



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:44 PM GMT

PDB ID : 4V5P
Title : The crystal structure of EF-Tu and A9C-tRNA-Trp bound to a near- cognate codon on the 70S ribosome
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

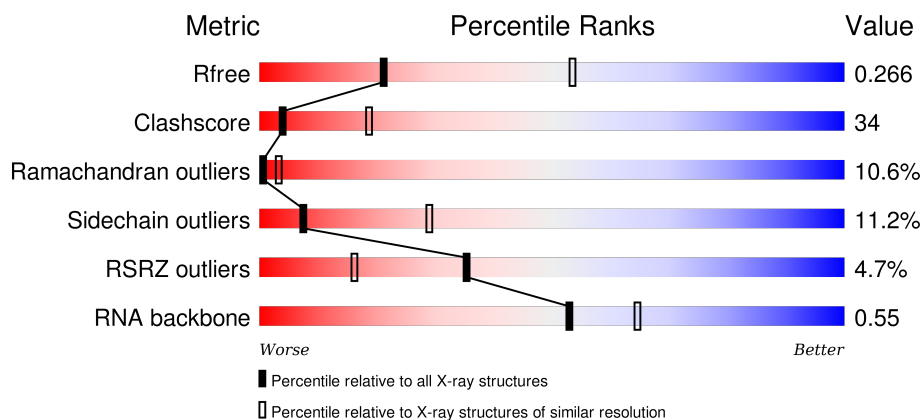
1 Overall quality at a glance

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.




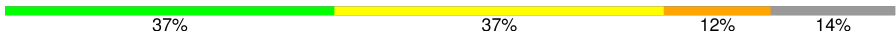
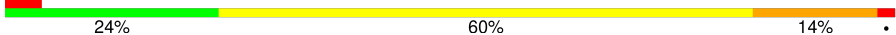



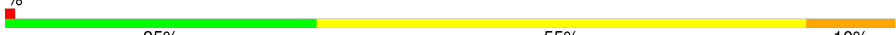
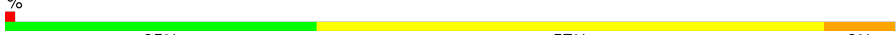



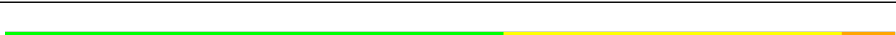

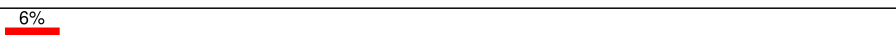
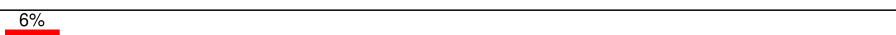
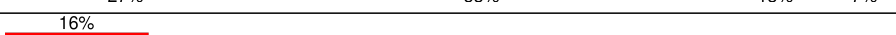
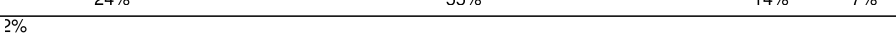
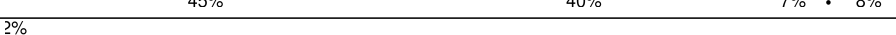

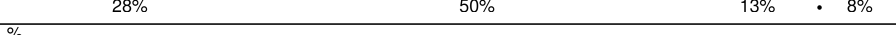
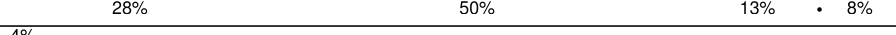




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	AA	1522	<div> <div>2%</div> <div>36% 49% 12% ..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>35% 51% 12% ..</div> </div>
2	AB	256	<div> <div>%</div> <div>30% 49% 12% • 9%</div> </div>
2	CB	256	<div> <div>3%</div> <div>28% 52% 11% • 9%</div> </div>


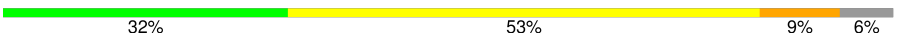



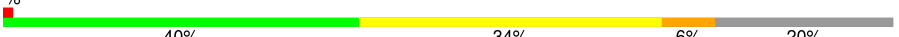
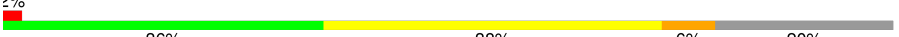
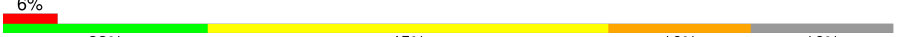
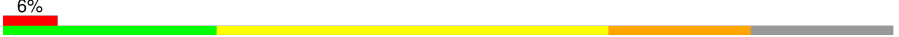

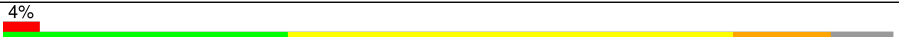


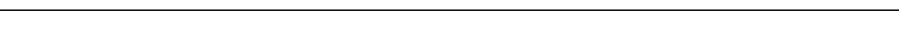
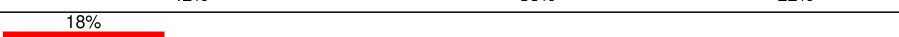
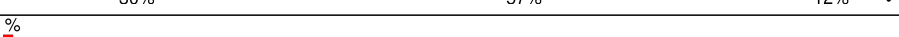



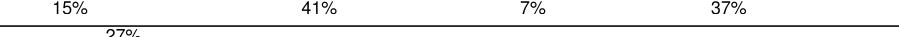
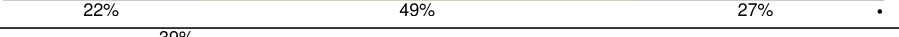
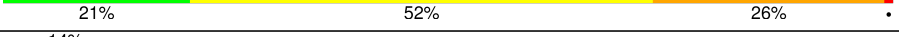
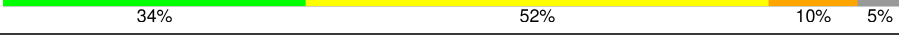


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	405	
25	CZ	405	
26	B0	85	
26	D0	85	

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Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	



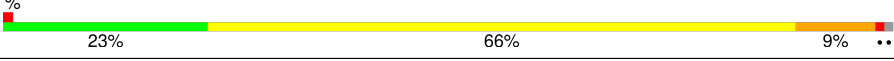
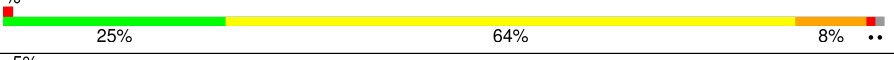
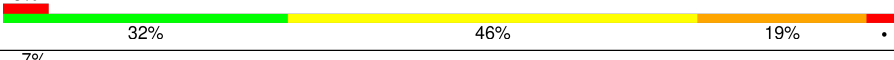
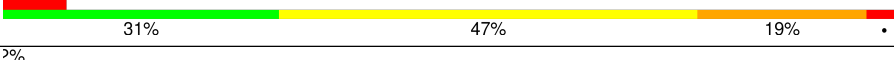
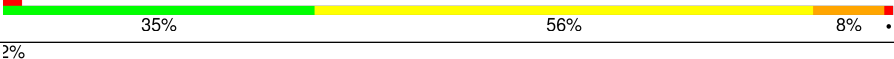
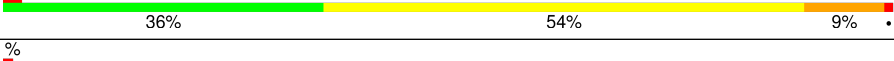
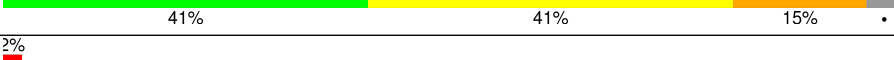

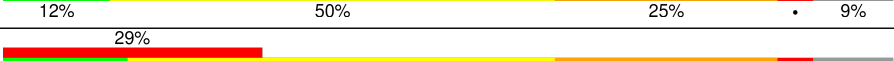
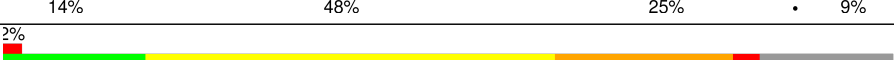
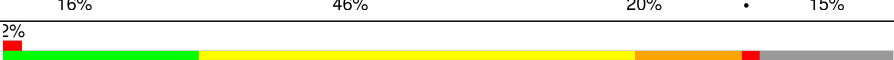
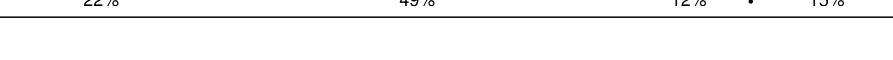
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Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

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Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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
24	PSU	AY	55	X	-	-	-
24	PSU	CY	55	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307322 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 RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			
1	CA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
12	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP Q5SHN3
AL	2	VAL	-	EXPRESSION TAG	UNP Q5SHN3
AL	3	ALA	-	EXPRESSION TAG	UNP Q5SHN3
AL	4	LEU	-	EXPRESSION TAG	UNP Q5SHN3
CL	1	MET	-	EXPRESSION TAG	UNP Q5SHN3
CL	2	VAL	-	EXPRESSION TAG	UNP Q5SHN3
CL	3	ALA	-	EXPRESSION TAG	UNP Q5SHN3
CL	4	LEU	-	EXPRESSION TAG	UNP Q5SHN3

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			
13	CM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			
23	CX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

- Molecule 24 is a RNA chain called A-SITE TRNA A9C TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1643	741	287	537	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1643	741	287	537	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AZ	385	Total	C	N	O	S		0	0	0
			2983	1886	522	563	12				
25	CZ	385	Total	C	N	O	S		0	0	0
			2983	1886	522	563	12				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	6	ILE	VAL	CONFLICT	UNP Q5SHN6
AZ	264	LYS	ARG	CONFLICT	UNP Q5SHN6
CZ	6	ILE	VAL	CONFLICT	UNP Q5SHN6
CZ	264	LYS	ARG	CONFLICT	UNP Q5SHN6

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S		0	0	0
			662	410	140	111	1				
26	D0	84	Total	C	N	O	S		0	0	0
			662	410	140	111	1				

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S		0	0	0
			731	460	145	125	1				
27	D1	93	Total	C	N	O	S		0	0	0
			731	460	145	125	1				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S		0	0	0
			598	370	121	106	1				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
29	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			
30	D4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
33	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
37	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
38	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
39	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
41	DF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
42	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
43	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O		0	0	0
			651	391	130	130				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	DJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			
45	DK	140	Total	C	N	O	0	0	0
			700	420	140	140			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
46	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
47	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
50	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			
51	DS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
52	DT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
54	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
56	DX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
57	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			
58	DZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

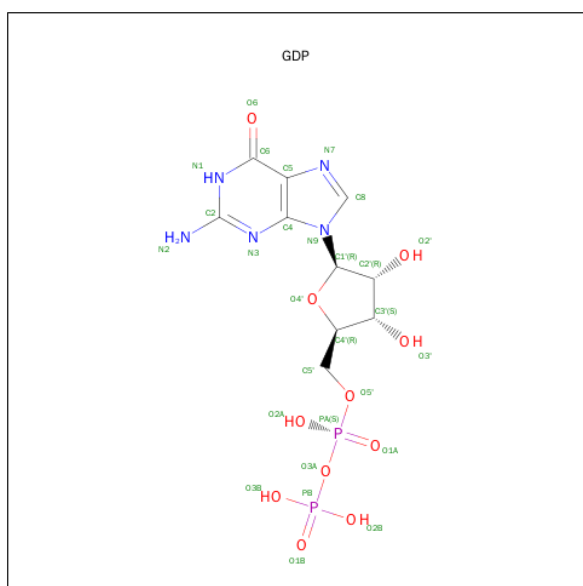
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

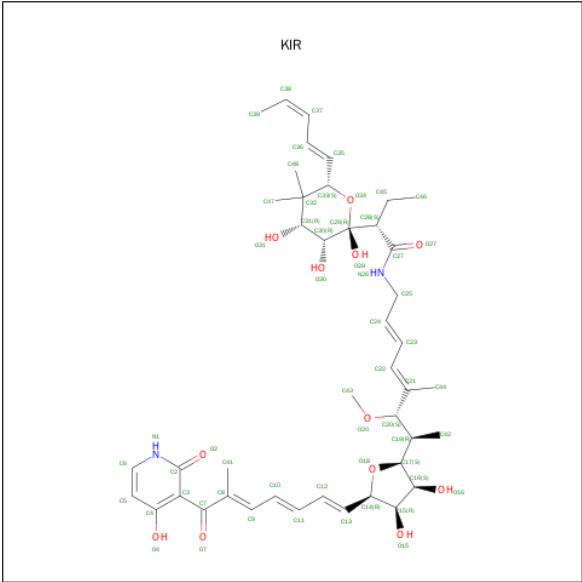
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



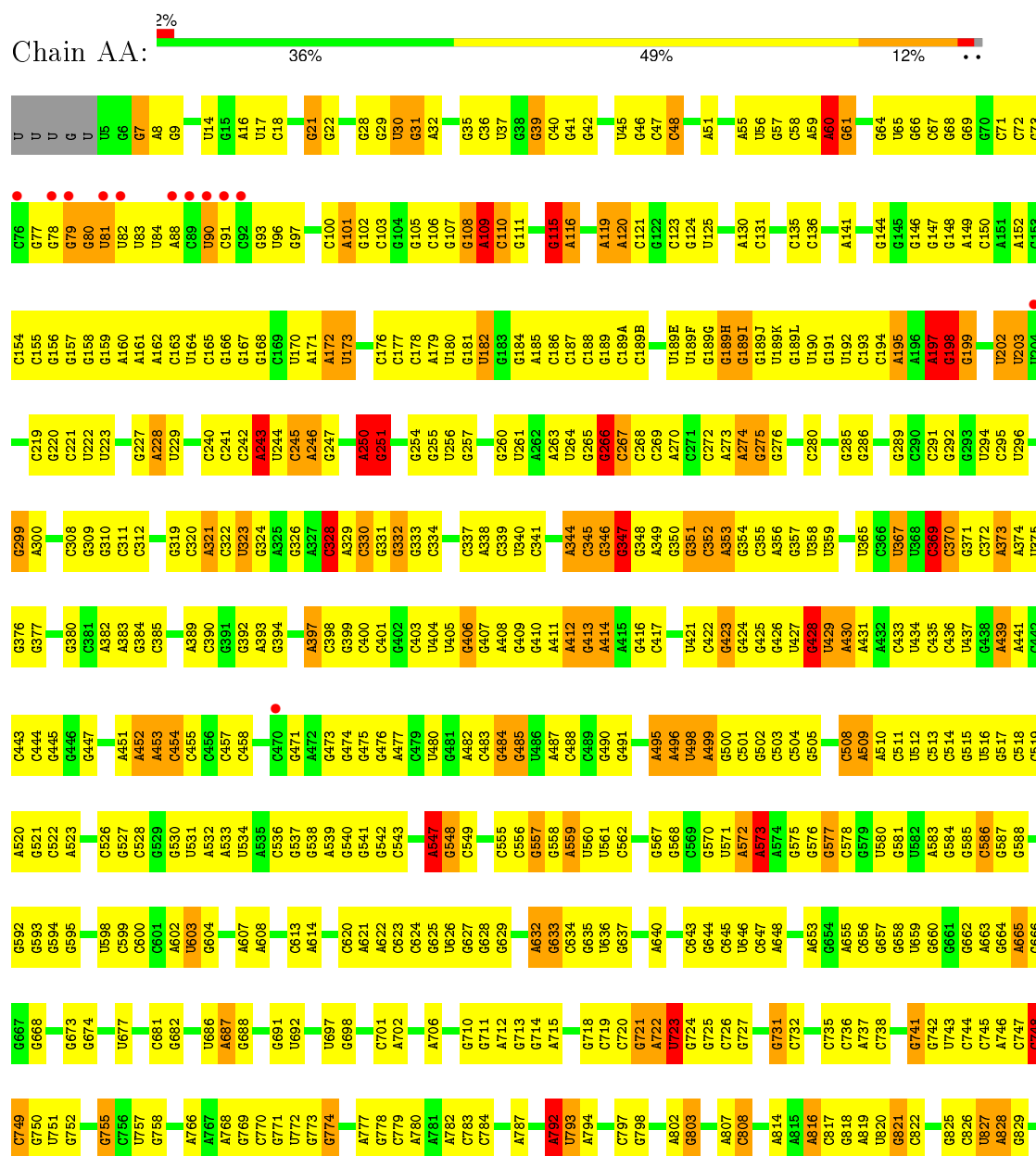


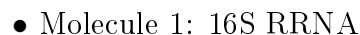
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

