



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:59 pm BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

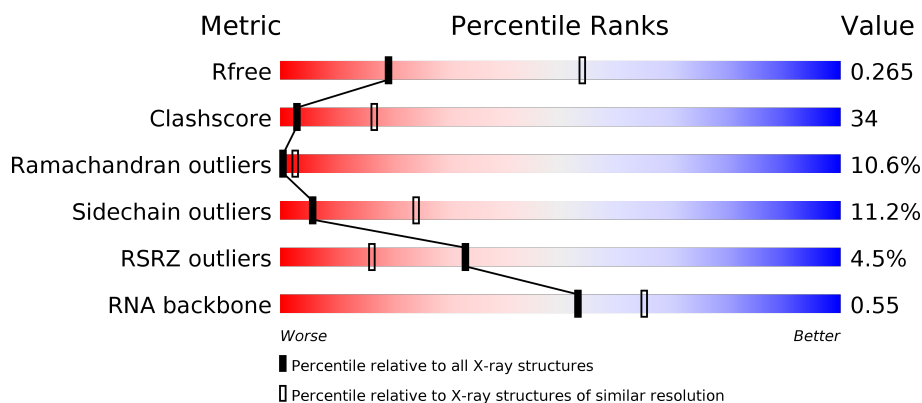
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






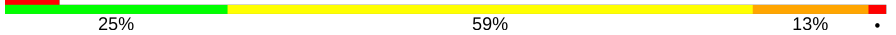
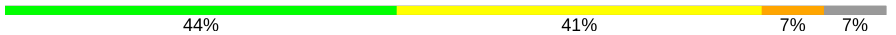
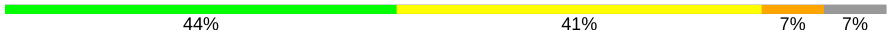
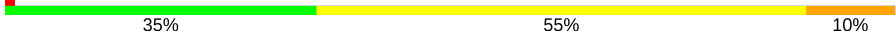
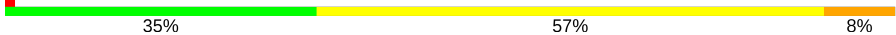
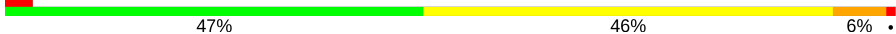



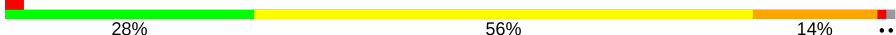

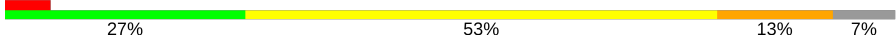
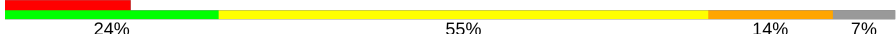



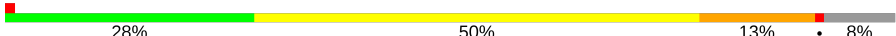





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	


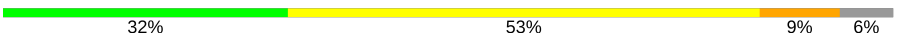
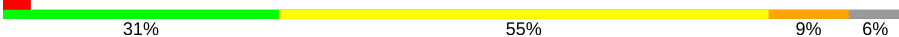


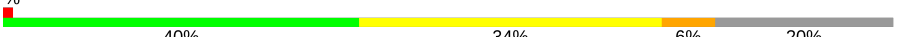
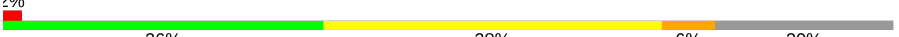
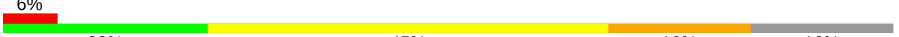
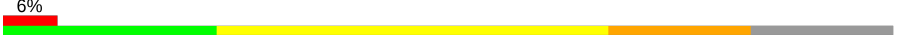

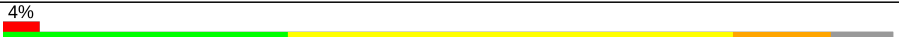


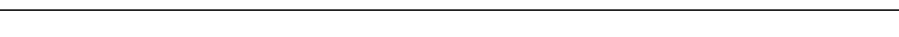






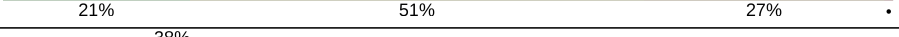

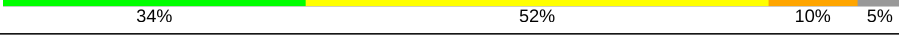


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
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	H2U	AY	16	-	-	-	X
24	H2U	AY	17	-	-	-	X
24	H2U	AY	20	-	-	-	X
24	PSU	AY	55	X	-	-	-
24	H2U	CY	16	-	-	-	X
24	H2U	CY	17	-	-	-	X
24	H2U	CY	20	-	-	-	X
24	7MG	CY	46	-	-	-	X
24	PSU	CY	55	X	-	-	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).

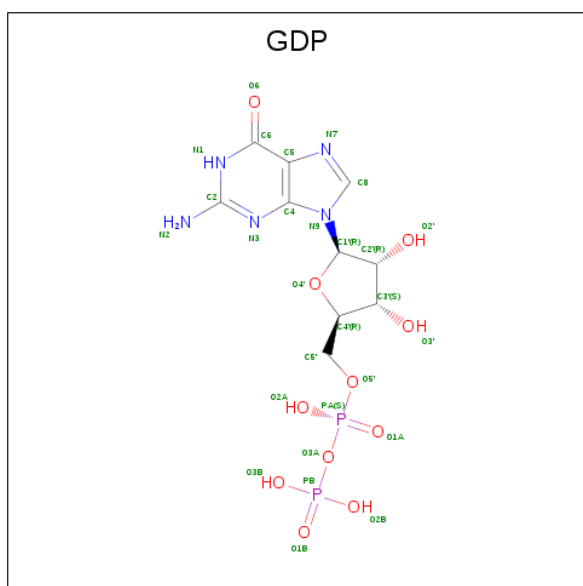
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

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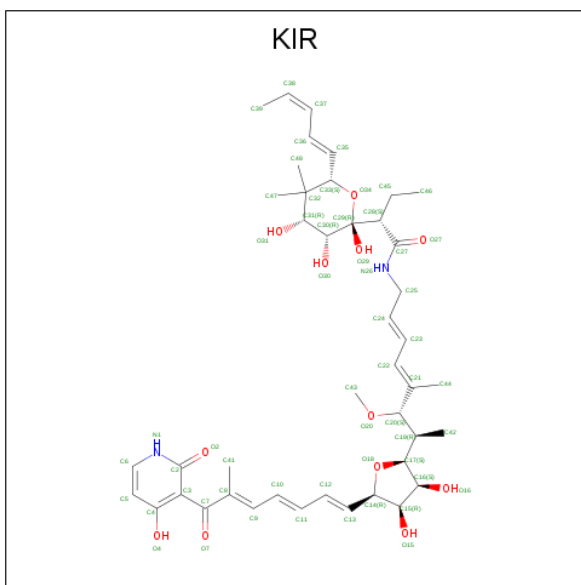
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- 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
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula:  $C_{43}H_{60}N_2O_{12}$ ).

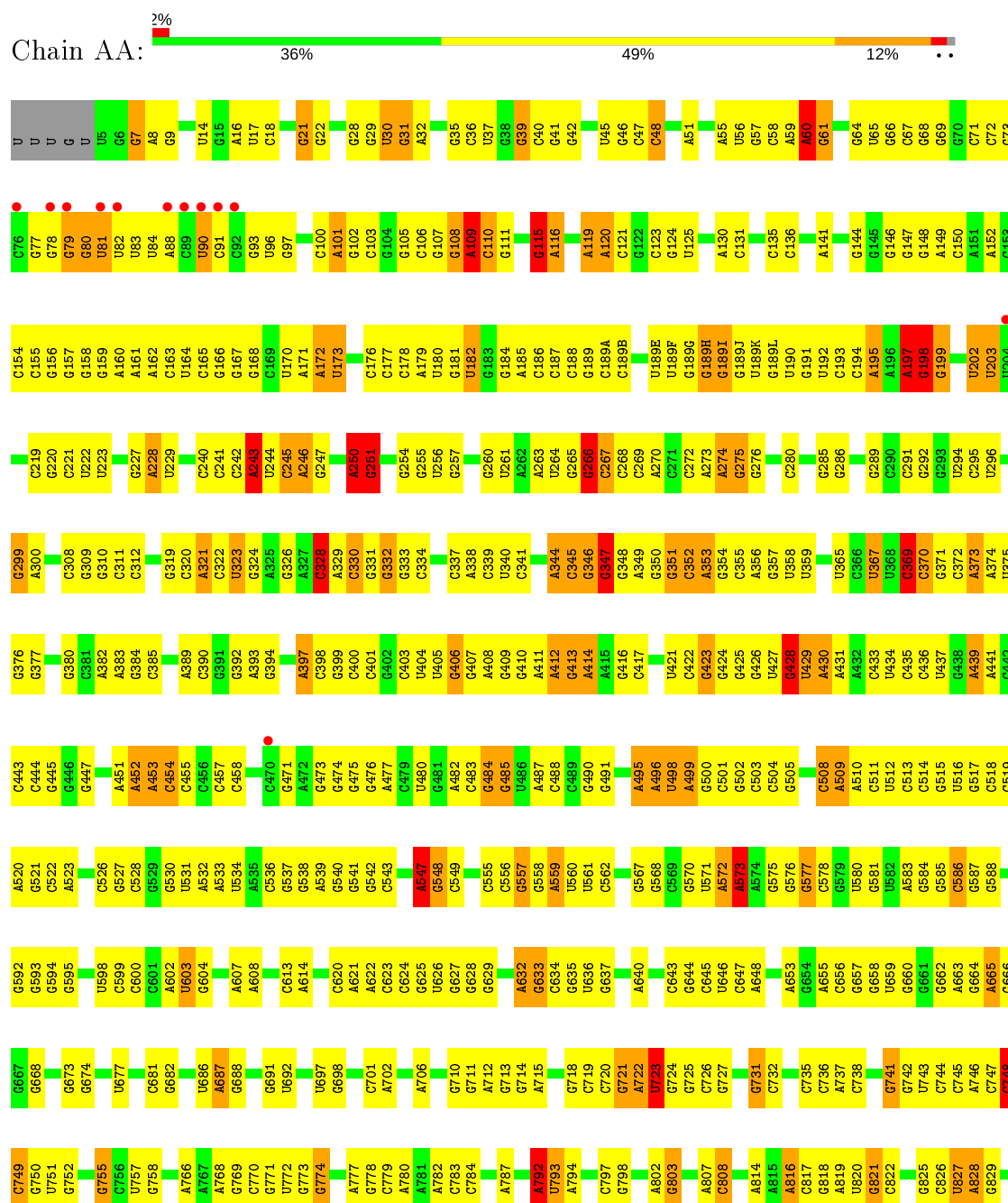


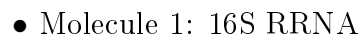
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total 57	C 43	N 2	O 12	0	0
61	CZ	1	Total 57	C 43	N 2	O 12	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

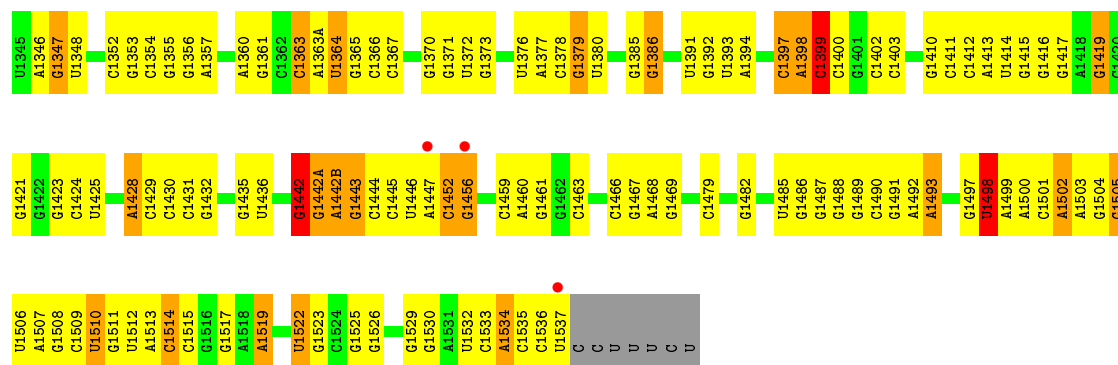
#### • Molecule 1: 16S rRNA



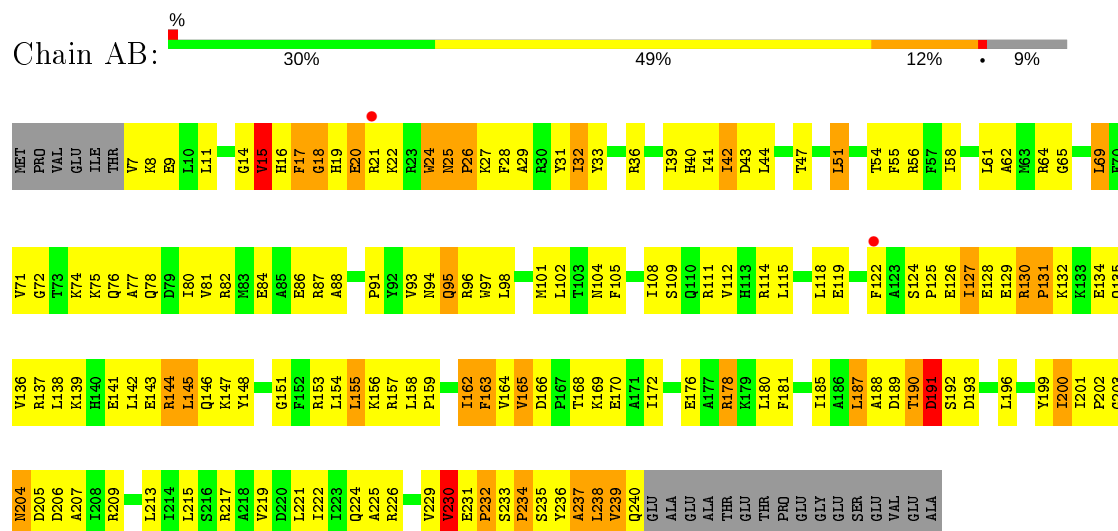


A1275	A1204	A983	A913	A819	C738	G661	G584	G515	C436	G370	G297	U204
G1276	U1205	C984	A914	U820	G741	G663	G585	U516	U437	G371	A298	C219
G1277	G1057	U991	A918	G921	G742	A663	G586	G517	A438	C372	G299	C219
U1211	G1058	U991	A918	C922	G743	G664	G587	G518	A439	A373	A300	G220
U1212	C1059	G992	A919	G825	U743	A665	G588	C519	A441	A374	G301	G221
U1213	C1060	U993	U920	G826	G744	G666	G589	A520	C442	U375	G302	U222
U1281	G1061	A994	A923	C926	G745	G667	G592	G521	C443	G376	C308	U223
C1282	U1062	C995	A924	U827	G746	G668	G593	C522	C444	G377	G309	G227
G1283	C1063	A996	C924	A928	G747	G669	G594	C523	C445	G311	A228	A228
G1284	U1064	U997	G925	G829	C748	G670	G595	A523	U446	C312	U229	U229
G1285	G1065	A1001	G926	U833	C749	G671	U598	C526	U447	C381	C240	C240
A1286	C1066	G1002	G927	C934	U751	U677	C599	G528	A451	A382	C241	C241
A1287	G1068	G1003	G933	U835	G756	G681	G600	G529	A452	A383	C242	C242
A1288	U1072	A1005	A935	G836	C757	G682	G601	G530	A453	C320	A243	A243
A1289	U1073	U1006	A936	G837	U757	G683	A602	U531	C454	A321	U244	U244
C1296	U1074	C1007	A937	U839	G758	U686	G603	A532	C455	C322	C245	C245
A1299	G1077	C1008	A938	C840	U766	A687	G604	U534	C456	A390	A246	A246
G1300	U1078	U1009	G939	U841	A767	G688	A607	A535	C457	G391	G247	G247
U1301	U1079	C940	C941	U842	G769	G689	A608	C536	U471	A392	A250	A250
U1302	A1080	G941	G942	C949	C770	U692	G613	G537	A472	C328	G251	G251
C1303	G1081	G942	G943	G853	U771	U693	A614	G538	G473	A329	G254	G254
U1234	U1086	G945	G946	G854	U772	G698	A621	A539	G474	C330	G255	G255
U1235	G1087	A947	A948	G855	U773	G699	A622	G540	G475	C331	U256	U256
A1236	U1088	G949	C949	U858	G774	G701	A623	G541	G476	C400	U257	U257
C1237	U1089	C950	G951	G859	G775	A702	G624	G542	G477	C401	G333	G333
U1307	U1090	U950	U951	A860	C776	A703	G625	U551	C479	G402	C334	C334
A1238	U1091	G952	U952	G861	U777	A704	G626	U552	U480	G403	G260	G260
A1239	U1092	U953	U953	G862	C778	A705	U626	C549	A481	U404	U261	U261
U1240	U1093	U954	U954	C863	U779	A706	U627	C550	A482	A405	A262	A262
G1241	U1094	U955	U955	G864	C780	A707	G628	U553	A483	C339	A263	A263
C1242	U1095	U956	U956	G865	U781	A708	U629	U554	A484	G407	U264	U264
C1243	U1096	U957	U957	C866	U782	A709	G632	U555	A485	A408	G265	G265
C1244	U1097	U958	U958	G867	C783	G710	A632	U556	U486	G409	G266	G266
A1245	A1101	U959	U959	U870	U784	G711	G633	C555	U487	G410	C267	C267
C1246	A1102	U960	U960	U871	C785	A712	G634	C556	A488	G411	C268	C268
U1247	C1103	U961	U961	G878	U786	A713	U635	C557	C489	A412	C269	C269
A1250	G1104	U962	U962	U879	U787	G714	U636	C558	C490	G413	A270	A270
A1251	U1105	U963	U963	C882	U792	A715	U637	A559	C491	A414	C271	C271
A1252	G1106	U964	U964	C883	U793	A716	U638	U560	U491	A415	A349	A349
C1320	C1107	U965	U965	U884	U794	G717	U639	U561	A495	G416	A273	A273
C1321	G1108	U966	U966	G885	C795	A718	U640	C562	A496	C417	A274	A274
G1255	C1109	U967	U967	U886	U796	G719	U641	C563	U497	C351	G275	G275
A1256	A1110	U968	U968	G887	G797	C720	U642	C564	U498	C352	G276	G276
U1257	C1116	A965	A965	G894	G798	G721	U643	C565	A499	U421	C280	C280
G1258	G1117	A966	A966	G895	A802	A722	G644	C566	C500	C422	G289	G289
C1259	C1118	A967	A967	C896	G803	U723	U645	C567	C501	G423	C291	C291
C1260	C1119	U968	U968	C897	U804	G724	U646	C568	G502	G424	G292	G292
A1261	C1120	C969	C969	C898	U805	G725	U647	C569	C503	G425	G293	G293
C1262	U1121	C970	C970	C899	A807	G726	U648	C570	C504	G426	U294	U294
C1263	U1122	G971	G971	C900	C808	G727	U649	C571	C505	U427	C295	C295
G1264	U1123	A972	A972	A901	C809	G728	U650	C572	U499	G428	G296	G296
G1265	G1124	A973	A973	G902	C810	A729	U651	C573	C506	A430	G297	G297
C1266	U1125	A974	A974	G903	C811	G730	U652	C574	A509	A431	G298	G298
C1267	U1126	A975	A975	G904	C812	A731	U653	C575	A510	A432	U299	U299
A1268	U1127	A976	A976	G905	U806	G732	U654	C576	A511	G433	C369	C369
A1269	U1128	A977	A977	G906	A814	A733	U655	C577	A512	U434	U296	U296
C1270	G1129	A978	A978	G907	A815	G734	U656	C578	C511	C435	U297	U297
G1271	C1130	C979	C979	A908	A816	G735	U657	C579	U512	U436	U298	U298
A1272	U1131	C980	C980	C910	A817	C736	U658	C580	C513	U437	U299	U299
C1273	U1132	U981	U981	C911	C817	C737	U659	C581	C514	C436	U296	U296
U1274	G1133	U982	U982	C912	G818	A737	U660	C582	C515	C437	U297	U297
G1131	C1132	A983	A983	U983	G819	A738	U661	C583	C516	C438	U298	U298
C1132	G1133	C984	C984	U984	G820	A739	U662	C584	C517	C439	U299	U299
G1133	G1134	U985	U985	U985	G821	A740	U663	C585	C518	C440	U296	U296
U1135	U1135	U986	U986	U986	G822	A741	U664	C586	C519	C441	U297	U297
U1136	U1136	U987	U987	U987	G823	A742	U665	C587	C520	C442	U298	U298
C1137	U1137	U988	U988	U988	G824	A743	U666	C588	C521	C443	U299	U299
G1138	G1138	U989	U989	U989	G825	A744	U667	C589	C522	C444	U296	U296
C1139	C1139	U990	U990	U990	G826	A745	U668	C590	C523	C445	U297	U297
C1140	U1140	U991	U991	U991	G827	A746	U669	C591	C524	C446	U298	U298
C1141	G1141	U992	U992	U992	G828	A747	U670	C592	C525	C447	U299	U299
G1142	U1142	U993	U993	U993	G829	A748	U671	C593	C526	C448	U296	U296
C1143	G1143	U994	U994	U994	G830	A749	U672	C594	C527	C449	U297	U297
G1144	G1144	U995	U995	U995	G831	A750	U673	C595	C528	C450	U298	U298
C1145	U1145	U996	U996	U996	G832	A751	U674	C596	C529	C451	U299	U299
A1146	A1146	U997	U997	U997	G833	A752	U675	C597	C530	C452	U296	U296
C1147	C1147	U998	U998	U998	G834	A753	U676	C598	C531	C453	U297	U297
U1148	U1148	U999	U999	U999	G835	A754	U677	C599	C532	C454	U298	U298
C1149	C1149	U1000	U1000	U1000	G836	A755	U678	C600	C533	C455	U299	U299
U1150	U1150	U1001	U1001	U1001	G837	A756	U679	C601	C534	C456	U296	U296
A1151	A1151	U1002	U1002	U1002	G838	A757	U680	C602	C535	C457	U297	U297
C1152	C1152	U1003	U1003	U1003	G839	A758	U681	C603	C536	C458	U298	U298
G1153	G1153	U1004	U1004	U1004	G840	A759	U682	C604	C537	C459	U299	U299
C1154	U1154	U1005	U1005	U1005	G841	A760	U683	C605	C538	C460	U296	U296
A1155	A1155	U1006	U1006	U1006	G842	A761	U684	C606	C539	C461	U297	U297
C1156	C1156	U1007	U1007	U1007	G843	A762	U685	C607	C540	C462	U298	U298
G1157	G1157	U1008	U1008	U1008	G844	A763	U686	C608	C541	C463	U299	U299
U1158	U1158	U1009	U1009	U1009	G845	A764	U687	C609	C542	C464	U296	U296
C1159	C1159	U1010	U1010	U1010	G846	A765	U688	C610	C543	C465	U297	U297
A1160	A1160	U1011	U1011	U1011	G847	A766	U689	C611	C544	C466	U298	U298
C1161	C1161	U1012	U1012	U1012	G848	A767	U690	C612	C545	C467	U299	U299
U1162	U1162	U1013	U1013	U1013	G849	A768	U691	C613	C546	C468	U296	U296
C1163	C1163	U1014	U1014	U1014	G850	A769	U692	C614	C547	C469	U297	U297
A1164	A1164	U1015	U1015	U1015	G851	A770	U693	C615	C548	C470	U298	U298
G1165	G1165	U1016	U1016	U1016	G852	A771	U694	C616	C549	C471	U299	U299
C1166	C1166	U1017	U1017	U1017	G853	A772	U695	C617	C550	C472	U296	U296
U1167	U1167	U1018	U1018	U1018	G854	A773	U696	C618	C551	C473	U297	U297
C1168	C1168	U1019	U1019	U1019	G855	A774	U697	C619	C552	C474	U298	U298
A1169	A1169	U1020	U1020	U1020	G856	A775	U698	C620	C553	C475	U299	U299
C1170	C1170	U1021	U1021	U1021	G857	A776	U699	C621	C554	C476	U296	U296
U1171	U1171	U1022	U1022	U1022	G858	A777	U700	C622	C555	C477	U297	U297
C1172	C1172	U1023	U1023	U1023	G859	A778	U701	C623	C556	C478	U298	U298
G1173	G1173	U1024	U1024	U1024	G860	A779	U702	C624	C557	C479	U299	U299
C1174	C1174	U1025	U1025	U1025	G861	A780	U703	C625	C558	C480	U296	U296
G1175	G1175	U1026	U1026	U1026	G862	A781	U704	C626	C559	C481	U297	U297
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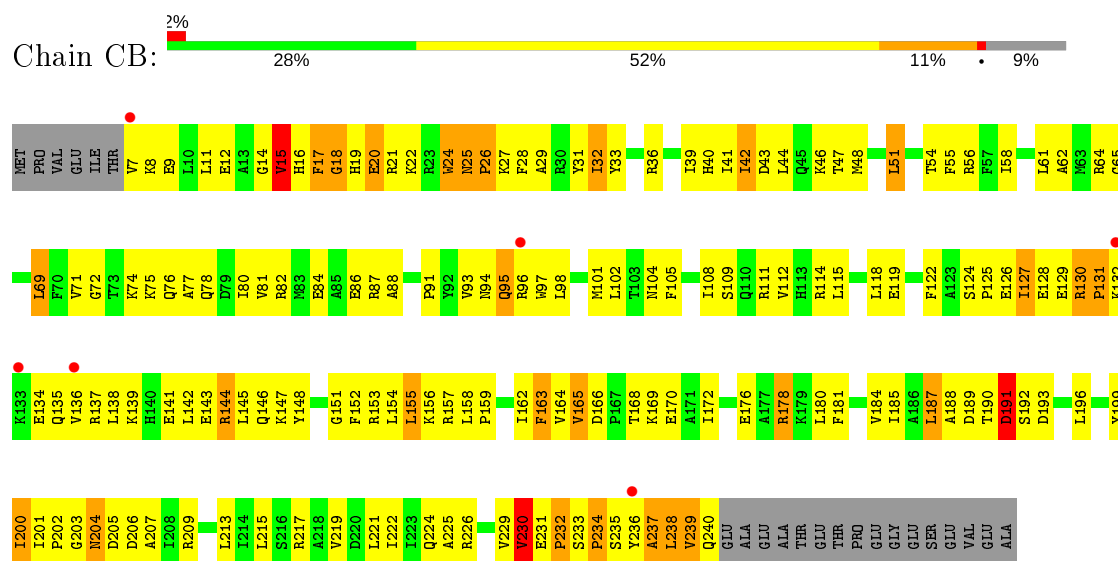




