ribosomal protein L10

Chain g:



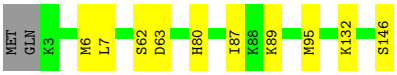
• Molecule 20: 50S ribosomal protein L11

Chain h:



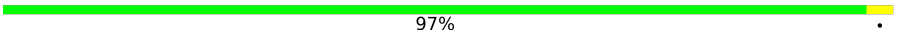
• Molecule 21: 50S ribosomal protein L13

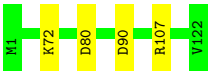
Chain i:



• Molecule 22: 50S ribosomal protein L14

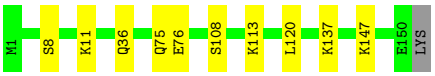
Chain j:





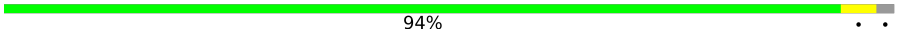
• Molecule 23: 50S ribosomal protein L15

Chain k:



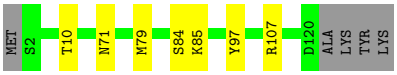
• Molecule 24: 50S ribosomal protein L16

Chain l:



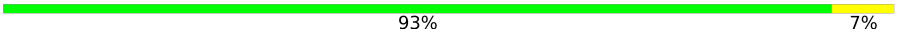
• Molecule 25: 50S ribosomal protein L17

Chain m:



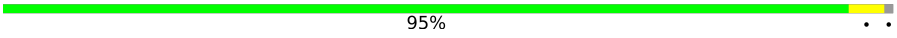
• Molecule 26: 50S ribosomal protein L18

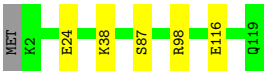
Chain n:



• Molecule 27: 50S ribosomal protein L19

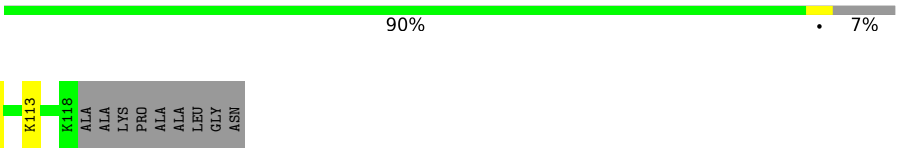
Chain o:





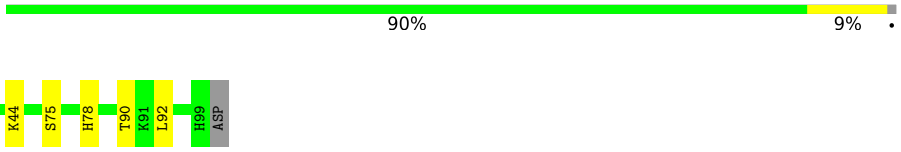
• Molecule 28: 50S ribosomal protein L20

Chain p:



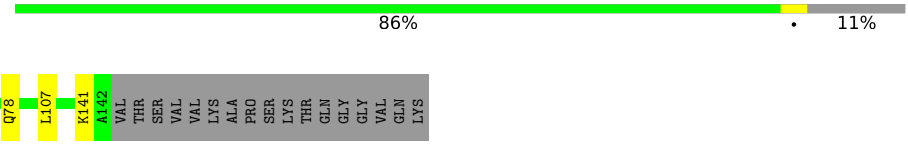
• Molecule 29: 50S ribosomal protein L21

Chain q:



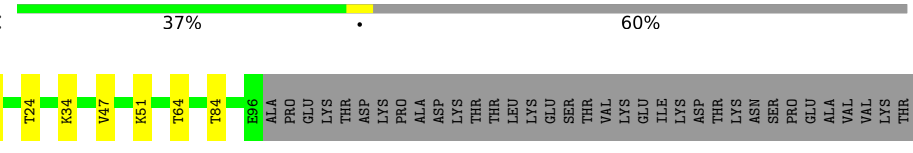
• Molecule 30: 50S ribosomal protein L22

