



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:36 AM BST

PDB ID : 6LKQ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

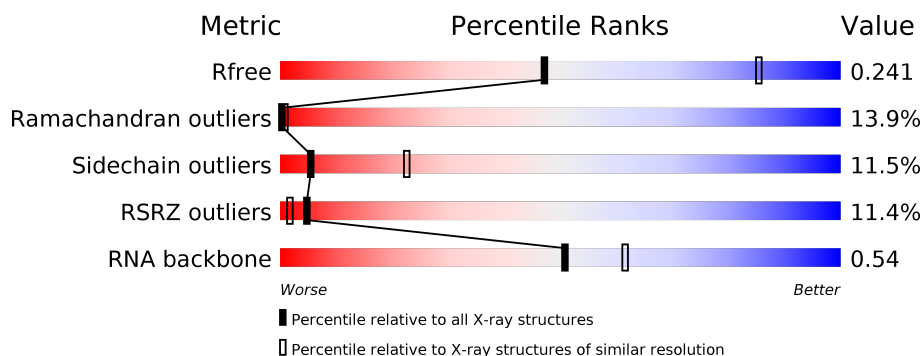
1 Overall quality at a glance

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}	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 on 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	<div> <div>26%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
2	B	206	<div> <div>7%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
3	C	205	<div> <div>22%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
4	D	150	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
5	E	100	<div> <div>14%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
6	F	151	<div> <div>42%</div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
30	3	136	
31	4	120	

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Mol	Chain	Length	Quality of chain
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	
52	t	2903	
53	u	118	

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Mol	Chain	Length	Quality of chain
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	UAL	7	5	-	-	-	X
56	5OH	7	6	-	-	-	X
56	KBE	AA	1	-	-	-	X
56	DPP	AA	2	-	-	-	X
56	5OH	AA	6	-	-	-	X
56	KBE	BA	1	-	-	-	X
56	DPP	BA	2	-	-	-	X
56	UAL	BA	5	-	-	-	X
56	KBE	y	1	-	-	-	X
56	KBE	z	1	-	-	-	X
56	5OH	z	6	-	-	-	X

2 Entry composition [i](#)

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			

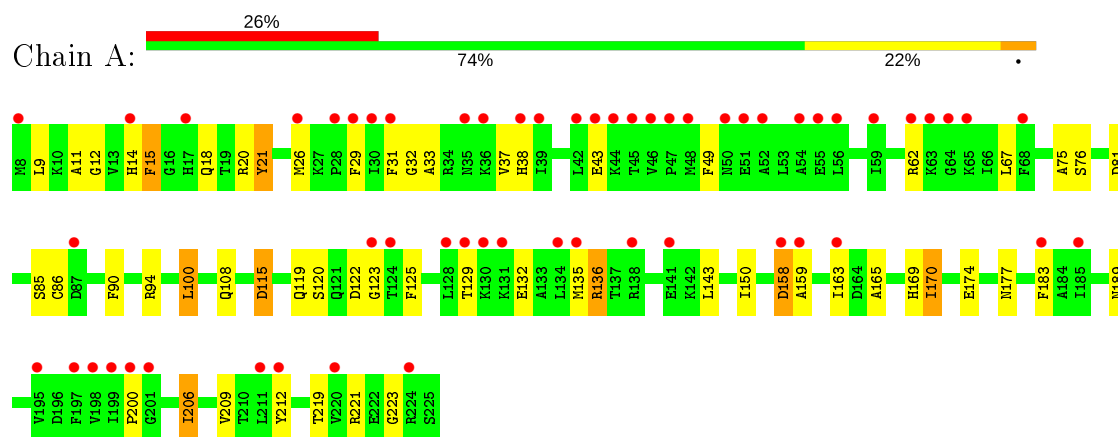
- Molecule 56 is a protein called Viomycin.

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			

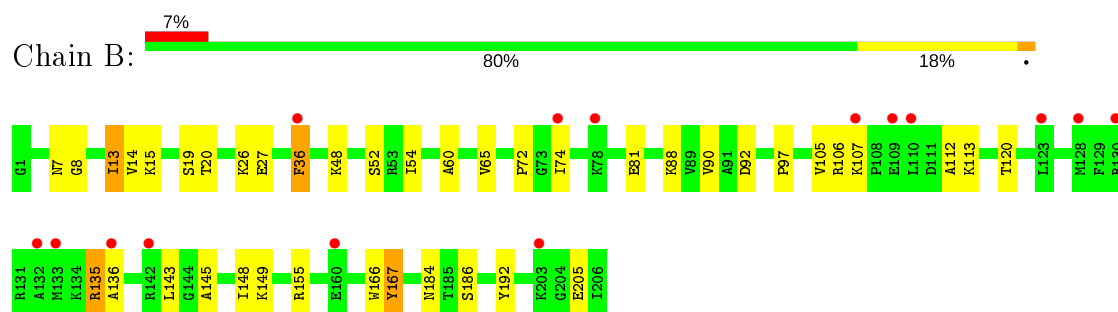
3 Residue-property plots [i](#)

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 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 ($\text{RSRZ} > 2$). 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.

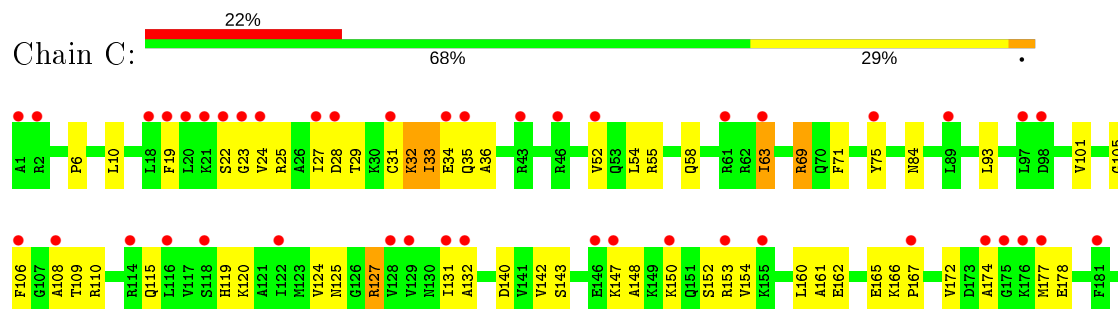
- Molecule 1: 30S ribosomal protein S2

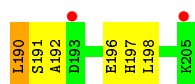


- Molecule 2: 30S ribosomal protein S3

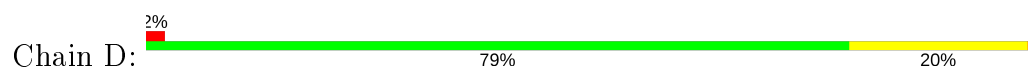


- Molecule 3: 30S ribosomal protein S4

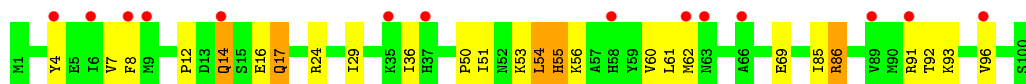




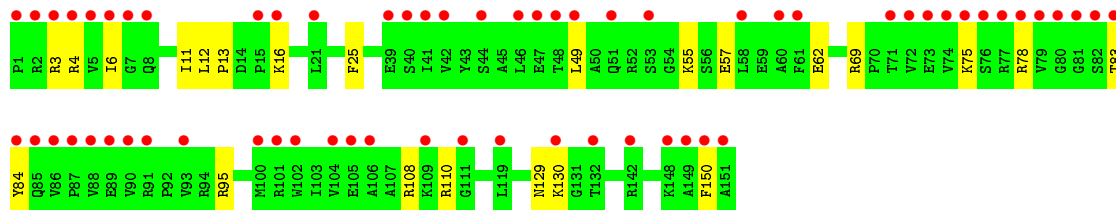
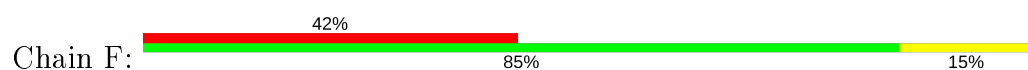
- Molecule 4: 30S ribosomal protein S5



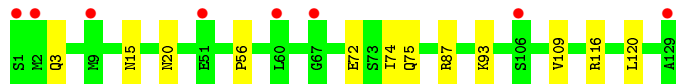
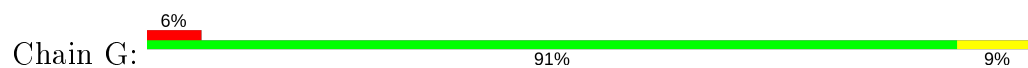
- Molecule 5: 30S ribosomal protein S6



