



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:51 PM UTC

PDB ID : 6LKQ / pdb_00006lkq
Title : The Structural Basis for Inhibition of Ribosomal Translocation by Viomycin
Authors : Zhang, L.; Wang, Y.H.; Lancaster, L.; Zhou, J.; Noller, H.F.
Deposited on : 2019-12-20
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

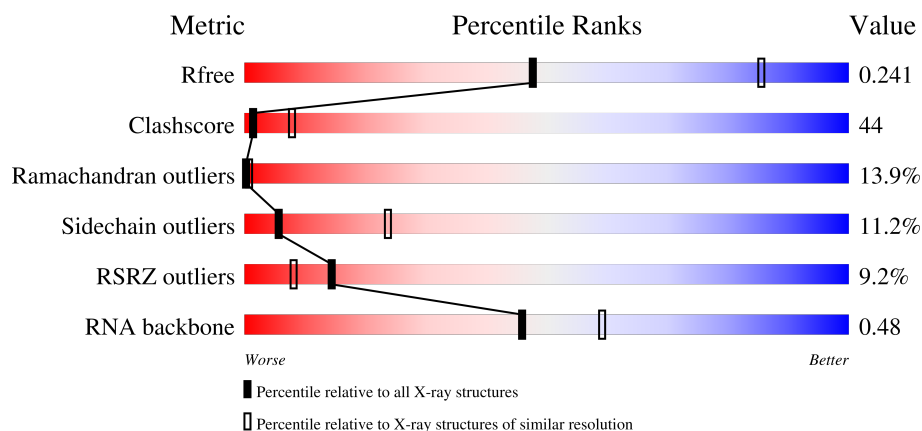
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	14% 21% 54% 22%
2	B	206	13% 17% 63% 18%
3	C	205	21% 18% 54% 26%
4	D	150	10% 28% 48% 21%

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Mol	Chain	Length	Quality of chain
5	E	100	
6	F	151	
7	G	129	
8	H	127	
9	I	98	
10	J	117	
11	K	123	
12	L	114	
13	M	100	
14	N	88	
15	O	82	
16	P	80	
17	Q	55	
18	R	79	
19	S	85	
20	T	51	
21	U	271	
22	V	209	
23	W	201	
24	X	177	
25	Y	176	
26	Z	141	
27	0	142	
28	1	122	
29	2	143	

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Mol	Chain	Length	Quality of chain
30	3	136	
31	4	120	
32	5	116	
33	6	114	
34	8	117	
35	9	103	
36	a	110	
37	b	93	
38	c	102	
39	d	94	
40	e	79	
41	f	77	
42	g	63	
43	h	58	
44	i	56	
45	j	50	
46	k	46	
47	l	64	
48	m	38	
49	n	163	
50	o	30	
50	p	30	
50	q	30	
50	r	30	
51	s	1532	

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Mol	Chain	Length	Quality of chain
52	t	2903	
53	u	118	
54	v	525	
55	w	6	
56	7	6	
56	AA	6	
56	BA	6	
56	y	6	
56	z	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	KBE	AA	1	-	-	-	X
56	UAL	AA	5	-	-	X	-
56	5OH	z	6	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 146817 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1702	1079	305	312	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	55	Total	C	N	O	0	0	0
			456	288	86	82			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 21 is a protein called 50S ribosomal protein L2.

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

- Molecule 22 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 23 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 24 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 25 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 26 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	0	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	5	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	8	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	9	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 36 is a protein called 50S ribosomal protein L22.

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

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	b	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	c	102	Total	C	N	O		0	0	0
			780	492	146	142				

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	d	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	e	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	f	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	g	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	h	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 44 is a protein called 50S ribosomal protein L32.

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

- Molecule 45 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	j	50	Total	C	N	O	S	0	0	0
			410	263	75	72				

- Molecule 46 is a protein called 50S ribosomal protein L34.

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

- Molecule 47 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	l	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 48 is a protein called 50S ribosomal protein L36.

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

- Molecule 49 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	n	163	Total	C	N	O	S	0	0	0
			1234	779	219	229	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	85	LEU	SER	conflict	UNP A0A1X3LA41
n	160	GLU	ASP	conflict	UNP A0A1X3LA41

- Molecule 50 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	o	30	Total	C	N	O	S	0	0	0
			228	144	33	48	3			
50	p	30	Total	C	N	O	S	0	0	0
			228	144	33	48	3			
50	q	30	Total	C	N	O	S	0	0	0
			228	144	33	48	3			
50	r	30	Total	C	N	O	S	0	0	0
			228	144	33	48	3			

- Molecule 51 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	s	1532	Total	C	N	O	P	0	0	0
			32870	14661	6031	10647	1531			

- Molecule 52 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	t	2850	Total	C	N	O	P	0	0	0
			61183	27295	11261	19778	2849			

- Molecule 53 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	u	118	Total	C	N	O	P	0	0	0
			2526	1126	464	819	117			

- Molecule 54 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	v	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	w	6	Total	C	N	O	P	0	0	0
			126	58	24	39	5			

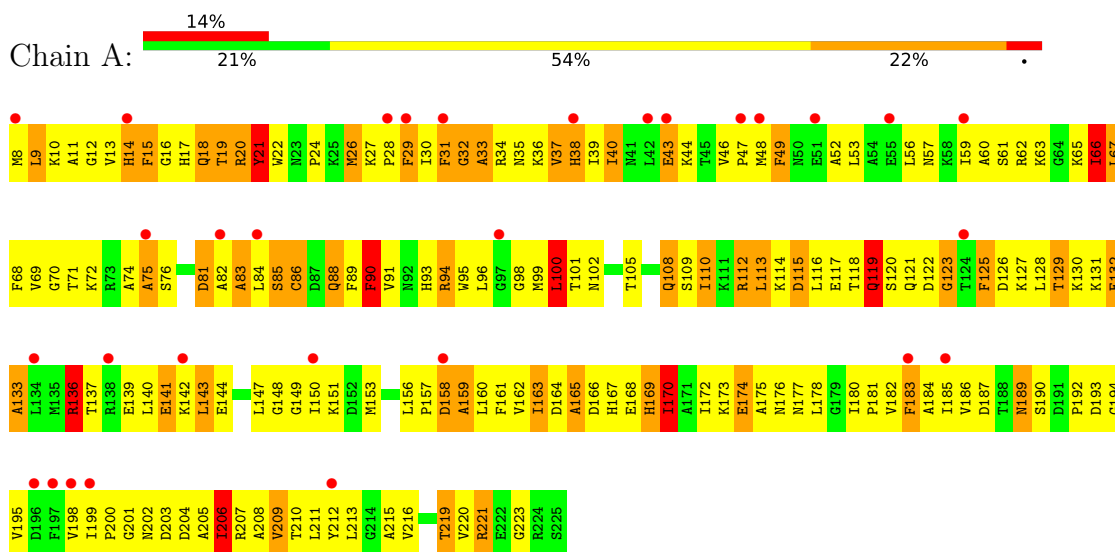
- Molecule 56 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	y	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	z	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	7	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	AA	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	BA	6	Total	C	N	O	0	0	0
			48	25	13	10			

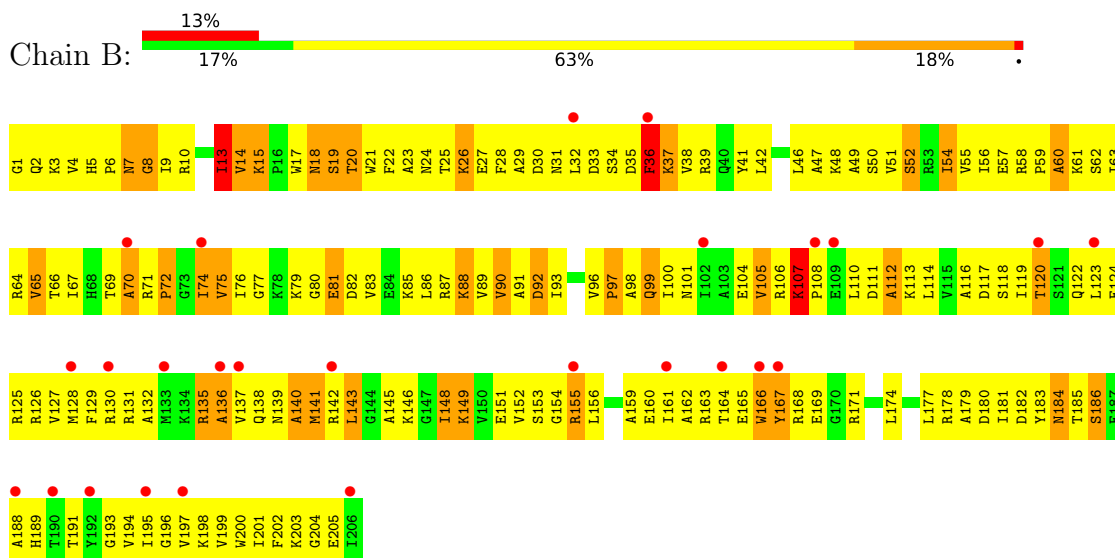
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

