



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 4V5F / pdb_00004v5f
Title : The structure of the ribosome with elongation factor G trapped in the post-translocational state
Authors : Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-09-01
Resolution : 3.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

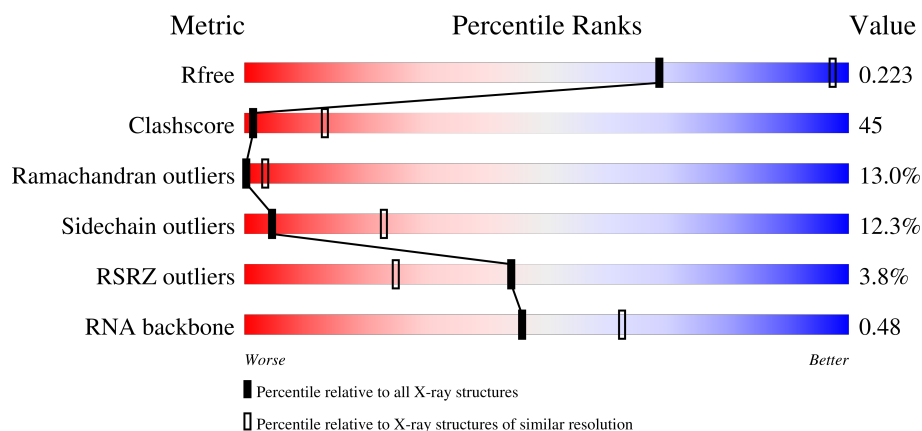
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 28% 55% 13% ..
1	CA	1522	3% 27% 57% 13% ..
2	AB	256	2% 20% 50% 19% . 8%

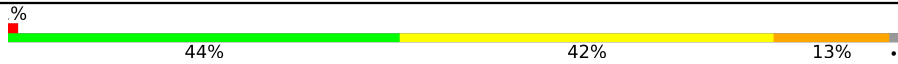
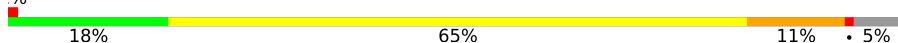
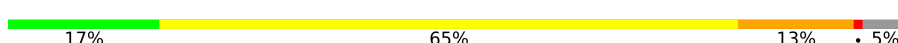
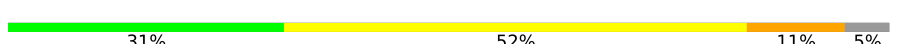
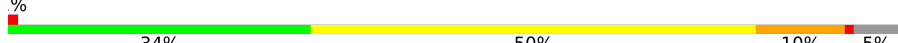
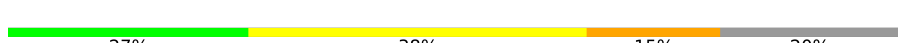
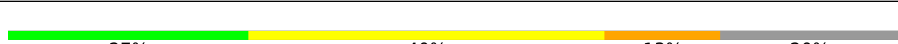
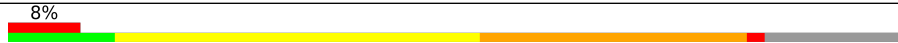
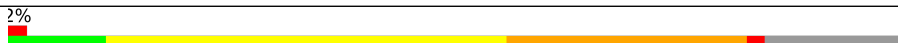
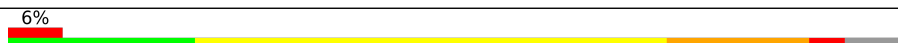
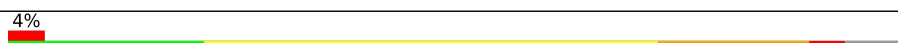
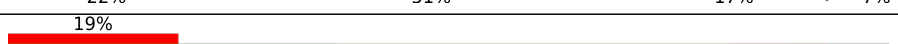
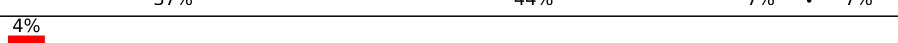
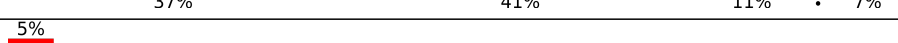
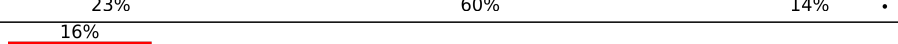
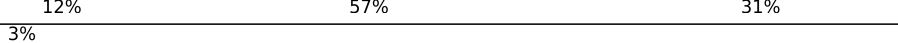
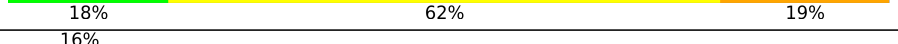
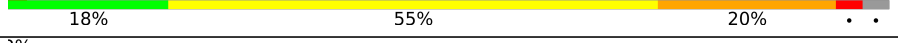
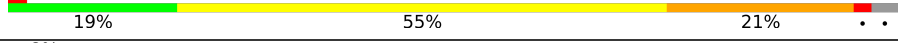
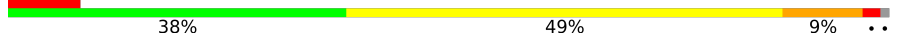
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Mol	Chain	Length	Quality of chain
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	