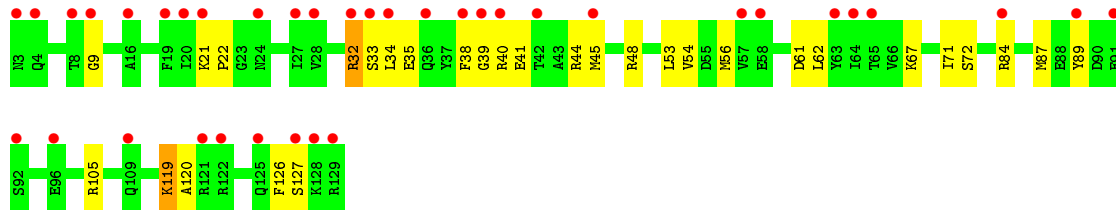
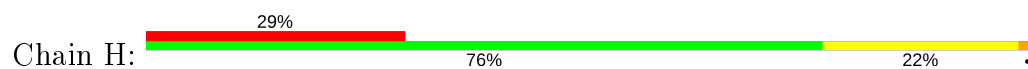
- Molecule 6: 30S ribosomal protein S7



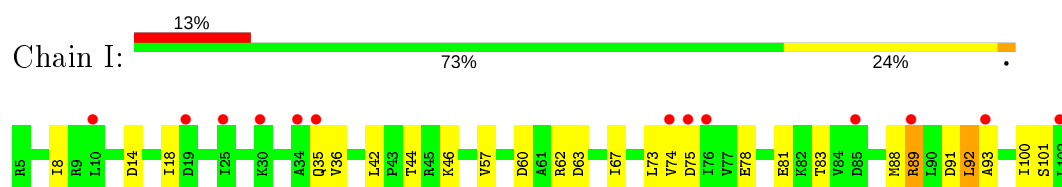
- Molecule 7: 30S ribosomal protein S8



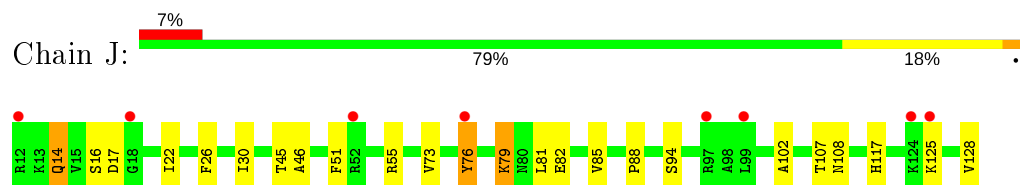
- Molecule 8: 30S ribosomal protein S9



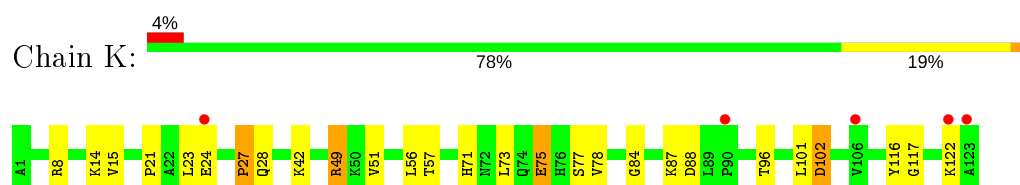
- Molecule 9: 30S ribosomal protein S10



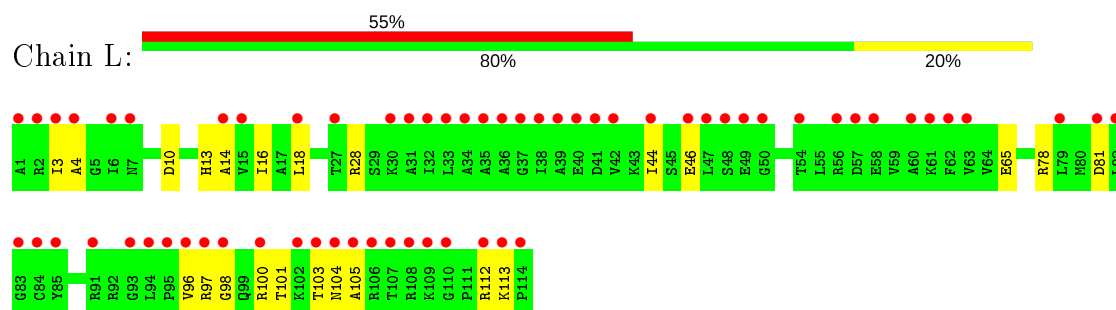
- Molecule 10: 30S ribosomal protein S11



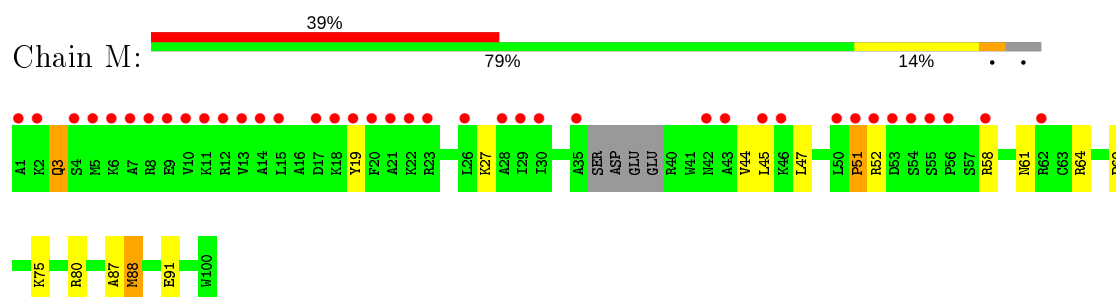
- Molecule 11: 30S ribosomal protein S12



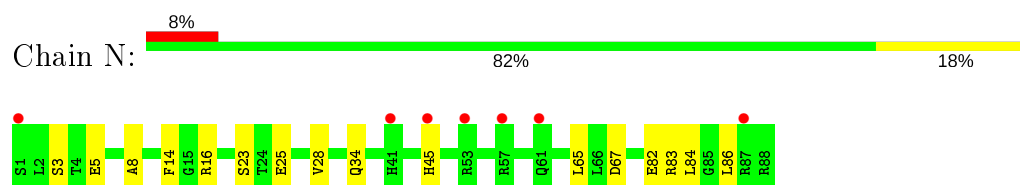
- Molecule 12: 30S ribosomal protein S13



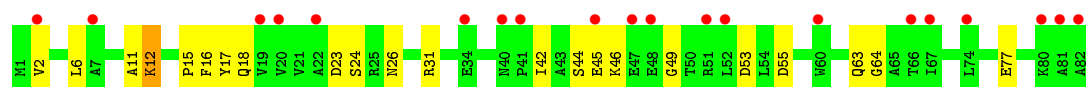
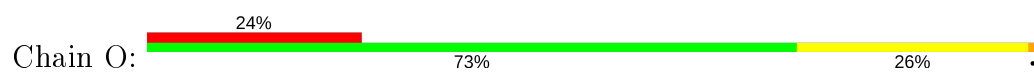
- Molecule 13: 30S ribosomal protein S14



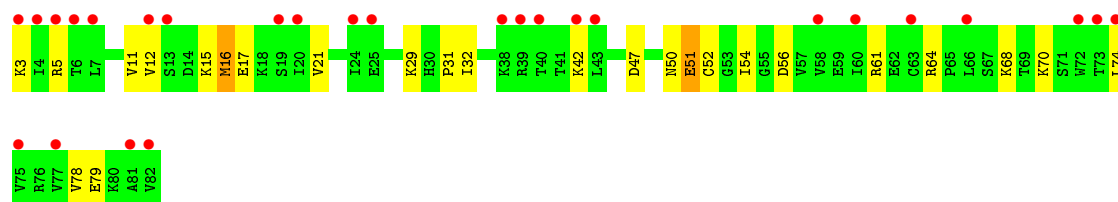
- Molecule 14: 30S ribosomal protein S15



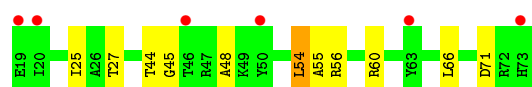
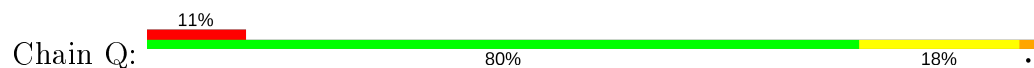
- Molecule 15: 30S ribosomal protein S16



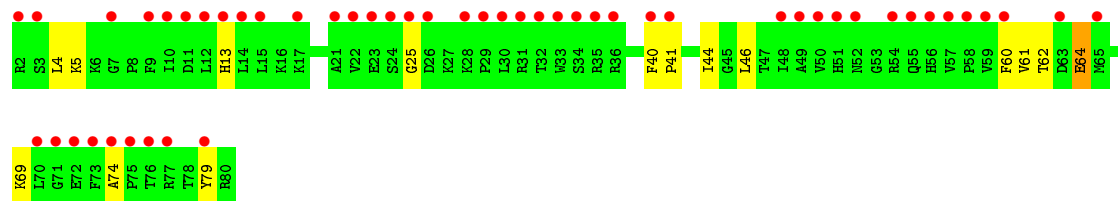
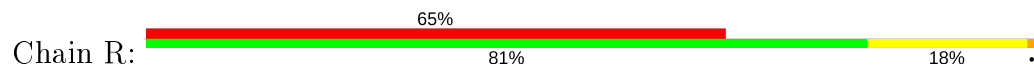
- Molecule 16: 30S ribosomal protein S17