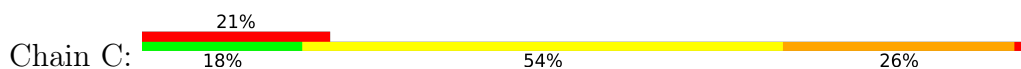
• Molecule 1: 30S ribosomal protein S2

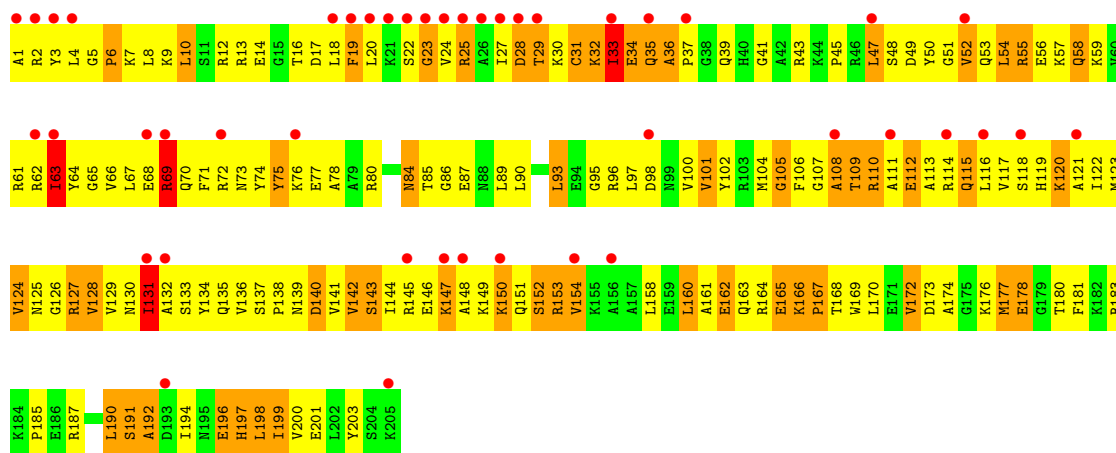


• Molecule 2: 30S ribosomal protein S3

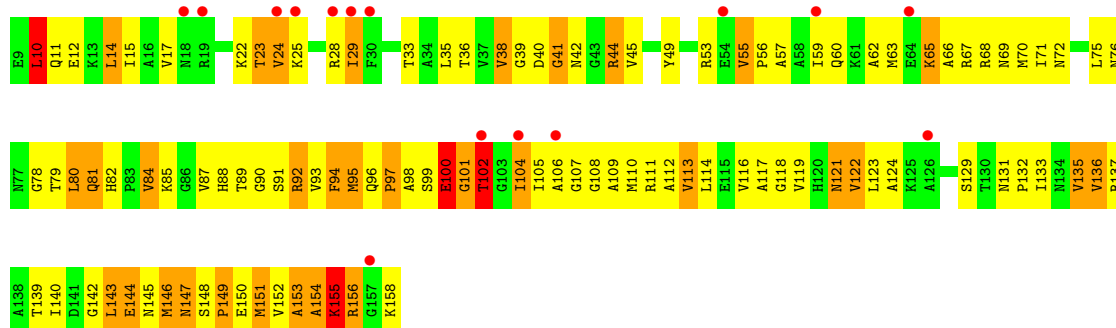


• Molecule 3: 30S ribosomal protein S4

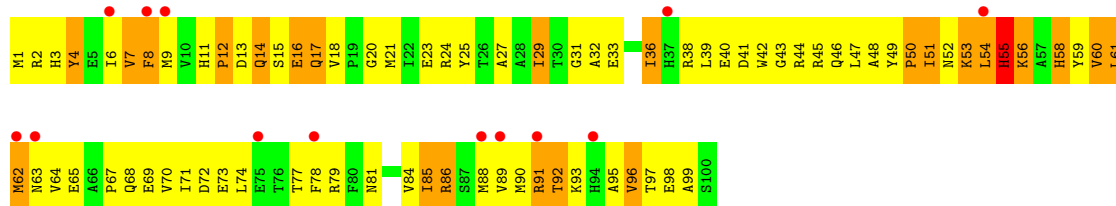




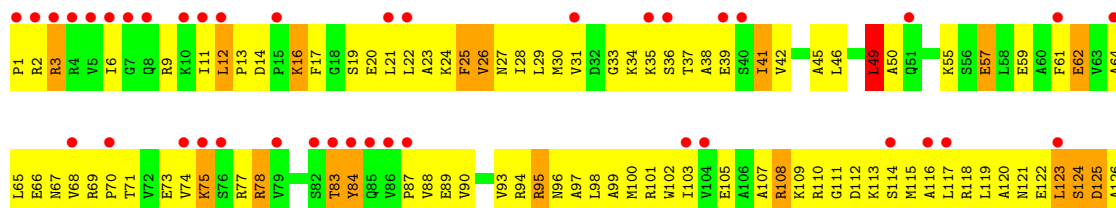
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

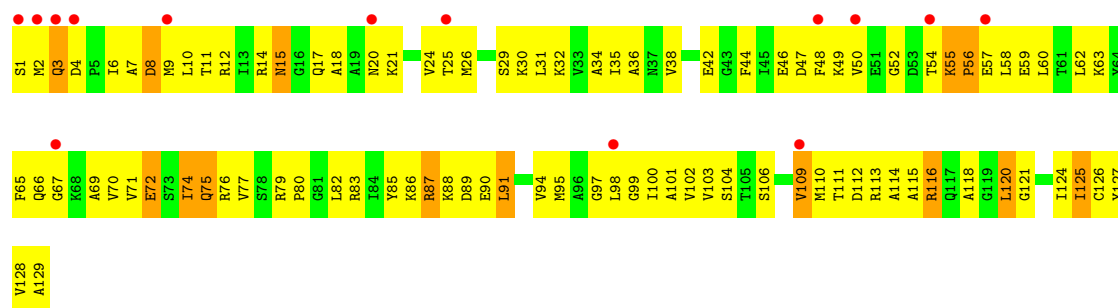


• Molecule 6: 30S ribosomal protein S7

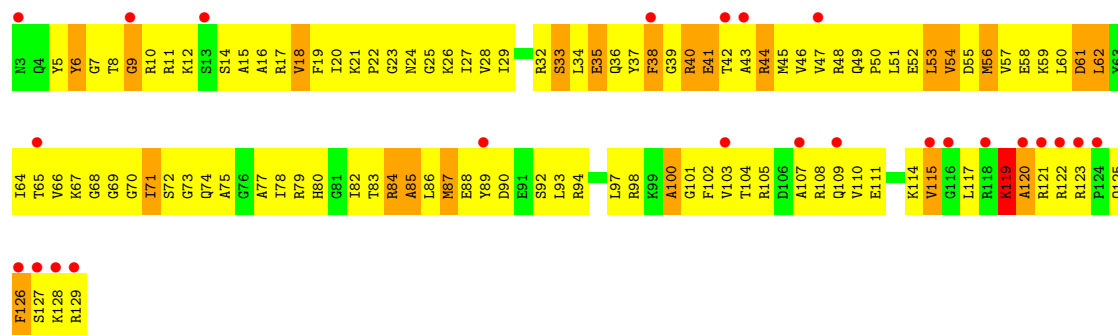




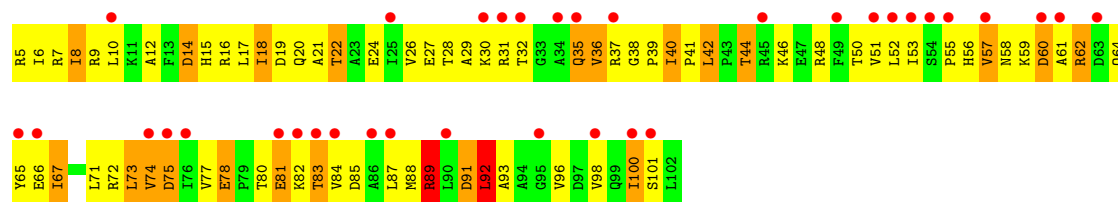
• Molecule 7: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

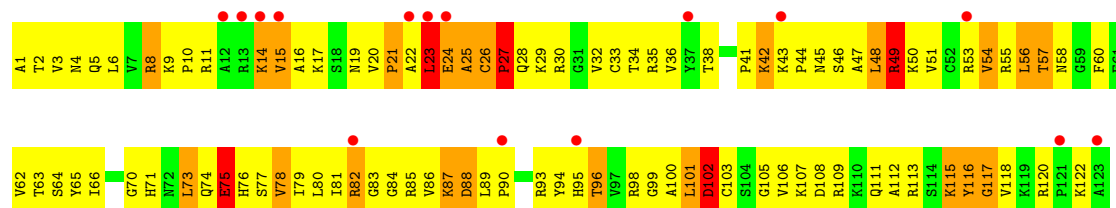


• Molecule 10: 30S ribosomal protein S11

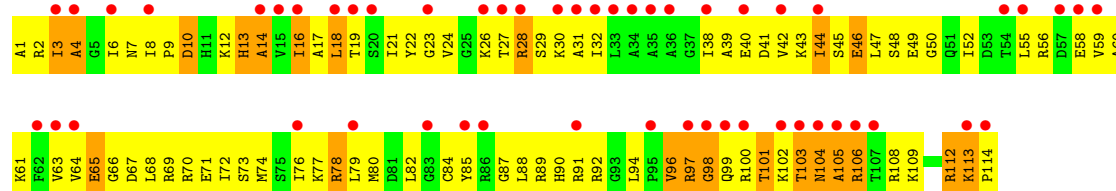




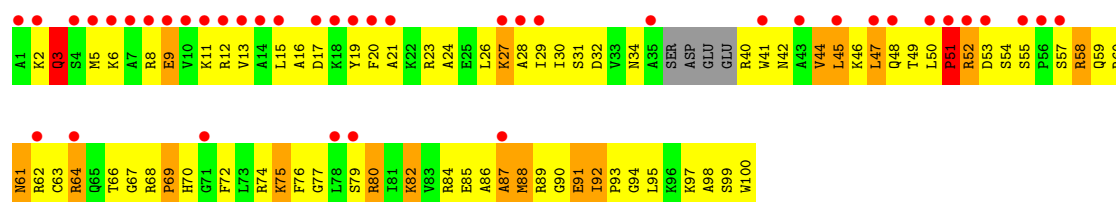
• Molecule 11: 30S ribosomal protein S12



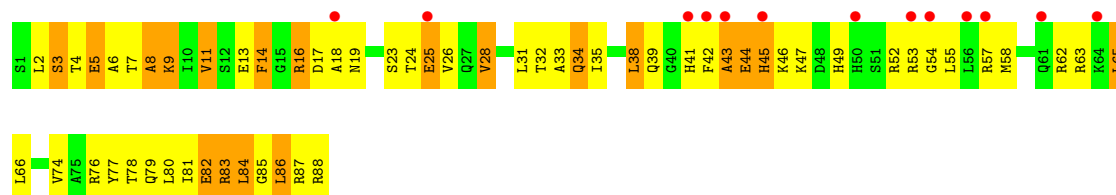
• Molecule 12: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S14

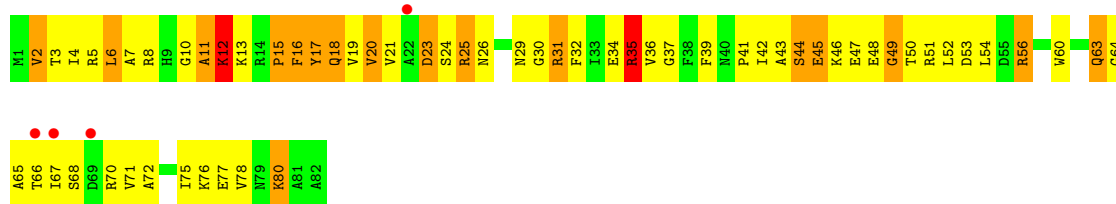


• Molecule 14: 30S ribosomal protein S15

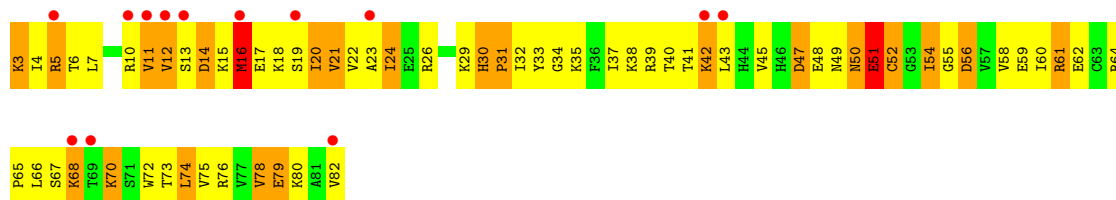
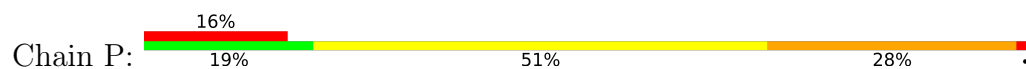


• Molecule 15: 30S ribosomal protein S16





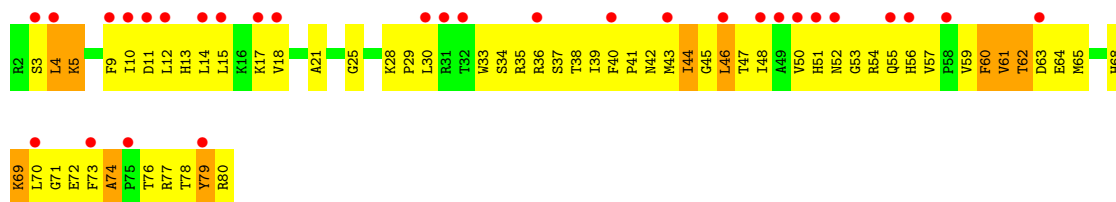
• Molecule 16: 30S ribosomal protein S17



