



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 04:44 am BST

PDB ID : 4V5R
Title : The crystal structure of EF-Tu and Trp-tRNA-Trp bound to a cognate codon on the 70S ribosome.
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

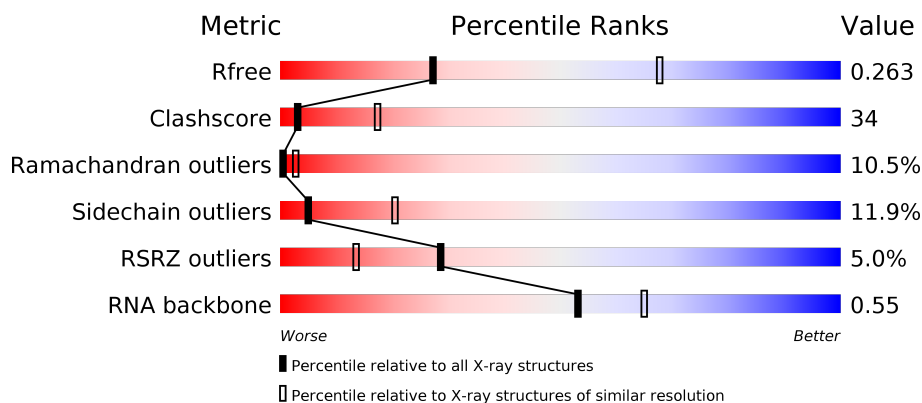
1 Overall quality at a glance

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 ≥ 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	<div> <div> <div></div> <div>38%</div> <div>48%</div> <div>11%</div> <div>••</div> </div> </div>
1	CA	1522	<div> <div> <div>2%</div> <div>42%</div> <div>45%</div> <div>10%</div> <div>••</div> </div> </div>
2	AB	256	<div> <div> <div>2%</div> <div>30%</div> <div>50%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
2	CB	256	<div> <div> <div></div> <div>33%</div> <div>46%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>



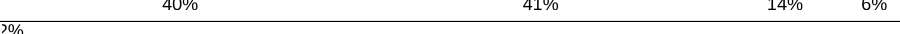
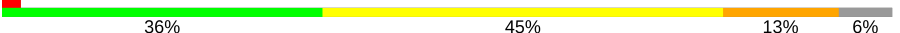

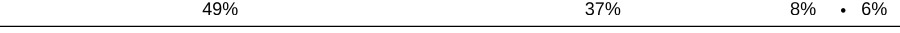

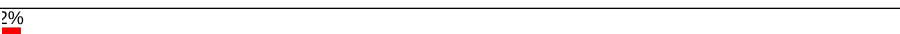
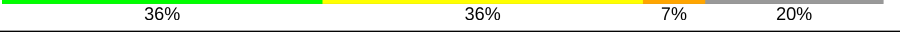
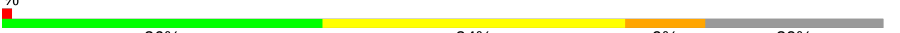
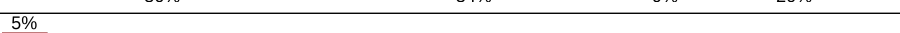


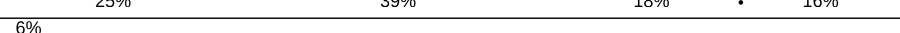
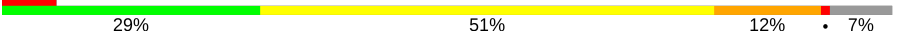

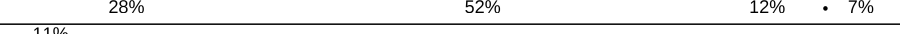


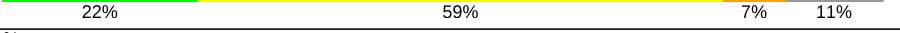

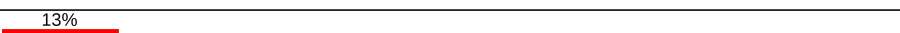
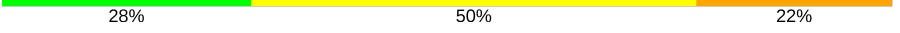


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
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	

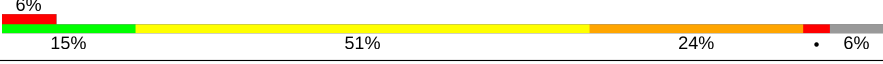


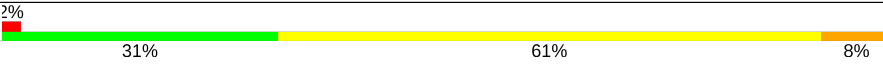
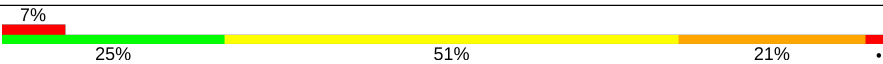
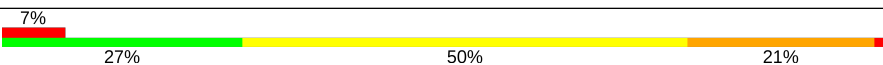
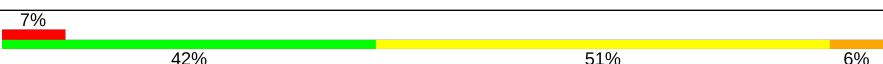
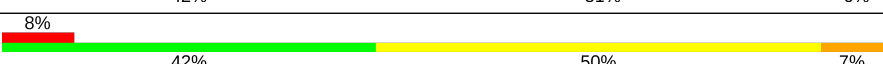
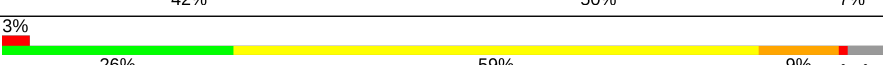
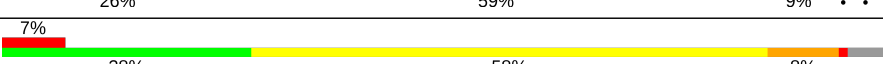
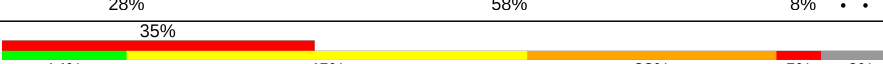
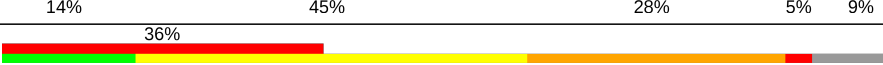
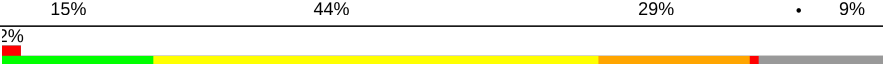
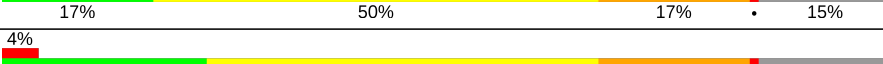
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Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	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	CY	16	-	-	-	X
24	H2U	CY	17	-	-	-	X
59	ZN	AD	301	-	-	X	-
59	ZN	AN	101	-	-	X	-
59	ZN	CD	301	-	-	X	-
59	ZN	CN	101	-	-	X	-
60	GDP	AZ	501	-	-	X	-
61	KIR	AZ	502	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307330 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			

- 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			
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
			362	164	68	114	16			
23	CX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	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
			2984	1885	524	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

- 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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

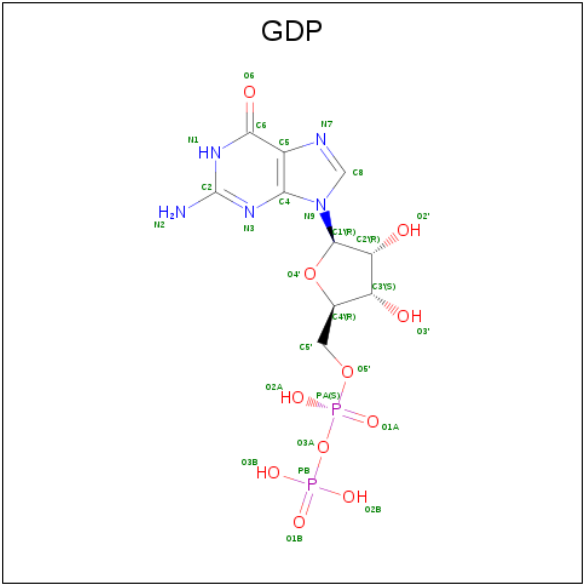
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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).

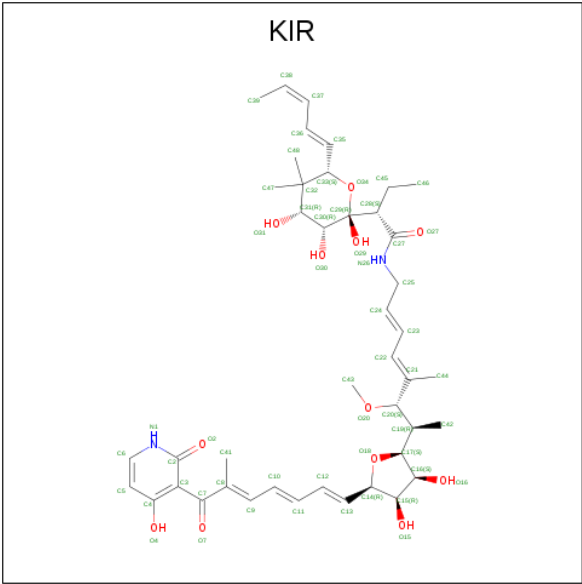
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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: C₄₃H₆₀N₂O₁₂).

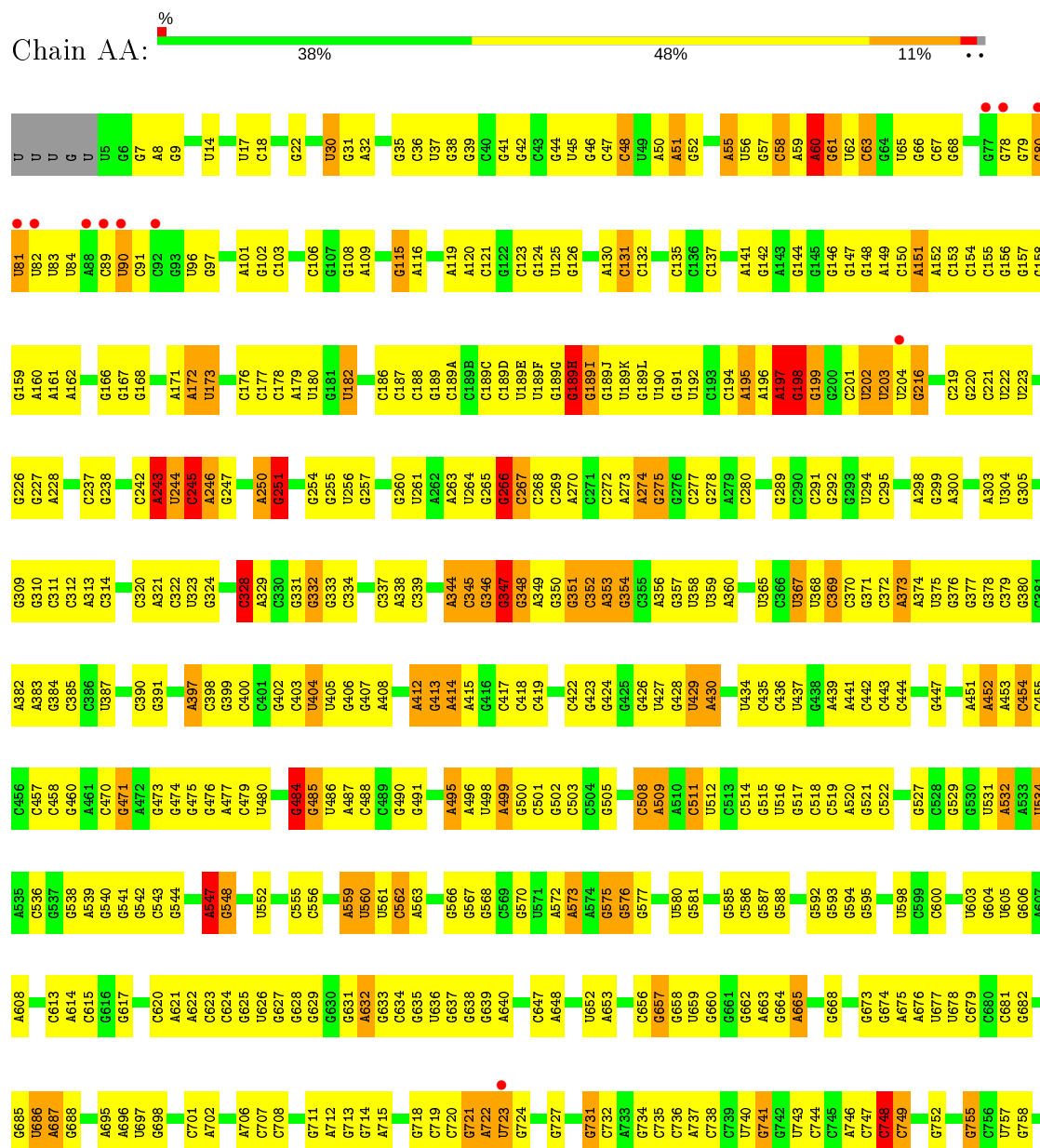


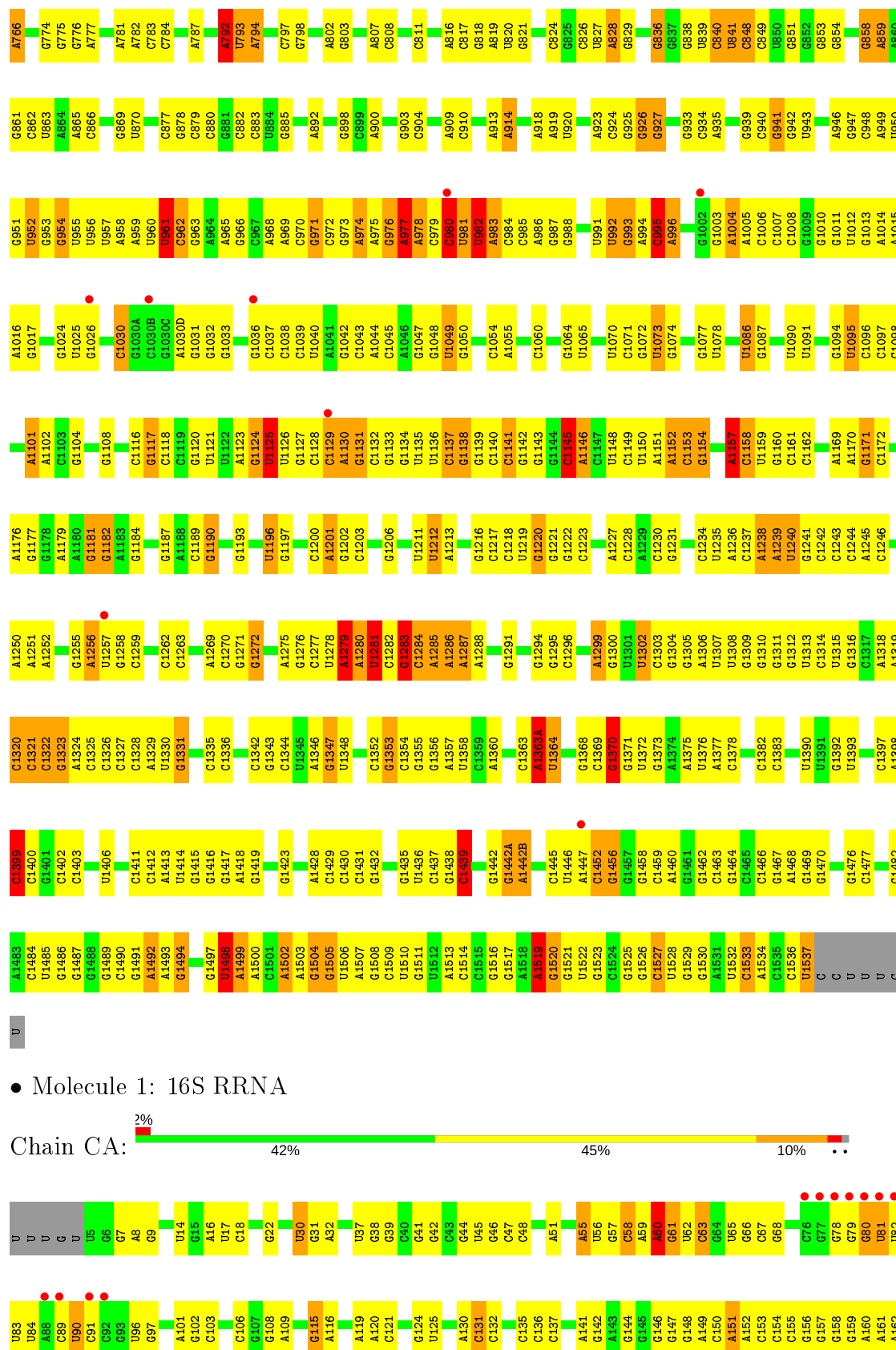
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

3 Residue-property plots

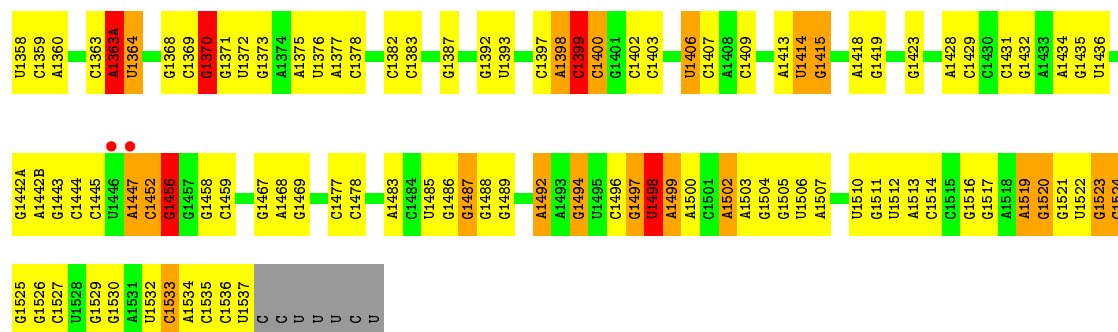
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

