



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2019 – 02:49 PM EDT

PDB ID : 4V8Q  
Title : Complex of SmpB, a tmRNA fragment and EF-Tu-GDP-Kirromycin with the 70S ribosome  
Authors : Neubauer, C.; Gillet, R.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2011-12-10  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

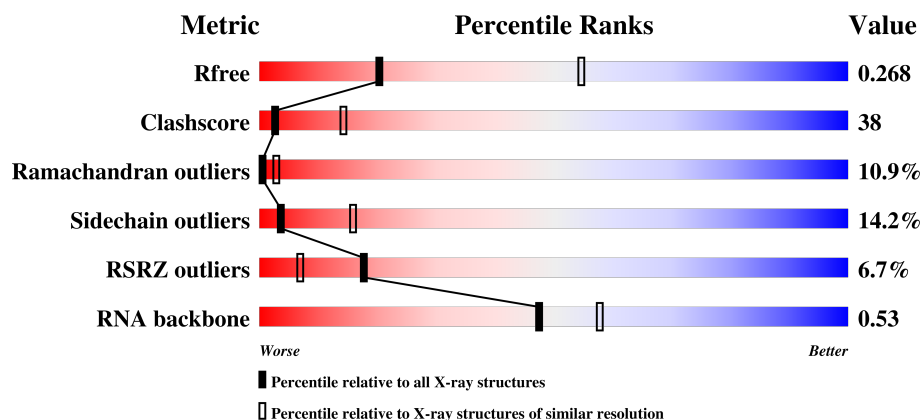
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)
RNA backbone	2636	1015 (3.44-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A0	85	<div> <div>11%</div> <div>27% 61% 8% ..</div> </div>
2	A1	98	<div> <div>2%</div> <div>38% 45% 12% ..</div> </div>
3	A2	72	<div> <div>3%</div> <div>18% 64% 17% .</div> </div>
4	A3	60	<div> <div>2%</div> <div>37% 55% 7% .</div> </div>

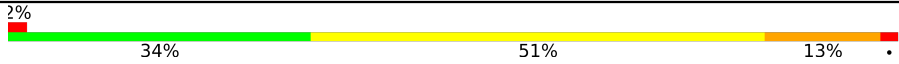


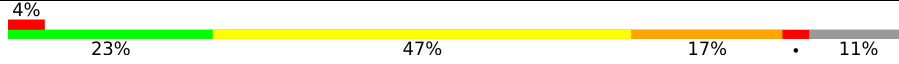
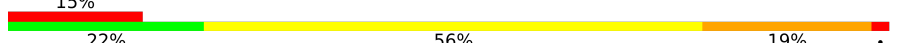
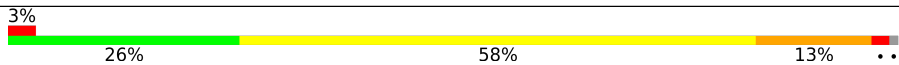
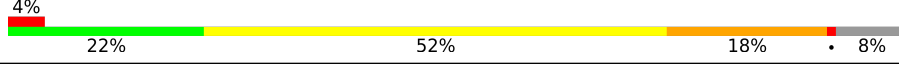
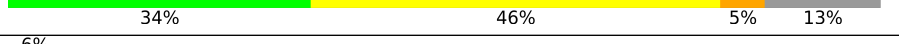
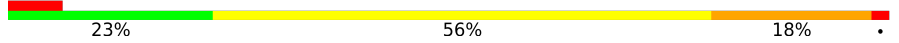
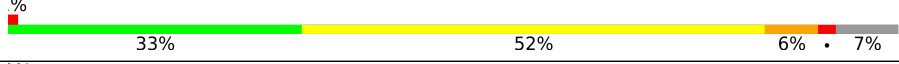
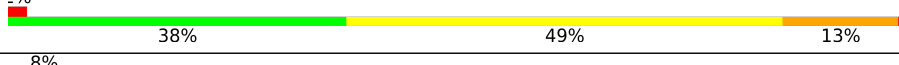
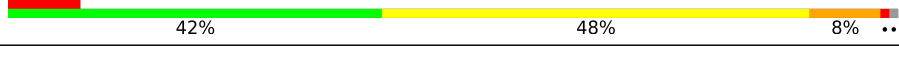
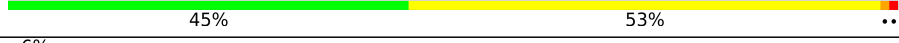
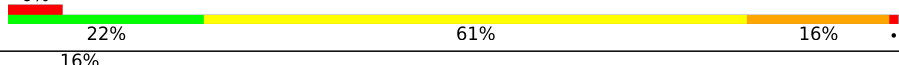
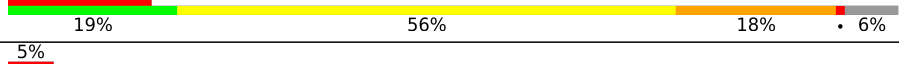

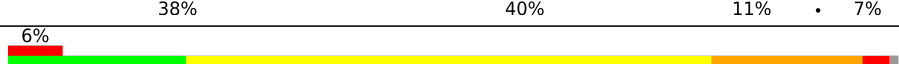
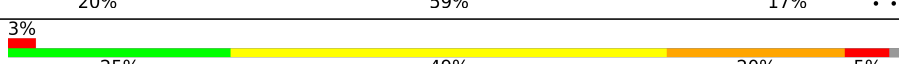
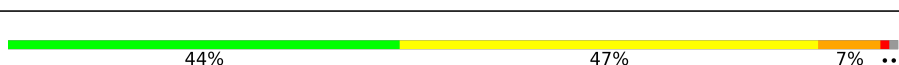
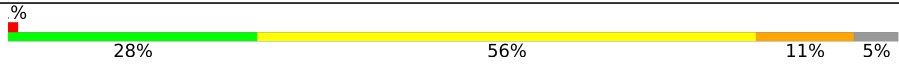

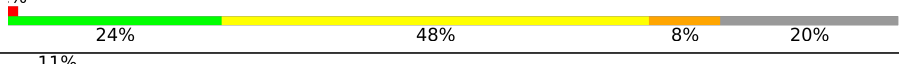



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Mol	Chain	Length	Quality of chain
5	A4	71	
6	A5	60	
7	A6	54	
8	A7	49	
9	A8	65	
10	A9	37	
11	AA	2915	
12	AB	122	
13	AC	229	
14	AD	276	
15	AE	206	
16	AF	210	
17	AG	182	
18	AH	180	
19	AJ	130	
20	AK	140	
21	AN	140	
22	AO	122	
23	AP	150	
24	AQ	141	
25	AR	118	
26	AS	112	
27	AT	146	
28	AU	118	
29	AV	101	

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Mol	Chain	Length	Quality of chain
30	AW	113	
31	AX	96	
32	AY	110	
33	AZ	206	
34	B2	144	
35	BA	1522	
36	BB	256	
37	BC	239	
38	BD	209	
39	BE	162	
40	BF	101	
41	BG	156	
42	BH	138	
43	BI	128	
44	BJ	105	
45	BK	129	
46	BL	135	
47	BM	126	
48	BN	61	
49	BO	89	
50	BP	88	
51	BQ	105	
52	BR	88	
53	BS	93	
54	BT	106	

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Mol	Chain	Length	Quality of chain
55	BU	27	<div><div></div><div>52%26%11%7%</div></div>
56	BV	77	<div><div>%</div><div>38%48%13%</div></div>
56	BW	77	<div><div>87%</div><div>27%58%10%</div></div>
57	BX	19	<div><div>5%16%5%</div><div>74%</div></div>
58	BY	90	<div><div>7%32%23%7%</div><div>31%</div></div>
59	BZ	405	<div><div>2%</div><div>32%50%10%7%</div></div>

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 154205 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 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	A7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	A8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AA	2901	Total	C	N	O	P	0	0	0
			62479	27808	11685	20086	2900			

- Molecule 12 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AC	228	Total	C	N	O	S	0	0	0
			1742	1101	318	319	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	19	ILE	VAL	conflict	UNP Q5SLP7
AC	27	HIS	ARG	conflict	UNP Q5SLP7
AC	127	MET	LEU	conflict	UNP Q5SLP7

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AJ	130	Total	C	N	O		0	0	0
			654	393	130	131				

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L11.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AK	140	Total	C	N	O	0	0	0
			701	420	140	141			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	AR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	AX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AZ	184	Total	C	N	O	S	0	0	1
			1460	932	261	265	2			

- Molecule 34 is a protein called SMALL PROTEIN B SMPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B2	144	Total	C	N	O	S	0	0	0
			1184	754	219	210	1			

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	1504	Total	C	N	O	P	0	0	0
			32330	14391	5994	10442	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1489	A	G	conflict	GB NC_006461
BA	1490	A	C	conflict	GB NC_006461

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	1	MET	-	expression tag	UNP Q5SHN3
BL	2	VAL	-	expression tag	UNP Q5SHN3
BL	3	ALA	-	expression tag	UNP Q5SHN3
BL	4	LEU	-	expression tag	UNP Q5SHN3

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 54 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 55 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 56 is a RNA chain called E-SITE or P-SITE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
56	BW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 57 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BX	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

- Molecule 58 is a RNA chain called TMRNA DELA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	62	Total	C	N	O	P	0	0	0
			1305	582	233	429	61			

- Molecule 59 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BZ	378	Total	C	N	O	S	0	0	1
			2929	1854	510	553	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	181	GLU	GLN	conflict	UNP Q5SHN6
BZ	184	LYS	ARG	conflict	UNP Q5SHN6
BZ	189	LYS	ARG	conflict	UNP Q5SHN6
BZ	264	LYS	ARG	conflict	UNP Q5SHN6
BZ	288	LEU	VAL	conflict	UNP Q5SHN6
BZ	322	ILE	VAL	conflict	UNP Q5SHN6
BZ	336	THR	SER	conflict	UNP Q5SHN6
BZ	354	ARG	GLN	conflict	UNP Q5SHN6
BZ	357	GLN	PRO	conflict	UNP Q5SHN6

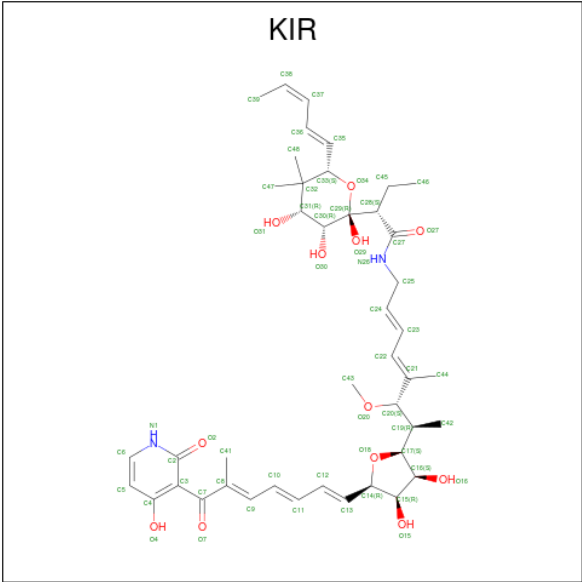
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	A9	1	Total Zn 1 1	0	0
60	BN	1	Total Zn 1 1	0	0
60	BD	1	Total Zn 1 1	0	0

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

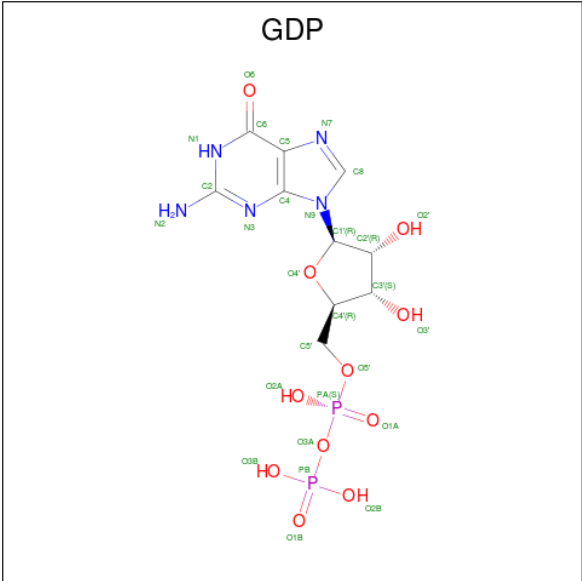
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BZ	1	Total Mg 1 1	0	0
61	AA	1	Total Mg 1 1	0	0

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
62	BZ	1	Total	C	N	O	0	0
			57	43	2	12		