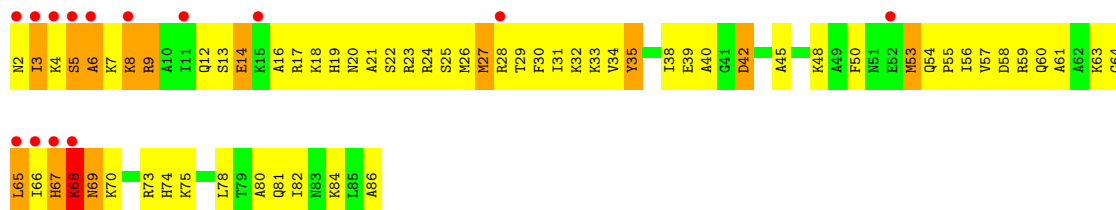
• Molecule 17: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S19

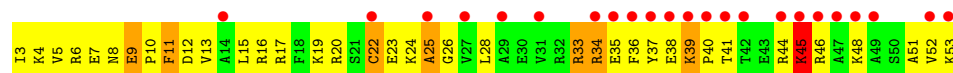


• Molecule 19: 30S ribosomal protein S20

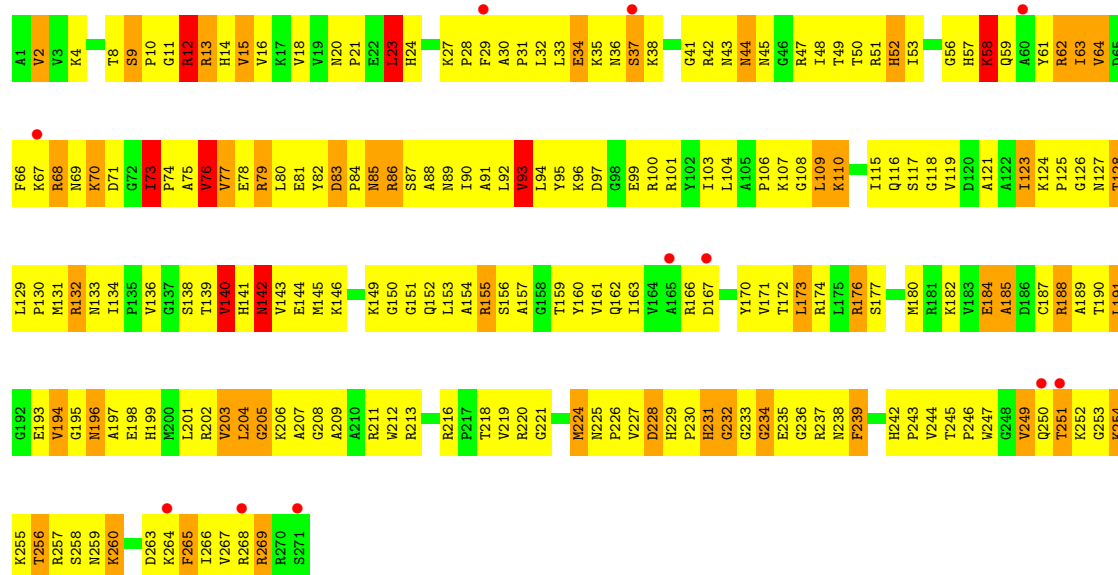


• Molecule 20: 30S ribosomal protein S21

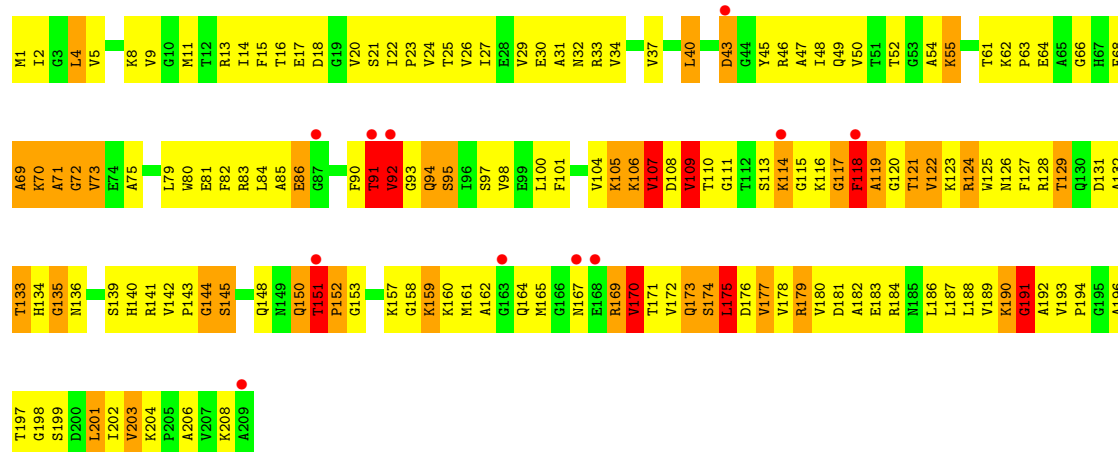




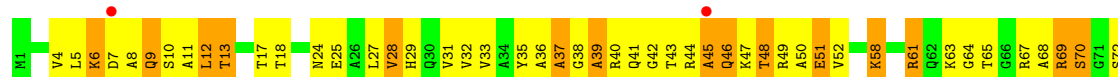
• Molecule 21: 50S ribosomal protein L2

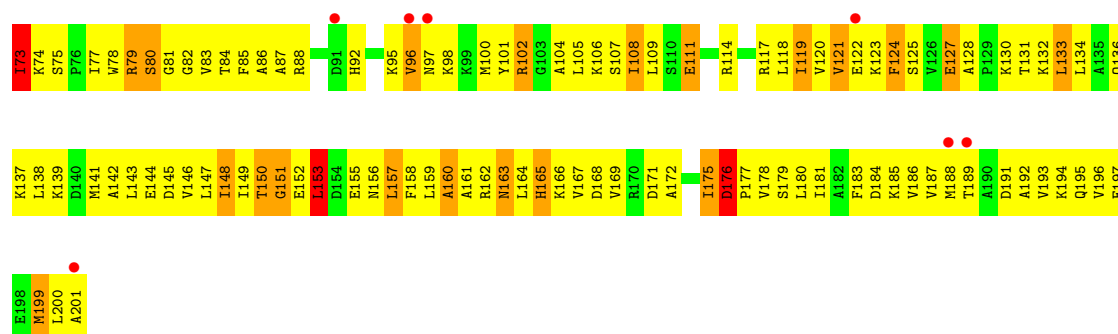


• Molecule 22: 50S ribosomal protein L3

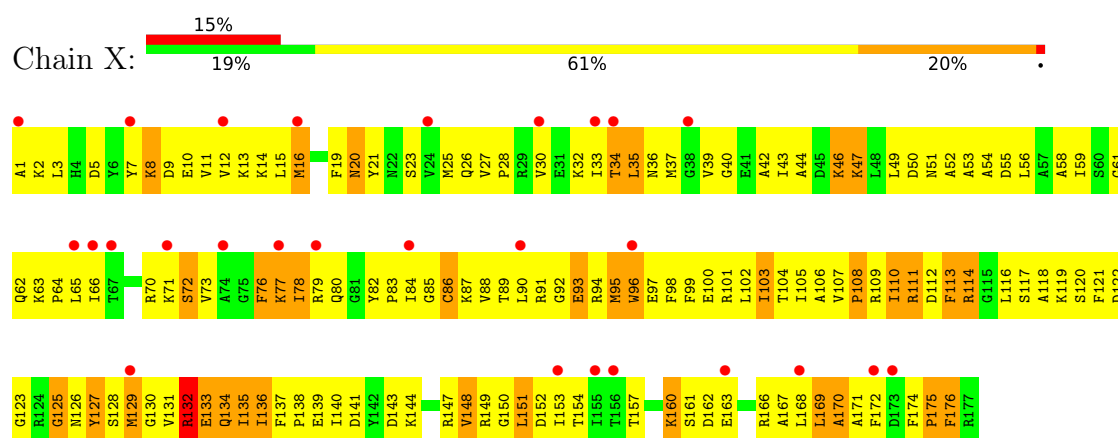


• Molecule 23: 50S ribosomal protein L4

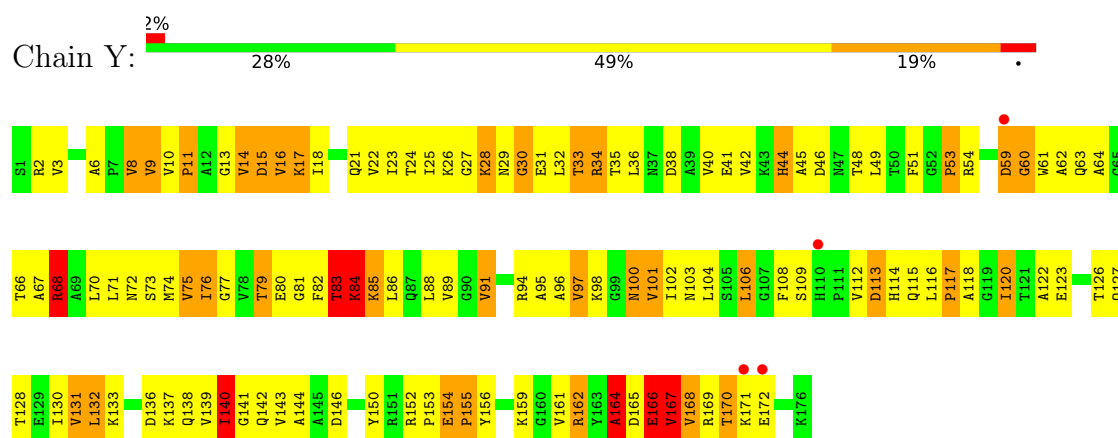




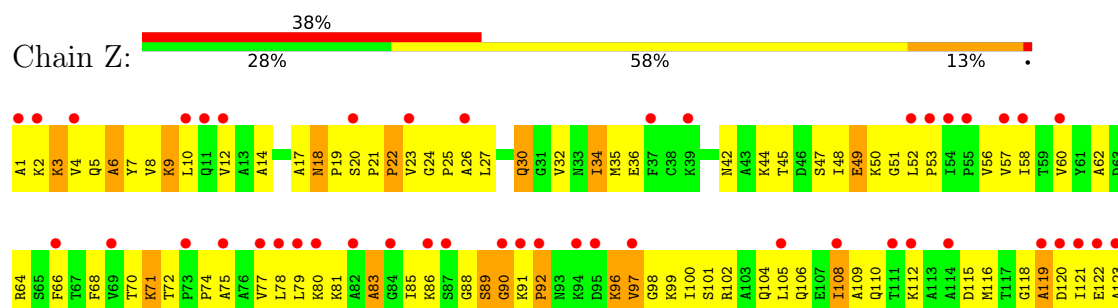
• Molecule 24: 50S ribosomal protein L5



• Molecule 25: 50S ribosomal protein L6

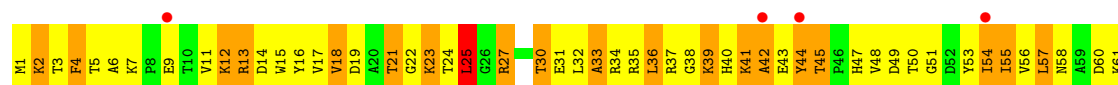


• Molecule 26: 50S ribosomal protein L11

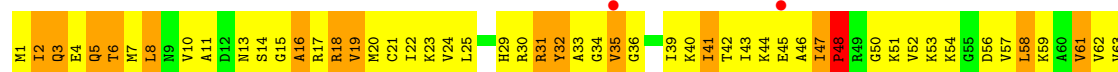




• Molecule 27: 50S ribosomal protein L13



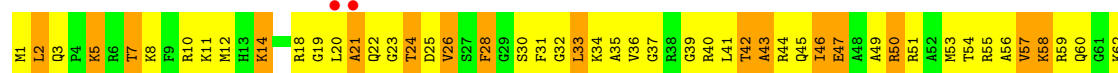
• Molecule 28: 50S ribosomal protein L14