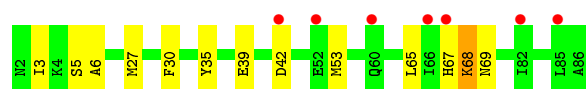
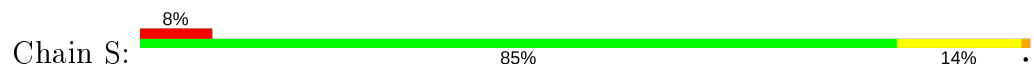
- Molecule 17: 30S ribosomal protein S18



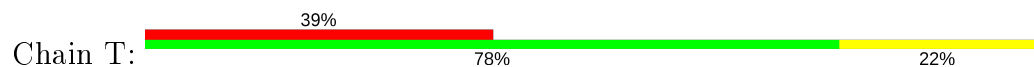
- Molecule 18: 30S ribosomal protein S19



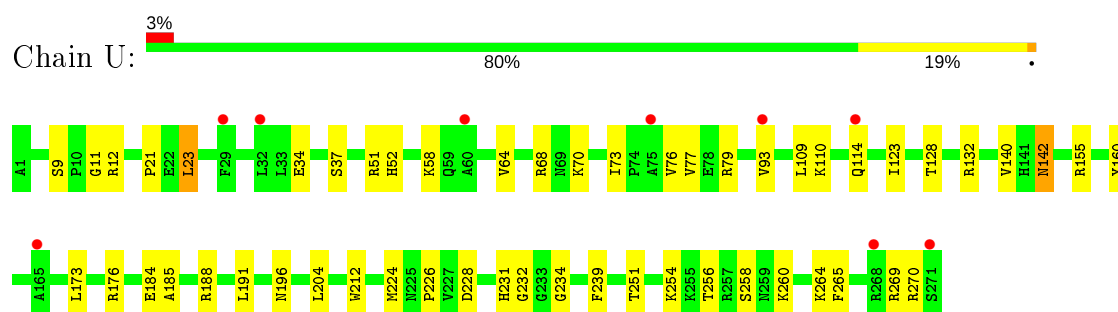
- Molecule 19: 30S ribosomal protein S20



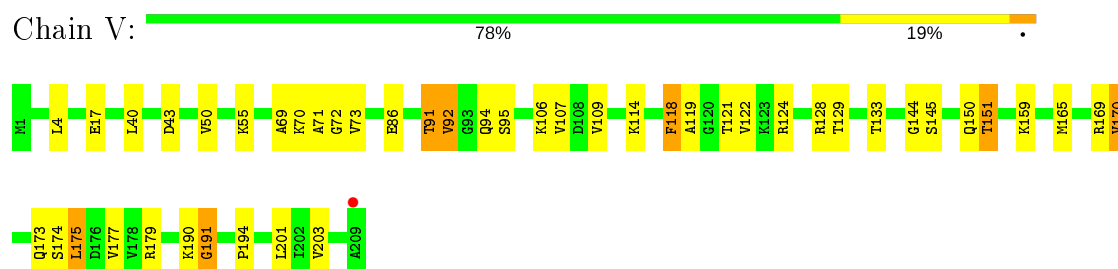
- Molecule 20: 30S ribosomal protein S21



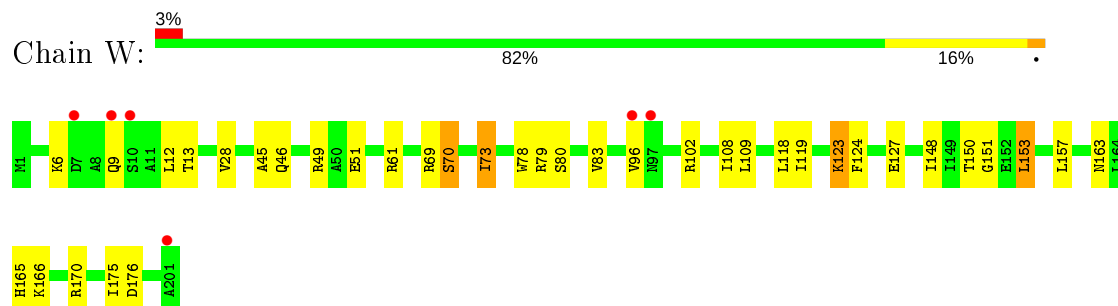
- Molecule 21: 50S ribosomal protein L2



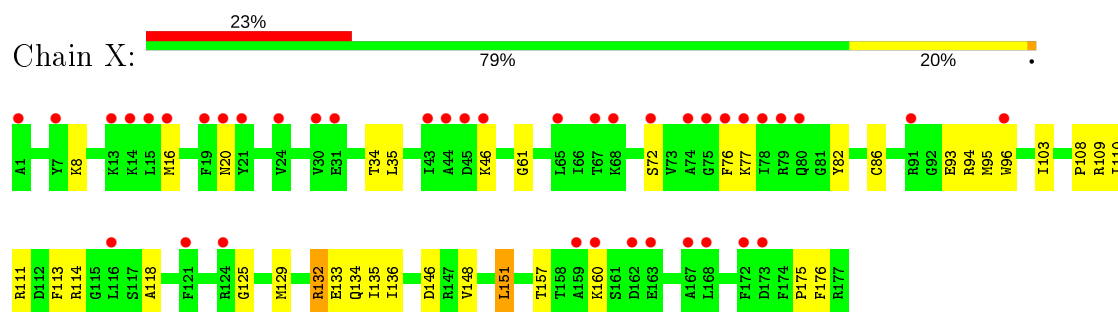
- Molecule 22: 50S ribosomal protein L3



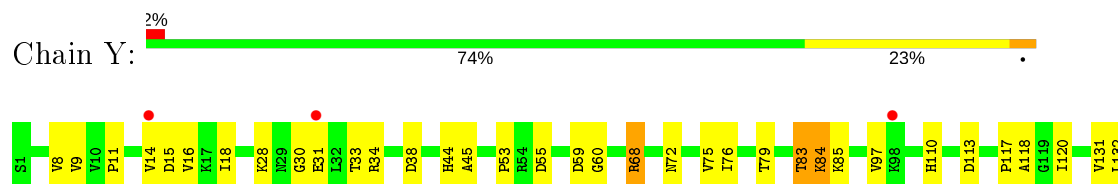
- Molecule 23: 50S ribosomal protein L4



- Molecule 24: 50S ribosomal protein L5

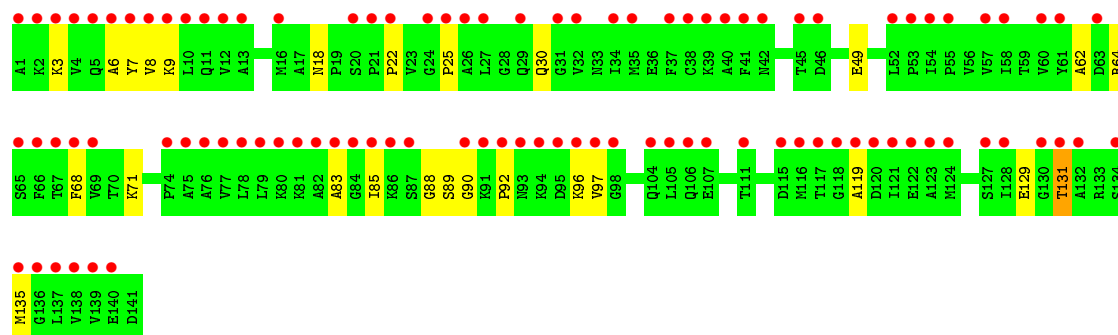
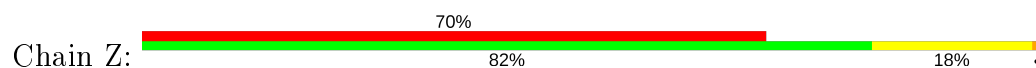


- Molecule 25: 50S ribosomal protein L6

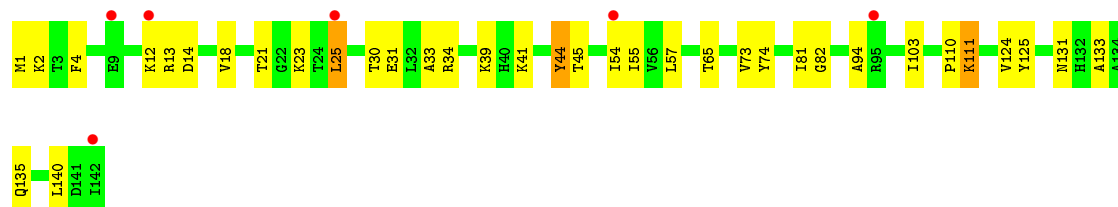
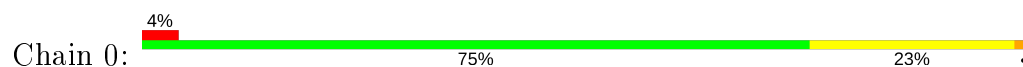