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Mol	Chain	Length	Quality of chain
15	AO	89	
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	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
23	CX	25	
24	AY	691	
24	CY	691	
25	B0	85	
25	D0	85	
26	B1	98	

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

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Mol	Chain	Length	Quality of chain
39	BE	206	
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BJ	173	
43	DJ	173	
44	BK	147	
44	DK	147	
45	BL	125	
45	BM	125	
45	Bl	125	
45	Bm	125	
45	DL	125	
45	DM	125	
45	DI	125	
45	Dm	125	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	

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Mol	Chain	Length	Quality of chain
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
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
61	FUA	CY	702	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 311552 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	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	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

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

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

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	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	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UN-MODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			
23	CX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			
24	CY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
29	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			
42	DH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				
43	DJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			
44	DK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	BM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bl	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bm	30	Total	C	N	O		0	0	1
			146	87	30	29				
45	DL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	DM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	DI	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Dm	30	Total	C	N	O		0	0	1
			146	87	30	29				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	0	0	1
			1142	710	235	196			
52	DT	138	Total	C	N	O	0	0	1
			1142	710	235	196			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			
57	DY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
58	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

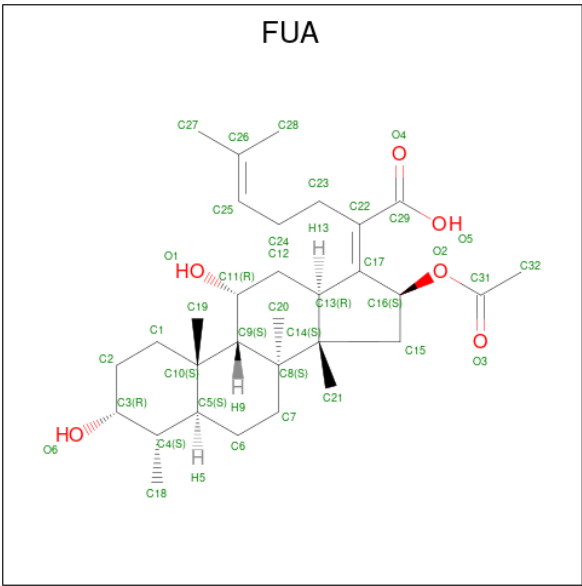
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

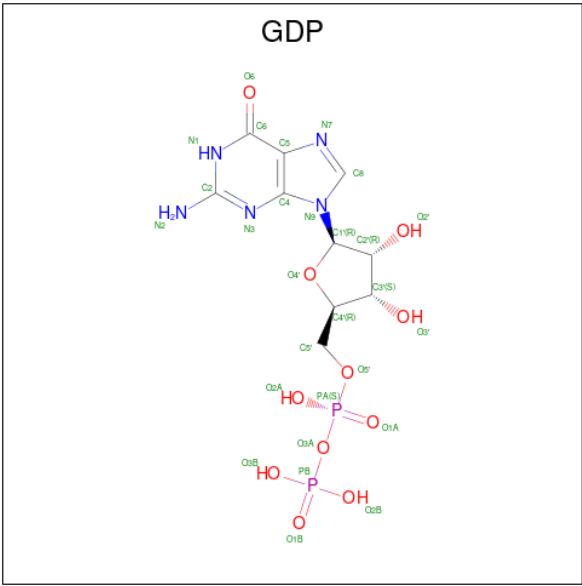
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Mg	0	0
			1	1		
60	CY	1	Total	Mg	0	0
			1	1		