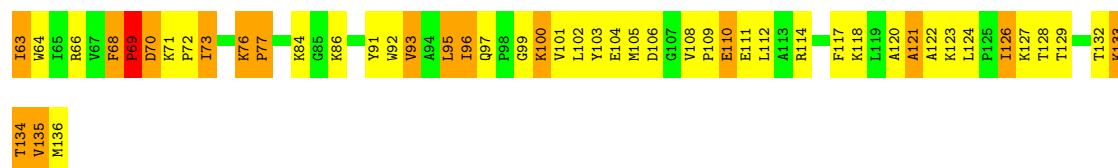


• Molecule 29: 50S ribosomal protein L15

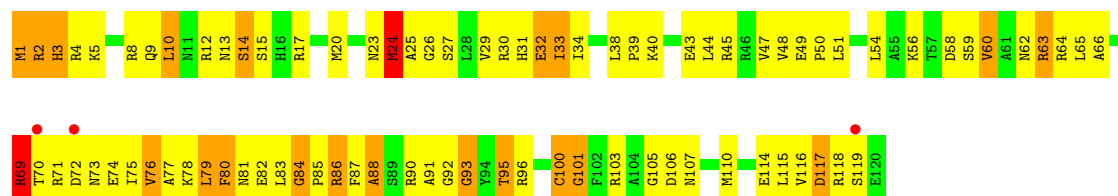


• Molecule 30: 50S ribosomal protein L16

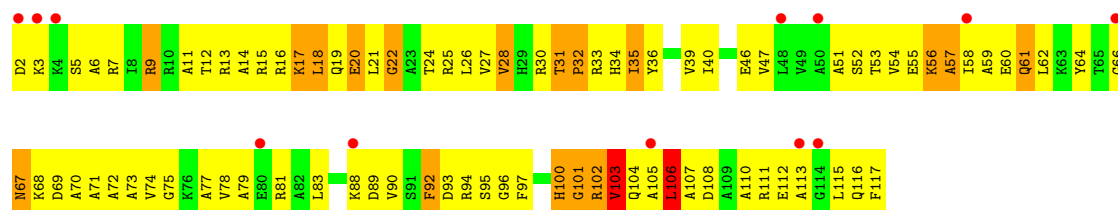




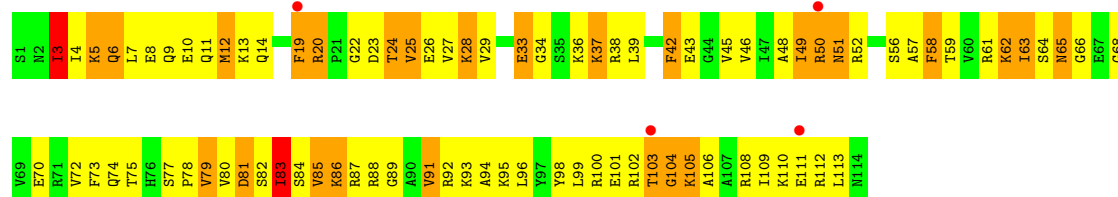
• Molecule 31: 50S ribosomal protein L17



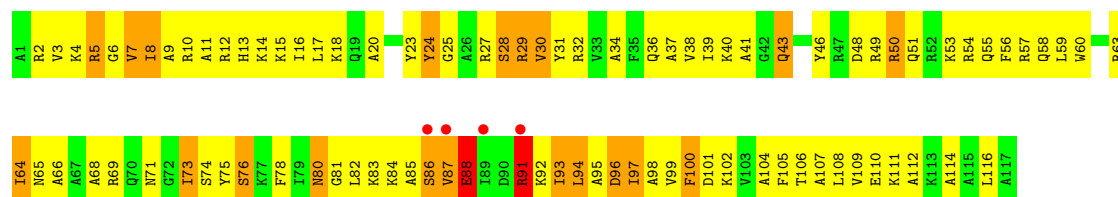
• Molecule 32: 50S ribosomal protein L18



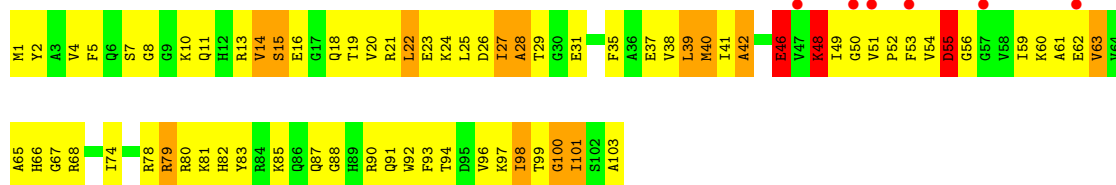
• Molecule 33: 50S ribosomal protein L19



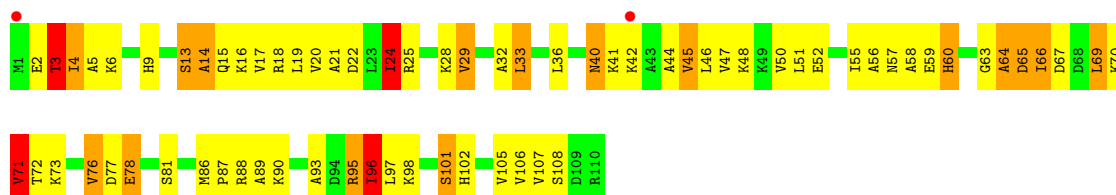
• Molecule 34: 50S ribosomal protein L20



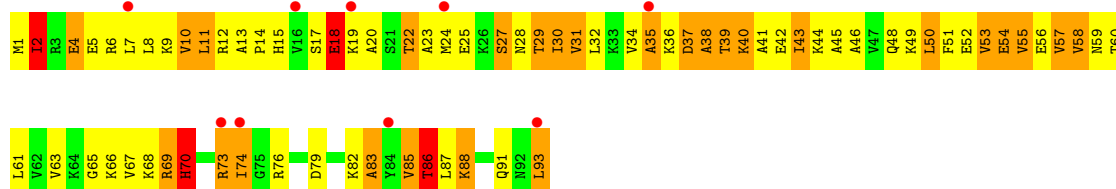
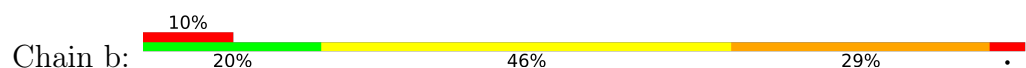
• Molecule 35: 50S ribosomal protein L21



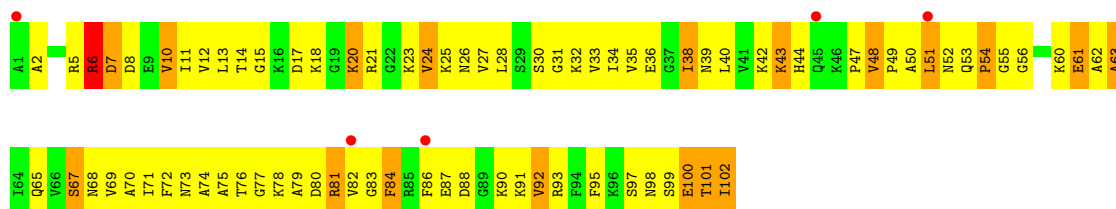
• Molecule 36: 50S ribosomal protein L22



• Molecule 37: 50S ribosomal protein L23



• Molecule 38: 50S ribosomal protein L24

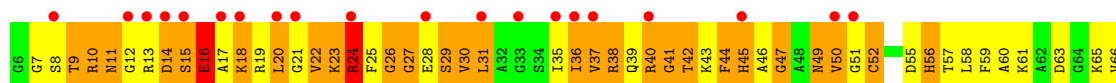


• Molecule 39: 50S ribosomal protein L25

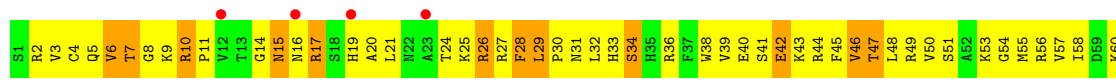
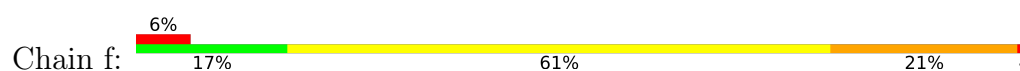




• Molecule 40: 50S ribosomal protein L27



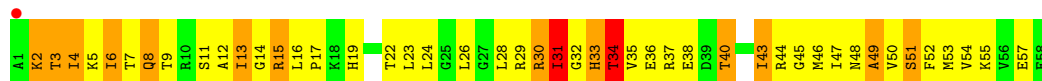
• Molecule 41: 50S ribosomal protein L28



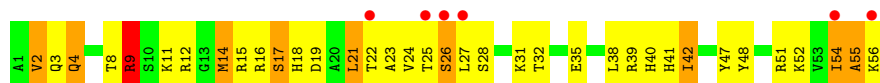
• Molecule 42: 50S ribosomal protein L29



• Molecule 43: 50S ribosomal protein L30



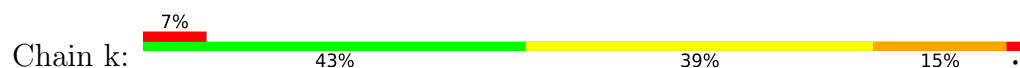
• Molecule 44: 50S ribosomal protein L32



• Molecule 45: 50S ribosomal protein L33



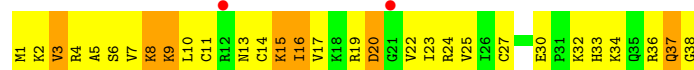
- Molecule 46: 50S ribosomal protein L34



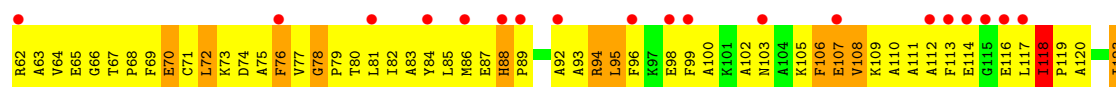
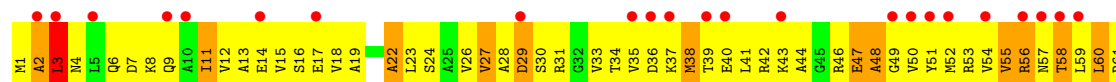
- Molecule 47: 50S ribosomal protein L35