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

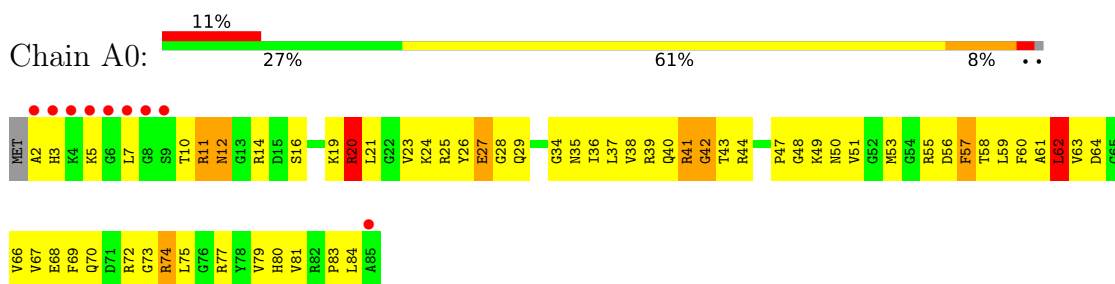




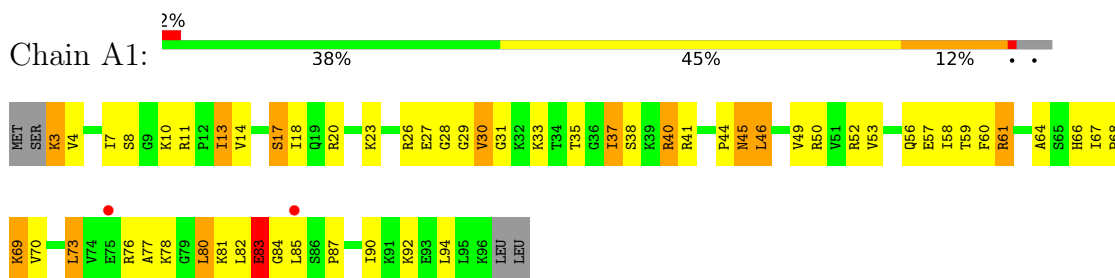
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

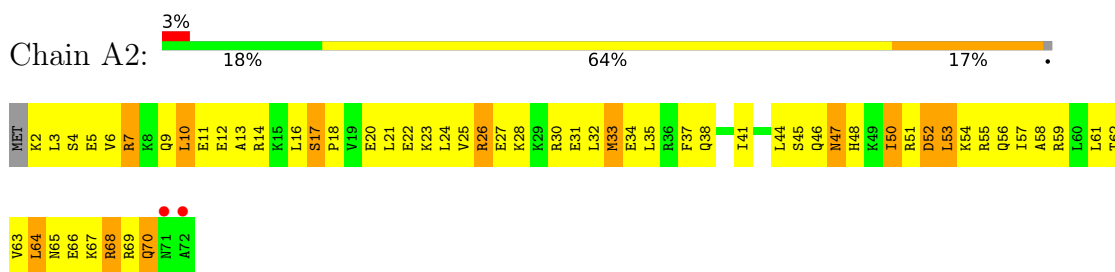
#### • Molecule 1: 50S RIBOSOMAL PROTEIN L27



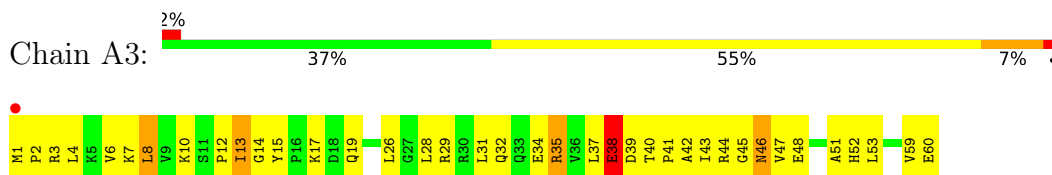
#### • Molecule 2: 50S RIBOSOMAL PROTEIN L28



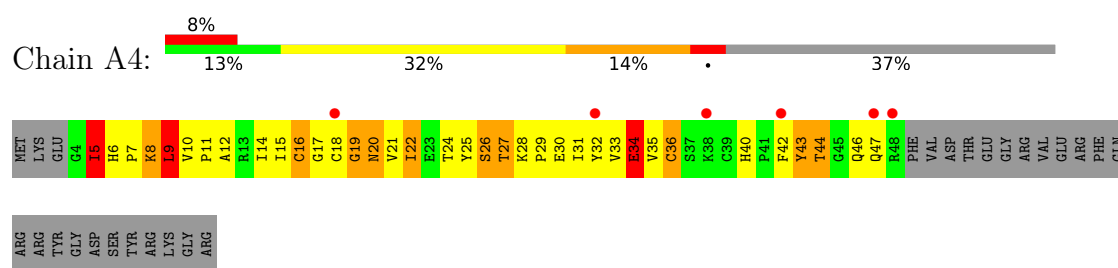
#### • Molecule 3: 50S RIBOSOMAL PROTEIN L29



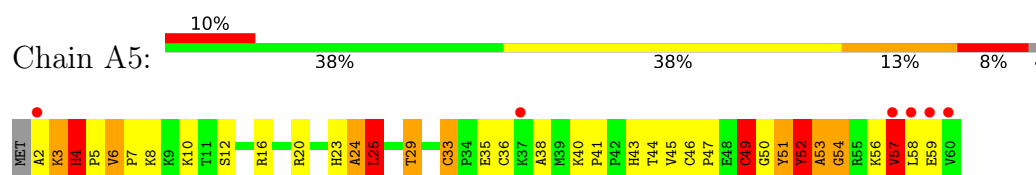
#### • Molecule 4: 50S RIBOSOMAL PROTEIN L30



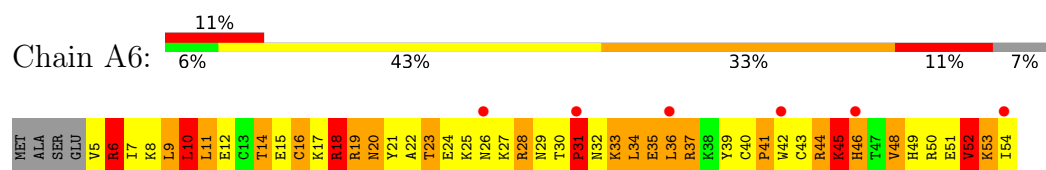
#### • Molecule 5: 50S RIBOSOMAL PROTEIN L31