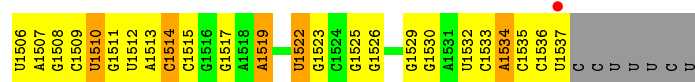
• Molecule 1: 16S rRNA



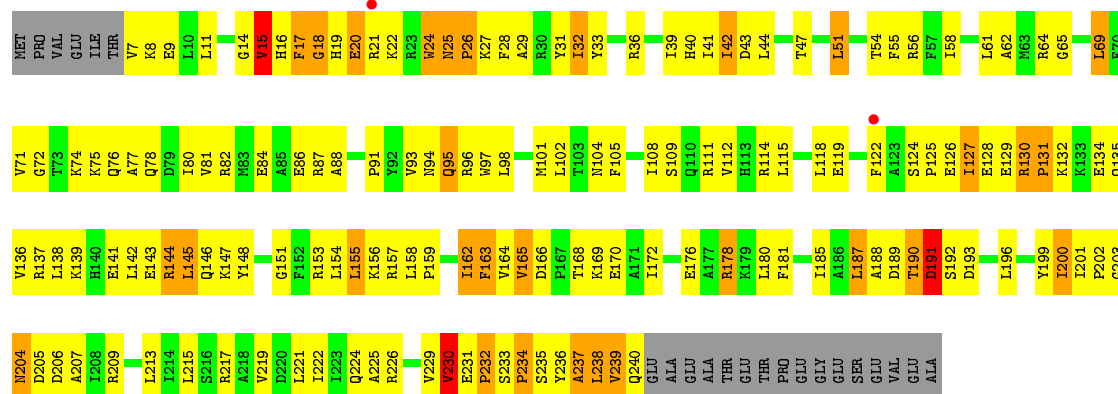


U2024	C154	C76	U
C219	C155	G77	U
G220	G156	G78	U
C221	G157	G79	G
U222	G158	G80	U
U223	G159	U81	U5
	A160	U82	G6
G227	A161	U83	G7
A228	A162	U84	A8
U229	U164	C83	G9
	C165	U90	U14
C240	G166	C91	G15
C241	G167	C92	A16
C242	G168	G93	U17
A243	G169	U96	C18
A244	U170	G97	
C245	A171		G21
A246	A172	C100	G22
G247	U173	A101	G28
		G102	G29
A250	G176	G103	U30
G251	C177	G104	G31
	C178	G105	A32
G254	A179	C106	
G255	U180	G107	G35
U256	G181	G108	C36
G257	U182	A109	U37
	G183	C110	G38
G260	G184	G111	G39
U261	A185		C40
A263	C186	G115	G41
G264	C187	A116	G42
U264	G188		
G265	G189	A119	U45
G266	C189A	A120	G46
G267	C189B	C121	C47
C268		G122	C48
G269	U189E	C123	
A270	U189F	G124	A51
	G189G	U125	
C272	G189H		A55
A273	G189I	A130	U56
A274	G189J	C131	G57
G275	U189K		C58
G276	G189L	G135	A59
	U190	C136	A60
C280	G191		G61
	U192	A141	
G285	C193		G64
G286	C194	G144	U65
G289	A195	G145	G66
G290	A196	G146	C67
C291	A197	G147	G68
G292	G198	G148	G69
G293	G199	A149	G70
U294	G200	C150	C71
C295	C201	A151	C72
U296	U202	A152	G73
	U203	G153	

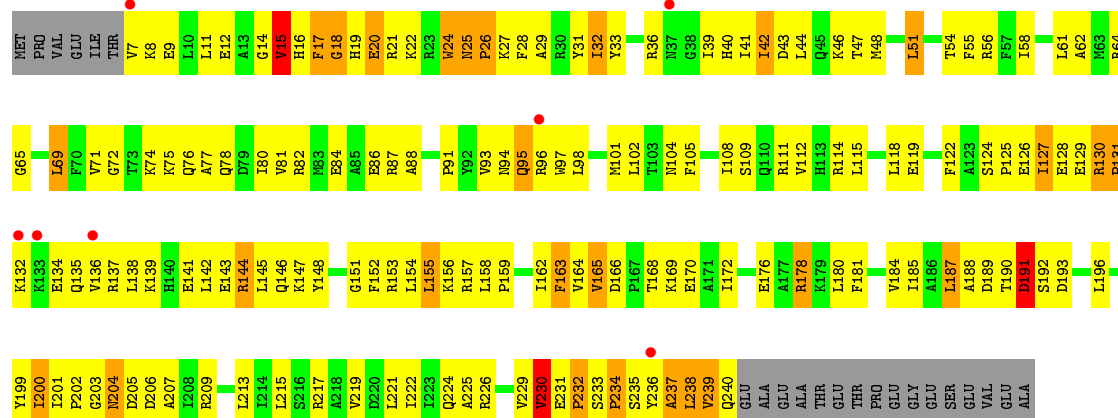




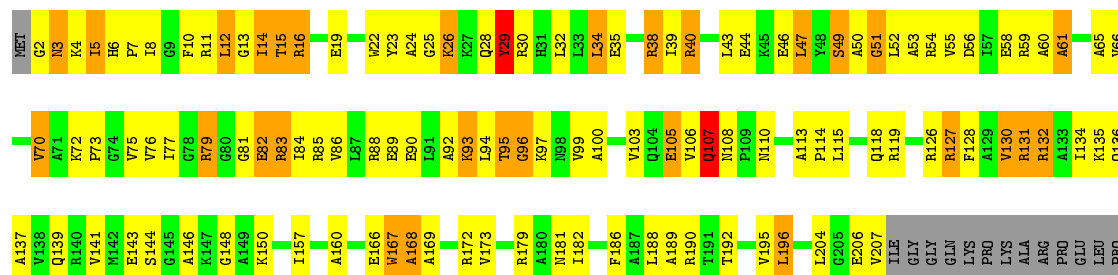
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



• Molecule 2: 30S RIBOSOMAL PROTEIN S2



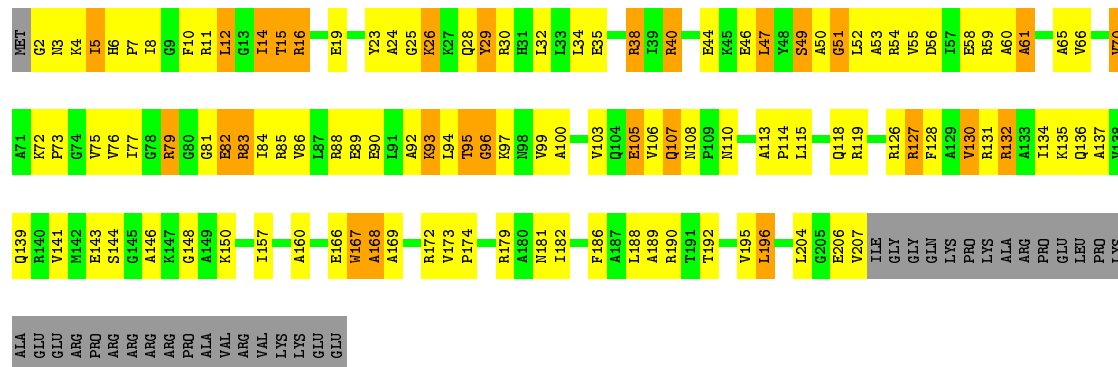
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



LYS
ALA
GLU
GLU
ARG
PRO
ARG
ARG
ARG
ARG
PRO
PRO
ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

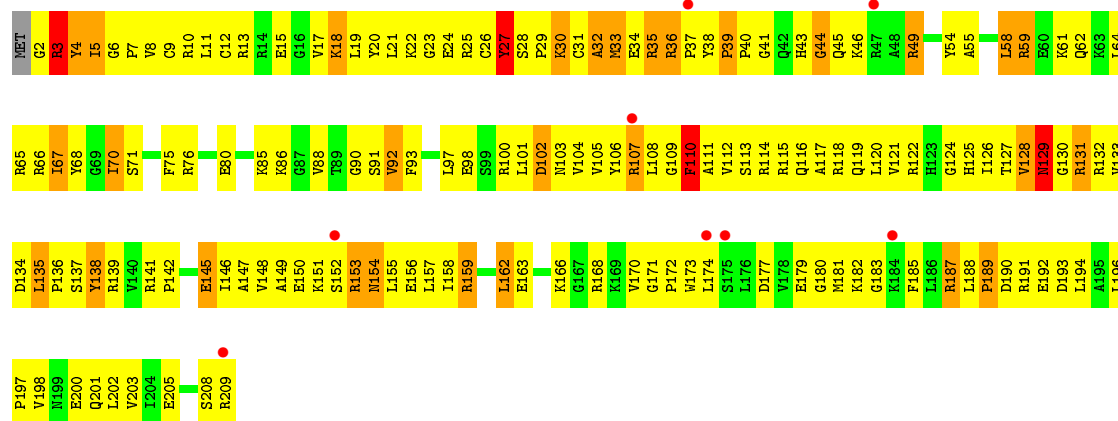
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 37% 37% 12% 14%



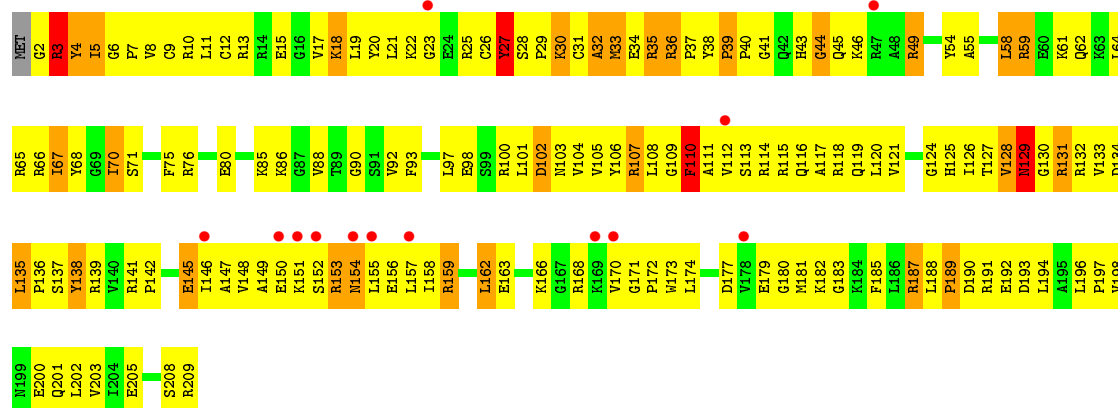
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

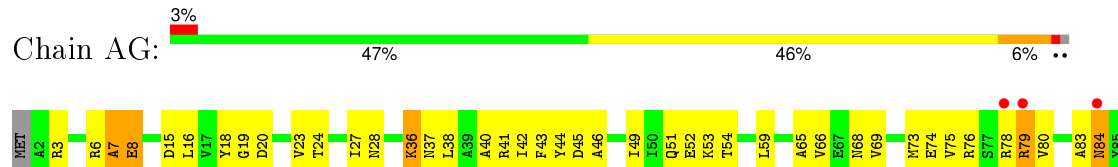
Chain AD: 4% 24% 60% 14%

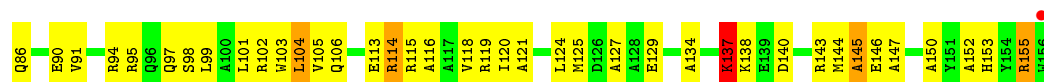


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

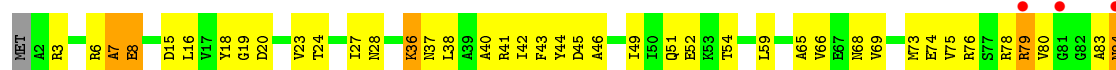
Chain CD: 6% 25% 59% 13%







• Molecule 7: 30S RIBOSOMAL PROTEIN S7



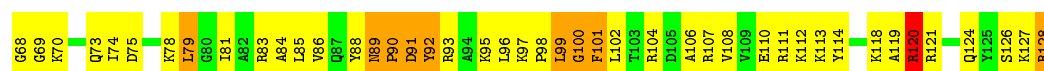
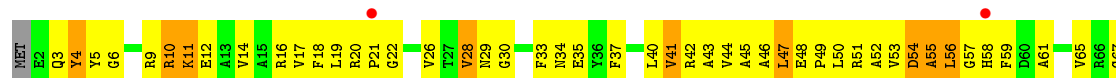
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



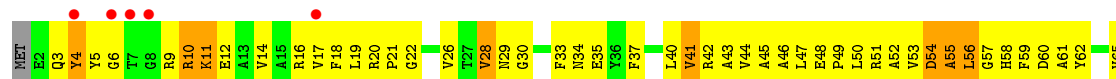
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

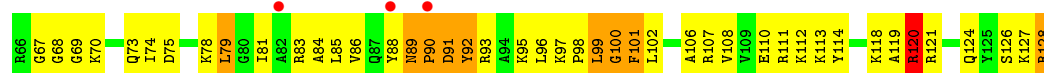


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

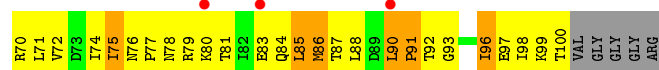


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

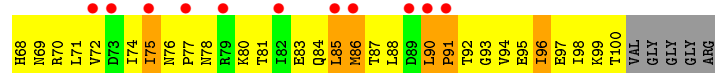
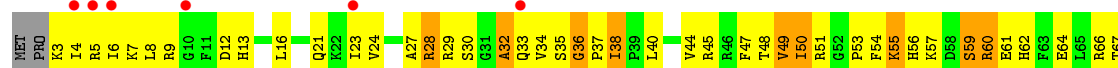




• Molecule 10: 30S RIBOSOMAL PROTEIN S10



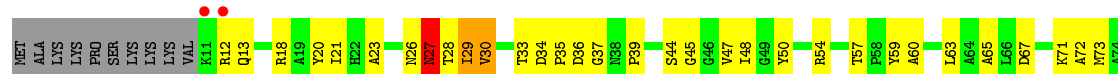
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



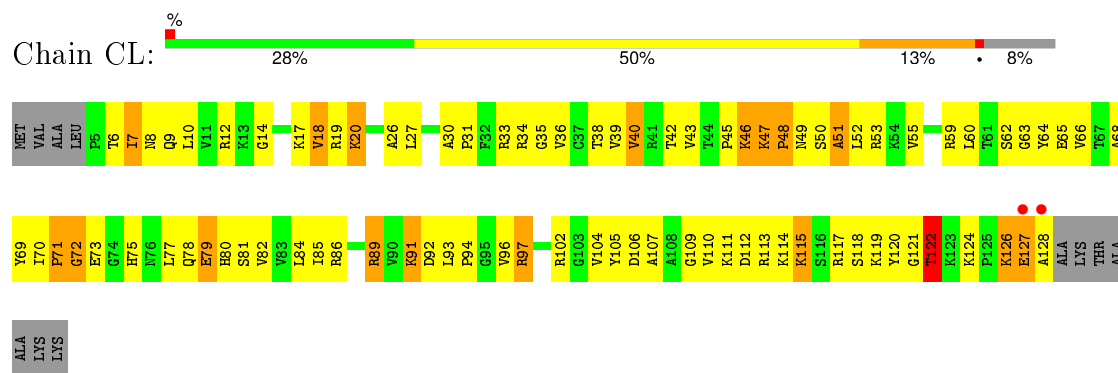
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



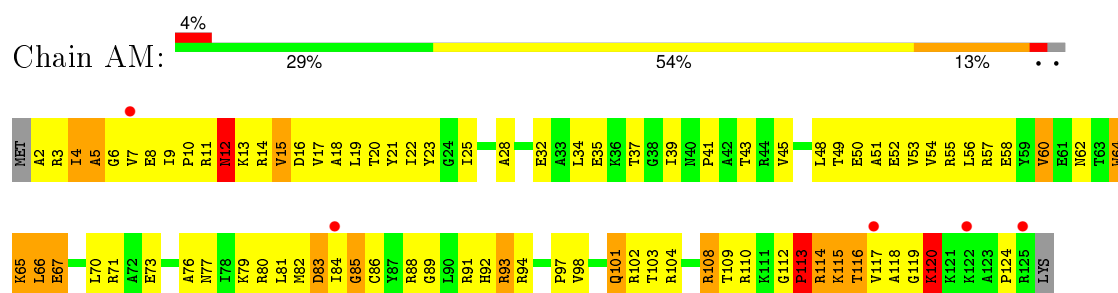
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



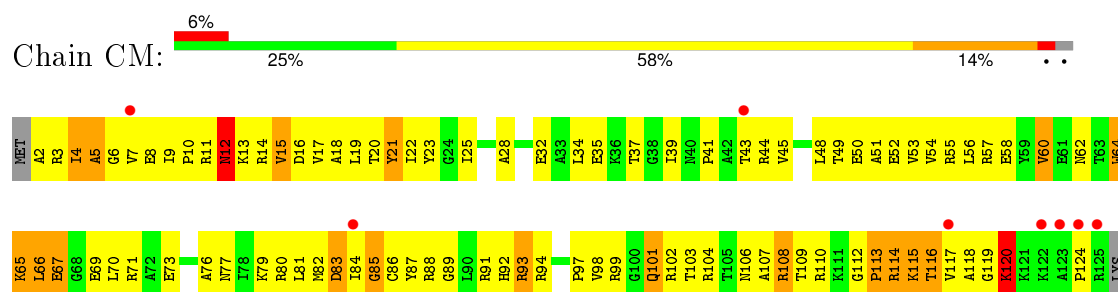
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



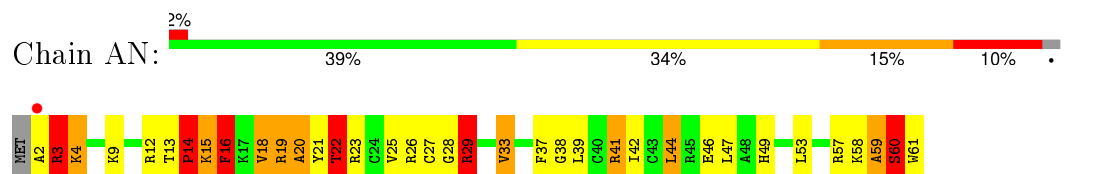
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



● Molecule 13: 30S RIBOSOMAL PROTEIN S13



● Molecule 14: 30S RIBOSOMAL PROTEIN S14



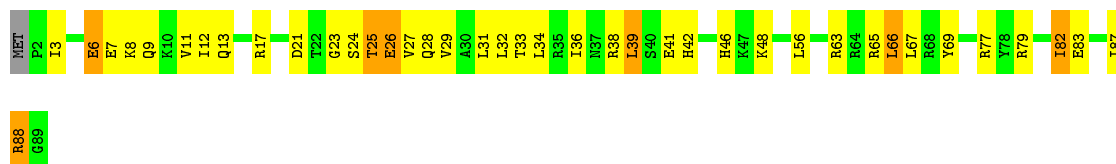
• Molecule 14: 30S RIBOSOMAL PROTEIN S14





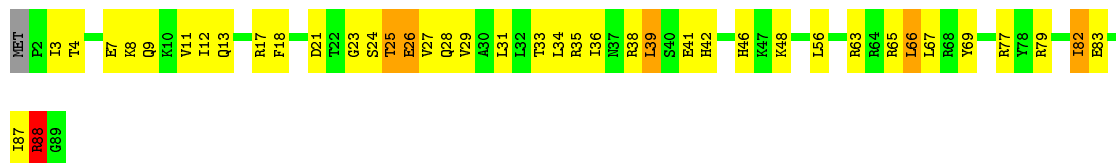
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 54% 37% 8% .