Chain r:



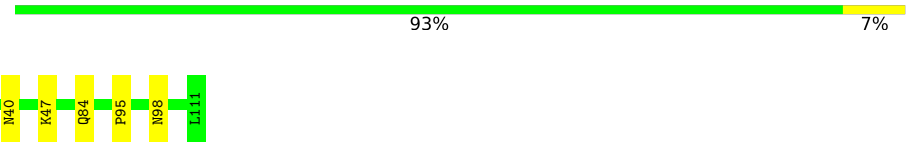
• Molecule 31: 50S ribosomal protein L23

Chain s:



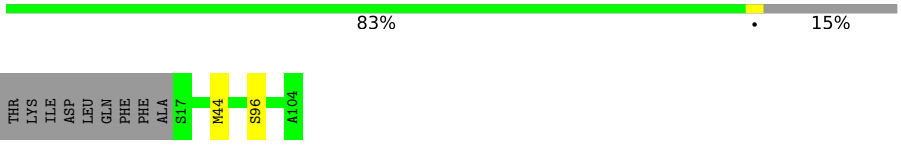
• Molecule 32: 50S ribosomal protein L24

Chain t:



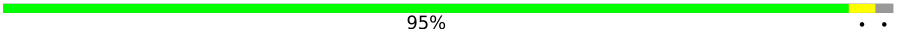
• Molecule 33: 50S ribosomal protein L27

Chain u:



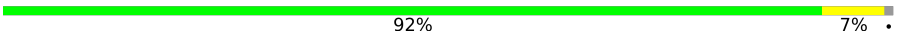
• Molecule 34: 50S ribosomal protein L28

Chain v:



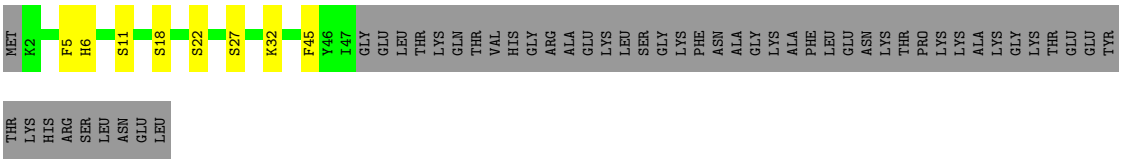
• Molecule 35: 50S ribosomal protein L29

Chain w:



• Molecule 36: 50S ribosomal protein L31

Chain x:

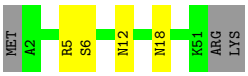


• Molecule 37: 50S ribosomal protein L32

Chain y:

• Molecule 38: 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	30774	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 1MG, CLM, PUT, B8T, ZN, MG, K, 2MA, SPD, SPM, N2P, 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	0.23	0/395	0.56	0/518
2	1	0.24	0/484	0.52	0/637
3	2	0.23	0/306	0.52	0/401
4	3	0.19	0/69363	0.71	8/108161 (0.0%)
5	4	0.17	0/2578	0.72	0/4016
6	5	0.17	0/715	0.71	0/1107
7	6	0.13	0/46	0.62	0/69
8	7	0.30	1/1785 (0.1%)	0.84	2/2779 (0.1%)
9	8	0.53	6/1804 (0.3%)	0.80	0/2807
10	X	0.29	0/245	0.79	1/325 (0.3%)
11	Y	0.28	0/218	0.79	0/338
12	Z	0.75	0/26	1.33	0/33
13	a	0.37	2/2267 (0.1%)	0.60	3/3044 (0.1%)
14	b	0.29	0/1812	0.55	1/2436 (0.0%)
15	c	0.30	0/1681	0.54	1/2257 (0.0%)
16	d	0.32	0/1437	0.66	0/1931
17	e	0.49	2/1420 (0.1%)	0.94	5/1912 (0.3%)
18	f	0.40	1/1233 (0.1%)	0.62	0/1653
19	g	0.32	0/960	0.60	0/1284
20	h	0.78	4/968 (0.4%)	1.19	7/1298 (0.5%)
21	i	0.25	0/1186	0.50	0/1592
22	j	0.27	0/953	0.61	1/1275 (0.1%)
23	k	0.29	0/1187	0.60	0/1581
24	l	0.29	0/1104	0.56	0/1481
25	m	0.29	0/973	0.52	1/1309 (0.1%)
26	n	0.28	0/927	0.58	0/1239
27	o	0.31	0/976	0.59	0/1296
28	p	0.26	0/996	0.54	0/1325
29	q	0.29	0/828	0.55	0/1111
30	r	0.26	0/1100	0.50	0/1471
31	s	0.27	0/752	0.58	0/1015
32	t	0.57	1/878 (0.1%)	0.96	4/1165 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	u	0.25	0/678	0.52	0/902
34	v	0.23	0/526	0.56	0/703
35	w	0.26	0/916	0.56	0/1222
36	x	0.26	0/375	0.46	0/502
37	y	0.28	0/457	0.63	0/601
38	z	0.23	0/412	0.54	0/547
All	All	0.25	17/104967 (0.0%)	0.70	34/157343 (0.0%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	52	PRO	CG-CD	-15.31	1.00	1.50
32	t	95	PRO	CG-CD	-13.85	1.04	1.50
17	e	30	PRO	CB-CG	-11.82	0.90	1.50
9	8	76	A	N9-C4	10.38	1.44	1.37
20	h	52	PRO	N-CD	10.15	1.62	1.47

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	h	52	PRO	N-CD-CG	-20.95	71.77	103.20
32	t	95	PRO	N-CD-CG	-19.84	73.44	103.20
17	e	30	PRO	N-CD-CG	-19.64	73.73	103.20
17	e	30	PRO	CB-CG-CD	18.83	179.95	106.50
17	e	30	PRO	CA-CB-CG	-16.62	72.43	104.00

There are no chirality outliers.

There are no planarity outliers.

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	0	392	0	442	8	0
2	1	477	0	530	7	0
3	2	304	0	348	3	0
4	3	61995	0	31115	341	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	2305	0	1164	12	0
6	5	683	0	339	4	0
7	6	42	0	23	0	0
8	7	1599	0	805	24	0
9	8	1615	0	816	19	0
10	X	242	0	263	9	0
11	Y	195	0	99	1	0
12	Z	187	0	68	5	0
13	a	2225	0	2301	0	0
14	b	1778	0	1821	0	0
15	c	1654	0	1744	0	0
16	d	1416	0	1500	0	0
17	e	1396	0	1481	0	0
18	f	1210	0	1259	0	0
19	g	951	0	1001	0	0
20	h	959	0	1039	0	0
21	i	1164	0	1192	0	0
22	j	944	0	1019	0	0
23	k	1170	0	1274	0	0
24	l	1079	0	1134	0	0
25	m	958	0	1011	0	0
26	n	918	0	979	0	0
27	o	966	0	1042	0	0
28	p	981	0	1062	0	0
29	q	811	0	858	0	0
30	r	1091	0	1178	0	0
31	s	740	0	819	0	0
32	t	871	0	972	0	0
33	u	670	0	704	0	0
34	v	520	0	565	0	0
35	w	906	0	981	0	0
36	x	366	0	356	0	0
37	y	452	0	471	0	0
38	z	408	0	436	0	0
39	2	1	0	0	0	0
39	x	1	0	0	0	0
39	y	1	0	0	0	0
39	z	1	0	0	0	0
40	3	20	0	11	4	0
41	3	1	0	0	0	0
42	3	219	0	0	0	0
42	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	6	1	0	0	0	0
42	7	1	0	0	0	0
42	8	2	0	0	0	0
42	b	2	0	0	0	0
42	i	1	0	0	0	0
42	y	2	0	0	0	0
43	3	42	0	84	1	0
44	3	42	0	78	7	0
44	b	14	0	26	0	0
45	3	160	0	304	3	0
46	3	21	0	42	0	0
47	8	9	0	12	0	0
All	All	97182	0	64768	416	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 7.