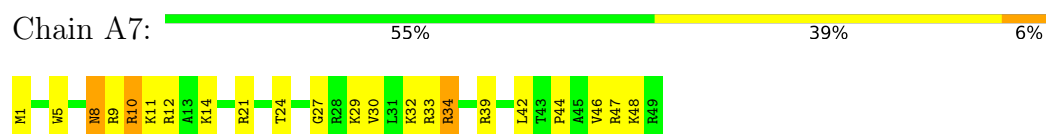
• Molecule 6: 50S RIBOSOMAL PROTEIN L32



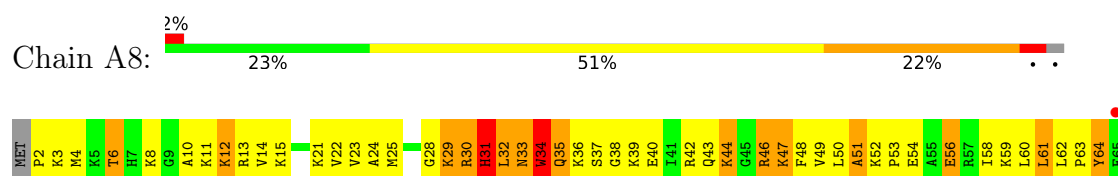
• Molecule 7: 50S RIBOSOMAL PROTEIN L33



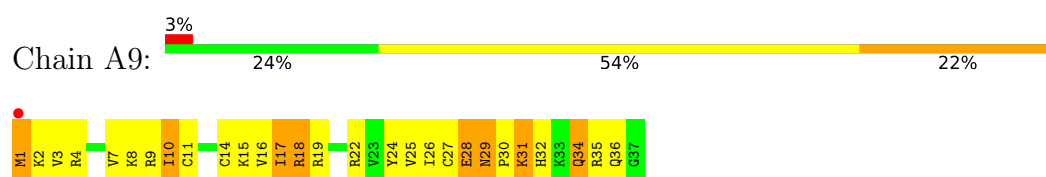
• Molecule 8: 50S RIBOSOMAL PROTEIN L34



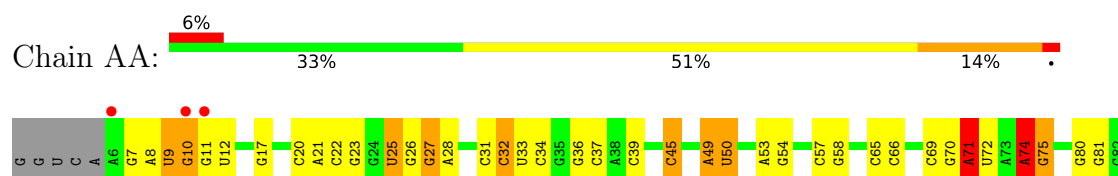
• Molecule 9: 50S RIBOSOMAL PROTEIN L35



• Molecule 10: 50S RIBOSOMAL PROTEIN L36



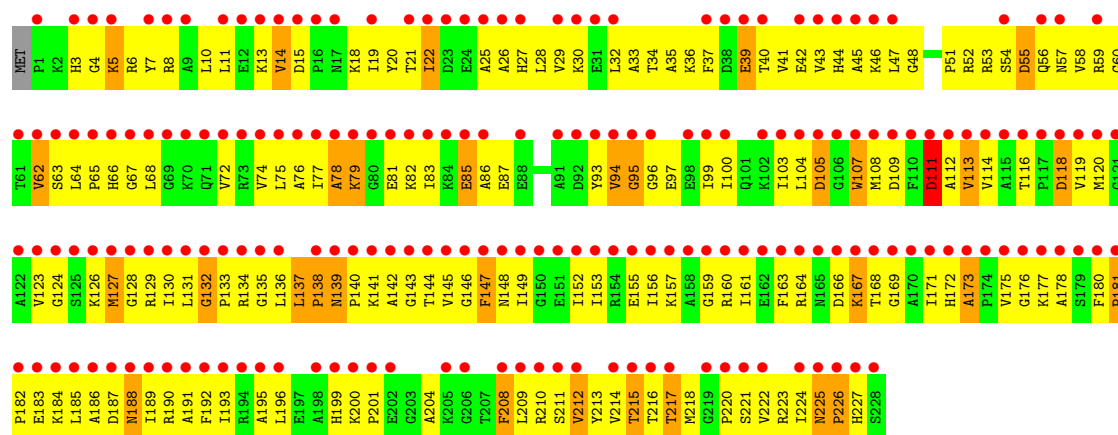
• Molecule 11: 23S ribosomal RNA



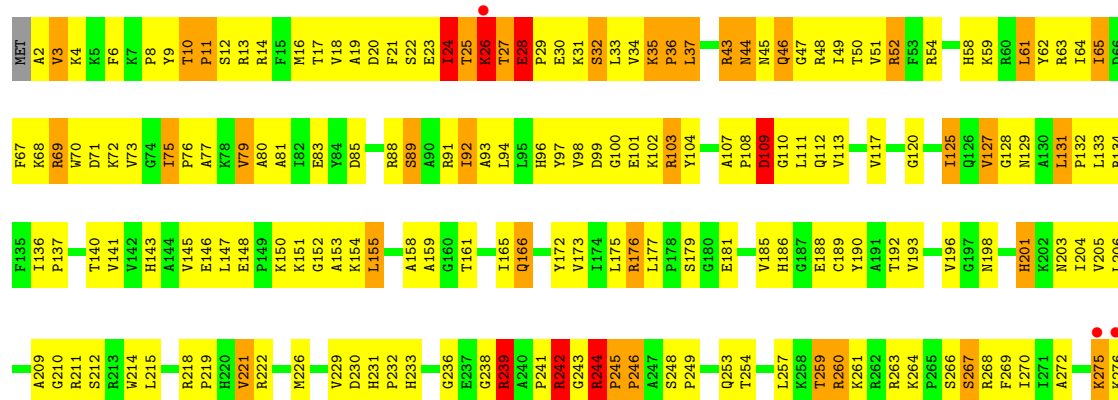




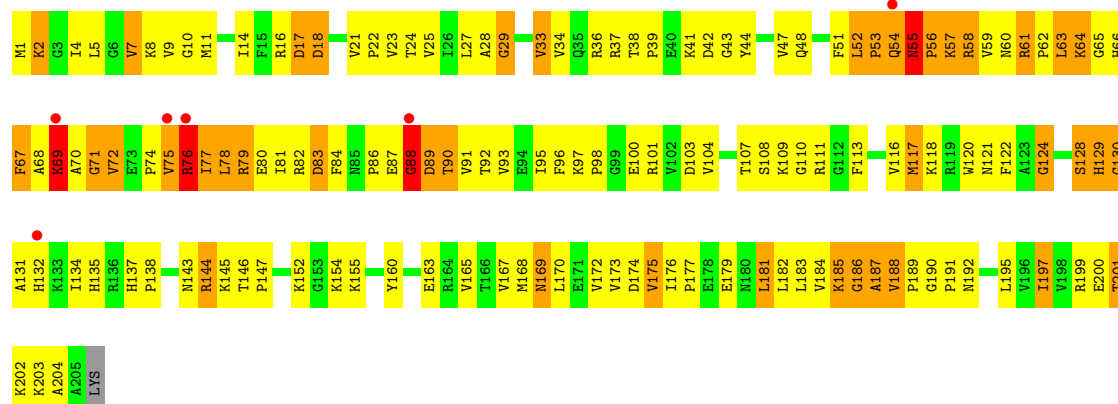




### • Molecule 14: 50S RIBOSOMAL PROTEIN L2

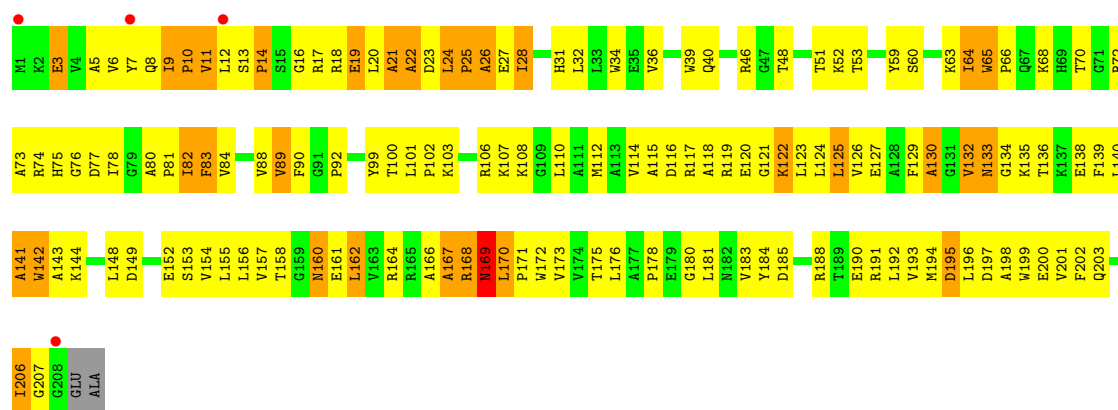


### • Molecule 15: 50S RIBOSOMAL PROTEIN L3

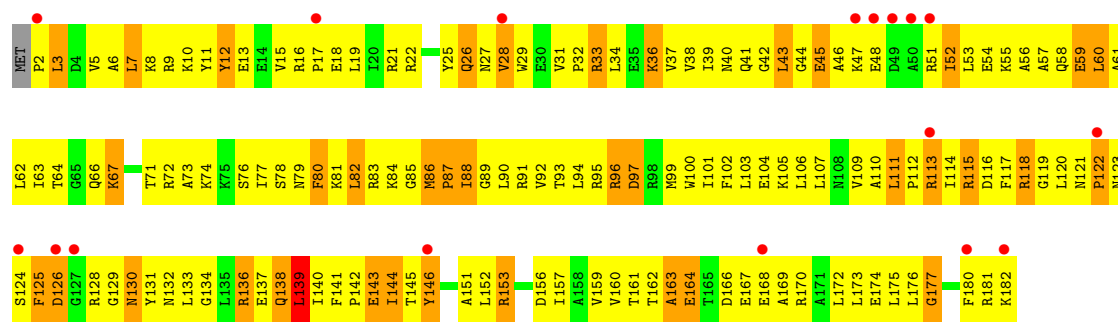


### • Molecule 16: 50S RIBOSOMAL PROTEIN L4

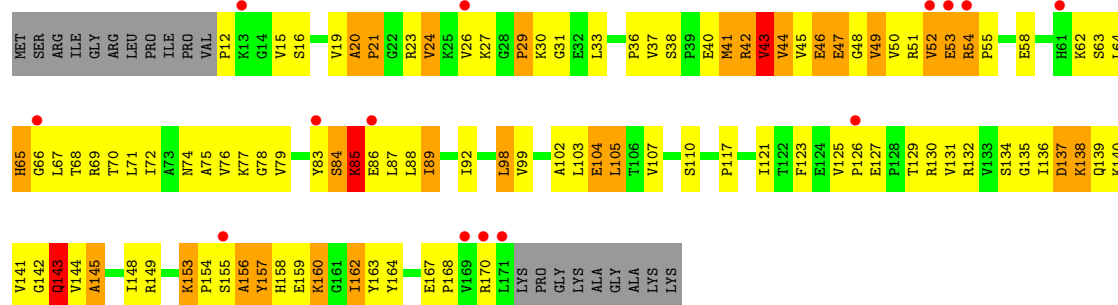




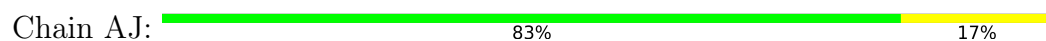
• Molecule 17: 50S RIBOSOMAL PROTEIN L5



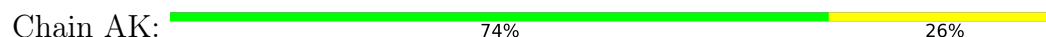
• Molecule 18: 50S RIBOSOMAL PROTEIN L6



• Molecule 19: 50S RIBOSOMAL PROTEIN L10

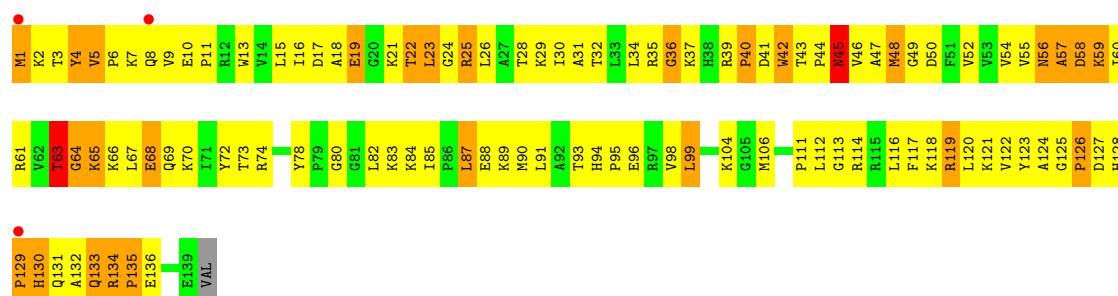


• Molecule 20: 50S RIBOSOMAL PROTEIN L11

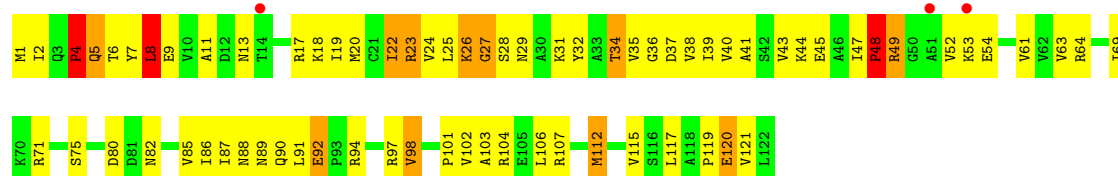




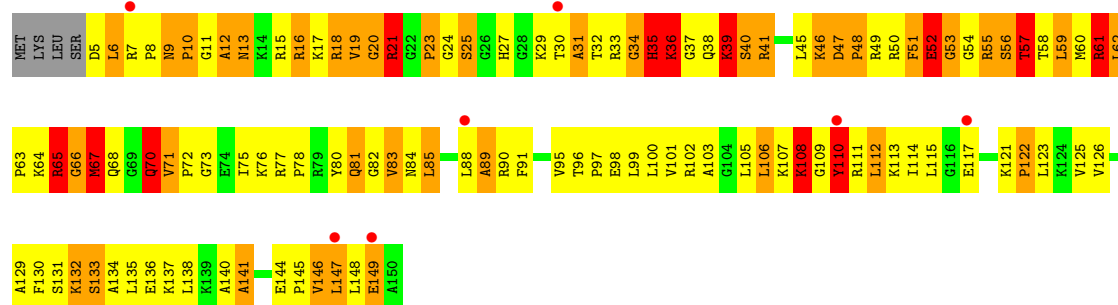
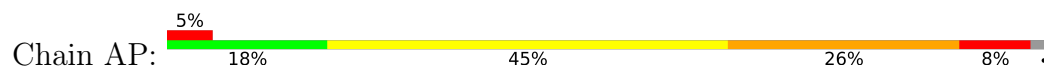
## ● Molecule 21: 50S RIBOSOMAL PROTEIN L13



## ● Molecule 22: 50S RIBOSOMAL PROTEIN L14



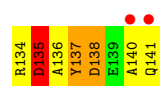
## ● Molecule 23: 50S RIBOSOMAL PROTEIN L15



## ● Molecule 24: 50S RIBOSOMAL PROTEIN L16

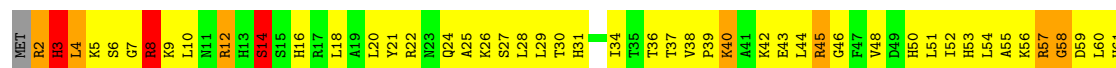






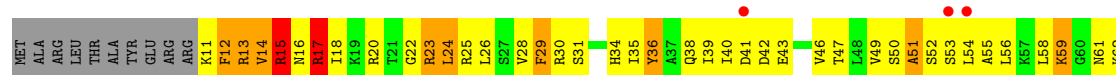
## • Molecule 25: 50S RIBOSOMAL PROTEIN L17

Chain AR:



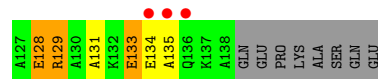
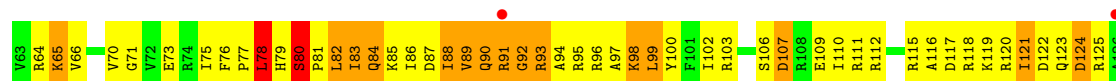
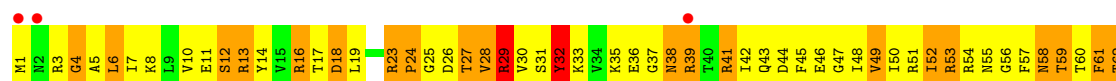
## • Molecule 26: 50S RIBOSOMAL PROTEIN L18

Chain AS:



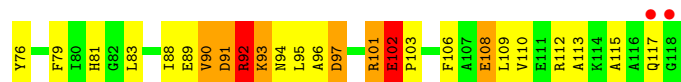
## • Molecule 27: 50S RIBOSOMAL PROTEIN L19

Chain AT:



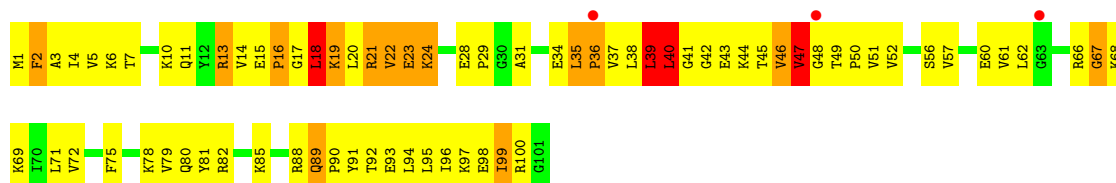
## • Molecule 28: 50S RIBOSOMAL PROTEIN L20

Chain AU:

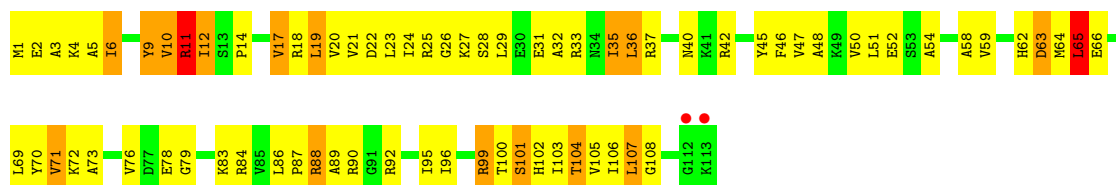


## • Molecule 29: 50S RIBOSOMAL PROTEIN L21

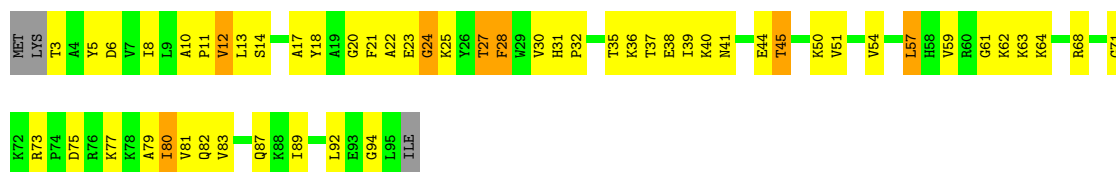
Chain AV:



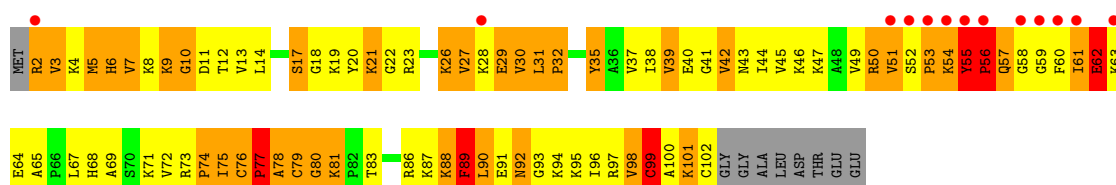
• Molecule 30: 50S RIBOSOMAL PROTEIN L22