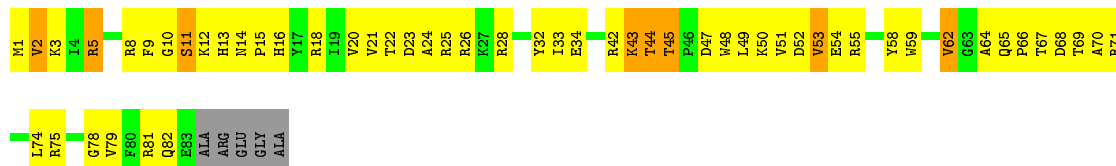
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 53% 39% 6% ..



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 32% 53% 9% 6%



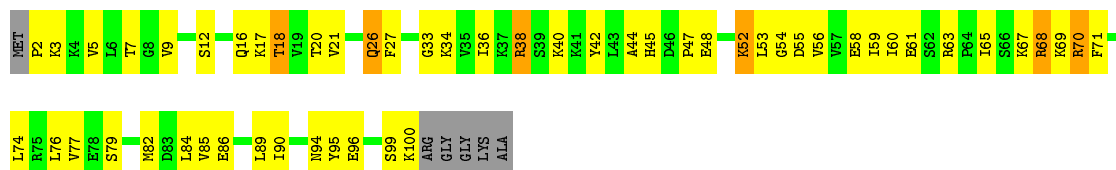
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 3% 31% 55% 9% 6%

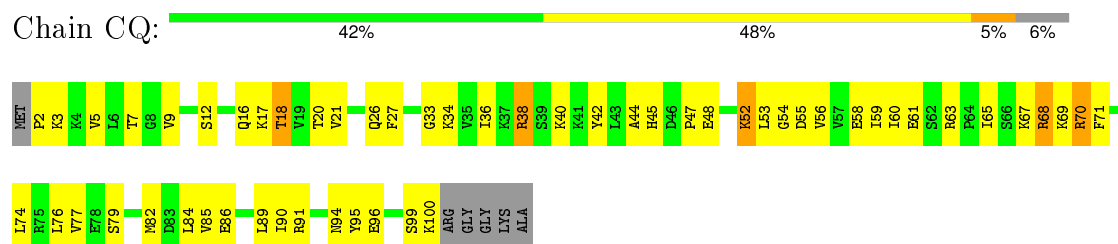


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

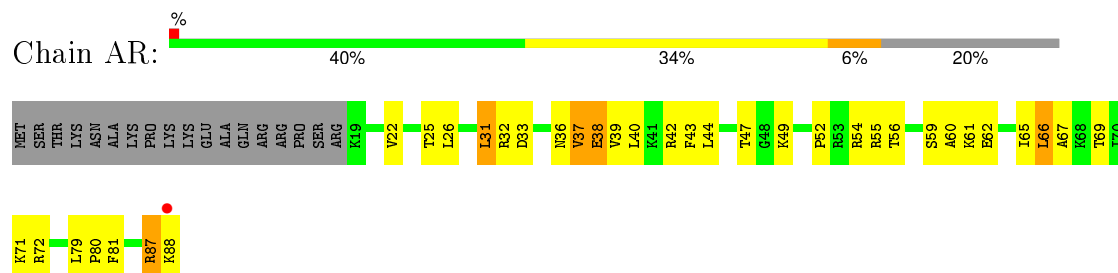
Chain AQ: 43% 46% 6% 6%



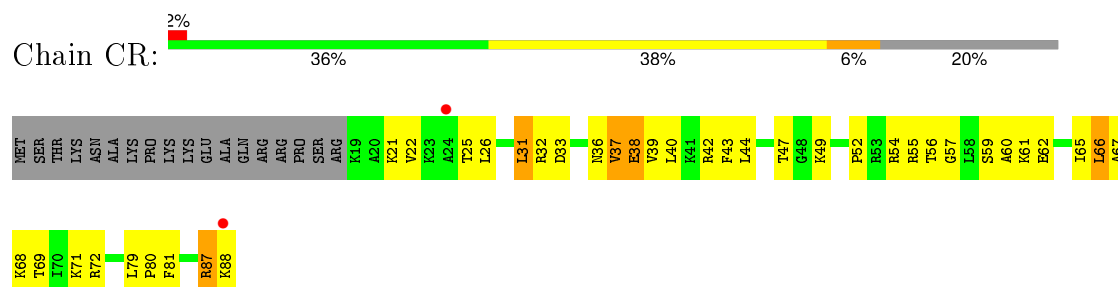
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



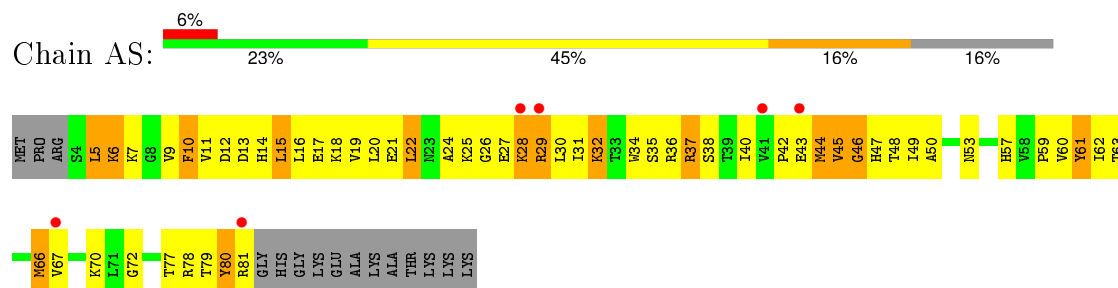
- Molecule 18: 30S RIBOSOMAL PROTEIN S18



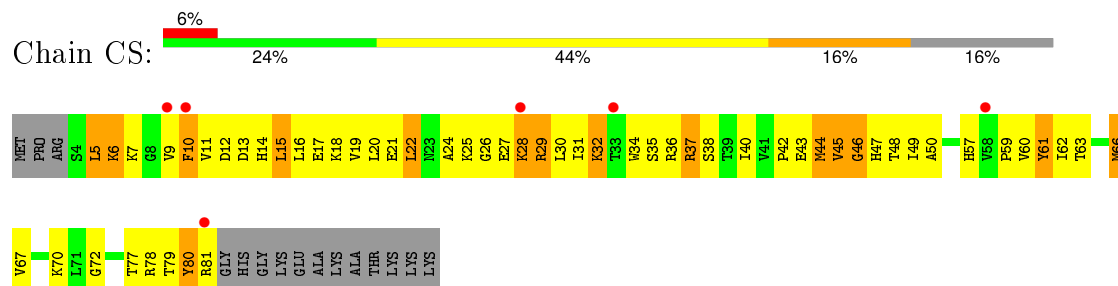
- Molecule 18: 30S RIBOSOMAL PROTEIN S18



- Molecule 19: 30S RIBOSOMAL PROTEIN S19



- Molecule 19: 30S RIBOSOMAL PROTEIN S19

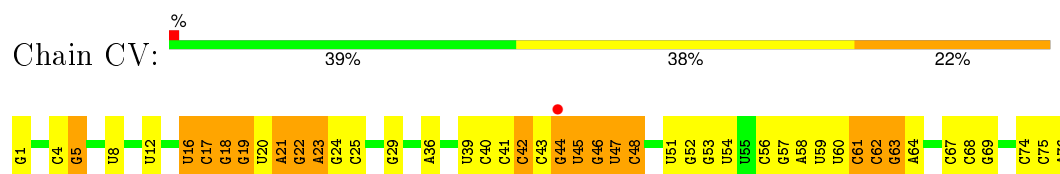


Chain AW:

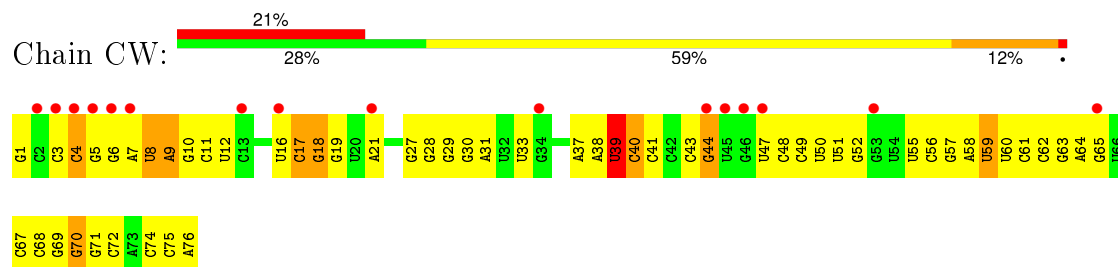
18% 30% 57% 12%

G69 G70 G71 G72 A76 A77

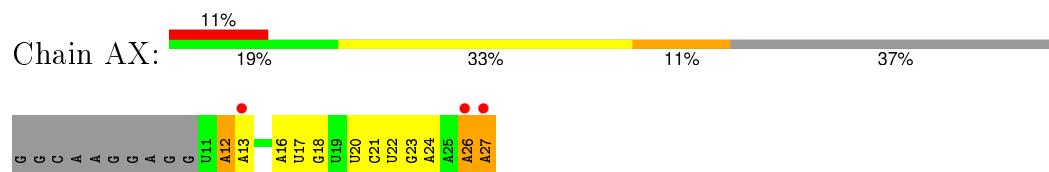
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



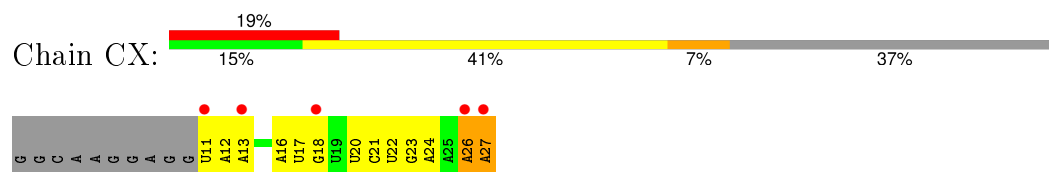
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



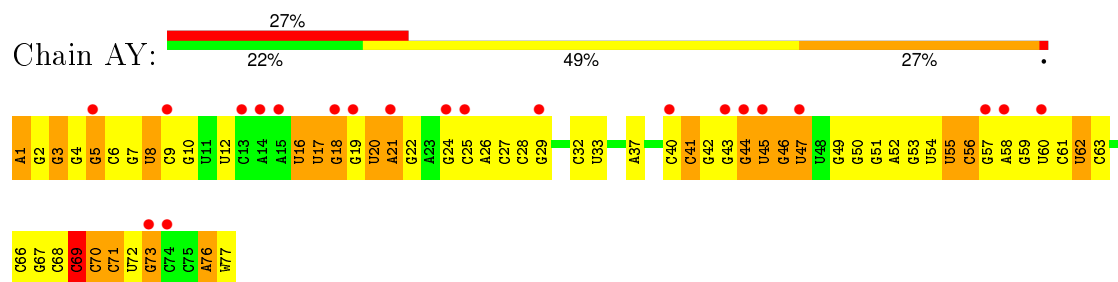
- Molecule 23: MRNA



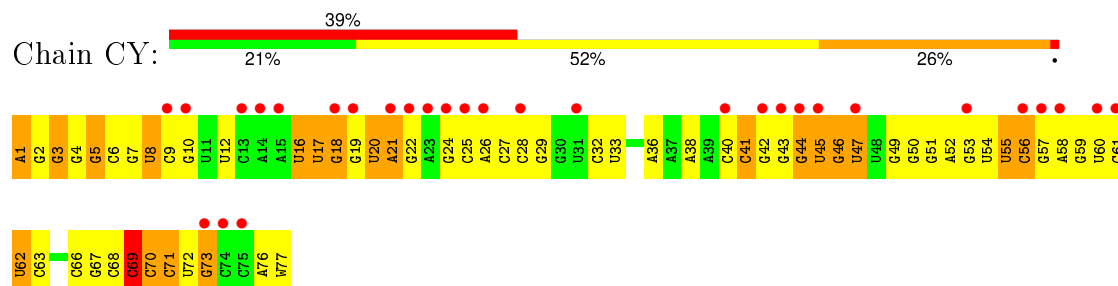
- Molecule 23: MRNA



- Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP



- Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP



Chain AZ:

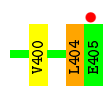
14% 34% 52% 10% 5%

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

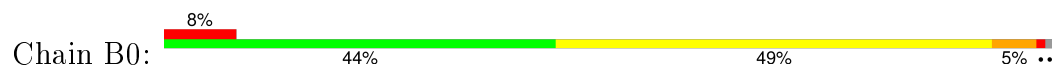
Chain CZ:

16% 33% 51% 10% 5%

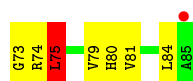
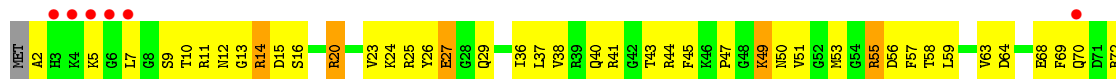
The chart displays the distribution of Chain CZ values across 50 categories. The categories are represented by colored squares, each with a label. The colors correspond to the segments in the bar chart above. The categories are: A1, A2, A3, A4, A5, A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, A20, A21, A22, A23, A24, A25, A26, A27, A28, A29, A30, A31, A32, A33, A34, A35, A36, A37, A38, A39, A40, A41, A42, A43, A44, A45, A46, A47, A48, A49, A50.



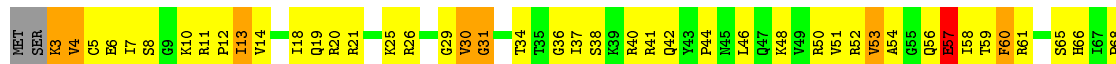
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



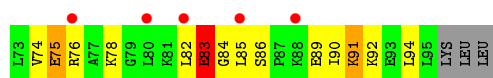
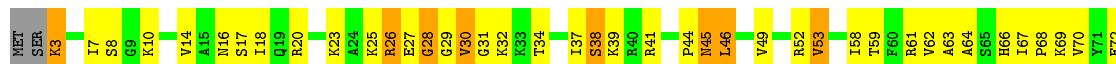
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



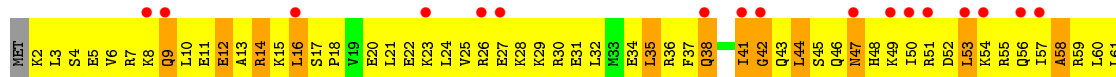
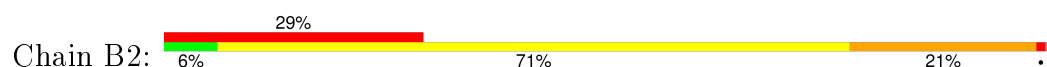
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L28

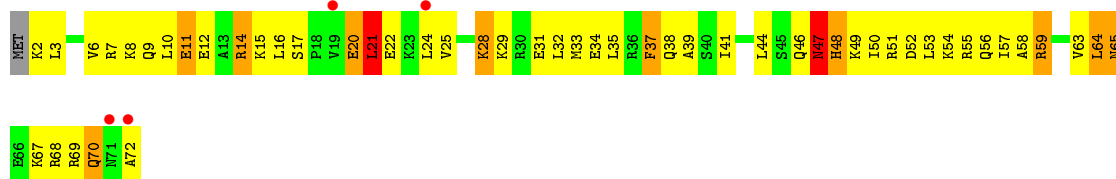


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

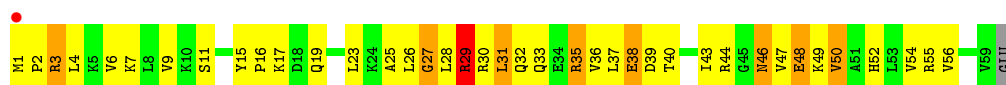




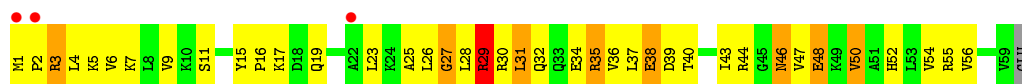
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



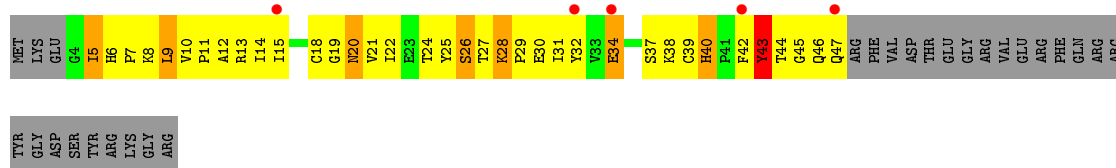
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