The worst 5 of 416 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)
9:8:50:G:H1	9:8:64:U:H3	1.21	0.88
4:3:2736:U:HO2'	4:3:2737:G:H8	1.24	0.85
10:X:29:LYS:HE3	10:X:30:GLN:HG2	1.60	0.82
3:2:4:ARG:NH2	4:3:2485:U:O2	2.12	0.82
10:X:38:MET:SD	10:X:57:LEU:HD22	2.20	0.81

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	
1	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
12	Z	3/36 (8%)	3 (100%)	0	0	100	100
13	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	60
14	b	229/287 (80%)	221 (96%)	8 (4%)	0	100	100
15	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
16	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
17	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
18	f	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	31
19	g	123/161 (76%)	116 (94%)	7 (6%)	0	100	100
20	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
21	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
23	k	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
24	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
25	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
26	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
27	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
28	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
29	q	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
30	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
31	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
32	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
33	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
34	v	62/65 (95%)	62 (100%)	0	0	100	100
35	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
36	x	44/97 (45%)	35 (80%)	8 (18%)	1 (2%)	5	20
37	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
38	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	3485/4359 (80%)	3310 (95%)	171 (5%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	a	128	ILE
18	f	12	LEU
18	f	74	GLN
36	x	18	SER

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%)	39 (95%)	2 (5%)	21 53
2	1	51/51 (100%)	49 (96%)	2 (4%)	27 62
3	2	35/35 (100%)	35 (100%)	0	100 100
10	X	27/406 (7%)	22 (82%)	5 (18%)	1 4
12	Z	2/2 (100%)	2 (100%)	0	100 100
13	a	241/243 (99%)	232 (96%)	9 (4%)	29 64
14	b	188/233 (81%)	180 (96%)	8 (4%)	25 57
15	c	183/184 (100%)	170 (93%)	13 (7%)	12 36
16	d	153/154 (99%)	143 (94%)	10 (6%)	14 40
17	e	153/159 (96%)	147 (96%)	6 (4%)	27 62
18	f	134/134 (100%)	129 (96%)	5 (4%)	29 64
19	g	100/129 (78%)	90 (90%)	10 (10%)	6 20
20	h	102/110 (93%)	97 (95%)	5 (5%)	21 53
21	i	126/128 (98%)	116 (92%)	10 (8%)	10 30
22	j	103/103 (100%)	100 (97%)	3 (3%)	37 72
23	k	125/126 (99%)	115 (92%)	10 (8%)	10 30
24	l	113/115 (98%)	108 (96%)	5 (4%)	24 57
25	m	105/109 (96%)	99 (94%)	6 (6%)	17 47
26	n	99/99 (100%)	91 (92%)	8 (8%)	9 29
27	o	104/105 (99%)	99 (95%)	5 (5%)	21 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	p	104/108 (96%)	100 (96%)	4 (4%)	28 63
29	q	90/91 (99%)	81 (90%)	9 (10%)	6 20
30	r	118/132 (89%)	113 (96%)	5 (4%)	25 59
31	s	84/208 (40%)	76 (90%)	8 (10%)	7 22
32	t	96/96 (100%)	89 (93%)	7 (7%)	11 34
33	u	70/85 (82%)	68 (97%)	2 (3%)	37 72
34	v	59/60 (98%)	57 (97%)	2 (3%)	32 67
35	w	97/98 (99%)	89 (92%)	8 (8%)	9 29
36	x	44/86 (51%)	37 (84%)	7 (16%)	2 6
37	y	48/49 (98%)	41 (85%)	7 (15%)	2 8
38	z	47/50 (94%)	43 (92%)	4 (8%)	8 27
All	All	3042/3729 (82%)	2857 (94%)	185 (6%)	18 43