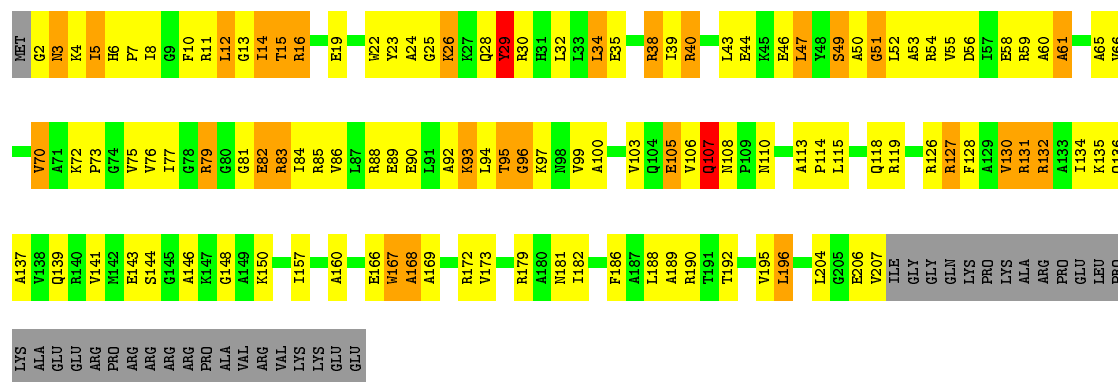
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

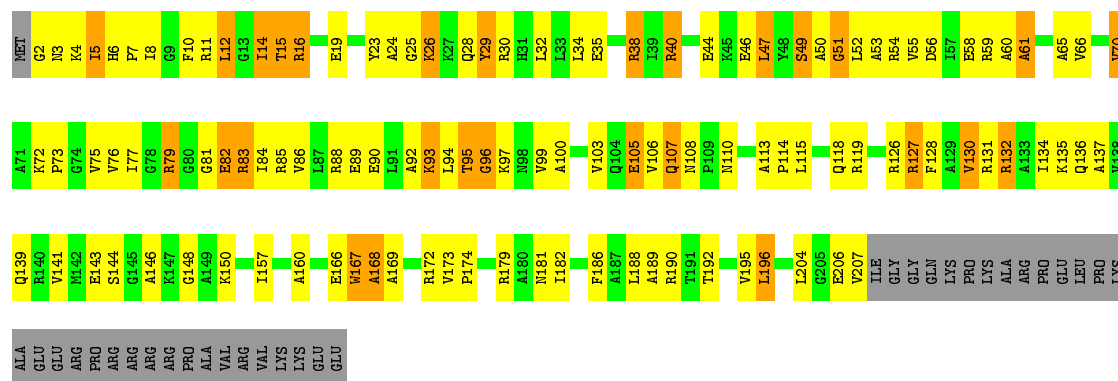


### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



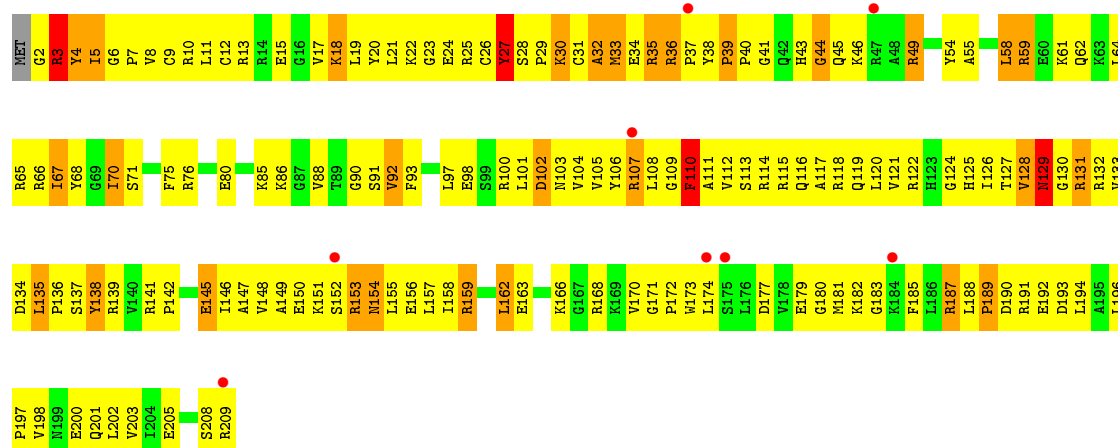
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 37% 37% 12% 14%



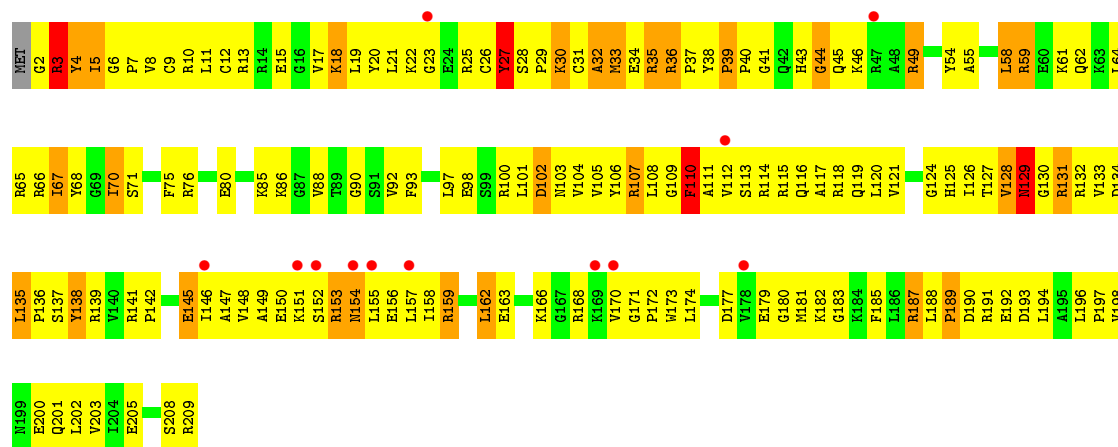
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 4% 24% 60% 14%



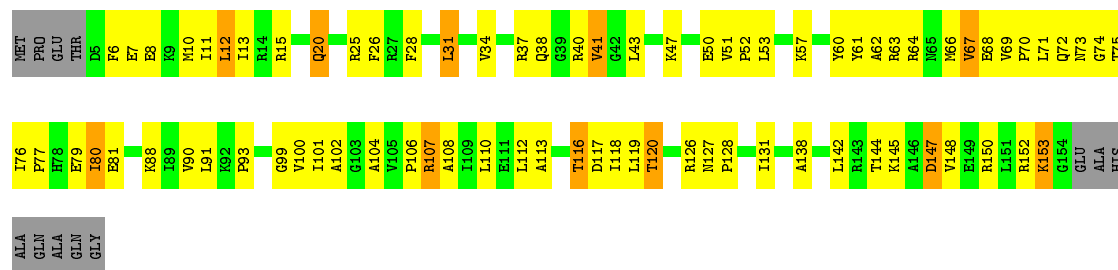
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD: 6% 25% 59% 13%



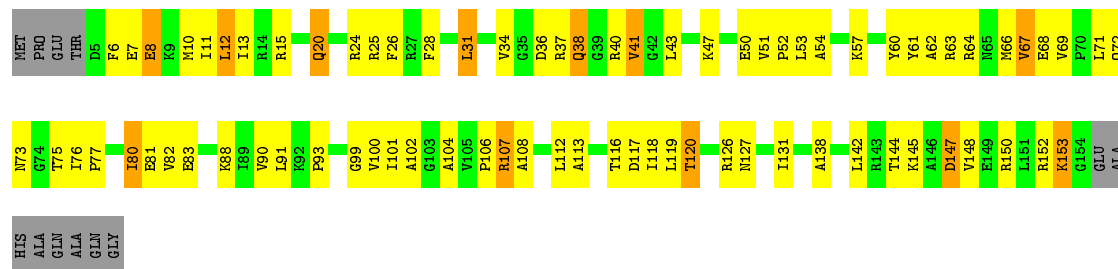
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 44% 41% 7% 7%



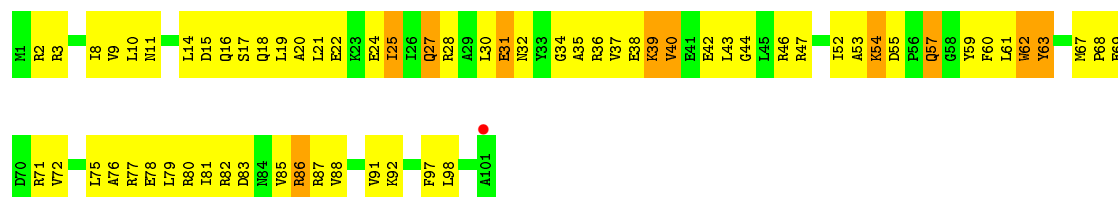
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE: 44% 41% 7% 7%

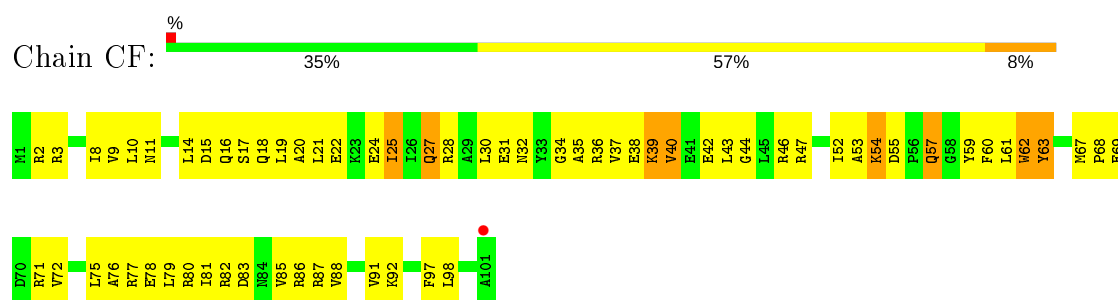


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

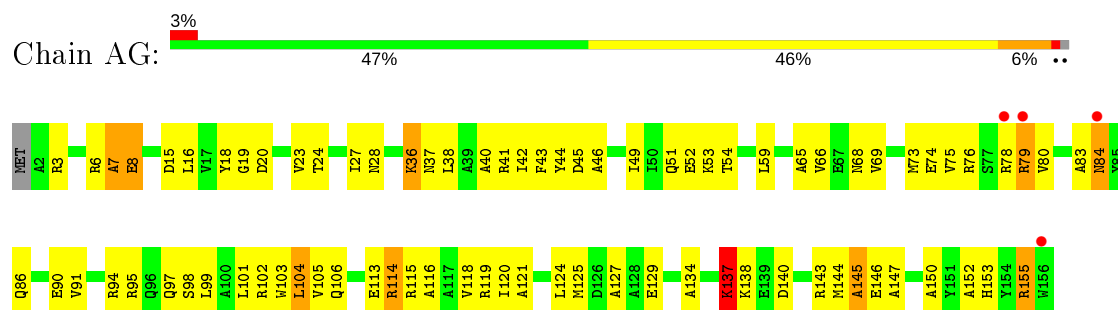
Chain AF: 35% 55% 10%



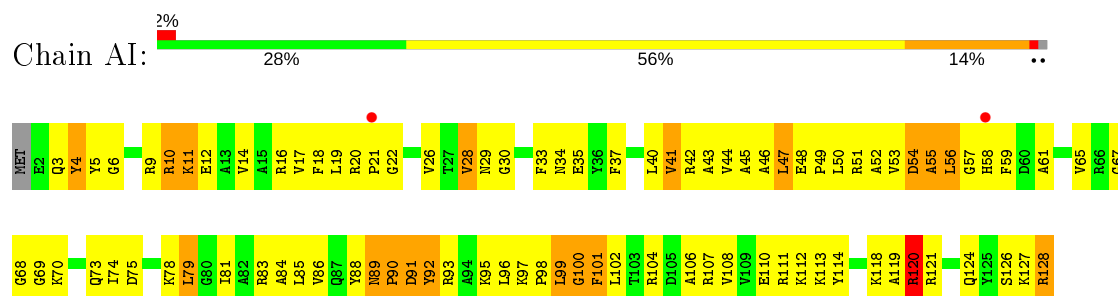
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



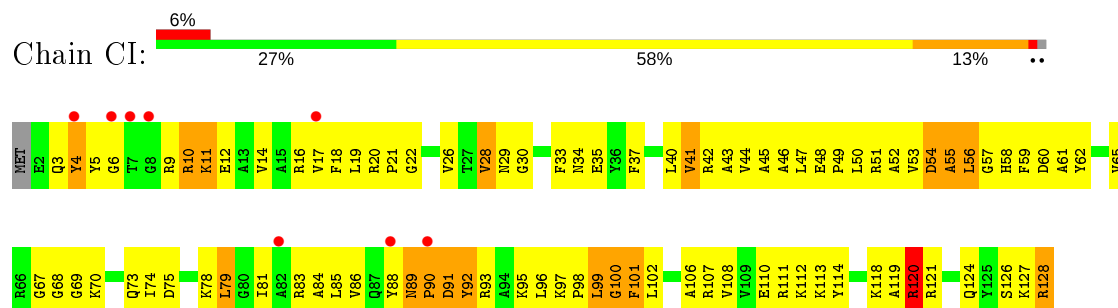
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



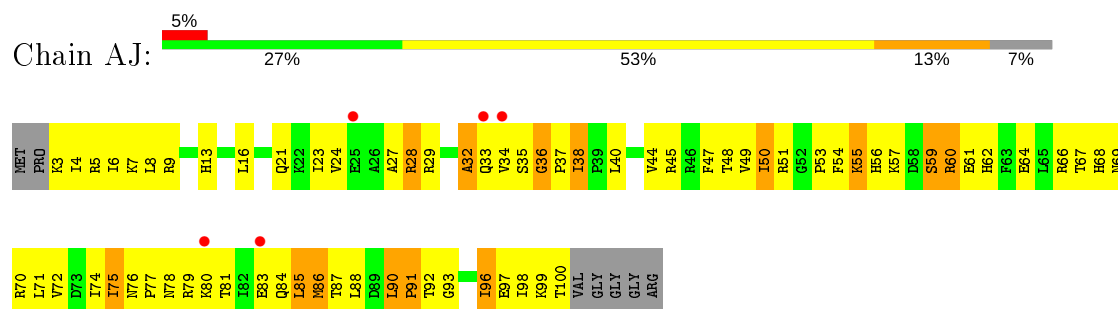
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



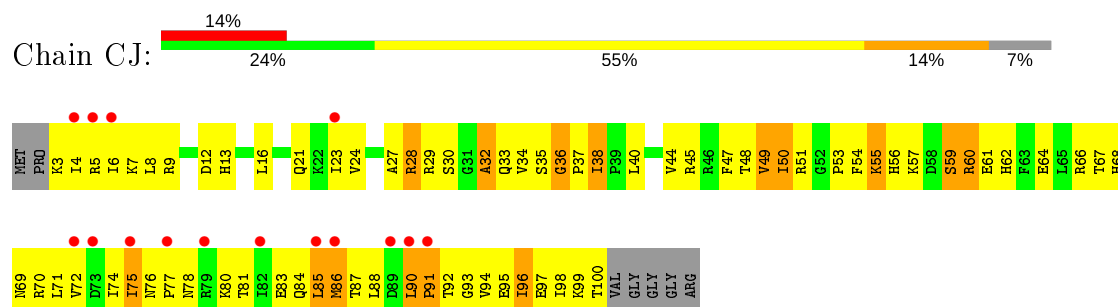
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



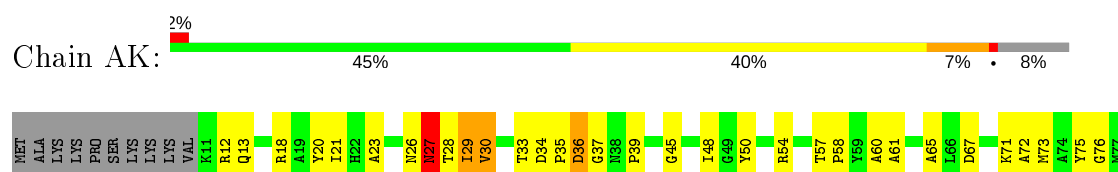
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

