wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 10:57 AM JST

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 (i) symbol.

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

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

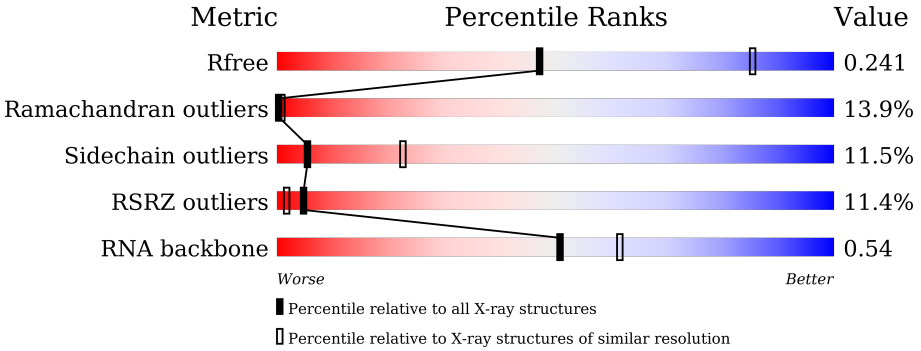
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

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Mol	Chain	Length	Quality of chain
7	G	129	6% 91% 9%
8	H	127	29% 76% 22%
9	I	98	13% 73% 24%
10	J	117	7% 79% 18%
11	K	123	4% 78% 19%
12	L	114	55% 80% 20%
13	M	100	39% 79% 14%
14	N	88	8% 82% 18%
15	O	82	24% 73% 26%
16	P	80	34% 69% 29%
17	Q	55	11% 80% 18%
18	R	79	65% 81% 18%
19	S	85	8% 85% 14%
20	T	51	39% 78% 22%
21	U	271	3% 80% 19%
22	V	209	78% 19%
23	W	201	3% 82% 16%
24	X	177	23% 79% 20%
25	Y	176	2% 74% 23%
26	Z	141	70% 82% 18%
27	0	142	4% 75% 23%
28	1	122	% 80% 19%
29	2	143	6% 75% 25%
30	3	136	% 79% 21%
31	4	120	2% 81% 18%

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Mol	Chain	Length	Quality of chain
32	5	116	31% 86% 13%
33	6	114	3% 76% 22%
34	8	117	3% 81% 18%
35	9	103	3% 88% 10%
36	a	110	% 82% 17%
37	b	93	14% 75% 22%
38	c	102	21% 74% 25%
39	d	94	9% 84% 16%
40	e	79	6% 58% 35% 6%
41	f	77	4% 82% 16%
42	g	63	5% 76% 22%
43	h	58	17% 74% 22%
44	i	56	5% 79% 21%
45	j	50	70% 90% 10%
46	k	46	4% 83% 17%
47	l	64	88% 12%
48	m	38	3% 74% 26%
49	n	163	69% 77% 20%
50	o	30	17% 70% 27%
50	p	30	27% 83% 17%
50	q	30	57% 93% 7%
50	r	30	37% 80% 20%
51	s	1532	6% 79% 19%
52	t	2903	3% 73% 21%
53	u	118	84% 16%

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Mol	Chain	Length	Quality of chain
54	v	525	11% 78% 18%
55	w	6	83% 67% 33%
56	7	6	17% 33% 67%
56	AA	6	33% 33% 67%
56	BA	6	17% 50% 50%
56	y	6	50% 50%
56	z	6	17% 33% 67%

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
			Total	C	N	O	S			
1	A	218	1702	1079	305	312	6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
50	o	30	228	144	33	48	3	0	0	0
50	p	30	228	144	33	48	3	0	0	0
50	q	30	228	144	33	48	3	0	0	0
50	r	30	228	144	33	48	3	0	0	0

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called messenger RNA.

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

- Molecule 56 is a protein called Viomycin.

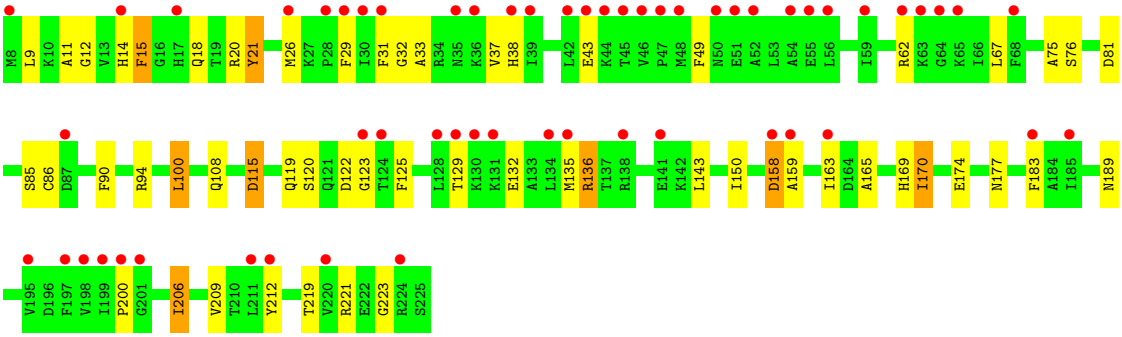
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	y	6	48	25	13	10	0	0	0
56	z	6	48	25	13	10	0	0	0
56	7	6	48	25	13	10	0	0	0
56	AA	6	48	25	13	10	0	0	0
56	BA	6	48	25	13	10	0	0	0

3 Residue-property plots (i)

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

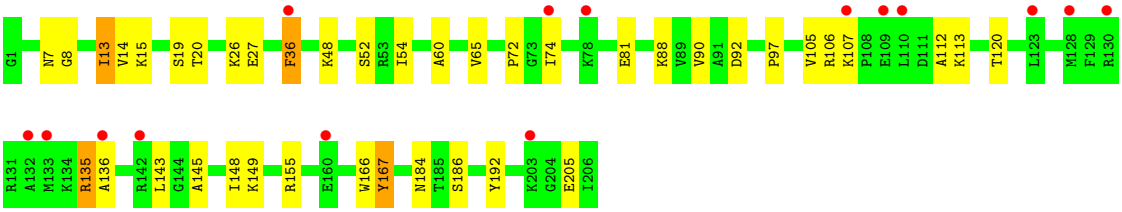
- Molecule 1: 30S ribosomal protein S2

Chain A:



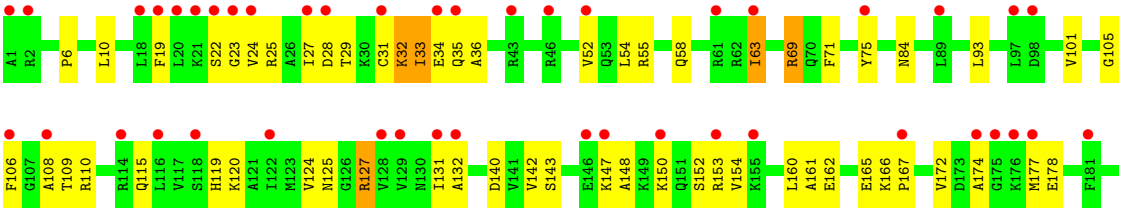
- Molecule 2: 30S ribosomal protein S3

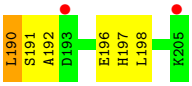
Chain B:



- Molecule 3: 30S ribosomal protein S4

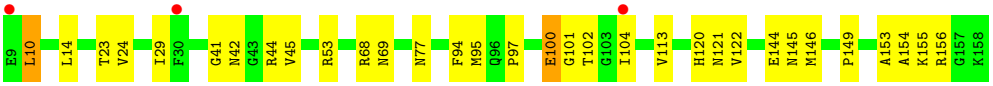
Chain C:





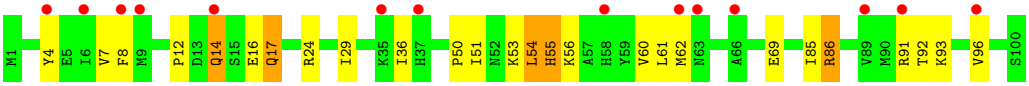
- Molecule 4: 30S ribosomal protein S5

Chain D:



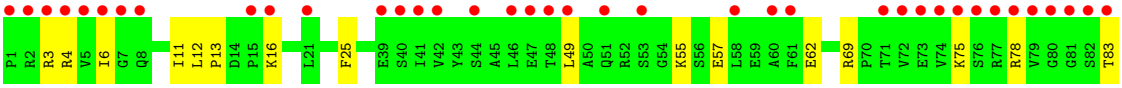
- Molecule 5: 30S ribosomal protein S6

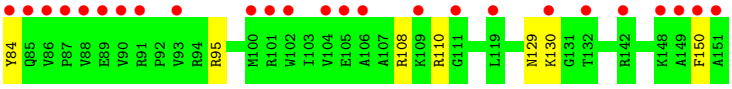
Chain E:



- Molecule 6: 30S ribosomal protein S7

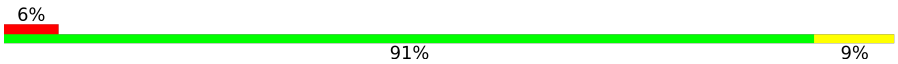
Chain F:

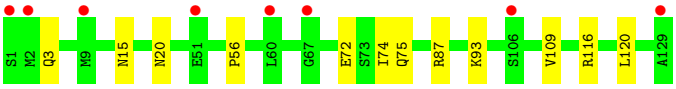




- Molecule 7: 30S ribosomal protein S8

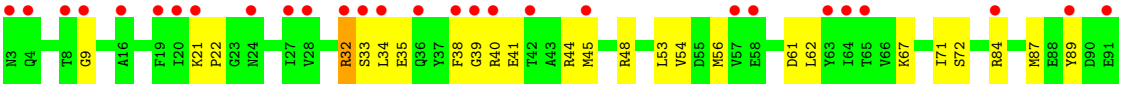
Chain G:

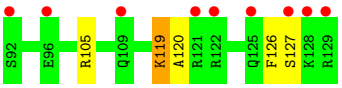




- Molecule 8: 30S ribosomal protein S9

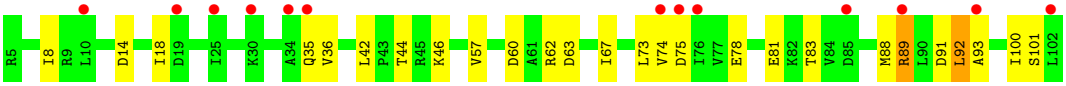
Chain H:





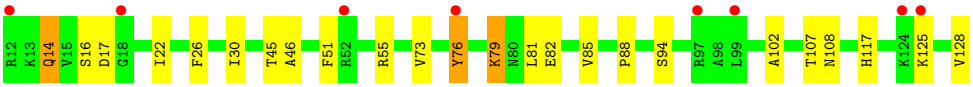
- Molecule 9: 30S ribosomal protein S10

Chain I: 13% 73% 24%



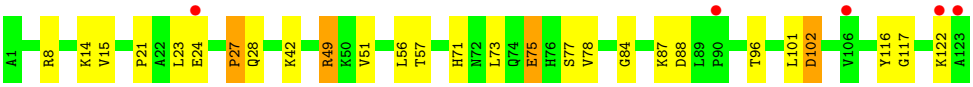
• Molecule 10: 30S ribosomal protein S11

Chain J: 7% 79% 18%



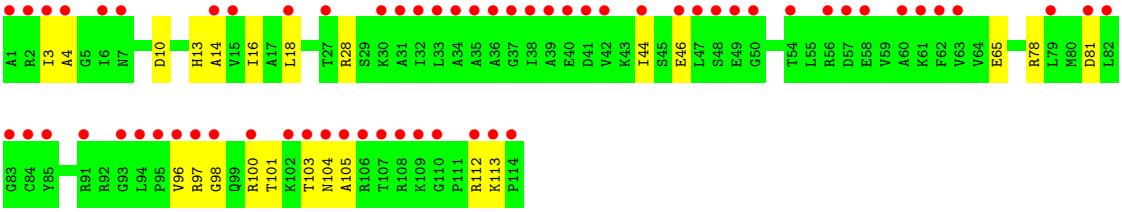
• Molecule 11: 30S ribosomal protein S12

Chain K: 4% 78% 19%



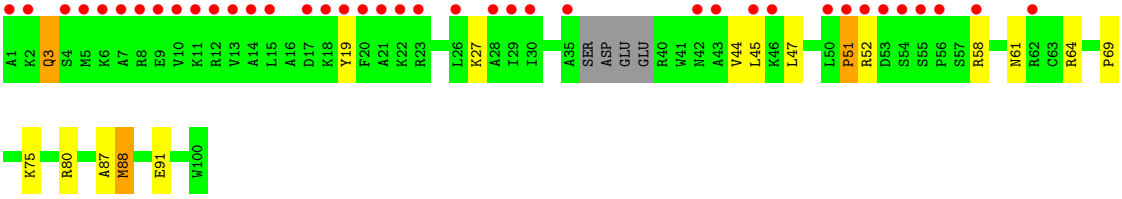
• Molecule 12: 30S ribosomal protein S13

Chain L: 55% 80% 20%



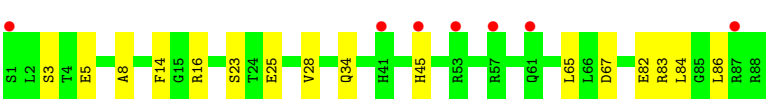
• Molecule 13: 30S ribosomal protein S14

Chain M: 39% 79% 14%



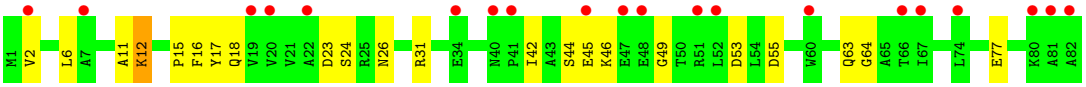
• Molecule 14: 30S ribosomal protein S15