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	n	66	ASN
31	s	34	LYS
27	o	87	SER
29	q	44	LYS
32	t	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
23	k	134	GLN
26	n	64	ASN
33	u	100	HIS
28	p	71	GLN
28	p	106	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Y	8/9 (88%)	4 (50%)	1 (12%)
4	3	2891/2907 (99%)	503 (17%)	12 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	4	107/108 (99%)	29 (27%)	0
6	5	29/1520 (1%)	6 (20%)	0
7	6	1/76 (1%)	0	0
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	3185/4771 (66%)	585 (18%)	15 (0%)

5 of 585 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 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	1583	G
8	7	46	U
4	3	1618	U
11	Y	42	U
4	3	2764	U

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

5 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	$\#\|Z\| > 2$
4	2MA	3	2511	42,4	17,25,26	2.62	5 (29%)	17,37,40	1.35	3 (17%)
4	OMG	3	2259	42,8,4	18,26,27	2.83	7 (38%)	19,38,41	1.57	4 (21%)
6	B8T	5	1377	6	19,22,23	3.28	8 (42%)	26,31,34	0.84	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	1MG	3	783	4	18,26,27	2.73	6 (33%)	19,39,42	1.50	3 (15%)
6	5MC	5	1375	6	18,22,23	4.07	7 (38%)	26,32,35	1.04	2 (7%)

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
4	2MA	3	2511	42,4	-	2/3/25/26	0/3/3/3
4	OMG	3	2259	42,8,4	-	3/5/27/28	0/3/3/3
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C6-C5	9.99	1.51	1.34
4	3	2511	2MA	C2-N3	7.81	1.47	1.31
6	5	1375	5MC	C4-N3	7.53	1.46	1.34
6	5	1377	B8T	C4-N3	7.25	1.45	1.32
4	3	2259	OMG	C2-N2	7.16	1.51	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3	783	1MG	C5-C6-N1	4.12	120.09	113.90
4	3	2259	OMG	C5-C6-N1	3.44	120.03	113.95
4	3	2511	2MA	C5-C6-N1	3.39	119.88	114.02
6	5	1375	5MC	C5-C6-N1	-3.16	120.09	123.34
4	3	2259	OMG	C2-N1-C6	-2.89	119.77	125.10

There are no chirality outliers.