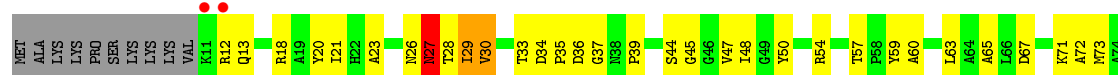


- Molecule 11: 30S RIBOSOMAL PROTEIN S11





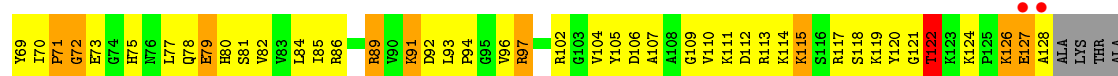
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



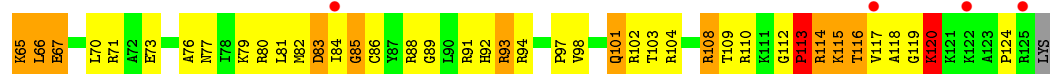
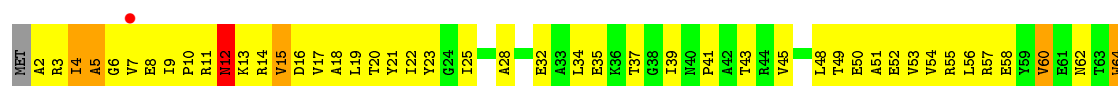
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



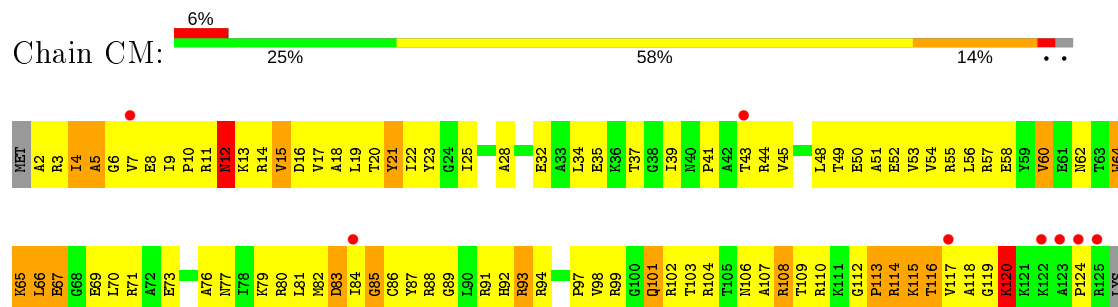
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



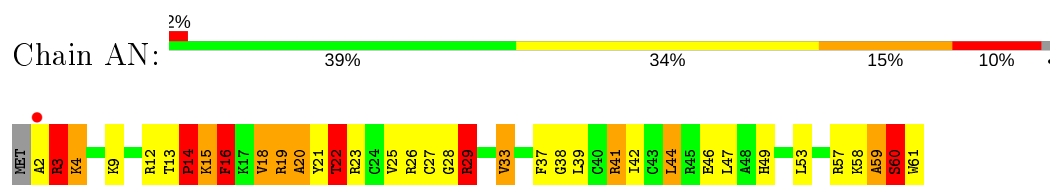
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



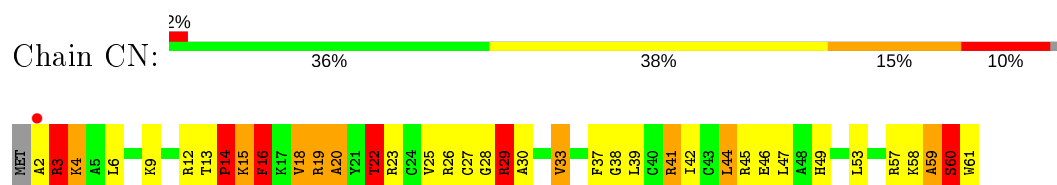
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



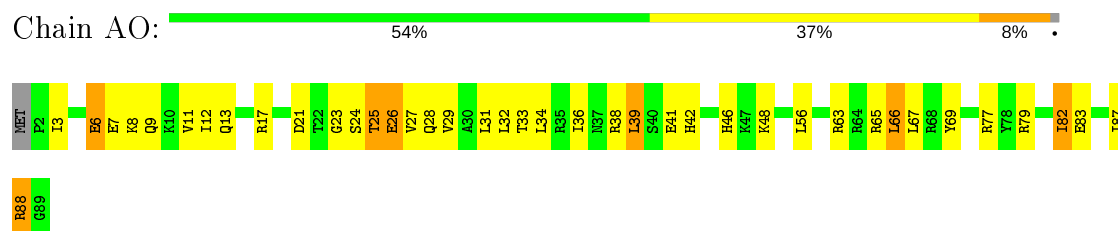
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



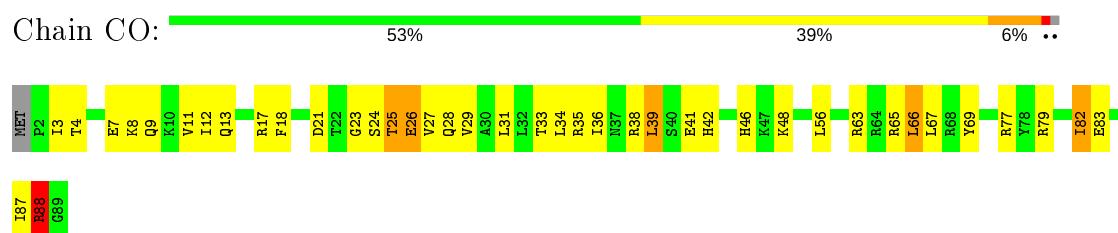
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



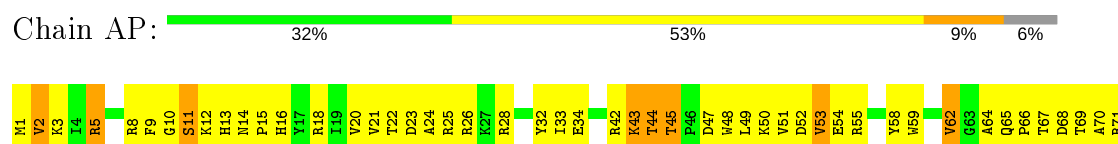
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

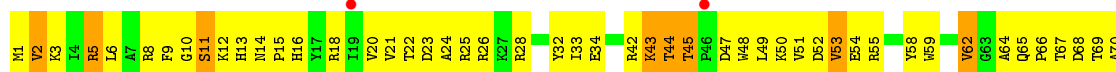


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

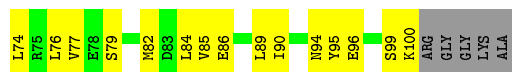
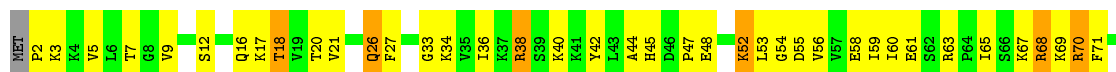




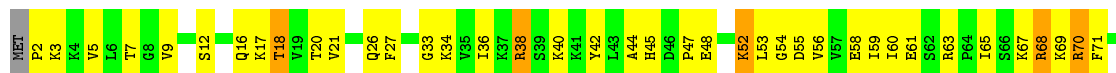
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



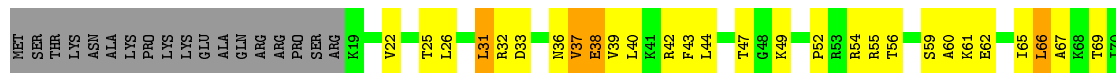
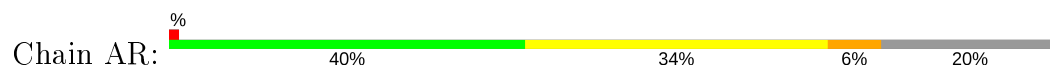
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

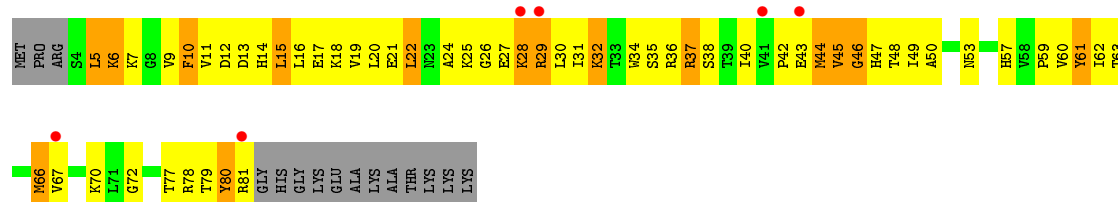


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

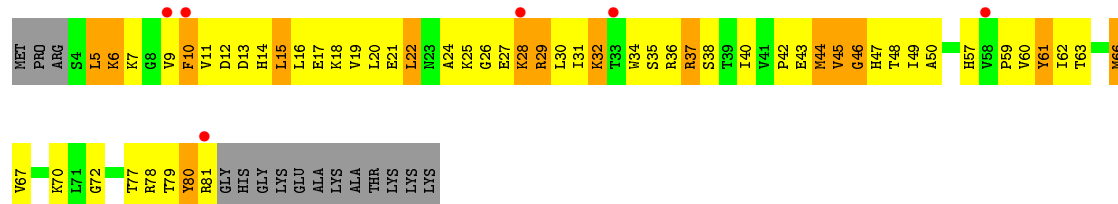




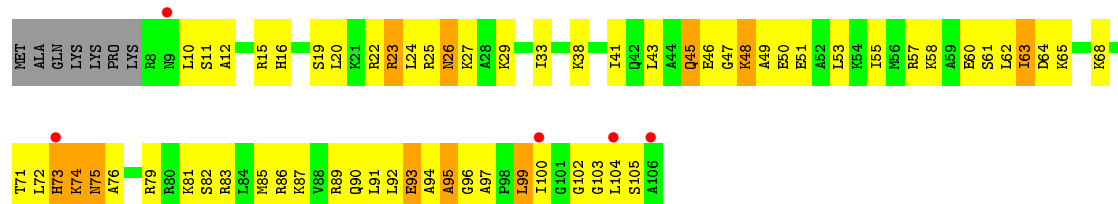
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



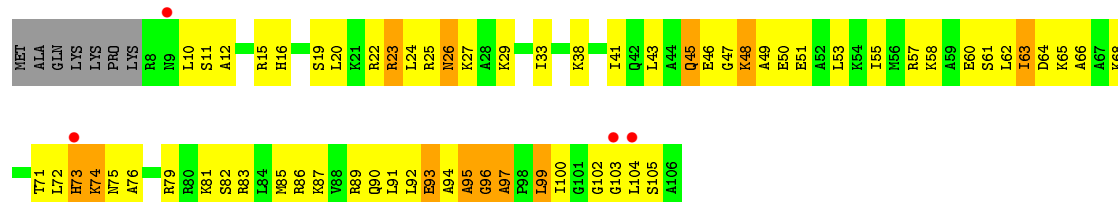
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



● Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



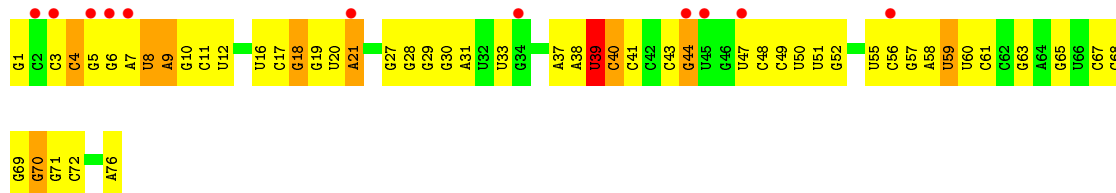
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



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



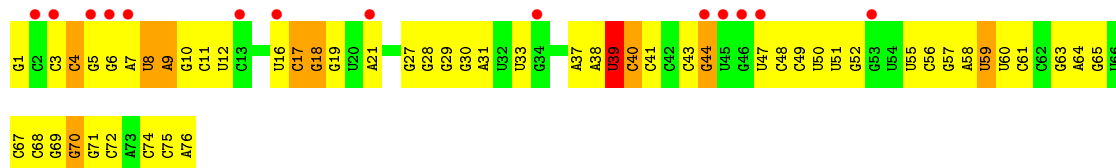
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



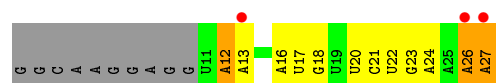
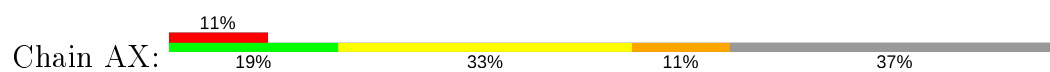
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



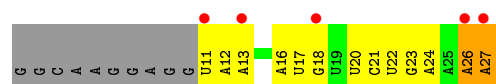
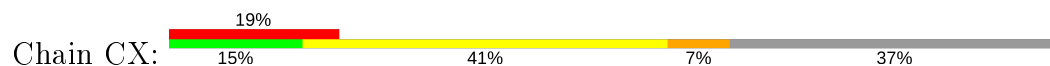
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



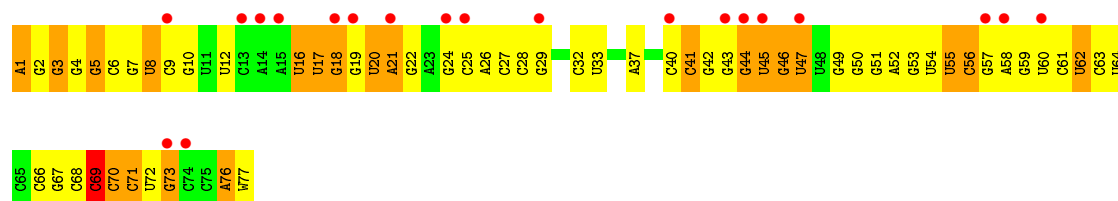
- Molecule 23: MRNA



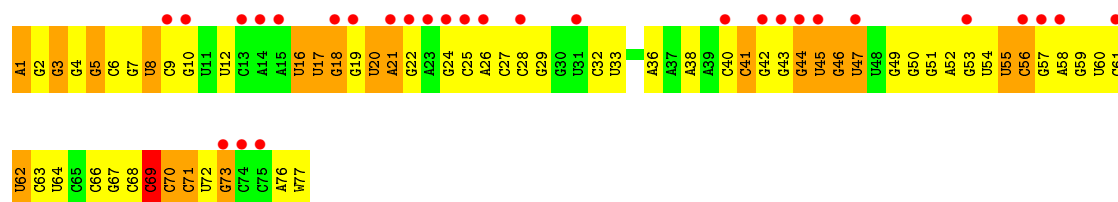
• Molecule 23: MRNA



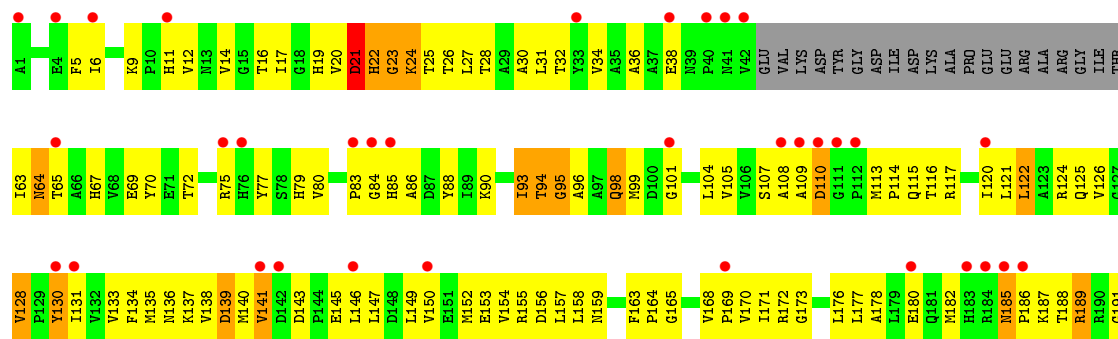
• Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

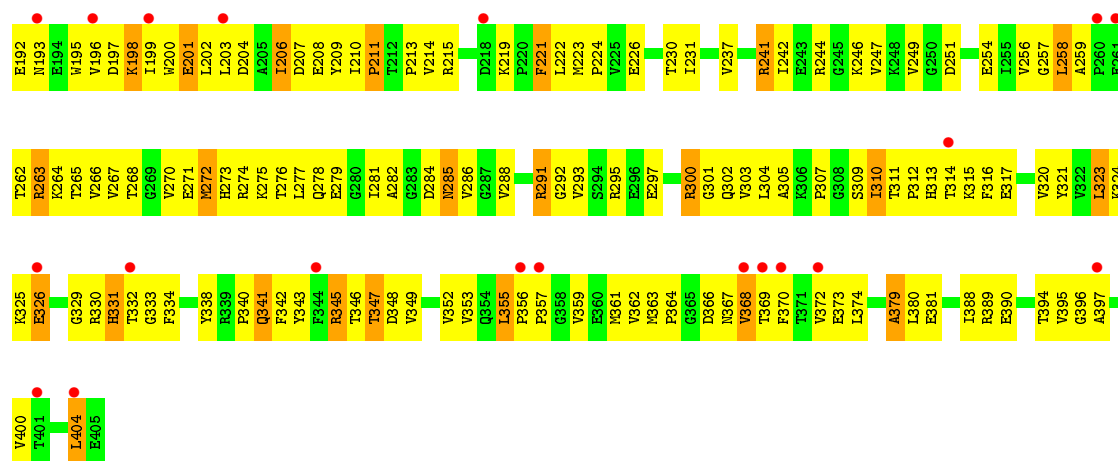


• Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

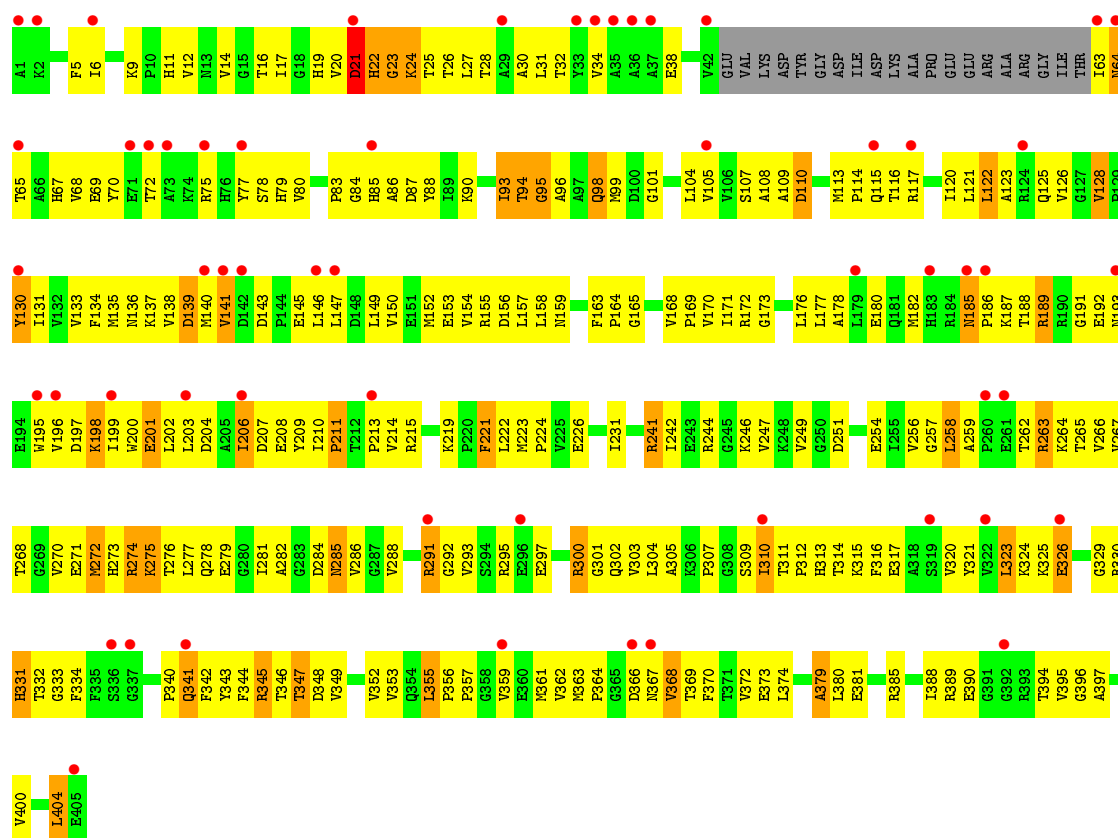


• Molecule 25: ELONGATION FACTOR TU

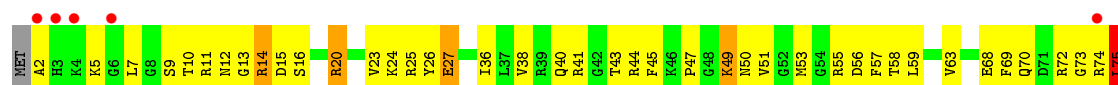




• Molecule 25: ELONGATION FACTOR TU

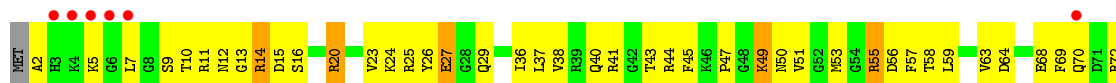
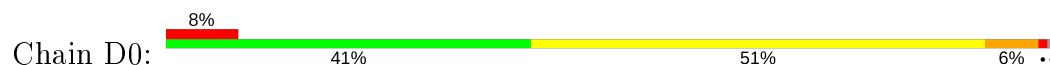