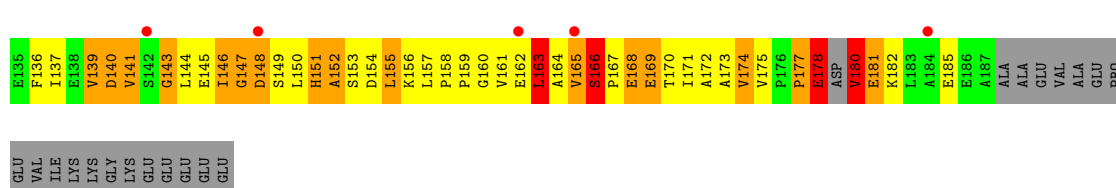
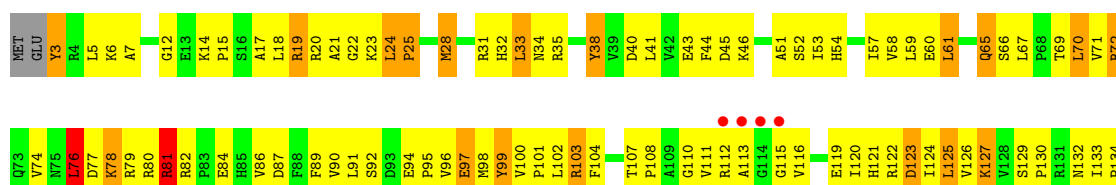
• Molecule 31: 50S RIBOSOMAL PROTEIN L23



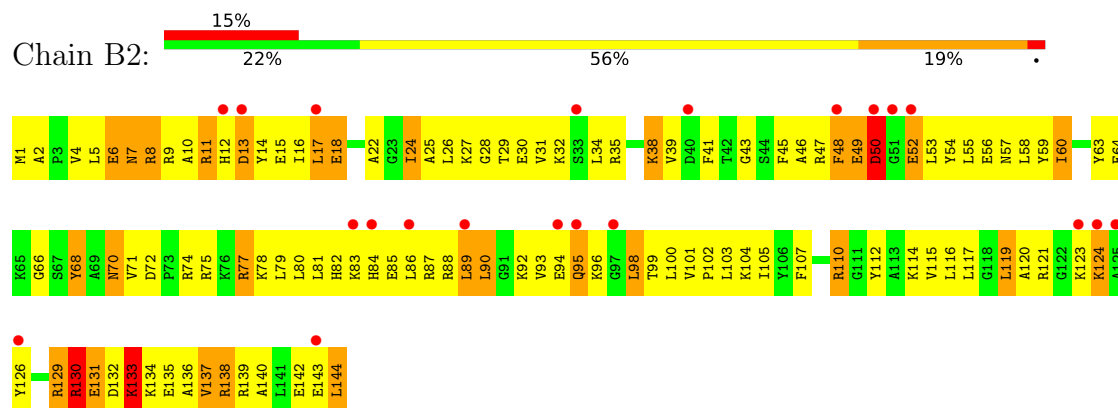
• Molecule 32: 50S RIBOSOMAL PROTEIN L24



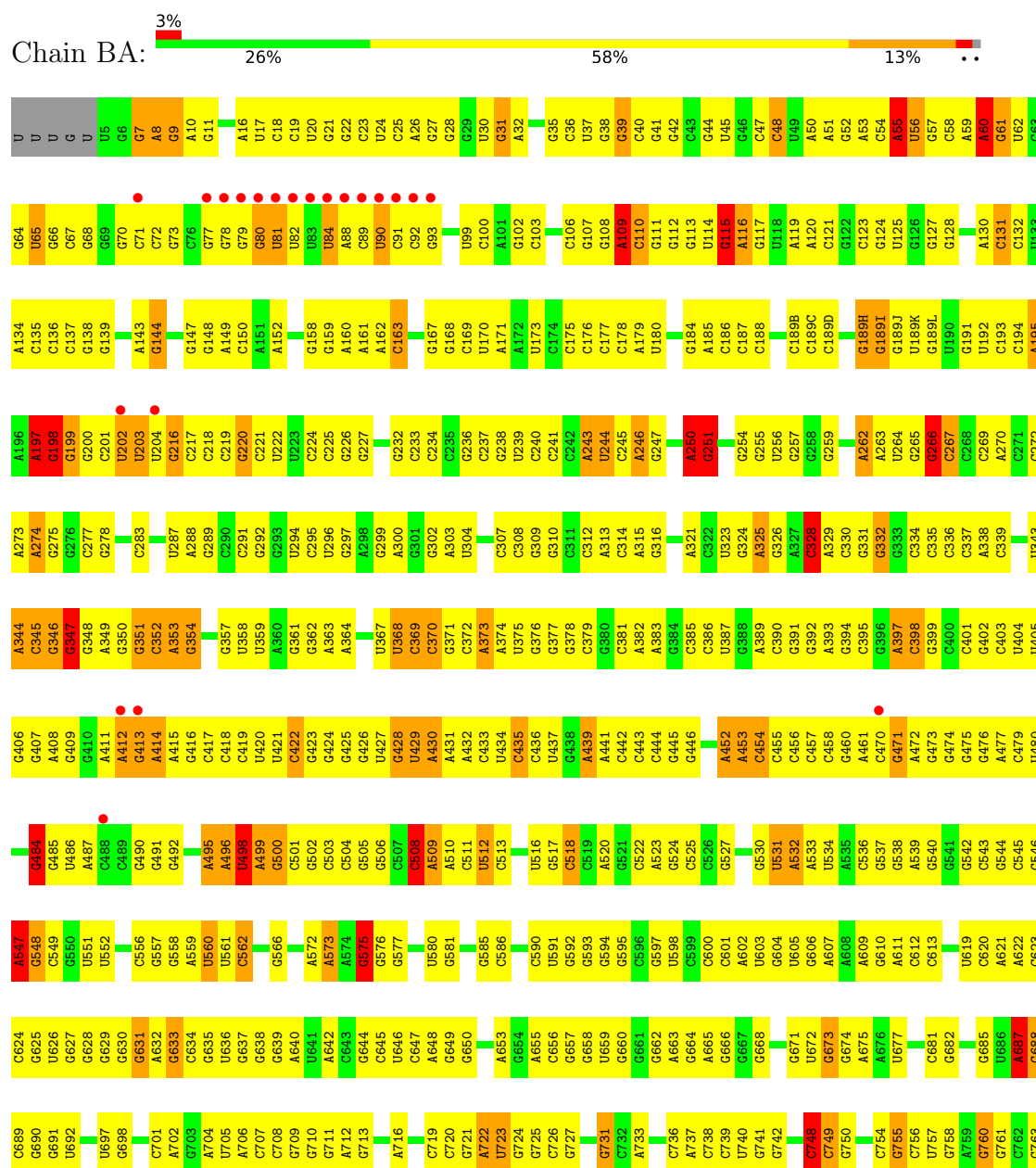
• Molecule 33: 50S RIBOSOMAL PROTEIN L25

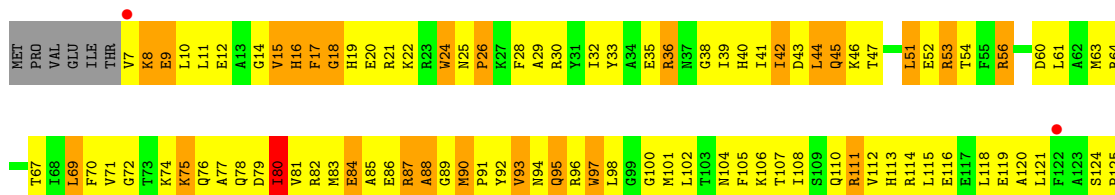


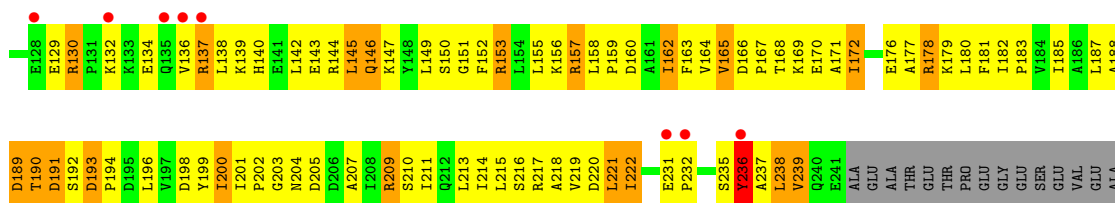
• Molecule 34: SMALL PROTEIN B SMPB



• Molecule 35: 16S ribosomal RNA

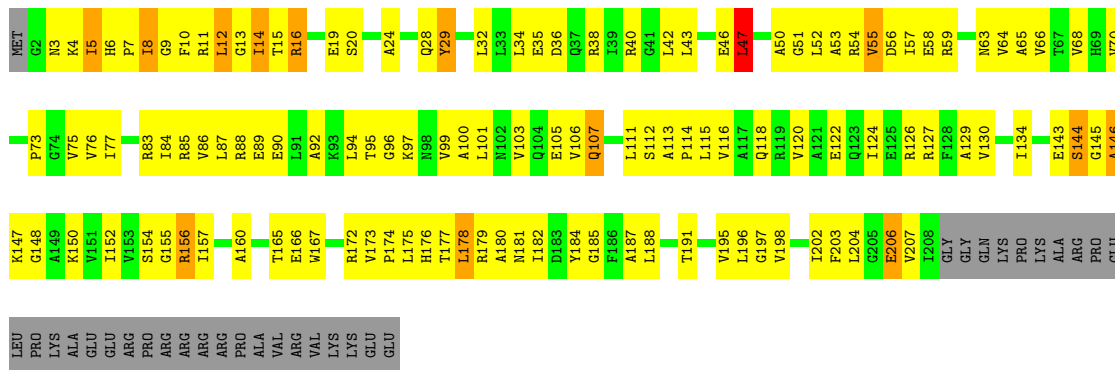






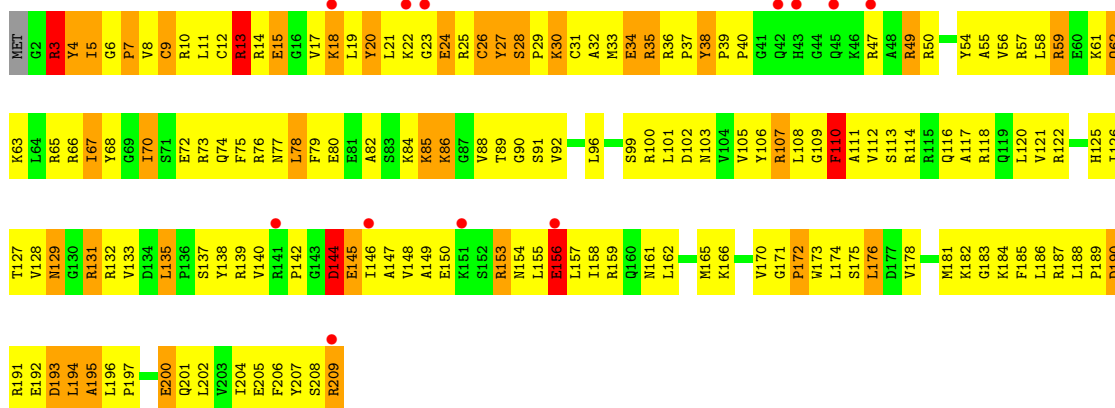
### • Molecule 37: 30S RIBOSOMAL PROTEIN S3

Chain BC: 34% 46% 5% 13%



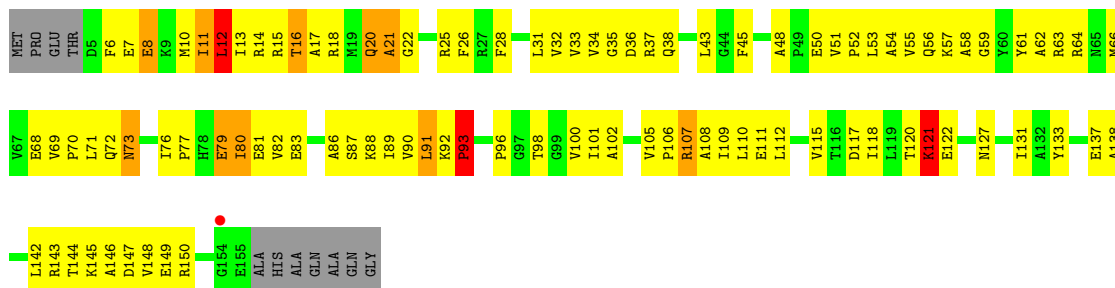
### • Molecule 38: 30S RIBOSOMAL PROTEIN S4