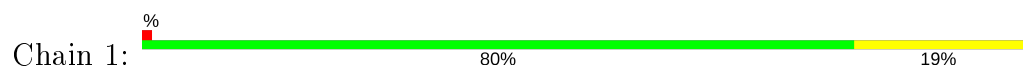
- Molecule 26: 50S ribosomal protein L11



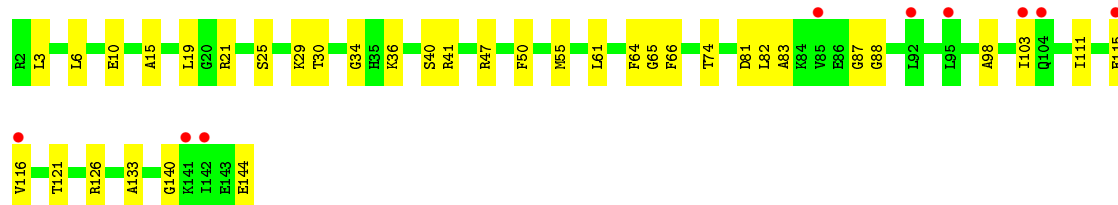
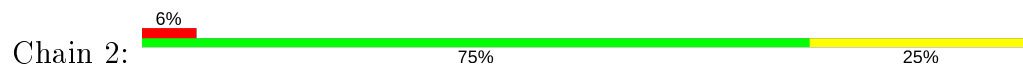
- Molecule 27: 50S ribosomal protein L13



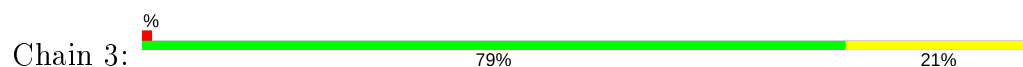
- Molecule 28: 50S ribosomal protein L14



- Molecule 29: 50S ribosomal protein L15

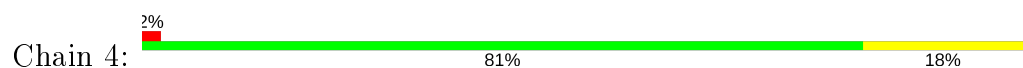


- Molecule 30: 50S ribosomal protein L16

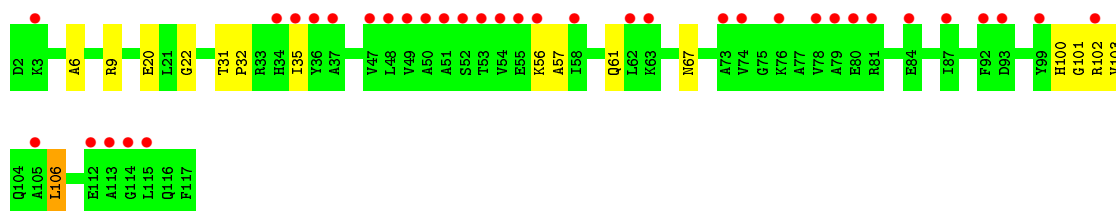
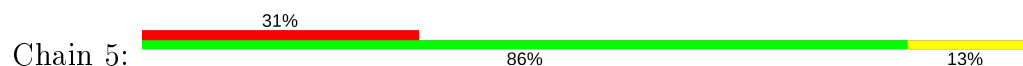




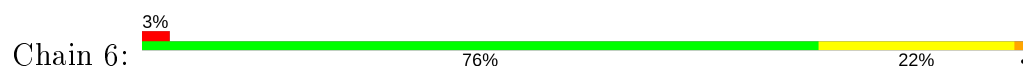
- Molecule 31: 50S ribosomal protein L17



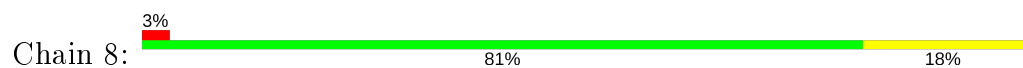
- Molecule 32: 50S ribosomal protein L18



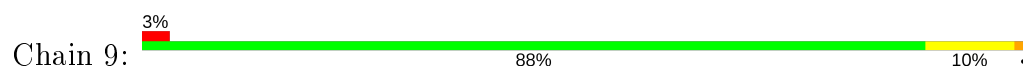
- Molecule 33: 50S ribosomal protein L19



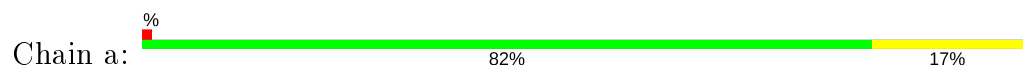
- Molecule 34: 50S ribosomal protein L20



- Molecule 35: 50S ribosomal protein L21

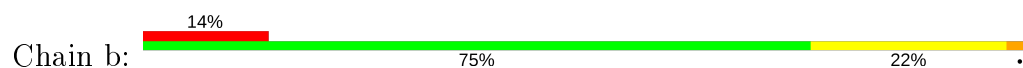


- Molecule 36: 50S ribosomal protein L22

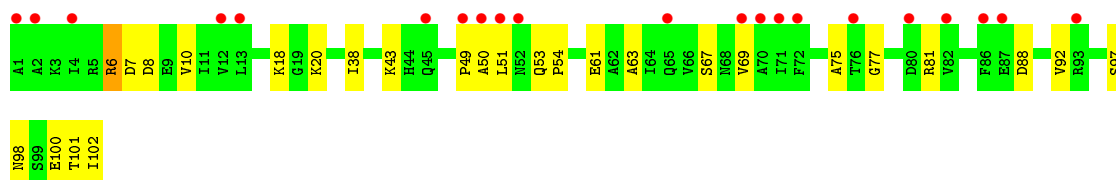




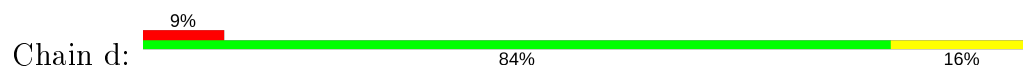
- Molecule 37: 50S ribosomal protein L23



- Molecule 38: 50S ribosomal protein L24



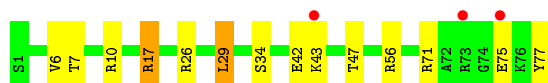
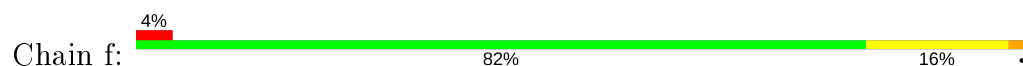
- Molecule 39: 50S ribosomal protein L25



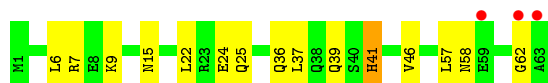
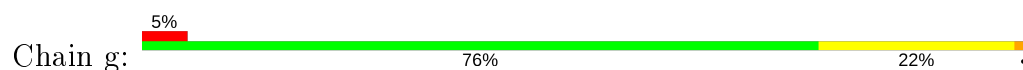
- Molecule 40: 50S ribosomal protein L27



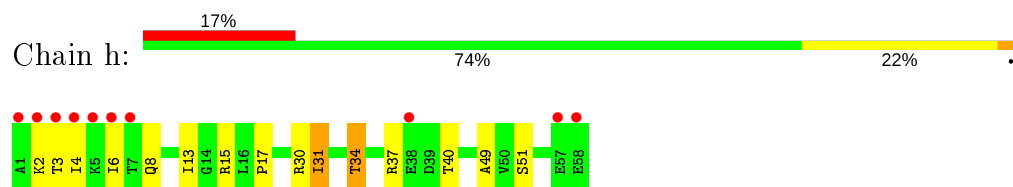
- Molecule 41: 50S ribosomal protein L28



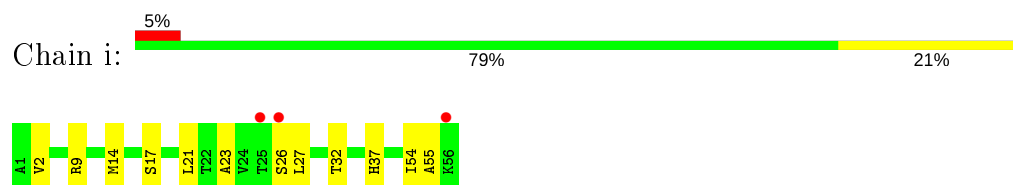
- Molecule 42: 50S ribosomal protein L29



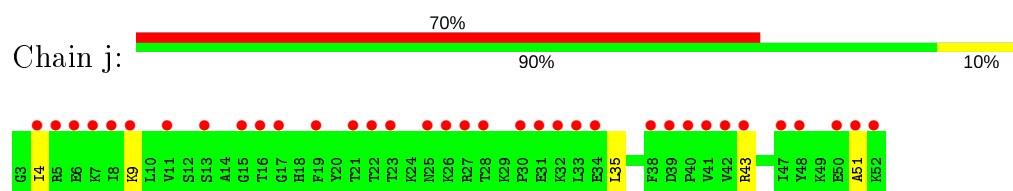
- Molecule 43: 50S ribosomal protein L30