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

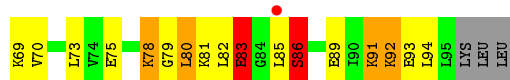
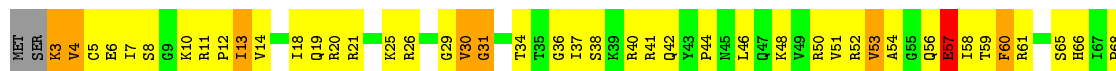




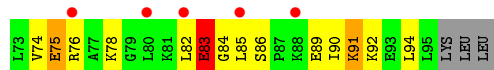
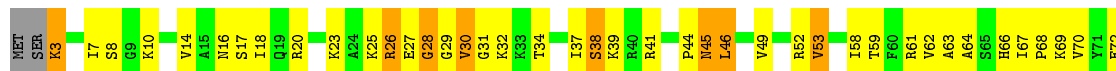
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



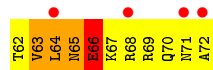
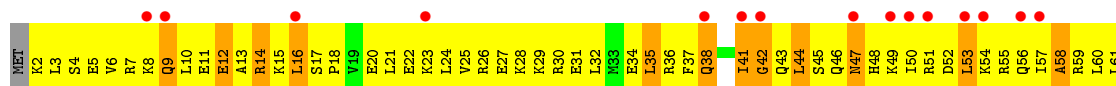
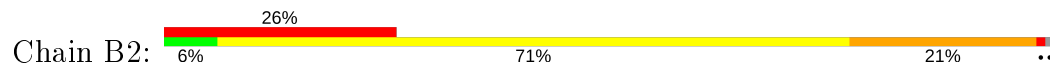
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L28



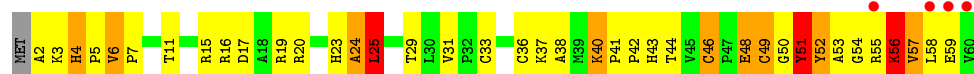
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



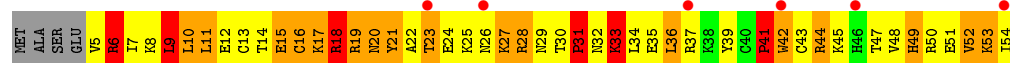
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



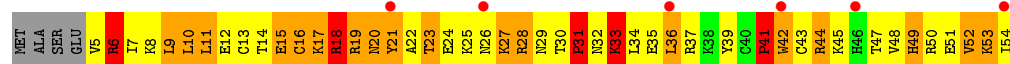




• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L33



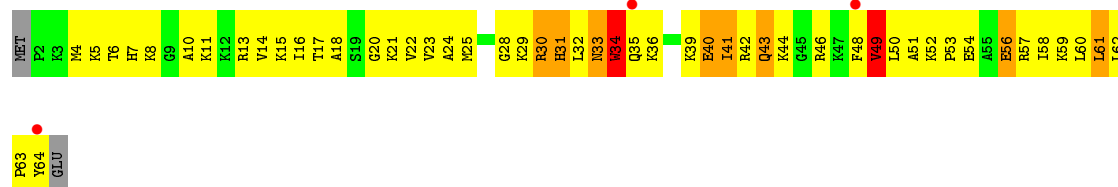
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



• Molecule 33: 50S RIBOSOMAL PROTEIN L34

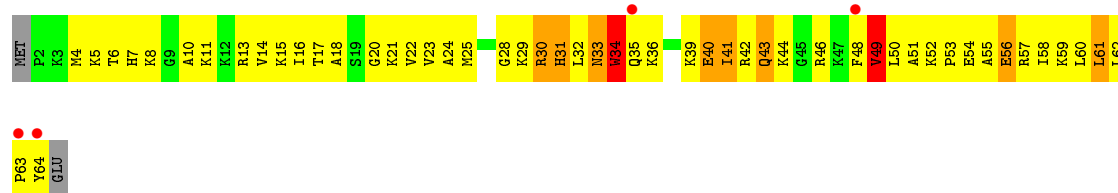


• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L35





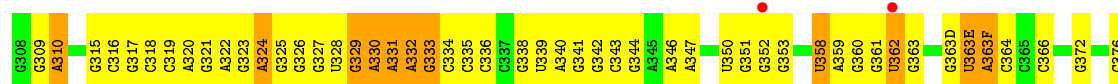
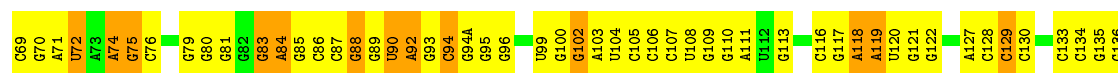
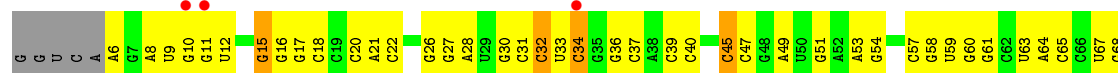
- Molecule 35: 50S RIBOSOMAL PROTEIN L36



- Molecule 35: 50S RIBOSOMAL PROTEIN L36



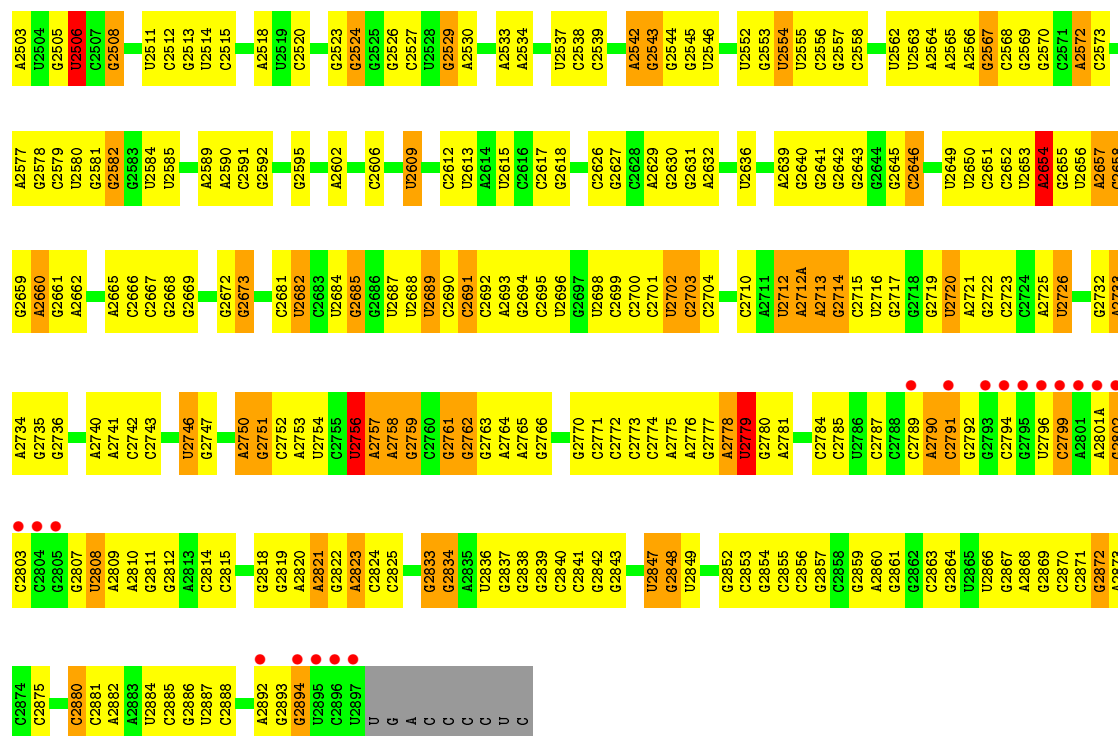
- Molecule 36: 23S RIBOSOMAL RNA



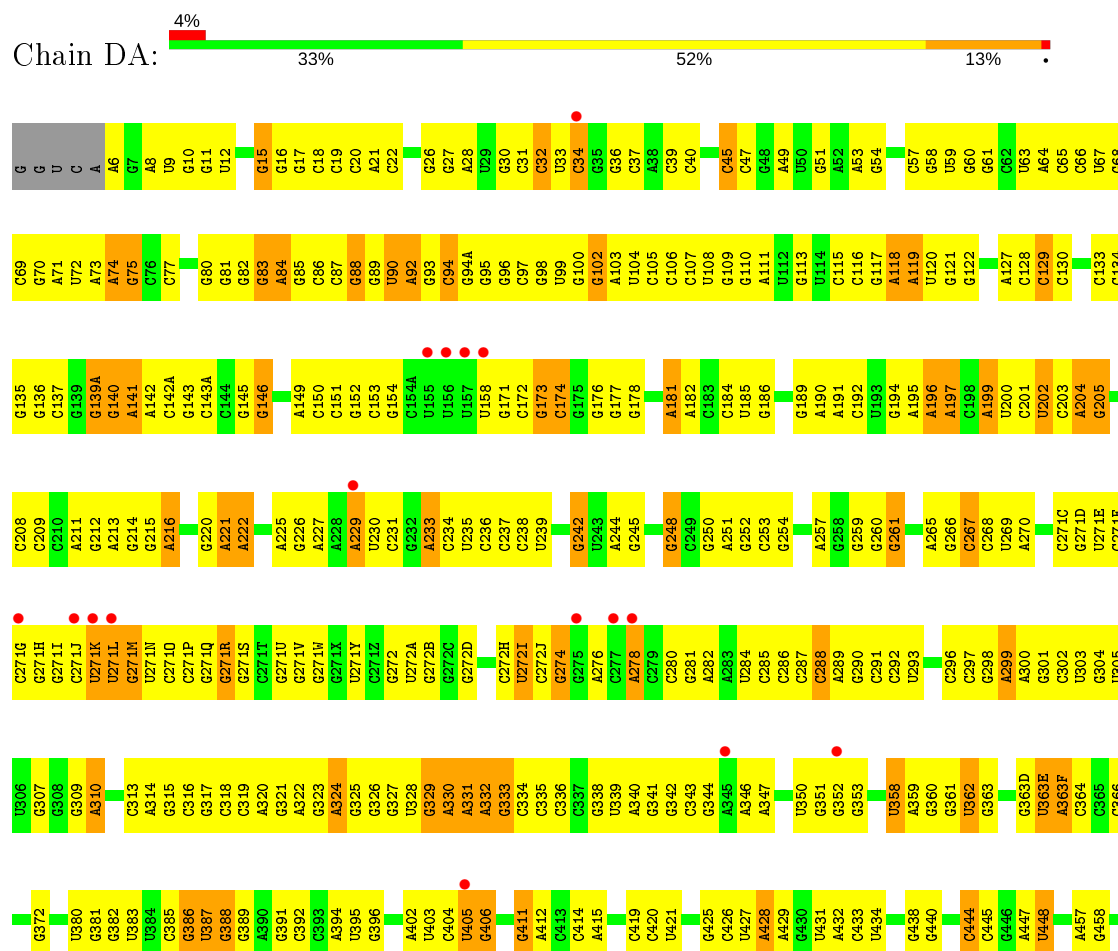


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A1346	A1275	G1206	G1138	G1070	G1007	G934	U860	G786	G715	C654K	U606	C531	G463
U1352	A1276	C1207	G1139	G1071	G1008	G935	A861	G787	U716	C654L	U607	G534	U464
A1353	G1278	G1208	G1140	C1072	A1009	C936	G862	A788	G717	C654M	A608	U534	G465
A1354	G1280	G1209	U1141	G1073	A1010	C937	A863	A789	A718	G654N	G610	C535	A466
G1355	G1281	U1210	U1142	G1074	G1011	G940	G864	C790	C719	G654O	C611	A536	G467
G1356	U1282	A1142A	A1143	G1075	U1012	G941	A865	G791	G722	C654P	C612	C537	G468
G1357	G1283	A1213	G1144	U1076	C1013	A942	G866	G792	U723	C654Q	G613	G469	A470
G1358	A1284	G1214	G1145	U1077	U1014	G943	G869	A793	A722	C654R	U614	C540	A471
G1359	G1285	G1215	G1146	U1078	G1018	U944	A870	G796	U724	C654S	U615	C543	A472
A1360	A1286	G1216	A1147	C1079	U1019	G945	A871	C797	U725	A654T	G616	G473	A473
A1361	A1287	G1217	A1148	C1080	A1020	G946	G875	G798	G729	A654U	A614C	A547	A474
C1362	U1288	G1218	G1149	U1081	G1021	G947	G876	G801	G730	A655	G815	A548	A475
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A1364	C1290	G1223	G1151	A1084	U1023	G949	A878	G805	G732	U657	G818	G551	A477
A1365	C1291	G1224	C1152	A1085	G1024	A953	G879	C812	C733	C658	G619	U555	A478
A1366	U1292	G1225	G1153	A1086	U1025	G954	G880	C813	U740	C659	G620	U556	A479
A1367	C1293	G1227	G1154	U1087	G1026	C955	G881	C814	G741	G660	G621	G557	A480
G1368	G1297	G1228	A1155	A1088	U1027	G956	G882	C815	G742	G661	G622	U558	A481
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G1370	C1299	C1230	G1160	U1090	G1029	U958	A886	C816	G744	G663	C624	G558	A483
C1371	U1300	G1231	C1161	G1091	G1030	A959	A887	C817	G745	C664	G625	C484	A484
A1372	A1301	G1232	G1162	C1092	G1031	A960	C888	C818	U746	C665	U626	C485	A485
A1373	A1302	G1233	G1163	G1093	A1032	G961	C889	C819	G747	G666	A627	U562	A486
A1374	G1305	G1234	U1164	U1094	U1033	G962	C890	A819	A751	U667	G628	G563	A487
A1375	C1306	G1235	G1165	A1095	G1034	U963	A890	G824	A752	G668	G629	G564	A488
A1376	G1310	U1240	C1166	A1096	U1035	C964	C891	C825	A753	G669	G630	C574	A489
A1377	G1311	A1241	U1167	U1097	G1036	U969	C892	U826	C753	A670	G631	U576	A490
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A1380	C1316	G1244	U1170	U1100	G1039	G972	C895	G832	C755	C673	A634	G578	A503
A1381	A1317	G1245	A1174	A1103	G1040	C973	C896	C833	U756	A674	A643	G580	A504
A1382	C1318	U1246	U1175	C1104	A1041	C974	A900	C834	G757	A675	A644	G581	A505
A1383	G1319	A1247	G1176	U1105	A1042	C975	C901	U839	G758	A676	C645	G582	A506
A1384	C1320	G1248	A1177	G1106	A1043	G977	C902	G842	A763	G684	A646	G583	A507
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A1392	C1328	G1255	C1185	G1114	A1053	C985	A919	C850	G775	U703	G654A	U519	A515
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A1397	C1333	C1260	U1188	G1118	A1058	A990	A917	G855	G780	C709	G654F	U524	A520
A1398	U1334	C1261	A1189	G1119	G1059	C991	A918	G856	A781	G710	C654G	G525	A521
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A1402	C1338	G1265	G1193	G1123	G1063	C995	C925	G860	G714	G714	G654K	G529	A525
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A1407	G1343	C1270	U1198	A1131	U1068	G997	C930	G865	G719	G719	G654P	G534	A530
A1408	U1344	G1271	U1199	A1132	U1069	G998	C931	G866	G720	G720	G654Q	G535	A531
A1409	A1345	A1272	G1203	C1135	A1067	U999	G932	C867	G721	G721	G654R	G536	A532
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A1415	U1347												
A1416	A1347												
A1417	G1349												

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G2429	A2286	G2193	C2128	G2056	A1981	G1888	G1801	C1709	A1634	A1558	U1489	A1419
A2430	A2287	G2194			G1982	A1889	G1807	C1710	C1638	G1559	U1420	G1421
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G2481	C2341	C2179	G2123	G2123	G2033	U1952	U1864	A1783	U1688	A1608		
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		G2191	A2136	A2136	G2052	G1973	C1886	U1798	C1548	G1485		
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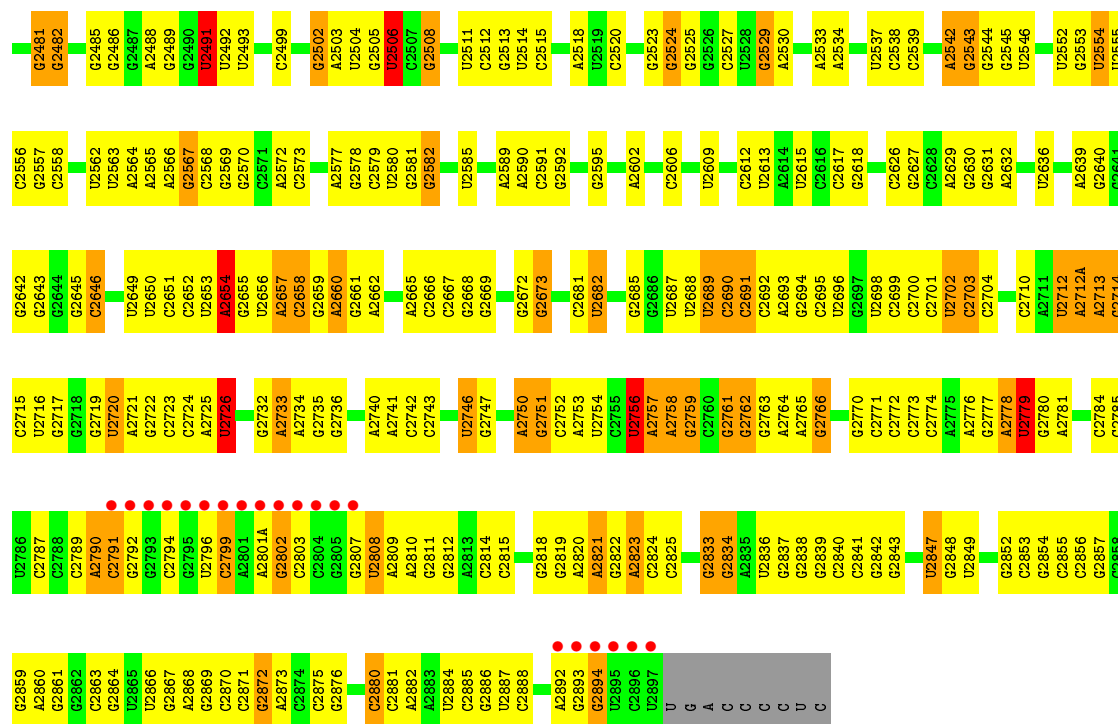


• Molecule 36: 23S RIBOSOMAL RNA



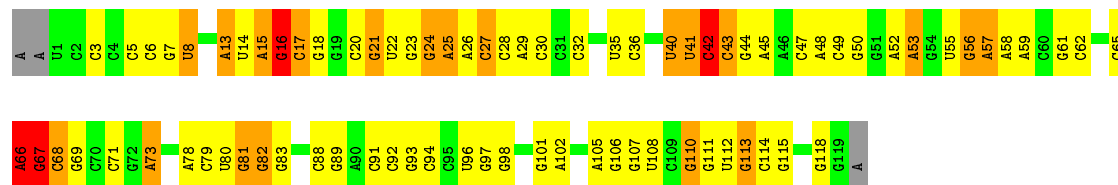






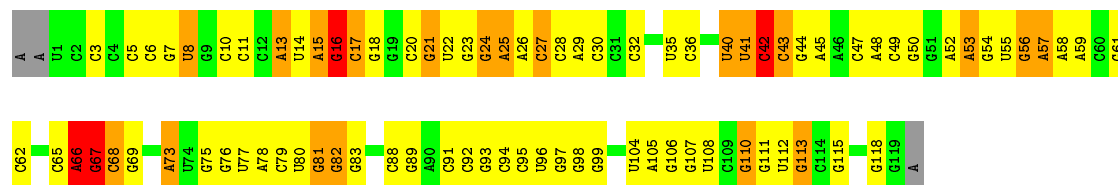
### • Molecule 37: 5S RIBOSOMAL RNA

Chain BB: 33% 45% 16%



### • Molecule 37: 5S RIBOSOMAL RNA

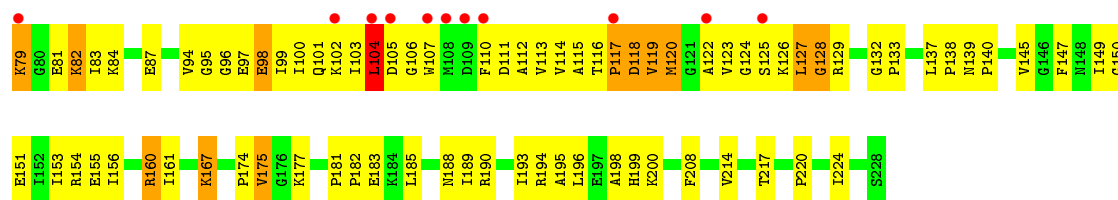
Chain DB: 29% 49% 16%



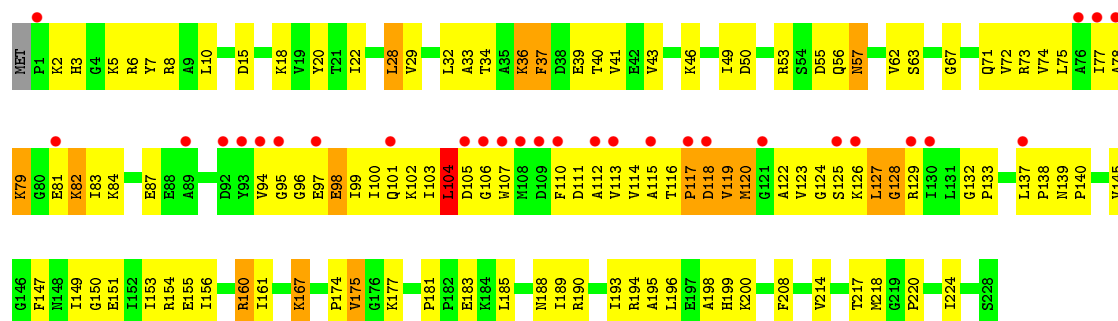
### • Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC: 6% 48% 45% 7%