- Molecule 61 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AY	1	Total	C	O	0	0
			37	31	6		
61	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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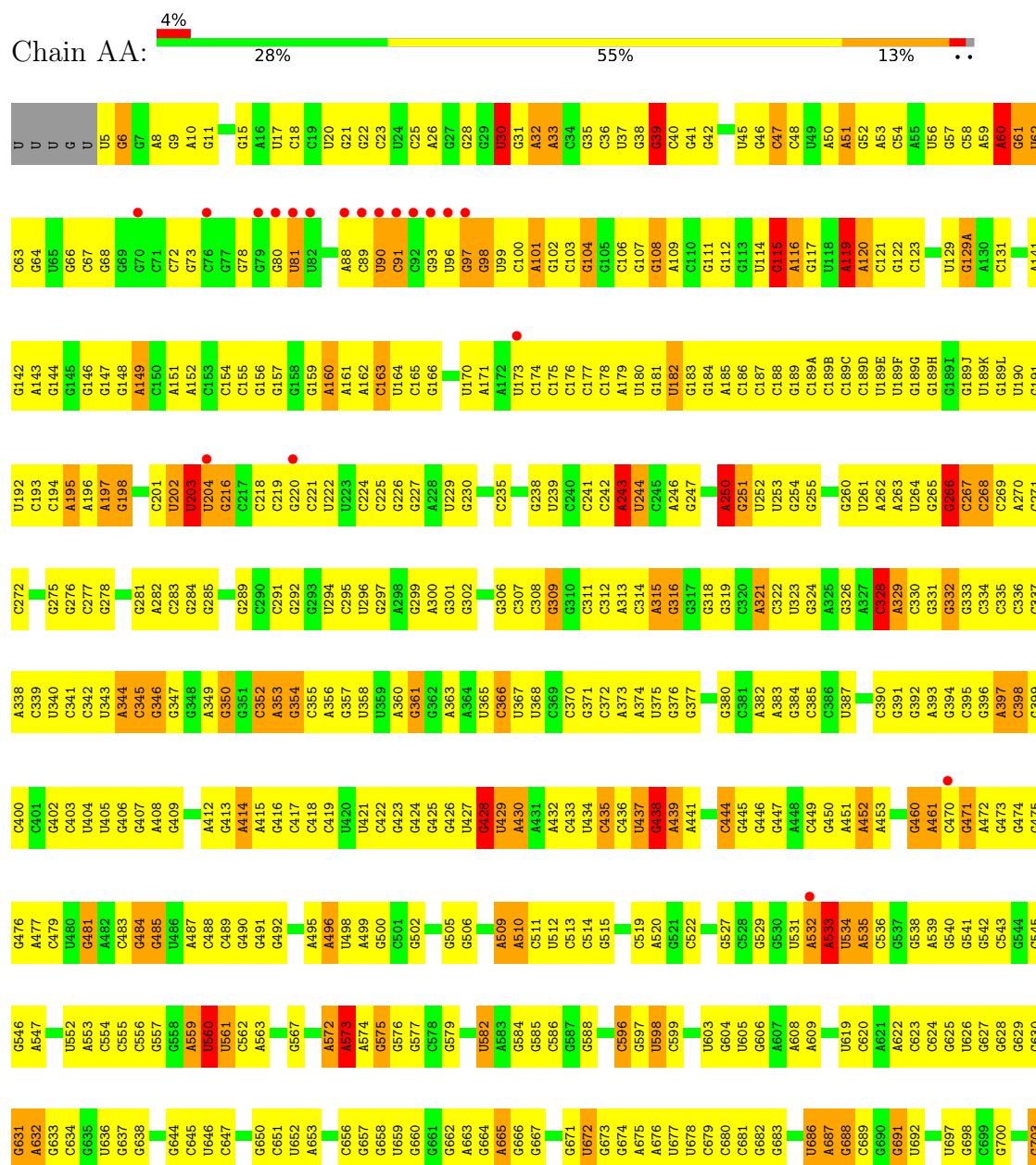
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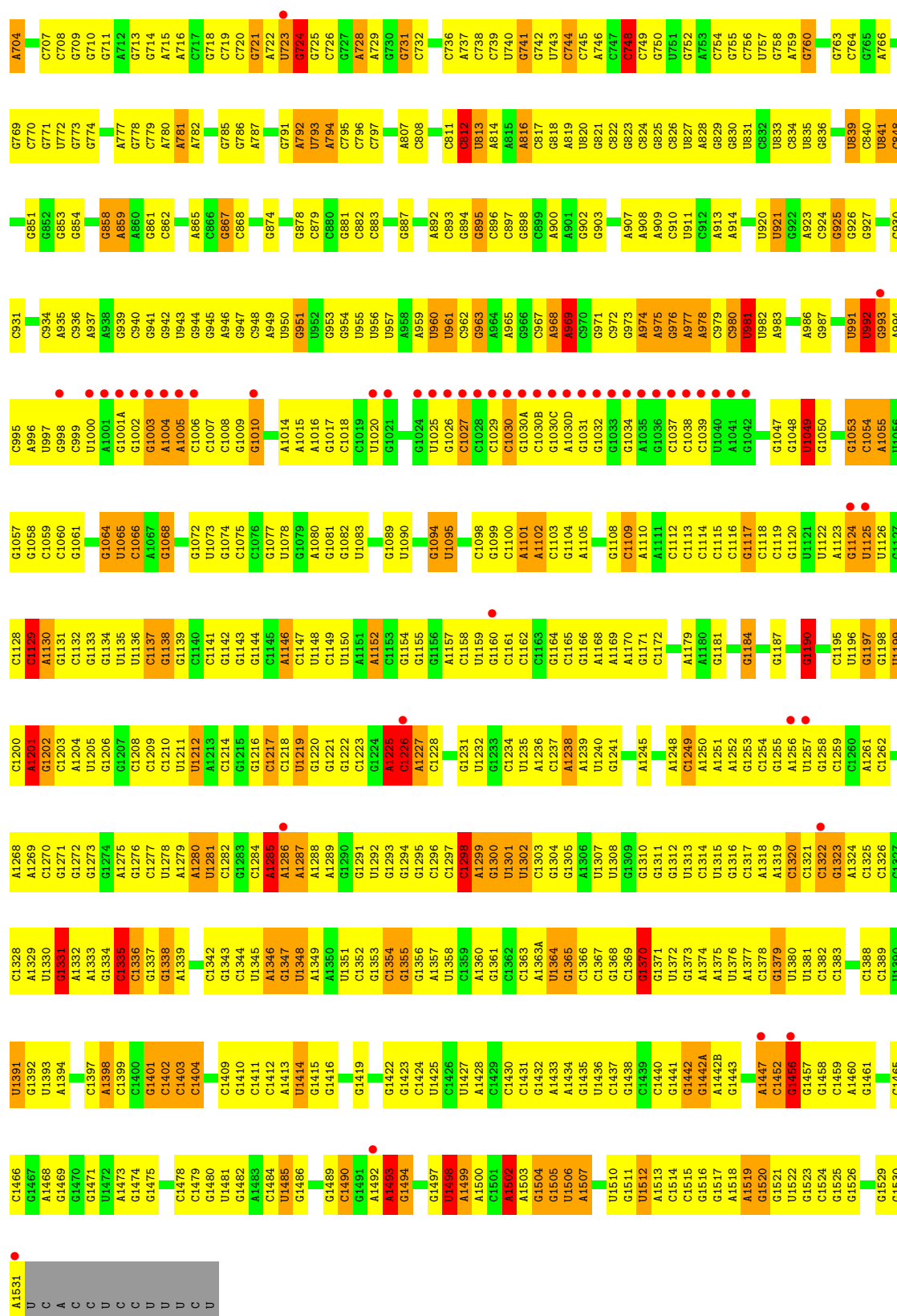
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