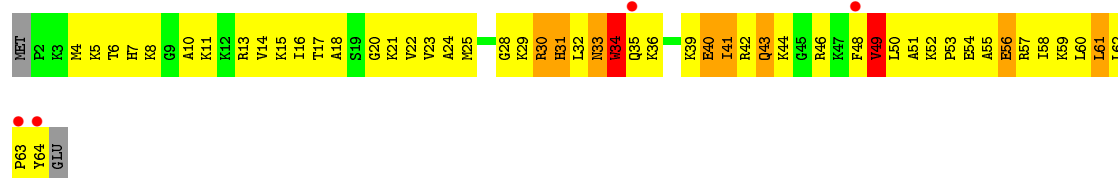
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



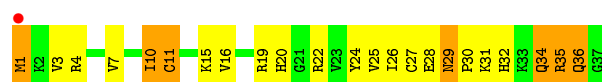
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



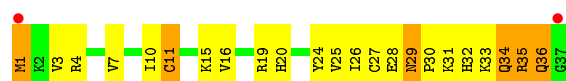




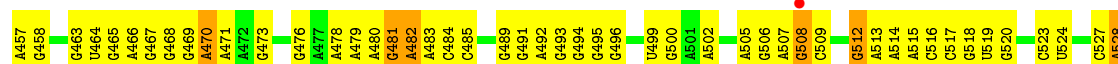
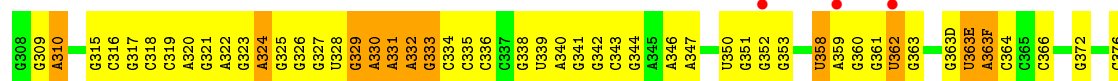
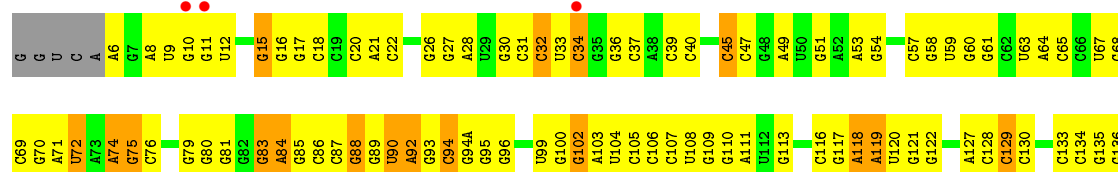
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36

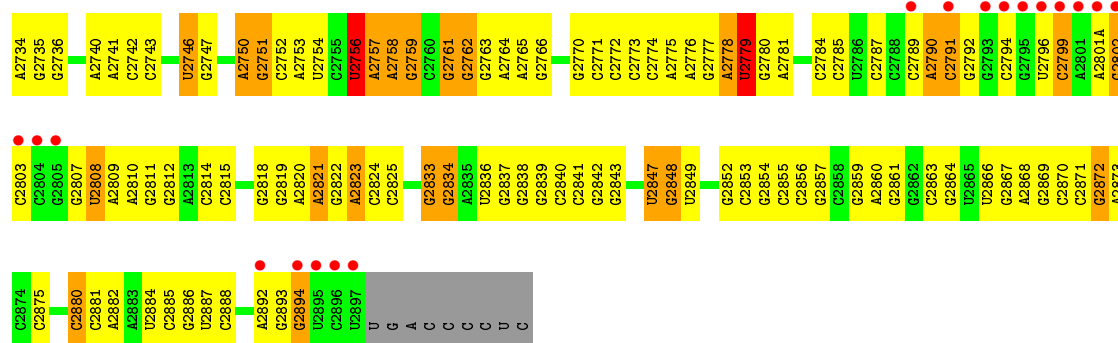


• Molecule 36: 23S RIBOSOMAL RNA

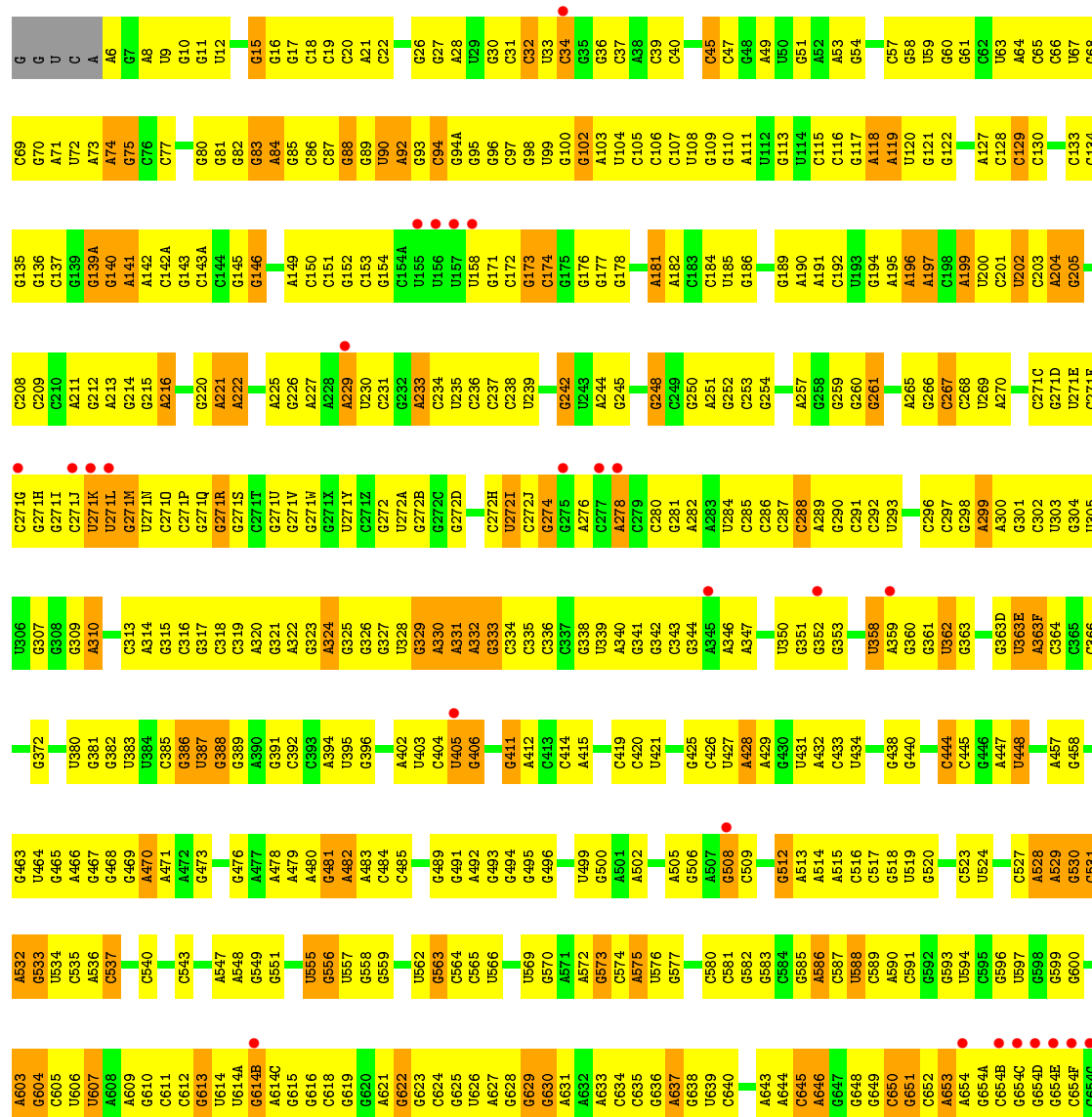




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G1800	G1801	G1807	U1808	G1809	A1810	G1811	G1812	G1813	G1816	G1817	U1818	A1819	U1820	A1821	G1826	G1827	G1828	G1831	G1835	G1836	G1837	U1841	G1842	G1843	G1844	U1847	U1851	G1852	A1853	U1854	G1858	G1859	G1860	G1861	G1862	G1863	U1864	G1865	G1866	A1876	U1877	G1878	C1879	U1880	G1881	U1882	G1883	A1884	U1885	G1886													
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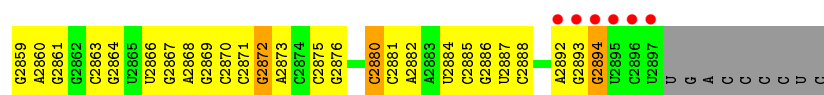


• Molecule 36: 23S RIBOSOMAL RNA

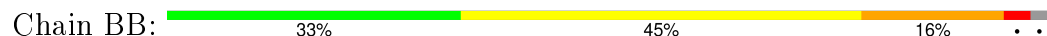




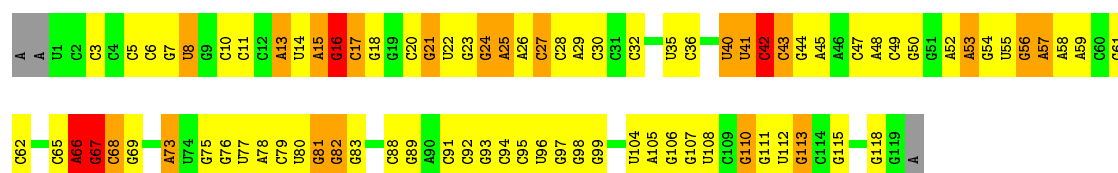
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C2795	C2724	C2652	A2565	G2490	G2420	G2351	C2283	C2196	U2132	C2067	C1908	G1817	A1722
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C2799	U2656	U2657	C2570		U2424	C2355	A2287	C2200	C2136		U1911	U1820	G1740
A2801	G2657	A2658	C2571	C2499	C2425		A2288	C2201	G2072		A1912	A1821	C1745A
A2802	C2658	C2659	A2572	G2502	G2428	G2358	A2289	C2202	C2073	C2073	A1913	A1821	G1746
C2803	G2659	G2660	C2573	A2503	G2429	C2359	G2290		C2074	U2075	A1914	G1826	G1747
C2804	A2660	G2661	G2574	U2504	A2430	A2360	C2291	G2206	G2146		G1915	G1827	G1747A
C2805	G2662	A2662	G2575	G2505	U2431	A2361	C2292	G2207	G2147		G1916	G1828	G1748
C2806	A2663	A2663	U2576	U2506	A2432	C2364	C2293	A2208	G2148		U1917		A1749
C2807	G2664	G2664	G2577	G2507	G2433	G2365	C2294	U2218	G2149	C2078	A2001	G1831	G1750
U2808	C2665	A2665	G2578	U2508	A2434	A2366	U2295	G2219	G2150	G2080	G1921	G1835	C1752
U2809	C2666	C2666	G2579	G2509	A2435	A2367	U2296	G2220	G2151		G1922	G1836	G1753
A2810	C2667	G2667	G2580	U2510	G2436	G2368	C2297	G2221	U2152		C2007	C1837	G1754
A2811	C2668	G2668	G2581	G2511	U2437	G2369	A2298	G2222	G2153	U2086	C1925	G1837	A1755
A2812	C2669	G2669	G2582	C2512	A2438	G2370	G2299	G2223	G2154	G2087	U1926		
C2813			U2583	G2513	A2439	G2371		G2224	G2155	U2088		U1841	A1762
C2814			C2584	U2514	G2440	G2372	G2303	A2225	G2156	U2089	G1929	G1842	G1763
C2815			G2585	C2515	G2441	G2373	G2304	G2226	G2157	U2090	G1930	G1843	G1764
C2816			U2586	G2516	G2442	G2374	A2305	A2227	G2158	U2091	U1931	G1844	
C2817			G2587	U2517	C2443	G2375	G2306	G2228	G2159		A1932	G1765	C1765
C2818			U2588	G2518	G2444	A2376	G2307	G2229	G2160		G1933	U1766	
C2819			C2589	C2519	G2445	A2377	G2308	G2230	A2158			A1847	
C2820			G2590	G2520	G2446	A2378	A2309	C2231	U2096		A1936		C1771
C2821			U2591	G2521	A2447	C2381	A2310	G2236	A2097		A1937	C1852	G1772
C2822			G2592	C2522	G2448	G2382	A2311	G2237	C2097		A1938	A1853	A1773
C2823			A2602	G2523	A2449	G2383	U2312	G2238	U2098		U1939	A1854	G1774
C2824			C2606	U2524	A2450	G2384	C2313	G2239	U2099		U1940		U1775
C2825			U2609	G2525	G2451	G2385	G2314	G2240	G2100		U1946	G1888	G1776
C2826			G2612	U2526	U2452	C2386	G2315	A2241	G2101		C1947	A1859	U1777
C2827			U2613	G2527	G2453	U2387	C2316	G2242	U2102		G1948	G1860	U1778
C2828			G2614	U2528	G2454	G2388	C2317	U2243	C2103			G1861	U1779
C2829			A2615	G2529	U2455	A2389	G2318	U2244	G2104		G1949	G1862	A1780
C2830			U2616	A2630	G2456	G2390	G2319	U2245	G2105			G1863	C1781
C2831			C2617	U2631	G2457	G2391	A2320	U2246	G2106		A1952	U1864	G1782
C2832			G2618	A2634	G2458	A2392		U2247			A1953	G1865	A1783
C2833			U2619	U2637	G2459	A2393	A2327	A2248	C2107		G1954	A1876	A1784
C2834			C2626	G2638	G2460	G2396	A2328	C2248	C2108		U1955	A1877	A1786
C2835			G2627	U2639	G2461	G2397	G2329	U2249	G2109			G1878	A1787
C2836			U2628	A2642	G2462	U2398	G2330		G2111		C1958	C1879	A1787
C2837			C2629	G2643	A2463	U2399	G2331	U2257	G2112		G1959	C1879	
C2838			A2630	U2644	G2464	G2402	U2332	C2258	U2113			C1880	C1790
C2839			G2632	G2645	G2465	C2403	A2333	C2259	A2114		U1963	A1791	A1791
C2840			U2633	U2646	G2466	C2404	G2334	C2261	G2115		C2039	C1882	
C2841			G2634	G2647	G2467	U2472	A2335	C2262	G2116		U2041	G1967	U1796
C2842			C2635	G2468	G2468	U2473	A2336	C2263	A2117		G1968	A1884	C1797
C2843			U2636	A2474	G2469	G2405	G2337	G2264	A2042		A1969	A1885	U1798
U2844			A2642	C2475	A2470	U2406		U2265	U2118		A1970	C1886	U1799
G2848			G2643	A2476	G2471	U2407	G2340	A2266	G2120			G1887	C1800
U2849			U2644	U2477	A2472	U2408	G2341	A2267	G2121			G1888	G1801
C2852			C2636	U2645	G2473	U2409		A2268					
C2853			U2637	U2646	G2474								
C2854			U2638	U2647	G2475								
C2855			U2639	U2648	G2476								
C2856			U2640	U2649	G2477								
C2857			U2641	U2650	G2478								
C2858			U2642	U2651	G2479								



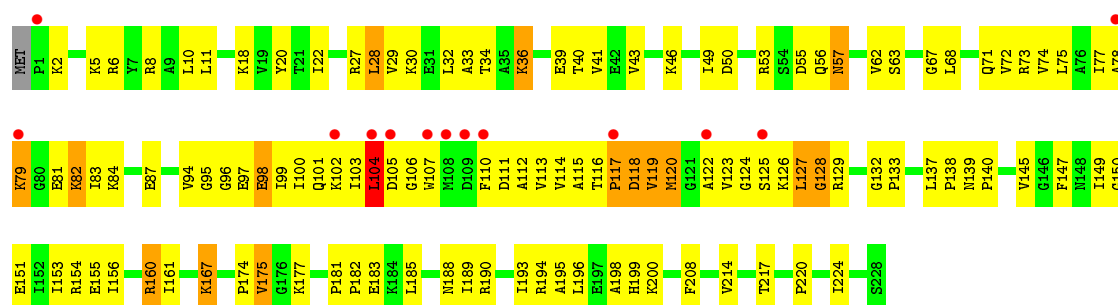
• Molecule 37: 5S RIBOSOMAL RNA



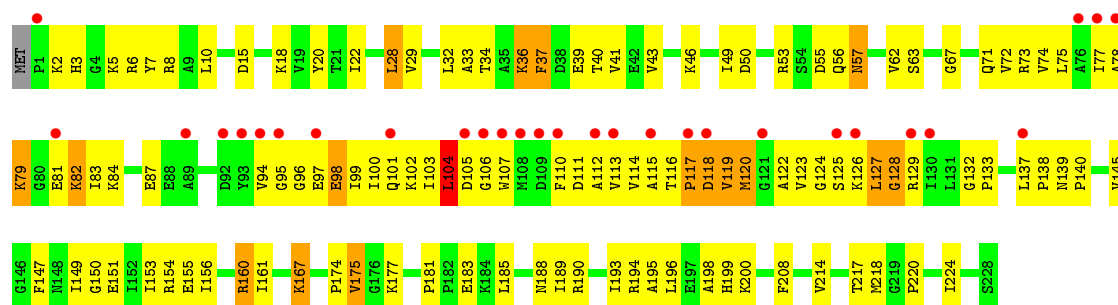
• Molecule 37: 5S RIBOSOMAL RNA



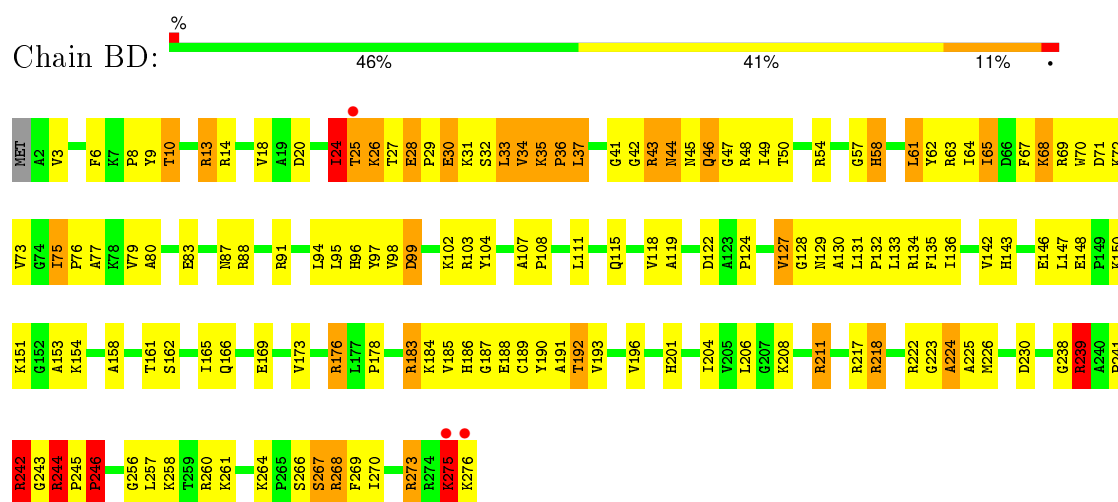
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