Chain BD: 6% 23% 56% 18%

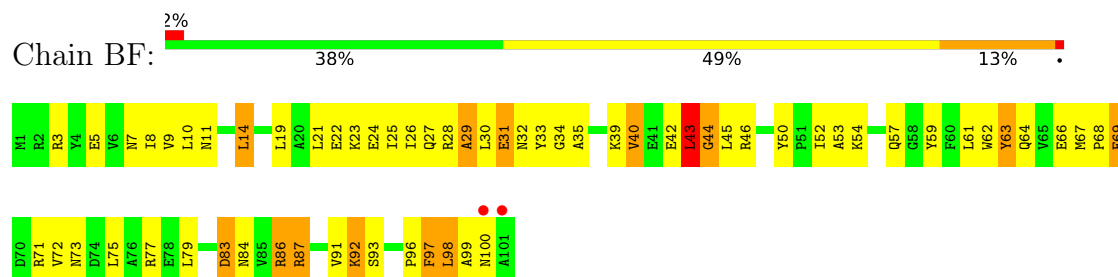


### • Molecule 39: 30S RIBOSOMAL PROTEIN S5

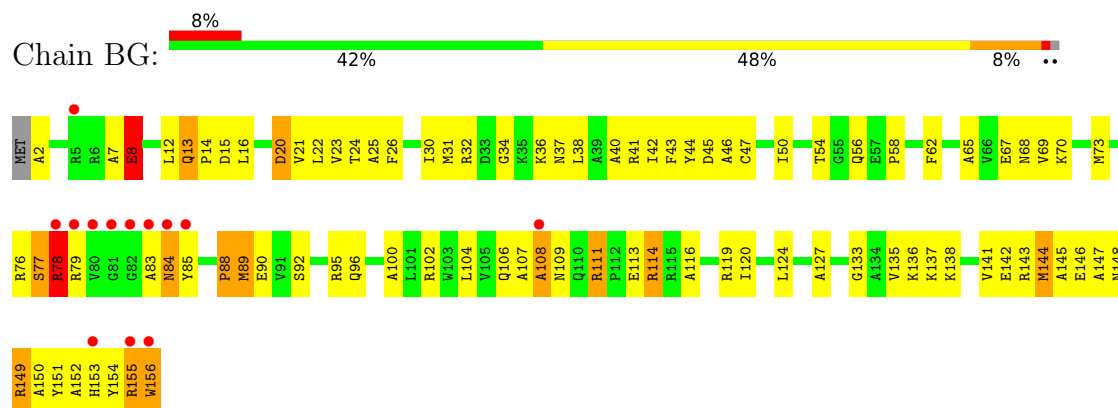
Chain BE: 33% 52% 6% 7%



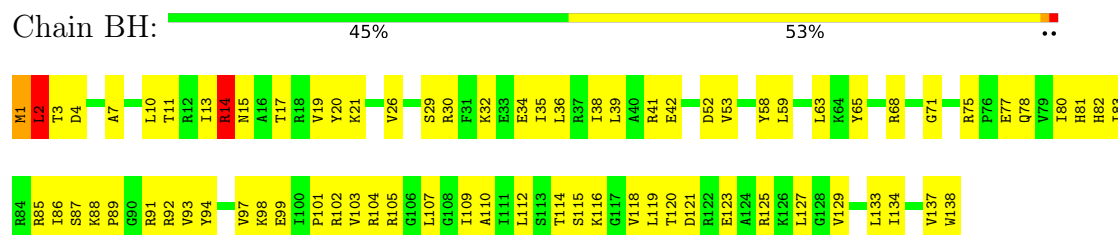
- Molecule 40: 30S RIBOSOMAL PROTEIN S6



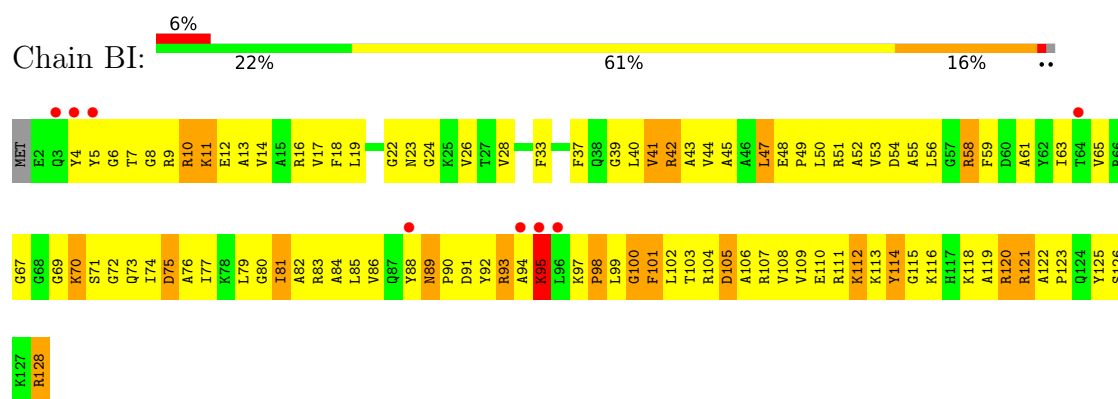
- Molecule 41: 30S RIBOSOMAL PROTEIN S7



- Molecule 42: 30S RIBOSOMAL PROTEIN S8

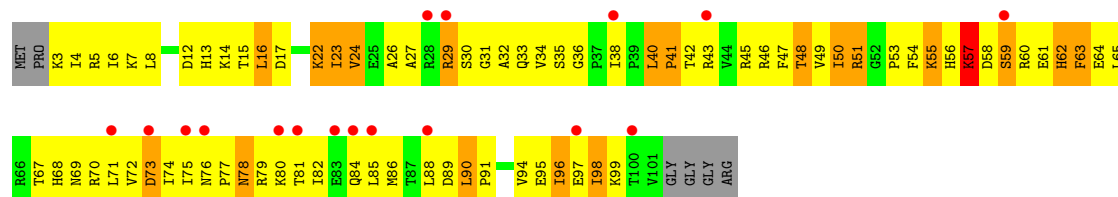


- Molecule 43: 30S RIBOSOMAL PROTEIN S9

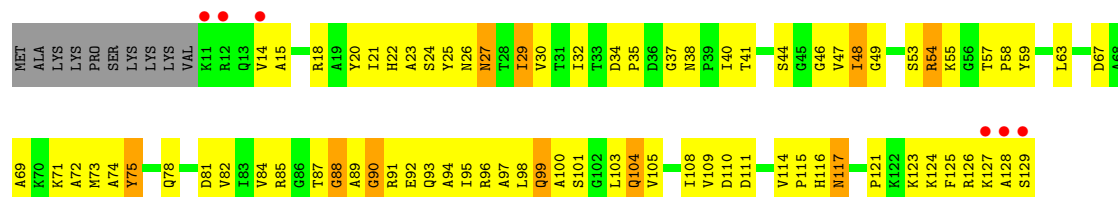


- Molecule 44: 30S RIBOSOMAL PROTEIN S10

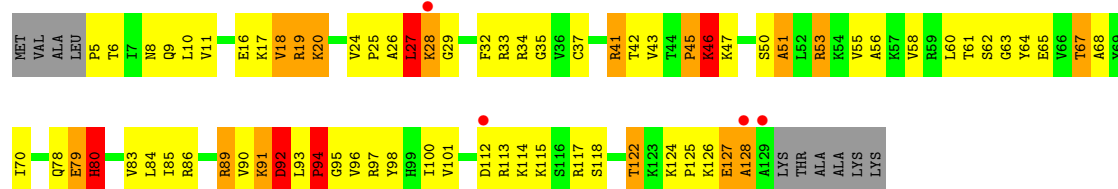




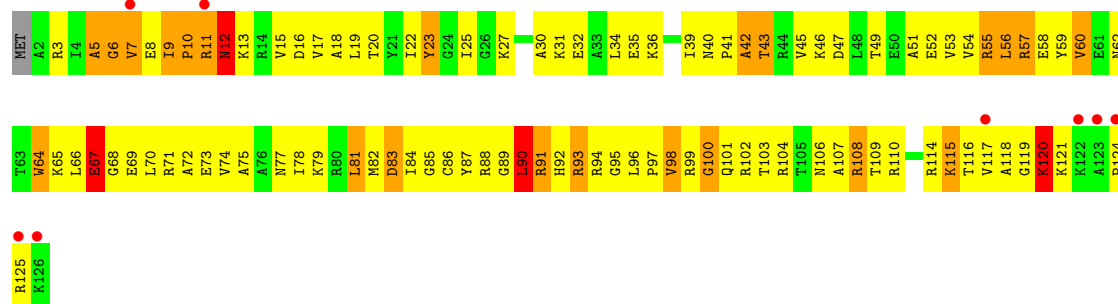
• Molecule 45: 30S RIBOSOMAL PROTEIN S11



• Molecule 46: 30S RIBOSOMAL PROTEIN S12



• Molecule 47: 30S RIBOSOMAL PROTEIN S13

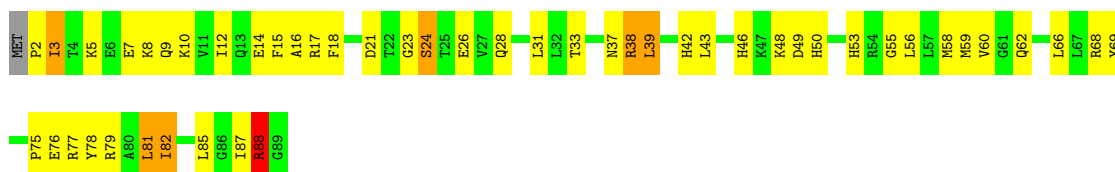


• Molecule 48: 30S RIBOSOMAL PROTEIN S14



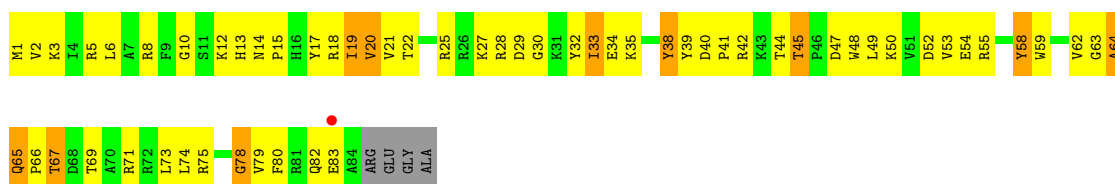
• Molecule 49: 30S RIBOSOMAL PROTEIN S15

Chain BO:  44% 47% 7% ..



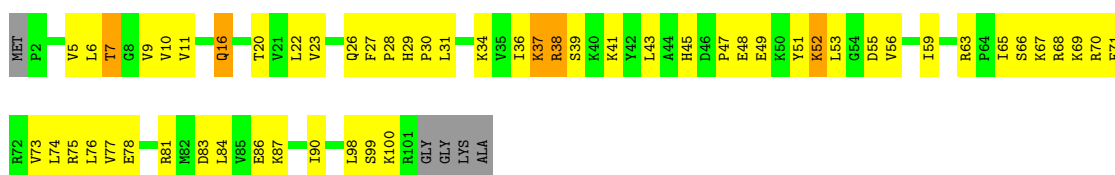
• Molecule 50: 30S RIBOSOMAL PROTEIN S16

Chain BP:  28% 56% 11% 5%



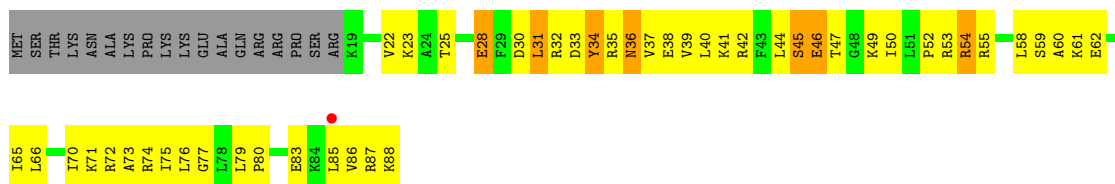
• Molecule 51: 30S RIBOSOMAL PROTEIN S17

Chain BQ:  42% 49% 5% 5%

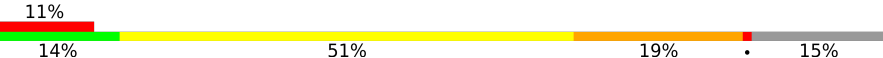


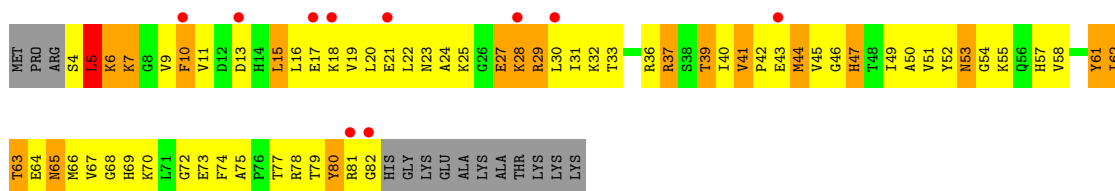
• Molecule 52: 30S RIBOSOMAL PROTEIN S18