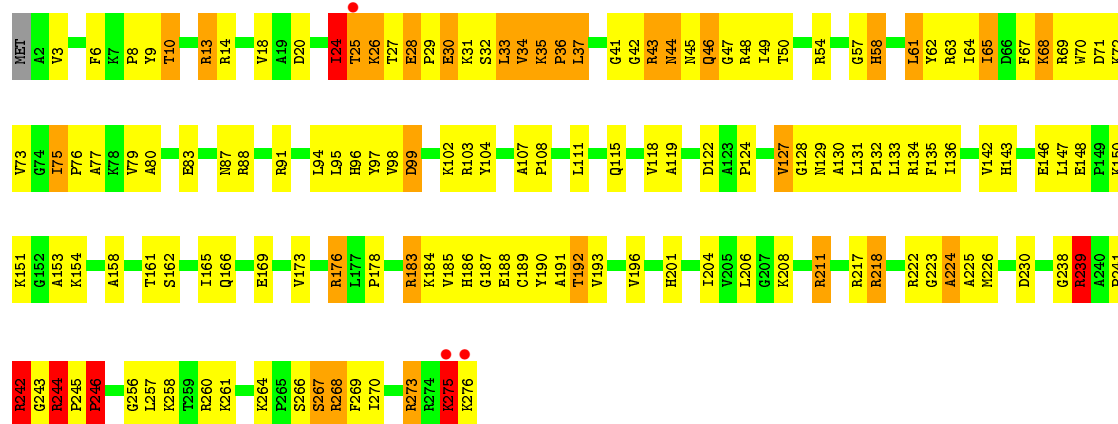




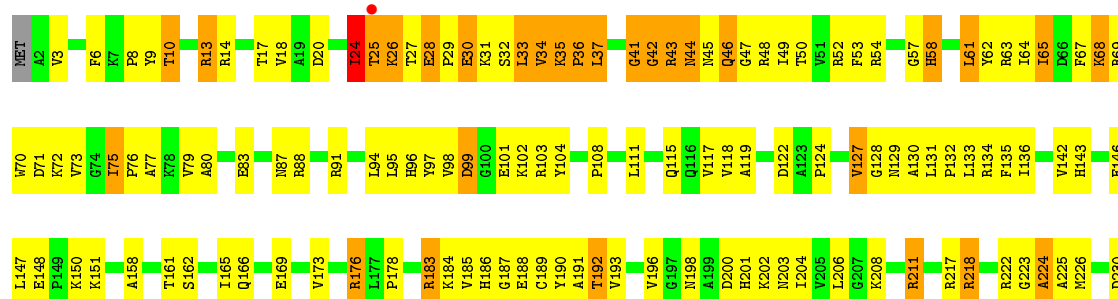
● Molecule 38: 50S RIBOSOMAL PROTEIN L1



● Molecule 39: 50S RIBOSOMAL PROTEIN L2

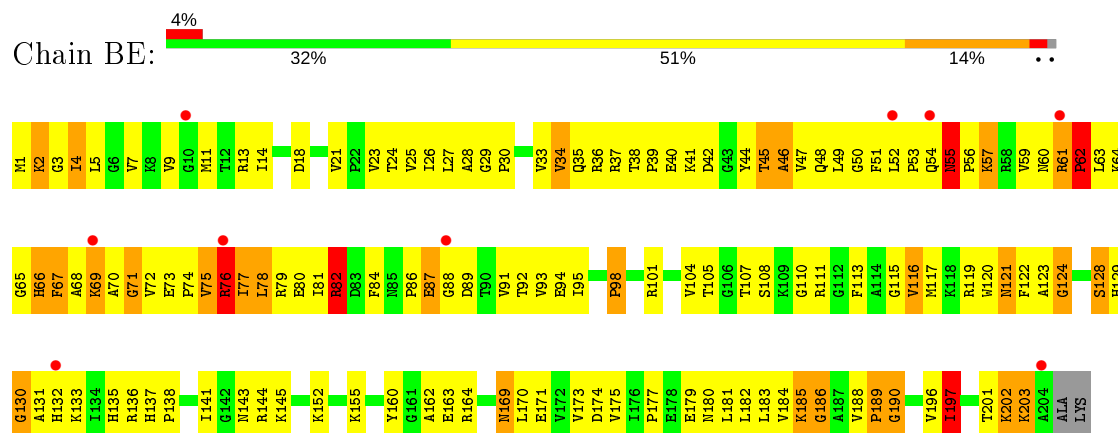


● Molecule 39: 50S RIBOSOMAL PROTEIN L2

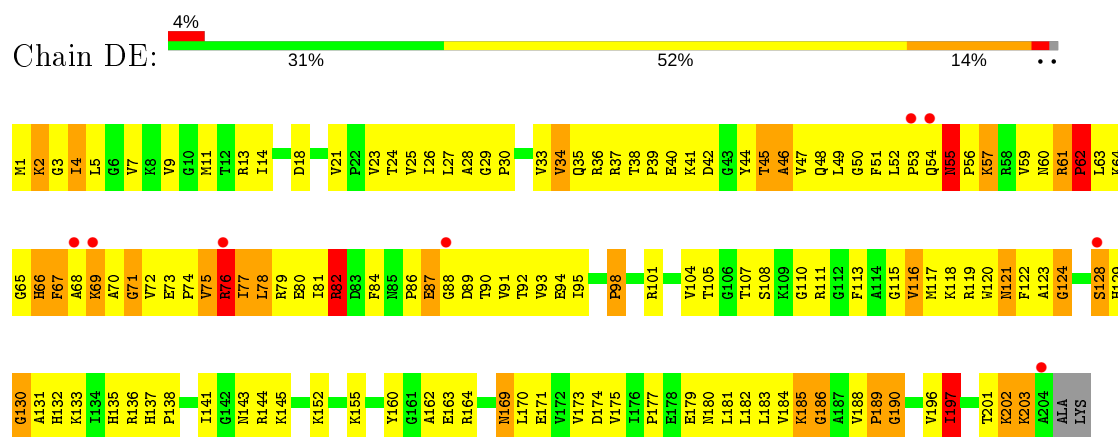




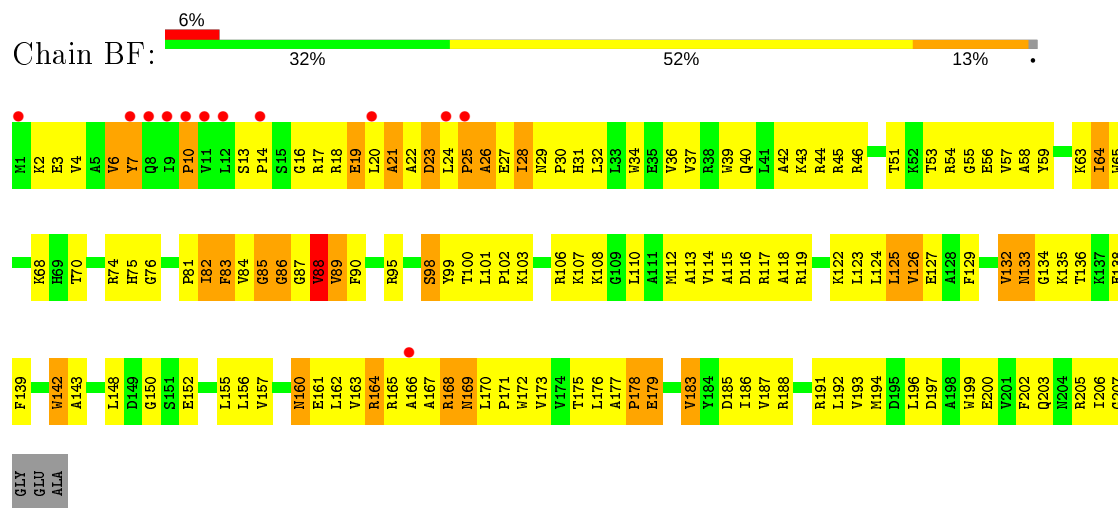
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L3

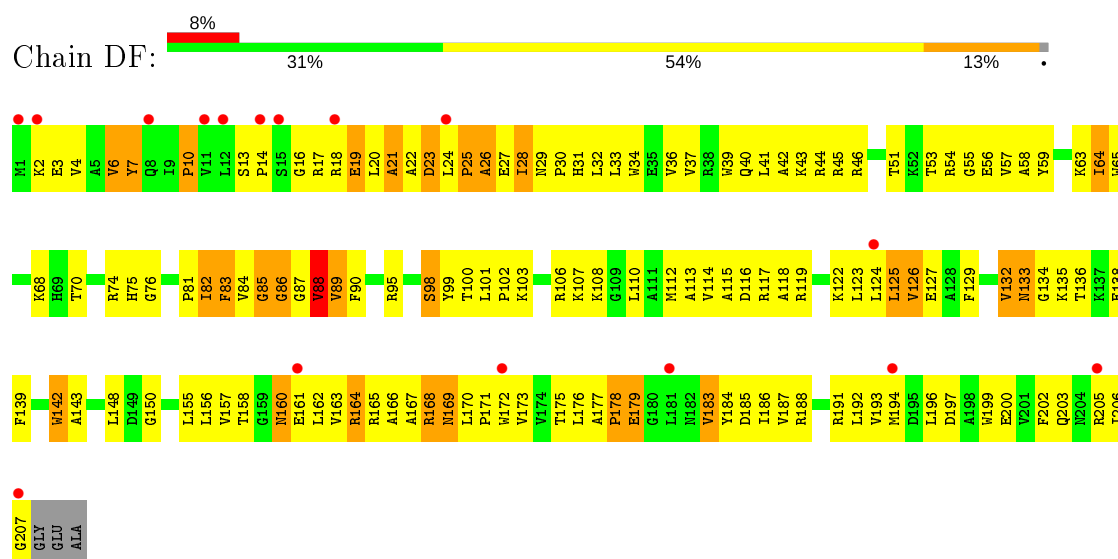


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

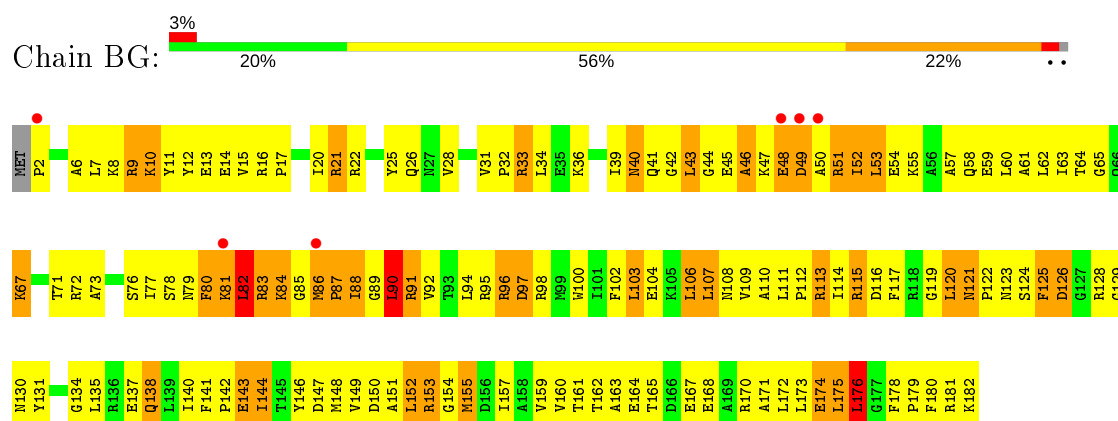


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

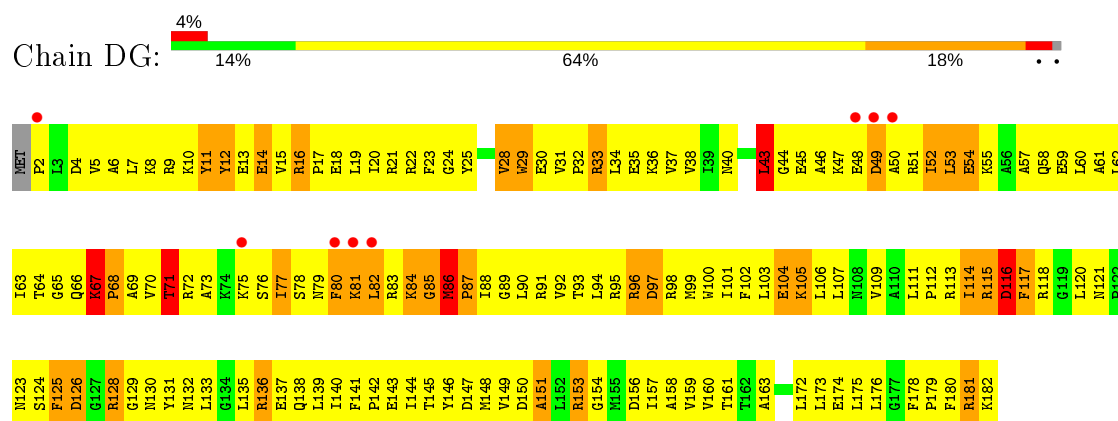




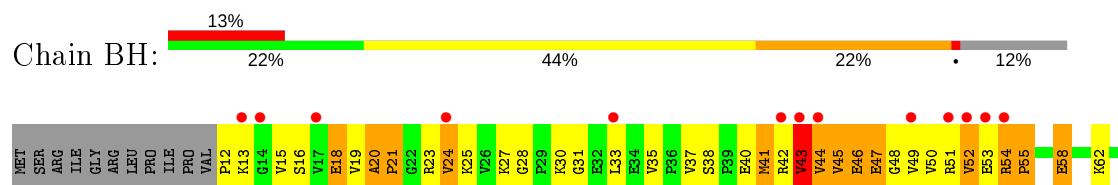
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

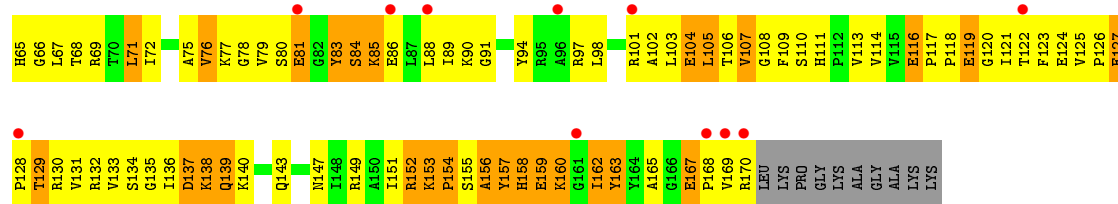


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

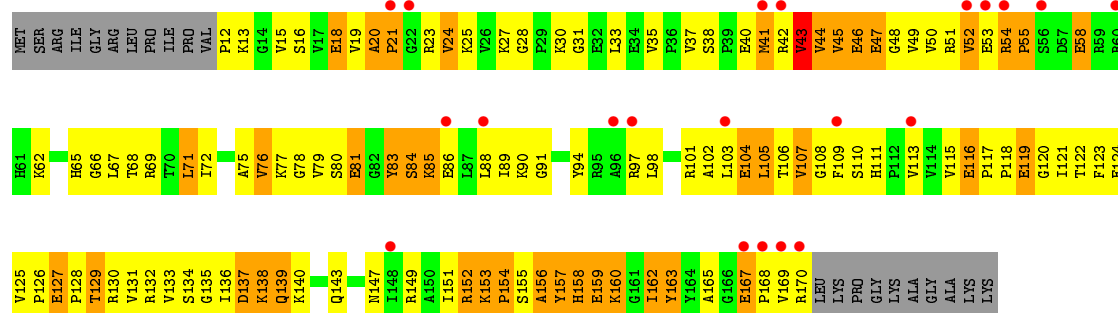


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

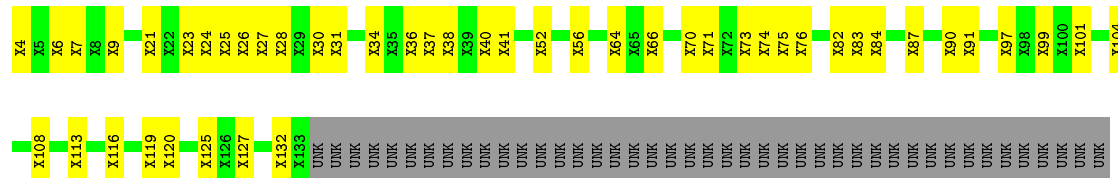





• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

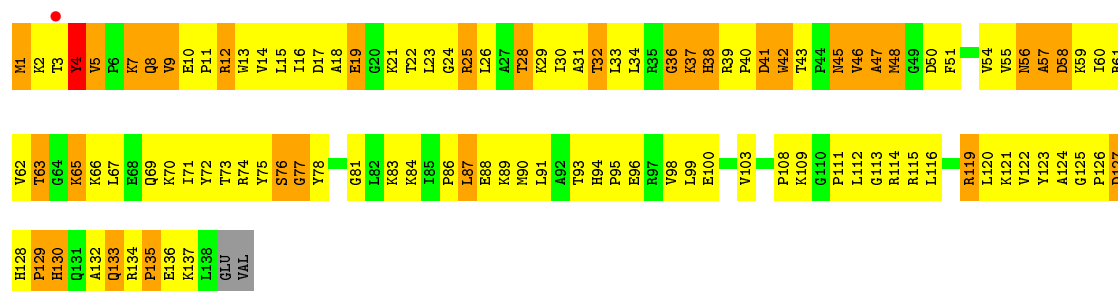


Chain DK: 



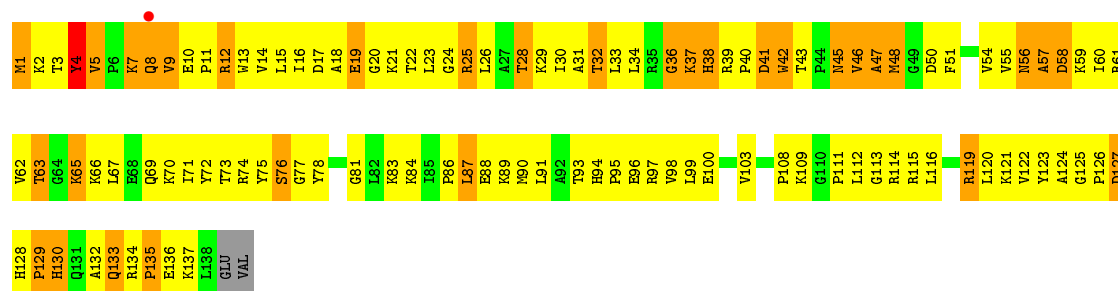
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 



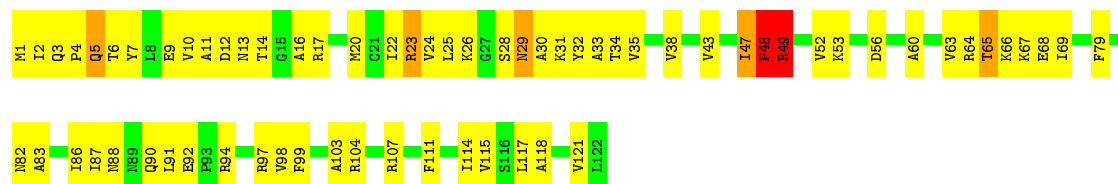
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 



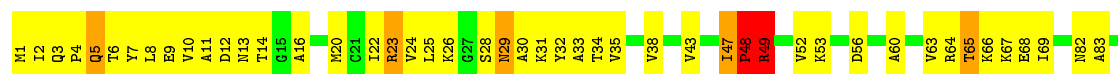
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 



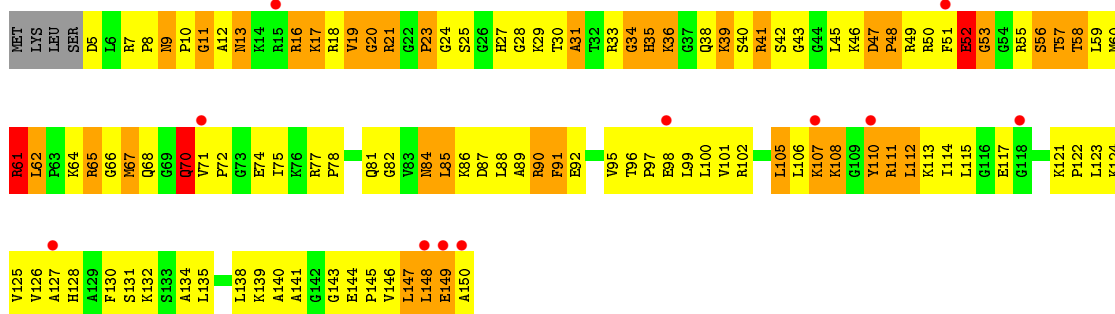
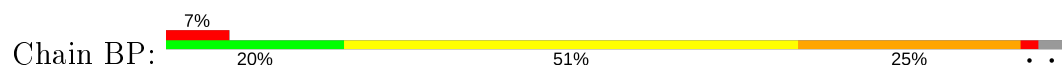
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 