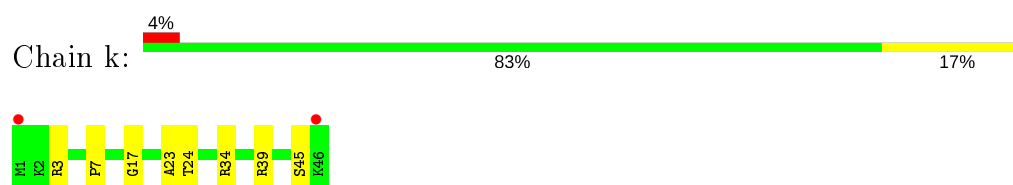
- Molecule 44: 50S ribosomal protein L32



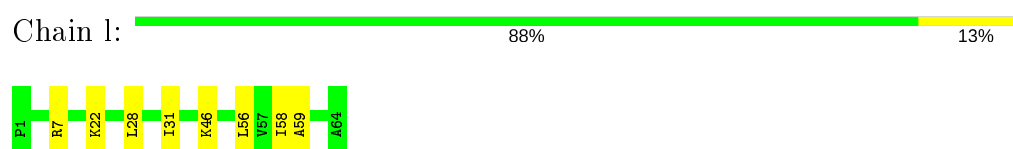
- Molecule 45: 50S ribosomal protein L33



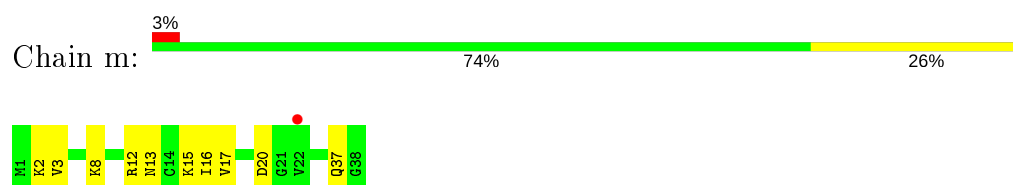
- Molecule 46: 50S ribosomal protein L34



- Molecule 47: 50S ribosomal protein L35

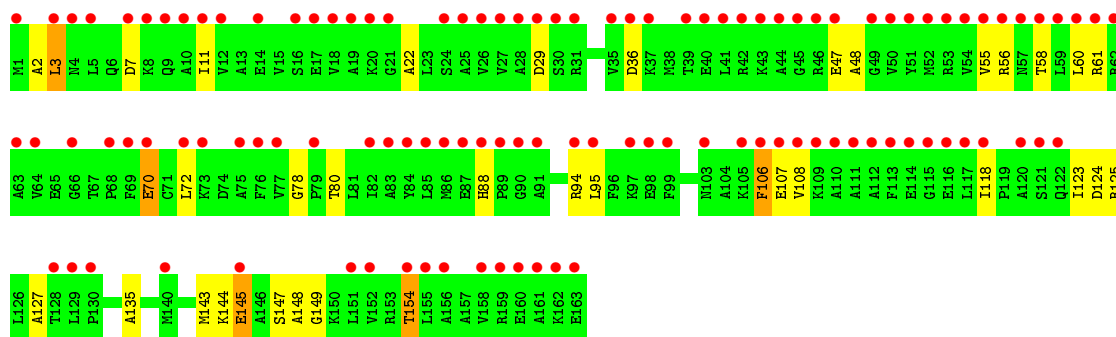


- Molecule 48: 50S ribosomal protein L36

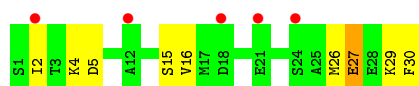


- Molecule 49: 50S ribosomal protein L10

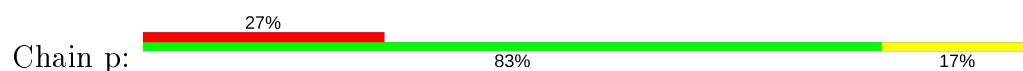




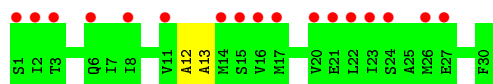
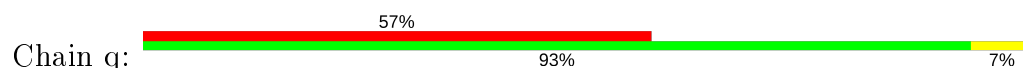
- Molecule 50: 50S ribosomal protein L7/L12



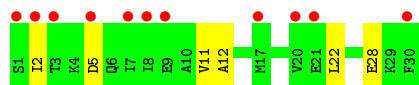
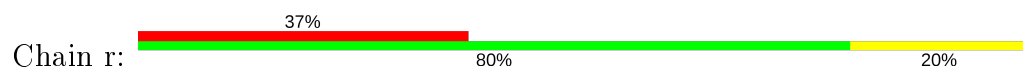
- Molecule 50: 50S ribosomal protein L7/L12



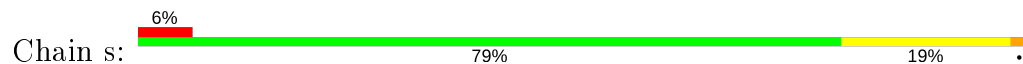
- Molecule 50: 50S ribosomal protein L7/L12

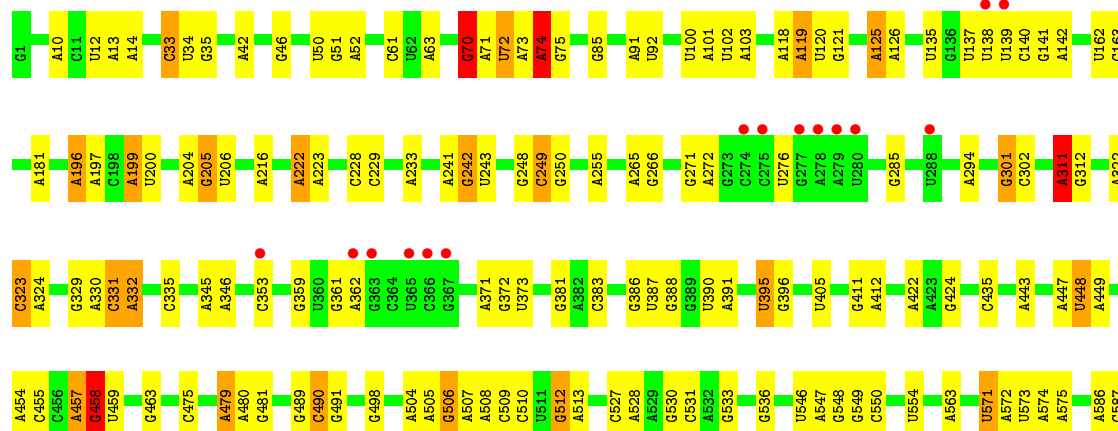
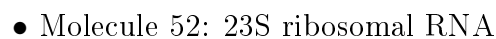