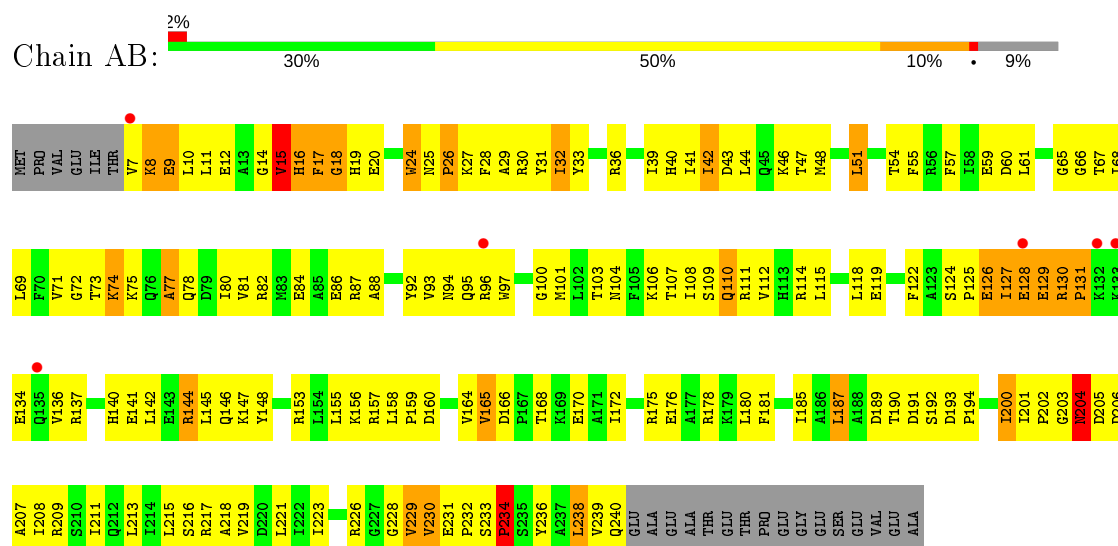




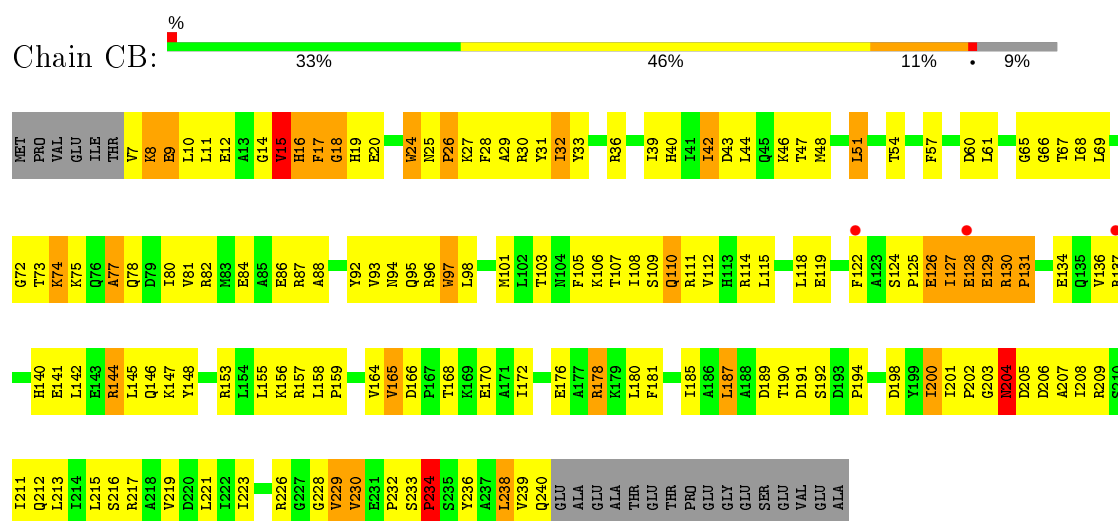
A1286	A1287	A1288	G1291	G1294	G1295	G1296	A1299	G1300	G1301	G1302	A1227	G1303	G1304	G1305	A1306	U1307	U1308	G1310	G1309	G1311	G1312	A1238	A1239	U1313	U1314	G1315	G1316	G1317	A1318	A1319	G1320	G1321	G1322	G1323	A1324	G1325	A1256	U1257	G1258	C1259	G1262	G1263	G1269	G1270	G1271	G1272	A1275	G1276	G1277	U1278	A1279	A1280	U1281	G1282	G1283	G1284	A1285
G1133	G1134	U1135	U1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	C1145	C1059	U1146	U1147	U1148	U1149	U1150	A1151	A1152	G1153	G1154	A1157	G1158	U1159	G1160	U1086	G1087	U1170	G1171	G1172	U1095	G1096	C1097	G1098	A1101	A1102	G1181	G1182	A1183	G1184	G1187	A1188	G1189	G1190	G1193	U1196	G1197	G1198	U1199	A1279	A1280	C1201	G1202	G1203	G1206	
A1044	C1045	A1046	G1047	U1048	G1049	G1050	G1053	G1054	A1055	G1058	C1059	G1064	U1065	U1070	C1071	U1072	U1073	G1074	G1077	U1078	U1086	G1087	G1094	U1095	C1096	C1097	G1098	A1101	A1102	G1181	G1182	A1183	G1184	A1179	A1180	G1181	G1182	A1183	G1184	C1116	G1117	C1118	G1119	G1120	U1121	A1123	G1124	U1125	U1126	G1127	C1128	A1201	G1202	G1203	G1206		
G976	A977	A978	G979	G980	U981	U982	A983	G984	G987	G988	U991	U992	G993	A994	G995	A996	A1001	G1001A	G1002	G1003	A1004	A1005	G1006	G1007	G1008	U1012	G1013	A1014	A1015	A1016	G1017	G1024	U1025	G1026	G1027	G1028	G1029	C1030	G1030A	G1030B	G1030C	A1030D	G1031	G1032	G1033	G1036	G1037	G1038	G1039	U1040	A1041	G1042	G1043	A1044			
A900	G903	C904	A909	C910	A913	A914	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	G933	C934	A935	G939	C940	G941	G942	G943	G944	G945	A946	G947	C948	G949	G958	A959	A960	G961	C962	G963	A964	A965	A968	A969	G970	G971	G972	G973	A974	A975	A976	A977	A978	A979							
A794	A802	G803	A807	C808	C811	C812	C817	G818	A819	U820	G821	G822	G823	C826	U827	A828	G829	G836	G837	G838	U839	C840	U841	C843	C849	G853	G854	G858	A859	A860	C861	C862	U863	A864	A865	C866	G869	C877	G878	C879	C880	G881	C882	C883	U884	G885	A892	A893	A894	A895							
A712	G713	G714	A715	G719	G720	G721	A722	G723	G724	G727	G731	A733	G734	G735	G736	A737	G738	U740	G741	G742	U743	G744	A745	A746	A747	C748	G752	G755	C756	U757	G758	G765	A766	A767	A768	G769	G775	G776	A777	A781	A782	C783	C784	A787	A792	U793	A794	A795									
G631	A632	G633	C634	U635	U636	G637	G638	G639	A640	G644	G645	U646	C647	A648	U652	A653	G657	G658	U659	G660	G662	A663	G664	A665	G668	G673	G674	A675	A676	U677	U678	C680	G681	G682	U686	A687	G688	A695	A696	U697	G698	C701	A702	A706	C707	C708	G711	G712	G713	G714							
C555	C556	A559	U560	U561	C562	A563	G566	G567	U568	C569	U570	A572	A573	A574	G575	G576	G577	U580	G581	G585	C586	G587	G592	G593	G594	G595	U598	U603	G604	U605	G606	A607	A608	C613	A614	C615	G616	G617	C620	A621	C624	G625	U626	G627	G628	G629	G630										
A321	C322	U323	G324	C328	A329	C330	G332	G333	C334	C337	A338	C339	A344	C345	U346	G347	G348	A349	G350	G351	C352	A353	C355	A356	G357	U358	U359	U367	U368	C370	G371	C372	A373	A452	U453	U454	C455	C456	C457	C458	G460	A461	C470	G471	A472	G473	G474	G475	G476	A477	C479	U480					
G238	C242	A243	U244	A245	A246	G247	A250	G251	C254	G255	G260	U261	A262	A263	U264	G265	G266	C267	C268	C269	A270	C272	A273	G275	G276	C277	G278	A279	C280	G289	C290	C291	G292	G293	U294	C295	A298	G299	C300	A303	U304	G305	G309	C312	A313	C314	C320										
G166	G167	G168	A171	A172	U173	C176	C177	G178	A179	U180	G186	C187	C188	G189	C189A	C189B	G189C	C189D	U189E	U189F	G189G	G189H	A189I	G189J	U189K	G189L	U190	G191	U192	G193	C194	A195	A196	A197	G198	G199	G200	C201	U202	U203	U204	G216	C219	G220	C221	U222	U223	G226	G227	C237							



• Molecule 2: 30S RIBOSOMAL PROBLEM S2

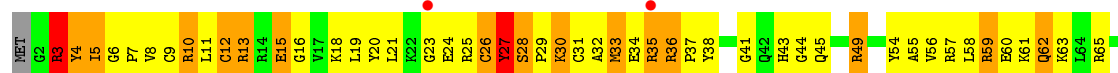


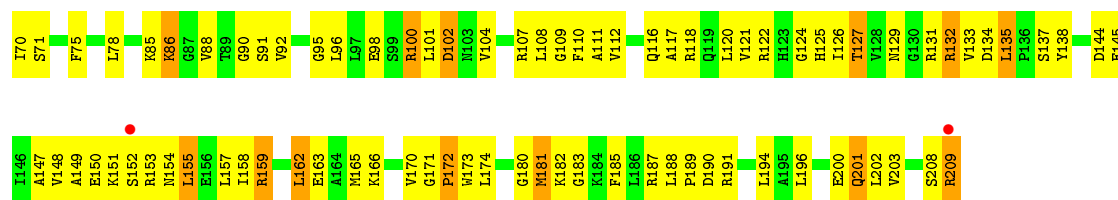
• Molecule 2: 30S RIBOSOMAL PROBLEM S2



• Molecule 3: 30S RIBOSOMAL PROBLEM S3

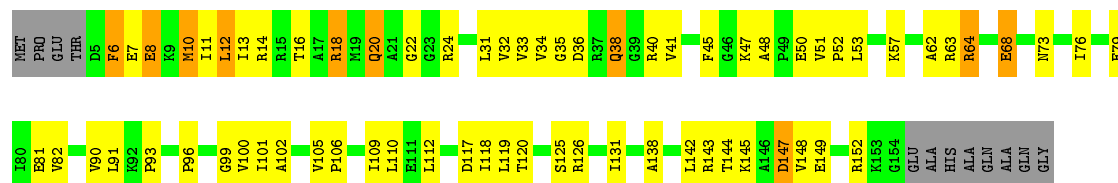






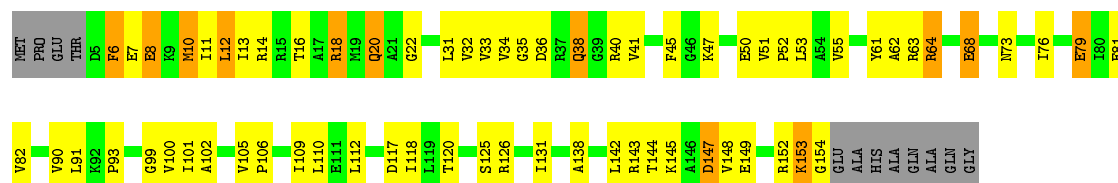
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 51% 36% 6% 7%



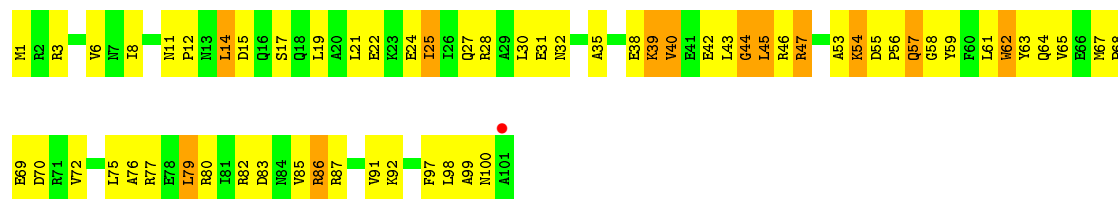
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE: 51% 34% 7% 7%



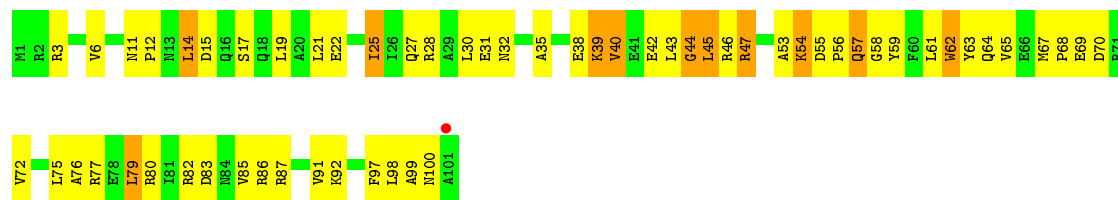
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 39% 50% 12%



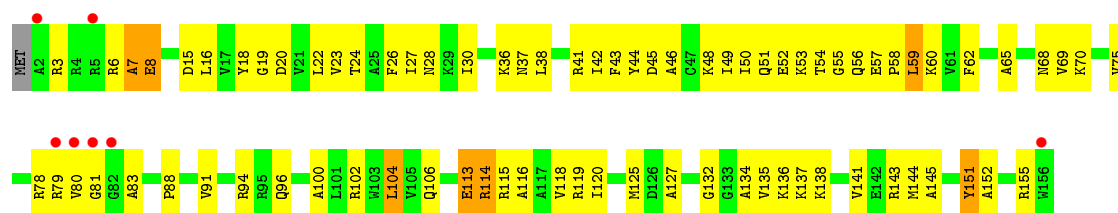
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF: 42% 48% 11%



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

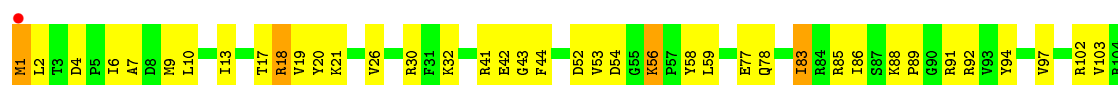
Chain AG: 4% 49% 46%



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



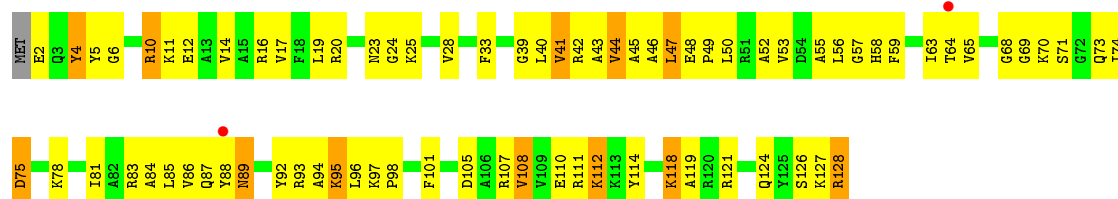
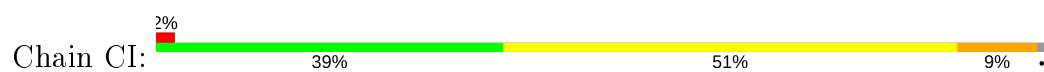
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



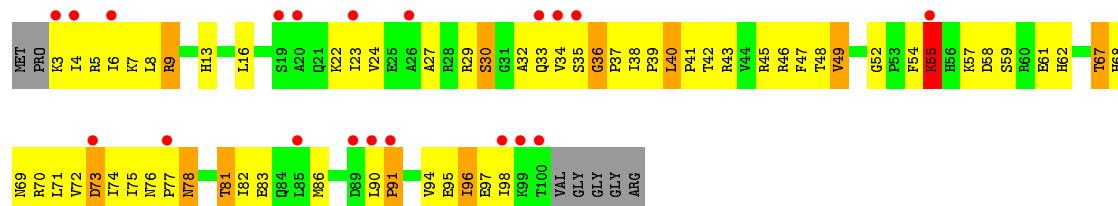
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



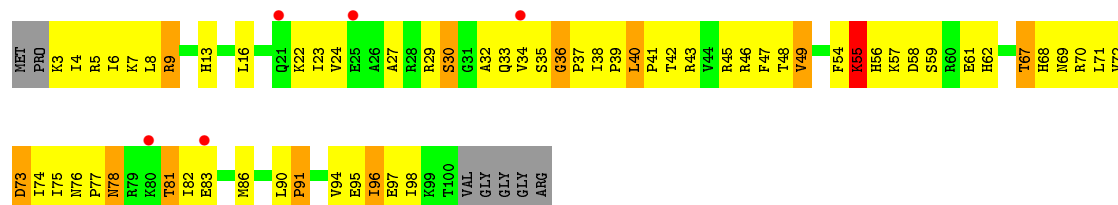
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



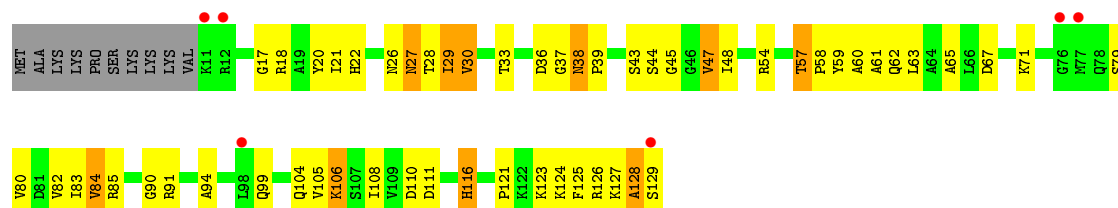
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



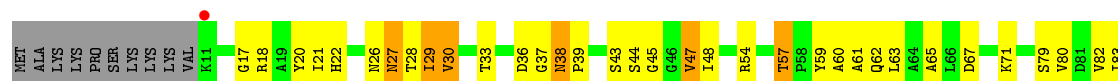
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

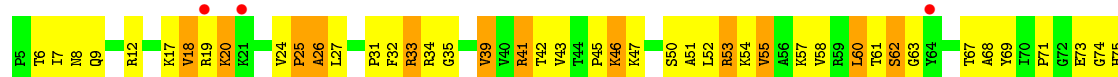


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

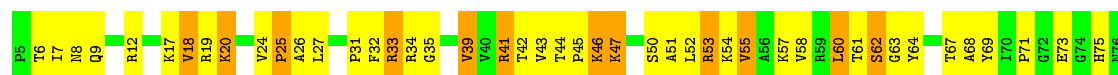




• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

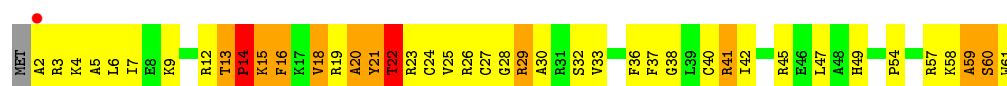


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

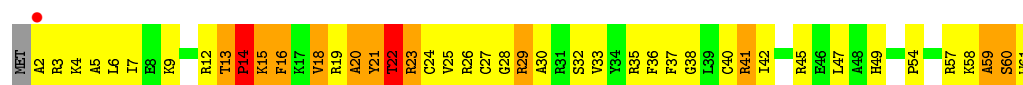


• Molecule 14: 30S RIBOSOMAL PROTEIN S14

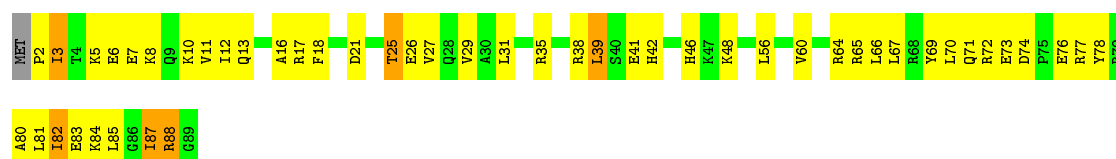




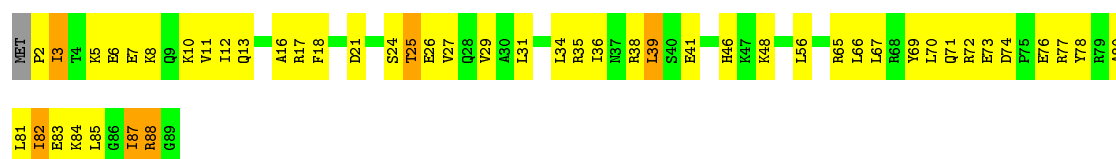
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



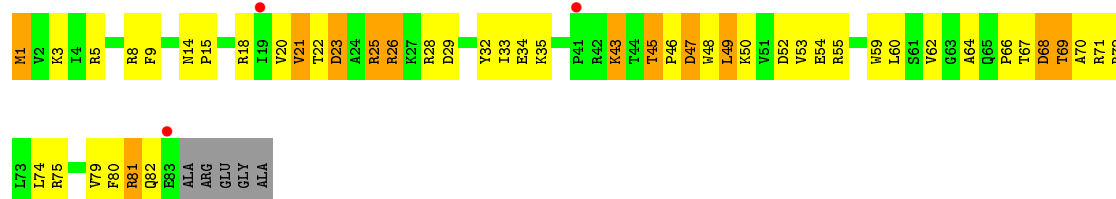
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



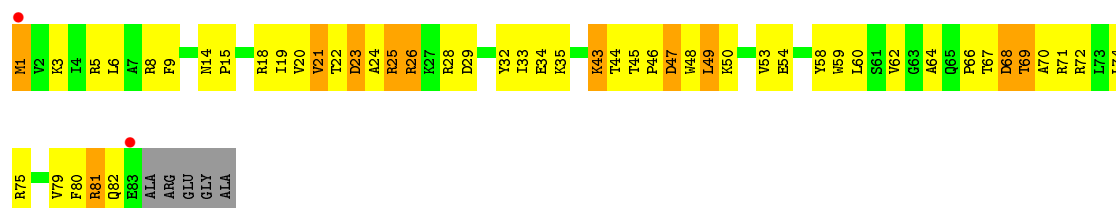
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



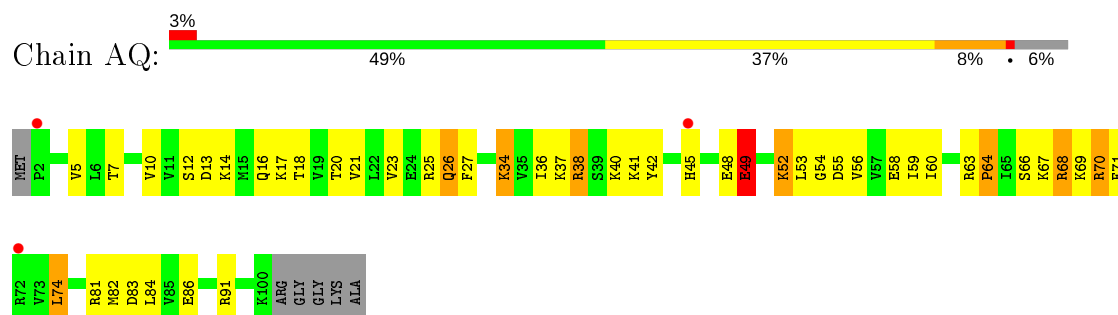
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



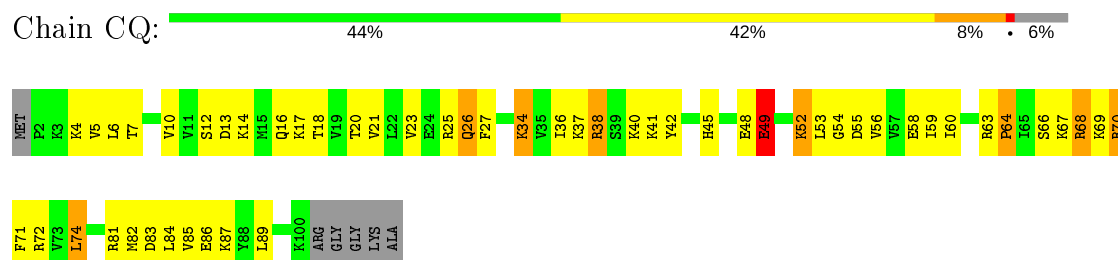
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



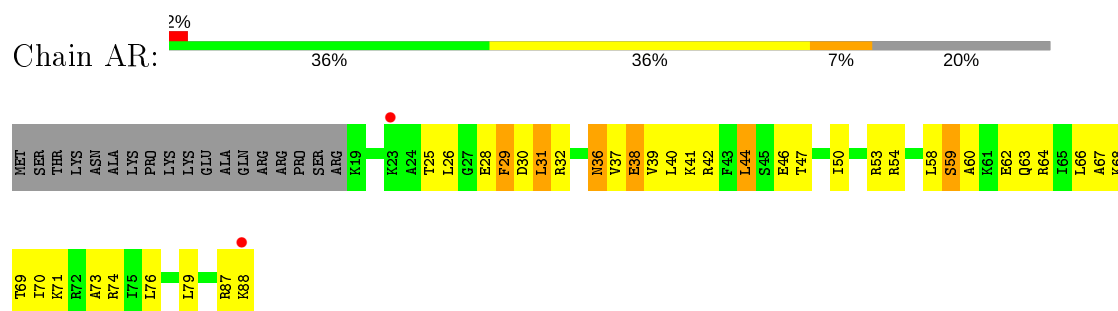
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



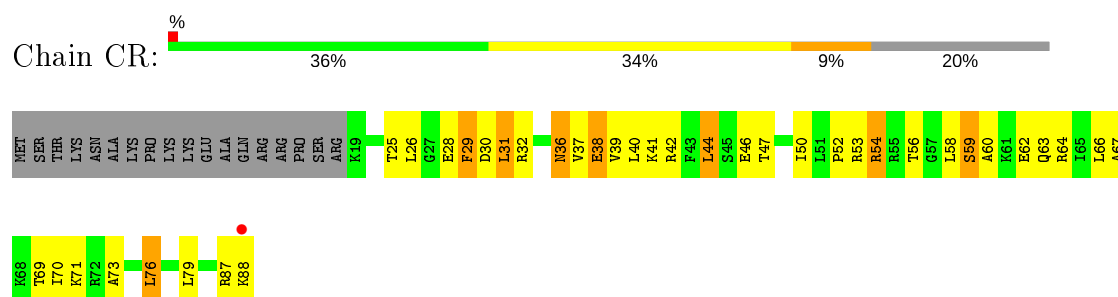
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



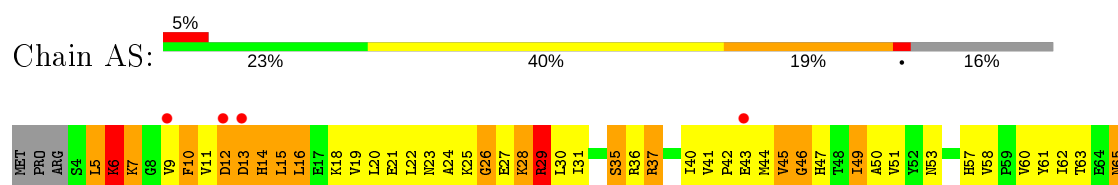
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