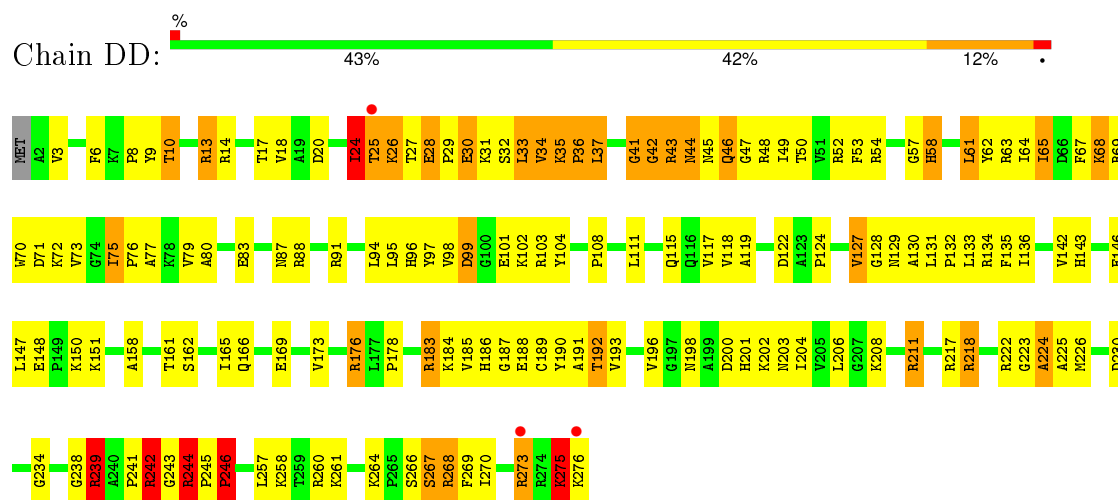
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



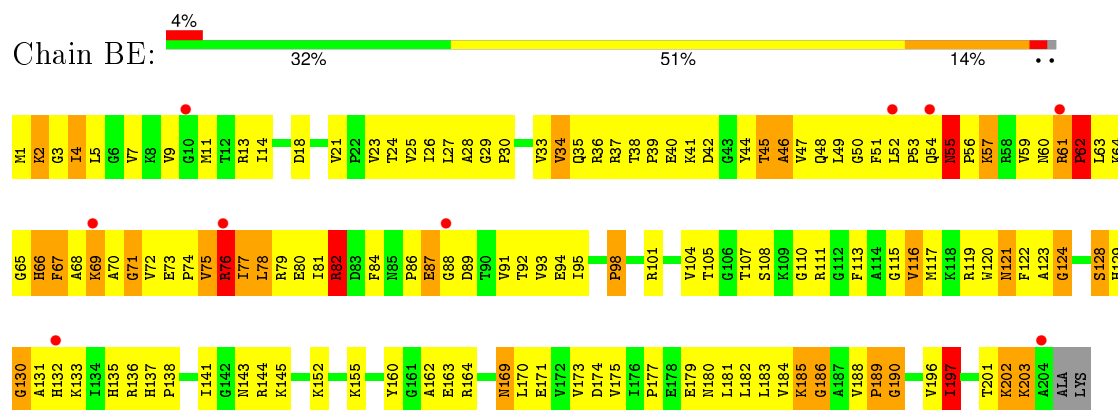
• Molecule 39: 50S RIBOSOMAL PROTEIN L2



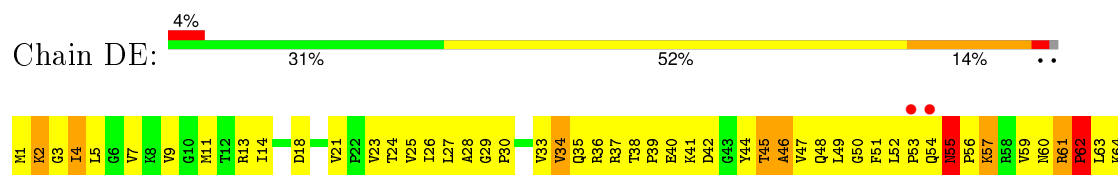
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

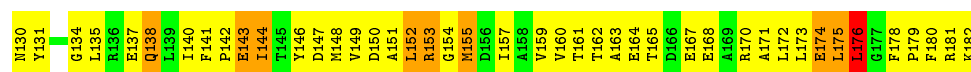


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

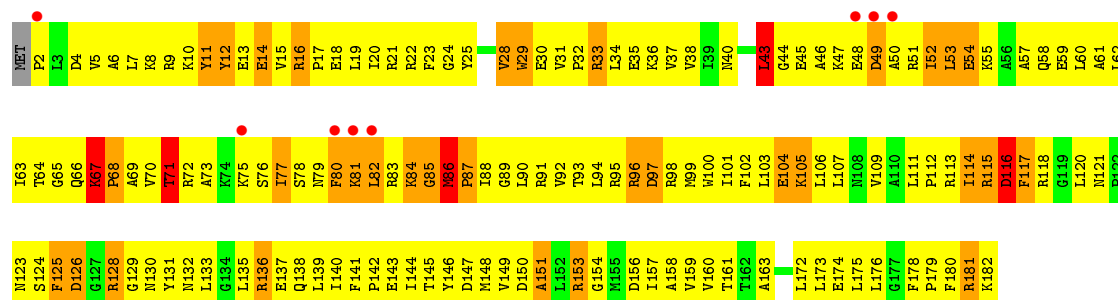


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

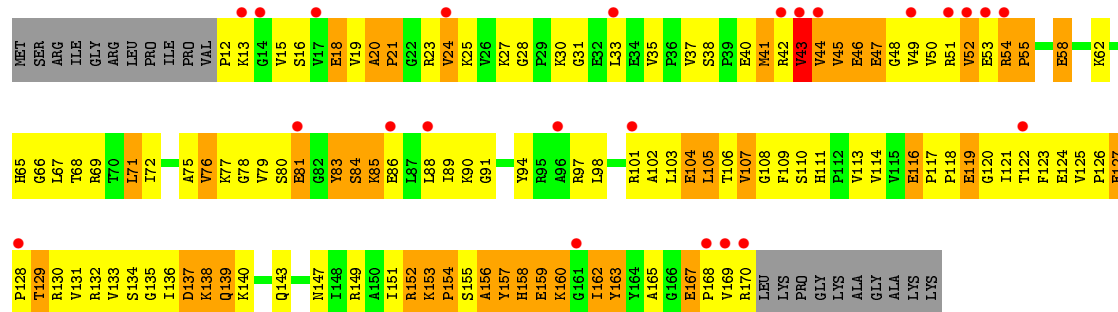
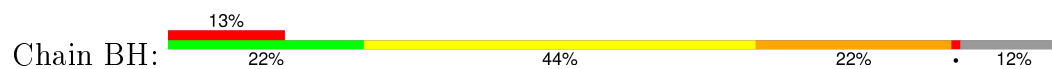




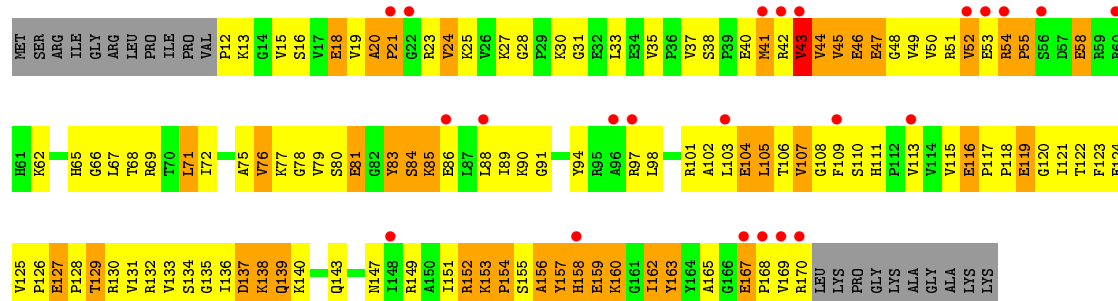
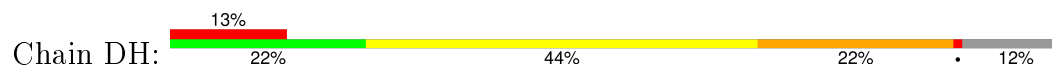
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



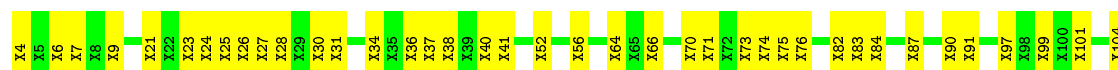
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L6

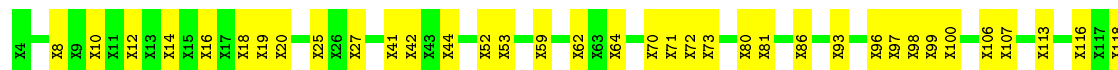


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

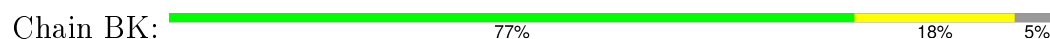




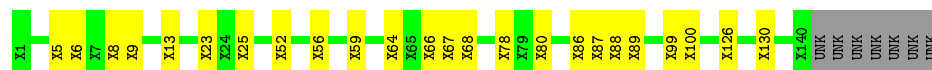
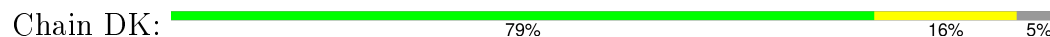
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



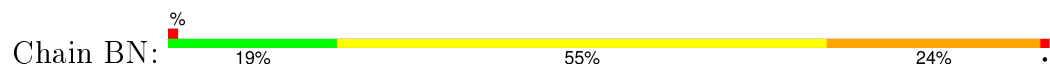
• Molecule 45: 50S RIBOSOMAL PROTEIN L11



• Molecule 45: 50S RIBOSOMAL PROTEIN L11

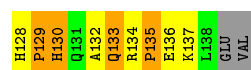


• Molecule 46: 50S RIBOSOMAL PROTEIN L13



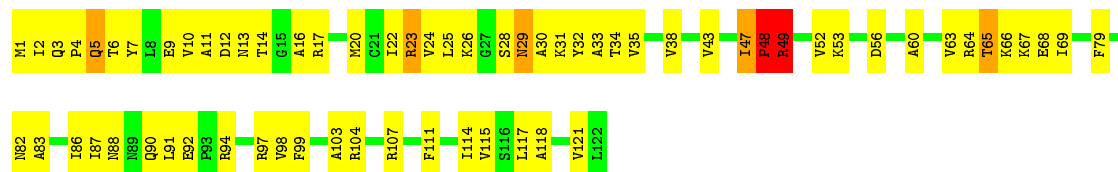
• Molecule 46: 50S RIBOSOMAL PROTEIN L13





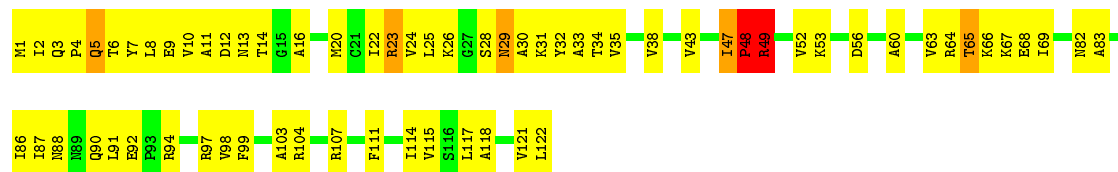
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 45% 49%



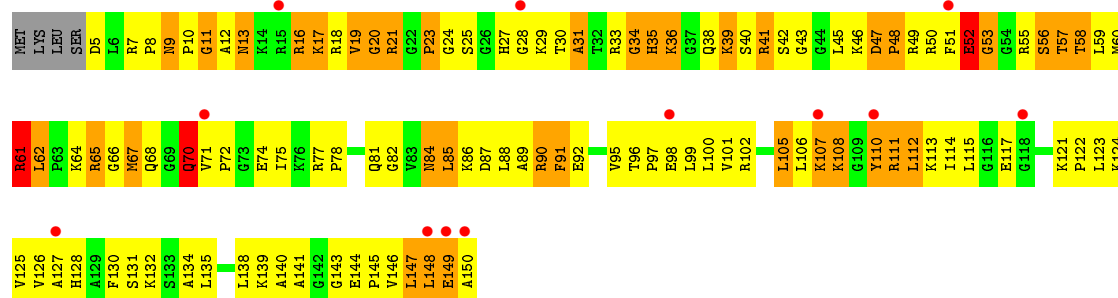
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 45% 49%



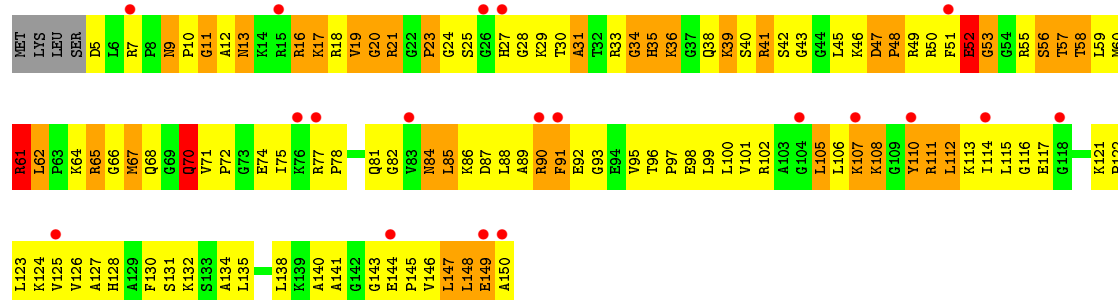
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 8% 20% 51% 25%



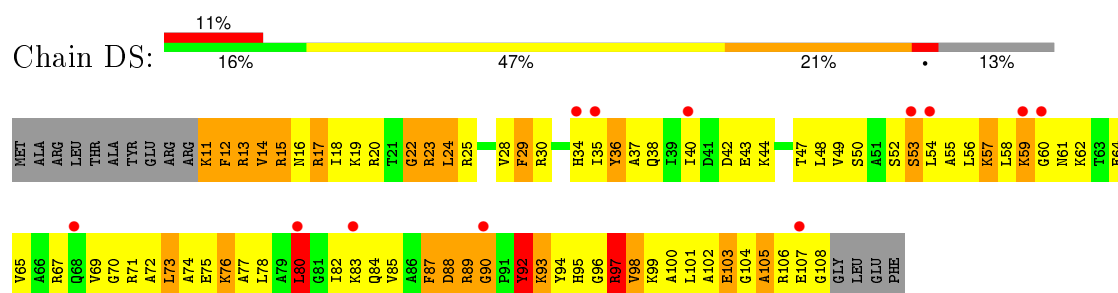
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 13% 20% 51% 25%