5 of 7 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

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Mol	Chain	Res	Type	Atoms
6	5	1377	B8T	O4'-C4'-C5'-O5'
4	3	2511	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	2511	2MA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 266 ligands modelled in this entry, 234 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
45	SPD	3	3239	-	9,9,9	0.32	0	8,8,8	0.88	0
45	SPD	3	3248	-	9,9,9	0.31	0	8,8,8	0.88	0
40	CLM	3	3001	-	19,20,20	0.55	1 (5%)	23,27,27	0.61	0
45	SPD	3	3234	-	9,9,9	0.32	0	8,8,8	0.78	0
46	N2P	3	3244	-	6,6,6	0.25	0	5,5,5	0.63	0
43	PUT	3	3231	-	5,5,5	0.25	0	4,4,4	0.51	0
45	SPD	3	3235	-	9,9,9	0.33	0	8,8,8	0.87	0
43	PUT	3	3223	-	5,5,5	0.23	0	4,4,4	0.56	0
45	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.80	0
45	SPD	3	3236	-	9,9,9	0.33	0	8,8,8	0.82	0
45	SPD	3	3229	-	9,9,9	0.32	0	8,8,8	0.87	0
46	N2P	3	3243	-	6,6,6	0.25	0	5,5,5	0.65	0
45	SPD	3	3245	-	9,9,9	0.32	0	8,8,8	0.89	0
44	SPM	3	3249	-	13,13,13	0.35	0	12,12,12	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	SPD	3	3240	-	9,9,9	0.32	0	8,8,8	0.86	0
44	SPM	3	3227	-	13,13,13	0.35	0	12,12,12	0.90	0
45	SPD	3	3238	-	9,9,9	0.32	0	8,8,8	0.85	0
45	SPD	3	3237	-	9,9,9	0.32	0	8,8,8	0.96	0
43	PUT	3	3226	-	5,5,5	0.26	0	4,4,4	0.52	0
45	SPD	3	3232	-	9,9,9	0.35	0	8,8,8	0.75	0
47	LYS	8	103	9	7,8,9	1.79	1 (14%)	3,8,10	0.37	0
45	SPD	3	3246	-	9,9,9	0.33	0	8,8,8	0.82	0
43	PUT	3	3222	-	5,5,5	0.24	0	4,4,4	0.55	0
43	PUT	3	3225	-	5,5,5	0.25	0	4,4,4	0.52	0
45	SPD	3	3228	-	9,9,9	0.32	0	8,8,8	0.87	0
46	N2P	3	3247	-	6,6,6	0.24	0	5,5,5	0.67	0
44	SPM	3	3241	-	13,13,13	0.34	0	12,12,12	0.93	0
45	SPD	3	3233	-	9,9,9	0.32	0	8,8,8	0.89	0
45	SPD	3	3250	-	9,9,9	0.17	0	8,8,8	0.19	0
44	SPM	b	303	-	13,13,13	0.16	0	12,12,12	0.32	0
43	PUT	3	3242	-	5,5,5	0.25	0	4,4,4	0.54	0
43	PUT	3	3224	-	5,5,5	0.25	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
45	SPD	3	3239	-	-	2/7/7/7	-
45	SPD	3	3248	-	-	0/7/7/7	-
40	CLM	3	3001	-	-	2/20/22/22	0/1/1/1
45	SPD	3	3234	-	-	1/7/7/7	-
46	N2P	3	3244	-	-	2/4/4/4	-
43	PUT	3	3231	-	-	0/3/3/3	-
45	SPD	3	3235	-	-	0/7/7/7	-
43	PUT	3	3223	-	-	0/3/3/3	-
45	SPD	3	3230	-	-	0/7/7/7	-
45	SPD	3	3236	-	-	0/7/7/7	-
45	SPD	3	3229	-	-	1/7/7/7	-
46	N2P	3	3243	-	-	1/4/4/4	-
45	SPD	3	3245	-	-	0/7/7/7	-
44	SPM	3	3249	-	-	1/11/11/11	-
45	SPD	3	3240	-	-	0/7/7/7	-
44	SPM	3	3227	-	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SPD	3	3238	-	-	0/7/7/7	-
45	SPD	3	3237	-	-	1/7/7/7	-
43	PUT	3	3226	-	-	0/3/3/3	-
45	SPD	3	3232	-	-	2/7/7/7	-
47	LYS	8	103	9	-	3/6/7/9	-
45	SPD	3	3246	-	-	1/7/7/7	-
43	PUT	3	3222	-	-	0/3/3/3	-
43	PUT	3	3225	-	-	1/3/3/3	-
45	SPD	3	3228	-	-	0/7/7/7	-
46	N2P	3	3247	-	-	1/4/4/4	-
44	SPM	3	3241	-	-	2/11/11/11	-
45	SPD	3	3233	-	-	0/7/7/7	-
45	SPD	3	3250	-	-	0/7/7/7	-
44	SPM	b	303	-	-	2/11/11/11	-
43	PUT	3	3242	-	-	0/3/3/3	-
43	PUT	3	3224	-	-	0/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	103	LYS	CB-CA	4.20	1.59	1.53
40	3	3001	CLM	C1-C2	-2.11	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	8	103	LYS	O-C-CA-CB
47	8	103	LYS	C-CA-CB-CG
46	3	3243	N2P	C2-C3-C4-C5
44	3	3227	SPM	C7-C8-C9-N10
40	3	3001	CLM	C5-C3-N2-C2

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	3	3248	SPD	1	0
40	3	3001	CLM	4	0