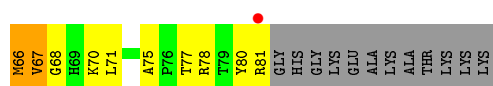


- Molecule 18: 30S RIBOSOMAL PROTEIN S18

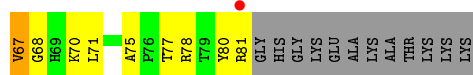


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

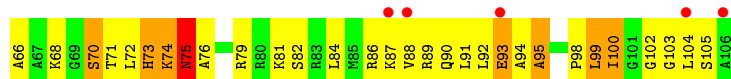




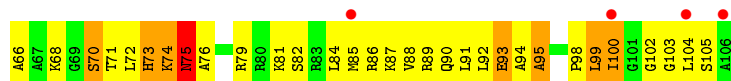
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



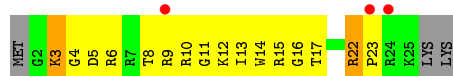
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



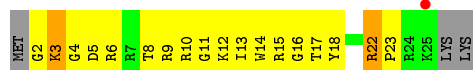
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



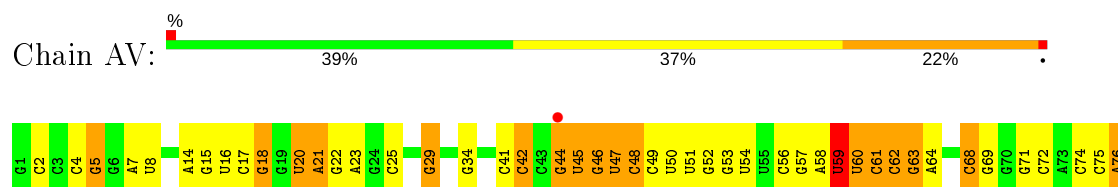
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



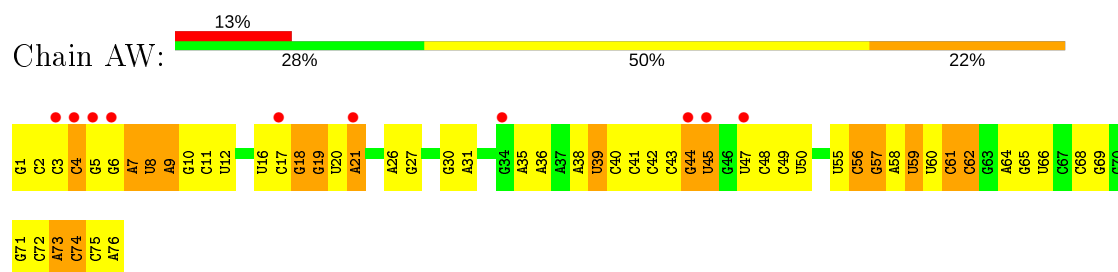
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



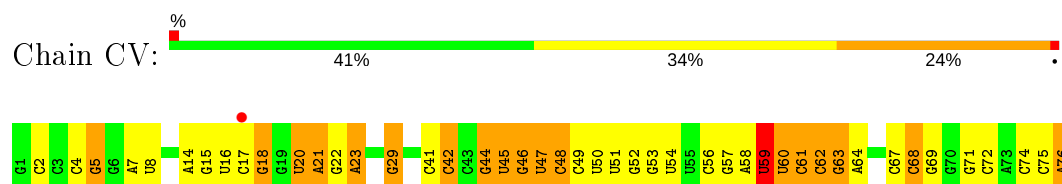
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



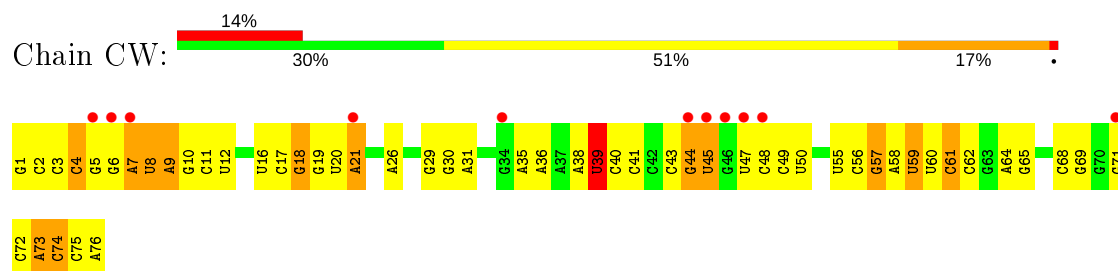
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



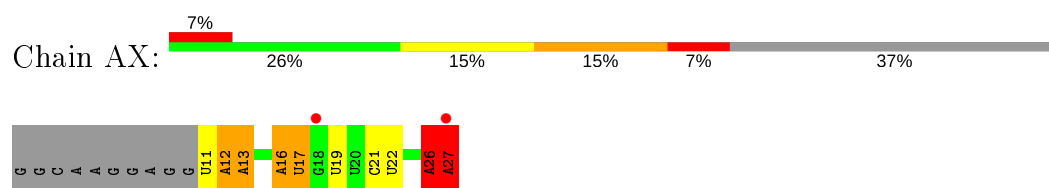
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



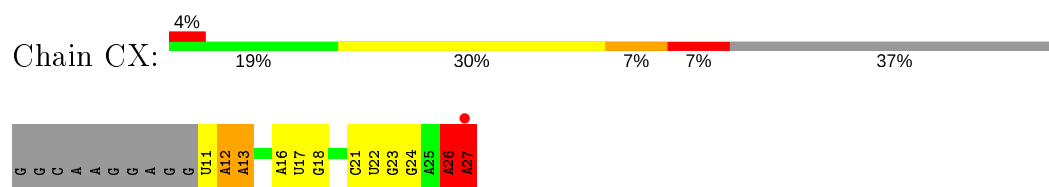
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



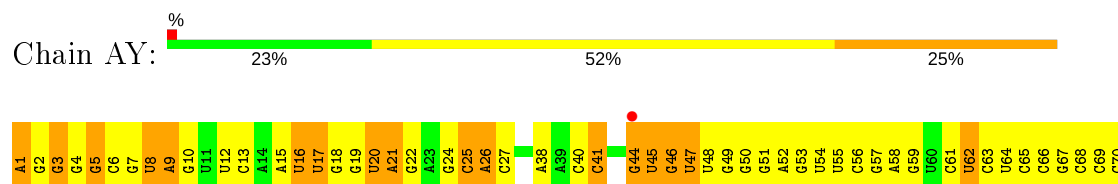
- Molecule 23: MRNA



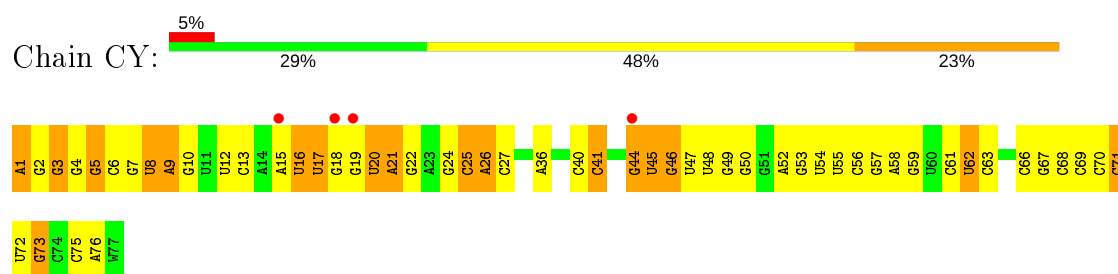
- Molecule 23: MRNA



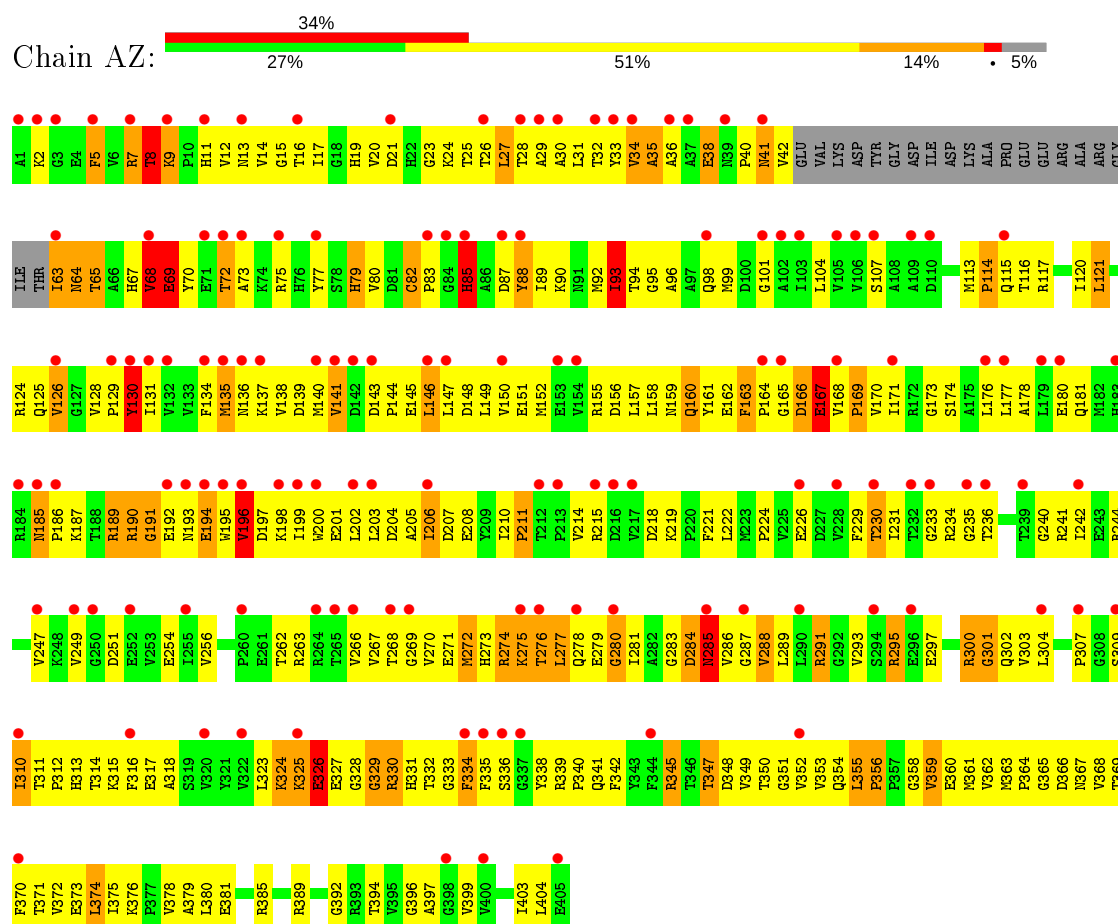
- Molecule 24: A-SITE TRNA TRP-TRNA TRP



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

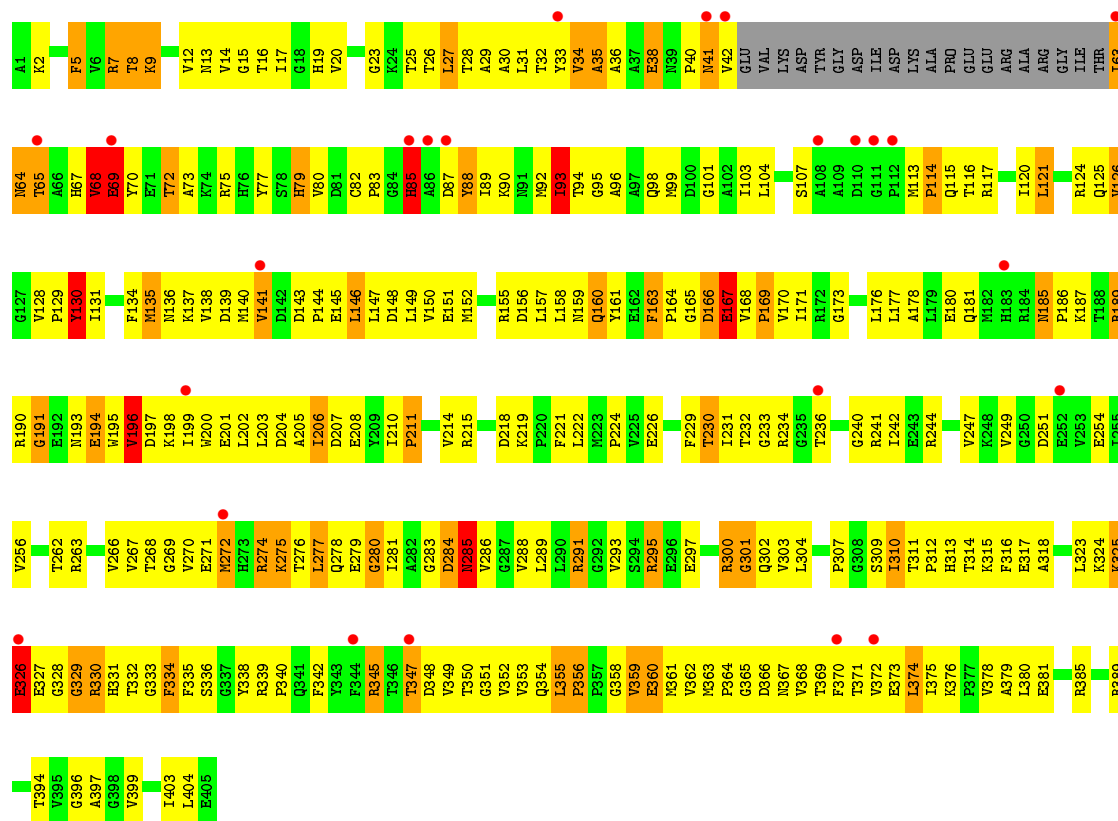


• Molecule 25: ELONGATION FACTOR TU



• Molecule 25: ELONGATION FACTOR TU





• Molecule 26: 50S RIBOSOMAL PROTEIN L27

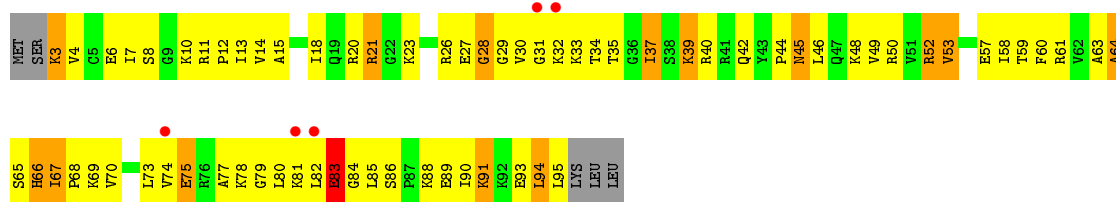


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

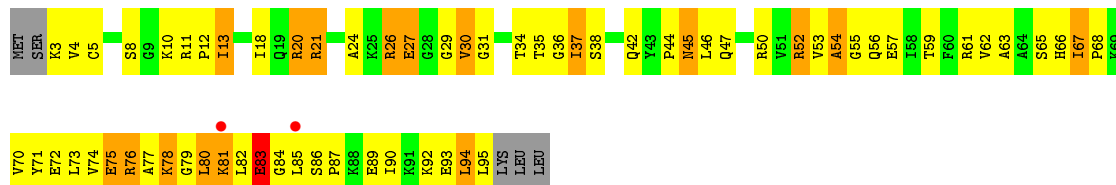


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

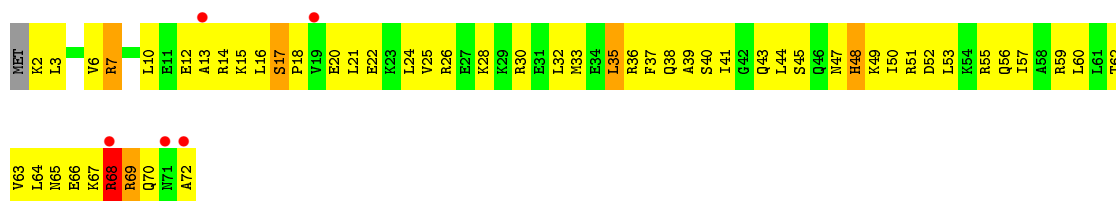




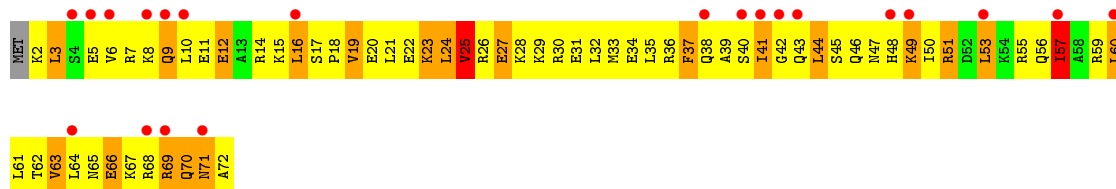
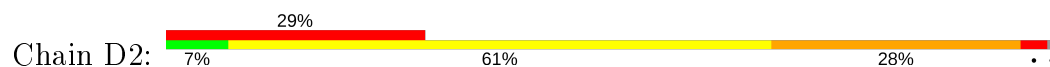
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



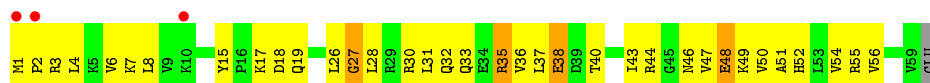
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



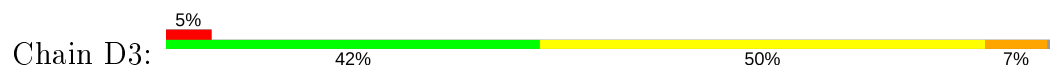
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

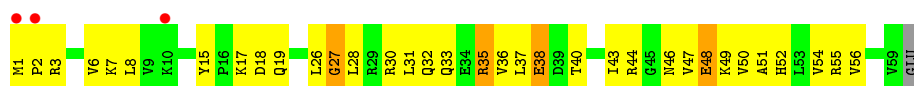


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

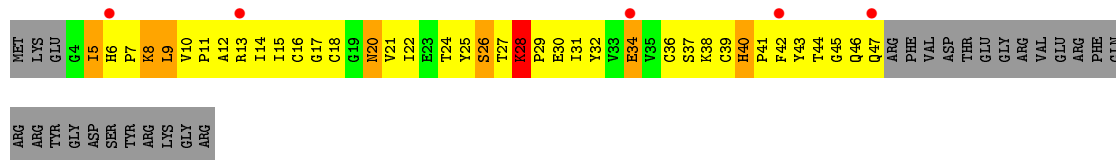


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

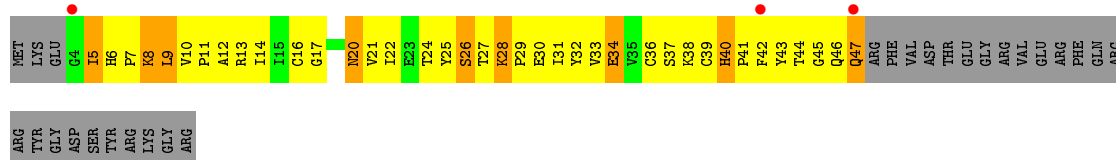




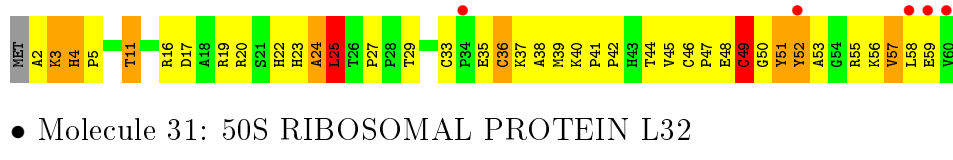
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



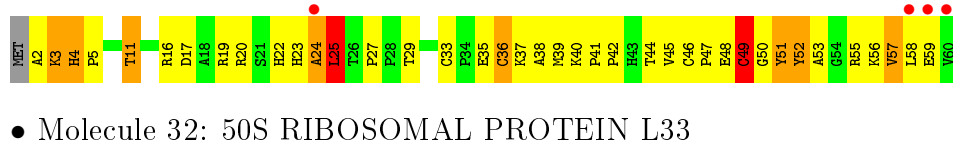
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



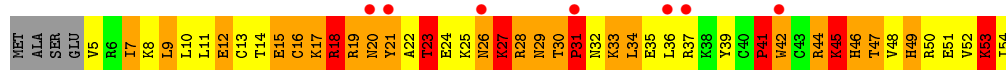
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



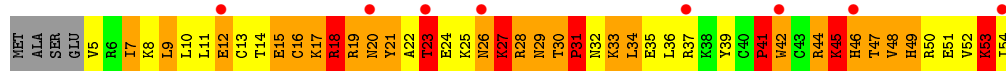
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L33



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7: 




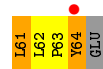
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7: 

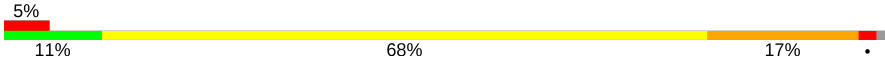


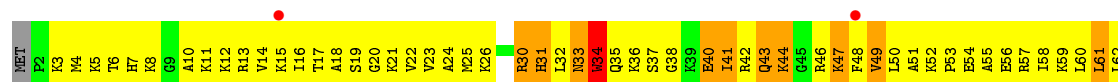
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



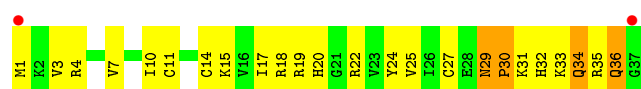
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



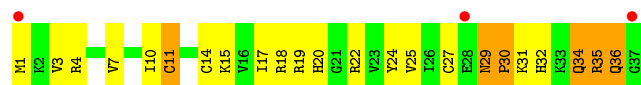
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9: 