- Molecule 50: 50S ribosomal protein L7/L12

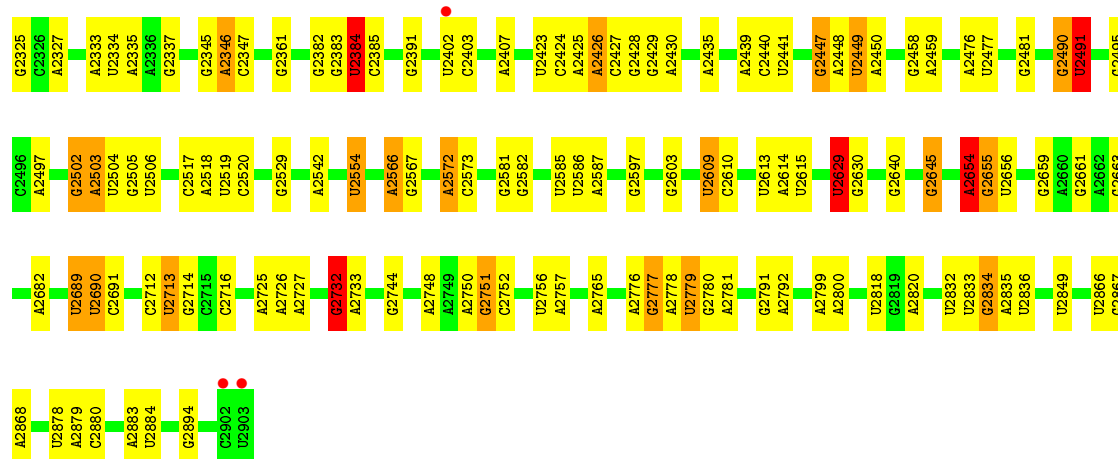


- Molecule 51: 16S ribosomal RNA

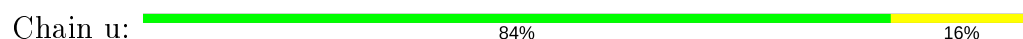




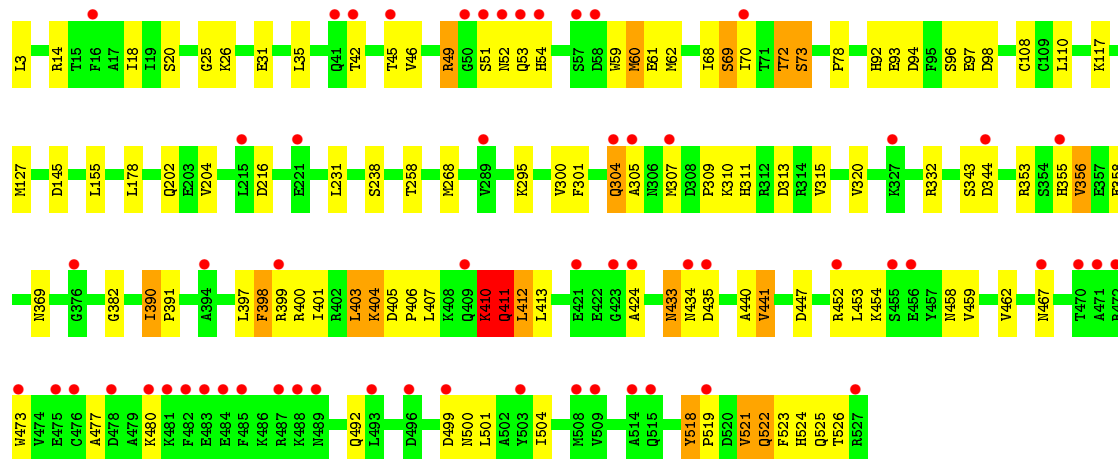
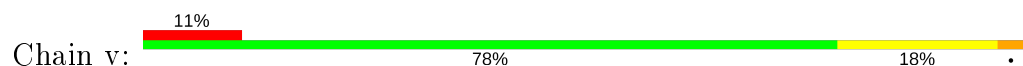
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A2211	C1914	A1609	A1453	A1144	C1012	A878	G603
G2213	A1918	C1610	C1289	A1151	A1021	G880	A613
G2220	A1919	A1611	G1300	A1156	G1022	A761	A614
A2225	A1927	G1613	A1301	G1157	G1023	G882	U615
C2226	G1930	A1616	A1302	G1162	G1024	U894	A616
G2238	A1937	G1617	G1303	G1168	G1026	C	G620
G2239	A1986	A1618	G1306	A1169	U1033	A	A621
U2243	U1939	G1619	G1311	G1170	U1034	C	A627
U2244	U1940	G1622	U1312	G1171	G1034	C	G628
U2249	C1941	A1626	U1313	C1172	A1046	G	C634
G2250	C1942	U1781	C1320	U1173	U1060	A892	G638
G2251	U1943	U1782	A1321	U1174	U1061	U894	G783
C2258	U1944	A1783	U1497	A1175	G1082	U895	U645
U2259	U1945	G1633	U1497	U1176	U1085	A896	U646
A2267	G1946	A1634	A1504	G1179	U1086	C897	G647
C2273	G1954	U1647	A1507	U1180	A1067	A789	A654
A2274	U1955	U1648	C1507	G1186	G1068	U790	A655
C2275	U1956	G1649	A1508	U1203	A1069	C901	G656
G2276	A1965	U1653	A1509	G1188	A1070	C902	A668
G2277	C1967	G1667	A1515	U1206	A1073	A910	G669
A2278	U1970	A1668	A1522	G1210	G1074	G914	A670
G2282	U1971	C1674	U1523	C1211	U1083	U932	C671
C2283	U1972	C1675	G1524	G1212	A1088	A933	A675
G2286	G1975	G1681	U1533	U1236	A1098	A941	A685
A2287	A1981	G1682	C1535	A1237	A1103	A945	U686
G2288	C1986	G1684	G1537	G1238	C1104	C946	C687
G2289	U1991	G1694	A1555	A1247	U1105	U958	G690
A2297	U1992	G1695	G1558	U1248	G1112	A819	A705
U2305	U1993	A1847	U1559	U1249	G1125	U827	C717
C2306	C1996	A1848	G1560	G1251	A1126	U828	G726
G2307	C1997	A1858	A1566	G1252	A1127	A829	A727
G2308	G2009	U1713	A1385	A1253	G1128	G973	G728
C2309	A2009	U1714	A1386	G1256	A1129	A975	G729
A2311	G2012	G1715	U1397	G1266	U1130	A979	A730
G2319	U2017	G1723	G1416	U1267	G1131	A845	A742
U2320	G2018	C1726	A1419	C1270	U1132	U846	U746
U2321	G2018	C1727	A1420	G1271	A1133	U847	U747
A2322	C2021	C1728	A1427	U1272	A1134	G858	G748
G2323	U2022	U1729	C1428	A1274	C1135	G859	A749
U2324	C2023	G1730	A1434	A1276	G1136	U860	A750
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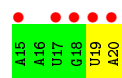
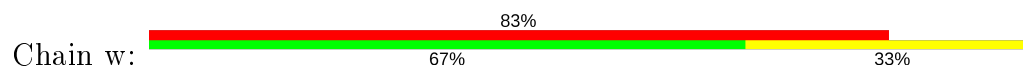
• Molecule 53: 5S ribosomal RNA



• Molecule 54: Peptide chain release factor 3



• Molecule 55: messenger RNA

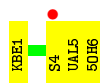


• Molecule 56: Viomycin

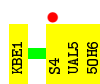




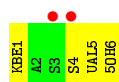
- Molecule 56: Viomycin



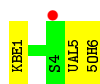
- Molecule 56: Viomycin



- 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 59.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.00-3.10) 99.9 (59.36-3.00)	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 0.236 , 0.241	Depositor DCC
R_{free} test set	26311 reflections (5.02%)	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)	0.32 , 86.0	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: 5OH, DPP, UAL, KBE

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	0.33	0/1732	0.59	0/2333
2	B	0.34	0/1652	0.61	0/2225
3	C	0.34	0/1665	0.61	0/2227
4	D	0.38	0/1119	0.70	0/1504
5	E	0.34	0/836	0.57	0/1128
6	F	0.27	0/1196	0.54	0/1602
7	G	0.34	0/989	0.61	0/1326
8	H	0.31	0/1034	0.59	0/1375
9	I	0.33	0/797	0.63	0/1077
10	J	0.34	0/893	0.61	0/1205
11	K	0.44	0/969	0.79	0/1300
12	L	0.24	0/893	0.54	0/1193
13	M	0.32	0/785	0.56	0/1043
14	N	0.32	0/722	0.60	0/964
15	O	0.39	0/659	0.63	0/884
16	P	0.35	0/658	0.65	0/881
17	Q	0.39	0/463	0.59	0/621
18	R	0.28	0/653	0.54	0/877
19	S	0.37	0/671	0.58	0/888
20	T	0.38	0/431	0.58	0/570
21	U	0.47	0/2122	0.83	1/2852 (0.0%)
22	V	0.52	0/1586	0.82	1/2134 (0.0%)
23	W	0.41	0/1571	0.70	0/2113
24	X	0.32	0/1435	0.57	0/1926
25	Y	0.42	0/1343	0.71	0/1816
26	Z	0.26	0/1046	0.52	0/1410
27	0	0.47	0/1152	0.78	1/1551 (0.1%)
28	1	0.53	0/948	0.81	0/1268
29	2	0.39	0/1054	0.76	0/1403
30	3	0.46	0/1093	0.72	0/1460
31	4	0.45	0/974	0.76	0/1301
32	5	0.32	0/902	0.60	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.46	0/929	0.79	1/1242 (0.1%)
34	8	0.45	0/960	0.68	0/1278
35	9	0.39	0/829	0.71	0/1107
36	a	0.48	0/864	0.75	0/1156
37	b	0.43	0/745	0.76	0/994
38	c	0.41	0/788	0.73	0/1051
39	d	0.36	0/766	0.57	0/1025
40	e	0.49	0/603	0.79	1/797 (0.1%)
41	f	0.39	0/635	0.74	1/848 (0.1%)
42	g	0.36	0/510	0.71	0/677
43	h	0.37	0/453	0.67	0/605
44	i	0.47	0/450	0.78	0/599
45	j	0.33	0/417	0.55	0/554
46	k	0.50	0/380	0.79	0/498
47	l	0.41	0/513	0.70	0/676
48	m	0.46	0/303	0.83	1/397 (0.3%)
49	n	0.30	0/1248	0.60	0/1679
50	o	0.34	0/228	0.66	0/304
50	p	0.29	0/228	0.49	0/304
50	q	0.31	0/228	0.58	0/304
50	r	0.31	0/228	0.58	0/304
51	s	0.40	0/36806	0.74	26/57419 (0.0%)
52	t	0.53	0/68523	0.83	141/106893 (0.1%)
53	u	0.36	0/2825	0.69	0/4406
54	v	0.47	2/4221 (0.0%)	0.73	5/5702 (0.1%)
55	w	0.27	0/141	0.70	0/218
56	7	1.41	0/11	1.06	0/13
56	AA	1.56	0/11	0.97	0/13
56	BA	1.40	0/11	0.64	0/13
56	y	1.33	0/11	0.91	0/13
56	z	1.48	0/11	1.40	0/13
All	All	0.46	2/158919 (0.0%)	0.76	179/236768 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	v	72	THR	C-O	6.02	1.34	1.23
54	v	73	SER	CB-OG	5.44	1.49	1.42