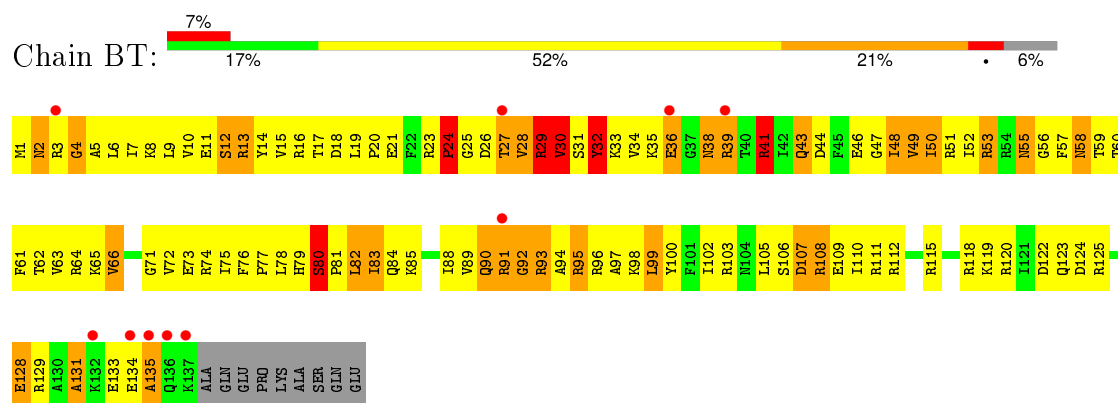


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

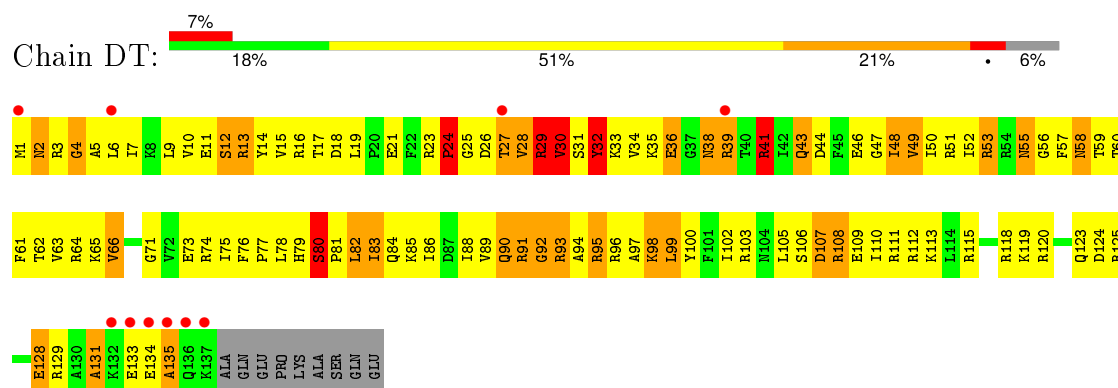




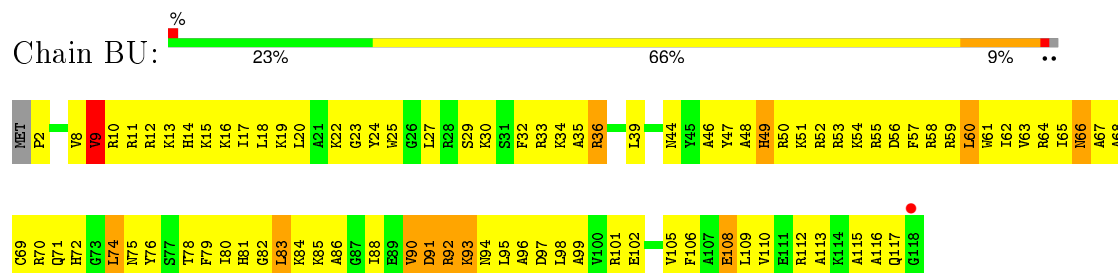
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

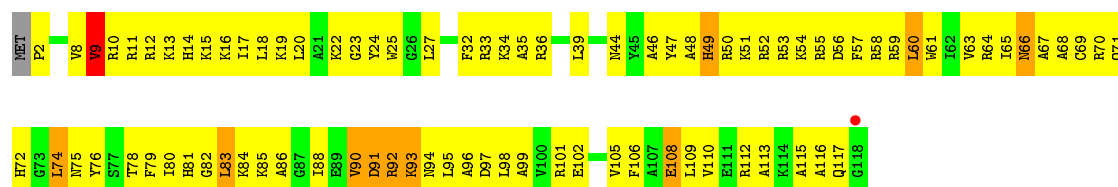


• Molecule 53: 50S RIBOSOMAL PROTEIN L20



• Molecule 53: 50S RIBOSOMAL PROTEIN L20





• Molecule 54: 50S RIBOSOMAL PROTEIN L21



• Molecule 54: 50S RIBOSOMAL PROTEIN L21



• Molecule 55: 50S RIBOSOMAL PROTEIN L22



• Molecule 55: 50S RIBOSOMAL PROTEIN L22



• Molecule 56: 50S RIBOSOMAL PROTEIN L23



GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

• Molecule 58: 50S RIBOSOMAL PROTEIN L25



MET
GLU
Y3
R4
L5
K6
A7
T8
Y9
R10
E11
G12
E13
K14
P15
S16
A17
L18
R19
R20
R23
L24
P25
R28
Y29
N30
R31
R34
R35
R36
V37
Y38
V39
D40
L41
V42
E43
F44
F48
A51
S52
I53
H54
H55
V56
I57
V58
L59
E60
L61
P62
R63
G64
Q65
S66

L67
F68
T69
L70
V71
R72
Q73
V74
N75
L76
D77
K78
R79
R80
R81
V86
D87
F88
F89
V90
L91
P95
V96
E97
M98
Y99
V100
P101
L102
R103
F104
V105
P108
A109
G110
V111
R112
A113
G114
G115
V116
E119
I120
H121
R122
D123
I124
L125
V126
K127
V128
S129
N132
I133
P134

E135
F136
I137
E138
V139
D140
Y141
S142
G143
L144
E145
I146
G147
D148
S149
L150
H151
A152
L155
K156
L157
P158
P159
G160
V161
E162
L163
A164
V165
S166
P167
E168
E169
T170
I171
A172
A173
P177
E178
ASP
VAL
GLU
LYS
LEU
ALA
GLU
GLU
ALA
ALA
ALA
VAL
VAL
ALA
GLU
PRO
GLU
VAL
ILE

LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	289.90Å 268.50Å 403.60Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.92 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.10) 90.5 (49.92-2.93)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.267 0.241 , 0.266	Depositor DCC
R_{free} test set	54322 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.0	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1195890 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	307322	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: OMC, GDP, ZN, H2U, KIR, MIA, 4SU, 7MG, 5MU, PSU

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	AA	0.57	4/36325 (0.0%)	0.75	46/56695 (0.1%)
1	CA	0.52	2/36325 (0.0%)	0.74	36/56695 (0.1%)
2	AB	0.44	0/1935	0.68	0/2609
2	CB	0.43	0/1935	0.69	0/2609
3	AC	0.49	0/1636	0.73	1/2205 (0.0%)
3	CC	0.45	0/1636	0.72	1/2205 (0.0%)
4	AD	0.39	0/1733	0.63	0/2318
4	CD	0.39	0/1733	0.63	0/2318
5	AE	0.54	0/1162	0.77	0/1564
5	CE	0.52	0/1162	0.76	0/1564
6	AF	0.39	0/856	0.65	0/1154
6	CF	0.39	0/856	0.66	0/1154
7	AG	0.45	0/1276	0.63	0/1709
7	CG	0.42	0/1276	0.63	1/1709 (0.1%)
8	AH	0.49	0/1136	0.73	0/1527
8	CH	0.45	0/1136	0.73	0/1527
9	AI	0.44	0/1029	0.68	0/1379
9	CI	0.42	0/1029	0.68	0/1379
10	AJ	0.41	0/807	0.68	0/1085
10	CJ	0.39	0/807	0.67	0/1085
11	AK	0.50	0/900	0.70	0/1213
11	CK	0.47	0/900	0.70	0/1213
12	AL	0.42	0/986	0.72	0/1320
12	CL	0.41	0/986	0.71	0/1320
13	AM	0.41	0/998	0.71	1/1336 (0.1%)
13	CM	0.38	0/998	0.71	1/1336 (0.1%)
14	AN	0.46	0/501	0.78	0/664
14	CN	0.45	0/501	0.79	0/664
15	AO	0.42	0/745	0.64	0/992
15	CO	0.43	0/745	0.64	0/992
16	AP	0.36	0/716	0.64	0/963
16	CP	0.35	0/716	0.64	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.45	0/836	0.67	0/1117
17	CQ	0.44	0/836	0.67	0/1117
18	AR	0.45	0/579	0.66	0/768
18	CR	0.46	0/579	0.67	0/768
19	AS	0.44	0/642	0.69	0/865
19	CS	0.41	0/642	0.69	0/865
20	AT	0.35	0/765	0.65	0/1007
20	CT	0.34	0/765	0.65	0/1007
21	AU	0.45	0/212	0.67	0/277
21	CU	0.50	0/212	0.66	0/277
22	AV	0.55	0/1809	0.73	1/2819 (0.0%)
22	AW	0.36	0/1809	0.73	2/2819 (0.1%)
22	CV	0.53	0/1809	0.73	1/2819 (0.0%)
22	CW	0.36	0/1809	0.73	2/2819 (0.1%)
23	AX	0.50	0/405	0.71	0/629
23	CX	0.49	0/405	0.70	0/629
24	AY	0.43	1/1616 (0.1%)	0.70	1/2511 (0.0%)
24	CY	0.45	1/1616 (0.1%)	0.70	1/2511 (0.0%)
25	AZ	0.31	0/3041	0.56	0/4127
25	CZ	0.32	0/3041	0.57	0/4127
26	B0	0.39	0/671	0.69	0/892
26	D0	0.41	0/671	0.70	0/892
27	B1	0.47	0/738	0.73	0/981
27	D1	0.40	0/738	0.68	0/981
28	B2	0.35	0/600	0.66	0/793
28	D2	0.33	0/600	0.64	1/793 (0.1%)
29	B3	0.37	0/472	0.61	0/634
29	D3	0.35	0/472	0.61	0/634
30	B4	0.38	0/349	0.65	0/474
30	D4	0.37	0/349	0.65	0/474
31	B5	0.38	0/473	0.72	0/639
31	D5	0.38	0/473	0.71	0/639
32	B6	0.60	0/440	0.82	0/586
32	D6	0.54	0/440	0.80	0/586
33	B7	0.42	0/426	0.68	0/561
33	D7	0.42	0/426	0.69	0/561
34	B8	0.56	0/515	0.87	1/679 (0.1%)
34	D8	0.53	0/515	0.87	1/679 (0.1%)
35	B9	0.42	0/310	0.65	0/407
35	D9	0.41	0/310	0.65	0/407
36	BA	0.51	3/69976 (0.0%)	0.72	33/109244 (0.0%)
36	DA	0.49	2/69976 (0.0%)	0.72	32/109244 (0.0%)
37	BB	0.43	0/2853	0.75	2/4451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.46	0/2853	0.75	2/4451 (0.0%)
38	BC	0.39	1/1774 (0.1%)	0.60	0/2391
38	DC	0.40	2/1774 (0.1%)	0.60	0/2391
39	BD	0.51	0/2195	0.81	1/2955 (0.0%)
39	DD	0.50	0/2195	0.80	1/2955 (0.0%)
40	BE	0.43	0/1596	0.75	0/2153
40	DE	0.43	0/1596	0.74	0/2153
41	BF	0.36	0/1658	0.65	0/2244
41	DF	0.37	0/1658	0.65	0/2244
42	BG	0.40	0/1499	0.74	1/2016 (0.0%)
42	DG	0.38	0/1499	0.68	0/2016
43	BH	0.32	0/1245	0.66	0/1682
43	DH	0.32	0/1245	0.66	0/1682
46	BN	0.37	0/1131	0.70	0/1525
46	DN	0.37	0/1131	0.69	0/1525
47	BO	0.47	0/943	0.68	0/1269
47	DO	0.46	0/943	0.67	0/1269
48	BP	0.43	0/1131	0.91	2/1504 (0.1%)
48	DP	0.42	0/1131	0.91	2/1504 (0.1%)
49	BQ	0.50	0/1143	0.71	0/1527
49	DQ	0.49	0/1143	0.72	0/1527
50	BR	0.38	0/974	0.71	1/1302 (0.1%)
50	DR	0.38	0/974	0.70	1/1302 (0.1%)
51	BS	0.36	0/778	0.76	0/1036
51	DS	0.37	0/778	0.75	0/1036
52	BT	0.43	0/1155	0.76	2/1542 (0.1%)
52	DT	0.41	0/1155	0.76	2/1542 (0.1%)
53	BU	0.41	0/975	0.68	0/1297
53	DU	0.43	0/975	0.68	0/1297
54	BV	0.37	0/790	0.68	0/1057
54	DV	0.39	0/790	0.68	0/1057
55	BW	0.35	0/907	0.67	0/1216
55	DW	0.36	0/907	0.67	0/1216
56	BX	0.40	0/739	0.65	0/993
56	DX	0.40	0/739	0.65	0/993
57	BY	0.36	0/788	0.73	1/1051 (0.1%)
57	DY	0.36	0/788	0.73	1/1051 (0.1%)
58	BZ	0.46	0/1435	0.81	1/1949 (0.1%)
58	DZ	0.44	0/1435	0.74	0/1949
All	All	0.49	16/330268 (0.0%)	0.72	183/493444 (0.0%)

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
1	AA	5	49
1	CA	4	49
22	AW	1	1
22	CW	1	1
24	AY	2	0
24	CY	2	0
36	BA	2	66
36	DA	2	67
37	BB	0	6
37	DB	0	6
All	All	19	245

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	761	A	C5-C6	-10.36	1.31	1.41
36	DA	761	A	C5-C6	-10.14	1.31	1.41
36	BA	2506	U	N1-C2	8.65	1.46	1.38
36	DA	2506	U	N1-C2	8.34	1.46	1.38
1	AA	858	G	C5-C6	-7.88	1.34	1.42

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	BD	244	ARG	C-N-CD	-11.04	96.32	120.60
39	DD	244	ARG	C-N-CD	-10.91	96.59	120.60
1	CA	1498	U	C2'-C3'-O3'	10.87	133.42	109.50
1	AA	1498	U	C2'-C3'-O3'	10.68	132.99	109.50
1	AA	508	C	C2'-C3'-O3'	9.74	130.93	109.50

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1239	A	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
1	AA	1531	A	C3'

5 of 245 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	21	G	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	AA	32451	0	16382	1017	0
1	CA	32451	0	16382	1043	0
2	AB	1900	0	1951	209	0
2	CB	1900	0	1951	211	0
3	AC	1612	0	1677	148	0
3	CC	1612	0	1677	155	0
4	AD	1703	0	1764	221	0
4	CD	1703	0	1763	226	0
5	AE	1146	0	1207	78	0
5	CE	1146	0	1207	89	0
6	AF	843	0	857	78	0
6	CF	843	0	857	77	0
7	AG	1257	0	1296	94	0
7	CG	1257	0	1296	89	0
8	AH	1116	0	1177	50	0
8	CH	1116	0	1177	52	0
9	AI	1010	0	1037	143	0
9	CI	1010	0	1037	142	0
10	AJ	794	0	840	113	0
10	CJ	794	0	840	118	0
11	AK	885	0	904	59	0
11	CK	885	0	904	61	0
12	AL	970	0	1057	112	0
12	CL	970	0	1057	111	0
13	AM	987	0	1059	136	0
13	CM	987	0	1059	139	0
14	AN	492	0	529	58	0
14	CN	492	0	529	61	0
15	AO	734	0	771	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	43	0
16	AP	700	0	720	72	0
16	CP	700	0	720	73	0
17	AQ	823	0	891	56	0
17	CQ	823	0	891	58	0
18	AR	574	0	644	35	0
18	CR	574	0	644	39	0
19	AS	629	0	652	77	0
19	CS	629	0	652	79	0
20	AT	763	0	861	78	0
20	CT	763	0	861	79	0
21	AU	208	0	221	12	0
21	CU	208	0	221	13	0
22	AV	1619	0	822	60	0
22	AW	1619	0	822	67	0
22	CV	1619	0	822	63	0
22	CW	1619	0	822	71	0
23	AX	361	0	184	7	0
23	CX	361	0	184	11	0
24	AY	1643	0	853	75	0
24	CY	1643	0	853	74	0
25	AZ	2983	0	2999	284	0
25	CZ	2983	0	2999	287	0
26	B0	662	0	688	63	0
26	D0	662	0	688	65	0
27	B1	731	0	808	69	0
27	D1	731	0	808	69	0
28	B2	598	0	653	158	0
28	D2	598	0	653	67	0
29	B3	467	0	523	49	0
29	D3	467	0	523	47	0
30	B4	340	0	336	51	0
30	D4	340	0	336	53	0
31	B5	459	0	480	62	0
31	D5	459	0	480	65	0
32	B6	433	0	461	135	0
32	D6	433	0	461	133	0
33	B7	418	0	467	29	0
33	D7	418	0	467	28	0
34	B8	507	0	576	124	0
34	D8	507	0	576	123	0
35	B9	307	0	336	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D9	307	0	335	42	0
36	BA	62477	0	31497	2141	0
36	DA	62477	0	31497	2212	0
37	BB	2551	0	1295	85	0
37	DB	2551	0	1295	97	0
38	BC	1742	0	1800	141	0
38	DC	1742	0	1800	132	0
39	BD	2145	0	2234	221	0
39	DD	2145	0	2234	234	0
40	BE	1563	0	1629	225	0
40	DE	1563	0	1629	222	0
41	BF	1623	0	1677	193	0
41	DF	1623	0	1677	197	0
42	BG	1474	0	1535	247	0
42	DG	1474	0	1535	232	0
43	BH	1222	0	1282	178	0
43	DH	1222	0	1282	184	0
44	BJ	651	0	164	27	0
44	DJ	651	0	164	31	0
45	BK	700	0	173	18	0
45	DK	700	0	173	15	0
46	BN	1104	0	1180	176	0
46	DN	1104	0	1180	171	0
47	BO	933	0	996	77	0
47	DO	933	0	996	78	0
48	BP	1114	0	1187	263	0
48	DP	1114	0	1187	265	0
49	BQ	1122	0	1179	112	0
49	DQ	1122	0	1179	106	0
50	BR	960	0	1021	133	0
50	DR	960	0	1021	128	0
51	BS	770	0	832	152	0
51	DS	770	0	832	150	0
52	BT	1141	0	1202	229	0
52	DT	1141	0	1202	223	0
53	BU	958	0	1015	132	0
53	DU	958	0	1015	130	0
54	BV	779	0	852	117	0
54	DV	779	0	852	120	0
55	BW	896	0	953	87	0
55	DW	896	0	953	86	0
56	BX	725	0	778	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DX	725	0	778	84	0
57	BY	775	0	870	162	0
57	DY	775	0	870	156	0
58	BZ	1403	0	1432	216	0
58	DZ	1403	0	1432	200	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	2	0
60	CZ	28	0	12	6	0
61	AZ	57	0	58	3	0
61	CZ	57	0	59	2	0
All	All	307322	0	208715	17683	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 34.