Chain N: 8% 82% 18%



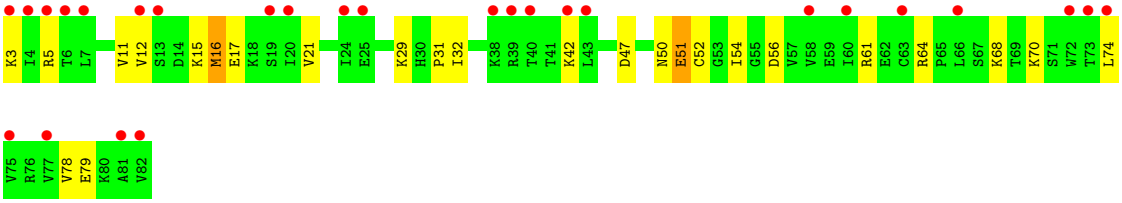
• Molecule 15: 30S ribosomal protein S16

Chain O:



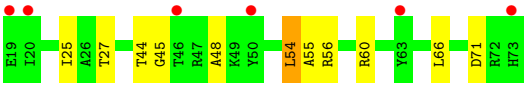
- Molecule 16: 30S ribosomal protein S17

Chain P:



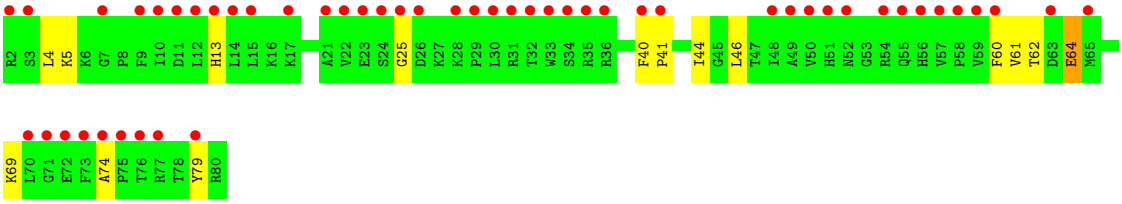
- Molecule 17: 30S ribosomal protein S18

Chain Q:



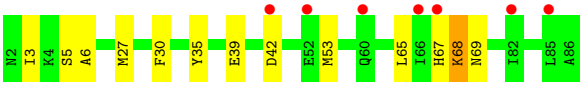
- Molecule 18: 30S ribosomal protein S19

Chain R:



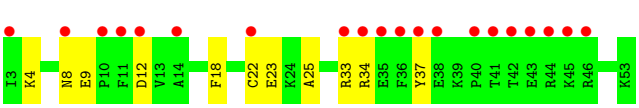
- Molecule 19: 30S ribosomal protein S20

Chain S:



- Molecule 20: 30S ribosomal protein S21

Chain T:



- Molecule 21: 50S ribosomal protein L2

Chain U: 3% 80% 19%

A1 S9 P10 G11 R12 P21 E22 L23 F29 L32 L33 E34 S37 R51 H52 K58 Q59 A60 V64 R68 N69 K70 I73 P74 A75 V76 V77 E78 R79 V93 L109 K110 Q114 I123 T128 R132 V140 H141 N142 R155 Y160

A165 L173 R176 E184 A185 R188 L191 N196 L204 W212 M224 N225 P226 V227 D228 H231 G232 G233 G234 F239 T251 K254 K255 T256 R257 S258 N259 K260 K264 F265 R268 R269 R270 S271

- Molecule 22: 50S ribosomal protein L3

Chain V: 78% 19%

M1 L4 E17 L40 D43 V50 K55 A69 K70 A71 G72 V73 E86 T91 V92 G93 Q94 S95 K106 V107 D108 V109 K114 F118 A119 G120 T121 V122 K123 R124 R128 T129 T133 G144 S145 Q150 T151 K159 M165 R169 V170

Q173 S174 L175 D176 V177 V178 R179 K190 G191 P194 L201 I202 V203 A209

- Molecule 23: 50S ribosomal protein L4

Chain W: 3% 82% 16%

M1 K6 D7 A8 Q9 S10 A11 L12 T13 V28 A45 Q46 R49 A50 E51 R61 R69 S70 I73 W78 R79 S80 V83 V96 N97 R102 I108 L109 L118 I119 K123 F124 E127 I148 I149 T150 G151 E152 L153 L157 N163 L164

H165 K166 R170 I175 D176 A201

- Molecule 24: 50S ribosomal protein L5

Chain X: 23% 79% 20%

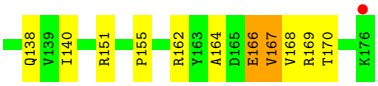
A1 Y7 K8 K13 K14 L15 M16 F19 N20 Y21 V24 V30 E31 T34 L35 I43 A44 D45 K46 G61 L65 I66 T67 K68 S72 V73 A74 G75 F76 K77 I78 R79 Q80 G81 Y82 C86 R91 G92 E93 R94 M95 W96 I103 P108 R109 I110

R111 D112 F113 R114 G115 L116 S117 A118 F121 R124 G125 M129 R132 E133 Q134 I135 I136 D146 R147 V148 L151 T157 T158 A159 K160 S161 D162 E163 A167 L168 F172 D173 F174 P175 F176 R177

- Molecule 25: 50S ribosomal protein L6

Chain Y: 2% 74% 23%

S1 V8 V9 V10 P11 V14 D15 V16 K17 I18 K28 W29 G30 E31 L32 T33 R34 D38 H44 A45 P53 R54 D55 D59 G60 R68 N72 V75 I76 T79 T83 K84 K85 V97 K98 H110 D113 P117 A118 G119 I120 V131 L132

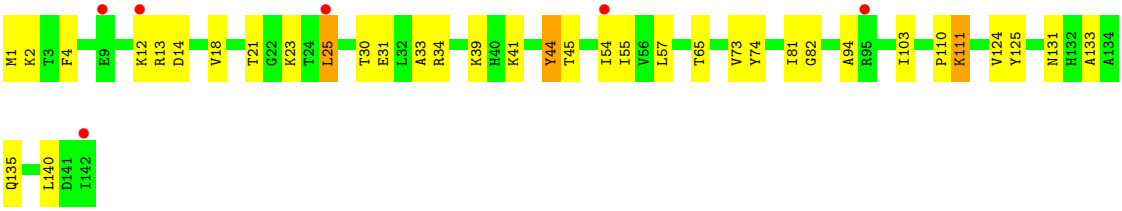


- Molecule 26: 50S ribosomal protein L11

Chain Z:

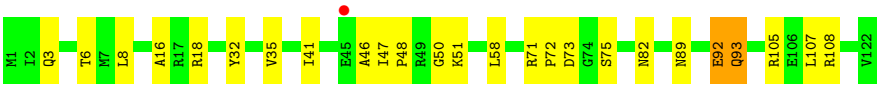
- Molecule 27: 50S ribosomal protein L13

Chain 0:



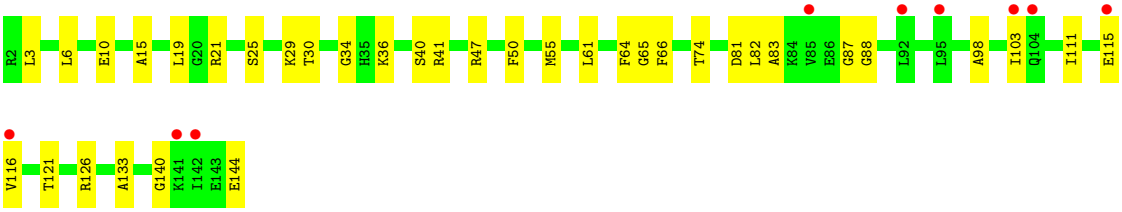
- Molecule 28: 50S ribosomal protein L14

Chain 1:



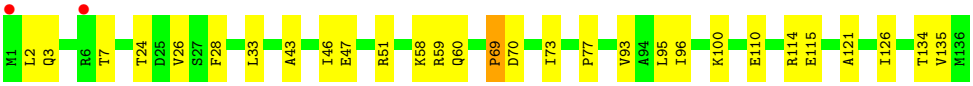
- Molecule 29: 50S ribosomal protein L15

Chain 2:



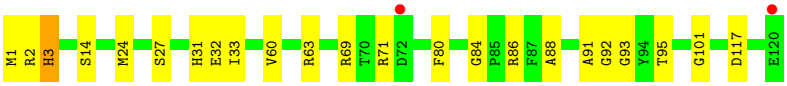
- Molecule 30: 50S ribosomal protein L16

Chain 3:



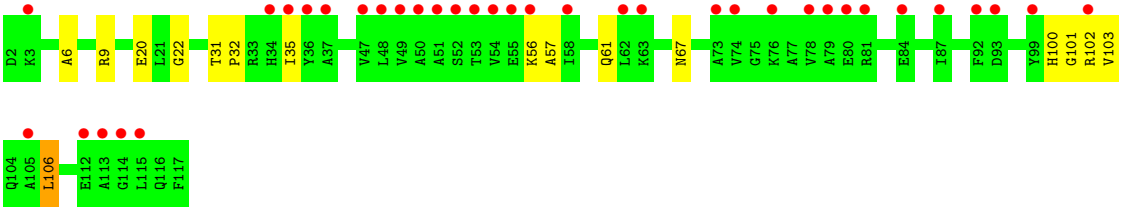
- Molecule 31: 50S ribosomal protein L17

Chain 4:



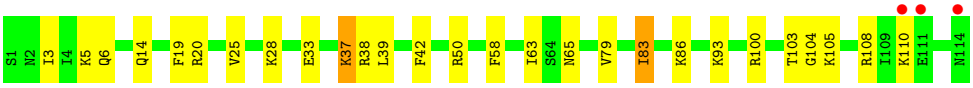
- Molecule 32: 50S ribosomal protein L18

Chain 5:



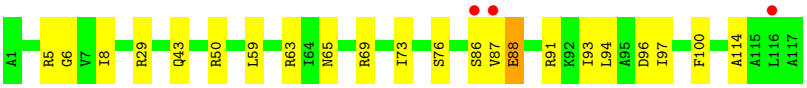
- Molecule 33: 50S ribosomal protein L19

Chain 6:



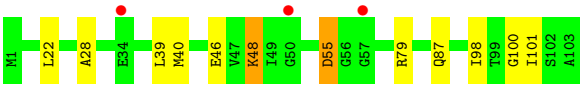
- Molecule 34: 50S ribosomal protein L20

Chain 8:



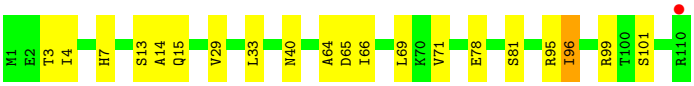
- Molecule 35: 50S ribosomal protein L21

Chain 9:



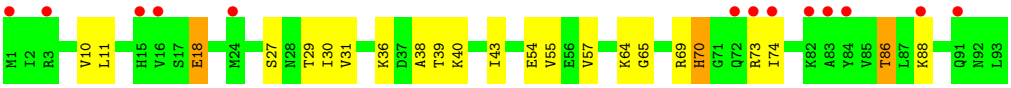
- Molecule 36: 50S ribosomal protein L22

Chain a:



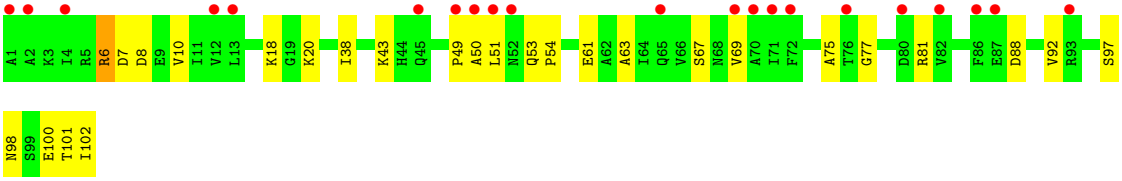
- Molecule 37: 50S ribosomal protein L23

Chain b:



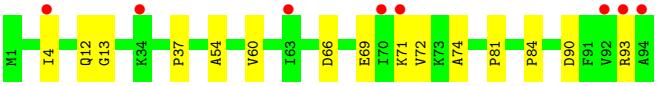
- Molecule 38: 50S ribosomal protein L24

Chain c:



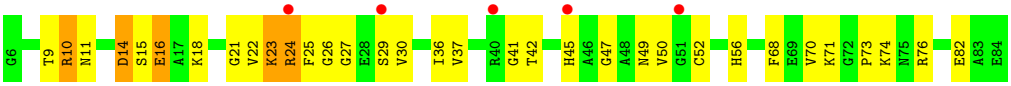
- Molecule 39: 50S ribosomal protein L25

Chain d:



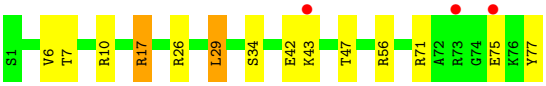
- Molecule 40: 50S ribosomal protein L27

Chain e:



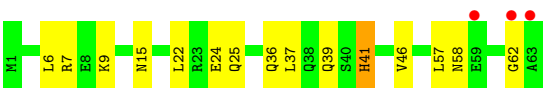
- Molecule 41: 50S ribosomal protein L28

Chain f:



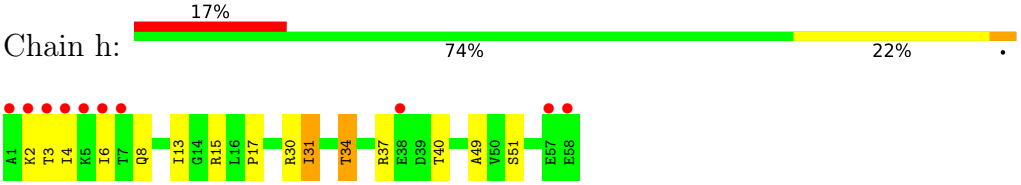
- Molecule 42: 50S ribosomal protein L29

Chain g:



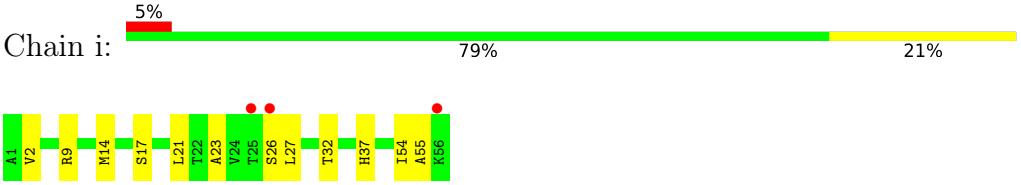
- Molecule 43: 50S ribosomal protein L30

Chain h:



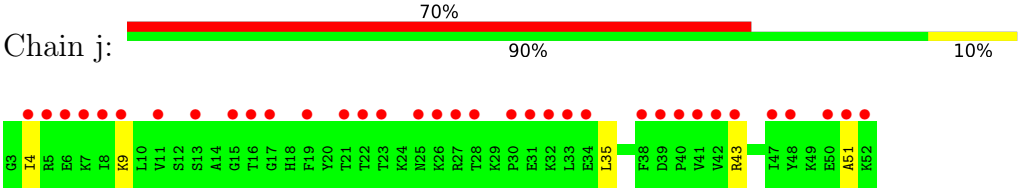
- Molecule 44: 50S ribosomal protein L32

Chain i:



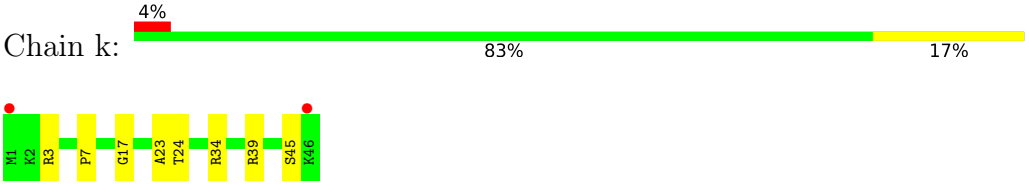
- Molecule 45: 50S ribosomal protein L33

Chain j:



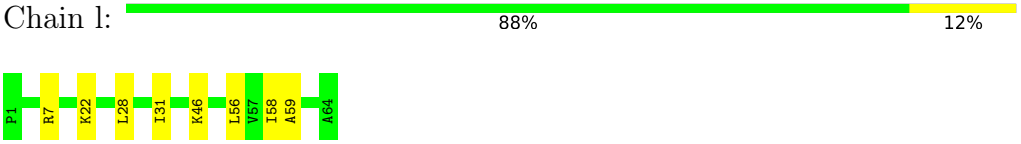
- Molecule 46: 50S ribosomal protein L34

Chain k:



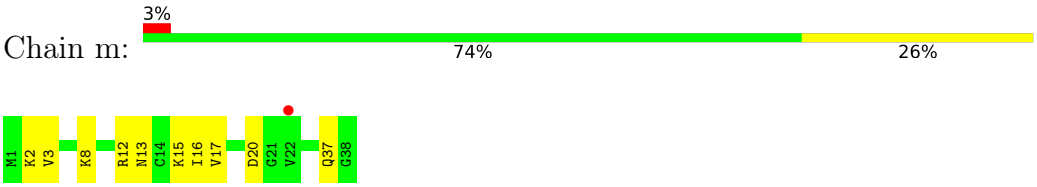
- Molecule 47: 50S ribosomal protein L35

Chain l:



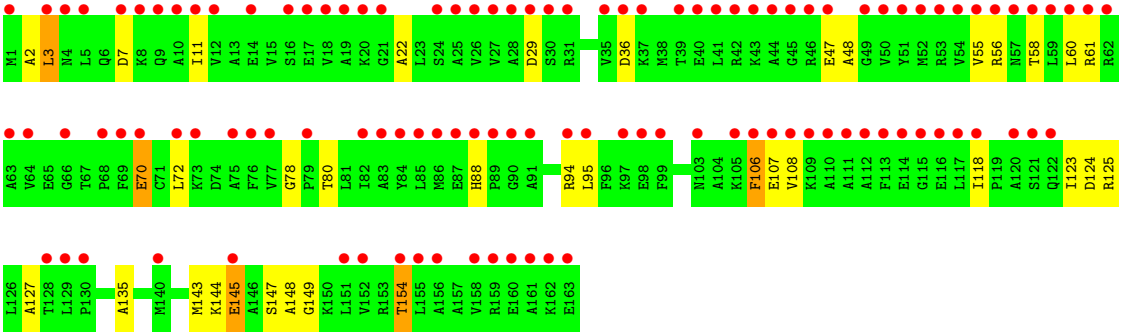
- Molecule 48: 50S ribosomal protein L36

Chain m:



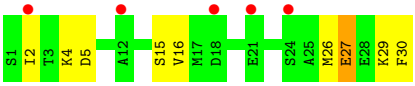
- Molecule 49: 50S ribosomal protein L10

Chain n:



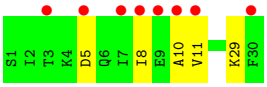
• Molecule 50: 50S ribosomal protein L7/L12

Chain o:



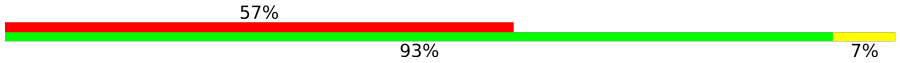
• Molecule 50: 50S ribosomal protein L7/L12

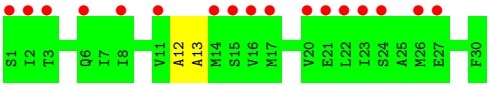
Chain p:



• Molecule 50: 50S ribosomal protein L7/L12

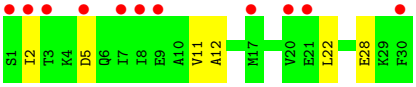
Chain q:





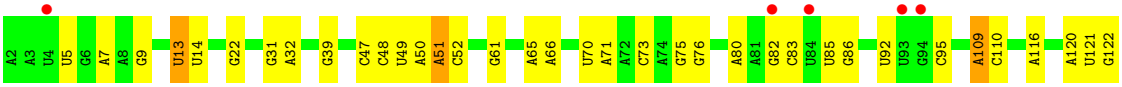
• Molecule 50: 50S ribosomal protein L7/L12