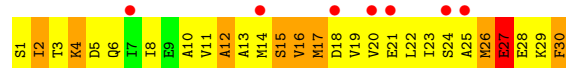
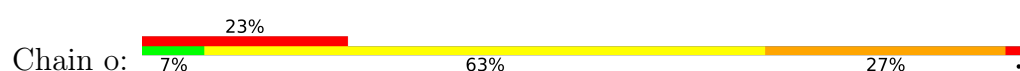
- Molecule 48: 50S ribosomal protein L36



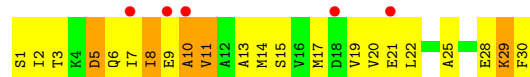
- Molecule 49: 50S ribosomal protein L10



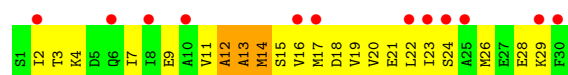
- Molecule 50: 50S ribosomal protein L7/L12



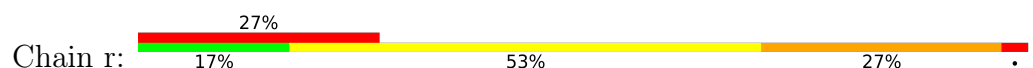
- Molecule 50: 50S ribosomal protein L7/L12



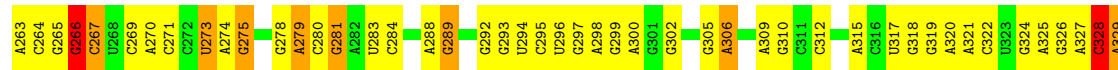
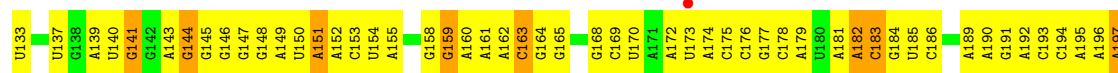
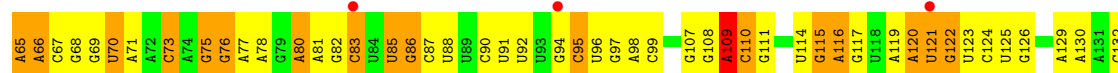
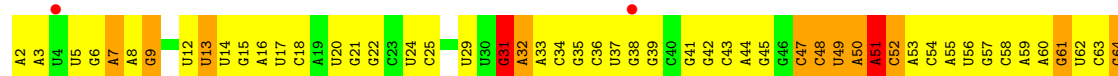
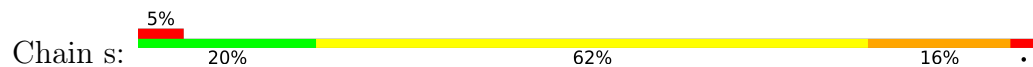
- Molecule 50: 50S ribosomal protein L7/L12



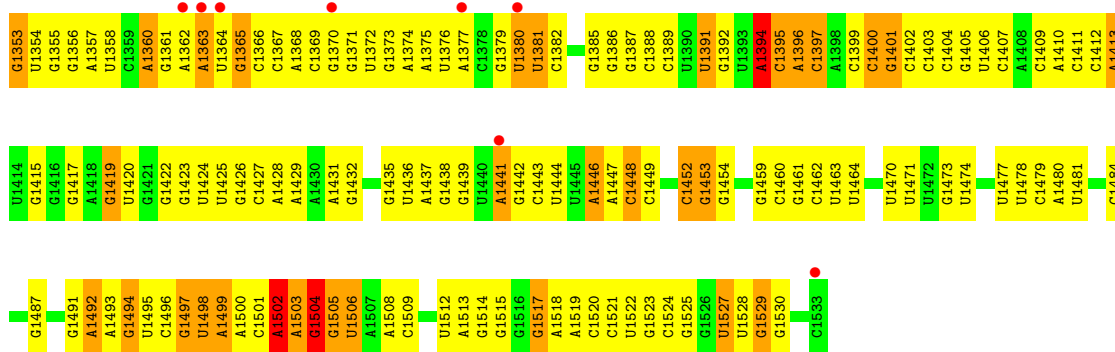
- Molecule 50: 50S ribosomal protein L7/L12