The worst 5 of 17683 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:DC:123:VAL:CG2	38:DC:127:LEU:HD23	1.33	1.53
38:BC:123:VAL:CG2	38:BC:127:LEU:HD23	1.33	1.51
38:DC:123:VAL:HG23	38:DC:127:LEU:CD2	1.50	1.42
38:BC:123:VAL:HG23	38:BC:127:LEU:CD2	1.50	1.41
36:DA:1899:G:N2	36:DA:1902:C:H41	1.34	1.24

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	
2	AB	232/256 (91%)	175 (75%)	39 (17%)	18 (8%)	1	6
2	CB	232/256 (91%)	173 (75%)	41 (18%)	18 (8%)	1	6
3	AC	204/239 (85%)	161 (79%)	23 (11%)	20 (10%)	1	4
3	CC	204/239 (85%)	159 (78%)	28 (14%)	17 (8%)	1	6
4	AD	206/209 (99%)	134 (65%)	46 (22%)	26 (13%)	0	1
4	CD	206/209 (99%)	133 (65%)	48 (23%)	25 (12%)	0	2
5	AE	148/162 (91%)	138 (93%)	5 (3%)	5 (3%)	5	25
5	CE	148/162 (91%)	138 (93%)	6 (4%)	4 (3%)	6	31
6	AF	99/101 (98%)	80 (81%)	12 (12%)	7 (7%)	1	8
6	CF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	8
7	AG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	2	15
7	CG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	2	15
8	AH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	65
8	CH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	65
9	AI	125/128 (98%)	85 (68%)	23 (18%)	17 (14%)	0	1
9	CI	125/128 (98%)	84 (67%)	24 (19%)	17 (14%)	0	1
10	AJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	1	4
10	CJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	1	4
11	AK	117/129 (91%)	100 (86%)	10 (8%)	7 (6%)	2	11
11	CK	117/129 (91%)	101 (86%)	9 (8%)	7 (6%)	2	11
12	AL	122/135 (90%)	94 (77%)	15 (12%)	13 (11%)	0	3
12	CL	122/135 (90%)	91 (75%)	18 (15%)	13 (11%)	0	3
13	AM	122/126 (97%)	82 (67%)	26 (21%)	14 (12%)	0	2
13	CM	122/126 (97%)	84 (69%)	24 (20%)	14 (12%)	0	2
14	AN	58/61 (95%)	41 (71%)	6 (10%)	11 (19%)	0	0
14	CN	58/61 (95%)	40 (69%)	7 (12%)	11 (19%)	0	0
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	CO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	16	52
16	AP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	5
16	CP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	9	37
17	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	9	37
18	AR	68/88 (77%)	56 (82%)	11 (16%)	1 (2%)	13	46
18	CR	68/88 (77%)	57 (84%)	10 (15%)	1 (2%)	13	46
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
20	AT	97/106 (92%)	64 (66%)	24 (25%)	9 (9%)	1	4
20	CT	97/106 (92%)	62 (64%)	26 (27%)	9 (9%)	1	4
21	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	3	17
21	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	3	17
25	AZ	381/405 (94%)	269 (71%)	82 (22%)	30 (8%)	1	6
25	CZ	381/405 (94%)	268 (70%)	83 (22%)	30 (8%)	1	6
26	B0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	4	23
26	D0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	4	23
27	B1	91/98 (93%)	70 (77%)	10 (11%)	11 (12%)	0	2
27	D1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	9
28	B2	69/72 (96%)	40 (58%)	15 (22%)	14 (20%)	0	0
28	D2	69/72 (96%)	44 (64%)	18 (26%)	7 (10%)	1	4
29	B3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	5
29	D3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	5
30	B4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	2
30	D4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	2
31	B5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
31	D5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
32	B6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
32	D6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
33	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	8	36
33	D7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	8	36
34	B8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	1	4
34	D8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	1	4
35	B9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	5
38	BC	226/229 (99%)	170 (75%)	45 (20%)	11 (5%)	3	16
38	DC	226/229 (99%)	171 (76%)	43 (19%)	12 (5%)	2	14
39	BD	273/276 (99%)	219 (80%)	31 (11%)	23 (8%)	1	6
39	DD	273/276 (99%)	217 (80%)	31 (11%)	25 (9%)	1	4
40	BE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	1
40	DE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	1
41	BF	205/210 (98%)	148 (72%)	35 (17%)	22 (11%)	0	3
41	DF	205/210 (98%)	149 (73%)	34 (17%)	22 (11%)	0	3
42	BG	179/182 (98%)	118 (66%)	33 (18%)	28 (16%)	0	0
42	DG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	0
43	BH	157/180 (87%)	93 (59%)	34 (22%)	30 (19%)	0	0
43	DH	157/180 (87%)	94 (60%)	33 (21%)	30 (19%)	0	0
46	BN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
46	DN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
47	BO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	3	16
47	DO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	3	16
48	BP	144/150 (96%)	78 (54%)	36 (25%)	30 (21%)	0	0
48	DP	144/150 (96%)	77 (54%)	37 (26%)	30 (21%)	0	0
49	BQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	4	24
49	DQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	4	24
50	BR	115/118 (98%)	83 (72%)	16 (14%)	16 (14%)	0	1
50	DR	115/118 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
51	BS	96/112 (86%)	50 (52%)	24 (25%)	22 (23%)	0	0
51	DS	96/112 (86%)	49 (51%)	23 (24%)	24 (25%)	0	0
52	BT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
52	DT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
53	BU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	2	11
53	DU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	2	11
54	BV	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	0
54	DV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BW	111/113 (98%)	87 (78%)	12 (11%)	12 (11%)	0	3
55	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	3
56	BX	90/96 (94%)	64 (71%)	20 (22%)	6 (7%)	1	9
56	DX	90/96 (94%)	65 (72%)	19 (21%)	6 (7%)	1	9
57	BY	98/110 (89%)	41 (42%)	31 (32%)	26 (26%)	0	0
57	DY	98/110 (89%)	43 (44%)	29 (30%)	26 (26%)	0	0
58	BZ	174/206 (84%)	109 (63%)	27 (16%)	38 (22%)	0	0
58	DZ	174/206 (84%)	109 (63%)	47 (27%)	18 (10%)	1	4
All	All	12256/13106 (94%)	8858 (72%)	2104 (17%)	1294 (11%)	0	3

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	190	THR
2	AB	191	ASP
2	AB	230	VAL

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	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	6	25
2	CB	202/220 (92%)	180 (89%)	22 (11%)	8	30
3	AC	160/188 (85%)	143 (89%)	17 (11%)	8	31
3	CC	160/188 (85%)	144 (90%)	16 (10%)	9	34
4	AD	180/181 (99%)	157 (87%)	23 (13%)	5	21
4	CD	180/181 (99%)	157 (87%)	23 (13%)	5	21
5	AE	115/123 (94%)	104 (90%)	11 (10%)	10	37
5	CE	115/123 (94%)	105 (91%)	10 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	90/90 (100%)	81 (90%)	9 (10%)	9	34
6	CF	90/90 (100%)	82 (91%)	8 (9%)	12	42
7	AG	126/127 (99%)	116 (92%)	10 (8%)	15	49
7	CG	126/127 (99%)	116 (92%)	10 (8%)	15	49
8	AH	119/119 (100%)	109 (92%)	10 (8%)	14	46
8	CH	119/119 (100%)	109 (92%)	10 (8%)	14	46
9	AI	98/99 (99%)	89 (91%)	9 (9%)	11	40
9	CI	98/99 (99%)	89 (91%)	9 (9%)	11	40
10	AJ	88/92 (96%)	80 (91%)	8 (9%)	12	40
10	CJ	88/92 (96%)	80 (91%)	8 (9%)	12	40
11	AK	90/99 (91%)	81 (90%)	9 (10%)	9	34
11	CK	90/99 (91%)	82 (91%)	8 (9%)	12	42
12	AL	104/111 (94%)	95 (91%)	9 (9%)	13	44
12	CL	104/111 (94%)	97 (93%)	7 (7%)	20	56
13	AM	99/101 (98%)	86 (87%)	13 (13%)	5	21
13	CM	99/101 (98%)	86 (87%)	13 (13%)	5	21
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	6
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	AO	79/80 (99%)	70 (89%)	9 (11%)	7	28
15	CO	79/80 (99%)	71 (90%)	8 (10%)	9	33
16	AP	72/74 (97%)	66 (92%)	6 (8%)	14	46
16	CP	72/74 (97%)	66 (92%)	6 (8%)	14	46
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	17	51
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	17	51
18	AR	61/77 (79%)	54 (88%)	7 (12%)	7	27
18	CR	61/77 (79%)	54 (88%)	7 (12%)	7	27
19	AS	69/80 (86%)	56 (81%)	13 (19%)	2	8
19	CS	69/80 (86%)	56 (81%)	13 (19%)	2	8
20	AT	76/82 (93%)	71 (93%)	5 (7%)	21	56
20	CT	76/82 (93%)	71 (93%)	5 (7%)	21	56
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	64
25	AZ	322/338 (95%)	299 (93%)	23 (7%)	18	54
25	CZ	322/338 (95%)	299 (93%)	23 (7%)	18	54
26	B0	66/67 (98%)	58 (88%)	8 (12%)	6	24
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	14
27	B1	78/83 (94%)	67 (86%)	11 (14%)	4	18
27	D1	78/83 (94%)	71 (91%)	7 (9%)	12	41
28	B2	66/67 (98%)	61 (92%)	5 (8%)	16	51
28	D2	66/67 (98%)	60 (91%)	6 (9%)	12	40
29	B3	51/52 (98%)	44 (86%)	7 (14%)	4	19
29	D3	51/52 (98%)	44 (86%)	7 (14%)	4	19
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	10
30	D4	39/63 (62%)	32 (82%)	7 (18%)	2	10
31	B5	51/52 (98%)	43 (84%)	8 (16%)	3	13
31	D5	51/52 (98%)	43 (84%)	8 (16%)	3	13
32	B6	49/52 (94%)	36 (74%)	13 (26%)	0	2
32	D6	49/52 (94%)	37 (76%)	12 (24%)	1	3
33	B7	41/42 (98%)	35 (85%)	6 (15%)	4	16
33	D7	41/42 (98%)	35 (85%)	6 (15%)	4	16
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	15
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	15
35	B9	34/34 (100%)	31 (91%)	3 (9%)	12	43
35	D9	34/34 (100%)	31 (91%)	3 (9%)	12	43
38	BC	180/181 (99%)	170 (94%)	10 (6%)	26	62
38	DC	180/181 (99%)	171 (95%)	9 (5%)	30	67
39	BD	217/218 (100%)	187 (86%)	30 (14%)	4	19
39	DD	217/218 (100%)	186 (86%)	31 (14%)	4	17
40	BE	165/166 (99%)	148 (90%)	17 (10%)	9	32
40	DE	165/166 (99%)	148 (90%)	17 (10%)	9	32
41	BF	165/166 (99%)	150 (91%)	15 (9%)	12	40
41	DF	165/166 (99%)	150 (91%)	15 (9%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BG	155/156 (99%)	132 (85%)	23 (15%)	4	16
42	DG	155/156 (99%)	138 (89%)	17 (11%)	8	30
43	BH	132/148 (89%)	116 (88%)	16 (12%)	6	24
43	DH	132/148 (89%)	116 (88%)	16 (12%)	6	24
46	BN	117/119 (98%)	102 (87%)	15 (13%)	5	21
46	DN	117/119 (98%)	102 (87%)	15 (13%)	5	21
47	BO	100/100 (100%)	95 (95%)	5 (5%)	30	67
47	DO	100/100 (100%)	95 (95%)	5 (5%)	30	67
48	BP	112/116 (97%)	97 (87%)	15 (13%)	5	20
48	DP	112/116 (97%)	97 (87%)	15 (13%)	5	20
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	5	20
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	22
50	BR	100/101 (99%)	89 (89%)	11 (11%)	8	30
50	DR	100/101 (99%)	90 (90%)	10 (10%)	9	34
51	BS	77/88 (88%)	68 (88%)	9 (12%)	7	26
51	DS	77/88 (88%)	68 (88%)	9 (12%)	7	26
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	8
52	DT	120/127 (94%)	98 (82%)	22 (18%)	2	9
53	BU	92/94 (98%)	83 (90%)	9 (10%)	10	36
53	DU	92/94 (98%)	84 (91%)	8 (9%)	13	44
54	BV	82/82 (100%)	66 (80%)	16 (20%)	2	7
54	DV	82/82 (100%)	66 (80%)	16 (20%)	2	7
55	BW	91/92 (99%)	86 (94%)	5 (6%)	27	63
55	DW	91/92 (99%)	86 (94%)	5 (6%)	27	63
56	BX	74/78 (95%)	64 (86%)	10 (14%)	5	20
56	DX	74/78 (95%)	64 (86%)	10 (14%)	5	20
57	BY	84/91 (92%)	70 (83%)	14 (17%)	3	11
57	DY	84/91 (92%)	70 (83%)	14 (17%)	3	11
58	BZ	155/179 (87%)	126 (81%)	29 (19%)	2	8
58	DZ	155/179 (87%)	135 (87%)	20 (13%)	5	21
All	All	10338/10860 (95%)	9176 (89%)	1162 (11%)	7	29

5 of 1162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	18	LEU
4	CD	138	TYR
52	DT	38	ASN
55	BW	82	LEU
58	BZ	127	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 301 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	94	ASN
6	CF	32	ASN
50	DR	24	GLN
55	BW	57	ASN
2	CB	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	240 (15%)	49 (3%)
1	CA	1509/1522 (99%)	234 (15%)	47 (3%)
22	AV	75/76 (98%)	19 (25%)	2 (2%)
22	AW	75/76 (98%)	17 (22%)	0
22	CV	75/76 (98%)	19 (25%)	1 (1%)
22	CW	75/76 (98%)	17 (22%)	0
23	AX	16/27 (59%)	6 (37%)	0
23	CX	16/27 (59%)	6 (37%)	0
24	AY	74/77 (96%)	25 (33%)	5 (6%)
24	CY	74/77 (96%)	25 (33%)	5 (6%)
36	BA	2900/2915 (99%)	510 (17%)	46 (1%)
36	DA	2900/2915 (99%)	508 (17%)	46 (1%)
37	BB	118/122 (96%)	25 (21%)	2 (1%)
37	DB	118/122 (96%)	25 (21%)	2 (1%)
All	All	9534/9630 (99%)	1676 (17%)	205 (2%)

5 of 1676 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G

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Mol	Chain	Res	Type
1	AA	32	A
1	AA	39	G

5 of 205 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2126	A
1	CA	250	A
36	DA	1970	A
36	BA	2282	G
1	CA	30	U

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

18 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$
24	H2U	AY	16	24	17,21,22	1.04	2 (11%)	23,30,33	1.85	4 (17%)
24	H2U	AY	17	24	17,21,22	0.97	1 (5%)	23,30,33	2.03	5 (21%)
24	H2U	AY	20	24	17,21,22	1.03	1 (5%)	23,30,33	1.93	4 (17%)
24	OMC	AY	32	24	13,22,23	0.76	0	20,31,34	1.04	2 (10%)
24	MIA	AY	37	24	21,31,32	1.25	2 (9%)	26,44,47	1.72	3 (11%)
24	7MG	AY	46	24	19,26,27	1.66	3 (15%)	24,39,42	2.29	4 (16%)
24	5MU	AY	54	24	12,22,23	1.32	3 (25%)	14,32,35	4.52	3 (21%)
24	PSU	AY	55	24	13,21,22	1.21	2 (15%)	18,30,33	3.63	5 (27%)
24	4SU	AY	8	24	11,21,22	1.52	3 (27%)	13,30,33	2.31	1 (7%)
24	H2U	CY	16	24	17,21,22	1.10	2 (11%)	23,30,33	1.85	4 (17%)
24	H2U	CY	17	24	17,21,22	0.98	1 (5%)	23,30,33	2.05	5 (21%)
24	H2U	CY	20	24	17,21,22	1.00	1 (5%)	23,30,33	1.92	4 (17%)
24	OMC	CY	32	24	13,22,23	0.73	0	20,31,34	1.02	2 (10%)
24	MIA	CY	37	24	21,31,32	1.05	1 (4%)	26,44,47	1.72	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	7MG	CY	46	24	19,26,27	1.64	3 (15%)	24,39,42	2.29	3 (12%)
24	5MU	CY	54	24	12,22,23	1.35	3 (25%)	14,32,35	4.49	3 (21%)
24	PSU	CY	55	24	13,21,22	1.21	2 (15%)	18,30,33	3.66	5 (27%)
24	4SU	CY	8	24	11,21,22	1.55	4 (36%)	13,30,33	2.30	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	20	24	-	0/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/5/27/28	0/2/2/2
24	MIA	AY	37	24	-	0/11/33/34	0/3/3/3
24	7MG	AY	46	24	-	0/7/37/38	0/3/3/3
24	5MU	AY	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AY	55	24	1/1/5/5	0/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/3/25/26	0/2/2/2
24	H2U	CY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	17	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/7/38/39	0/2/2/2
24	OMC	CY	32	24	-	0/5/27/28	0/2/2/2
24	MIA	CY	37	24	-	0/11/33/34	0/3/3/3
24	7MG	CY	46	24	-	0/7/37/38	0/3/3/3
24	5MU	CY	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CY	55	24	1/1/5/5	0/7/25/26	0/2/2/2
24	4SU	CY	8	24	-	0/3/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-4.67	1.38	1.45
24	AY	46	7MG	C8-N9	-4.67	1.38	1.45
24	AY	46	7MG	C8-N7	-2.74	1.31	1.43
24	CY	46	7MG	C8-N7	-2.72	1.31	1.43
24	AY	54	5MU	C6-C5	-2.16	1.34	1.40