- Molecule 36: 23S RIBOSOMAL RNA



C1881	A1803	G1719	A1477	G1410	A1336	G1258	C1179	U1105	G1041	C961	C888
C1882	C1894	U1720	G1478	C1411	G1337	G1259	C1180	G1106	G1042		C889
G1883	U1805	G1721	G1479	A1412	G1338	G1260		U1107	C1043		A890
A1884	G1806	A1722	G1480	G1413	G1339	C1261	G1186	U1108	G1044		G892
A1886	G1807	U1739	U1481		U1340		G1187	A1045	A1045		C893
G1886	G1638	C1547	G1482	G1416	C1341	G1264	U1188	G1110	A1046		C894
C1887	U1639	C1549	G1484	C1417	G1344	A1265	A1189	A1111	G1047		U895
G1888	U1639		G1484	G1418			G1190	G1112	A1048		A896
A1889	A1641	G1552	G1486	A1419	G1344	A1268	G1191	U1113	C1049		C897
	G1642	A1553	A1486	U1420		A1269	G1192	G1114	A1050		A898
	G1643	A1554		U1420		C1270	G1193	G1115	A1051		A899
			A1490		G1348	G1271			A983		A900
			G1491	G1425	U1352	A1272	U1199	C1116	C1052		A901
			G1492	G1425	A1353	U1273			C1053		A902
			C1493	G1426	A1353	A1274	C1200	G1120	A1054		C902
			A1494	A1427	G1355			C1121	G1055		C903
			A1495	C1428		A1278	G1203	G1124	G1056		U905
			A1496	G1429	U1356	G1279	A1204	C1125	A1057		G906
			U1497	C1430	G1358		U1205	G1125	C991		U907
			C1498	U1431	U1358				G1059		C908
			C1499	C1432	A1359	A1286	C1208	G1131	U1060		A909
			G1500	U1433	A1360	A1287	G1209	A1132	U1061		
			C1501	A1434	G1361	U1288	A1210	U1133	G1062		A910
			C1502	G1435	C1362	C1289	U1211	C1135	C995		A911
			U1503	G1436	G1363	C1290	G1212	G1136	G1063		G912
			C1504	G1437	G1364	C1291	A1213	G1137	C1064		C913
			C1505	U1438	A1365	U1292	A1214	G1138	U1065		C914
			C1506	A1439	A1366	U1293	G1215		U1066		C915
			A1507	G1440	A1367	C1294		C1139	A1067		G916
			A1508	G1441	G1368	U1294	C1221	U1141	A1069		A917
			C1509			G1297	C1221A	U1142	U1070		
			A1509A	A1445	G1374	C1298	C1222	A1142A	G1071		U922
			A1509B	C1445A	C1375	C1299	G1223	A1143	C1072		
			G1510	G1446	C1376	U1300			A1073		C925
			C1511	G1447	G1377	A1301	G1227	C1146	G1074		A926
			U1512	G1448	A1378	A1302		A1147	A1009		G927
			C1513	A1449	A1379	G1303	G1231	A1148	C1075		G928
			U1514	G1450	G1380	C1304	G1232	G1149	C1076		
			G1515	C1450A		C1305	G1233	C1150	U1012		G932
			C1516		A1384		U1234	G1151	C1013		A933
			G1517	U1453	G1385		G1235	C1152	U1014		
			U1518	G1455	C1387		G1236	C1153			G940
					C1387	G1311	A1237	G1154	A1084		A941
			U1523	C1458	G1388	U1313	G1238	A1155	G1087		G942
			G1524	G1459	G1389	C1314	G1239	A1156	A1088		U943
			U1525	A1460	U1390	C1315	U1240	G1157	G1089		G944
			G1526	G1461		U1316	A1241		U1090		A945
			G1527		A1393	A1317	A1242	G1162	U1091		G946
			A1528A	G1465	U1396	G1318	G1243	G1163	G1024		G947
			G1529	G1466		C1319	G1244	G1164	C1092		G948
				C1467	G1400	C1320	G1245	U1165	U1094		C949
					G1401		A1246	C1166	A1095		G950
			U1534	C1468	A1401	G1327	A1247		A1096		
			A1535	A1469	C1402	G1328	G1248	G1170	U1097		A953
			C1536	C1470	C1403	U1329		G1171	A1098		G954
			G1537	A1471	A1404	C1330	G1251	U1035	G1034		C955
			U1538	A1472	U1405	A1331	G1252	G1036	U1035		G956
			G1539	A1473	U1406	G1332	A1253	U1175	C1100		A957
			U1540	C1474	A1407	C1333		G1176	G1038		U958
			G1541	G1475	C1408	G1334	G1256	A1177	A1102		A959
			A1542	C1476	C1409	U1335	C1257	C1178	C1104		A960
C1543	C1544	A1544	G1478	C1411	A1336	G1258	C1179	U1105	G1041		C888
A1544	A1545	G1479	A1412	G1413	G1337	G1259	C1180	G1106	G1042		C889
C1546	C1547	G1480	G1481		G1338	G1260		U1107	C1043		A890
C1548	C1549	G1482	U1481	G1416	U1341	G1264	G1186	U1108	G1044		G892
C1549		G1484	G1485	C1417	G1344	A1265	U1187	G1109	A1045		C893
	G1552	G1486	A1486	G1418			A1189	G1110	A1046		C894
	A1553	A1486		A1419	G1344	A1268	G1190	A1111	G1047		U895
	A1554			U1420		A1269	G1191	G1112	A1048		A896
			A1490		G1348	C1270	G1192	U1113	C1049		C897
			G1491	G1425	A1348	G1271	G1193	G1114	A1050		A898
			G1492	G1425	G1349	A1272		G1115	G1051		A899
			C1493	G1426	U1352	G1273	U1199	C1116	C1052		A900
			A1494	A1427	A1353	U1273			C1053		A901
			A1495	C1428	G1355	A1274	C1200	G1120	A1054		C902
			A1496	G1429	U1356		G1203	C1121	G1055		C903
			U1497	C1430	G1358	A1278	A1204	G1124	A1057		U905
			C1498	U1431	U1358	G1279	U1205	G1125	C991		G906
			C1499	C1432	A1359				G1059		U907
			G1500	U1433	A1360	A1286	C1208	G1131	U1060		C908
			C1501	A1434	G1361	A1287	G1209	A1132	U1061		A909
			U1503	G1435	C1362	U1288	A1210	U1133	G1062		A910
			C1504	G1436	G1363	C1289	U1211	C1135	C995		A911
			C1505	G1437	G1364	C1290	G1212	G1136	G1063		G912
			C1506	U1438	A1365	C1291	A1213	G1137	C1064		C913
			A1507	A1439	A1366	U1292	A1214	G1138	U1065		C914
			A1508	G1440	A1367	U1293	G1215		U1066		C915
			C1509	G1441	G1368	U1294	C1221	U1141	A1067		G916
			A1509A	A1445		G1297	C1221A	U1142	A1069		A917
			A1509B	C1445A	G1374	C1298	C1222	A1142A	U1070		
			G1510	G1446	C1375	C1299	G1223	A1143	C1072		U922
			C1511	G1447	C1376	U1300			A1073		C925
			U1512	G1448	G1377	A1301	G1227	C1146	G1074		A926
			C1513	A1449	A1378	A1302		A1147	A1009		G927
			U1514	G1450	A1379	G1303	G1231	A1148	C1075		G928
			G1515	C1450A	G1380	C1304	G1232	G1149	C1076		
			C1516			C1305	G1233	C1150	U1012		G932
			G1517	U1453	A1384		U1234	G1151	C1013		A933
			U1518	G1455	G1385		G1235	C1152	U1014		
					C1387	G1311	G1236	C1153			G940
			U1523	C1458	G1388	U1313	A1237	G1154	A1084		A941
			G1524	G1459	G1389	C1314	G1238	A1155	G1087		G942
			U1525	A1460	U1390	C1315	G1239	A1156	A1088		U943
			G1526	G1461		U1316	U1240	G1157	G1089		G944
			G1527		A1393	A1317	A1241		U1090		A945
			A1528A	G1465	U1396	G1318	G1242	G1162	G1091		G946
			G1529	G1466		C1319	G1243	G1163	G1024		G947
				C1467	G1400	C1320	G1245	U1165	C1092		G948
					G1401		A1246	C1166	U1094		C949
			U1534	C1468	A1401	G1327	A1247		A1095		G950
			A1535	A1469	C1402	G1328	G1248	G1170	A1096		
			C1536	C1470	C1403	U1329		G1171	U1097		A953
			G1537	A1471	A1404	C1330	G1251	U1035	G1034		G954
			U1538	A1472	U1405	A1331	G1252	G1036	U1035		C955
			G1539	A1473	U1406	G1332	A1253	U1175	G1037		G956
			U1540	C1474	A1407	C1333		G1176	G1038		A957
			G1541	G1475	C1408	G1334	G1256	A1177	A1102		U958
			A1542	C1476	C1409	U1335	C1257	C1178	C1104		A959
											A960



C897	C898	U822	C665	U626	G549	G396	G325	G271Q	G220	C142A	G
C898	A824	G823	G666	A627	G551	A402	G326	G271R	A221	G143	G
A899	C825	C826	G669	G628	G566	G327	G327	G271S	A222	C143A	U
A900	A905	C827	A670	G629	A478	U403	U328	C271T	A78	C144	C
A901	C902	U826	G671	A630	A479	C404	G329	G271U	G79	G226	A
C902	C903	U827	G672	G631	A480	U405	A330	G271V	G80	G146	A6
C903	C904	U828	C673	A632	C481	C406	A331	G271W	G81	G227	G7
A829	U905	A829	C674	A633	A482	G407	A332	G271X	G82	A149	A8
G830	G906	G830	G675	A634	A483	C408	G333	U272A	G83	G228	A8
G831	G907	G831	A676	C635	G563	C409	G334	G272B	A84	G229	U9
G832	U907	G832	A676	C636	C564	C410	G335	G272C	G85	C153	G10
U833	C908	U833	A637	G637	C565	G411	C336	G272D	G86	C154	G11
C834	A909	C834	G638	G638	G491	C414	C337	U272E	G88	U156	U12
A910	A910	G657	C667	U639	A492	A415	G338	C272H	G89	U157	G15
C911	C912	C766	U688	C840	G493	A415	G339	U272I	U90	U158	G16
U913	U913	U767	A689	C941	G573	G494	A340	C272J	A92	G171	G17
C846	C914	U773	G690	G642	C574	C419	G341	G274	G93	C172	C18
U847	C915	A774	G691	A643	A575	C420	G342	G275	G94	G173	C19
C916	C916	A775	C692	A644	U499	U421	G342	A276	G94A	C174	C20
A917	A917	G775	C693	C645	G500	G424	G352	C277	G95	G175	A21
U922	U922	G776	U694	G646	A501	G425	G353	A277	G96	G176	A22
G850	U851	A777	G695	G647	A502	G426	G354	C279	G97	G177	G22
G852	G852	G778	G696	G648	A503	U427	G355	C280	G98	G178	U25
G853	G853	U779	G700	G649	A505	U428	G356	G281	G99	C246	G26
C924	C925	G780	G700	C650	G506	A428	A357	G281	G100	A181	G27
C925	A926	A781	G703	G651	A507	A428	U358	U284	G102	A182	A28
A926	G927	A782	U704	C652	G508	C436	A359	C285	C105	G183	U29
G928	G928	A783	G704	A653	C509	G437	G360	C286	C106	C184	G30
U858	U858	A784	A706	A654	C510	C438	G361	C287	C107	U185	C31
G859	U860	G785	G707	G654A	A511	C440	U362	C288	C108	C107	C32
U860	A861	G786	C708	C654B	G512	U441	G363	A289	U108	G189	U33
A861	G862	A787	G709	G654C	A513	G442	A363A	G290	G109	A190	C34
A863	G863	G788	G710	G654D	A514	A443	G363B	C291	G110	A191	C37
G864	C941	G791	G711	G654E	A515	C444	U363E	U292	A111	C192	C37
C944	A866	G792	G720	C654G	U519	C445	A363F	U293	U114	A195	A38
U875	U875	A793	C721	C654H	G520	A447	C364	G296	C115	A196	A39
C946	C946	A796	A722	A654J	G521	U448	G365	C297	C116	A197	C40
G947	G947	C796	G723	C654K	G522	C451	C366	G298	G117	C198	A43
U877	U877	C797	U724	G654L	U524	G452	G370	A300	A118	U200	G44
C949	C949	A802	G725	C654M	C527	C453	U373	G301	A119	C201	C45
G950	G950	U803	G729	G654N	A528	A454	A374	C302	G121	U202	C47
A953	A953	A804	C730	C654P	A529	C455	C375	U303	G122	C203	G57
G954	G954	G805	C731	C654Q	A530	C456	G379	G304	C204	A204	G58
C955	C955	C806	C732	C654R	C531	A457	U380	C271B	G205	G206	U59
G956	G956	U807	G733	G654S	A532	U459	G381	C271C	U206	U207	G60
A957	A957	G808	C736	C654T	G533	A460	G382	G271E	C129	C208	G61
U958	U958	G809	C737	A654U	U534	C461	U383	C271F	C130	C209	A64
A959	A959	U810	U740	A654V	C535	G462	U384	C271G	G133	G210	C65
C960	C960	C811	G741	G654W	A536	G463	C385	G271H	C134	A211	C66
C961	C961	U813	G742	U657	C537	U464	G386	C271I	G135	G212	U67
A960	A960	C814	G743	C658	C541	C465	U387	G271J	C136	A213	G68
G969	G969	C815	G744	C659	C542	A466	G388	C319	G137	G214	C69
C970	C970	C819	G745	G660	C543	C467	G389	A320	G139	G215	G70
C971	C971	A819	A746	C661	C543	G468	A390	G271K	G139A	A216	A71
G974	G974	A820	C664	G623	A547	A470	C392	G271L	G140	G217	U72
		A821		G625	A548	A471	G392	C271P	A142	G219	A74

U1993	C1902	U1818	G1748	C1648	A1567	G1491	G1439	G1348	A1268	U1188	G1112	C975
C1906	G1906	A1819	A1749	G1649	G1568	G1492	U1420	A1349	A1269	A1189	U1113	A1049
G1907	G1907	U1820	G1750	G1650	A1569	C1493	G1425	A1349	G1270	A1189	G1114	A1050
G1908	C1908	A1821	G1751	G1651	G1573	A1494	G1425	A1349	G1271	G1190	G1115	G1051
G1909	G1909	G1822	G1752	G1652	A1495	A1496	A1427	A1352	A1272	G1191	C1116	C1052
G2000	G1910	G1826	G1753	G1653	G1574	A1497	C1428	A1353	U1273	A1054	G1055	C1053
A2001	U1911	C1827	G1754	A1654	C1575	C1498	G1429	A1354	A1274	G1120	G1056	A984
C2006	C1914	U1828	G1755	C1657	U1578	C1499	G1430	G1355	A1278	U1199	G1057	C985
C2007	U1915	G1828	U1757	C1658	A1579	C1499	U1431	G1356	G1279	C1200	A1057	C986
C2008	A1916	G1831	G1758	U1659	A1580	G1500	C1432	U1357	G1279	G1124	G1058	G987
C2009	U1917	G1835	A1762	A1665	C1582	C1502	U1433	A1359	A1286	G1203	U1061	A990
G2010	G1921	C1836	G1763	G1666	A1583	U1503	A1434	A1360	A1287	A1204	U1061	C991
U2011	G1922	C1837	G1764	G1667	C1584	C1504	G1435	G1361	U1288	U1205	G1062	C992
G2012	G1922	C1838	A1668	A1668	A1586	C1506	G1437	C1362	C1289	C1208	G1063	C994
A2013	C1928	G1839	G1767	A1669	G1588	A1507	U1438	C1363	C1290	G1209	G1064	C995
A2014	A1928	G1840	U1768	G1670	C1589	A1508	U1439	G1364	C1291	A1210	U1065	A996
U2022	G1929	U1841	G1769	G1674	U1590	C1509	A1445	A1366	U1292	G1212	U1066	G997
G2023	G1930	G1842	C1771	G1674	G1591	A1509A	A1445	A1367	U1294	A1213	A1067	C998
C2024	U1931	C1843	G1772	A1677	C1592	A1509B	C1445A	A1367	A1297	G1214	G1068	U999
C2025	A1932	C1844	C1773	G1678	G1593	C1511	G1447	G1374	C1298	G1215	A1070	A1000
C2026	G1933	G1845	C1774	G1679	G1595	U1512	G1448	C1375	G1299	C1221	U1071	A1001
C2027	A1936	A1846	U1777	U1679	A1596	C1513	A1449	C1376	U1300	G1222	G1072	C1005
U2028	A1937	A1848	U1778	G1681	A1597	U1514	G1450	G1377	A1301	G1223	A1073	C1006
C2029	U1938	G1849	U1779	G1682	C1598	G1515	U1451	A1378	G1302	G1227	G1074	C1075
A2030	U1939	U1851	A1780	C1683	C1599	G1516	U1452	A1379	C1304	G1227	C1076	A1010
A2031	U1940	C1782	C1781	C1684	G1600	U1517	G1455	G1380	C1305	G1231	A1077	U1011
C2032	C1946	A1854	U1782	U1688	G1601	U1518	G1458	A1384	C1306	G1232	C1078	U1012
A2033	U1947	G1855	A1783	A1689	U1602	U1523	G1459	G1385	G1311	G1235	G1087	U1013
U2034	C1947	G1856	A1784	G1697	A1603	G1524	A1460	C1386	U1312	G1236	U1081	U1014
G2035	G1948	G1857	A1785	G1697	C1607	G1525	G1461	C1387	G1313	G1236	U1082	C1018
C2036	C1952	A1858	A1786	A1698	A1608	G1526	G1462	G1388	C1314	U1240	G1088	A1020
C2039	A1953	G1859	C1788	G1699	A1609	G1527	G1463	G1389	C1315	A1241	A1089	A1021
G1954	G1954	G1860	A1789	A1700	A1610	A1528A	G1464	U1390	U1316	A1242	U1090	G1022
U1955	U1955	U1864	C1790	A1701	G1614	G1529	G1465	A1393	A1317	G1243	G1091	G1023
C2043	G1959	G1865	A1791	U1709	C1615	U1534	G1466	U1396	C1318	G1244	G1092	U1025
C2044	A1960	A1876	U1796	C1710	A1616	A1535	A1469	G1400	G1319	G1245	G1093	U1026
C2045	C2045	A1877	C1797	C1711	C1617	U1536	A1470	C1401	C1320	U1246	U1094	A1029
G2046	U1963	G1878	U1798	C1712	A1618	G1537	A1471	C1402	G1327	A1247	A1095	A1030
C2050	C1967	C1879	C1799	G1713	G1619	G1538	A1472	C1403	G1328	G1248	A1096	G1036
A2051	G1968	C1880	G1801	G1717	G1620	U1539	A1473	C1404	U1329	C1251	U1097	G1034
G2052	C1968	C1881	A1802	G1718	G1630	U1540	C1474	U1405	C1330	G1257	A1098	U1035
G2053	A1969	G1882	A1803	G1719	A1634	G1541	G1475	A1406	A1331	A1253	G1099	G1036
A2054	A1970	G1883	C1804	G1720	G1635	A1542	G1476	C1407	G1332	G1256	C1100	G1037
C2055	A1971	A1884	U1805	G1721	C1636	A1543	A1477	C1408	C1333	G1257	U1101	G1038
G2056	A1972	C1885	C1806	A1722	A1637	A1544	G1478	C1409	G1334	C1257	G1176	G1039
A2060	G1981	G1887	G1807	U1739	A1637	C1547	G1479	G1410	U1335	G1258	A1177	A1040
G2061	C1982	A1888	A1810	A1740	C1638	U1481	G1480	G1411	A1336	G1259	C1178	G1041
A2062	A1889	G1889	G1811	A1741	C1639	A1554	U1481	C1412	G1337	G1260	U1175	G1042
C2063	G1987	C1893	A1812	G1743	C1640	G1482	G1484	G1413	G1338	C1261	G1102	G1043
G2064	A1987	G1894	C1743	G1744	G1642	G1485	G1486	G1416	U1339	G1264	G1107	G1044
C2065	G1988	G1895	G1745	G1745	G1643	A1486	A1486	G1417	U1341	A1265	U1108	A1045
U2068	G1989	G1899	G1816	G1745	G1643	A1486	A1486	G1418	G1344	G1265	U1109	A1046
G2069	G1992	A1901	G1817	G1747A	G1647	A1490	A1490	G1418	G1344	G1265	G1110	G1047
											A1048	A1048



Category	Percentage
Very bad	33%
Bad	48%
Good	15%
Very good	4%





- Molecule 37: 5S RIBOSOMAL RNA

Chain DB: 32% 49% 14%



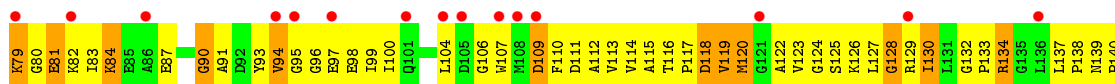
- Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC: 14% 42% 49% 8%