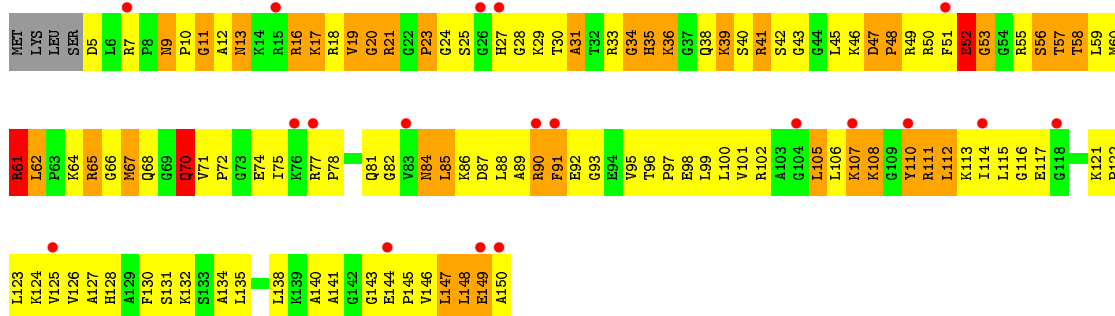
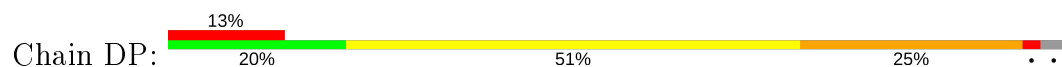




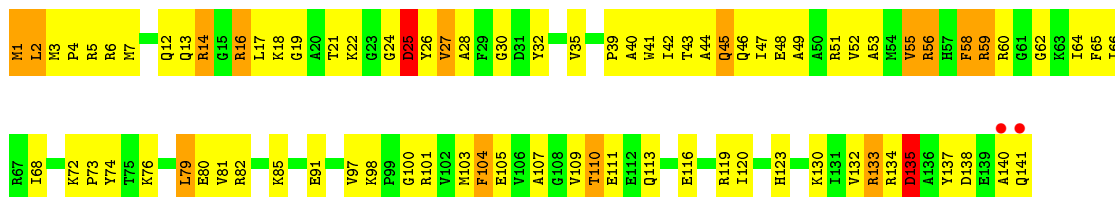
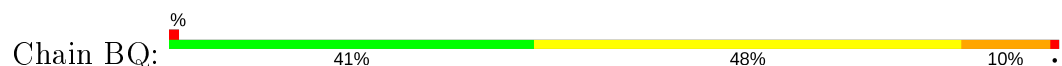
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

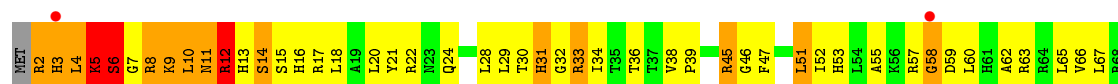




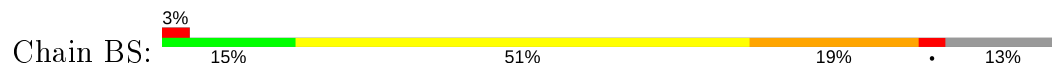
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



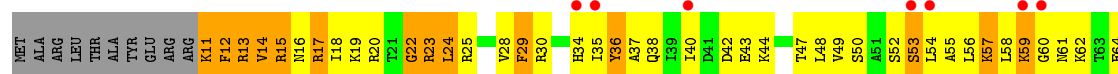
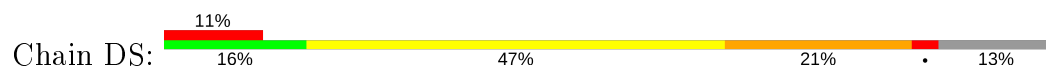
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



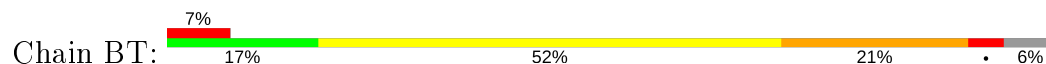
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

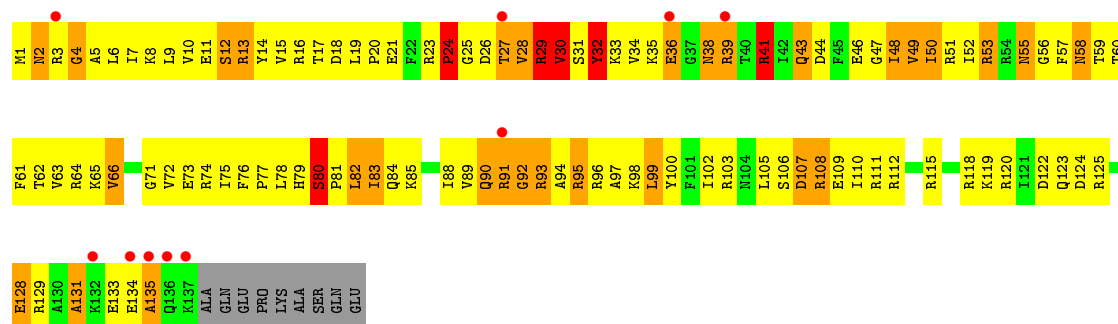


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

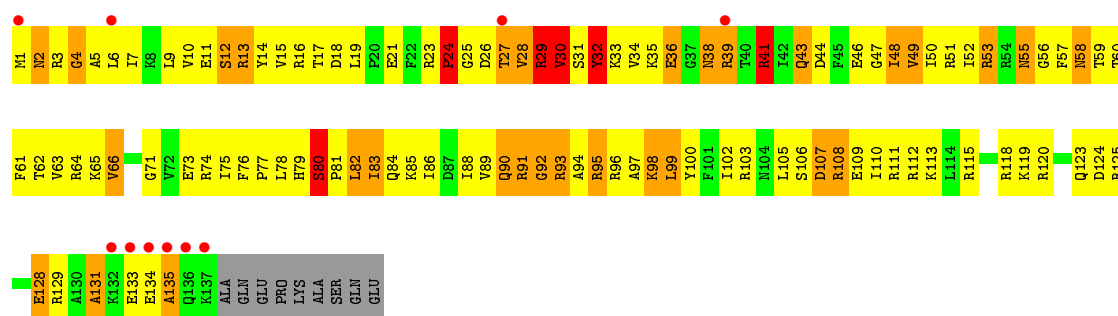
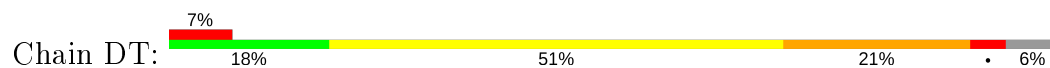


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

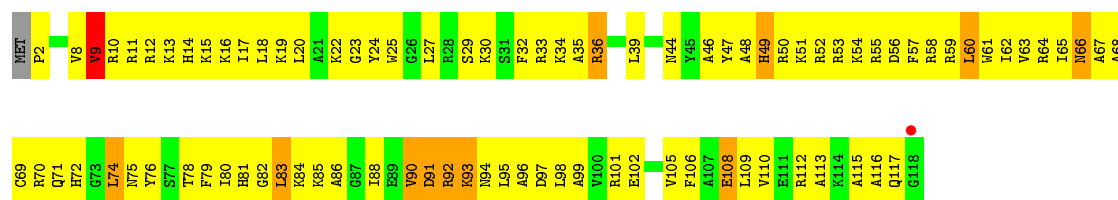




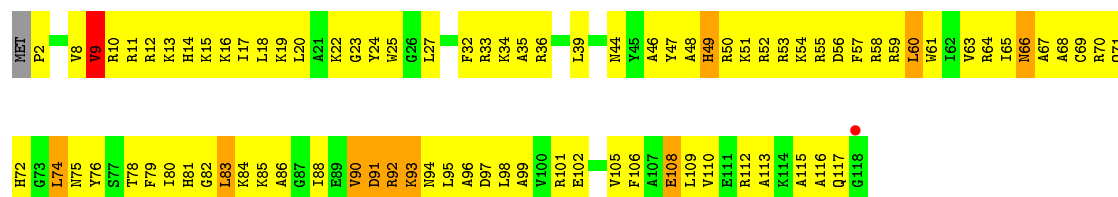
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



• Molecule 53: 50S RIBOSOMAL PROTEIN L20

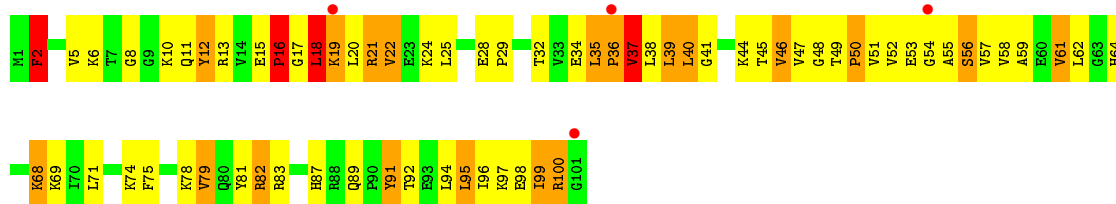


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

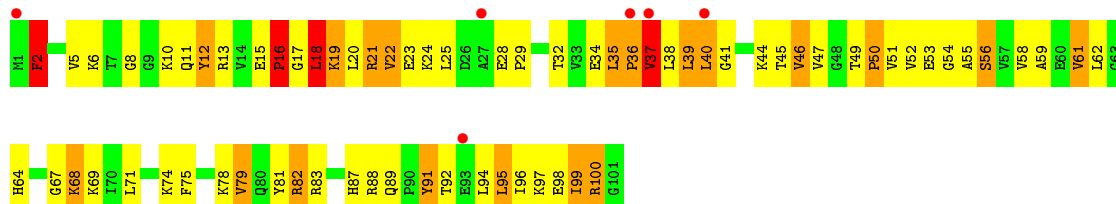


• Molecule 54: 50S RIBOSOMAL PROTEIN L21

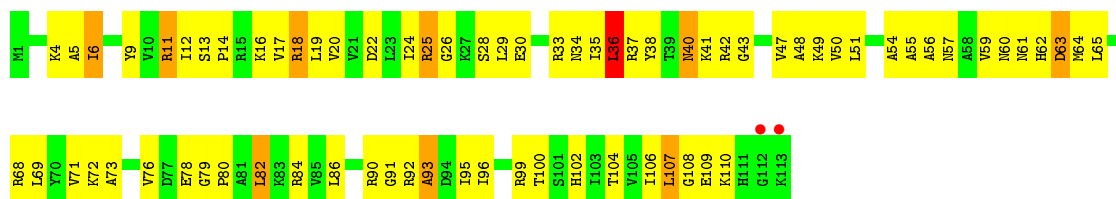




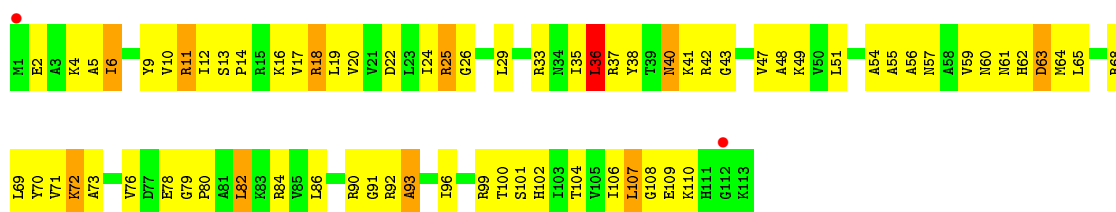
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



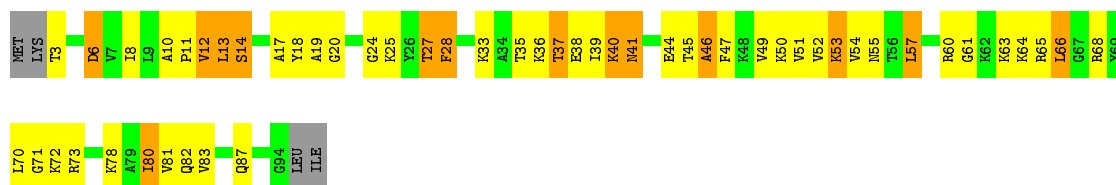
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



• Molecule 55: 50S RIBOSOMAL PROTEIN L22

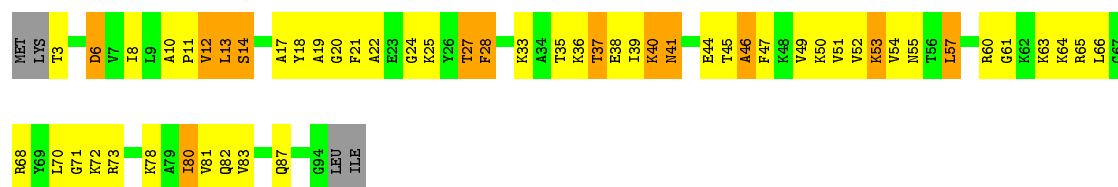


• Molecule 56: 50S RIBOSOMAL PROTEIN L23




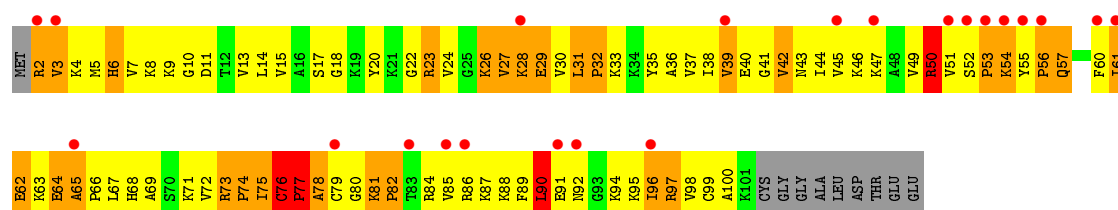
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX: 




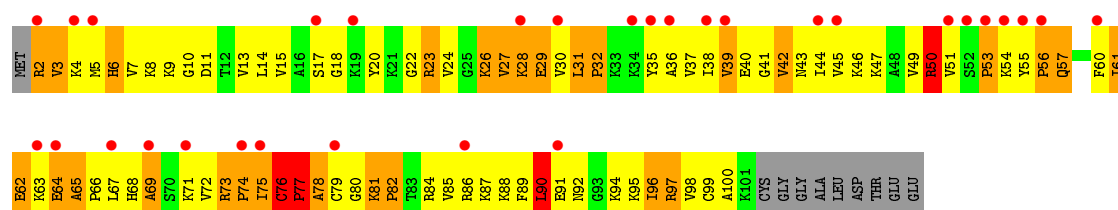
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY: 




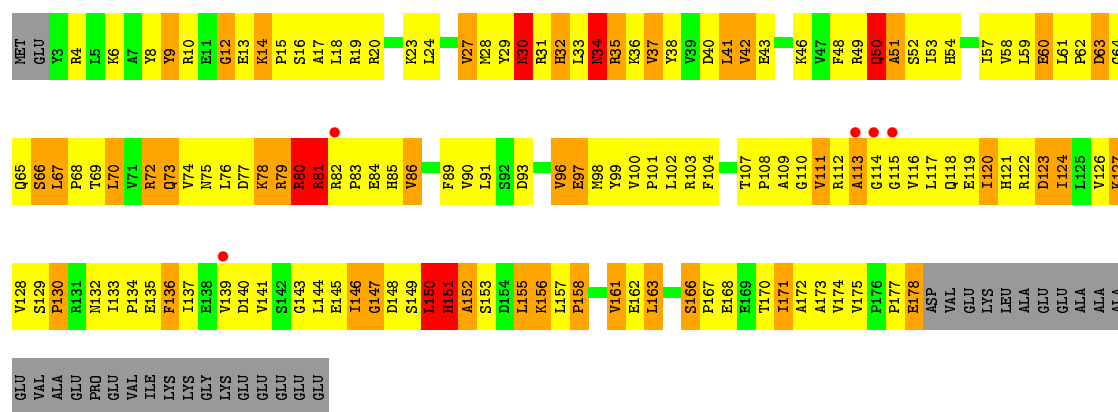
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY: 

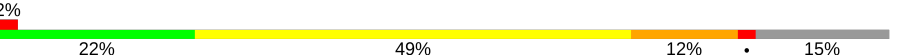


• Molecule 58: 50S RIBOSOMAL PROTEIN L25

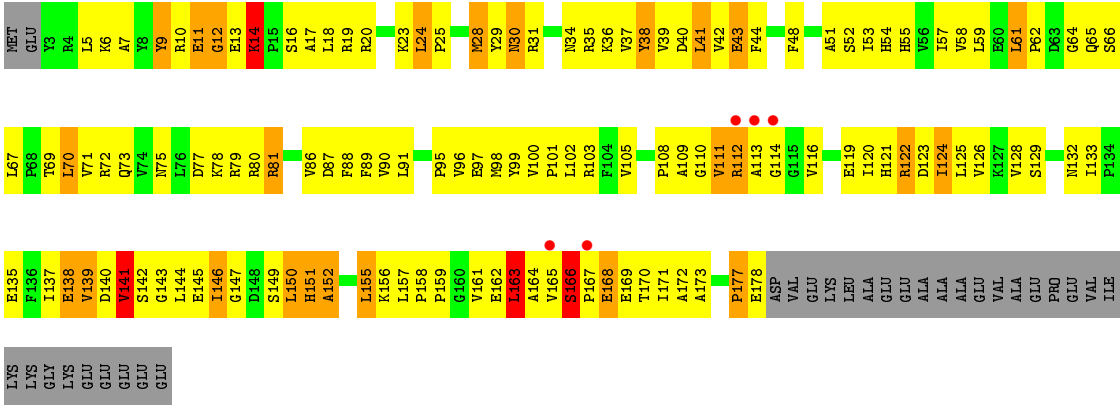
Chain BZ: 



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.243 , 0.267 0.241 , 0.265	Depositor DCC
$R_{free}$ test set	59600 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	307322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	65	0
22	CV	1619	0	822	63	0
22	CW	1619	0	822	69	0
23	AX	361	0	184	7	0
23	CX	361	0	184	11	0
24	AY	1643	0	853	76	0
24	CY	1643	0	853	75	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