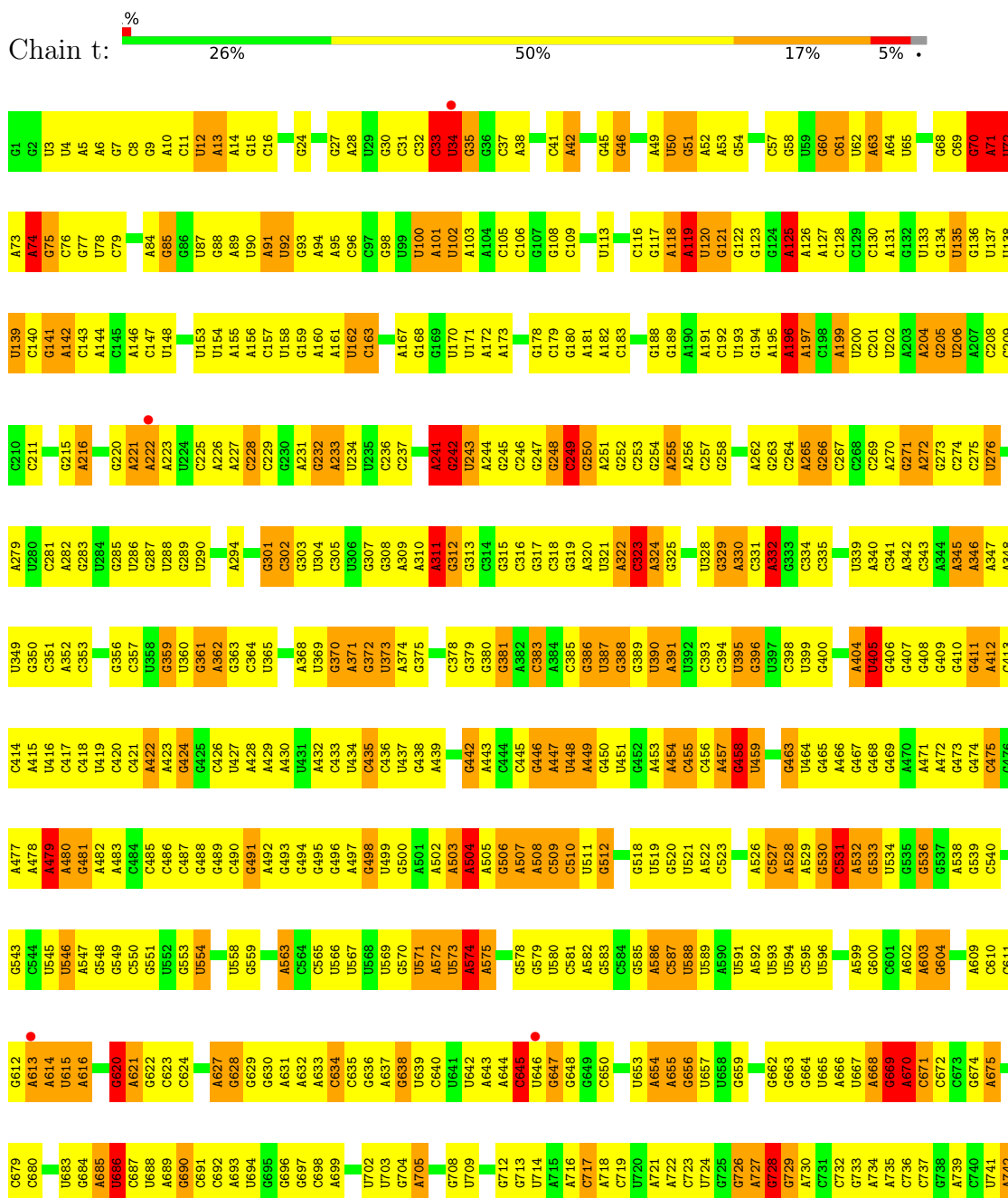
- Molecule 51: 16S ribosomal RNA





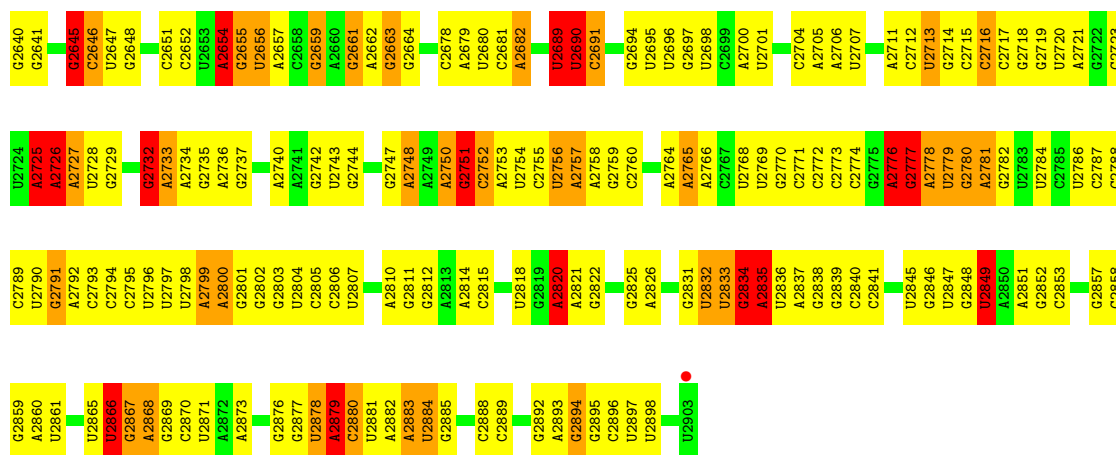


• Molecule 52: 23S ribosomal RNA

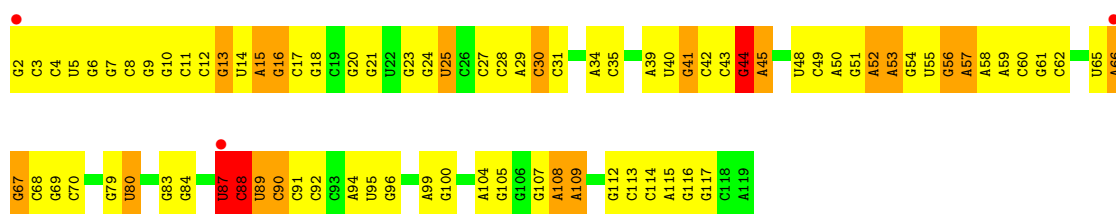




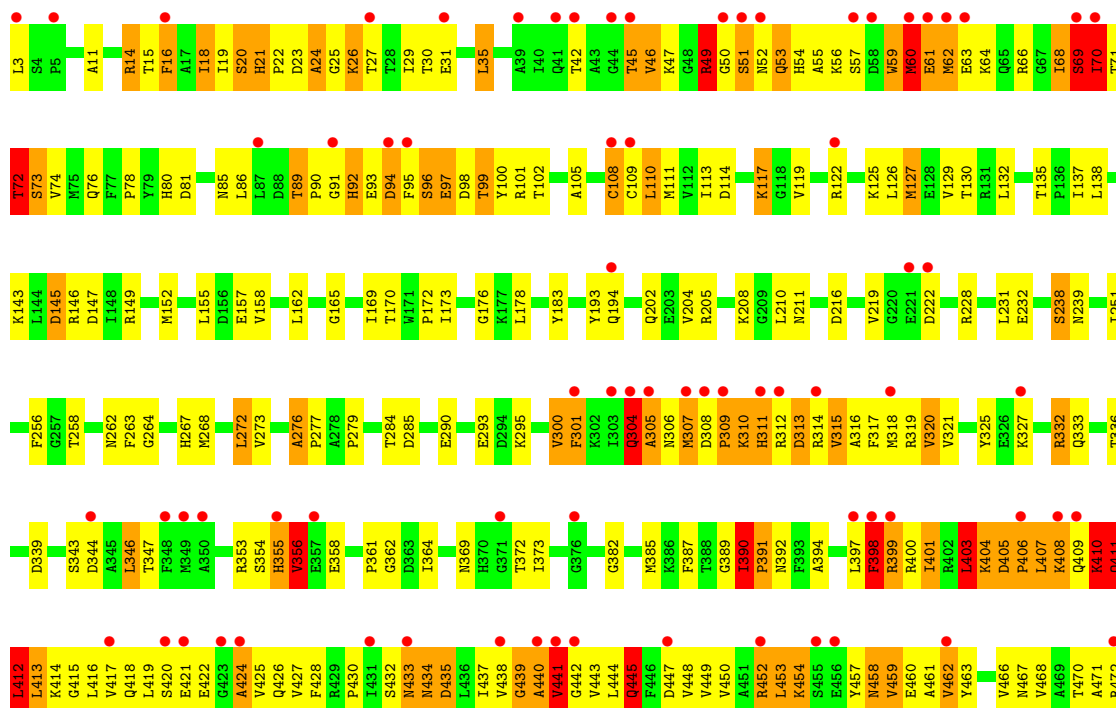


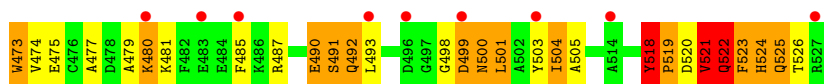


• Molecule 53: 5S ribosomal RNA

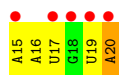
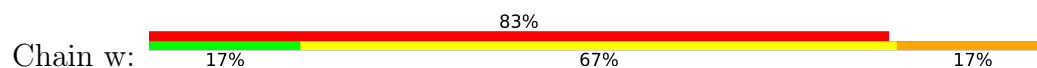


• Molecule 54: Peptide chain release factor 3

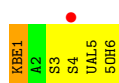




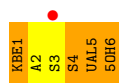
● Molecule 55: messenger RNA



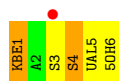
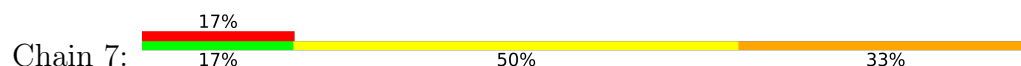
● Molecule 56: Viomycin



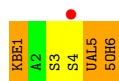
● Molecule 56: Viomycin



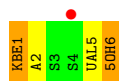
● Molecule 56: Viomycin



● Molecule 56: Viomycin



● Molecule 56: Viomycin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.10 100.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.00-3.10) 100.0 (100.00-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6	Depositor
R, R_{free}	0.210 , 0.240 0.238 , 0.241	Depositor DCC
R_{free} test set	26311 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	146817	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DPP, KBE, 5OH, UAL

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	A	0.42	1/1732 (0.1%)	0.98	10/2333 (0.4%)
2	B	0.42	0/1652	0.99	10/2225 (0.4%)
3	C	0.43	0/1665	0.97	7/2227 (0.3%)
4	D	0.49	0/1119	1.04	9/1504 (0.6%)
5	E	0.41	0/836	0.83	0/1128
6	F	0.35	0/1196	0.95	7/1602 (0.4%)
7	G	0.41	0/989	1.02	8/1326 (0.6%)
8	H	0.37	0/1034	0.91	4/1375 (0.3%)
9	I	0.45	0/797	0.95	3/1077 (0.3%)
10	J	0.41	0/893	0.94	2/1205 (0.2%)
11	K	0.55	0/969	1.19	7/1300 (0.5%)
12	L	0.34	0/893	0.87	1/1193 (0.1%)
13	M	0.38	0/785	0.93	2/1043 (0.2%)
14	N	0.37	0/722	0.89	2/964 (0.2%)
15	O	0.46	0/659	1.00	4/884 (0.5%)
16	P	0.40	0/658	1.03	5/881 (0.6%)
17	Q	0.45	0/463	0.95	2/621 (0.3%)
18	R	0.36	0/653	0.90	0/877
19	S	0.43	0/671	0.95	2/888 (0.2%)
20	T	0.44	0/431	1.03	3/570 (0.5%)
21	U	0.59	0/2122	1.27	22/2852 (0.8%)
22	V	0.65	0/1586	1.16	10/2134 (0.5%)
23	W	0.51	0/1571	1.07	12/2113 (0.6%)
24	X	0.35	0/1435	0.92	5/1926 (0.3%)
25	Y	0.51	0/1343	1.08	11/1816 (0.6%)
26	Z	0.36	0/1046	0.91	3/1410 (0.2%)
27	0	0.61	0/1152	1.13	11/1551 (0.7%)
28	1	0.67	0/948	1.17	9/1268 (0.7%)
29	2	0.49	0/1054	1.16	11/1403 (0.8%)
30	3	0.56	0/1093	1.14	12/1460 (0.8%)
31	4	0.59	0/974	1.18	7/1301 (0.5%)
32	5	0.39	0/902	0.97	3/1209 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.56	0/929	1.19	12/1242 (1.0%)
34	8	0.57	0/960	1.08	7/1278 (0.5%)
35	9	0.47	0/829	1.04	4/1107 (0.4%)
36	a	0.63	0/864	1.12	4/1156 (0.3%)
37	b	0.58	0/745	1.17	7/994 (0.7%)
38	c	0.47	0/788	1.11	7/1051 (0.7%)
39	d	0.43	0/766	0.86	1/1025 (0.1%)
40	e	0.60	0/603	1.14	6/797 (0.8%)
41	f	0.48	0/635	1.09	4/848 (0.5%)
42	g	0.43	0/510	1.08	6/677 (0.9%)
43	h	0.51	0/453	1.05	1/605 (0.2%)
44	i	0.61	0/450	1.12	3/599 (0.5%)
45	j	0.45	0/417	0.82	0/554
46	k	0.62	0/380	1.19	5/498 (1.0%)
47	l	0.47	0/513	0.93	2/676 (0.3%)
48	m	0.61	0/303	1.27	2/397 (0.5%)
49	n	0.37	0/1248	0.99	11/1679 (0.7%)
50	o	0.42	0/228	1.02	1/304 (0.3%)
50	p	0.36	0/228	0.72	0/304
50	q	0.41	0/228	0.98	2/304 (0.7%)
50	r	0.37	0/228	1.29	6/304 (2.0%)
51	s	0.36	0/36806	0.75	63/57419 (0.1%)
52	t	0.43	0/68523	0.86	206/106893 (0.2%)
53	u	0.34	0/2825	0.70	7/4406 (0.2%)
54	v	0.62	7/4221 (0.2%)	1.10	29/5702 (0.5%)
55	w	0.30	0/141	0.72	0/218
56	7	1.17	0/11	1.13	0/13
56	AA	1.70	0/11	1.38	0/13
56	BA	1.24	0/11	0.99	0/13
56	y	1.50	0/11	1.14	0/13
56	z	1.58	0/11	2.10	0/13
All	All	0.44	8/158919 (0.0%)	0.89	600/236768 (0.3%)

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
51	s	0	29
52	t	0	109
53	u	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
54	v	0	2
All	All	0	141

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	v	25	GLY	C-N	9.66	1.45	1.33
54	v	72	THR	C-O	8.58	1.34	1.24
54	v	26	LYS	C-N	-6.56	1.25	1.34
54	v	72	THR	CA-CB	6.09	1.63	1.53
54	v	70	ILE	CA-CB	5.82	1.62	1.54

The worst 5 of 600 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	24	ILE	N-CA-C	13.29	123.24	111.81
21	U	44	ASN	N-CA-C	-12.86	97.62	113.18
48	m	15	LYS	N-CA-C	11.64	129.37	111.56
50	r	7	ILE	N-CA-C	-10.41	103.82	113.71
21	U	63	ILE	N-CA-C	10.23	120.04	110.42

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	s	266	G	Sidechain
51	s	362	G	Sidechain
51	s	388	G	Sidechain
51	s	51	A	Sidechain
51	s	7	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1724	276	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1625	0	1699	239	0
3	C	1643	0	1710	297	0
4	D	1106	0	1148	191	0
5	E	818	0	808	136	0
6	F	1182	0	1240	156	0
7	G	979	0	1034	152	0
8	H	1022	0	1070	176	0
9	I	787	0	828	134	0
10	J	877	0	887	139	0
11	K	955	0	1019	169	0
12	L	884	0	944	155	0
13	M	774	0	827	149	0
14	N	714	0	737	69	0
15	O	649	0	666	91	0
16	P	649	0	691	110	0
17	Q	456	0	478	70	0
18	R	638	0	665	97	0
19	S	665	0	714	102	0
20	T	426	0	449	78	0
21	U	2083	0	2157	302	0
22	V	1565	0	1616	238	0
23	W	1552	0	1619	241	0
24	X	1411	0	1447	219	0
25	Y	1323	0	1374	181	0
26	Z	1032	0	1088	134	0
27	0	1129	0	1162	185	0
28	1	939	0	1012	127	0
29	2	1045	0	1117	151	0
30	3	1074	0	1157	130	0
31	4	961	0	1000	114	0
32	5	892	0	923	113	0
33	6	917	0	965	128	0
34	8	947	0	1022	185	0
35	9	816	0	839	117	0
36	a	857	0	922	105	0
37	b	739	0	807	140	0
38	c	780	0	834	89	0
39	d	753	0	780	83	0
40	e	596	0	610	193	0
41	f	625	0	655	79	0
42	g	509	0	543	73	0
43	h	449	0	491	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	444	0	461	37	0
45	j	410	0	440	51	0
46	k	377	0	418	40	0
47	l	504	0	574	61	0
48	m	302	0	340	55	0
49	n	1234	0	1290	283	0
50	o	228	0	237	68	0
50	p	228	0	237	38	0
50	q	228	0	237	44	0
50	r	228	0	237	57	0
51	s	32870	0	16543	1809	0
52	t	61183	0	30777	2580	0
53	u	2526	0	1282	125	0
54	v	4144	0	4129	283	0
55	w	126	0	66	5	0
56	7	48	0	40	8	0
56	AA	48	0	40	7	0
56	BA	48	0	41	4	0
56	y	48	0	40	5	0
56	z	48	0	41	13	0
All	All	146817	0	100948	10896	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 44.