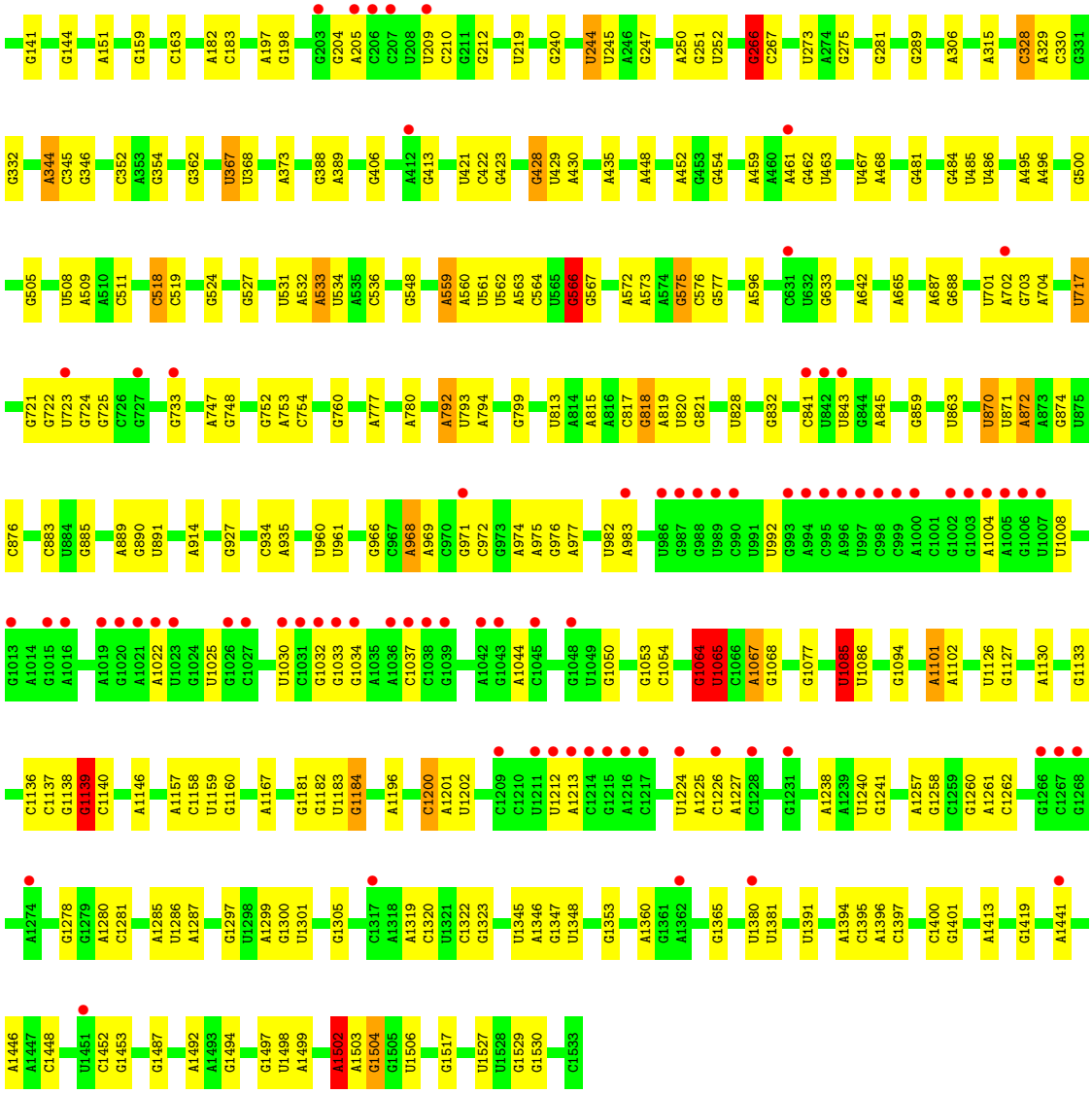
Chain r:



• Molecule 51: 16S ribosomal RNA

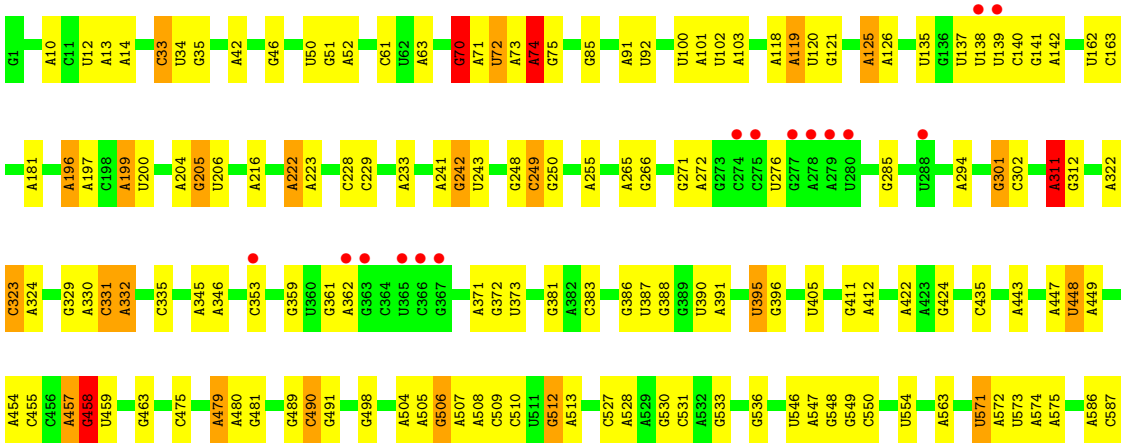
Chain s:

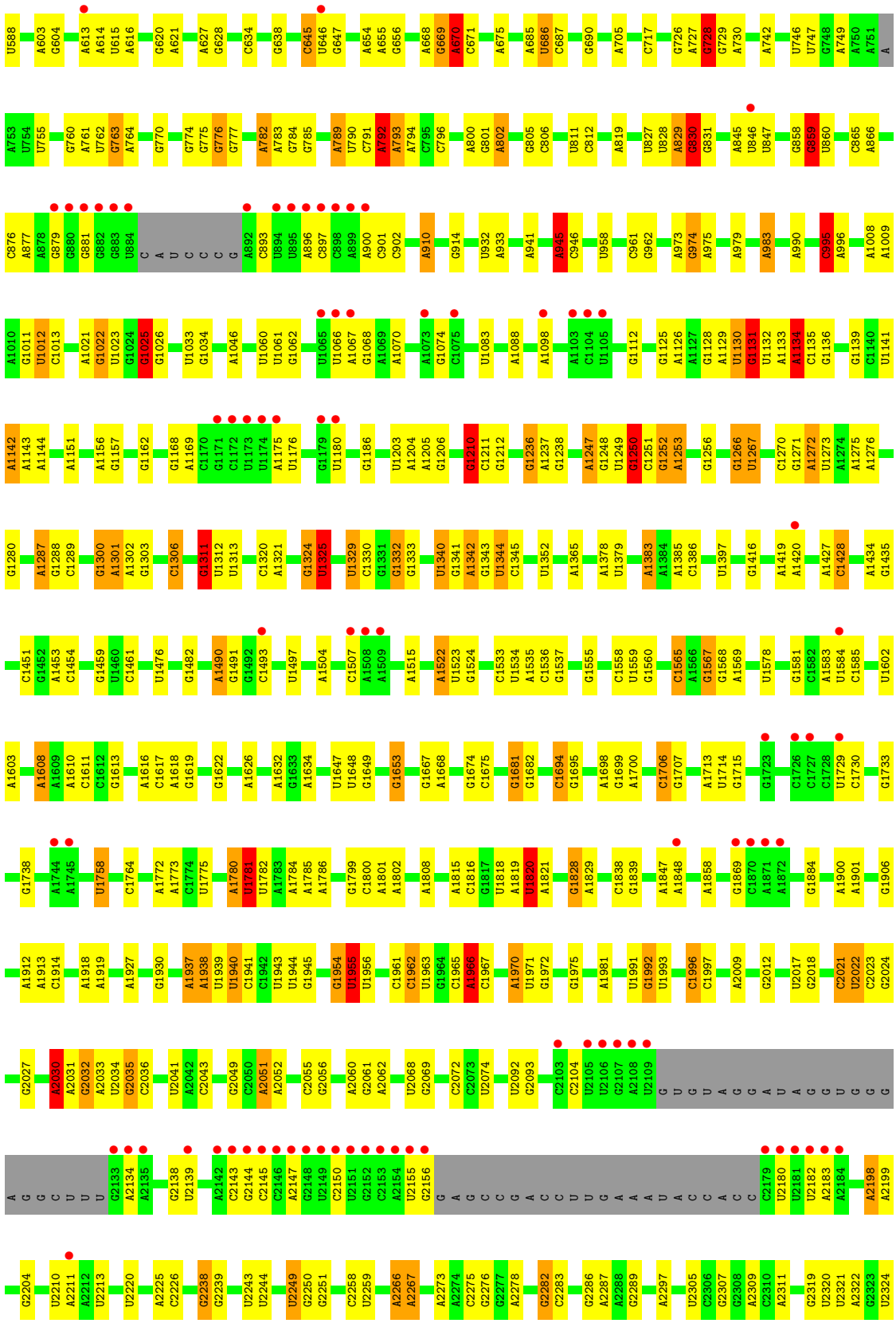


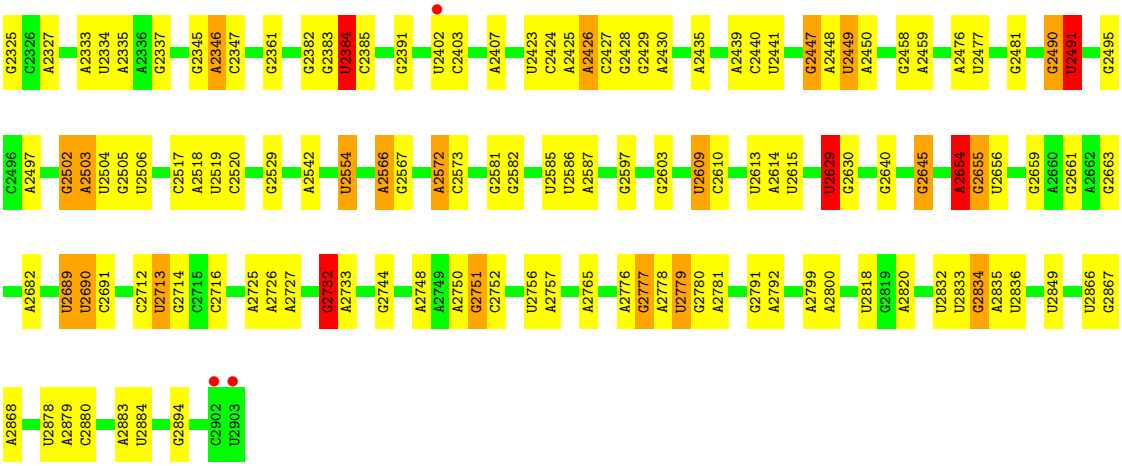


• Molecule 52: 23S ribosomal RNA

Chain t:




U588 A603 G604 A613 A614 U615 A616 G620 A621 A627 G628 C634 G638 C645 U646 G647 A654 A655 G656 A668 G669 A670 C671 A675 A685 U686 C687 G690 A705 C717 G726 A727 G728 G729 A730 A742 U746 U747 G748 A749 A750 A751 A
A753 U754 U755 G760 A761 U762 G763 A764 G770 G774 G775 G776 G777 A782 A783 G784 G785 A789 U790 C791 A792 A793 A794 C795 C796 A800 G801 A802 G805 C806 U811 C812 A819 U827 U828 A829 G830 G831 A845 U846 U847 G858 G859 U860 C865 A866
C876 A877 A878 G879 G880 G881 G882 G883 U884 C A U C C C G A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 A910 G914 U932 A933 A941 A945 C946 U958 C961 G962 A973 G974 A975 A979 A983 A990 C995 A996 A1008 A1009
A1010 G1011 U1012 C1013 A1021 G1022 U1023 G1024 G1025 G1026 U1033 G1034 A1046 U1060 U1061 G1062 U1065 U1066 A1067 G1068 A1069 A1070 A1073 G1074 C1075 U1083 A1088 A1098 A1103 C1104 U1105 G1112 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141
A1142 A1143 A1144 A1151 A1156 G1157 G1162 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1179 U1180 G1186 U1203 A1204 A1205 G1206 G1210 C1211 G1212 G1236 A1237 G1238 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 A1276
G1280 A1287 G1288 C1289 G1300 A1301 A1302 G1303 C1306 G1311 U1312 U1313 C1320 A1321 G1324 U1325 U1329 C1330 G1331 G1332 G1333 U1340 G1341 A1342 G1343 U1344 C1345 U1352 A1365 A1378 U1379 A1383 A1384 A1385 C1386 U1397 G1416 A1419 A1420 A1427 C1428 A1434 G1435
C1451 G1452 A1453 C1454 G1459 U1460 C1461 U1476 G1482 A1490 G1491 G1492 C1493 U1497 A1504 C1507 A1508 A1509 A1515 A1522 U1523 G1524 C1533 U1534 A1535 C1536 G1537 G1555 C1558 U1559 G1560 C1565 A1566 G1567 G1568 A1569 U1578 G1581 C1582 A1583 U1584 C1585 U1602
A1603 A1608 A1609 A1610 C1611 C1612 G1613 A1616 C1617 A1618 G1619 G1622 A1626 A1632 G1633 A1634 U1647 U1648 G1649 G1653 G1667 A1668 G1674 C1675 G1681 G1682 C1694 G1695 A1698 G1699 A1700 C1706 G1707 A1713 U1714 G1715 G1723 C1726 C1727 C1728 U1729 C1730 G1733
G1738 A1744 A1745 U1758 C1764 A1772 A1773 C1774 U1775 A1780 U1781 U1782 A1783 A1784 A1785 A1786 G1799 C1800 A1801 A1802 A1808 A1815 C1816 G1817 U1818 A1819 U1820 A1821 G1828 A1829 C1838 G1839 A1847 A1848 A1858 G1869 C1870 A1871 A1872 G1884 A1900 A1901 G1906
A1912 A1913 C1914 A1918 A1919 A1927 G1930 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 G1954 U1955 U1956 C1961 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1975 A1981 U1991 G1992 U1993 C1996 C1997 A2009 G2012 U2017 G2018 C2021 U2022 C2023 G2024
G2027 A2030 A2031 G2032 A2033 U2034 G2035 C2036 U2041 A2042 C2043 G2049 C2050 A2051 A2052 C2055 G2056 A2060 G2061 A2062 U2068 G2069 C2072 C2073 U2074 U2092 G2093 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G U G U A G G A U A G G U G G G
A G G C U U U G2133 A2134 A2135 G2138 U2139 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G A G C C G A C C U U G A A A U A C C A C C C2179 U2180 U2181 U2182 A2183 A2184 A2198 A2199
G2204 U2210 A2211 A2212 U2213 U2220 A2225 C2226 G2238 G2239 U2243 U2244 U2249 G2250 G2251 C2258 U2259 A2266 A2267 A2273 A2274 C2275 G2276 G2277 A2278 G2282 C2283 G2286 A2287 A2288 G2289 A2297 U2305 C2306 G2307 G2308 A2309 C2310 A2311 G2319 U2320 U2321 A2322 G2323 U2324