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	t	1340	U	N1-C1'-C2'	10.45	127.59	114.00
52	t	974	G	N9-C1'-C2'	9.82	126.77	114.00
52	t	70	G	N9-C1'-C2'	9.73	126.65	114.00
52	t	2447	G	N9-C1'-C2'	9.40	126.22	114.00
52	t	2732	G	N9-C1'-C2'	9.32	126.12	114.00

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](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	1	4
7	G	127/129 (98%)	92 (72%)	29 (23%)	6 (5%)	2	14
8	H	125/127 (98%)	81 (65%)	26 (21%)	18 (14%)	0	1
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	3
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	7
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	4	118/120 (98%)	83 (70%)	20 (17%)	15 (13%)	0	1
32	5	114/116 (98%)	79 (69%)	25 (22%)	10 (9%)	1	4
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	5
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	7
42	g	61/63 (97%)	34 (56%)	15 (25%)	12 (20%)	0	0
43	h	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	4
44	i	54/56 (96%)	44 (82%)	5 (9%)	5 (9%)	0	3
45	j	48/50 (96%)	32 (67%)	14 (29%)	2 (4%)	3	16
46	k	44/46 (96%)	36 (82%)	4 (9%)	4 (9%)	1	4
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	6
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	2
56	7	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
56	AA	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
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%)	152 (85%)	27 (15%)	3	12
2	B	170/170 (100%)	153 (90%)	17 (10%)	7	28
3	C	172/172 (100%)	150 (87%)	22 (13%)	4	18
4	D	113/113 (100%)	101 (89%)	12 (11%)	6	26
5	E	87/87 (100%)	76 (87%)	11 (13%)	4	18
6	F	124/124 (100%)	114 (92%)	10 (8%)	11	39
7	G	104/104 (100%)	98 (94%)	6 (6%)	20	51
8	H	105/105 (100%)	91 (87%)	14 (13%)	4	16
9	I	86/86 (100%)	73 (85%)	13 (15%)	3	12
10	J	90/90 (100%)	75 (83%)	15 (17%)	2	9
11	K	103/103 (100%)	93 (90%)	10 (10%)	8	30
12	L	92/92 (100%)	86 (94%)	6 (6%)	17	47
13	M	79/83 (95%)	73 (92%)	6 (8%)	13	41
14	N	76/76 (100%)	66 (87%)	10 (13%)	4	17
15	O	65/65 (100%)	56 (86%)	9 (14%)	3	16
16	P	74/74 (100%)	60 (81%)	14 (19%)	1	6
17	Q	48/48 (100%)	42 (88%)	6 (12%)	4	18
18	R	70/70 (100%)	65 (93%)	5 (7%)	14	44
19	S	65/65 (100%)	59 (91%)	6 (9%)	9	33
20	T	44/44 (100%)	40 (91%)	4 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	216/216 (100%)	188 (87%)	28 (13%)	4	18
22	V	164/164 (100%)	144 (88%)	20 (12%)	5	19
23	W	165/165 (100%)	148 (90%)	17 (10%)	7	27
24	X	148/148 (100%)	135 (91%)	13 (9%)	10	36
25	Y	137/137 (100%)	116 (85%)	21 (15%)	2	12
26	Z	109/109 (100%)	104 (95%)	5 (5%)	27	59
27	0	116/116 (100%)	97 (84%)	19 (16%)	2	10
28	1	103/103 (100%)	90 (87%)	13 (13%)	4	18
29	2	102/102 (100%)	90 (88%)	12 (12%)	5	21
30	3	109/109 (100%)	95 (87%)	14 (13%)	4	18
31	4	100/100 (100%)	91 (91%)	9 (9%)	9	34
32	5	86/86 (100%)	79 (92%)	7 (8%)	11	39
33	6	99/99 (100%)	89 (90%)	10 (10%)	7	28
34	8	89/89 (100%)	77 (86%)	12 (14%)	4	16
35	9	84/84 (100%)	78 (93%)	6 (7%)	14	44
36	a	93/93 (100%)	82 (88%)	11 (12%)	5	21
37	b	80/80 (100%)	73 (91%)	7 (9%)	10	36
38	c	83/83 (100%)	75 (90%)	8 (10%)	8	31
39	d	78/78 (100%)	74 (95%)	4 (5%)	24	56
40	e	59/59 (100%)	49 (83%)	10 (17%)	2	9
41	f	67/67 (100%)	57 (85%)	10 (15%)	3	13
42	g	55/55 (100%)	51 (93%)	4 (7%)	14	43
43	h	48/48 (100%)	36 (75%)	12 (25%)	0	2
44	i	47/47 (100%)	40 (85%)	7 (15%)	3	13
45	j	45/45 (100%)	42 (93%)	3 (7%)	16	46
46	k	38/38 (100%)	34 (90%)	4 (10%)	7	26
47	l	51/51 (100%)	49 (96%)	2 (4%)	32	65
48	m	34/34 (100%)	29 (85%)	5 (15%)	3	13
49	n	123/123 (100%)	112 (91%)	11 (9%)	9	34
50	o	26/26 (100%)	23 (88%)	3 (12%)	5	22
50	p	26/26 (100%)	25 (96%)	1 (4%)	33	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	q	26/26 (100%)	26 (100%)	0	100	100
50	r	26/26 (100%)	23 (88%)	3 (12%)	5	22
54	v	447/449 (100%)	381 (85%)	66 (15%)	3	13
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%)	4635 (88%)	600 (12%)	5	22

5 of 600 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	W	12	LEU
27	0	39	LYS
54	v	145	ASP
23	W	109	LEU
25	Y	34	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	136	ASN
27	0	128	ASN
49	n	9	GLN
22	V	140	HIS
23	W	136	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	s	1531/1532 (99%)	298 (19%)	0
52	t	2845/2903 (98%)	660 (23%)	0
53	u	117/118 (99%)	18 (15%)	0
55	w	5/6 (83%)	2 (40%)	0
All	All	4498/4559 (98%)	978 (21%)	0

5 of 978 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	DPP	AA	2	56	3,5,6	1.13	0	1,5,7	1.21	0
56	KBE	BA	1	56	8,8,9	1.21	1 (12%)	7,8,10	1.32	1 (14%)
56	KBE	7	1	56	8,8,9	0.73	0	7,8,10	1.22	1 (14%)
56	DPP	z	2	56	3,5,6	0.78	0	1,5,7	0.36	0
56	UAL	AA	5	56	7,8,9	2.53	1 (14%)	5,9,11	1.33	1 (20%)
56	KBE	z	1	56	8,8,9	1.22	1 (12%)	7,8,10	2.16	1 (14%)
56	5OH	BA	6	56	8,12,13	1.17	0	3,16,18	2.21	2 (66%)
56	5OH	AA	6	56	8,12,13	1.33	1 (12%)	3,16,18	1.68	1 (33%)
56	DPP	7	2	56	3,5,6	0.50	0	1,5,7	0.90	0
56	UAL	z	5	56	7,8,9	1.82	3 (42%)	5,9,11	2.61	1 (20%)
56	KBE	AA	1	56	8,8,9	1.66	2 (25%)	7,8,10	3.54	1 (14%)
56	5OH	y	6	56	8,12,13	0.92	0	3,16,18	2.40	2 (66%)
56	UAL	BA	5	56	7,8,9	2.69	1 (14%)	5,9,11	1.62	1 (20%)
56	DPP	BA	2	56	3,5,6	1.30	0	1,5,7	0.08	0
56	KBE	y	1	56	8,8,9	1.36	1 (12%)	7,8,10	2.04	1 (14%)
56	UAL	7	5	56	7,8,9	2.72	1 (14%)	5,9,11	1.18	0
56	5OH	7	6	56	8,12,13	1.77	2 (25%)	3,16,18	2.93	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	UAL	y	5	56	7,8,9	2.26	2 (28%)	5,9,11	1.39	1 (20%)
56	5OH	z	6	56	8,12,13	1.13	1 (12%)	3,16,18	1.13	0
56	DPP	y	2	56	3,5,6	0.39	0	1,5,7	0.30	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	DPP	AA	2	56	-	0/2/4/6	-
56	KBE	BA	1	56	-	4/7/7/8	-
56	KBE	7	1	56	-	3/7/7/8	-
56	DPP	z	2	56	-	0/2/4/6	-
56	UAL	AA	5	56	-	0/3/7/9	-
56	KBE	z	1	56	-	2/7/7/8	-
56	5OH	BA	6	56	-	2/2/18/20	0/1/1/1
56	5OH	AA	6	56	-	0/2/18/20	0/1/1/1
56	DPP	7	2	56	-	0/2/4/6	-
56	UAL	z	5	56	-	0/3/7/9	-
56	KBE	AA	1	56	-	0/7/7/8	-
56	5OH	y	6	56	-	0/2/18/20	0/1/1/1
56	UAL	BA	5	56	-	0/3/7/9	-
56	DPP	BA	2	56	-	0/2/4/6	-
56	KBE	y	1	56	-	2/7/7/8	-
56	UAL	7	5	56	-	0/3/7/9	-
56	5OH	7	6	56	-	0/2/18/20	0/1/1/1
56	UAL	y	5	56	-	0/3/7/9	-
56	5OH	z	6	56	-	1/2/18/20	0/1/1/1
56	DPP	y	2	56	-	0/2/4/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	7	5	UAL	C-CA	6.99	1.56	1.45
56	BA	5	UAL	C-CA	6.80	1.56	1.45
56	AA	5	UAL	C-CA	6.04	1.54	1.45
56	y	5	UAL	C-CA	5.10	1.53	1.45
56	AA	1	KBE	CA-CB	3.46	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	9.12	125.67	112.25
56	z	5	UAL	O-C-CA	-5.34	118.61	125.39
56	z	1	KBE	CB-CA-C	5.23	119.95	112.25
56	y	1	KBE	CB-CA-C	5.05	119.68	112.25
56	7	6	5OH	CR-CB-CA	4.99	117.99	112.61