Chain BR:  24% 48% 8% 20%



• Molecule 53: 30S RIBOSOMAL PROTEIN S19

Chain BS:  11% 14% 51% 19% 15%

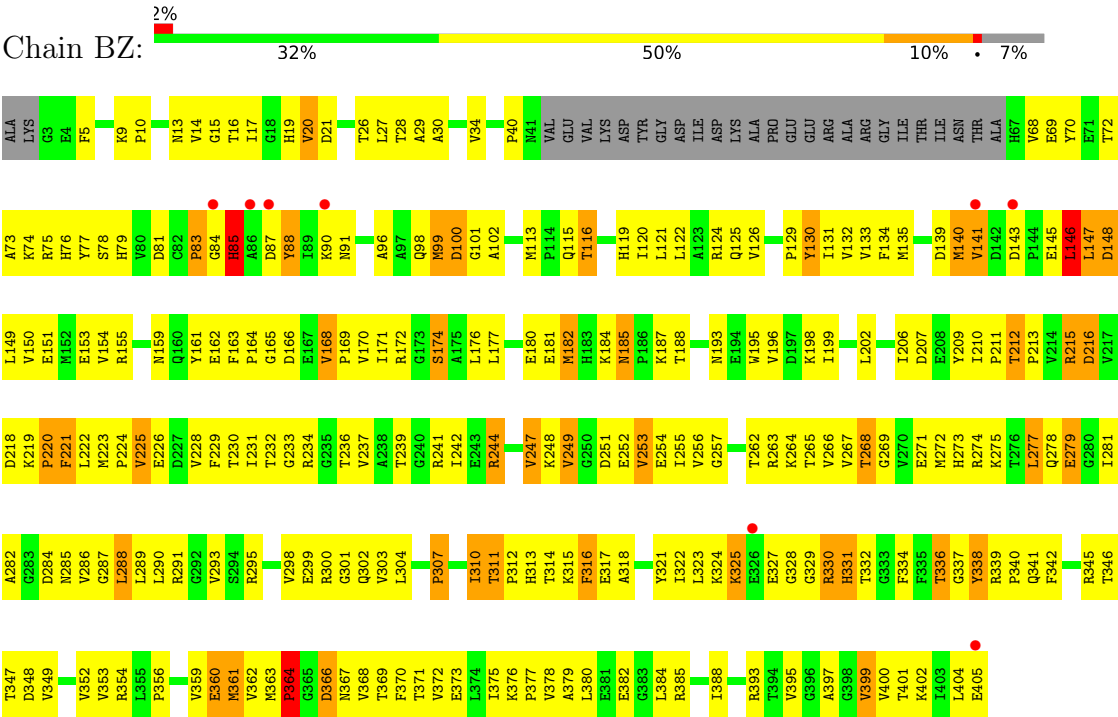


• Molecule 54: 30S RIBOSOMAL PROTEIN S20

Chain BT:  4% 25% 58% 11% 7%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.17Å 290.76Å 250.65Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.10) 97.4 (49.68-3.10)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.230 , 0.270 0.228 , 0.268	Depositor DCC
$R_{free}$ test set	24443 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	154205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GDP, KIR, ZN, MG

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	A0	0.46	0/671	0.72	1/892 (0.1%)
2	A1	0.46	0/739	0.74	0/983
3	A2	0.43	0/600	0.73	0/793
4	A3	0.45	0/473	0.70	0/636
5	A4	0.47	0/350	0.62	0/476
6	A5	0.53	0/473	0.86	1/639 (0.2%)
7	A6	0.69	0/440	0.99	1/586 (0.2%)
8	A7	0.49	0/427	0.69	0/563
9	A8	0.59	0/516	0.94	1/681 (0.1%)
10	A9	0.48	0/310	0.75	0/407
11	AA	0.57	5/69979 (0.0%)	0.81	83/109249 (0.1%)
12	AB	0.44	0/2853	0.79	2/4451 (0.0%)
13	AC	0.46	1/1775 (0.1%)	0.65	0/2392
14	AD	0.53	0/2195	0.83	2/2955 (0.1%)
15	AE	0.54	0/1597	0.84	1/2155 (0.0%)
16	AF	0.45	0/1659	0.78	1/2246 (0.0%)
17	AG	0.38	0/1499	0.69	1/2016 (0.0%)
18	AH	0.44	0/1246	0.77	0/1684
21	AN	0.49	0/1132	0.82	0/1527
22	AO	0.50	0/943	0.77	1/1269 (0.1%)
23	AP	0.54	0/1131	1.06	6/1504 (0.4%)
24	AQ	0.51	0/1143	0.74	0/1527
25	AR	0.45	0/974	0.82	1/1302 (0.1%)
26	AS	0.43	0/779	0.75	0/1038
27	AT	0.54	0/1156	0.88	2/1544 (0.1%)
28	AU	0.56	0/975	0.80	0/1297
29	AV	0.49	0/790	0.86	1/1057 (0.1%)
30	AW	0.54	0/907	0.83	2/1216 (0.2%)
31	AX	0.52	0/740	0.74	0/995
32	AY	0.59	0/789	0.95	3/1053 (0.3%)
33	AZ	0.47	0/1492	0.76	0/2026
34	B2	0.49	0/1203	0.71	1/1606 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	BA	0.48	1/36192 (0.0%)	0.78	39/56489 (0.1%)
36	BB	0.46	0/1936	0.72	0/2611
37	BC	0.43	0/1637	0.69	0/2207
38	BD	0.40	0/1733	0.68	0/2318
39	BE	0.49	0/1163	0.72	0/1566
40	BF	0.43	0/856	0.68	1/1154 (0.1%)
41	BG	0.36	0/1276	0.61	0/1709
42	BH	0.45	0/1136	0.75	0/1527
43	BI	0.41	0/1029	0.67	0/1378
44	BJ	0.42	0/808	0.69	0/1087
45	BK	0.39	0/900	0.65	0/1213
46	BL	0.45	0/987	0.74	0/1322
47	BM	0.38	0/999	0.71	0/1338
48	BN	0.45	0/501	0.75	0/664
49	BO	0.45	0/745	0.70	0/992
50	BP	0.42	0/717	0.65	0/965
51	BQ	0.42	0/837	0.67	0/1119
52	BR	0.42	0/579	0.70	0/768
53	BS	0.45	0/643	0.67	1/867 (0.1%)
54	BT	0.37	0/765	0.65	0/1007
55	BU	0.48	0/213	0.63	0/279
56	BV	0.45	0/1832	0.79	1/2855 (0.0%)
56	BW	0.45	0/1832	0.81	3/2855 (0.1%)
57	BX	0.71	0/116	0.89	0/179
58	BY	0.80	4/1454 (0.3%)	0.97	5/2258 (0.2%)
59	BZ	0.42	0/2986	0.69	0/4050
All	All	0.52	11/165828 (0.0%)	0.79	161/247542 (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
11	AA	9	95
12	AB	0	3
14	AD	0	1
30	AW	0	1
33	AZ	0	1
35	BA	4	40
56	BV	0	1
56	BW	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
58	BY	0	3
All	All	13	148

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BY	12	G	C2-N2	-13.61	1.21	1.34
11	AA	761	A	C5-C6	-11.47	1.30	1.41
58	BY	1	G	OP3-P	-6.81	1.52	1.61
11	AA	761	A	C6-N6	-6.64	1.28	1.33
11	AA	1332	G	N9-C4	-6.30	1.32	1.38

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1992	G	C2'-C3'-O3'	10.04	131.59	109.50
35	BA	115	G	C2'-C3'-O3'	9.61	130.64	109.50
11	AA	1786	A	N9-C1'-C2'	9.57	126.44	114.00
11	AA	527	C	O4'-C1'-N1	9.54	115.83	108.20
35	BA	966	G	N9-C1'-C2'	-9.47	101.58	112.00

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	AA	614(C)	A	C3'
11	AA	1300	U	C3'
11	AA	1378	A	C3'
11	AA	1427	A	C3'
11	AA	1799	G	C3'

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AA	122	G	Sidechain
11	AA	25	U	Sidechain
11	AA	27	G	Sidechain
11	AA	50	U	Sidechain
11	AA	90	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	662	0	688	113	0
2	A1	732	0	808	72	0
3	A2	598	0	653	74	0
4	A3	468	0	523	35	0
5	A4	341	0	339	67	0
6	A5	459	0	480	71	0
7	A6	433	0	461	148	0
8	A7	419	0	467	30	0
9	A8	508	0	576	97	0
10	A9	307	0	335	40	0
11	AA	62479	0	31495	2218	0
12	AB	2551	0	1295	109	0
13	AC	1742	0	1794	315	0
14	AD	2145	0	2234	279	0
15	AE	1564	0	1629	224	0
16	AF	1624	0	1677	194	0
17	AG	1474	0	1535	276	0
18	AH	1223	0	1282	159	0
19	AJ	654	0	142	11	0
20	AK	701	0	163	25	0
21	AN	1105	0	1180	160	0
22	AO	933	0	996	95	0
23	AP	1114	0	1187	270	0
24	AQ	1122	0	1179	154	0
25	AR	960	0	1021	136	0
26	AS	771	0	832	122	0
27	AT	1142	0	1202	267	0
28	AU	958	0	1015	128	0
29	AV	779	0	852	147	0
30	AW	896	0	953	83	0
31	AX	726	0	778	77	0
32	AY	776	0	870	193	0
33	AZ	1460	0	1488	183	0
34	B2	1184	0	1235	205	0
35	BA	32330	0	16318	1299	0
36	BB	1901	0	1951	255	0
37	BC	1613	0	1677	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	1703	0	1764	265	0
39	BE	1147	0	1207	135	0
40	BF	843	0	857	69	0
41	BG	1257	0	1296	103	0
42	BH	1116	0	1177	77	0
43	BI	1011	0	1043	155	0
44	BJ	795	0	840	176	0
45	BK	885	0	904	83	0
46	BL	971	0	1057	105	0
47	BM	988	0	1059	186	0
48	BN	492	0	529	90	0
49	BO	734	0	771	61	0
50	BP	701	0	720	70	0
51	BQ	824	0	891	54	0
52	BR	574	0	644	62	0
53	BS	630	0	652	103	0
54	BT	763	0	861	83	0
55	BU	209	0	221	14	0
56	BV	1640	0	837	44	0
56	BW	1640	0	837	160	0
57	BX	104	0	55	4	0
58	BY	1305	0	663	87	0
59	BZ	2929	0	2941	341	0
60	A9	1	0	0	0	0
60	BD	1	0	0	1	0
60	BN	1	0	0	0	0
61	AA	1	0	0	0	0
61	BZ	1	0	0	0	0
62	BZ	57	0	58	7	0
63	BZ	28	0	12	2	0
All	All	154205	0	105206	9943	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 9943 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:20:TYR:HA	38:BD:26:CYS:SG	1.82	1.19
14:AD:44:ASN:HB3	14:AD:49:ILE:HA	1.21	1.18
1:A0:40:GLN:HE22	1:A0:43:THR:HA	1.02	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A6:11:LEU:HD22	7:A6:12:GLU:H	1.08	1.15
13:AC:167:LYS:HB2	56:BW:18:U:H5''	1.18	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A0	82/85 (96%)	62 (76%)	14 (17%)	6 (7%)	1	7
2	A1	92/98 (94%)	80 (87%)	7 (8%)	5 (5%)	2	13
3	A2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	1
4	A3	58/60 (97%)	46 (79%)	8 (14%)	4 (7%)	1	8
5	A4	43/71 (61%)	23 (54%)	10 (23%)	10 (23%)	0	0
6	A5	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
7	A6	48/54 (89%)	18 (38%)	15 (31%)	15 (31%)	0	0
8	A7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
9	A8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	0
10	A9	35/37 (95%)	27 (77%)	6 (17%)	2 (6%)	2	12
13	AC	226/229 (99%)	159 (70%)	46 (20%)	21 (9%)	1	4
14	AD	273/276 (99%)	210 (77%)	39 (14%)	24 (9%)	1	5
15	AE	203/206 (98%)	136 (67%)	40 (20%)	27 (13%)	0	1
16	AF	206/210 (98%)	147 (71%)	34 (16%)	25 (12%)	0	2
17	AG	179/182 (98%)	110 (62%)	46 (26%)	23 (13%)	0	1
18	AH	158/180 (88%)	98 (62%)	35 (22%)	25 (16%)	0	0
21	AN	137/140 (98%)	89 (65%)	27 (20%)	21 (15%)	0	0
22	AO	120/122 (98%)	103 (86%)	9 (8%)	8 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AP	144/150 (96%)	74 (51%)	28 (19%)	42 (29%)	0	0
24	AQ	139/141 (99%)	104 (75%)	27 (19%)	8 (6%)	2	11
25	AR	115/118 (98%)	80 (70%)	21 (18%)	14 (12%)	0	1
26	AS	97/112 (87%)	57 (59%)	20 (21%)	20 (21%)	0	0
27	AT	136/146 (93%)	89 (65%)	28 (21%)	19 (14%)	0	1
28	AU	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	6
29	AV	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	0
30	AW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	7
31	AX	91/96 (95%)	78 (86%)	8 (9%)	5 (6%)	2	13
32	AY	99/110 (90%)	47 (48%)	18 (18%)	34 (34%)	0	0
33	AZ	182/206 (88%)	107 (59%)	40 (22%)	35 (19%)	0	0
34	B2	142/144 (99%)	124 (87%)	14 (10%)	4 (3%)	5	28
36	BB	233/256 (91%)	153 (66%)	55 (24%)	25 (11%)	0	3
37	BC	205/239 (86%)	141 (69%)	49 (24%)	15 (7%)	1	7
38	BD	206/209 (99%)	126 (61%)	52 (25%)	28 (14%)	0	1
39	BE	149/162 (92%)	121 (81%)	21 (14%)	7 (5%)	2	16
40	BF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	14
41	BG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	9
42	BH	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	11	43
43	BI	125/128 (98%)	73 (58%)	33 (26%)	19 (15%)	0	0
44	BJ	97/105 (92%)	69 (71%)	18 (19%)	10 (10%)	0	3
45	BK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	6
46	BL	123/135 (91%)	84 (68%)	23 (19%)	16 (13%)	0	1
47	BM	123/126 (98%)	76 (62%)	28 (23%)	19 (15%)	0	0
48	BN	58/61 (95%)	43 (74%)	5 (9%)	10 (17%)	0	0
49	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	4	23
50	BP	82/88 (93%)	53 (65%)	23 (28%)	6 (7%)	1	7
51	BQ	98/105 (93%)	76 (78%)	20 (20%)	2 (2%)	8	35
52	BR	68/88 (77%)	53 (78%)	10 (15%)	5 (7%)	1	7
53	BS	77/93 (83%)	53 (69%)	14 (18%)	10 (13%)	0	1
54	BT	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	5
59	BZ	374/405 (92%)	295 (79%)	58 (16%)	21 (6%)	2	12
All	All	6294/6697 (94%)	4435 (70%)	1170 (19%)	689 (11%)	0	3