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	55	PSU	N1-C2-N3	-12.54	120.33	128.33
24	AY	55	PSU	N1-C2-N3	-12.39	120.43	128.33
24	AY	54	5MU	C5-C4-N3	-8.99	115.12	125.14
24	CY	54	5MU	C5-C4-N3	-8.94	115.19	125.14
24	AY	8	4SU	C5-C4-N3	-8.16	115.63	123.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	CY	55	PSU	C3'
24	AY	55	PSU	C3'

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	16	H2U	3	0
24	AY	17	H2U	5	0
24	AY	20	H2U	2	0
24	AY	32	OMC	1	0
24	AY	37	MIA	1	0
24	AY	46	7MG	4	0
24	AY	54	5MU	1	0
24	AY	55	PSU	3	0
24	AY	8	4SU	1	0
24	CY	16	H2U	3	0
24	CY	17	H2U	5	0
24	CY	20	H2U	2	0
24	CY	32	OMC	1	0
24	CY	46	7MG	4	0
24	CY	54	5MU	1	0
24	CY	55	PSU	2	0
24	CY	8	4SU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
60	GDP	AZ	501	-	23,30,30	1.38	3 (13%)	30,47,47	1.90	8 (26%)
61	KIR	AZ	502	-	55,59,59	3.77	21 (38%)	53,84,84	1.73	11 (20%)
60	GDP	CZ	501	-	23,30,30	1.43	3 (13%)	30,47,47	1.80	7 (23%)
61	KIR	CZ	502	-	55,59,59	3.73	21 (38%)	53,84,84	1.72	12 (22%)

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
60	GDP	AZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	AZ	502	-	-	0/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	CZ	502	-	-	0/54/98/98	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.73	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.46	1.22	1.44
61	AZ	502	KIR	O30-C30	-11.91	1.17	1.42
61	CZ	502	KIR	O30-C30	-11.85	1.17	1.42
61	AZ	502	KIR	O34-C33	-11.13	1.29	1.44

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	N3-C2-N1	-5.49	119.08	127.44
61	AZ	502	KIR	O29-C29-O34	-4.80	102.25	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CZ	502	KIR	O29-C29-O34	-4.66	102.48	110.18
60	CZ	501	GDP	N3-C2-N1	-4.64	120.38	127.44
61	CZ	502	KIR	C11-C10-C9	-4.09	114.34	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	2	0
61	AZ	502	KIR	3	0
60	CZ	501	GDP	6	0
61	CZ	502	KIR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1510/1522 (99%)	0.05	32 (2%) 67 44	17, 54, 143, 200	0
1	CA	1510/1522 (99%)	-0.15	28 (1%) 70 48	26, 58, 145, 200	0
2	AB	234/256 (91%)	-0.12	2 (0%) 85 72	34, 64, 130, 141	0
2	CB	234/256 (91%)	-0.10	7 (2%) 54 29	36, 65, 130, 142	0
3	AC	206/239 (86%)	-0.29	0 100 100	27, 48, 81, 86	0
3	CC	206/239 (86%)	-0.40	0 100 100	32, 52, 82, 88	0
4	AD	208/209 (99%)	0.32	8 (3%) 44 21	55, 89, 119, 122	0
4	CD	208/209 (99%)	0.25	13 (6%) 23 9	55, 90, 119, 122	0
5	AE	150/162 (92%)	-0.41	0 100 100	23, 41, 62, 84	0
5	CE	150/162 (92%)	-0.41	0 100 100	30, 44, 64, 86	0
6	AF	101/101 (100%)	-0.23	1 (0%) 84 69	48, 72, 88, 94	0
6	CF	101/101 (100%)	0.07	1 (0%) 84 69	52, 74, 90, 95	0
7	AG	155/156 (99%)	-0.11	4 (2%) 59 35	40, 64, 100, 115	0
7	CG	155/156 (99%)	-0.08	4 (2%) 59 35	45, 67, 101, 115	0
8	AH	138/138 (100%)	-0.39	0 100 100	30, 44, 61, 71	0
8	CH	138/138 (100%)	-0.49	0 100 100	31, 47, 62, 72	0
9	AI	127/128 (99%)	0.29	2 (1%) 74 55	33, 73, 113, 120	0
9	CI	127/128 (99%)	0.37	8 (6%) 23 9	40, 77, 114, 120	0
10	AJ	98/105 (93%)	0.50	6 (6%) 25 10	41, 80, 133, 136	0
10	CJ	98/105 (93%)	0.76	17 (17%) 2 1	44, 84, 134, 137	0
11	AK	119/129 (92%)	-0.11	3 (2%) 61 37	28, 49, 80, 104	0
11	CK	119/129 (92%)	-0.15	3 (2%) 61 37	32, 53, 82, 104	0
12	AL	124/135 (91%)	0.02	2 (1%) 74 55	28, 66, 87, 125	0
12	CL	124/135 (91%)	0.13	2 (1%) 74 55	30, 67, 88, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.11	5 (4%) 42 20	50, 73, 100, 137	0
13	CM	124/126 (98%)	0.20	8 (6%) 22 8	53, 76, 101, 137	0
14	AN	60/61 (98%)	-0.02	1 (1%) 73 52	33, 48, 76, 79	0
14	CN	60/61 (98%)	-0.16	1 (1%) 73 52	39, 53, 76, 80	0
15	AO	88/89 (98%)	-0.34	0 100 100	36, 51, 73, 81	0
15	CO	88/89 (98%)	-0.20	0 100 100	37, 53, 73, 81	0
16	AP	83/88 (94%)	0.31	0 100 100	62, 78, 99, 125	0
16	CP	83/88 (94%)	0.37	3 (3%) 46 23	62, 80, 100, 124	0
17	AQ	99/105 (94%)	-0.18	0 100 100	33, 55, 72, 83	0
17	CQ	99/105 (94%)	-0.15	0 100 100	39, 56, 73, 83	0
18	AR	70/88 (79%)	-0.23	1 (1%) 78 60	37, 55, 87, 99	0
18	CR	70/88 (79%)	-0.13	2 (2%) 55 31	43, 59, 88, 99	0
19	AS	78/93 (83%)	0.41	6 (7%) 16 5	61, 81, 116, 125	0
19	CS	78/93 (83%)	0.57	6 (7%) 16 5	63, 83, 117, 125	0
20	AT	99/106 (93%)	0.23	5 (5%) 32 13	49, 77, 112, 115	0
20	CT	99/106 (93%)	0.33	4 (4%) 42 20	52, 78, 113, 115	0
21	AU	24/27 (88%)	0.35	1 (4%) 40 19	43, 55, 76, 93	0
21	CU	24/27 (88%)	0.60	3 (12%) 5 2	46, 59, 78, 92	0
22	AV	76/76 (100%)	-0.11	0 100 100	34, 64, 95, 113	0
22	AW	76/76 (100%)	0.95	14 (18%) 2 1	60, 165, 193, 200	0
22	CV	76/76 (100%)	-0.20	1 (1%) 79 62	38, 66, 97, 114	0
22	CW	76/76 (100%)	1.09	16 (21%) 1 0	63, 166, 193, 200	0
23	AX	17/27 (62%)	0.82	3 (17%) 2 1	27, 87, 137, 139	0
23	CX	17/27 (62%)	0.89	5 (29%) 1 0	32, 89, 137, 140	0
24	AY	68/77 (88%)	1.57	21 (30%) 1 0	70, 145, 175, 178	0
24	CY	68/77 (88%)	1.85	30 (44%) 0 0	72, 146, 174, 178	0
25	AZ	385/405 (95%)	0.90	56 (14%) 3 1	84, 129, 155, 177	0
25	CZ	385/405 (95%)	1.01	64 (16%) 2 1	85, 129, 155, 177	0
26	B0	84/85 (98%)	0.31	7 (8%) 14 5	47, 64, 95, 108	0
26	D0	84/85 (98%)	0.42	7 (8%) 14 5	50, 66, 95, 108	0
27	B1	93/98 (94%)	0.05	2 (2%) 65 42	38, 55, 114, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.34	5 (5%) 29 12	54, 71, 121, 129	0
28	B2	71/72 (98%)	1.40	21 (29%) 1 0	108, 136, 147, 149	0
28	D2	71/72 (98%)	0.59	4 (5%) 28 11	88, 107, 126, 142	0
29	B3	59/60 (98%)	0.25	1 (1%) 73 52	50, 71, 91, 116	0
29	D3	59/60 (98%)	0.56	3 (5%) 32 13	51, 72, 91, 116	0
30	B4	44/71 (61%)	1.03	5 (11%) 7 2	109, 148, 172, 176	0
30	D4	44/71 (61%)	0.57	4 (9%) 11 4	110, 148, 172, 176	0
31	B5	59/60 (98%)	0.13	3 (5%) 32 13	45, 71, 131, 148	0
31	D5	59/60 (98%)	0.22	4 (6%) 20 7	46, 73, 130, 148	0
32	B6	50/54 (92%)	1.08	7 (14%) 4 2	50, 80, 106, 112	0
32	D6	50/54 (92%)	0.96	8 (16%) 3 1	54, 82, 106, 114	0
33	B7	48/49 (97%)	0.09	1 (2%) 67 44	45, 53, 90, 110	0
33	D7	48/49 (97%)	-0.03	0 100 100	47, 55, 89, 110	0
34	B8	63/65 (96%)	0.32	4 (6%) 23 9	49, 63, 79, 101	0
34	D8	63/65 (96%)	0.32	4 (6%) 23 9	51, 65, 80, 101	0
35	B9	37/37 (100%)	0.40	1 (2%) 58 34	62, 75, 96, 98	0
35	D9	37/37 (100%)	0.65	2 (5%) 29 12	61, 77, 96, 98	0
36	BA	2901/2915 (99%)	0.15	118 (4%) 41 19	21, 65, 173, 200	0
36	DA	2901/2915 (99%)	0.08	112 (3%) 43 21	26, 67, 173, 200	0
37	BB	119/122 (97%)	-0.14	0 100 100	52, 81, 104, 123	0
37	DB	119/122 (97%)	-0.25	0 100 100	55, 82, 104, 123	0
38	BC	228/229 (99%)	0.24	13 (5%) 27 11	47, 78, 152, 166	0
38	DC	228/229 (99%)	0.67	29 (12%) 5 2	51, 80, 152, 167	0
39	BD	275/276 (99%)	-0.26	3 (1%) 82 66	27, 44, 71, 96	0
39	DD	275/276 (99%)	-0.28	3 (1%) 82 66	29, 46, 71, 96	0
40	BE	204/206 (99%)	0.16	9 (4%) 38 17	40, 65, 114, 124	0
40	DE	204/206 (99%)	0.14	8 (3%) 43 21	41, 65, 114, 124	0
41	BF	207/210 (98%)	0.34	13 (6%) 23 9	45, 96, 152, 159	0
41	DF	207/210 (98%)	0.43	18 (8%) 13 4	45, 97, 152, 159	0
42	BG	181/182 (99%)	-0.07	6 (3%) 50 26	50, 73, 111, 132	0
42	DG	181/182 (99%)	0.24	8 (4%) 38 17	78, 100, 124, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	1.07	24 (15%) 3 1	84, 119, 144, 150	0
43	DH	159/180 (88%)	0.99	23 (14%) 3 1	83, 119, 144, 151	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.06	1 (0%) 89 78	51, 74, 118, 123	0
46	DN	138/140 (98%)	0.06	1 (0%) 89 78	51, 75, 118, 123	0
47	BO	122/122 (100%)	-0.31	0 100 100	35, 49, 62, 66	0
47	DO	122/122 (100%)	-0.38	0 100 100	35, 50, 62, 65	0
48	BP	146/150 (97%)	0.77	12 (8%) 14 5	47, 93, 118, 139	0
48	DP	146/150 (97%)	0.87	19 (13%) 5 2	49, 95, 118, 139	0
49	BQ	141/141 (100%)	-0.06	2 (1%) 78 60	35, 54, 75, 117	0
49	DQ	141/141 (100%)	-0.07	2 (1%) 78 60	39, 54, 76, 117	0
50	BR	117/118 (99%)	0.16	1 (0%) 85 72	51, 70, 88, 93	0
50	DR	117/118 (99%)	0.15	4 (3%) 49 24	52, 71, 89, 93	0
51	BS	98/112 (87%)	0.40	3 (3%) 52 28	69, 89, 114, 118	0
51	DS	98/112 (87%)	0.76	12 (12%) 5 2	71, 90, 114, 117	0
52	BT	137/146 (93%)	0.23	10 (7%) 18 6	50, 71, 133, 164	0
52	DT	137/146 (93%)	0.20	10 (7%) 18 6	51, 72, 134, 164	0
53	BU	117/118 (99%)	0.02	1 (0%) 85 72	51, 68, 90, 112	0
53	DU	117/118 (99%)	-0.04	1 (0%) 85 72	52, 69, 89, 112	0
54	BV	101/101 (100%)	0.39	5 (4%) 32 13	52, 98, 113, 116	0
54	DV	101/101 (100%)	0.44	7 (6%) 20 7	52, 98, 113, 116	0
55	BW	113/113 (100%)	0.07	2 (1%) 71 50	56, 71, 102, 133	0
55	DW	113/113 (100%)	0.22	2 (1%) 71 50	56, 72, 103, 134	0
56	BX	92/96 (95%)	0.31	1 (1%) 82 66	64, 83, 101, 111	0
56	DX	92/96 (95%)	0.26	2 (2%) 65 42	65, 84, 102, 112	0
57	BY	100/110 (90%)	1.41	23 (23%) 1 0	93, 114, 151, 160	0
57	DY	100/110 (90%)	1.56	32 (32%) 1 0	93, 114, 151, 160	0
58	BZ	176/206 (85%)	0.08	5 (2%) 56 32	44, 71, 117, 123	0
58	DZ	176/206 (85%)	0.20	5 (2%) 56 32	56, 78, 111, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21994/23376 (94%)	0.16	1042 (4%) 35 16	17, 69, 146, 200	0

The worst 5 of 1042 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	2802	G	12.4
49	DQ	141	GLN	11.2
58	DZ	113	ALA	11.1
36	DA	2802	G	10.6
42	DG	2	PRO	9.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
24	5MU	CY	54	21/22	0.80	0.39	-	144,149,151,153	0
24	MIA	AY	37	29/30	0.90	0.32	-	71,88,103,104	0
24	7MG	CY	46	24/25	0.50	0.47	-	170,172,175,176	0
24	4SU	AY	8	20/21	0.62	0.34	-	145,147,149,149	0
24	OMC	CY	32	21/22	0.82	0.50	-	107,112,121,122	0
24	PSU	CY	55	20/21	0.71	0.43	-	154,160,160,160	0
24	7MG	AY	46	24/25	0.59	0.38	-	170,172,175,176	0
24	H2U	CY	20	20/21	0.59	0.44	-	178,179,179,180	0
24	5MU	AY	54	21/22	0.78	0.32	-	145,149,150,153	0
24	MIA	CY	37	29/30	0.93	0.25	-	74,88,101,102	0
24	H2U	AY	20	20/21	0.71	0.51	-	178,179,179,179	0
24	H2U	CY	16	20/21	0.53	0.58	-	170,173,173,174	0
24	H2U	AY	17	20/21	0.67	0.63	-	170,174,175,176	0
24	OMC	AY	32	21/22	0.90	0.31	-	107,112,120,121	0
24	PSU	AY	55	20/21	0.74	0.39	-	154,159,160,161	0
24	H2U	CY	17	20/21	0.64	0.52	-	170,173,175,176	0
24	H2U	AY	16	20/21	0.54	0.59	-	169,173,173,174	0
24	4SU	CY	8	20/21	0.74	0.35	-	146,147,148,149	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
61	KIR	CZ	502	57/57	0.84	0.35	0.28	118,120,121,123	0
59	ZN	CD	301	1/1	1.00	0.26	0.20	72,72,72,72	0
61	KIR	AZ	502	57/57	0.85	0.31	0.02	117,119,121,122	0
60	GDP	AZ	501	28/28	0.78	0.31	-0.04	130,136,140,141	0
59	ZN	CN	101	1/1	0.99	0.17	-0.10	60,60,60,60	0
59	ZN	AD	301	1/1	0.99	0.25	-0.48	59,59,59,59	0
60	GDP	CZ	501	28/28	0.86	0.17	-1.10	129,136,140,140	0
59	ZN	D4	101	1/1	0.94	0.10	-1.16	115,115,115,115	0
59	ZN	B4	101	1/1	0.97	0.17	-1.22	90,90,90,90	0
59	ZN	B9	101	1/1	0.99	0.11	-1.33	82,82,82,82	0
59	ZN	AN	101	1/1	1.00	0.16	-1.39	34,34,34,34	0
59	ZN	D9	101	1/1	0.97	0.11	-1.56	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.