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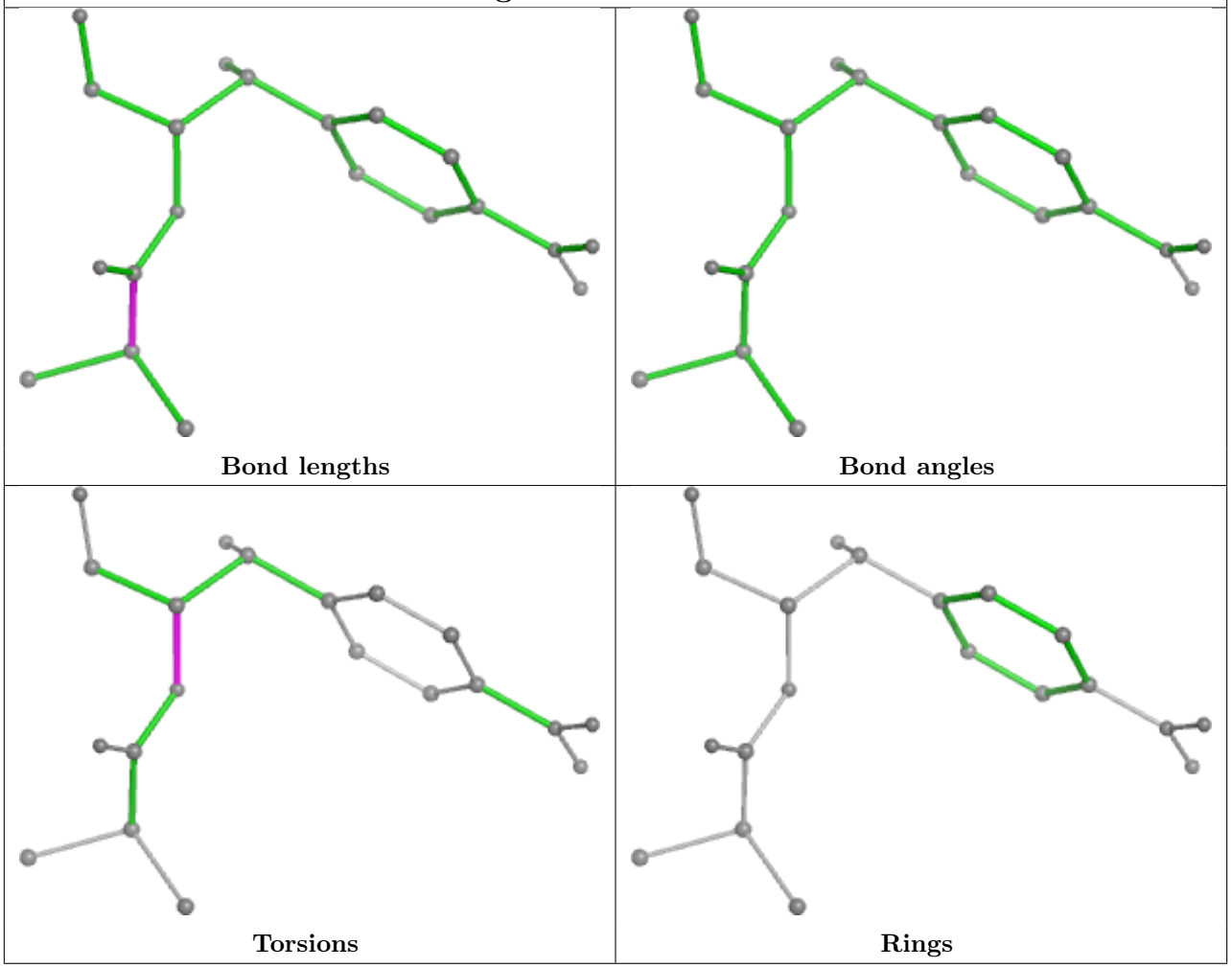
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	3	3231	PUT	1	0
44	3	3249	SPM	2	0
44	3	3227	SPM	4	0
45	3	3237	SPD	1	0
44	3	3241	SPM	1	0
45	3	3250	SPD	1	0

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.