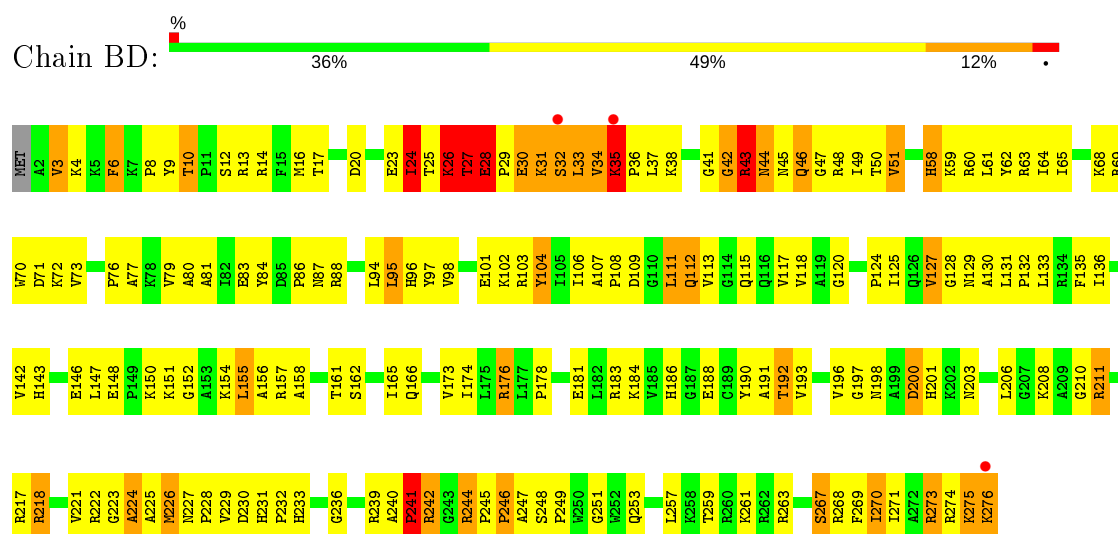


- Molecule 38: 50S RIBOSOMAL PROTEIN L1

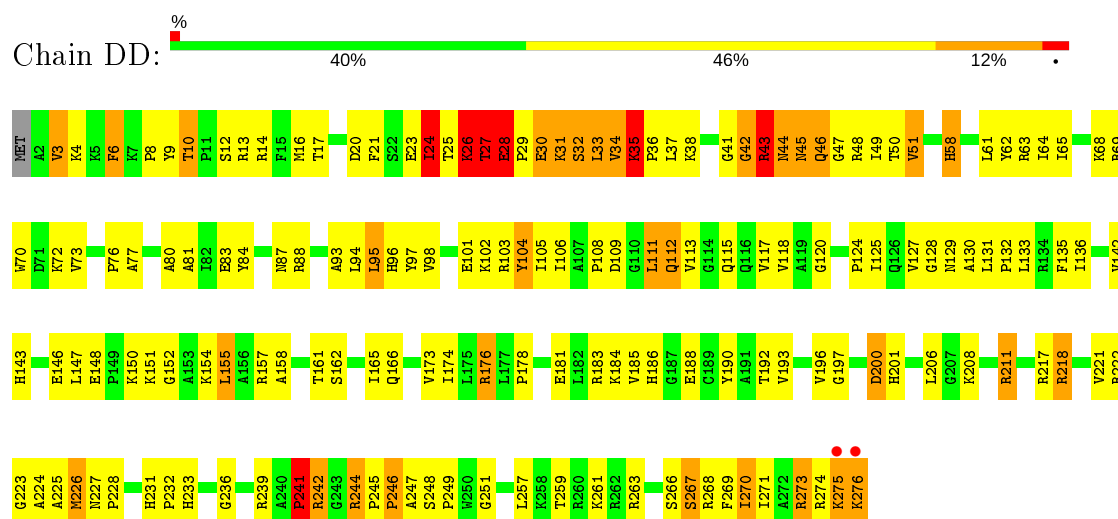
Chain DC: 9% 41% 49% 8%



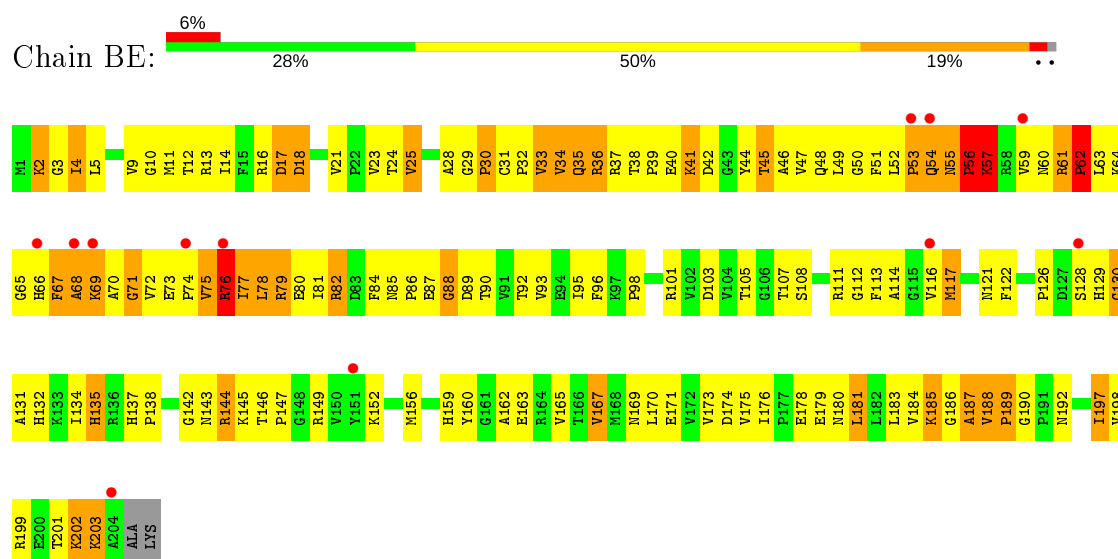
- Molecule 39: 50S RIBOSOMAL PROTEIN L2



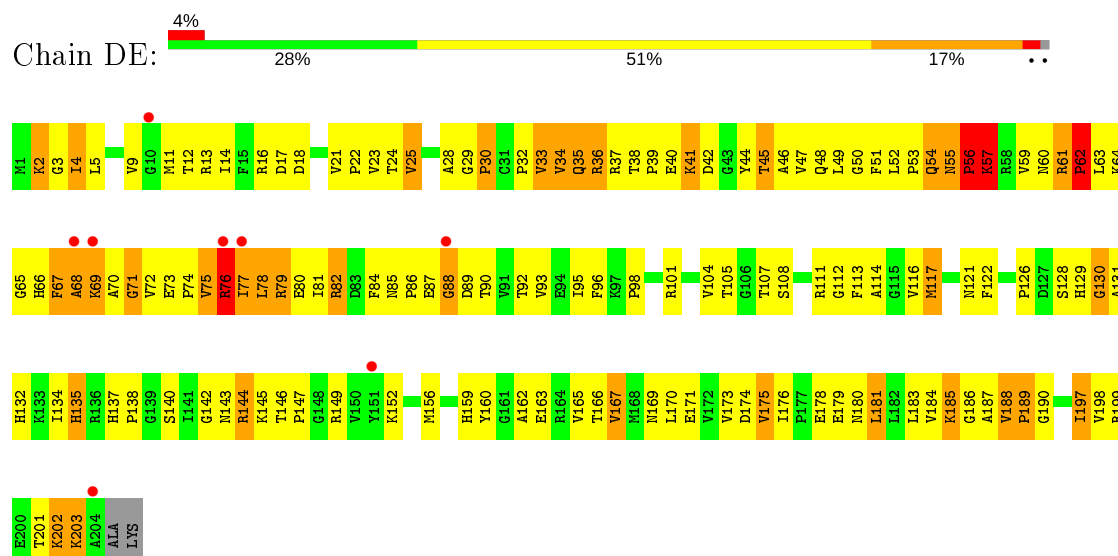
• Molecule 39: 50S RIBOSOMAL PROTEIN L2



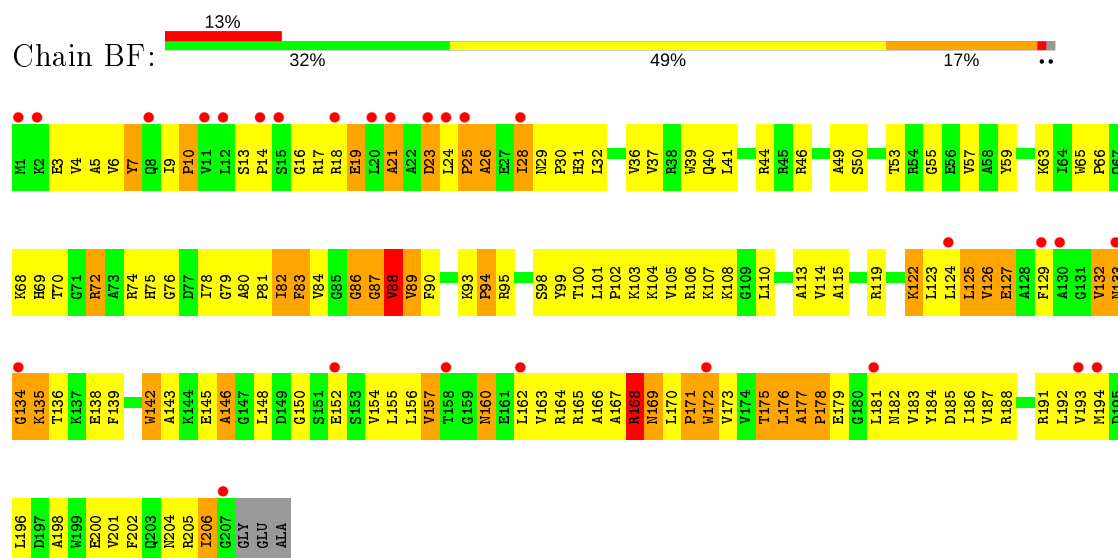
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



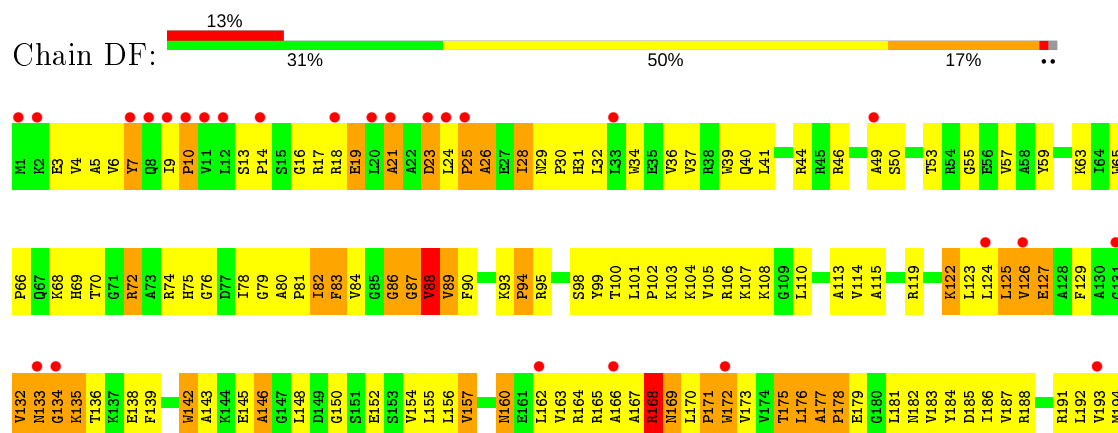
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

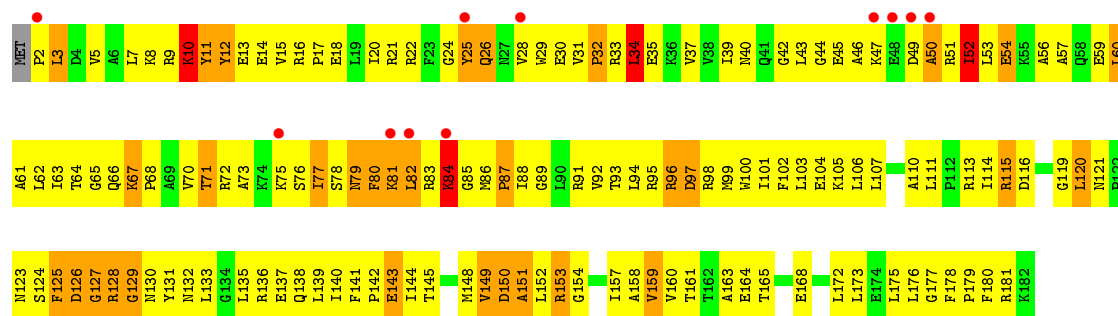


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

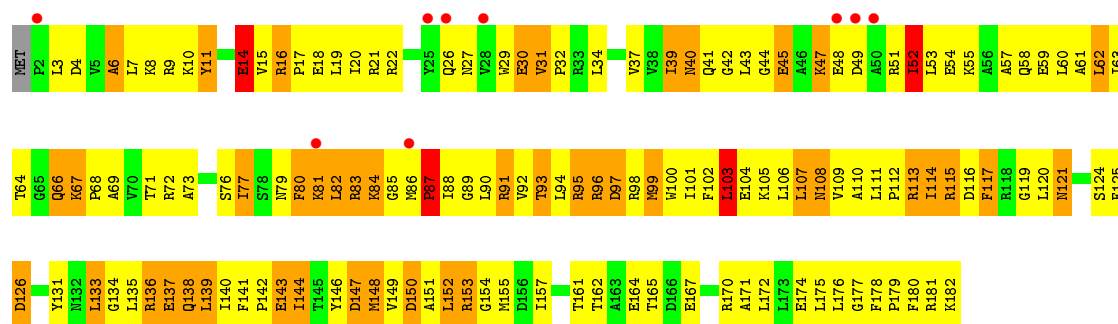




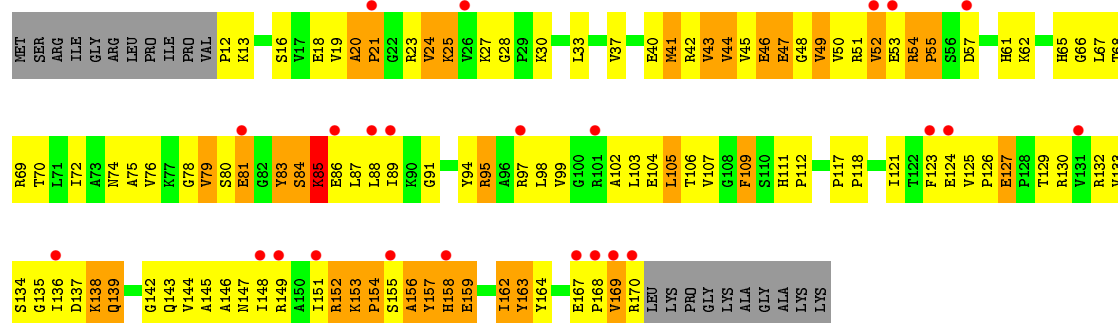
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



• Molecule 42: 50S RIBOSOMAL PROTEIN L5

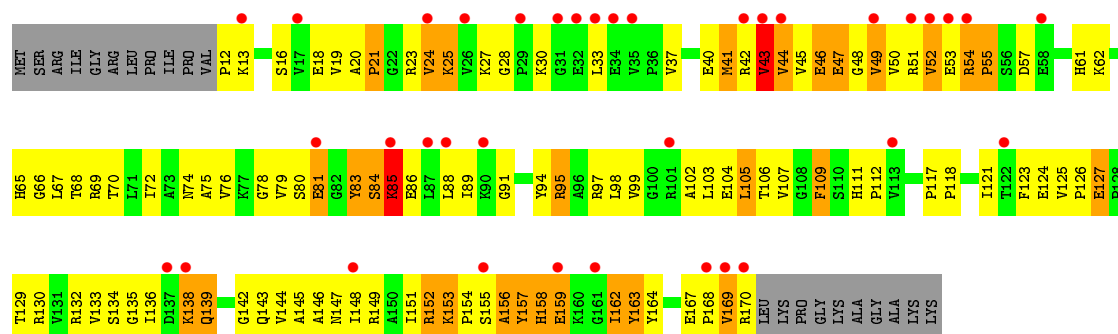


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

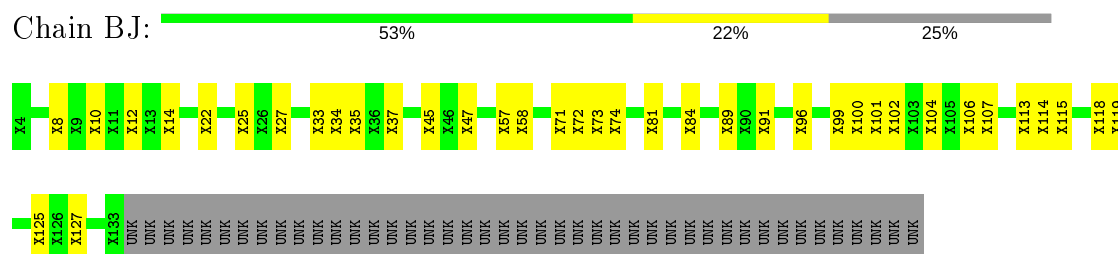


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

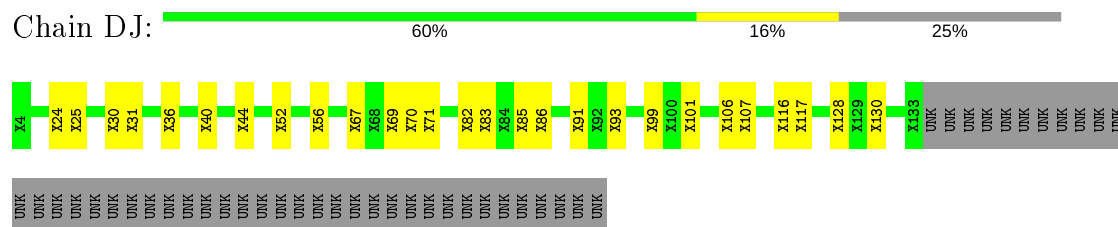




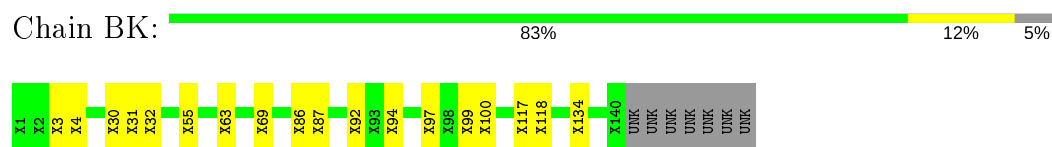
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



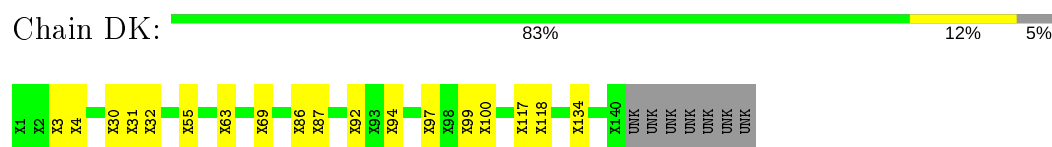
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



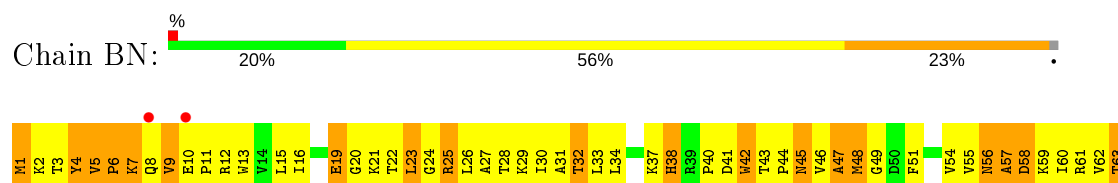
- Molecule 45: 50S RIBOSOMAL PROTEIN L11



- Molecule 45: 50S RIBOSOMAL PROTEIN L11

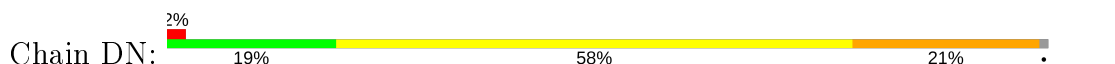


- Molecule 46: 50S RIBOSOMAL PROTEIN L13



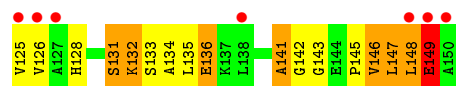
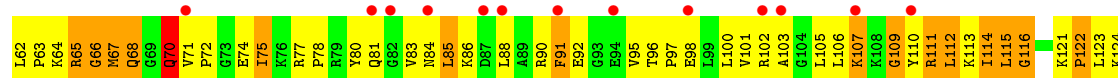
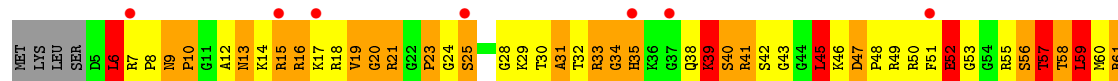
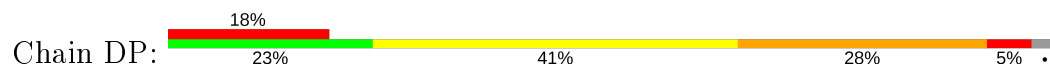


• Molecule 46: 50S RIBOSOMAL PROTEIN L13

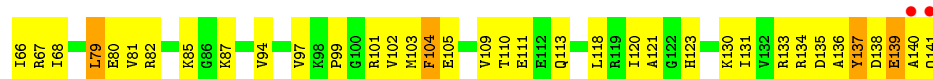
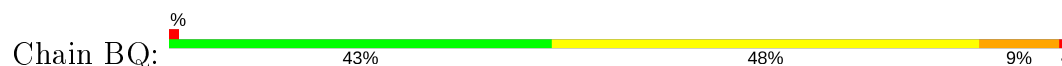




• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

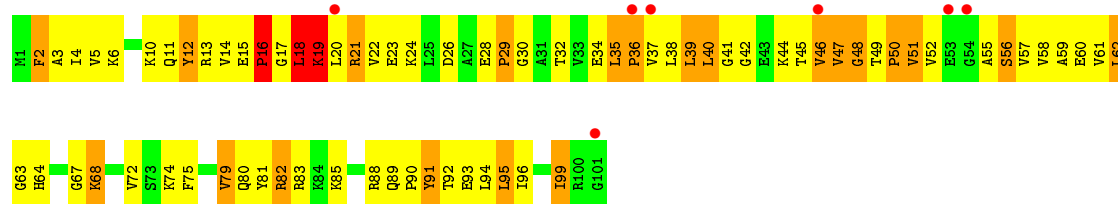


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

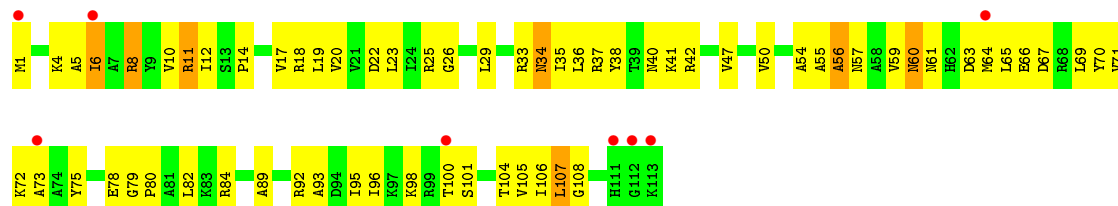
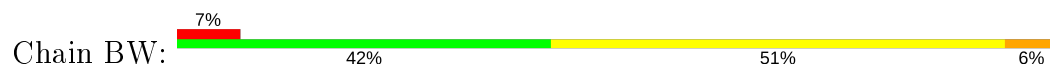


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

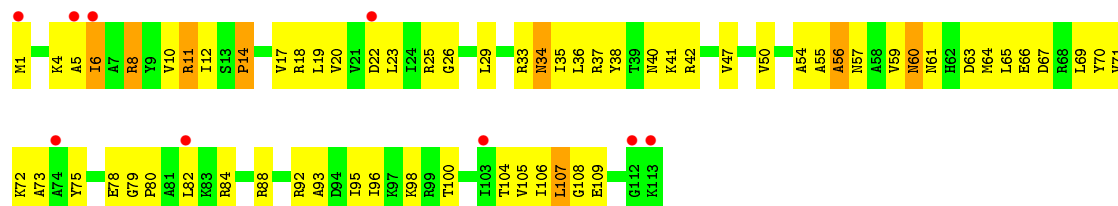
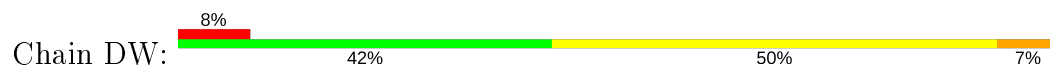




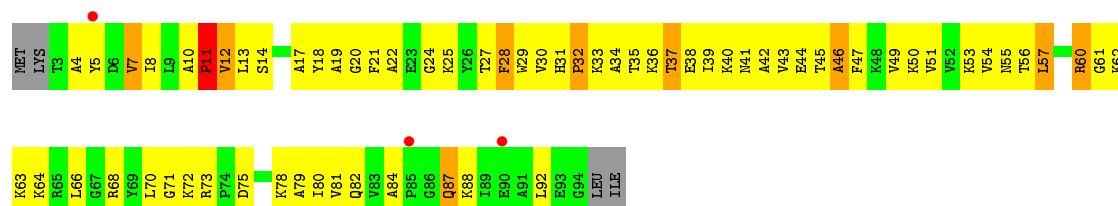
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