*Continued on next page...*



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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	2140	0
36	DA	62477	0	31497	2211	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	17679	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 17679 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	5
2	CB	232/256 (91%)	173 (75%)	41 (18%)	18 (8%)	1	5
3	AC	204/239 (85%)	161 (79%)	23 (11%)	20 (10%)	0	3
3	CC	204/239 (85%)	159 (78%)	28 (14%)	17 (8%)	1	5
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	1
5	AE	148/162 (91%)	138 (93%)	5 (3%)	5 (3%)	3	21
5	CE	148/162 (91%)	138 (93%)	6 (4%)	4 (3%)	5	25
6	AF	99/101 (98%)	80 (81%)	12 (12%)	7 (7%)	1	6
6	CF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	6
7	AG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	2	12
7	CG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	2	12
8	AH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	57
8	CH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	57
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%)	0	3
10	CJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0	3
11	AK	117/129 (91%)	100 (86%)	10 (8%)	7 (6%)	1	9
11	CK	117/129 (91%)	101 (86%)	9 (8%)	7 (6%)	1	9
12	AL	122/135 (90%)	94 (77%)	15 (12%)	13 (11%)	0	2
12	CL	122/135 (90%)	91 (75%)	18 (15%)	13 (11%)	0	2
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%)	13	44
16	AP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	4
16	CP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	7	30
17	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	7	30
18	AR	68/88 (77%)	56 (82%)	11 (16%)	1 (2%)	10	39
18	CR	68/88 (77%)	57 (84%)	10 (15%)	1 (2%)	10	39
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%)	0	3
20	CT	97/106 (92%)	62 (64%)	26 (27%)	9 (9%)	0	3
21	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2	15
21	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2	15
25	AZ	381/405 (94%)	269 (71%)	82 (22%)	30 (8%)	1	5
25	CZ	381/405 (94%)	268 (70%)	83 (22%)	30 (8%)	1	5
26	B0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	3	19
26	D0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	3	19
27	B1	91/98 (93%)	70 (77%)	10 (11%)	11 (12%)	0	1
27	D1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	7
28	B2	69/72 (96%)	40 (58%)	15 (22%)	14 (20%)	0	0
28	D2	69/72 (96%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	B3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	4
29	D3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	4
30	B4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	1
30	D4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	1
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%)	6	29
33	D7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	6	29
34	B8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	0	3
34	D8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	0	3
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	4
38	BC	226/229 (99%)	170 (75%)	45 (20%)	11 (5%)	2	14
38	DC	226/229 (99%)	171 (76%)	43 (19%)	12 (5%)	2	12
39	BD	273/276 (99%)	219 (80%)	31 (11%)	23 (8%)	1	5
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	2
41	DF	205/210 (98%)	149 (73%)	34 (17%)	22 (11%)	0	2
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%)	2	13
47	DO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	2	13
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%)	3	20
49	DQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	20
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%)	1	9
53	DU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	1	9
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	2
55	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	2
56	BX	90/96 (94%)	64 (71%)	20 (22%)	6 (7%)	1	7
56	DX	90/96 (94%)	65 (72%)	19 (21%)	6 (7%)	1	7
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%)	0	3
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%)	5	20
2	CB	202/220 (92%)	180 (89%)	22 (11%)	6	25
3	AC	160/188 (85%)	143 (89%)	17 (11%)	6	26
3	CC	160/188 (85%)	144 (90%)	16 (10%)	7	28
4	AD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	CD	180/181 (99%)	157 (87%)	23 (13%)	4	18
5	AE	115/123 (94%)	104 (90%)	11 (10%)	8	31
5	CE	115/123 (94%)	105 (91%)	10 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	90/90 (100%)	81 (90%)	9 (10%)	7	28
6	CF	90/90 (100%)	82 (91%)	8 (9%)	9	34
7	AG	126/127 (99%)	116 (92%)	10 (8%)	12	40
7	CG	126/127 (99%)	116 (92%)	10 (8%)	12	40
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	38
8	CH	119/119 (100%)	109 (92%)	10 (8%)	11	38
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	33
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	33
10	AJ	88/92 (96%)	80 (91%)	8 (9%)	9	33
10	CJ	88/92 (96%)	80 (91%)	8 (9%)	9	33
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	28
11	CK	90/99 (91%)	82 (91%)	8 (9%)	9	34
12	AL	104/111 (94%)	95 (91%)	9 (9%)	10	36
12	CL	104/111 (94%)	97 (93%)	7 (7%)	16	46
13	AM	99/101 (98%)	86 (87%)	13 (13%)	4	17
13	CM	99/101 (98%)	86 (87%)	13 (13%)	4	17
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	5
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	23
15	CO	79/80 (99%)	71 (90%)	8 (10%)	7	28
16	AP	72/74 (97%)	66 (92%)	6 (8%)	11	38
16	CP	72/74 (97%)	66 (92%)	6 (8%)	11	38
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	22
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	AS	69/80 (86%)	56 (81%)	13 (19%)	1	6
19	CS	69/80 (86%)	56 (81%)	13 (19%)	1	6
20	AT	76/82 (93%)	71 (93%)	5 (7%)	16	47
20	CT	76/82 (93%)	71 (93%)	5 (7%)	16	47
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	54
25	AZ	322/338 (95%)	299 (93%)	23 (7%)	14	44
25	CZ	322/338 (95%)	299 (93%)	23 (7%)	14	44
26	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	12
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	71 (91%)	7 (9%)	9	34
28	B2	66/67 (98%)	61 (92%)	5 (8%)	13	41
28	D2	66/67 (98%)	60 (91%)	6 (9%)	9	33
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	16
29	D3	51/52 (98%)	44 (86%)	7 (14%)	3	16
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	8
30	D4	39/63 (62%)	32 (82%)	7 (18%)	2	8
31	B5	51/52 (98%)	43 (84%)	8 (16%)	2	11
31	D5	51/52 (98%)	43 (84%)	8 (16%)	2	11
32	B6	49/52 (94%)	36 (74%)	13 (26%)	0	1
32	D6	49/52 (94%)	37 (76%)	12 (24%)	0	2
33	B7	41/42 (98%)	35 (85%)	6 (15%)	3	13
33	D7	41/42 (98%)	35 (85%)	6 (15%)	3	13
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	12
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	12
35	B9	34/34 (100%)	31 (91%)	3 (9%)	10	36
35	D9	34/34 (100%)	31 (91%)	3 (9%)	10	36
38	BC	180/181 (99%)	170 (94%)	10 (6%)	21	52
38	DC	180/181 (99%)	171 (95%)	9 (5%)	24	57
39	BD	217/218 (100%)	187 (86%)	30 (14%)	3	16
39	DD	217/218 (100%)	186 (86%)	31 (14%)	3	14
40	BE	165/166 (99%)	148 (90%)	17 (10%)	7	27
40	DE	165/166 (99%)	148 (90%)	17 (10%)	7	27
41	BF	165/166 (99%)	150 (91%)	15 (9%)	9	33
41	DF	165/166 (99%)	150 (91%)	15 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BG	155/156 (99%)	132 (85%)	23 (15%)	3	13
42	DG	155/156 (99%)	138 (89%)	17 (11%)	6	25
43	BH	132/148 (89%)	116 (88%)	16 (12%)	5	20
43	DH	132/148 (89%)	116 (88%)	16 (12%)	5	20
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	18
47	BO	100/100 (100%)	95 (95%)	5 (5%)	24	57
47	DO	100/100 (100%)	95 (95%)	5 (5%)	24	57
48	BP	112/116 (97%)	97 (87%)	15 (13%)	4	16
48	DP	112/116 (97%)	97 (87%)	15 (13%)	4	16
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
50	BR	100/101 (99%)	89 (89%)	11 (11%)	6	25
50	DR	100/101 (99%)	90 (90%)	10 (10%)	7	28
51	BS	77/88 (88%)	68 (88%)	9 (12%)	5	22
51	DS	77/88 (88%)	68 (88%)	9 (12%)	5	22
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	6
52	DT	120/127 (94%)	98 (82%)	22 (18%)	1	7
53	BU	92/94 (98%)	83 (90%)	9 (10%)	8	29
53	DU	92/94 (98%)	84 (91%)	8 (9%)	10	36
54	BV	82/82 (100%)	66 (80%)	16 (20%)	1	6
54	DV	82/82 (100%)	66 (80%)	16 (20%)	1	6
55	BW	91/92 (99%)	86 (94%)	5 (6%)	21	53
55	DW	91/92 (99%)	86 (94%)	5 (6%)	21	53
56	BX	74/78 (95%)	64 (86%)	10 (14%)	4	16
56	DX	74/78 (95%)	64 (86%)	10 (14%)	4	16
57	BY	84/91 (92%)	70 (83%)	14 (17%)	2	9
57	DY	84/91 (92%)	70 (83%)	14 (17%)	2	9
58	BZ	155/179 (87%)	126 (81%)	29 (19%)	1	7
58	DZ	155/179 (87%)	135 (87%)	20 (13%)	4	18
All	All	10338/10860 (95%)	9176 (89%)	1162 (11%)	6	24

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	OMC	CY	32	24	15,22,23	0.75	0	17,31,34	1.19	2 (11%)
24	H2U	AY	20	24	18,21,22	0.87	0	21,30,33	1.92	4 (19%)
24	7MG	CY	46	24	22,26,27	1.23	2 (9%)	28,39,42	2.28	5 (17%)
24	MIA	AY	37	24	24,31,32	1.19	2 (8%)	26,44,47	1.71	4 (15%)
24	4SU	AY	8	24	14,21,22	1.50	3 (21%)	15,30,33	2.63	2 (13%)
24	PSU	CY	55	24	17,21,22	1.19	2 (11%)	20,30,33	3.28	6 (30%)
24	7MG	AY	46	24	22,26,27	1.25	2 (9%)	28,39,42	2.27	5 (17%)
24	5MU	CY	54	24	15,22,23	1.17	2 (13%)	16,32,35	3.71	1 (6%)
24	H2U	CY	20	24	18,21,22	0.85	0	21,30,33	1.92	4 (19%)
24	5MU	AY	54	24	15,22,23	1.15	2 (13%)	16,32,35	3.73	1 (6%)
24	H2U	CY	16	24	18,21,22	0.94	0	21,30,33	1.79	4 (19%)
24	MIA	CY	37	24	24,31,32	1.02	1 (4%)	26,44,47	1.71	4 (15%)
24	H2U	AY	17	24	18,21,22	0.86	0	21,30,33	2.01	5 (23%)
24	OMC	AY	32	24	15,22,23	0.79	0	17,31,34	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	AY	55	24	17,21,22	1.20	2 (11%)	20,30,33	3.27	6 (30%)
24	H2U	CY	17	24	18,21,22	0.86	0	21,30,33	2.02	6 (28%)
24	H2U	AY	16	24	18,21,22	0.89	0	21,30,33	1.79	4 (19%)
24	4SU	CY	8	24	14,21,22	1.52	4 (28%)	15,30,33	2.62	2 (13%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C6-N1	4.04	1.40	1.33
24	CY	46	7MG	C6-N1	3.99	1.40	1.33
24	CY	8	4SU	C5-C4	3.94	1.42	1.38
24	AY	8	4SU	C5-C4	3.91	1.42	1.38
24	AY	37	MIA	C2-S10	3.49	1.78	1.75

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	54	5MU	C4-N3-C2	14.57	127.44	115.14
24	CY	54	5MU	C4-N3-C2	14.47	127.36	115.14
24	CY	55	PSU	N1-C2-N3	-10.19	120.33	128.43
24	AY	55	PSU	N1-C2-N3	-10.07	120.43	128.43
24	AY	8	4SU	C2-N3-C4	7.95	126.67	115.15

All (2) chirality outliers are listed below:

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

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	37	MIA	C5-C6-N6-C12
24	CY	37	MIA	C5-C6-N6-C12
24	AY	17	H2U	C4'-C5'-O5'-P
24	CY	17	H2U	C4'-C5'-O5'-P
24	AY	17	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 32 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	24,30,30	1.37	3 (12%)	31,47,47	2.14	9 (29%)
61	KIR	CZ	502	-	56,59,59	3.45	23 (41%)	62,84,84	1.67	13 (20%)
61	KIR	AZ	502	-	56,59,59	3.48	23 (41%)	62,84,84	1.68	13 (20%)
60	GDP	CZ	501	-	24,30,30	1.41	3 (12%)	31,47,47	1.96	7 (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	CZ	502	-	-	3/54/98/98	0/3/3/3
61	KIR	AZ	502	-	-	4/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/12/32/32	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.83	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.56	1.22	1.44
61	AZ	502	KIR	O30-C30	-12.56	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.50	1.17	1.42
61	AZ	502	KIR	C22-C21	5.64	1.39	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	N3-C2-N1	-6.10	119.08	127.22
60	AZ	501	GDP	C2-N3-C4	5.90	122.10	115.36
60	CZ	501	GDP	C2-N3-C4	5.62	121.77	115.36
60	CZ	501	GDP	N3-C2-N1	-5.13	120.38	127.22
61	AZ	502	KIR	O29-C29-O34	-4.75	102.25	110.21

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AZ	502	KIR	C11-C10-C9-C8
61	CZ	502	KIR	C11-C10-C9-C8
61	AZ	502	KIR	C36-C37-C38-C39
61	CZ	502	KIR	C36-C37-C38-C39
61	AZ	502	KIR	C19-C20-O20-C43

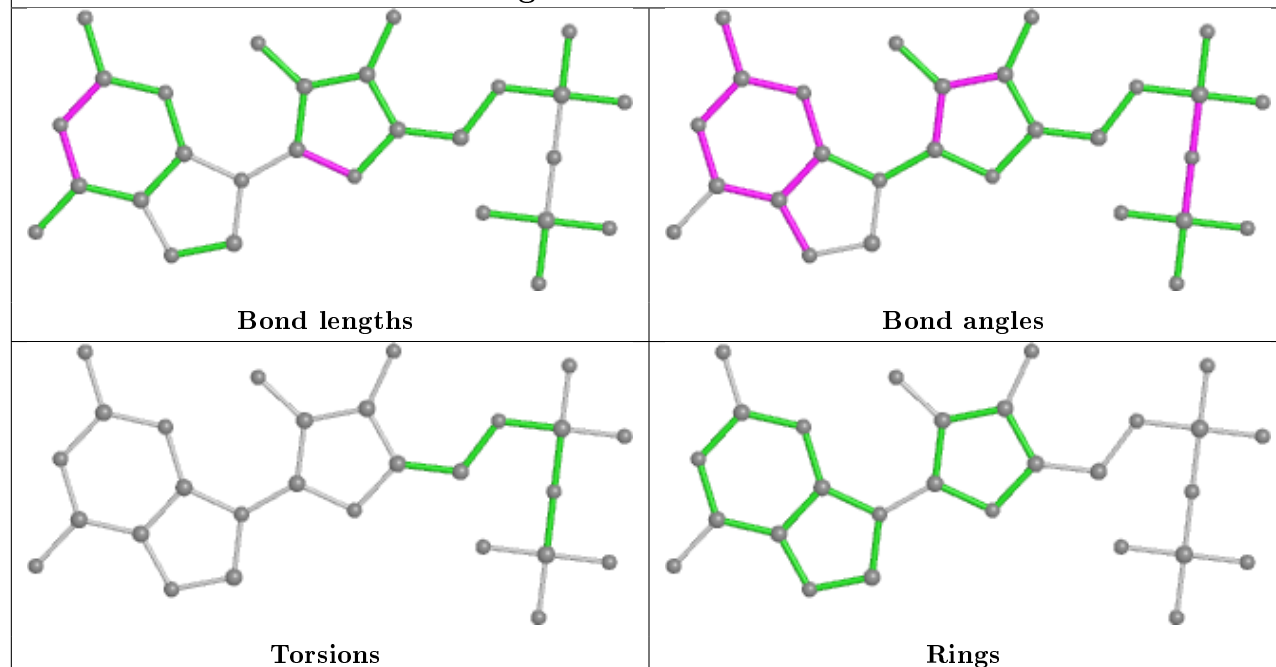
There are no ring outliers.

4 monomers are involved in 13 short contacts:

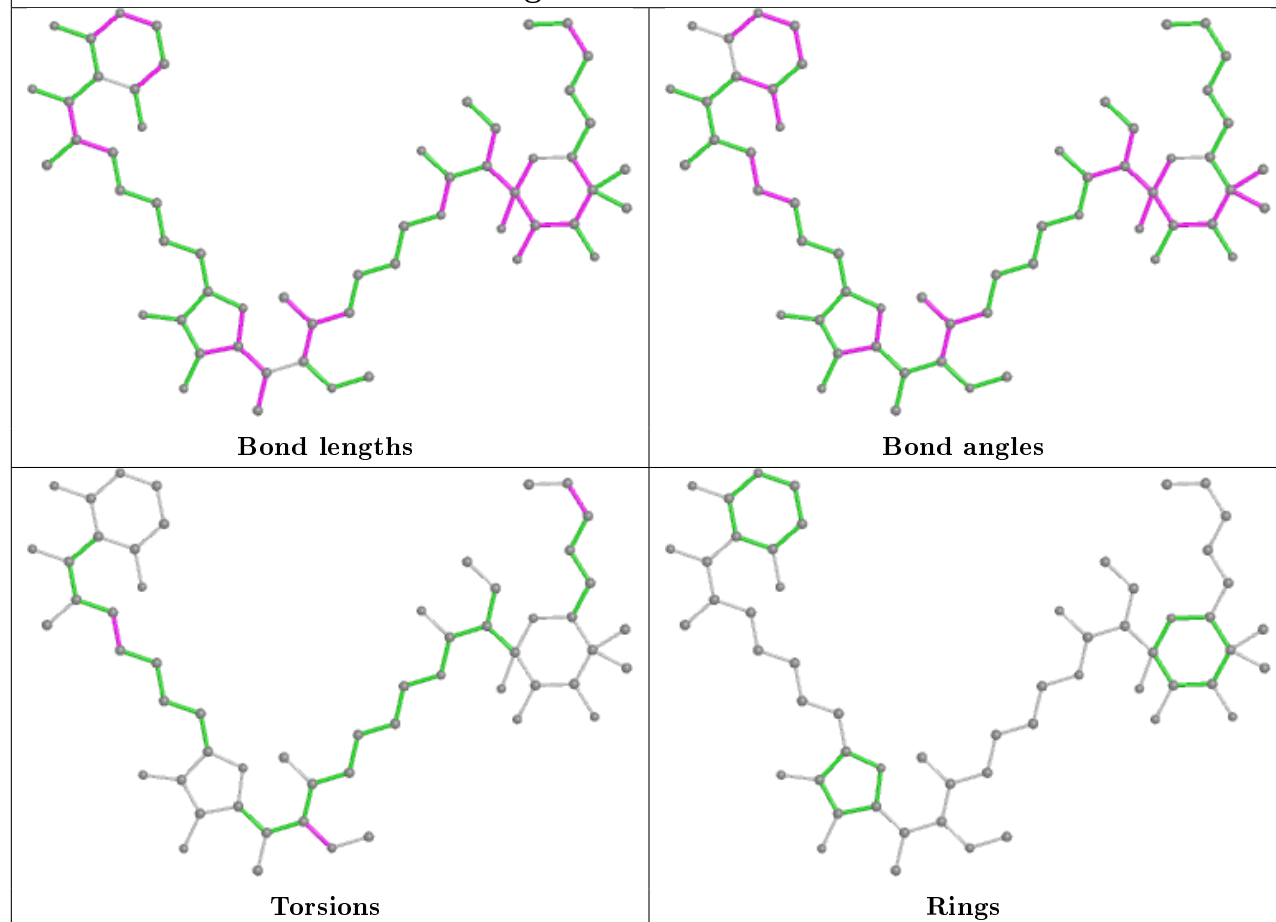
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	2	0
61	CZ	502	KIR	2	0
61	AZ	502	KIR	3	0
60	CZ	501	GDP	6	0