5 of 689 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A1	30	VAL
2	A1	83	GLU
3	A2	47	ASN
3	A2	70	GLN
4	A3	13	ILE

### 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	A0	66/67 (98%)	57 (86%)	9 (14%)	4	17
2	A1	78/83 (94%)	63 (81%)	15 (19%)	1	7
3	A2	66/67 (98%)	57 (86%)	9 (14%)	4	17
4	A3	51/52 (98%)	46 (90%)	5 (10%)	9	32
5	A4	39/63 (62%)	30 (77%)	9 (23%)	1	3
6	A5	51/52 (98%)	41 (80%)	10 (20%)	1	6
7	A6	49/52 (94%)	34 (69%)	15 (31%)	0	1
8	A7	41/42 (98%)	35 (85%)	6 (15%)	3	15
9	A8	53/55 (96%)	42 (79%)	11 (21%)	1	5
10	A9	34/34 (100%)	26 (76%)	8 (24%)	1	3
13	AC	180/181 (99%)	164 (91%)	16 (9%)	11	38
14	AD	217/218 (100%)	183 (84%)	34 (16%)	3	12
15	AE	165/166 (99%)	138 (84%)	27 (16%)	2	11
16	AF	165/166 (99%)	150 (91%)	15 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AG	155/156 (99%)	135 (87%)	20 (13%)	5	20
18	AH	132/148 (89%)	116 (88%)	16 (12%)	5	21
21	AN	117/119 (98%)	101 (86%)	16 (14%)	4	17
22	AO	100/100 (100%)	88 (88%)	12 (12%)	5	22
23	AP	112/116 (97%)	89 (80%)	23 (20%)	1	6
24	AQ	111/111 (100%)	90 (81%)	21 (19%)	1	7
25	AR	100/101 (99%)	85 (85%)	15 (15%)	3	14
26	AS	77/88 (88%)	67 (87%)	10 (13%)	4	19
27	AT	120/127 (94%)	91 (76%)	29 (24%)	1	2
28	AU	92/94 (98%)	82 (89%)	10 (11%)	7	28
29	AV	82/82 (100%)	72 (88%)	10 (12%)	5	21
30	AW	91/92 (99%)	77 (85%)	14 (15%)	3	13
31	AX	74/78 (95%)	67 (90%)	7 (10%)	9	34
32	AY	84/91 (92%)	69 (82%)	15 (18%)	2	9
33	AZ	161/179 (90%)	132 (82%)	29 (18%)	2	8
34	B2	120/120 (100%)	81 (68%)	39 (32%)	0	0
36	BB	202/220 (92%)	172 (85%)	30 (15%)	3	14
37	BC	160/188 (85%)	149 (93%)	11 (7%)	17	50
38	BD	180/181 (99%)	152 (84%)	28 (16%)	3	12
39	BE	115/123 (94%)	99 (86%)	16 (14%)	4	17
40	BF	90/90 (100%)	76 (84%)	14 (16%)	3	12
41	BG	126/127 (99%)	115 (91%)	11 (9%)	11	40
42	BH	119/119 (100%)	108 (91%)	11 (9%)	10	36
43	BI	98/99 (99%)	87 (89%)	11 (11%)	6	26
44	BJ	88/92 (96%)	74 (84%)	14 (16%)	3	12
45	BK	90/99 (91%)	84 (93%)	6 (7%)	18	50
46	BL	104/111 (94%)	91 (88%)	13 (12%)	5	20
47	BM	99/101 (98%)	84 (85%)	15 (15%)	3	13
48	BN	49/50 (98%)	41 (84%)	8 (16%)	2	11
49	BO	79/80 (99%)	72 (91%)	7 (9%)	11	38
50	BP	72/74 (97%)	64 (89%)	8 (11%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	BQ	94/97 (97%)	89 (95%)	5 (5%)	25	59
52	BR	61/77 (79%)	56 (92%)	5 (8%)	12	42
53	BS	69/80 (86%)	57 (83%)	12 (17%)	2	9
54	BT	76/82 (93%)	68 (90%)	8 (10%)	7	29
55	BU	19/22 (86%)	16 (84%)	3 (16%)	3	12
59	BZ	316/338 (94%)	275 (87%)	41 (13%)	4	19
All	All	5289/5550 (95%)	4537 (86%)	752 (14%)	3	16

5 of 752 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	AT	65	LYS
33	AZ	87	ASP
53	BS	39	THR
27	AT	133	GLU
30	AW	99	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
27	AT	79	HIS
31	AX	87	GLN
51	BQ	16	GLN
28	AU	14	HIS
30	AW	34	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	2900/2915 (99%)	536 (18%)	63 (2%)
12	AB	118/122 (96%)	27 (22%)	4 (3%)
35	BA	1503/1522 (98%)	248 (16%)	56 (3%)
56	BV	76/77 (98%)	12 (15%)	2 (2%)
56	BW	76/77 (98%)	11 (14%)	2 (2%)
57	BX	4/19 (21%)	1 (25%)	0
58	BY	60/90 (66%)	22 (36%)	13 (21%)
All	All	4737/4822 (98%)	857 (18%)	140 (2%)

5 of 857 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	9	U
11	AA	10	G
11	AA	32	C
11	AA	34	C
11	AA	45	C

5 of 140 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	AB	16	G
35	BA	266	G
58	BY	11	C
12	AB	42	C
35	BA	109	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	KIR	BZ	1002	-	55,59,59	3.28	20 (36%)	62,84,84	1.92	19 (30%)
63	GDP	BZ	1003	61	24,30,30	1.37	2 (8%)	27,47,47	2.07	7 (25%)

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
62	KIR	BZ	1002	-	-	9/54/98/98	0/3/3/3
63	GDP	BZ	1003	61	-	2/12/32/32	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	1002	KIR	O18-C17	-13.46	1.24	1.44
62	BZ	1002	KIR	O30-C30	-12.89	1.16	1.42
62	BZ	1002	KIR	C5-C4	5.14	1.48	1.39
62	BZ	1002	KIR	C27-N26	4.20	1.43	1.33
63	BZ	1003	GDP	C6-N1	4.18	1.40	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	1002	KIR	O29-C29-O34	-5.94	100.64	110.28
62	BZ	1002	KIR	C4-C3-C7	5.72	133.90	120.25
63	BZ	1003	GDP	N3-C2-N1	-5.24	120.16	127.25
63	BZ	1003	GDP	C2-N3-C4	4.96	121.02	115.36
62	BZ	1002	KIR	C20-C21-C22	-4.05	115.28	119.13

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

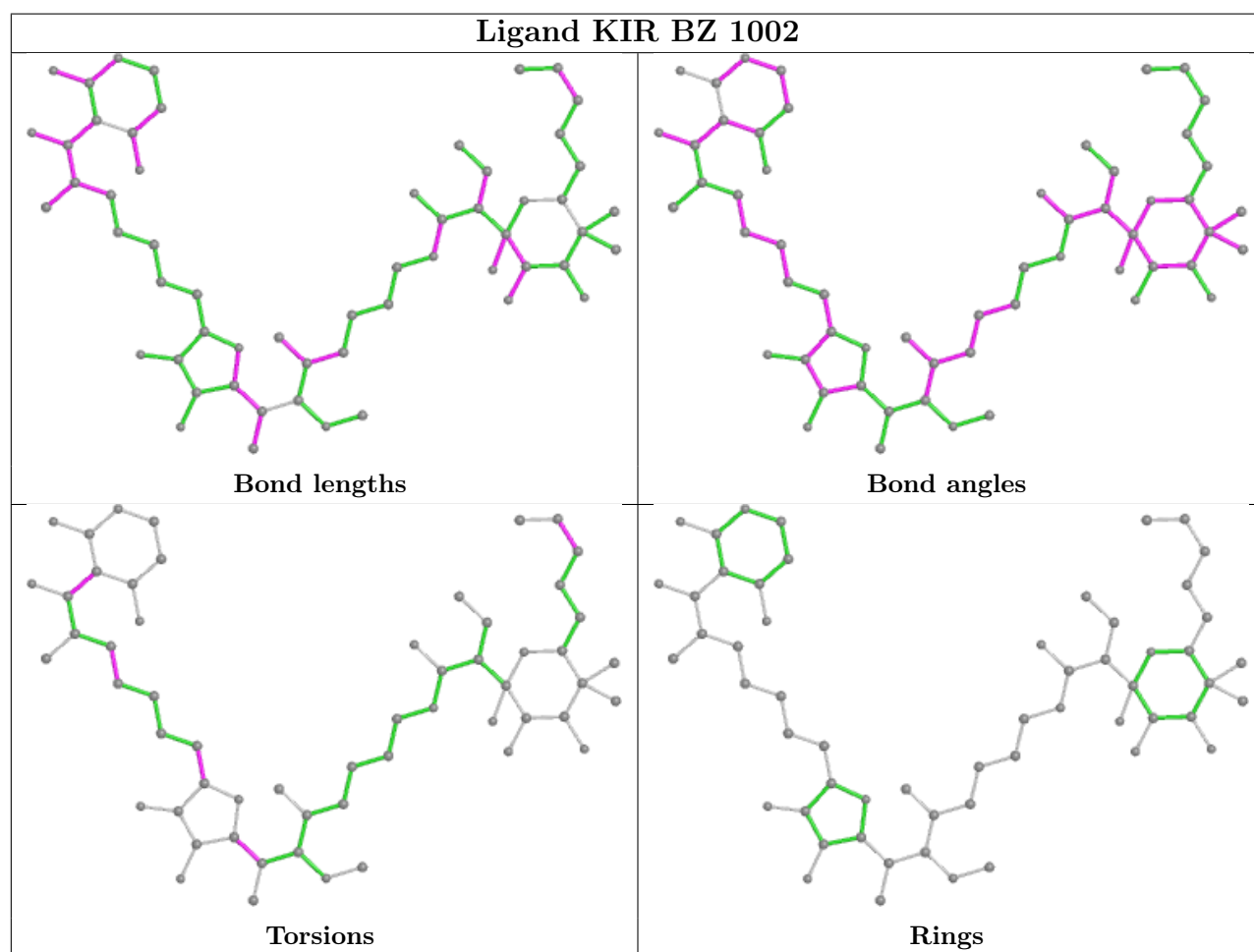
Mol	Chain	Res	Type	Atoms
62	BZ	1002	KIR	C12-C13-C14-O18
62	BZ	1002	KIR	C16-C17-C19-C20
62	BZ	1002	KIR	C16-C17-C19-C42
62	BZ	1002	KIR	O18-C17-C19-C20
62	BZ	1002	KIR	O18-C17-C19-C42

There are no ring outliers.