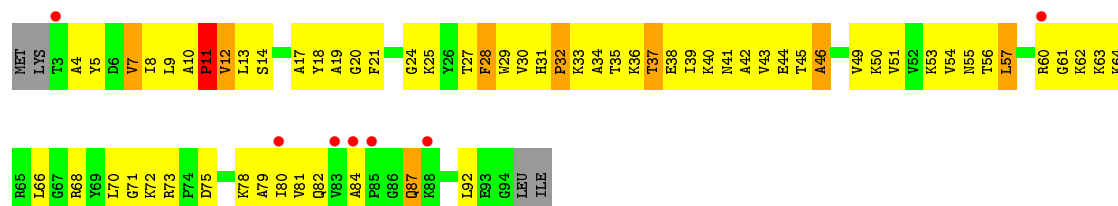
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



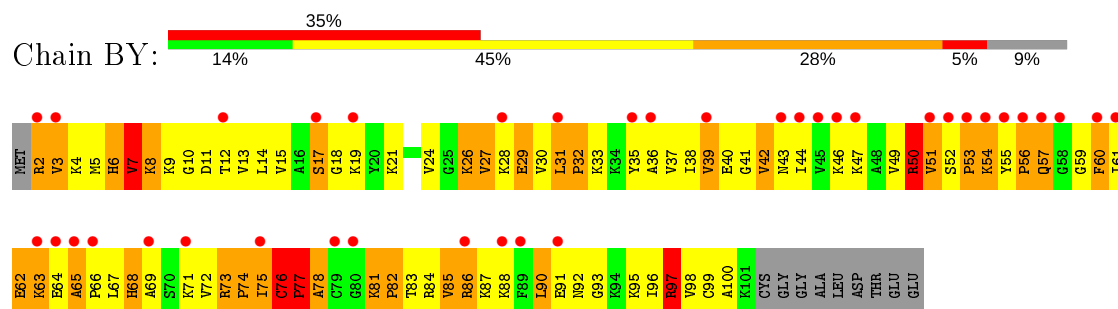
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



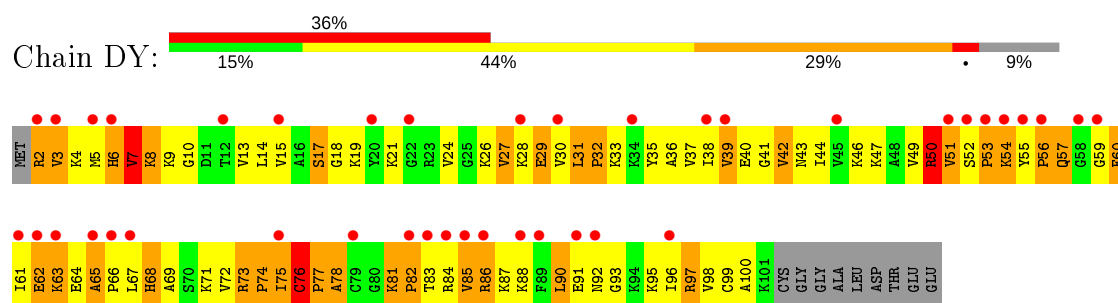
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



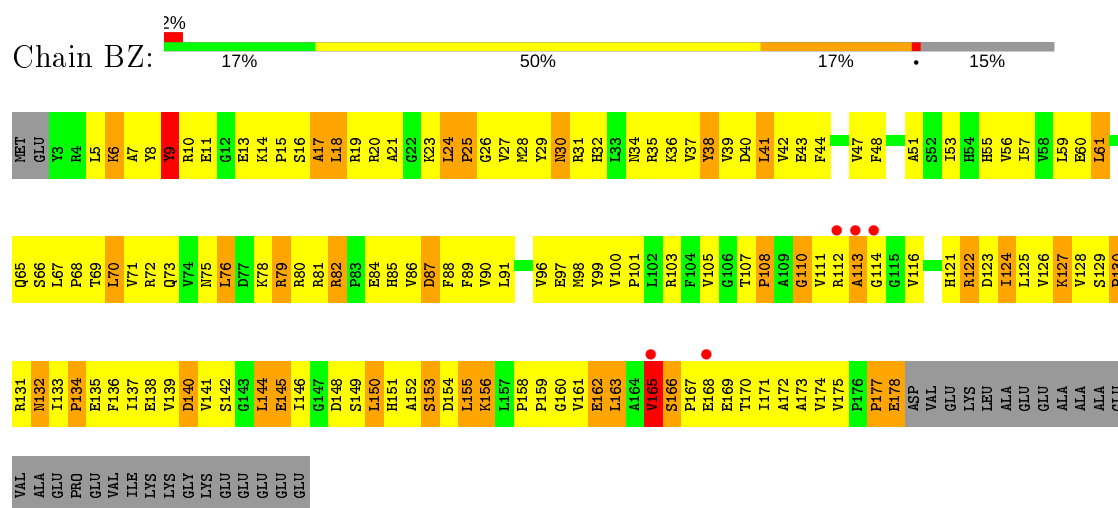
● Molecule 57: 50S RIBOSOMAL PROTEIN L24



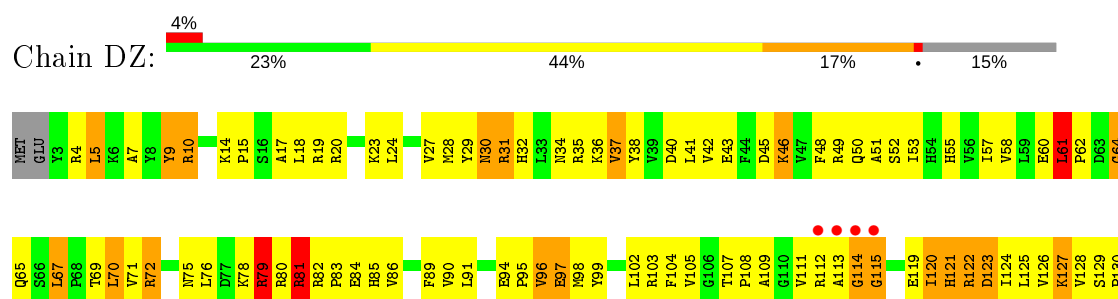
● Molecule 57: 50S RIBOSOMAL PROTEIN L24

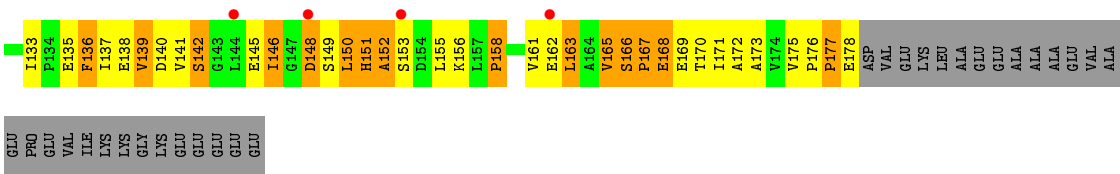


● Molecule 58: 50S RIBOSOMAL PROTEIN L25



● Molecule 58: 50S RIBOSOMAL PROTEIN L25





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 92.4 (49.51-2.90)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.264 0.236 , 0.263	Depositor DCC
R_{free} test set	62894 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	307330	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	6/36325 (0.0%)	0.75	35/56695 (0.1%)
1	CA	0.64	11/36325 (0.0%)	0.76	45/56695 (0.1%)
2	AB	0.49	0/1935	0.69	0/2609
2	CB	0.49	0/1935	0.69	0/2609
3	AC	0.53	0/1636	0.72	1/2205 (0.0%)
3	CC	0.58	0/1636	0.73	1/2205 (0.0%)
4	AD	0.45	0/1733	0.69	1/2318 (0.0%)
4	CD	0.43	0/1733	0.68	1/2318 (0.0%)
5	AE	0.56	0/1162	0.75	0/1564
5	CE	0.59	0/1162	0.76	0/1564
6	AF	0.43	0/856	0.68	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.45	0/1276	0.64	0/1709
7	CG	0.47	0/1276	0.64	0/1709
8	AH	0.48	0/1136	0.73	0/1527
8	CH	0.49	0/1136	0.75	0/1527
9	AI	0.45	0/1029	0.68	0/1379
9	CI	0.46	0/1029	0.68	0/1379
10	AJ	0.44	0/807	0.73	0/1085
10	CJ	0.47	0/807	0.74	0/1085
11	AK	0.49	0/900	0.72	0/1213
11	CK	0.52	0/900	0.72	0/1213
12	AL	0.49	0/986	0.77	0/1320
12	CL	0.51	0/986	0.78	0/1320
13	AM	0.45	0/998	0.73	0/1336
13	CM	0.46	0/998	0.73	0/1336
14	AN	0.62	0/501	0.81	0/664
14	CN	0.56	0/501	0.80	0/664
15	AO	0.47	0/745	0.67	0/992
15	CO	0.47	0/745	0.67	0/992
16	AP	0.43	0/716	0.70	0/963
16	CP	0.43	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.50	0/836	0.70	0/1117
17	CQ	0.50	0/836	0.70	0/1117
18	AR	0.50	0/579	0.66	0/768
18	CR	0.47	0/579	0.65	0/768
19	AS	0.47	0/642	0.71	0/865
19	CS	0.49	0/642	0.72	0/865
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.42	0/765	0.67	0/1007
21	AU	0.51	0/212	0.65	0/277
21	CU	0.47	0/212	0.64	0/277
22	AV	0.66	0/1809	0.83	1/2819 (0.0%)
22	AW	0.55	0/1809	0.75	0/2819
22	CV	0.72	0/1809	0.82	1/2819 (0.0%)
22	CW	0.57	1/1809 (0.1%)	0.76	0/2819
23	AX	0.69	0/406	0.87	2/631 (0.3%)
23	CX	0.80	0/406	0.90	3/631 (0.5%)
24	AY	0.49	1/1619 (0.1%)	0.70	0/2516
24	CY	0.50	1/1619 (0.1%)	0.70	0/2516
25	AZ	0.67	3/3042 (0.1%)	0.76	7/4129 (0.2%)
25	CZ	0.65	4/3042 (0.1%)	0.76	6/4129 (0.1%)
26	B0	0.45	0/671	0.70	0/892
26	D0	0.44	0/671	0.70	0/892
27	B1	0.43	0/738	0.72	0/981
27	D1	0.51	0/738	0.83	0/981
28	B2	0.35	0/600	0.63	0/793
28	D2	0.40	0/600	0.82	0/793
29	B3	0.35	0/472	0.60	0/634
29	D3	0.36	0/472	0.61	0/634
30	B4	0.41	0/349	0.64	0/474
30	D4	0.42	0/349	0.65	0/474
31	B5	0.40	0/473	0.64	0/639
31	D5	0.39	0/473	0.63	0/639
32	B6	0.62	0/440	0.95	0/586
32	D6	0.67	0/440	0.97	0/586
33	B7	0.45	0/426	0.71	0/561
33	D7	0.43	0/426	0.72	0/561
34	B8	0.55	0/515	0.77	0/679
34	D8	0.58	0/515	0.77	0/679
35	B9	0.53	0/310	0.70	0/407
35	D9	0.50	0/310	0.69	0/407
36	BA	0.52	5/69976 (0.0%)	0.72	27/109244 (0.0%)
36	DA	0.53	5/69976 (0.0%)	0.72	35/109244 (0.0%)
37	BB	0.49	0/2853	0.74	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.44	0/2853	0.74	1/4451 (0.0%)
38	BC	0.42	1/1774 (0.1%)	0.74	3/2391 (0.1%)
38	DC	0.43	2/1774 (0.1%)	0.75	3/2391 (0.1%)
39	BD	0.52	0/2195	0.88	4/2955 (0.1%)
39	DD	0.54	0/2195	0.90	4/2955 (0.1%)
40	BE	0.43	0/1596	0.71	0/2153
40	DE	0.44	0/1596	0.71	0/2153
41	BF	0.38	0/1658	0.74	3/2244 (0.1%)
41	DF	0.36	0/1658	0.74	3/2244 (0.1%)
42	BG	0.39	0/1499	0.70	1/2016 (0.0%)
42	DG	0.47	0/1499	0.80	0/2016
43	BH	0.35	0/1245	0.67	0/1682
43	DH	0.35	0/1245	0.67	0/1682
46	BN	0.39	0/1131	0.71	1/1525 (0.1%)
46	DN	0.39	0/1131	0.71	1/1525 (0.1%)
47	BO	0.52	1/943 (0.1%)	0.71	0/1269
47	DO	0.51	0/943	0.72	0/1269
48	BP	0.43	0/1131	0.89	3/1504 (0.2%)
48	DP	0.44	0/1131	0.90	4/1504 (0.3%)
49	BQ	0.51	0/1143	0.72	1/1527 (0.1%)
49	DQ	0.54	0/1143	0.72	1/1527 (0.1%)
50	BR	0.38	0/974	0.72	1/1302 (0.1%)
50	DR	0.39	0/974	0.72	1/1302 (0.1%)
51	BS	0.43	0/778	0.75	0/1036
51	DS	0.41	0/778	0.75	0/1036
52	BT	0.44	0/1155	0.76	2/1542 (0.1%)
52	DT	0.45	0/1155	0.77	2/1542 (0.1%)
53	BU	0.44	0/975	0.67	0/1297
53	DU	0.42	0/975	0.67	0/1297
54	BV	0.38	0/790	0.67	0/1057
54	DV	0.36	0/790	0.67	0/1057
55	BW	0.38	0/907	0.64	0/1216
55	DW	0.37	0/907	0.65	0/1216
56	BX	0.43	0/739	0.91	3/993 (0.3%)
56	DX	0.42	0/739	0.89	3/993 (0.3%)
57	BY	0.37	0/788	0.68	1/1051 (0.1%)
57	DY	0.37	0/788	0.68	1/1051 (0.1%)
58	BZ	0.46	0/1435	0.74	0/1949
58	DZ	0.49	0/1435	0.79	3/1949 (0.2%)
All	All	0.53	41/330278 (0.0%)	0.73	216/493462 (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	4	59
1	CA	4	49
22	AV	0	3
22	CV	0	2
23	AX	0	2
23	CX	0	1
36	BA	2	63
36	DA	2	72
37	BB	0	2
37	DB	0	2
49	BQ	0	1
49	DQ	0	1
All	All	12	257

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CZ	68	VAL	C-O	-20.43	0.84	1.23
25	AZ	68	VAL	C-O	-19.95	0.85	1.23
36	DA	761	A	C5-C6	-10.79	1.31	1.41
36	BA	761	A	C5-C6	-10.15	1.31	1.41
1	CA	858	G	C5-C6	-10.08	1.32	1.42

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	DC	134	ARG	NE-CZ-NH2	-14.36	113.12	120.30
39	DD	43	ARG	NE-CZ-NH1	14.15	127.37	120.30
41	BF	168	ARG	NE-CZ-NH2	-13.66	113.47	120.30
38	DC	134	ARG	NE-CZ-NH1	13.54	127.07	120.30
38	BC	134	ARG	NE-CZ-NH2	-13.34	113.63	120.30

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1363(A)	A	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
36	BA	1819	A	C3'

5 of 257 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	30	U	Sidechain
1	AA	37	U	Sidechain
1	AA	60	A	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	929	0
1	CA	32451	0	16382	850	0
2	AB	1900	0	1951	185	2
2	CB	1900	0	1951	176	2
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	141	0
4	AD	1703	0	1765	170	0
4	CD	1703	0	1765	157	0
5	AE	1146	0	1207	69	0
5	CE	1146	0	1207	69	0
6	AF	843	0	857	64	0
6	CF	843	0	857	59	0
7	AG	1257	0	1296	70	0
7	CG	1257	0	1296	63	0
8	AH	1116	0	1177	55	0
8	CH	1116	0	1177	49	0
9	AI	1010	0	1037	109	0
9	CI	1010	0	1037	109	0
10	AJ	794	0	840	116	0
10	CJ	794	0	840	116	0
11	AK	885	0	904	58	0
11	CK	885	0	904	57	0
12	AL	970	0	1057	99	0
12	CL	970	0	1057	97	0
13	AM	987	0	1059	116	0
13	CM	987	0	1059	116	0
14	AN	492	0	530	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	530	63	0
15	AO	734	0	771	44	0
15	CO	734	0	771	43	0
16	AP	700	0	720	75	0
16	CP	700	0	720	80	0
17	AQ	823	0	891	60	0
17	CQ	823	0	891	62	0
18	AR	574	0	644	46	0
18	CR	574	0	644	50	0
19	AS	629	0	652	76	0
19	CS	629	0	652	73	0
20	AT	763	0	861	97	0
20	CT	763	0	861	99	0
21	AU	208	0	221	25	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	59	0
22	AW	1619	0	822	79	0
22	CV	1619	0	822	58	0
22	CW	1619	0	822	73	0
23	AX	362	0	184	15	0
23	CX	362	0	184	14	0
24	AY	1645	0	853	132	0
24	CY	1645	0	853	89	0
25	AZ	2984	0	2997	475	0
25	CZ	2984	0	2997	384	0
26	B0	662	0	688	66	0
26	D0	662	0	688	65	0
27	B1	731	0	808	84	0
27	D1	731	0	808	80	0
28	B2	598	0	653	87	0
28	D2	598	0	653	215	0
29	B3	467	0	523	35	0
29	D3	467	0	523	35	0
30	B4	340	0	337	53	0
30	D4	340	0	336	58	0
31	B5	459	0	480	84	0
31	D5	459	0	480	76	0
32	B6	433	0	461	123	0
32	D6	433	0	461	121	0
33	B7	418	0	467	38	0
33	D7	418	0	467	37	0
34	B8	507	0	576	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D8	507	0	576	128	0
35	B9	307	0	337	33	0
35	D9	307	0	335	31	0
36	BA	62477	0	31497	2071	0
36	DA	62477	0	31497	2074	0
37	BB	2551	0	1295	93	0
37	DB	2551	0	1295	101	0
38	BC	1742	0	1800	162	2
38	DC	1742	0	1800	153	2
39	BD	2145	0	2234	254	0
39	DD	2145	0	2234	240	0
40	BE	1563	0	1629	237	0
40	DE	1563	0	1629	235	0
41	BF	1623	0	1677	214	0
41	DF	1623	0	1677	216	0
42	BG	1474	0	1535	236	0
42	DG	1474	0	1535	269	0
43	BH	1222	0	1282	159	0
43	DH	1222	0	1282	155	0
44	BJ	651	0	156	23	0
44	DJ	651	0	166	16	0
45	BK	700	0	167	9	0
45	DK	700	0	167	9	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	157	0
47	BO	933	0	996	86	0
47	DO	933	0	996	88	0
48	BP	1114	0	1187	267	0
48	DP	1114	0	1187	264	0
49	BQ	1122	0	1179	119	0
49	DQ	1122	0	1179	128	0
50	BR	960	0	1021	151	0
50	DR	960	0	1021	150	0
51	BS	770	0	832	135	0
51	DS	770	0	832	138	0
52	BT	1141	0	1202	207	0
52	DT	1141	0	1202	207	0
53	BU	958	0	1015	129	0
53	DU	958	0	1015	132	0
54	BV	779	0	852	139	0
54	DV	779	0	852	141	0
55	BW	896	0	953	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	84	0
56	BX	725	0	778	100	0
56	DX	725	0	778	92	0
57	BY	775	0	870	177	0
57	DY	775	0	870	169	0
58	BZ	1403	0	1432	211	0
58	DZ	1403	0	1432	189	0
59	AD	1	0	0	3	0
59	AN	1	0	0	2	0
59	B4	1	0	0	1	0
59	B9	1	0	0	1	0
59	CD	1	0	0	2	0
59	CN	1	0	0	2	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	15	0
60	CZ	28	0	12	8	0
61	AZ	57	0	58	13	0
61	CZ	57	0	58	9	0
All	All	307330	0	208699	17314	4

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 17314 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)
25:AZ:355:LEU:CD2	25:AZ:370:PHE:HB3	1.63	1.28
25:CZ:355:LEU:CD2	25:CZ:370:PHE:HB3	1.63	1.24
39:DD:35:LYS:HG3	39:DD:104:TYR:CE2	1.73	1.23
25:AZ:2:LYS:O	25:AZ:275:LYS:HE3	1.42	1.20
25:CZ:355:LEU:HD23	25:CZ:370:PHE:CB	1.73	1.19

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_445]	1.97	0.23
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_646]	2.02	0.18
2:CB:66:GLY:CA	38:DC:27:ARG:NH2[2_445]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:66:GLY:CA	38:BC:27:ARG:NH2[2_646]	2.18	0.02