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	1.26	57 (26%) 0 0	96, 133, 180, 198	0
2	B	206/206 (100%)	0.40	15 (7%) 15 6	73, 120, 145, 151	0
3	C	205/205 (100%)	1.14	46 (22%) 0 0	88, 115, 150, 205	0
4	D	150/150 (100%)	0.02	3 (2%) 65 44	73, 94, 139, 171	0
5	E	100/100 (100%)	0.78	14 (14%) 2 1	101, 135, 155, 159	0
6	F	151/151 (100%)	2.06	63 (41%) 0 0	111, 187, 225, 236	0
7	G	129/129 (100%)	0.51	8 (6%) 20 9	77, 101, 133, 142	0
8	H	127/127 (100%)	1.45	37 (29%) 0 0	82, 134, 190, 220	0
9	I	98/98 (100%)	0.91	13 (13%) 3 1	90, 110, 193, 210	0
10	J	117/117 (100%)	0.52	8 (6%) 17 7	76, 111, 147, 165	0
11	K	123/123 (100%)	0.53	5 (4%) 37 18	53, 76, 115, 156	0
12	L	114/114 (100%)	2.96	63 (55%) 0 0	166, 207, 253, 272	0
13	M	96/100 (96%)	2.11	39 (40%) 0 0	79, 143, 196, 206	0
14	N	88/88 (100%)	0.49	7 (7%) 12 5	76, 104, 140, 149	0
15	O	82/82 (100%)	1.45	20 (24%) 0 0	78, 101, 164, 212	0
16	P	80/80 (100%)	1.59	27 (33%) 0 0	79, 119, 168, 183	0
17	Q	55/55 (100%)	1.06	6 (10%) 5 2	80, 100, 133, 190	0
18	R	79/79 (100%)	3.64	51 (64%) 0 0	156, 207, 226, 233	0
19	S	85/85 (100%)	0.70	7 (8%) 11 4	82, 111, 136, 153	0
20	T	51/51 (100%)	1.88	20 (39%) 0 0	119, 147, 188, 197	0
21	U	271/271 (100%)	0.17	9 (3%) 46 24	37, 65, 82, 107	0
22	V	209/209 (100%)	-0.06	1 (0%) 91 81	31, 58, 94, 119	0
23	W	201/201 (100%)	0.09	6 (2%) 50 27	39, 76, 115, 160	0
24	X	177/177 (100%)	1.10	40 (22%) 0 0	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%)	0.30	4 (2%) 60 39	58, 82, 124, 141	0
26	Z	141/141 (100%)	3.49	98 (69%) 0 0	185, 260, 305, 346	0
27	0	142/142 (100%)	0.42	6 (4%) 36 18	49, 64, 94, 128	0
28	1	122/122 (100%)	0.18	1 (0%) 86 72	46, 61, 88, 115	0
29	2	143/143 (100%)	0.54	9 (6%) 20 8	45, 85, 123, 154	0
30	3	136/136 (100%)	0.36	2 (1%) 73 54	44, 70, 103, 137	0
31	4	120/120 (100%)	0.21	2 (1%) 70 49	41, 57, 71, 171	0
32	5	116/116 (100%)	1.37	36 (31%) 0 0	85, 106, 130, 136	0
33	6	114/114 (100%)	0.19	3 (2%) 56 33	48, 72, 115, 141	0
34	8	117/117 (100%)	0.08	3 (2%) 56 33	34, 60, 98, 119	0
35	9	103/103 (100%)	0.26	3 (2%) 51 28	46, 88, 128, 139	0
36	a	110/110 (100%)	-0.12	1 (0%) 84 69	41, 55, 86, 138	0
37	b	93/93 (100%)	0.88	13 (13%) 2 1	49, 81, 143, 167	0
38	c	102/102 (100%)	1.14	21 (20%) 1 0	65, 85, 153, 167	0
39	d	94/94 (100%)	0.64	8 (8%) 10 4	69, 98, 121, 143	0
40	e	79/79 (100%)	0.77	5 (6%) 20 8	66, 90, 125, 136	0
41	f	77/77 (100%)	0.46	3 (3%) 39 20	57, 72, 124, 133	0
42	g	63/63 (100%)	-0.00	3 (4%) 30 14	73, 99, 138, 170	0
43	h	58/58 (100%)	0.73	10 (17%) 1 0	63, 76, 133, 144	0
44	i	56/56 (100%)	0.19	3 (5%) 25 12	38, 61, 105, 136	0
45	j	50/50 (100%)	2.98	35 (70%) 0 0	128, 148, 161, 206	0
46	k	46/46 (100%)	0.22	2 (4%) 35 17	43, 55, 74, 119	0
47	l	64/64 (100%)	0.31	0 100 100	55, 67, 82, 89	0
48	m	38/38 (100%)	0.50	1 (2%) 56 33	62, 77, 89, 107	0
49	n	163/163 (100%)	4.42	112 (68%) 0 0	136, 200, 265, 312	1 (0%)
50	o	30/30 (100%)	1.02	5 (16%) 1 1	148, 184, 209, 215	0
50	p	30/30 (100%)	1.39	8 (26%) 0 0	170, 194, 226, 233	0
50	q	30/30 (100%)	3.14	17 (56%) 0 0	160, 205, 254, 264	0
50	r	30/30 (100%)	2.33	11 (36%) 0 0	148, 191, 224, 232	0
51	s	1532/1532 (100%)	0.35	85 (5%) 25 11	50, 102, 211, 316	0
52	t	2850/2903 (98%)	0.18	100 (3%) 44 23	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%)	-0.04	0 100 100	60, 110, 147, 189	0
54	v	525/525 (100%)	0.70	60 (11%) 5 2	47, 99, 188, 267	0
55	w	6/6 (100%)	3.84	5 (83%) 0 0	186, 194, 202, 203	0
56	7	2/6 (33%)	2.01	1 (50%) 0 0	103, 103, 103, 112	0
56	AA	2/6 (33%)	3.05	2 (100%) 0 0	103, 103, 103, 108	0
56	BA	2/6 (33%)	2.80	1 (50%) 0 0	100, 100, 100, 101	0
56	y	2/6 (33%)	-0.21	0 100 100	99, 99, 99, 102	0
56	z	2/6 (33%)	1.90	1 (50%) 0 0	93, 93, 93, 103	0
All	All	10896/10973 (99%)	0.65	1245 (11%) 5 2	31, 90, 212, 419	1 (0%)

The worst 5 of 1245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	n	50	VAL	24.7
49	n	88	HIS	20.5
18	R	55	GLN	19.4
49	n	112	ALA	19.4
49	n	89	PRO	19.1

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

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	0.28	0.42	97,99,99,100	0
56	KBE	BA	1	9/10	0.37	0.52	73,86,98,100	0
56	UAL	7	5	9/10	0.50	0.87	117,119,122,122	0
56	KBE	AA	1	9/10	0.51	0.57	74,80,92,93	0
56	5OH	7	6	12/13	0.55	0.58	107,109,112,116	0
56	KBE	y	1	9/10	0.64	0.53	105,106,108,108	0
56	5OH	z	6	12/13	0.67	0.84	100,106,109,110	0
56	KBE	z	1	9/10	0.72	0.45	86,90,94,94	0
56	DPP	AA	2	6/7	0.74	0.51	95,100,101,102	0
56	5OH	AA	6	12/13	0.76	0.54	101,103,104,105	0
56	UAL	BA	5	9/10	0.79	0.61	96,100,100,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	DPP	z	2	6/7	0.80	0.38	94,95,98,101	0
56	KBE	7	1	9/10	0.83	0.60	86,89,93,95	0
56	UAL	AA	5	9/10	0.85	0.65	103,105,106,106	0
56	5OH	BA	6	12/13	0.85	0.38	99,102,103,103	0
56	UAL	z	5	9/10	0.87	0.39	99,100,101,102	0
56	UAL	y	5	9/10	0.87	0.21	102,103,109,109	0
56	DPP	7	2	6/7	0.87	0.42	98,103,106,109	0
56	DPP	y	2	6/7	0.92	0.23	98,99,100,104	0
56	5OH	y	6	12/13	0.94	0.32	99,102,105,109	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.