The worst 5 of 10896 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)
25:Y:84:LYS:HG3	25:Y:132:LEU:N	1.52	1.24
51:s:158:G:H2'	51:s:159:G:H5''	1.24	1.19
52:t:1784:A:H4'	52:t:1785:A:O5'	1.44	1.18
52:t:1073:A:H3'	52:t:1074:G:H5''	1.17	1.16
12:L:27:THR:HG21	51:s:1328:C:H5''	1.27	1.14

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	216/218 (99%)	122 (56%)	56 (26%)	38 (18%)	0	0
2	B	204/206 (99%)	140 (69%)	36 (18%)	28 (14%)	0	1
3	C	203/205 (99%)	108 (53%)	46 (23%)	49 (24%)	0	0
4	D	148/150 (99%)	90 (61%)	36 (24%)	22 (15%)	0	0
5	E	98/100 (98%)	52 (53%)	26 (26%)	20 (20%)	0	0
6	F	149/151 (99%)	95 (64%)	41 (28%)	13 (9%)	0	4
7	G	127/129 (98%)	92 (72%)	29 (23%)	6 (5%)	2	11
8	H	125/127 (98%)	81 (65%)	26 (21%)	18 (14%)	0	0
9	I	96/98 (98%)	64 (67%)	17 (18%)	15 (16%)	0	0
10	J	115/117 (98%)	82 (71%)	21 (18%)	12 (10%)	0	2
11	K	121/123 (98%)	80 (66%)	20 (16%)	21 (17%)	0	0
12	L	112/114 (98%)	62 (55%)	33 (30%)	17 (15%)	0	0
13	M	92/100 (92%)	51 (55%)	27 (29%)	14 (15%)	0	0
14	N	86/88 (98%)	52 (60%)	28 (33%)	6 (7%)	1	5
15	O	80/82 (98%)	48 (60%)	18 (22%)	14 (18%)	0	0
16	P	78/80 (98%)	55 (70%)	10 (13%)	13 (17%)	0	0
17	Q	53/55 (96%)	30 (57%)	17 (32%)	6 (11%)	0	2
18	R	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	1
19	S	83/85 (98%)	51 (61%)	24 (29%)	8 (10%)	0	3
20	T	49/51 (96%)	25 (51%)	17 (35%)	7 (14%)	0	1
21	U	269/271 (99%)	204 (76%)	39 (14%)	26 (10%)	0	3
22	V	207/209 (99%)	138 (67%)	37 (18%)	32 (16%)	0	0
23	W	199/201 (99%)	135 (68%)	40 (20%)	24 (12%)	0	1
24	X	175/177 (99%)	114 (65%)	34 (19%)	27 (15%)	0	0
25	Y	174/176 (99%)	108 (62%)	36 (21%)	30 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	139/141 (99%)	66 (48%)	51 (37%)	22 (16%)	0	0
27	0	140/142 (99%)	94 (67%)	27 (19%)	19 (14%)	0	1
28	1	120/122 (98%)	82 (68%)	24 (20%)	14 (12%)	0	1
29	2	141/143 (99%)	94 (67%)	23 (16%)	24 (17%)	0	0
30	3	134/136 (98%)	95 (71%)	23 (17%)	16 (12%)	0	1
31	4	118/120 (98%)	83 (70%)	20 (17%)	15 (13%)	0	1
32	5	114/116 (98%)	79 (69%)	25 (22%)	10 (9%)	0	3
33	6	112/114 (98%)	71 (63%)	23 (20%)	18 (16%)	0	0
34	8	115/117 (98%)	73 (64%)	31 (27%)	11 (10%)	0	3
35	9	101/103 (98%)	73 (72%)	20 (20%)	8 (8%)	1	4
36	a	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	0	3
37	b	91/93 (98%)	54 (59%)	18 (20%)	19 (21%)	0	0
38	c	100/102 (98%)	63 (63%)	17 (17%)	20 (20%)	0	0
39	d	92/94 (98%)	62 (67%)	19 (21%)	11 (12%)	0	1
40	e	77/79 (98%)	29 (38%)	21 (27%)	27 (35%)	0	0
41	f	75/77 (97%)	54 (72%)	16 (21%)	5 (7%)	1	6
42	g	61/63 (97%)	34 (56%)	15 (25%)	12 (20%)	0	0
43	h	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	0	3
44	i	54/56 (96%)	44 (82%)	5 (9%)	5 (9%)	0	3
45	j	48/50 (96%)	32 (67%)	14 (29%)	2 (4%)	2	13
46	k	44/46 (96%)	36 (82%)	4 (9%)	4 (9%)	0	3
47	l	62/64 (97%)	45 (73%)	11 (18%)	6 (10%)	0	3
48	m	36/38 (95%)	30 (83%)	2 (6%)	4 (11%)	0	2
49	n	161/163 (99%)	77 (48%)	53 (33%)	31 (19%)	0	0
50	o	28/30 (93%)	12 (43%)	9 (32%)	7 (25%)	0	0
50	p	28/30 (93%)	16 (57%)	8 (29%)	4 (14%)	0	1
50	q	28/30 (93%)	14 (50%)	12 (43%)	2 (7%)	1	5
50	r	28/30 (93%)	19 (68%)	6 (21%)	3 (11%)	0	2
54	v	523/525 (100%)	381 (73%)	82 (16%)	60 (12%)	0	1
56	7	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
56	AA	2/6 (33%)	1 (50%)	0	1 (50%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	BA	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
56	y	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
56	z	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	6280/6414 (98%)	4060 (65%)	1346 (21%)	874 (14%)	0	1

5 of 874 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ALA
1	A	67	LEU
1	A	75	ALA
1	A	94	ARG
1	A	120	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	179/180 (99%)	151 (84%)	28 (16%)	2	12
2	B	170/170 (100%)	157 (92%)	13 (8%)	12	39
3	C	172/172 (100%)	154 (90%)	18 (10%)	6	26
4	D	113/113 (100%)	99 (88%)	14 (12%)	4	19
5	E	87/87 (100%)	78 (90%)	9 (10%)	7	27
6	F	124/124 (100%)	115 (93%)	9 (7%)	13	40
7	G	104/104 (100%)	100 (96%)	4 (4%)	29	60
8	H	105/105 (100%)	96 (91%)	9 (9%)	10	34
9	I	86/86 (100%)	74 (86%)	12 (14%)	3	15
10	J	90/90 (100%)	75 (83%)	15 (17%)	2	10
11	K	103/103 (100%)	93 (90%)	10 (10%)	8	30
12	L	92/92 (100%)	88 (96%)	4 (4%)	26	57
13	M	79/83 (95%)	73 (92%)	6 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	76/76 (100%)	63 (83%)	13 (17%)	2	10
15	O	65/65 (100%)	57 (88%)	8 (12%)	4	20
16	P	74/74 (100%)	63 (85%)	11 (15%)	3	13
17	Q	48/48 (100%)	43 (90%)	5 (10%)	7	27
18	R	70/70 (100%)	68 (97%)	2 (3%)	37	66
19	S	65/65 (100%)	58 (89%)	7 (11%)	6	25
20	T	44/44 (100%)	41 (93%)	3 (7%)	14	42
21	U	216/216 (100%)	189 (88%)	27 (12%)	4	19
22	V	164/164 (100%)	145 (88%)	19 (12%)	5	22
23	W	165/165 (100%)	148 (90%)	17 (10%)	7	27
24	X	148/148 (100%)	137 (93%)	11 (7%)	13	40
25	Y	137/137 (100%)	115 (84%)	22 (16%)	2	11
26	Z	109/109 (100%)	106 (97%)	3 (3%)	38	66
27	0	116/116 (100%)	99 (85%)	17 (15%)	3	14
28	1	103/103 (100%)	87 (84%)	16 (16%)	2	12
29	2	102/102 (100%)	89 (87%)	13 (13%)	4	18
30	3	109/109 (100%)	93 (85%)	16 (15%)	3	14
31	4	100/100 (100%)	93 (93%)	7 (7%)	14	41
32	5	86/86 (100%)	75 (87%)	11 (13%)	4	18
33	6	99/99 (100%)	90 (91%)	9 (9%)	9	32
34	8	89/89 (100%)	80 (90%)	9 (10%)	7	28
35	9	84/84 (100%)	76 (90%)	8 (10%)	8	30
36	a	93/93 (100%)	78 (84%)	15 (16%)	2	11
37	b	80/80 (100%)	67 (84%)	13 (16%)	2	11
38	c	83/83 (100%)	76 (92%)	7 (8%)	10	35
39	d	78/78 (100%)	74 (95%)	4 (5%)	21	52
40	e	59/59 (100%)	52 (88%)	7 (12%)	5	21
41	f	67/67 (100%)	57 (85%)	10 (15%)	3	13
42	g	55/55 (100%)	52 (94%)	3 (6%)	19	50
43	h	48/48 (100%)	36 (75%)	12 (25%)	0	2
44	i	47/47 (100%)	39 (83%)	8 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	j	45/45 (100%)	43 (96%)	2 (4%)	25	56
46	k	38/38 (100%)	35 (92%)	3 (8%)	11	37
47	l	51/51 (100%)	48 (94%)	3 (6%)	18	48
48	m	34/34 (100%)	28 (82%)	6 (18%)	2	9
49	n	123/123 (100%)	116 (94%)	7 (6%)	18	49
50	o	26/26 (100%)	23 (88%)	3 (12%)	5	23
50	p	26/26 (100%)	25 (96%)	1 (4%)	29	60
50	q	26/26 (100%)	26 (100%)	0	100	100
50	r	26/26 (100%)	23 (88%)	3 (12%)	5	23
54	v	447/449 (100%)	372 (83%)	75 (17%)	2	10
56	7	2/2 (100%)	2 (100%)	0	100	100
56	AA	2/2 (100%)	2 (100%)	0	100	100
56	BA	2/2 (100%)	2 (100%)	0	100	100
56	y	2/2 (100%)	2 (100%)	0	100	100
56	z	2/2 (100%)	2 (100%)	0	100	100
All	All	5235/5242 (100%)	4648 (89%)	587 (11%)	6	24

5 of 587 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	g	47	ARG
54	v	447	ASP
44	i	2	VAL
42	g	39	GLN
54	v	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	26	GLN
54	v	306	ASN
32	5	61	GLN
54	v	267	HIS
44	i	37	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	s	1531/1532 (99%)	300 (19%)	0
52	t	2845/2903 (98%)	685 (24%)	0
53	u	117/118 (99%)	18 (15%)	0
55	w	5/6 (83%)	2 (40%)	0
All	All	4498/4559 (98%)	1005 (22%)	0

5 of 1005 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	s	5	U
51	s	9	G
51	s	13	U
51	s	14	U
51	s	22	G

There are no RNA pucker outliers to report.