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%)	161 (69%)	48 (21%)	23 (10%)	0	3
2	CB	232/256 (91%)	164 (71%)	45 (19%)	23 (10%)	0	3
3	AC	204/239 (85%)	169 (83%)	22 (11%)	13 (6%)	1	8
3	CC	204/239 (85%)	171 (84%)	21 (10%)	12 (6%)	1	10
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	4
4	CD	206/209 (99%)	149 (72%)	38 (18%)	19 (9%)	1	4
5	AE	148/162 (91%)	136 (92%)	10 (7%)	2 (1%)	11	40
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	7	31
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	4
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	1	4
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	5	26
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	7	31
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	1	8
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	2	11
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	1	8
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	1	8
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	17	52
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	7
12	CL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	7
13	AM	122/126 (97%)	85 (70%)	27 (22%)	10 (8%)	1	5
13	CM	122/126 (97%)	85 (70%)	28 (23%)	9 (7%)	1	6
14	AN	58/61 (95%)	42 (72%)	9 (16%)	7 (12%)	0	1
14	CN	58/61 (95%)	43 (74%)	7 (12%)	8 (14%)	0	1
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	1	6
16	CP	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	6
17	AQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	12
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	12
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	4	24
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	4	24
19	AS	76/93 (82%)	48 (63%)	15 (20%)	13 (17%)	0	0
19	CS	76/93 (82%)	47 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	22 (23%)	8 (8%)	1	5
20	CT	97/106 (92%)	67 (69%)	21 (22%)	9 (9%)	0	3
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	15
21	CU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	15
25	AZ	381/405 (94%)	263 (69%)	80 (21%)	38 (10%)	0	3
25	CZ	381/405 (94%)	266 (70%)	77 (20%)	38 (10%)	0	3
26	B0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	14
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	14
27	B1	91/98 (93%)	68 (75%)	13 (14%)	10 (11%)	0	2
27	D1	91/98 (93%)	63 (69%)	10 (11%)	18 (20%)	0	0
28	B2	69/72 (96%)	46 (67%)	17 (25%)	6 (9%)	1	4
28	D2	69/72 (96%)	37 (54%)	16 (23%)	16 (23%)	0	0
29	B3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	4
29	D3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	4
30	B4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0
31	B5	57/60 (95%)	41 (72%)	7 (12%)	9 (16%)	0	0
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	0
32	B6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
33	D7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	43 (70%)	12 (20%)	6 (10%)	0	3
34	D8	61/65 (94%)	45 (74%)	10 (16%)	6 (10%)	0	3
35	B9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	4
35	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	4
38	BC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	6
38	DC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	6
39	BD	273/276 (99%)	214 (78%)	33 (12%)	26 (10%)	0	3
39	DD	273/276 (99%)	214 (78%)	34 (12%)	25 (9%)	1	4
40	BE	202/206 (98%)	125 (62%)	46 (23%)	31 (15%)	0	0
40	DE	202/206 (98%)	125 (62%)	47 (23%)	30 (15%)	0	0
41	BF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	1
41	DF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	1
42	BG	179/182 (98%)	103 (58%)	45 (25%)	31 (17%)	0	0
42	DG	179/182 (98%)	111 (62%)	40 (22%)	28 (16%)	0	0
43	BH	157/180 (87%)	105 (67%)	28 (18%)	24 (15%)	0	0
43	DH	157/180 (87%)	105 (67%)	29 (18%)	23 (15%)	0	1
46	BN	136/140 (97%)	85 (62%)	32 (24%)	19 (14%)	0	1
46	DN	136/140 (97%)	86 (63%)	32 (24%)	18 (13%)	0	1
47	BO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	16
47	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	16
48	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
48	DP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
49	BQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	16
49	DQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	82 (71%)	14 (12%)	19 (16%)	0	0
51	BS	96/112 (86%)	44 (46%)	31 (32%)	21 (22%)	0	0
51	DS	96/112 (86%)	44 (46%)	32 (33%)	20 (21%)	0	0
52	BT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0
52	DT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0
53	BU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	2	16
53	DU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	2	16
54	BV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
55	BW	111/113 (98%)	82 (74%)	23 (21%)	6 (5%)	2	12
55	DW	111/113 (98%)	84 (76%)	21 (19%)	6 (5%)	2	12
56	BX	90/96 (94%)	63 (70%)	16 (18%)	11 (12%)	0	1
56	DX	90/96 (94%)	64 (71%)	15 (17%)	11 (12%)	0	1
57	BY	98/110 (89%)	32 (33%)	36 (37%)	30 (31%)	0	0
57	DY	98/110 (89%)	32 (33%)	37 (38%)	29 (30%)	0	0
58	BZ	174/206 (84%)	111 (64%)	36 (21%)	27 (16%)	0	0
58	DZ	174/206 (84%)	119 (68%)	31 (18%)	24 (14%)	0	1
All	All	12256/13098 (94%)	8805 (72%)	2168 (18%)	1283 (10%)	0	3

5 of 1283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	130	ARG
2	AB	234	PRO
3	AC	12	LEU

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%)	181 (90%)	21 (10%)	7	27
2	CB	202/220 (92%)	180 (89%)	22 (11%)	6	25
3	AC	160/188 (85%)	141 (88%)	19 (12%)	5	20
3	CC	160/188 (85%)	142 (89%)	18 (11%)	6	23
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	28
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	28
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	23
5	CE	115/123 (94%)	102 (89%)	13 (11%)	6	23
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6	24
6	CF	90/90 (100%)	80 (89%)	10 (11%)	6	24
7	AG	126/127 (99%)	118 (94%)	8 (6%)	18	48
7	CG	126/127 (99%)	118 (94%)	8 (6%)	18	48
8	AH	119/119 (100%)	107 (90%)	12 (10%)	7	28
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7	28
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	38
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	33
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6	24
11	CK	90/99 (91%)	80 (89%)	10 (11%)	6	24
12	AL	104/108 (96%)	92 (88%)	12 (12%)	5	22
12	CL	104/108 (96%)	92 (88%)	12 (12%)	5	22
13	AM	99/101 (98%)	88 (89%)	11 (11%)	6	24
13	CM	99/101 (98%)	88 (89%)	11 (11%)	6	24
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	14
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	14
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	23
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	23
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	24
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	48
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	10
18	CR	61/77 (79%)	51 (84%)	10 (16%)	2	10
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%)	68 (90%)	8 (10%)	7	26
20	CT	76/82 (93%)	68 (90%)	8 (10%)	7	26
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	54
25	AZ	322/338 (95%)	279 (87%)	43 (13%)	4	16
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	4	18
26	B0	66/67 (98%)	59 (89%)	7 (11%)	6	26
26	D0	66/67 (98%)	59 (89%)	7 (11%)	6	26
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	68 (87%)	10 (13%)	4	18
28	B2	66/67 (98%)	64 (97%)	2 (3%)	41	71
28	D2	66/67 (98%)	57 (86%)	9 (14%)	3	16
29	B3	51/52 (98%)	45 (88%)	6 (12%)	5	21
29	D3	51/52 (98%)	45 (88%)	6 (12%)	5	21
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	8
30	D4	39/63 (62%)	33 (85%)	6 (15%)	2	11
31	B5	51/52 (98%)	45 (88%)	6 (12%)	5	21
31	D5	51/52 (98%)	45 (88%)	6 (12%)	5	21
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	31 (63%)	18 (37%)	0	0
33	B7	41/42 (98%)	38 (93%)	3 (7%)	14	43
33	D7	41/42 (98%)	38 (93%)	3 (7%)	14	43
34	B8	53/55 (96%)	44 (83%)	9 (17%)	2	9
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	9
35	B9	34/34 (100%)	31 (91%)	3 (9%)	10	36
35	D9	34/34 (100%)	31 (91%)	3 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	172 (96%)	8 (4%)	28	61
38	DC	180/181 (99%)	172 (96%)	8 (4%)	28	61
39	BD	217/218 (100%)	186 (86%)	31 (14%)	3	14
39	DD	217/218 (100%)	187 (86%)	30 (14%)	3	16
40	BE	165/166 (99%)	145 (88%)	20 (12%)	5	20
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	16
41	BF	165/166 (99%)	152 (92%)	13 (8%)	12	40
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	40
42	BG	155/156 (99%)	135 (87%)	20 (13%)	4	18
42	DG	155/156 (99%)	124 (80%)	31 (20%)	1	5
43	BH	132/148 (89%)	118 (89%)	14 (11%)	6	26
43	DH	132/148 (89%)	118 (89%)	14 (11%)	6	26
46	BN	117/119 (98%)	101 (86%)	16 (14%)	3	16
46	DN	117/119 (98%)	101 (86%)	16 (14%)	3	16
47	BO	100/100 (100%)	93 (93%)	7 (7%)	15	45
47	DO	100/100 (100%)	93 (93%)	7 (7%)	15	45
48	BP	112/116 (97%)	93 (83%)	19 (17%)	2	9
48	DP	112/116 (97%)	93 (83%)	19 (17%)	2	9
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
49	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
50	BR	100/101 (99%)	87 (87%)	13 (13%)	4	18
50	DR	100/101 (99%)	85 (85%)	15 (15%)	3	12
51	BS	77/88 (88%)	65 (84%)	12 (16%)	2	11
51	DS	77/88 (88%)	65 (84%)	12 (16%)	2	11
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	6
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	6
53	BU	92/94 (98%)	86 (94%)	6 (6%)	17	47
53	DU	92/94 (98%)	86 (94%)	6 (6%)	17	47
54	BV	82/82 (100%)	67 (82%)	15 (18%)	1	7
54	DV	82/82 (100%)	67 (82%)	15 (18%)	1	7
55	BW	91/92 (99%)	87 (96%)	4 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DW	91/92 (99%)	86 (94%)	5 (6%)	21	53
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	31
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	71 (84%)	13 (16%)	2	11
57	DY	84/91 (92%)	72 (86%)	12 (14%)	3	14
58	BZ	155/179 (87%)	130 (84%)	25 (16%)	2	10
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	11
All	All	10338/10854 (95%)	9112 (88%)	1226 (12%)	5	20

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	95	LEU
7	CG	24	THR
51	DS	97	ARG
57	BY	7	VAL
2	CB	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 325 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	49	HIS
5	CE	20	GLN
49	DQ	141	GLN
55	BW	57	ASN
2	CB	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	227 (15%)	43 (2%)
1	CA	1509/1522 (99%)	222 (14%)	46 (3%)
22	AV	75/76 (98%)	22 (29%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	23 (30%)	1 (1%)
22	CW	75/76 (98%)	21 (28%)	3 (4%)
23	AX	16/27 (59%)	6 (37%)	1 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CX	16/27 (59%)	5 (31%)	1 (6%)
24	AY	74/77 (96%)	25 (33%)	3 (4%)
24	CY	74/77 (96%)	25 (33%)	3 (4%)
36	BA	2900/2915 (99%)	494 (17%)	45 (1%)
36	DA	2900/2915 (99%)	492 (16%)	45 (1%)
37	BB	118/122 (96%)	22 (18%)	3 (2%)
37	DB	118/122 (96%)	22 (18%)	3 (2%)
All	All	9534/9630 (99%)	1627 (17%)	200 (2%)

5 of 1627 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2689	U
1	CA	353	A
36	DA	2033	A
36	BA	2762	G
1	CA	115	G

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

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	MIA	CY	37	24	24,31,32	1.08	3 (12%)	26,44,47	1.70	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	5MU	AY	54	24	15,22,23	1.21	2 (13%)	16,32,35	3.74	1 (6%)
24	H2U	CY	20	24	18,21,22	0.73	0	21,30,33	1.92	5 (23%)
24	7MG	AY	46	24	22,26,27	1.25	2 (9%)	28,39,42	2.32	5 (17%)
24	4SU	CY	8	24	14,21,22	1.44	3 (21%)	15,30,33	2.60	2 (13%)
24	PSU	AY	55	24	17,21,22	1.16	2 (11%)	20,30,33	3.37	8 (40%)
24	7MG	CY	46	24	22,26,27	1.27	2 (9%)	28,39,42	2.30	5 (17%)
24	OMC	AY	32	24	15,22,23	0.76	0	17,31,34	1.19	2 (11%)
24	H2U	AY	20	24	18,21,22	0.73	0	21,30,33	1.91	5 (23%)
24	5MU	CY	54	24	15,22,23	1.24	2 (13%)	16,32,35	3.73	1 (6%)
24	PSU	CY	55	24	17,21,22	1.14	2 (11%)	20,30,33	3.30	8 (40%)
24	MIA	AY	37	24	24,31,32	0.97	2 (8%)	26,44,47	1.69	4 (15%)
24	OMC	CY	32	24	15,22,23	0.75	0	17,31,34	1.21	2 (11%)
24	H2U	AY	16	24	18,21,22	0.99	1 (5%)	21,30,33	1.82	4 (19%)
24	H2U	CY	17	24	18,21,22	0.97	0	21,30,33	1.90	5 (23%)
24	H2U	AY	17	24	18,21,22	0.98	0	21,30,33	1.90	5 (23%)
24	H2U	CY	16	24	18,21,22	0.98	1 (5%)	21,30,33	1.79	4 (19%)
24	4SU	AY	8	24	14,21,22	1.50	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	MIA	CY	37	24	-	2/11/33/34	0/3/3/3
24	5MU	AY	54	24	-	0/5/25/26	0/2/2/2
24	H2U	CY	20	24	-	1/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	2/7/37/38	0/3/3/3
24	4SU	CY	8	24	-	1/5/25/26	0/2/2/2
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
24	7MG	CY	46	24	-	2/7/37/38	0/3/3/3
24	OMC	AY	32	24	-	0/7/27/28	0/2/2/2
24	H2U	AY	20	24	-	1/7/38/39	0/2/2/2
24	5MU	CY	54	24	-	0/5/25/26	0/2/2/2
24	PSU	CY	55	24	-	0/7/25/26	0/2/2/2
24	MIA	AY	37	24	-	2/11/33/34	0/3/3/3
24	OMC	CY	32	24	-	0/7/27/28	0/2/2/2
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	CY	17	24	-	3/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	3/7/38/39	0/2/2/2
24	H2U	CY	16	24	-	0/7/38/39	0/2/2/2
24	4SU	AY	8	24	-	1/5/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C6-N1	4.12	1.40	1.33
24	AY	8	4SU	C5-C4	4.00	1.42	1.38
24	CY	46	7MG	C6-N1	3.74	1.39	1.33
24	CY	8	4SU	C5-C4	3.71	1.42	1.38
24	CY	54	5MU	C4-N3	3.44	1.39	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	54	5MU	C4-N3-C2	14.56	127.43	115.14
24	CY	54	5MU	C4-N3-C2	14.51	127.39	115.14
24	AY	55	PSU	N1-C2-N3	-10.45	120.12	128.43
24	CY	55	PSU	N1-C2-N3	-10.19	120.33	128.43
24	AY	8	4SU	C2-N3-C4	7.92	126.63	115.15

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	54	5MU	1	0
24	CY	20	H2U	1	0
24	AY	46	7MG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	8	4SU	1	0
24	AY	55	PSU	1	0
24	CY	46	7MG	3	0
24	AY	20	H2U	1	0
24	CY	54	5MU	1	0
24	CY	55	PSU	1	0
24	AY	16	H2U	3	0
24	CY	17	H2U	4	0
24	AY	17	H2U	3	0
24	CY	16	H2U	4	0
24	AY	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
61	KIR	CZ	502	-	56,59,59	3.39	22 (39%)	62,84,84	1.66	13 (20%)
60	GDP	CZ	501	-	24,30,30	1.54	4 (16%)	31,47,47	2.16	7 (22%)
60	GDP	AZ	501	-	24,30,30	1.63	5 (20%)	31,47,47	1.59	6 (19%)
61	KIR	AZ	502	-	56,59,59	3.42	22 (39%)	62,84,84	1.63	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/12/32/32	0/3/3/3
60	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3
61	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.49	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.21	1.23	1.44
61	AZ	502	KIR	O30-C30	-12.64	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.30	1.18	1.42
60	AZ	501	GDP	C6-N1	5.52	1.42	1.33

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C2-N3-C4	5.78	121.96	115.36
60	CZ	501	GDP	N3-C2-N1	-5.33	120.11	127.22
61	AZ	502	KIR	O29-C29-O34	-5.09	101.68	110.21
61	CZ	502	KIR	O29-C29-O34	-5.02	101.79	110.21
61	CZ	502	KIR	C48-C32-C47	-4.41	101.43	107.72

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

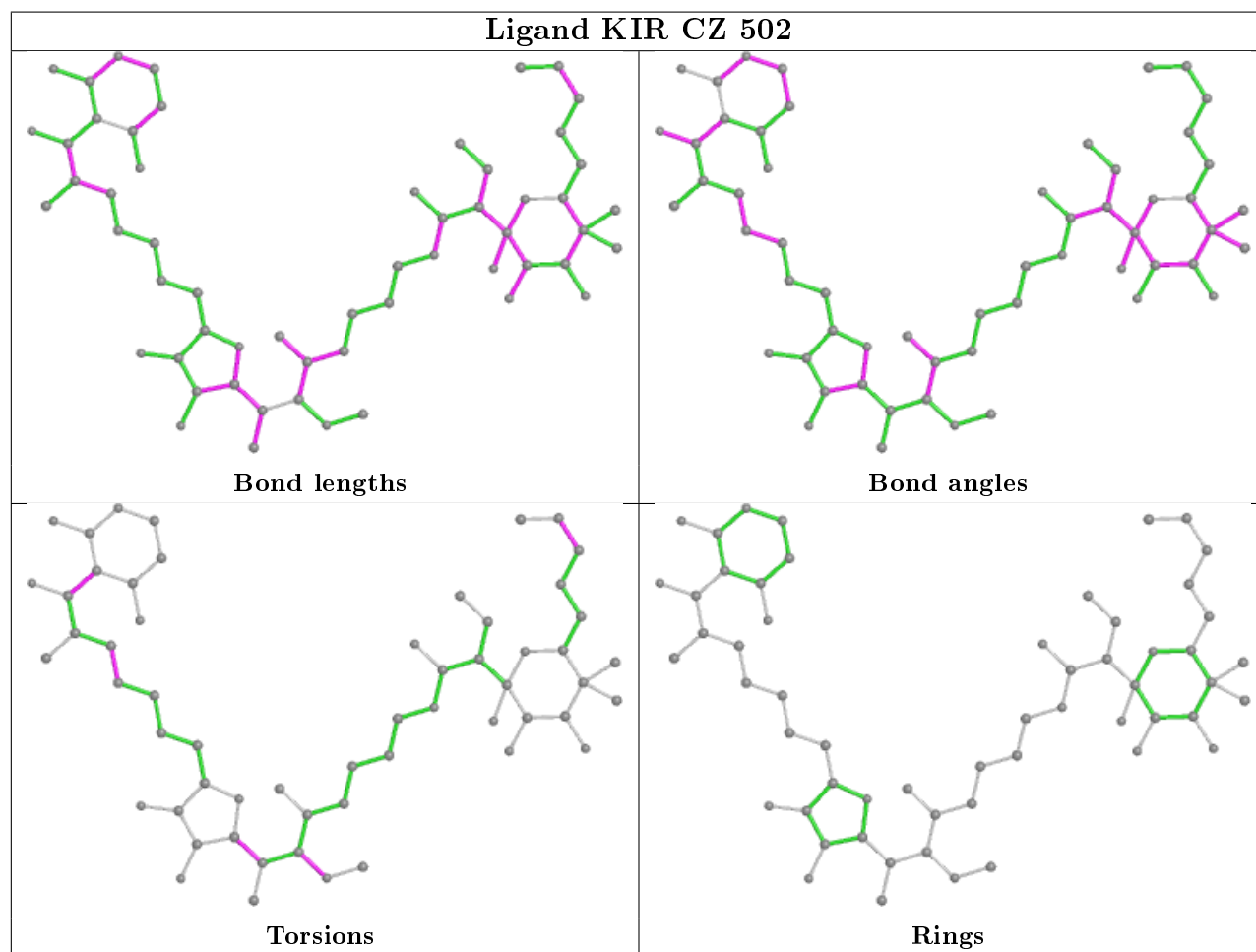
Mol	Chain	Res	Type	Atoms
61	CZ	502	KIR	O18-C17-C19-C42
61	AZ	502	KIR	O18-C17-C19-C42
60	AZ	501	GDP	PA-O3A-PB-O2B
61	CZ	502	KIR	C11-C10-C9-C8
61	AZ	502	KIR	C11-C10-C9-C8

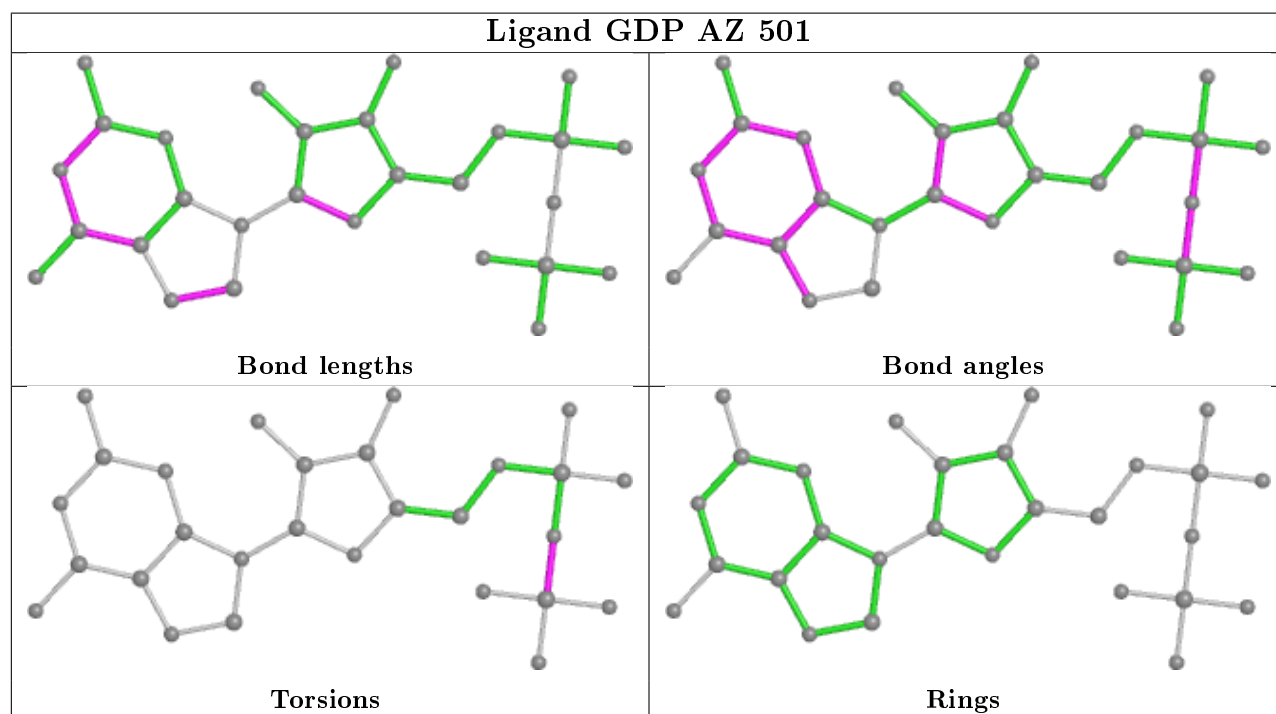
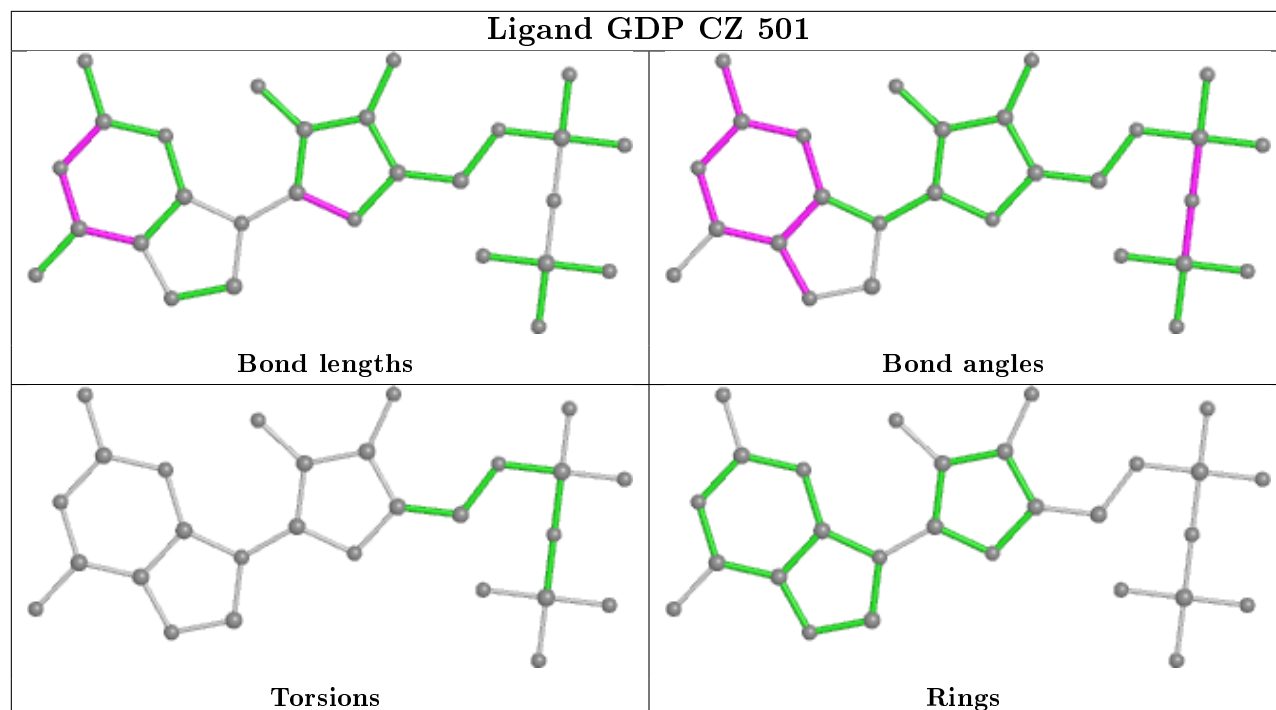
There are no ring outliers.