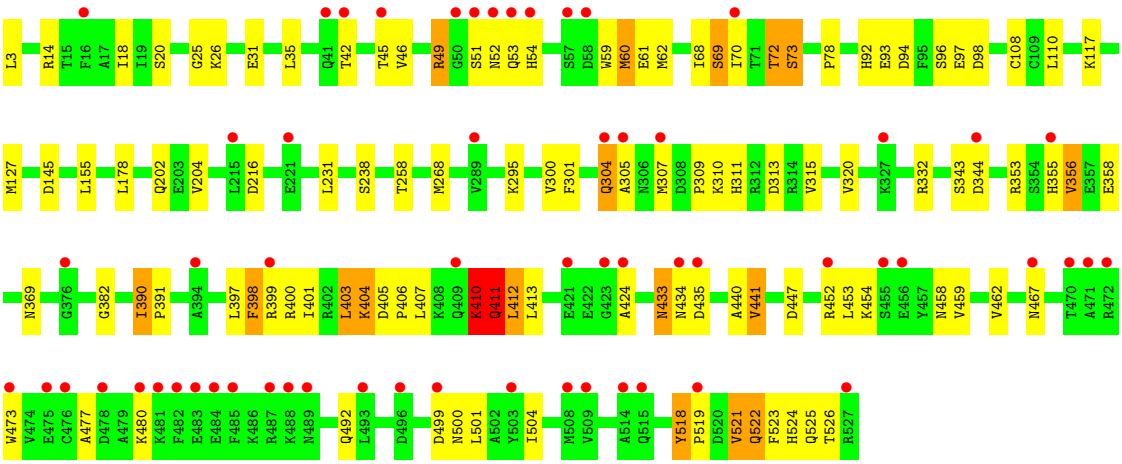


• Molecule 53: 5S ribosomal RNA

Chain u:

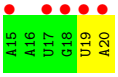
• Molecule 54: Peptide chain release factor 3

Chain v:



• Molecule 55: messenger RNA

Chain w:



• Molecule 56: Viomycin

Chain y:

• Molecule 56: Viomycin

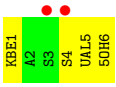
Chain z:

• Molecule 56: Viomycin

Chain 7:

• Molecule 56: Viomycin

Chain AA:



• Molecule 56: Viomycin

Chain BA:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 (i)

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
40	e	23	LYS
54	v	356	VAL
41	f	56	ARG
40	e	22	VAL
49	n	61	ARG

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

Mol	Chain	Res	Type
36	a	57	ASN
43	h	33	HIS
37	b	70	HIS
40	e	39	GLN
49	n	4	ASN

5.3.3 RNA (i)

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 (i)

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	UAL	7	5	56	7,8,9	2.72	1 (14%)	5,9,11	1.18	0
56	KBE	7	1	56	8,8,9	0.73	0	7,8,10	1.22	1 (14%)
56	5OH	BA	6	56	8,12,13	1.17	0	3,16,18	2.21	2 (66%)
56	DPP	z	2	56	3,5,6	0.78	0	1,5,7	0.36	0
56	UAL	z	5	56	7,8,9	1.82	3 (42%)	5,9,11	2.61	1 (20%)
56	DPP	y	2	56	3,5,6	0.39	0	1,5,7	0.30	0
56	UAL	BA	5	56	7,8,9	2.69	1 (14%)	5,9,11	1.62	1 (20%)
56	KBE	BA	1	56	8,8,9	1.21	1 (12%)	7,8,10	1.32	1 (14%)
56	KBE	z	1	56	8,8,9	1.22	1 (12%)	7,8,10	2.16	1 (14%)
56	KBE	y	1	56	8,8,9	1.36	1 (12%)	7,8,10	2.04	1 (14%)
56	5OH	AA	6	56	8,12,13	1.33	1 (12%)	3,16,18	1.68	1 (33%)
56	5OH	z	6	56	8,12,13	1.13	1 (12%)	3,16,18	1.13	0
56	DPP	AA	2	56	3,5,6	1.13	0	1,5,7	1.21	0
56	DPP	BA	2	56	3,5,6	1.30	0	1,5,7	0.08	0
56	UAL	AA	5	56	7,8,9	2.53	1 (14%)	5,9,11	1.33	1 (20%)
56	5OH	y	6	56	8,12,13	0.92	0	3,16,18	2.40	2 (66%)
56	KBE	AA	1	56	8,8,9	1.66	2 (25%)	7,8,10	3.54	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	5OH	7	6	56	8,12,13	1.77	2 (25%)	3,16,18	2.93	1 (33%)
56	DPP	7	2	56	3,5,6	0.50	0	1,5,7	0.90	0
56	UAL	y	5	56	7,8,9	2.26	2 (28%)	5,9,11	1.39	1 (20%)

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	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	DPP	z	2	56	-	0/2/4/6	-
56	UAL	z	5	56	-	0/3/7/9	-
56	DPP	y	2	56	-	0/2/4/6	-
56	UAL	BA	5	56	-	0/3/7/9	-
56	KBE	BA	1	56	-	4/7/7/8	-
56	KBE	z	1	56	-	2/7/7/8	-
56	KBE	y	1	56	-	2/7/7/8	-
56	5OH	AA	6	56	-	0/2/18/20	0/1/1/1
56	5OH	z	6	56	-	1/2/18/20	0/1/1/1
56	DPP	AA	2	56	-	0/2/4/6	-
56	DPP	BA	2	56	-	0/2/4/6	-
56	UAL	AA	5	56	-	0/3/7/9	-
56	5OH	y	6	56	-	0/2/18/20	0/1/1/1
56	KBE	AA	1	56	-	0/7/7/8	-
56	5OH	7	6	56	-	0/2/18/20	0/1/1/1
56	DPP	7	2	56	-	0/2/4/6	-
56	UAL	y	5	56	-	0/3/7/9	-

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(^{o})	Ideal(^{o})
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	y	1	KBE	CA-CB-CG-CD
56	z	1	KBE	C-CA-CB-N
56	z	1	KBE	C-CA-CB-CG
56	7	1	KBE	C-CA-CB-N
56	7	1	KBE	C-CA-CB-CG

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	38, 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, 70, 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, 84, 153, 167	0
39	d	94/94 (100%)	0.64	8 (8%) 10 4	69, 98, 120, 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 (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	0.28	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(Å^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	y	5	9/10	0.87	0.21	102,103,109,109	0
56	UAL	z	5	9/10	0.87	0.39	99,100,101,102	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.