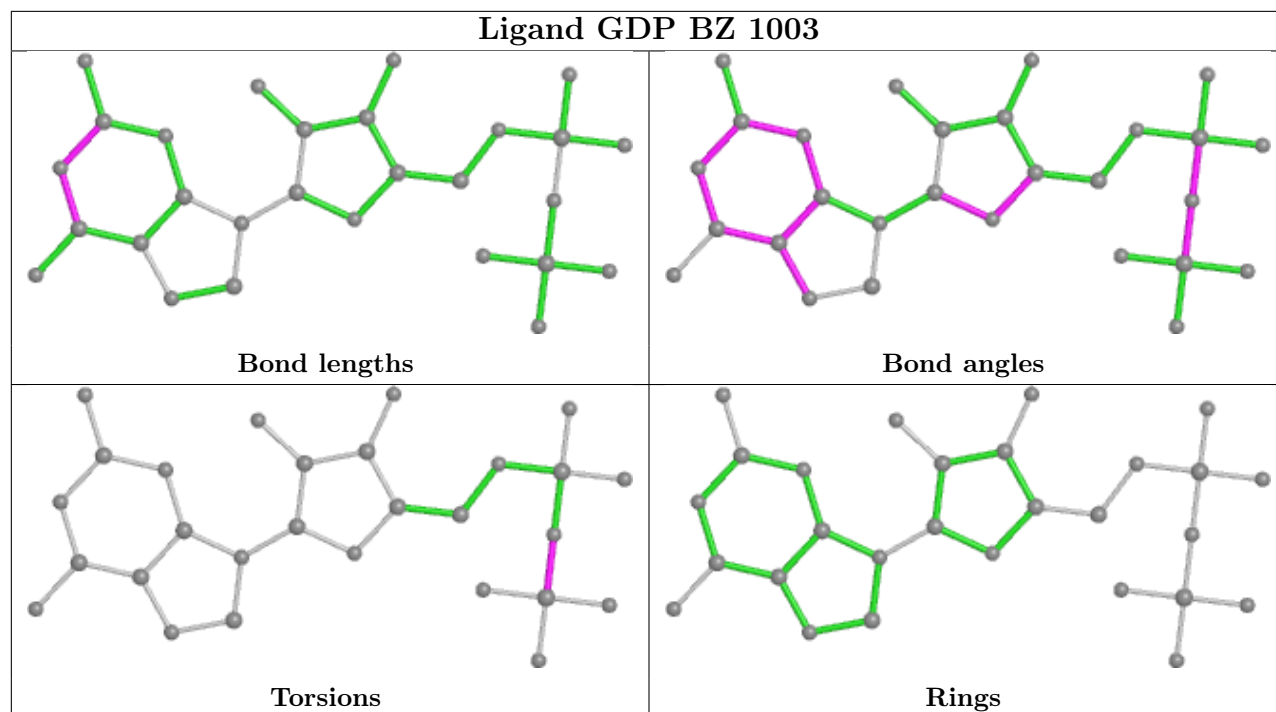
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	1002	KIR	7	0
63	BZ	1003	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A0	84/85 (98%)	0.48	9 (10%) 6 2	25, 44, 110, 136	0
2	A1	94/98 (95%)	0.19	2 (2%) 63 42	23, 43, 88, 95	0
3	A2	71/72 (98%)	0.14	2 (2%) 53 29	34, 61, 88, 98	0
4	A3	60/60 (100%)	-0.00	1 (1%) 70 48	21, 36, 55, 87	0
5	A4	45/71 (63%)	0.68	6 (13%) 3 1	98, 118, 132, 138	0
6	A5	59/60 (98%)	0.41	6 (10%) 7 2	14, 39, 121, 137	0
7	A6	50/54 (92%)	0.69	6 (12%) 4 2	31, 61, 79, 82	0
8	A7	49/49 (100%)	-0.22	0 100 100	14, 24, 77, 93	0
9	A8	64/65 (98%)	-0.05	1 (1%) 72 50	21, 40, 55, 83	0
10	A9	37/37 (100%)	0.33	1 (2%) 54 30	33, 49, 68, 72	0
11	AA	2901/2915 (99%)	0.12	167 (5%) 23 10	8, 36, 159, 189	0
12	AB	119/122 (97%)	0.01	0 100 100	26, 77, 104, 137	0
13	AC	228/229 (99%)	4.97	195 (85%) 0 0	131, 151, 164, 168	0
14	AD	275/276 (99%)	-0.38	3 (1%) 80 64	8, 27, 53, 87	0
15	AE	205/206 (99%)	-0.09	6 (2%) 51 28	10, 29, 75, 88	0
16	AF	208/210 (99%)	-0.11	4 (1%) 66 45	11, 49, 116, 129	0
17	AG	181/182 (99%)	0.53	17 (9%) 8 3	55, 86, 112, 132	0
18	AH	160/180 (88%)	0.61	14 (8%) 10 3	39, 83, 124, 134	0
19	AJ	0/130	-	-	-	-
20	AK	0/140	-	-	-	-
21	AN	139/140 (99%)	-0.19	3 (2%) 62 40	17, 37, 86, 94	0
22	AO	122/122 (100%)	-0.32	3 (2%) 57 34	15, 31, 49, 66	0
23	AP	146/150 (97%)	0.48	7 (4%) 30 13	18, 60, 93, 119	0
24	AQ	141/141 (100%)	-0.23	2 (1%) 75 56	22, 32, 57, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	AR	117/118 (99%)	-0.34	0 100 100	19, 31, 54, 67	0
26	AS	99/112 (88%)	0.51	4 (4%) 38 18	53, 76, 107, 109	0
27	AT	138/146 (94%)	0.11	8 (5%) 23 10	15, 48, 124, 143	0
28	AU	117/118 (99%)	-0.25	2 (1%) 70 48	15, 30, 57, 97	0
29	AV	101/101 (100%)	0.25	3 (2%) 50 26	9, 56, 76, 82	0
30	AW	113/113 (100%)	-0.29	2 (1%) 68 46	12, 29, 61, 106	0
31	AX	93/96 (96%)	-0.30	0 100 100	22, 41, 61, 75	0
32	AY	101/110 (91%)	0.77	13 (12%) 3 1	25, 56, 108, 128	0
33	AZ	184/206 (89%)	0.23	9 (4%) 29 13	28, 63, 98, 115	0
34	B2	144/144 (100%)	0.92	21 (14%) 2 1	49, 78, 118, 124	0
35	BA	1504/1522 (98%)	0.03	51 (3%) 45 23	14, 52, 128, 187	0
36	BB	235/256 (91%)	0.09	10 (4%) 35 17	27, 51, 114, 128	0
37	BC	207/239 (86%)	-0.07	0 100 100	36, 59, 86, 96	0
38	BD	208/209 (99%)	0.53	12 (5%) 23 10	47, 74, 111, 116	0
39	BE	151/162 (93%)	-0.34	1 (0%) 87 75	23, 40, 70, 92	0
40	BF	101/101 (100%)	-0.21	2 (1%) 65 43	33, 56, 71, 95	0
41	BG	155/156 (99%)	0.25	13 (8%) 11 4	52, 75, 107, 129	0
42	BH	138/138 (100%)	-0.36	0 100 100	17, 36, 54, 67	0
43	BI	127/128 (99%)	0.49	8 (6%) 20 8	46, 82, 107, 111	0
44	BJ	99/105 (94%)	0.89	17 (17%) 1 1	42, 82, 119, 122	0
45	BK	119/129 (92%)	0.22	6 (5%) 29 13	26, 56, 90, 107	0
46	BL	125/135 (92%)	0.03	4 (3%) 47 25	24, 50, 69, 112	0
47	BM	125/126 (99%)	0.53	8 (6%) 19 7	42, 80, 107, 139	0
48	BN	60/61 (98%)	0.07	2 (3%) 46 24	38, 48, 70, 77	0
49	BO	88/89 (98%)	-0.16	0 100 100	22, 41, 64, 69	0
50	BP	84/88 (95%)	0.19	1 (1%) 79 61	39, 58, 77, 102	0
51	BQ	100/105 (95%)	-0.27	0 100 100	27, 47, 68, 73	0
52	BR	70/88 (79%)	0.16	1 (1%) 75 56	28, 46, 71, 79	0
53	BS	79/93 (84%)	0.52	10 (12%) 3 2	55, 73, 101, 111	0
54	BT	99/106 (93%)	0.33	4 (4%) 38 18	46, 65, 101, 104	0
55	BU	25/27 (92%)	0.60	0 100 100	52, 65, 83, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BV	77/77 (100%)	0.02	1 (1%) 77 59	36, 57, 97, 104	0
56	BW	77/77 (100%)	5.39	67 (87%) 0 0	95, 192, 197, 199	0
57	BX	5/19 (26%)	0.76	0 100 100	34, 36, 69, 80	0
58	BY	62/90 (68%)	0.14	0 100 100	55, 85, 125, 135	0
59	BZ	378/405 (93%)	-0.04	8 (2%) 63 42	23, 56, 92, 124	0
All	All	11143/11789 (94%)	0.24	743 (6%) 18 7	8, 50, 137, 199	0

The worst 5 of 743 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AC	111	ASP	20.3
13	AC	173	ALA	18.7
13	AC	73	ARG	18.7
11	AA	2182	G	18.0
13	AC	172	HIS	17.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
62	KIR	BZ	1002	57/57	0.89	0.36	101,117,134,134	0
63	GDP	BZ	1003	28/28	0.97	0.14	36,43,44,45	0
61	MG	BZ	1001	1/1	0.97	0.14	25,25,25,25	0
60	ZN	BD	1001	1/1	0.98	0.19	59,59,59,59	0
60	ZN	BN	1001	1/1	0.98	0.13	51,51,51,51	0
60	ZN	A9	1001	1/1	0.99	0.07	58,58,58,58	0

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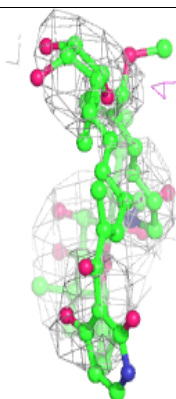
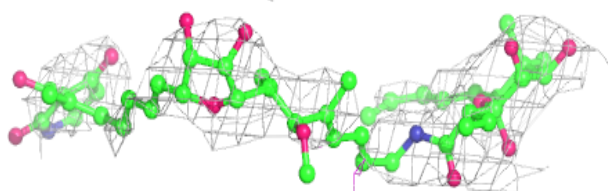
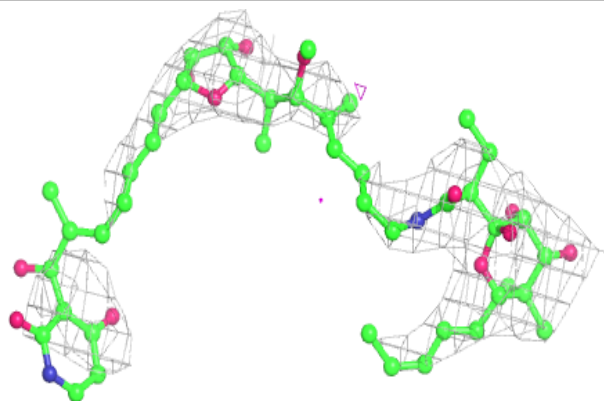
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	AA	3001	1/1	0.99	0.22	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

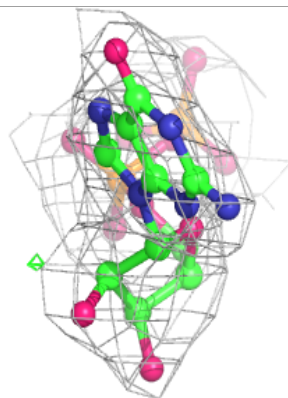
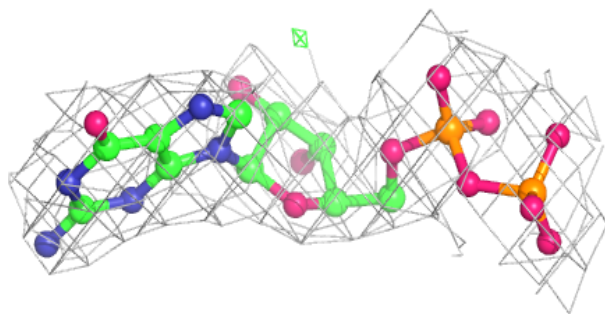
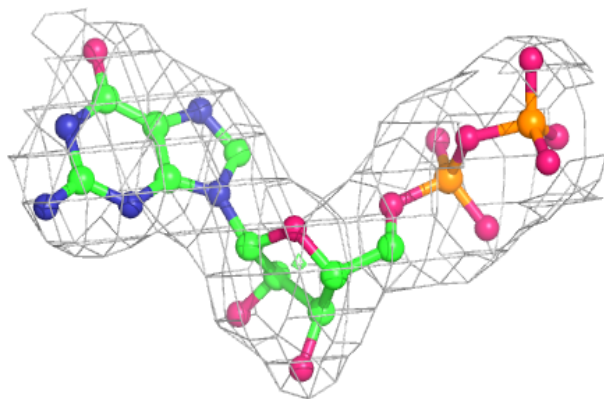
**Electron density around KIR BZ 1002:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP BZ 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.