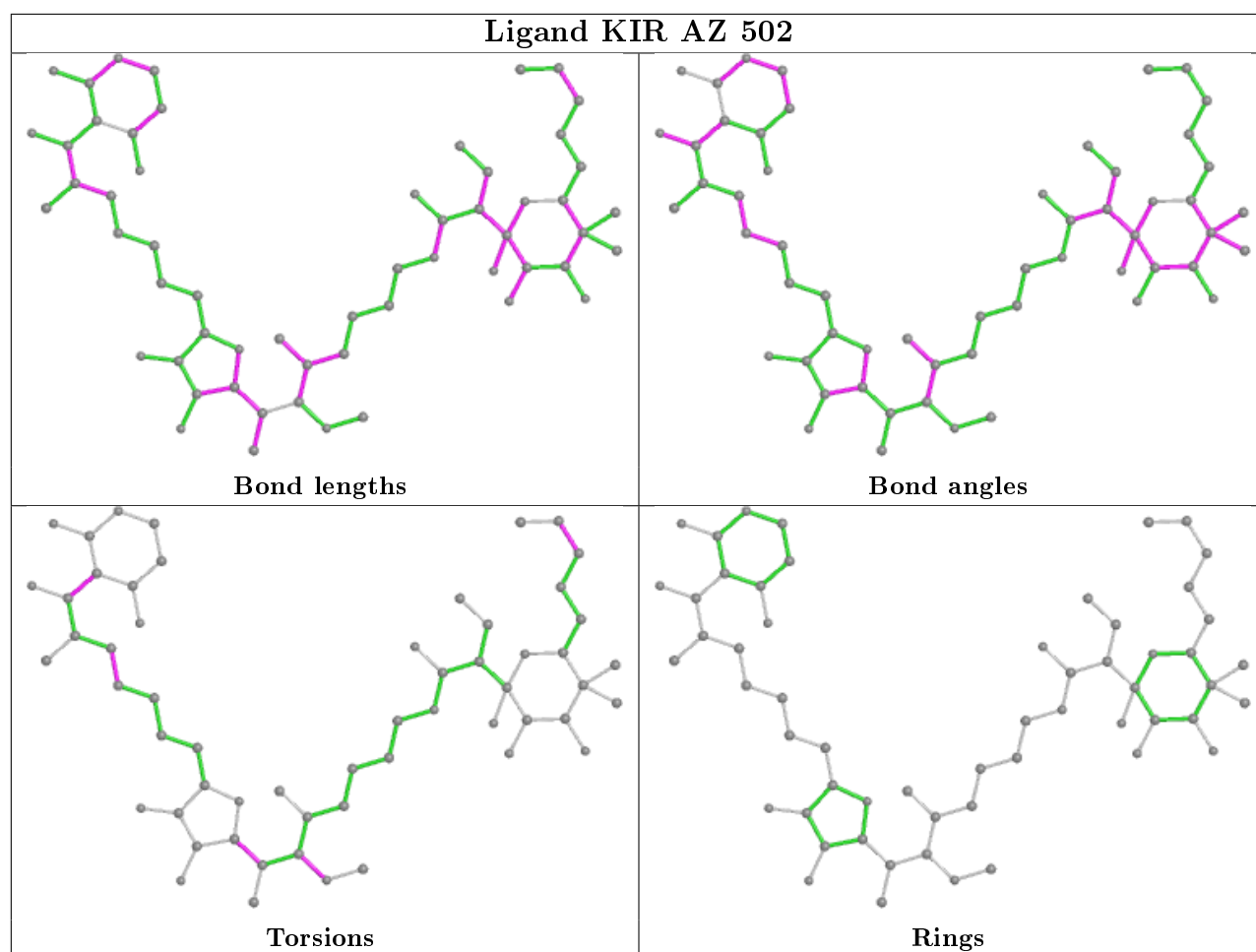
4 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CZ	502	KIR	9	0
60	CZ	501	GDP	8	0
60	AZ	501	GDP	15	0
61	AZ	502	KIR	13	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1510/1522 (99%)	-0.29	19 (1%) 77 59	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	-0.07	31 (2%) 63 43	37, 73, 161, 200	0
2	AB	234/256 (91%)	-0.10	6 (2%) 56 33	58, 88, 152, 164	0
2	CB	234/256 (91%)	-0.19	3 (1%) 77 59	54, 86, 151, 164	0
3	AC	206/239 (86%)	-0.30	1 (0%) 91 81	52, 75, 101, 110	0
3	CC	206/239 (86%)	-0.30	0 100 100	46, 70, 100, 109	0
4	AD	208/209 (99%)	0.11	10 (4%) 30 14	71, 97, 124, 132	0
4	CD	208/209 (99%)	0.05	4 (1%) 66 46	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.35	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.35	0 100 100	49, 63, 88, 109	0
6	AF	101/101 (100%)	0.04	1 (0%) 82 67	71, 99, 115, 122	0
6	CF	101/101 (100%)	-0.15	1 (0%) 82 67	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.18	7 (4%) 33 16	66, 89, 113, 130	0
7	CG	155/156 (99%)	-0.11	2 (1%) 77 59	59, 86, 112, 129	0
8	AH	138/138 (100%)	-0.28	1 (0%) 87 75	54, 70, 87, 95	0
8	CH	138/138 (100%)	-0.30	0 100 100	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.64	15 (11%) 4 2	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.23	2 (1%) 72 51	54, 93, 127, 139	0
10	AJ	98/105 (93%)	0.81	20 (20%) 1 0	59, 99, 141, 145	0
10	CJ	98/105 (93%)	0.35	5 (5%) 28 13	54, 95, 140, 144	0
11	AK	119/129 (92%)	0.04	6 (5%) 28 13	55, 73, 107, 134	0
11	CK	119/129 (92%)	-0.04	4 (3%) 45 24	51, 68, 108, 133	0
12	AL	124/131 (94%)	0.02	5 (4%) 38 19	55, 70, 94, 132	0
12	CL	124/131 (94%)	-0.12	1 (0%) 86 72	51, 68, 93, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.34	13 (10%) 6 2	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.13	7 (5%) 24 11	67, 95, 123, 152	0
14	AN	60/61 (98%)	-0.17	1 (1%) 70 49	57, 72, 93, 96	0
14	CN	60/61 (98%)	-0.02	1 (1%) 70 49	49, 66, 91, 96	0
15	AO	88/89 (98%)	-0.08	0 100 100	57, 75, 99, 105	0
15	CO	88/89 (98%)	-0.05	0 100 100	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.40	3 (3%) 42 22	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.38	2 (2%) 59 37	72, 89, 108, 136	0
17	AQ	99/105 (94%)	-0.00	3 (3%) 50 27	60, 79, 95, 108	0
17	CQ	99/105 (94%)	-0.06	0 100 100	57, 78, 93, 107	0
18	AR	70/88 (79%)	-0.05	2 (2%) 51 28	58, 82, 106, 119	0
18	CR	70/88 (79%)	-0.30	1 (1%) 75 56	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.43	5 (6%) 19 8	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.45	4 (5%) 28 13	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.44	6 (6%) 21 9	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.43	5 (5%) 28 13	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.77	3 (12%) 3 1	66, 84, 103, 115	0
21	CU	24/27 (88%)	0.37	1 (4%) 36 18	64, 78, 99, 115	0
22	AV	76/76 (100%)	-0.29	1 (1%) 77 59	56, 91, 128, 148	0
22	AW	76/76 (100%)	0.78	10 (13%) 3 1	103, 172, 200, 200	0
22	CV	76/76 (100%)	-0.22	1 (1%) 77 59	50, 89, 128, 147	0
22	CW	76/76 (100%)	0.70	11 (14%) 2 1	100, 172, 200, 200	0
23	AX	17/27 (62%)	0.58	2 (11%) 4 2	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.53	1 (5%) 22 10	45, 95, 156, 157	0
24	AY	68/77 (88%)	0.04	1 (1%) 73 54	61, 140, 171, 190	0
24	CY	68/77 (88%)	-0.01	4 (5%) 22 10	57, 140, 170, 190	0
25	AZ	385/405 (95%)	1.76	136 (35%) 0 0	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.44	24 (6%) 20 9	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.62	8 (9%) 8 2	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.55	7 (8%) 11 4	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.43	5 (5%) 25 12	74, 95, 134, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.24	2 (2%) 62 41	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.45	5 (7%) 16 7	110, 133, 148, 157	0
28	D2	71/72 (98%)	1.39	21 (29%) 0 0	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.66	3 (5%) 28 13	81, 99, 120, 142	0
29	D3	59/60 (98%)	0.54	3 (5%) 28 13	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.21	5 (11%) 5 2	124, 149, 160, 163	0
30	D4	44/71 (61%)	0.38	3 (6%) 17 7	123, 147, 158, 163	0
31	B5	59/60 (98%)	0.31	5 (8%) 10 4	73, 105, 158, 176	0
31	D5	59/60 (98%)	0.14	4 (6%) 17 7	72, 104, 158, 176	0
32	B6	50/54 (92%)	0.81	7 (14%) 2 1	74, 106, 116, 125	0
32	D6	50/54 (92%)	0.85	8 (16%) 1 1	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.43	0 100 100	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.58	2 (4%) 36 18	68, 78, 119, 140	0
34	B8	63/65 (96%)	0.49	3 (4%) 30 14	80, 90, 104, 131	0
34	D8	63/65 (96%)	0.41	3 (4%) 30 14	78, 88, 104, 131	0
35	B9	37/37 (100%)	0.63	2 (5%) 25 12	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.29	3 (8%) 12 5	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	-0.10	73 (2%) 57 34	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	-0.02	70 (2%) 59 37	46, 93, 190, 200	0
37	BB	119/122 (97%)	-0.46	0 100 100	78, 108, 134, 157	0
37	DB	119/122 (97%)	-0.37	0 100 100	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.71	32 (14%) 2 1	69, 99, 177, 187	0
38	DC	228/229 (99%)	0.33	20 (8%) 10 4	67, 97, 177, 187	0
39	BD	275/276 (99%)	-0.15	3 (1%) 80 64	50, 68, 98, 123	0
39	DD	275/276 (99%)	-0.16	2 (0%) 87 75	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.28	12 (5%) 22 10	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.25	8 (3%) 39 20	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.76	27 (13%) 3 1	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.68	27 (13%) 3 1	71, 127, 176, 184	0
42	BG	181/182 (99%)	0.25	11 (6%) 21 9	97, 125, 147, 157	0
42	DG	181/182 (99%)	0.08	9 (4%) 28 13	75, 96, 125, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	0.79	24 (15%) 2 1	106, 142, 163, 165	0
43	DH	159/180 (88%)	1.16	36 (22%) 0 0	106, 142, 163, 165	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.20	2 (1%) 75 56	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.17	3 (2%) 62 41	77, 104, 144, 147	0
47	BO	122/122 (100%)	-0.16	1 (0%) 86 72	58, 76, 90, 97	0
47	DO	122/122 (100%)	-0.06	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	0.95	20 (13%) 3 1	73, 121, 146, 162	0
48	DP	146/150 (97%)	0.96	27 (18%) 1 0	72, 120, 145, 162	0
49	BQ	141/141 (100%)	0.02	2 (1%) 75 56	61, 78, 107, 138	0
49	DQ	141/141 (100%)	0.05	4 (2%) 53 30	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.32	4 (3%) 45 24	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.31	3 (2%) 56 33	75, 98, 115, 129	0
51	BS	98/112 (87%)	0.87	18 (18%) 1 0	89, 112, 137, 141	0
51	DS	98/112 (87%)	0.46	5 (5%) 28 13	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.13	9 (6%) 18 7	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.23	12 (8%) 10 4	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.14	3 (2%) 56 33	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.13	2 (1%) 70 49	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.56	7 (6%) 16 7	79, 130, 146, 150	0
54	DV	101/101 (100%)	0.50	7 (6%) 16 7	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.47	8 (7%) 16 6	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.39	9 (7%) 12 5	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.49	3 (3%) 46 24	83, 109, 125, 134	0
56	DX	92/96 (95%)	0.40	7 (7%) 13 5	83, 108, 124, 134	0
57	BY	100/110 (90%)	1.80	38 (38%) 0 0	127, 146, 179, 187	0
57	DY	100/110 (90%)	1.76	40 (40%) 0 0	126, 146, 179, 187	0
58	BZ	176/206 (85%)	0.09	5 (2%) 53 30	75, 103, 135, 144	0
58	DZ	176/206 (85%)	0.05	8 (4%) 33 16	64, 94, 140, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21994/23368 (94%)	0.13	1092 (4%) 28 13	37, 93, 162, 200	0

The worst 5 of 1092 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	141	GLN	14.3
49	BQ	141	GLN	12.8
38	BC	1	PRO	11.6
43	DH	170	ARG	11.5
53	DU	118	GLY	11.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	H2U	CY	16	20/21	0.56	0.69	181,191,191,193	0
24	H2U	AY	16	20/21	0.58	0.66	181,191,192,193	0
24	7MG	AY	46	24/25	0.65	0.39	166,169,171,171	0
24	H2U	AY	20	20/21	0.74	0.35	186,186,188,188	0
24	4SU	AY	8	20/21	0.76	0.30	140,143,144,144	0
24	PSU	CY	55	20/21	0.79	0.18	158,166,168,168	0
24	H2U	CY	20	20/21	0.79	0.38	185,186,187,187	0
24	H2U	AY	17	20/21	0.80	0.54	194,195,195,195	0
24	H2U	CY	17	20/21	0.80	0.58	194,195,195,195	0
24	PSU	AY	55	20/21	0.80	0.19	157,166,168,168	0
24	7MG	CY	46	24/25	0.84	0.23	166,168,170,170	0
24	4SU	CY	8	20/21	0.85	0.24	140,141,142,142	0
24	5MU	CY	54	21/22	0.89	0.15	142,153,154,156	0
24	OMC	CY	32	21/22	0.90	0.17	96,103,108,109	0
24	OMC	AY	32	21/22	0.92	0.29	98,106,112,113	0
24	5MU	AY	54	21/22	0.92	0.20	143,153,153,156	0
24	MIA	CY	37	29/30	0.93	0.28	60,80,107,108	0
24	MIA	AY	37	29/30	0.94	0.26	63,84,108,108	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

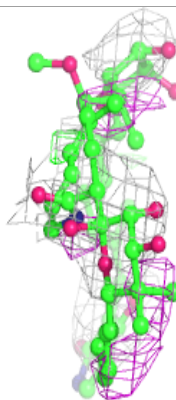
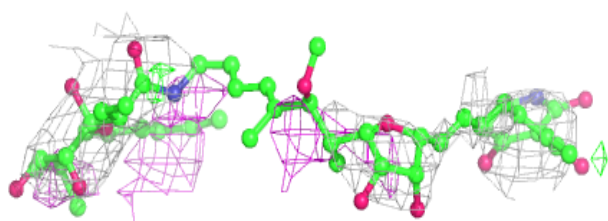
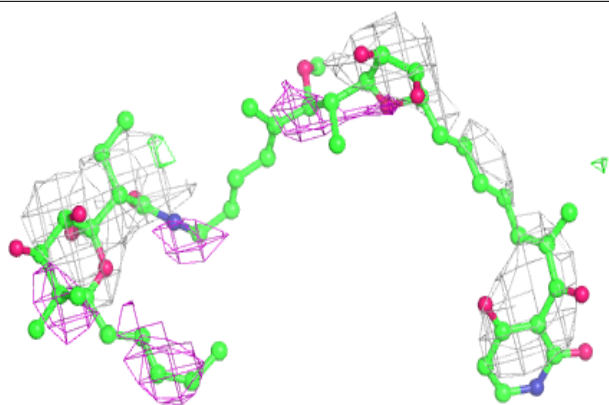
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
61	KIR	AZ	502	57/57	0.74	0.57	139,147,150,150	0
60	GDP	CZ	501	28/28	0.81	0.25	141,145,153,153	0
61	KIR	CZ	502	57/57	0.84	0.34	139,145,150,151	0
60	GDP	AZ	501	28/28	0.84	0.23	151,157,158,158	0
59	ZN	B4	101	1/1	0.88	0.08	200,200,200,200	0
59	ZN	B9	101	1/1	0.94	0.14	200,200,200,200	0
59	ZN	D9	101	1/1	0.97	0.11	133,133,133,133	0
59	ZN	AD	301	1/1	0.99	0.29	99,99,99,99	0
59	ZN	AN	101	1/1	0.99	0.16	84,84,84,84	0
59	ZN	D4	101	1/1	0.99	0.14	129,129,129,129	0
59	ZN	CD	301	1/1	0.99	0.31	85,85,85,85	0
59	ZN	CN	101	1/1	1.00	0.17	63,63,63,63	0

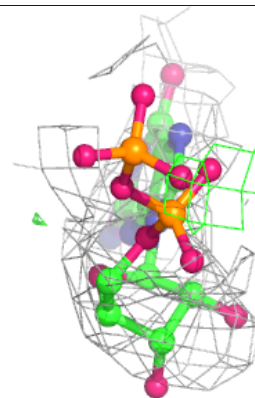
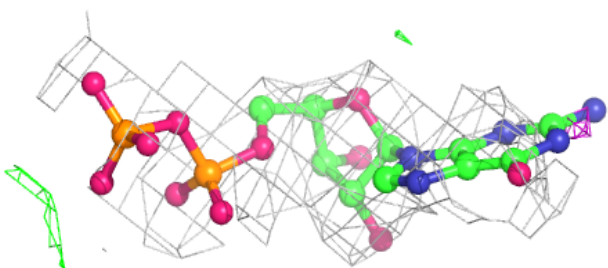
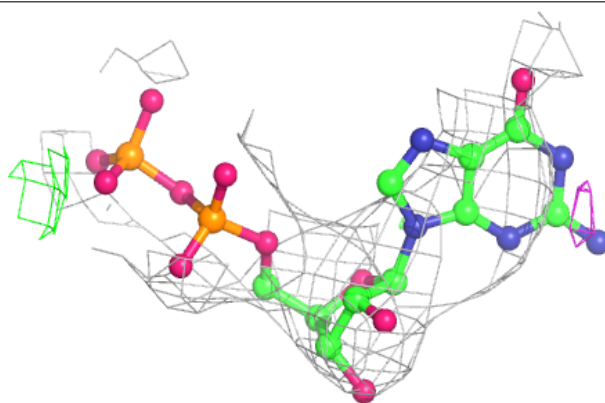
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KIR 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)

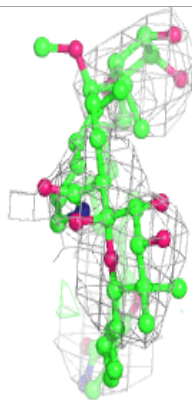
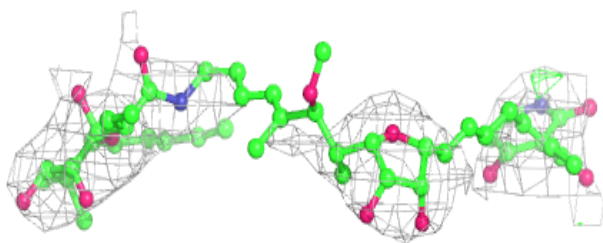
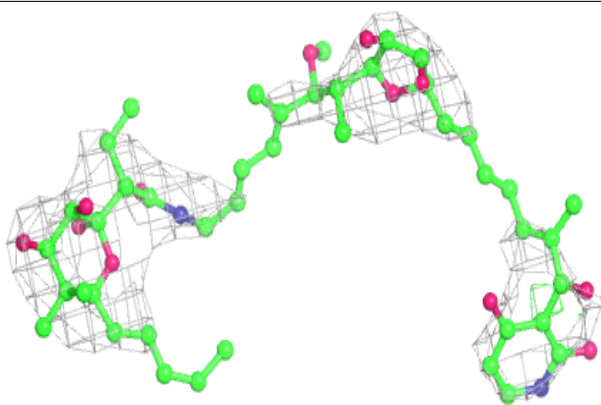
**Electron density around GDP CZ 501:**

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

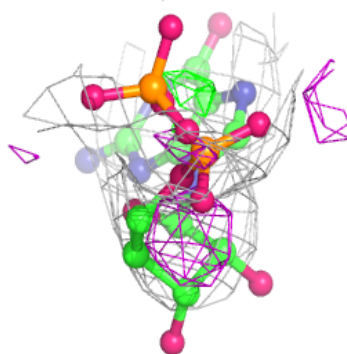
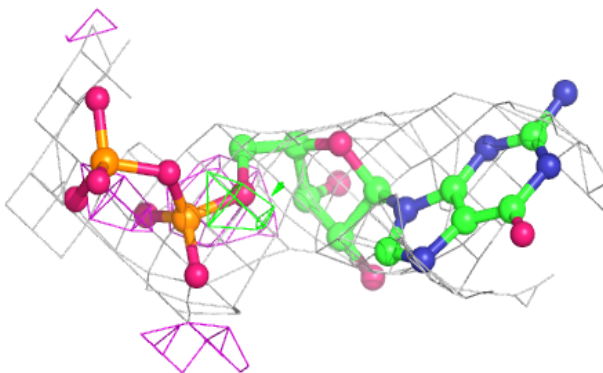
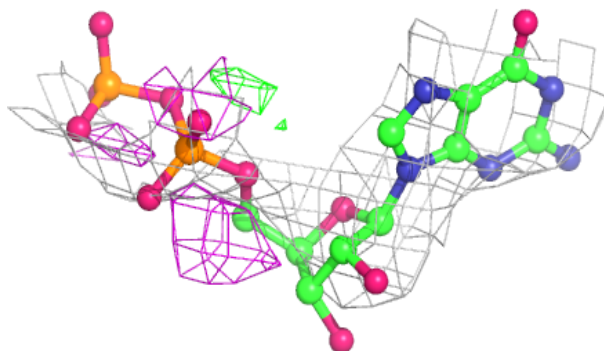


Electron density around KIR CZ 502:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.