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

20 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	$\# Z > 2$
56	5OH	y	6	56	7,12,13	0.89	0	4,16,18	2.13	2 (50%)
56	5OH	7	6	56	7,12,13	1.90	2 (28%)	4,16,18	2.58	1 (25%)
56	UAL	7	5	56	6,8,9	2.80	1 (16%)	4,9,11	1.16	0
56	KBE	7	1	56	8,8,9	0.71	0	6,8,10	1.22	1 (16%)
56	5OH	BA	6	56	7,12,13	1.21	1 (14%)	4,16,18	1.94	2 (50%)
56	UAL	BA	5	56	6,8,9	2.81	1 (16%)	4,9,11	1.78	1 (25%)
56	KBE	y	1	56	8,8,9	1.36	1 (12%)	6,8,10	2.04	1 (16%)
56	KBE	BA	1	56	8,8,9	1.19	1 (12%)	6,8,10	1.35	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	DPP	y	2	56	4,5,6	0.36	0	1,5,7	0.32	0
56	UAL	y	5	56	6,8,9	2.39	2 (33%)	4,9,11	1.38	1 (25%)
56	5OH	z	6	56	7,12,13	1.10	1 (14%)	4,16,18	1.00	0
56	DPP	z	2	56	4,5,6	0.64	0	1,5,7	0.39	0
56	DPP	AA	2	56	4,5,6	1.14	0	1,5,7	1.27	0
56	UAL	AA	5	56	6,8,9	2.65	1 (16%)	4,9,11	1.47	1 (25%)
56	UAL	z	5	56	6,8,9	1.89	3 (50%)	4,9,11	2.84	1 (25%)
56	KBE	z	1	56	8,8,9	1.22	1 (12%)	6,8,10	2.15	1 (16%)
56	KBE	AA	1	56	8,8,9	1.65	2 (25%)	6,8,10	3.50	1 (16%)
56	DPP	7	2	56	4,5,6	0.94	0	1,5,7	0.94	0
56	5OH	AA	6	56	7,12,13	1.39	1 (14%)	4,16,18	1.51	1 (25%)
56	DPP	BA	2	56	4,5,6	1.47	0	1,5,7	0.09	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
56	5OH	y	6	56	-	0/2/18/20	0/1/1/1
56	5OH	7	6	56	-	0/2/18/20	0/1/1/1
56	UAL	7	5	56	-	0/3/7/9	-
56	KBE	7	1	56	-	3/7/7/8	-
56	5OH	BA	6	56	-	2/2/18/20	0/1/1/1
56	UAL	BA	5	56	-	0/3/7/9	-
56	KBE	y	1	56	-	2/7/7/8	-
56	KBE	BA	1	56	-	4/7/7/8	-
56	DPP	y	2	56	-	0/2/4/6	-
56	UAL	y	5	56	-	0/3/7/9	-
56	5OH	z	6	56	-	1/2/18/20	0/1/1/1
56	DPP	z	2	56	-	0/2/4/6	-
56	DPP	AA	2	56	-	0/2/4/6	-
56	UAL	AA	5	56	-	0/3/7/9	-
56	UAL	z	5	56	-	0/3/7/9	-
56	KBE	z	1	56	-	2/7/7/8	-
56	KBE	AA	1	56	-	0/7/7/8	-
56	DPP	7	2	56	-	0/2/4/6	-
56	5OH	AA	6	56	-	0/2/18/20	0/1/1/1
56	DPP	BA	2	56	-	0/2/4/6	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	7	5	UAL	C-CA	6.71	1.56	1.45
56	BA	5	UAL	C-CA	6.52	1.56	1.45
56	AA	5	UAL	C-CA	5.79	1.54	1.45
56	y	5	UAL	C-CA	4.88	1.53	1.45
56	AA	1	KBE	CA-CB	3.50	1.57	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	1	KBE	CB-CA-C	8.37	125.67	112.17
56	z	5	UAL	O-C-CA	-5.41	118.61	125.39
56	7	6	5OH	CR-CB-CA	5.07	117.99	112.61
56	z	1	KBE	CB-CA-C	4.82	119.95	112.17
56	y	1	KBE	CB-CA-C	4.65	119.68	112.17

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	y	1	KBE	CA-CB-CG-CD
56	z	1	KBE	C-CA-CB-N
56	7	1	KBE	C-CA-CB-N
56	7	1	KBE	CA-CB-CG-CD
56	BA	1	KBE	C-CA-CB-CG

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	7	1	KBE	3	0
56	BA	6	5OH	2	0
56	y	1	KBE	2	0
56	BA	1	KBE	1	0
56	z	6	5OH	6	0
56	z	2	DPP	2	0
56	AA	5	UAL	4	0
56	z	5	UAL	3	0
56	z	1	KBE	1	0
56	AA	1	KBE	1	0
56	AA	6	5OH	2	0
56	BA	2	DPP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/218 (100%)	1.11	30 (13%) 6 4	96, 133, 180, 198	0
2	B	206/206 (100%)	0.98	26 (12%) 8 4	73, 120, 145, 151	0
3	C	205/205 (100%)	1.38	44 (21%) 2 1	88, 115, 150, 205	0
4	D	150/150 (100%)	0.87	15 (10%) 12 6	73, 94, 139, 171	0
5	E	100/100 (100%)	1.00	13 (13%) 7 4	101, 135, 155, 159	0
6	F	151/151 (100%)	1.71	41 (27%) 1 1	111, 187, 225, 236	0
7	G	129/129 (100%)	0.79	14 (10%) 10 5	77, 101, 133, 142	0
8	H	127/127 (100%)	1.33	24 (18%) 3 1	82, 134, 190, 220	0
9	I	98/98 (100%)	1.78	35 (35%) 1 0	90, 110, 193, 210	0
10	J	117/117 (100%)	0.74	4 (3%) 48 28	76, 111, 147, 165	0
11	K	123/123 (100%)	0.81	15 (12%) 8 5	53, 76, 115, 156	0
12	L	114/114 (100%)	2.24	52 (45%) 0 0	166, 207, 253, 272	0
13	M	96/100 (96%)	2.27	41 (42%) 0 0	79, 143, 196, 206	0
14	N	88/88 (100%)	0.97	13 (14%) 5 3	76, 104, 140, 149	0
15	O	82/82 (100%)	0.94	4 (4%) 35 18	78, 101, 164, 212	0
16	P	80/80 (100%)	1.24	13 (16%) 4 2	79, 119, 168, 183	0
17	Q	55/55 (100%)	1.01	8 (14%) 6 3	80, 100, 133, 190	0
18	R	79/79 (100%)	2.00	30 (37%) 1 0	156, 207, 226, 233	0
19	S	85/85 (100%)	1.03	14 (16%) 4 2	82, 111, 136, 153	0
20	T	51/51 (100%)	2.13	23 (45%) 0 0	119, 147, 188, 197	0
21	U	271/271 (100%)	0.34	11 (4%) 41 23	37, 65, 82, 107	0
22	V	209/209 (100%)	0.34	11 (5%) 32 17	31, 58, 94, 119	0
23	W	201/201 (100%)	0.49	9 (4%) 38 20	38, 76, 115, 160	0
24	X	177/177 (100%)	1.16	27 (15%) 5 3	113, 142, 190, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	176/176 (100%)	0.52	4 (2%) 61 39	58, 82, 124, 141	0
26	Z	141/141 (100%)	1.87	53 (37%) 1 0	185, 260, 305, 346	0
27	0	142/142 (100%)	0.36	11 (7%) 19 10	49, 64, 94, 128	0
28	1	122/122 (100%)	0.28	4 (3%) 49 29	46, 61, 88, 115	0
29	2	143/143 (100%)	0.75	11 (7%) 19 10	45, 85, 123, 154	0
30	3	136/136 (100%)	0.30	2 (1%) 72 52	44, 70, 103, 137	0
31	4	120/120 (100%)	-0.01	3 (2%) 58 37	41, 57, 70, 171	0
32	5	116/116 (100%)	0.97	12 (10%) 12 6	85, 106, 130, 136	0
33	6	114/114 (100%)	0.38	4 (3%) 47 27	48, 72, 115, 141	0
34	8	117/117 (100%)	0.21	4 (3%) 48 28	34, 60, 98, 119	0
35	9	103/103 (100%)	0.53	6 (5%) 29 16	46, 88, 128, 139	0
36	a	110/110 (100%)	0.08	2 (1%) 67 47	41, 55, 86, 138	0
37	b	93/93 (100%)	0.74	9 (9%) 13 7	49, 81, 143, 167	0
38	c	102/102 (100%)	0.66	5 (4%) 35 18	65, 84, 153, 167	0
39	d	94/94 (100%)	0.49	3 (3%) 50 30	69, 98, 120, 143	0
40	e	79/79 (100%)	1.55	23 (29%) 1 1	66, 90, 125, 136	0
41	f	77/77 (100%)	0.76	5 (6%) 25 13	57, 72, 124, 133	0
42	g	63/63 (100%)	0.79	8 (12%) 8 4	73, 99, 138, 170	0
43	h	58/58 (100%)	0.59	1 (1%) 69 48	63, 76, 133, 144	0
44	i	56/56 (100%)	0.39	6 (10%) 11 6	38, 61, 105, 136	0
45	j	50/50 (100%)	1.19	4 (8%) 18 10	128, 148, 161, 206	0
46	k	46/46 (100%)	0.26	3 (6%) 25 13	43, 55, 74, 119	0
47	l	64/64 (100%)	0.57	4 (6%) 26 14	55, 67, 82, 89	0
48	m	38/38 (100%)	0.71	2 (5%) 32 17	62, 77, 89, 107	0
49	n	163/163 (100%)	1.88	53 (32%) 1 0	133, 200, 265, 312	1 (0%)
50	o	30/30 (100%)	1.61	7 (23%) 2 1	148, 184, 209, 215	0
50	p	30/30 (100%)	1.40	5 (16%) 4 2	170, 194, 226, 233	0
50	q	30/30 (100%)	2.20	12 (40%) 1 0	160, 205, 254, 264	0
50	r	30/30 (100%)	1.73	8 (26%) 1 1	148, 191, 224, 232	0
51	s	1532/1532 (100%)	0.46	80 (5%) 33 17	50, 102, 211, 316	0
52	t	2850/2903 (98%)	-0.12	40 (1%) 73 53	36, 66, 212, 419	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
53	u	118/118 (100%)	0.21	3 (2%) 58 37	60, 110, 147, 189	0
54	v	525/525 (100%)	1.01	83 (15%) 5 2	47, 99, 188, 267	0
55	w	6/6 (100%)	3.30	5 (83%) 0 0	186, 194, 202, 203	0
56	7	2/6 (33%)	2.24	1 (50%) 0 0	103, 103, 103, 112	0
56	AA	2/6 (33%)	3.59	1 (50%) 0 0	103, 103, 103, 108	0
56	BA	2/6 (33%)	1.34	1 (50%) 0 0	100, 100, 100, 101	0
56	y	2/6 (33%)	1.72	1 (50%) 0 0	99, 99, 99, 102	0
56	z	2/6 (33%)	2.68	1 (50%) 0 0	93, 93, 93, 103	0
All	All	10896/10973 (99%)	0.58	1007 (9%) 14 8	31, 90, 212, 419	1 (0%)

The worst 5 of 1007 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	4	ARG	15.9
6	F	5	VAL	11.0
13	M	11	LYS	10.8
50	q	22	LEU	9.3
6	F	7	GLY	9.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	DPP	BA	2	6/7	0.31	0.24	97,99,99,100	0
56	KBE	AA	1	9/10	0.51	0.44	74,80,92,93	0
56	KBE	BA	1	9/10	0.57	0.31	73,86,98,100	0
56	KBE	z	1	9/10	0.60	0.29	86,90,94,94	0
56	UAL	7	5	9/10	0.63	0.30	117,119,122,122	0
56	DPP	AA	2	6/7	0.77	0.23	95,100,101,102	0
56	UAL	z	5	9/10	0.81	0.22	99,100,101,102	0
56	UAL	BA	5	9/10	0.81	0.16	96,100,100,101	0
56	5OH	z	6	12/13	0.81	0.34	100,106,109,110	0
56	5OH	AA	6	12/13	0.81	0.20	101,103,104,105	0
56	5OH	7	6	12/13	0.82	0.19	107,109,112,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	DPP	z	2	6/7	0.82	0.23	94,95,98,101	0
56	KBE	y	1	9/10	0.83	0.29	105,106,108,108	0
56	KBE	7	1	9/10	0.85	0.26	86,89,93,95	0
56	5OH	BA	6	12/13	0.86	0.14	99,102,103,103	0
56	DPP	7	2	6/7	0.90	0.21	98,103,106,109	0
56	UAL	y	5	9/10	0.91	0.14	102,103,109,109	0
56	5OH	y	6	12/13	0.91	0.19	99,102,105,109	0
56	UAL	AA	5	9/10	0.92	0.17	103,105,106,106	0
56	DPP	y	2	6/7	0.94	0.17	98,99,100,104	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.