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

## Ligand GDP AZ 501

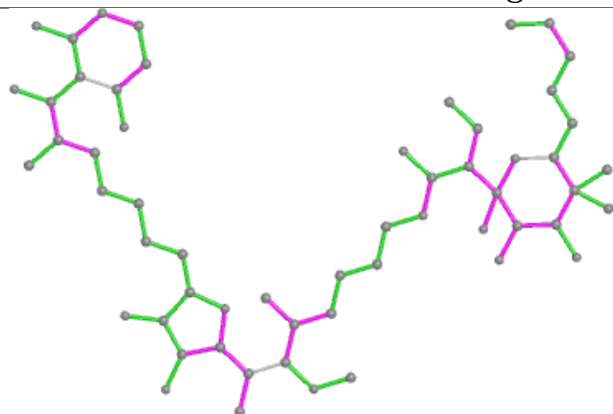


## Ligand KIR CZ 502

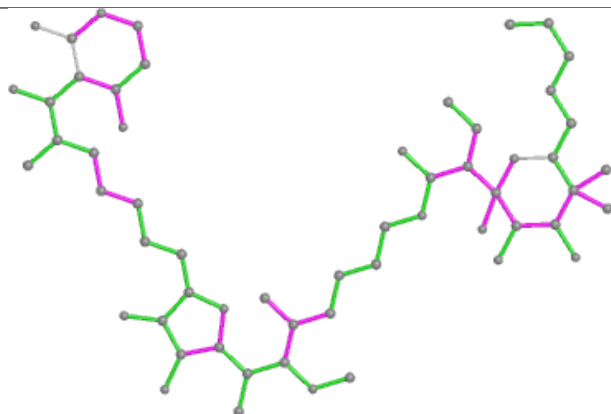




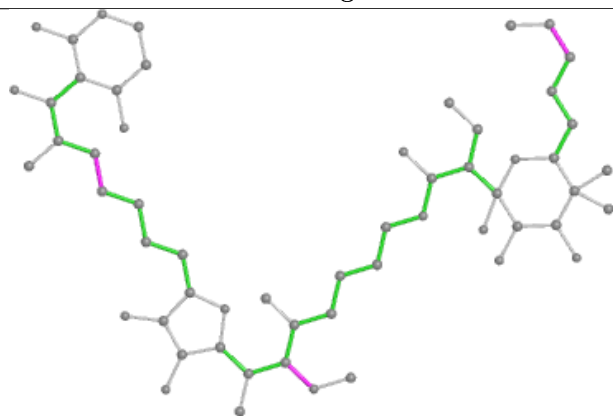
## Ligand KIR AZ 502



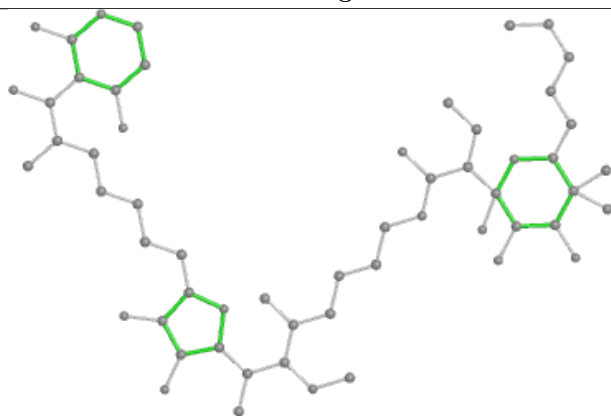
Bond lengths



Bond angles

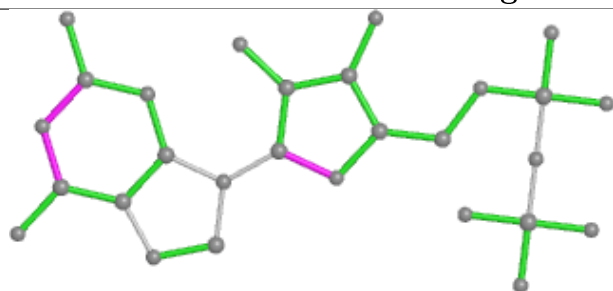


Torsions

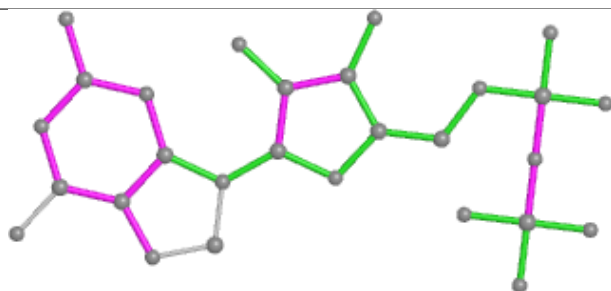


Rings

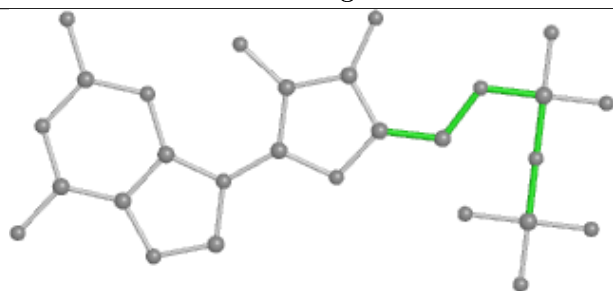
## Ligand GDP CZ 501



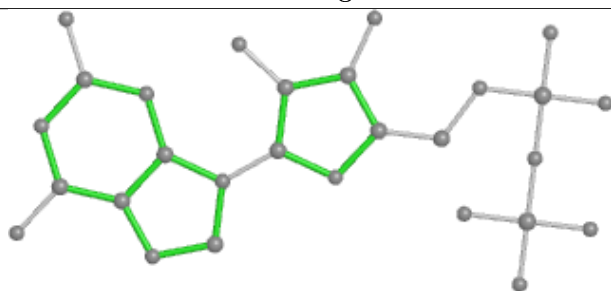
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1510/1522 (99%)	0.02	32 (2%) 63 43	17, 54, 143, 200	0
1	CA	1510/1522 (99%)	-0.17	26 (1%) 70 49	26, 58, 145, 200	0
2	AB	234/256 (91%)	-0.14	2 (0%) 84 69	34, 64, 130, 141	0
2	CB	234/256 (91%)	-0.12	6 (2%) 56 33	36, 65, 130, 142	0
3	AC	206/239 (86%)	-0.30	0 100 100	27, 48, 81, 86	0
3	CC	206/239 (86%)	-0.41	0 100 100	32, 52, 82, 88	0
4	AD	208/209 (99%)	0.29	8 (3%) 40 20	55, 89, 119, 122	0
4	CD	208/209 (99%)	0.22	12 (5%) 23 10	55, 90, 119, 122	0
5	AE	150/162 (92%)	-0.43	0 100 100	23, 41, 62, 84	0
5	CE	150/162 (92%)	-0.43	0 100 100	30, 44, 64, 86	0
6	AF	101/101 (100%)	-0.25	1 (0%) 82 67	48, 72, 88, 94	0
6	CF	101/101 (100%)	0.04	1 (0%) 82 67	52, 74, 90, 95	0
7	AG	155/156 (99%)	-0.13	4 (2%) 56 33	40, 64, 100, 115	0
7	CG	155/156 (99%)	-0.10	4 (2%) 56 33	45, 67, 101, 115	0
8	AH	138/138 (100%)	-0.41	0 100 100	30, 44, 61, 71	0
8	CH	138/138 (100%)	-0.50	0 100 100	31, 47, 62, 72	0
9	AI	127/128 (99%)	0.26	2 (1%) 72 51	33, 73, 113, 120	0
9	CI	127/128 (99%)	0.34	8 (6%) 20 8	40, 77, 114, 120	0
10	AJ	98/105 (93%)	0.47	5 (5%) 28 13	41, 80, 133, 136	0
10	CJ	98/105 (93%)	0.72	15 (15%) 2 1	44, 84, 134, 137	0
11	AK	119/129 (92%)	-0.13	3 (2%) 57 34	28, 49, 80, 104	0
11	CK	119/129 (92%)	-0.17	3 (2%) 57 34	32, 53, 82, 104	0
12	AL	124/135 (91%)	-0.01	2 (1%) 72 51	28, 66, 87, 125	0
12	CL	124/135 (91%)	0.10	2 (1%) 72 51	30, 67, 88, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	0.09	5 (4%) 38 19	50, 73, 100, 137	0
13	CM	124/126 (98%)	0.17	8 (6%) 18 8	53, 76, 101, 137	0
14	AN	60/61 (98%)	-0.04	1 (1%) 70 49	33, 48, 76, 79	0
14	CN	60/61 (98%)	-0.19	1 (1%) 70 49	39, 53, 76, 80	0
15	AO	88/89 (98%)	-0.35	0 100 100	36, 51, 73, 81	0
15	CO	88/89 (98%)	-0.22	0 100 100	37, 53, 73, 81	0
16	AP	83/88 (94%)	0.28	0 100 100	62, 78, 99, 125	0
16	CP	83/88 (94%)	0.34	3 (3%) 42 22	62, 80, 100, 124	0
17	AQ	99/105 (94%)	-0.20	0 100 100	33, 55, 72, 83	0
17	CQ	99/105 (94%)	-0.17	0 100 100	39, 56, 73, 83	0
18	AR	70/88 (79%)	-0.25	1 (1%) 75 56	37, 55, 87, 99	0
18	CR	70/88 (79%)	-0.15	2 (2%) 51 28	43, 59, 88, 99	0
19	AS	78/93 (83%)	0.38	6 (7%) 13 5	61, 81, 116, 125	0
19	CS	78/93 (83%)	0.53	6 (7%) 13 5	63, 83, 117, 125	0
20	AT	99/106 (93%)	0.20	5 (5%) 28 13	49, 77, 112, 115	0
20	CT	99/106 (93%)	0.30	4 (4%) 38 19	52, 78, 113, 115	0
21	AU	24/27 (88%)	0.31	1 (4%) 36 18	43, 55, 76, 93	0
21	CU	24/27 (88%)	0.56	3 (12%) 3 1	46, 59, 78, 92	0
22	AV	76/76 (100%)	-0.13	0 100 100	34, 64, 95, 113	0
22	AW	76/76 (100%)	0.89	11 (14%) 2 1	60, 165, 193, 200	0
22	CV	76/76 (100%)	-0.21	0 100 100	38, 66, 97, 114	0
22	CW	76/76 (100%)	1.03	14 (18%) 1 0	63, 166, 193, 200	0
23	AX	17/27 (62%)	0.76	3 (17%) 1 0	27, 87, 137, 139	0
23	CX	17/27 (62%)	0.83	5 (29%) 0 0	32, 89, 137, 140	0
24	AY	68/77 (88%)	1.50	20 (29%) 0 0	70, 145, 175, 178	0
24	CY	68/77 (88%)	1.77	29 (42%) 0 0	72, 146, 174, 178	0
25	AZ	385/405 (95%)	0.86	54 (14%) 2 1	84, 129, 155, 177	0
25	CZ	385/405 (95%)	0.97	57 (14%) 2 1	85, 129, 155, 177	0
26	B0	84/85 (98%)	0.28	7 (8%) 11 4	47, 64, 95, 108	0
26	D0	84/85 (98%)	0.38	7 (8%) 11 4	50, 66, 95, 108	0
27	B1	93/98 (94%)	0.03	1 (1%) 80 64	38, 55, 114, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.31	5 (5%) 25 12	54, 71, 121, 129	0
28	B2	71/72 (98%)	1.35	19 (26%) 0 0	108, 136, 147, 149	0
28	D2	71/72 (98%)	0.55	4 (5%) 24 11	88, 107, 126, 142	0
29	B3	59/60 (98%)	0.23	1 (1%) 70 49	50, 71, 91, 116	0
29	D3	59/60 (98%)	0.53	3 (5%) 28 13	51, 72, 91, 116	0
30	B4	44/71 (61%)	0.98	5 (11%) 5 2	109, 148, 172, 176	0
30	D4	44/71 (61%)	0.53	3 (6%) 17 7	110, 148, 172, 176	0
31	B5	59/60 (98%)	0.10	3 (5%) 28 13	45, 71, 131, 148	0
31	D5	59/60 (98%)	0.19	4 (6%) 17 7	46, 73, 130, 148	0
32	B6	50/54 (92%)	1.03	6 (12%) 4 2	50, 80, 106, 112	0
32	D6	50/54 (92%)	0.92	6 (12%) 4 2	54, 82, 106, 114	0
33	B7	48/49 (97%)	0.07	1 (2%) 63 43	45, 53, 90, 110	0
33	D7	48/49 (97%)	-0.05	0 100 100	47, 55, 89, 110	0
34	B8	63/65 (96%)	0.29	3 (4%) 30 14	49, 63, 79, 101	0
34	D8	63/65 (96%)	0.29	4 (6%) 20 8	51, 65, 80, 101	0
35	B9	37/37 (100%)	0.37	1 (2%) 54 31	62, 75, 96, 98	0
35	D9	37/37 (100%)	0.61	2 (5%) 25 12	61, 77, 96, 98	0
36	BA	2901/2915 (99%)	0.12	116 (3%) 38 19	21, 65, 173, 200	0
36	DA	2901/2915 (99%)	0.05	107 (3%) 41 21	26, 67, 173, 200	0
37	BB	119/122 (97%)	-0.16	0 100 100	52, 81, 104, 123	0
37	DB	119/122 (97%)	-0.27	0 100 100	55, 82, 104, 123	0
38	BC	228/229 (99%)	0.21	13 (5%) 23 11	47, 78, 152, 166	0
38	DC	228/229 (99%)	0.63	29 (12%) 3 1	51, 80, 152, 167	0
39	BD	275/276 (99%)	-0.27	3 (1%) 80 64	27, 44, 71, 96	0
39	DD	275/276 (99%)	-0.30	2 (0%) 87 75	29, 46, 71, 96	0
40	BE	204/206 (99%)	0.14	9 (4%) 34 17	40, 65, 114, 124	0
40	DE	204/206 (99%)	0.11	8 (3%) 39 20	41, 65, 114, 124	0
41	BF	207/210 (98%)	0.30	12 (5%) 23 10	45, 96, 152, 159	0
41	DF	207/210 (98%)	0.40	16 (7%) 13 5	45, 97, 152, 159	0
42	BG	181/182 (99%)	-0.09	6 (3%) 46 24	50, 73, 111, 132	0
42	DG	181/182 (99%)	0.21	8 (4%) 34 17	78, 100, 124, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	1.03	24 (15%) 2 1	84, 119, 144, 150	0
43	DH	159/180 (88%)	0.94	21 (13%) 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%)	0.03	1 (0%) 87 75	51, 74, 118, 123	0
46	DN	138/140 (98%)	0.04	1 (0%) 87 75	51, 75, 118, 123	0
47	BO	122/122 (100%)	-0.32	0 100 100	35, 49, 62, 66	0
47	DO	122/122 (100%)	-0.40	0 100 100	35, 50, 62, 65	0
48	BP	146/150 (97%)	0.73	11 (7%) 14 5	47, 93, 118, 139	0
48	DP	146/150 (97%)	0.83	19 (13%) 3 1	49, 95, 118, 139	0
49	BQ	141/141 (100%)	-0.08	2 (1%) 75 56	35, 54, 75, 117	0
49	DQ	141/141 (100%)	-0.09	2 (1%) 75 56	39, 54, 76, 117	0
50	BR	117/118 (99%)	0.14	1 (0%) 84 69	51, 70, 88, 93	0
50	DR	117/118 (99%)	0.12	4 (3%) 45 24	52, 71, 89, 93	0
51	BS	98/112 (87%)	0.37	3 (3%) 49 26	69, 89, 114, 118	0
51	DS	98/112 (87%)	0.72	12 (12%) 4 1	71, 90, 114, 117	0
52	BT	137/146 (93%)	0.20	10 (7%) 15 6	50, 71, 133, 164	0
52	DT	137/146 (93%)	0.17	10 (7%) 15 6	51, 72, 134, 164	0
53	BU	117/118 (99%)	-0.00	1 (0%) 84 69	51, 68, 90, 112	0
53	DU	117/118 (99%)	-0.07	1 (0%) 84 69	52, 69, 89, 112	0
54	BV	101/101 (100%)	0.35	4 (3%) 38 19	52, 98, 113, 116	0
54	DV	101/101 (100%)	0.41	6 (5%) 22 10	52, 98, 113, 116	0
55	BW	113/113 (100%)	0.05	2 (1%) 68 47	56, 71, 102, 133	0
55	DW	113/113 (100%)	0.19	2 (1%) 68 47	56, 72, 103, 134	0
56	BX	92/96 (95%)	0.28	0 100 100	64, 83, 101, 111	0
56	DX	92/96 (95%)	0.23	0 100 100	65, 84, 102, 112	0
57	BY	100/110 (90%)	1.35	22 (22%) 0 0	93, 114, 151, 160	0
57	DY	100/110 (90%)	1.50	31 (31%) 0 0	93, 114, 151, 160	0
58	BZ	176/206 (85%)	0.06	5 (2%) 53 30	44, 71, 117, 123	0
58	DZ	176/206 (85%)	0.17	5 (2%) 53 30	56, 78, 111, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21994/23376 (94%)	0.14	989 (4%) 33 16	17, 69, 146, 200	0

The worst 5 of 989 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	2802	G	12.0
49	DQ	141	GLN	10.9
58	DZ	113	ALA	10.7
36	DA	2802	G	10.3
42	DG	2	PRO	9.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	7MG	CY	46	24/25	0.50	0.47	170,172,175,176	0
24	H2U	CY	16	20/21	0.53	0.58	170,173,173,174	0
24	H2U	AY	16	20/21	0.54	0.60	169,173,173,174	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	4SU	AY	8	20/21	0.63	0.34	145,147,149,149	0
24	H2U	CY	17	20/21	0.65	0.52	170,173,175,176	0
24	H2U	AY	17	20/21	0.67	0.62	170,174,175,176	0
24	PSU	CY	55	20/21	0.70	0.43	154,160,160,160	0
24	H2U	AY	20	20/21	0.71	0.52	178,179,179,179	0
24	PSU	AY	55	20/21	0.74	0.39	154,159,160,161	0
24	4SU	CY	8	20/21	0.74	0.34	146,147,148,149	0
24	5MU	AY	54	21/22	0.78	0.32	145,149,150,153	0
24	5MU	CY	54	21/22	0.80	0.39	144,149,151,153	0
24	OMC	CY	32	21/22	0.82	0.50	107,112,121,122	0
24	MIA	AY	37	29/30	0.90	0.32	71,88,103,104	0
24	OMC	AY	32	21/22	0.90	0.31	107,112,120,121	0
24	MIA	CY	37	29/30	0.93	0.25	74,88,101,102	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

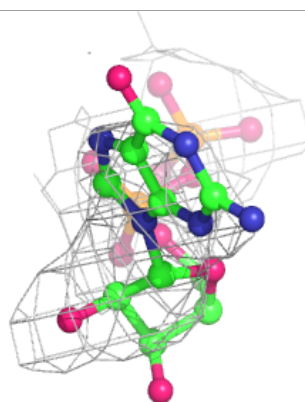
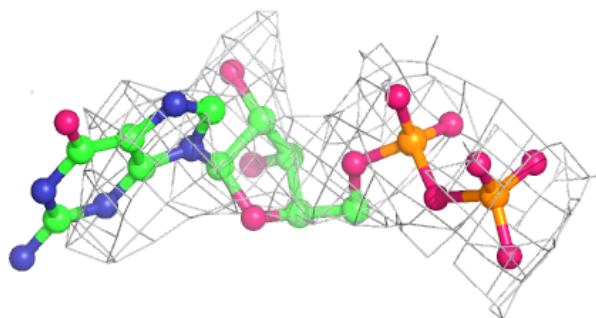
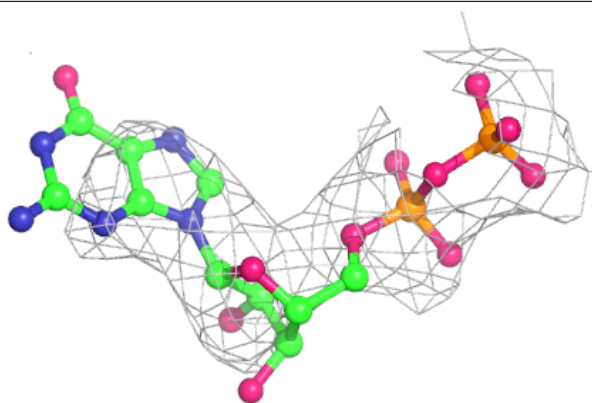
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	GDP	AZ	501	28/28	0.78	0.31	130,136,140,141	0
61	KIR	CZ	502	57/57	0.84	0.35	118,120,121,123	0
61	KIR	AZ	502	57/57	0.85	0.31	117,119,121,122	0
60	GDP	CZ	501	28/28	0.86	0.17	129,136,140,140	0
59	ZN	D4	101	1/1	0.94	0.10	115,115,115,115	0
59	ZN	B4	101	1/1	0.97	0.17	90,90,90,90	0
59	ZN	D9	101	1/1	0.97	0.11	81,81,81,81	0
59	ZN	B9	101	1/1	0.99	0.11	82,82,82,82	0
59	ZN	AD	301	1/1	0.99	0.25	59,59,59,59	0
59	ZN	CN	101	1/1	0.99	0.17	60,60,60,60	0
59	ZN	AN	101	1/1	1.00	0.16	34,34,34,34	0
59	ZN	CD	301	1/1	1.00	0.26	72,72,72,72	0

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

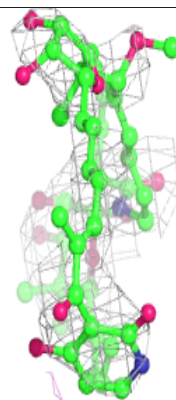
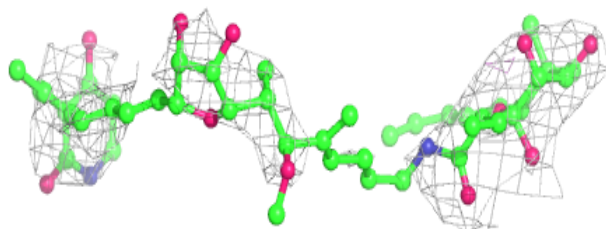
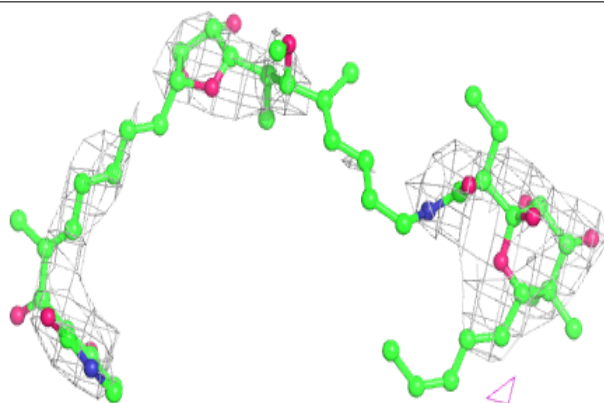


**Electron density around GDP AZ 501:**

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

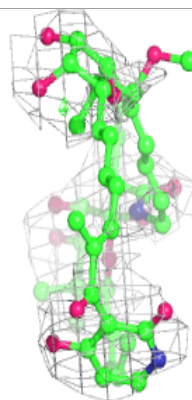
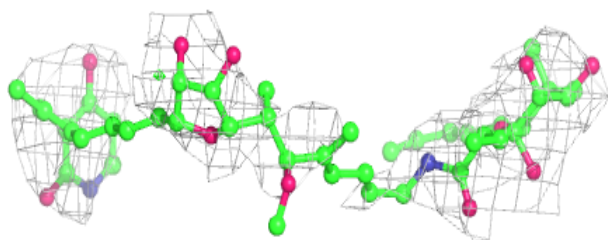
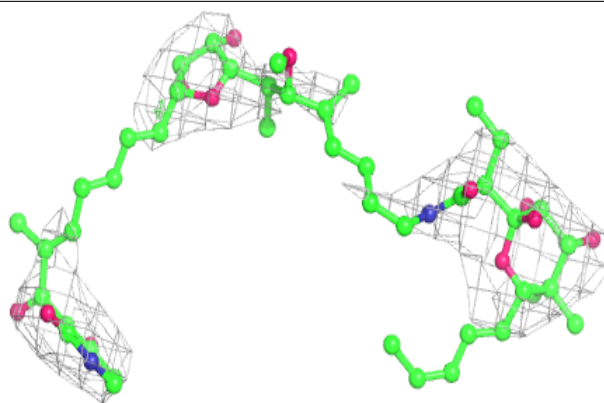
**Electron density around KIR CZ 502:**

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

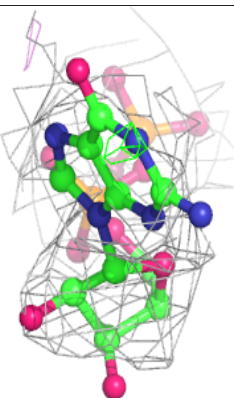
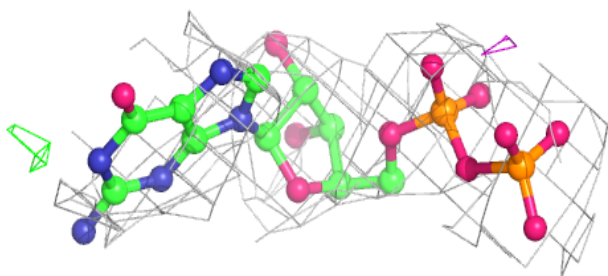
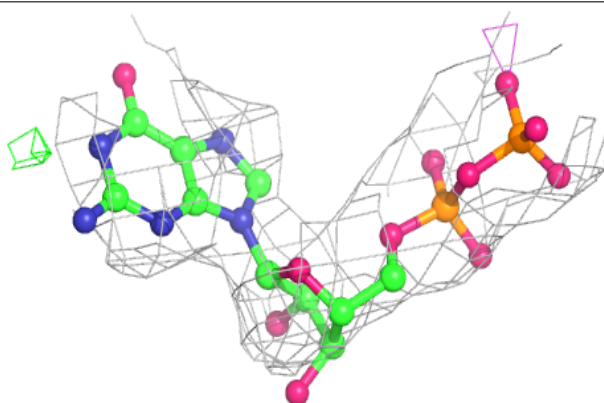


**Electron density around KIR AZ 502:**

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

**Electron density around GDP CZ 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.