3 Residue-property plots

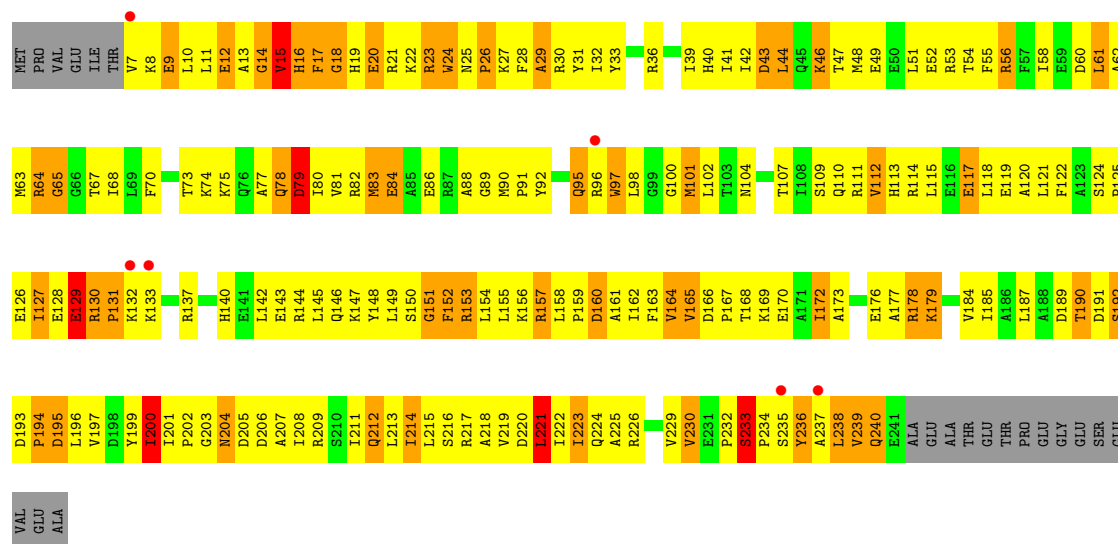
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S ribosomal RNA

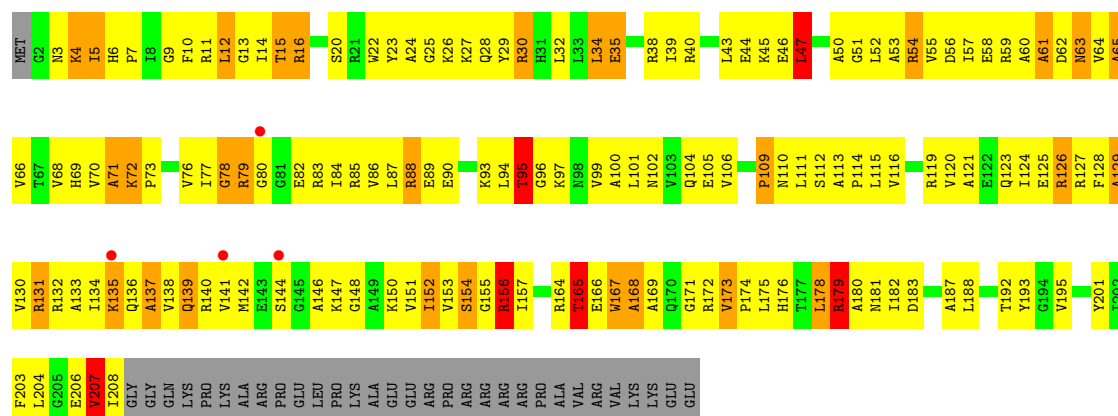




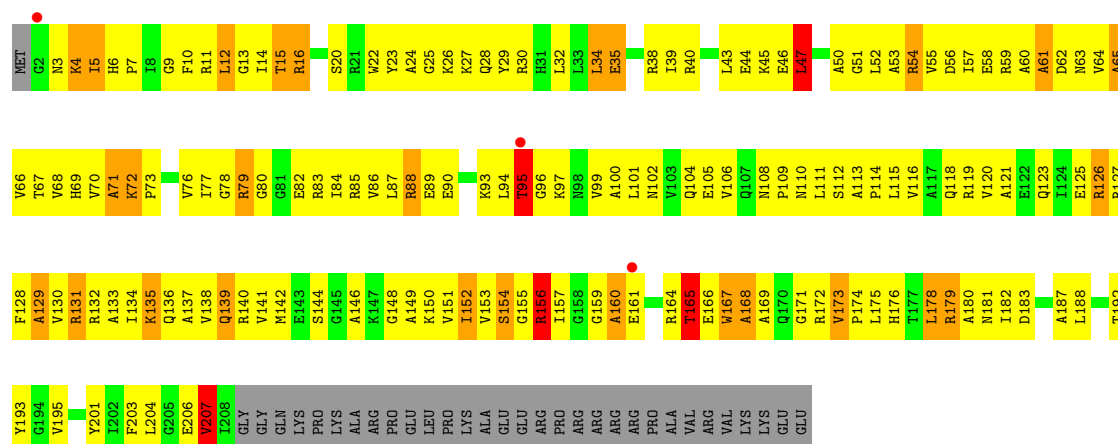




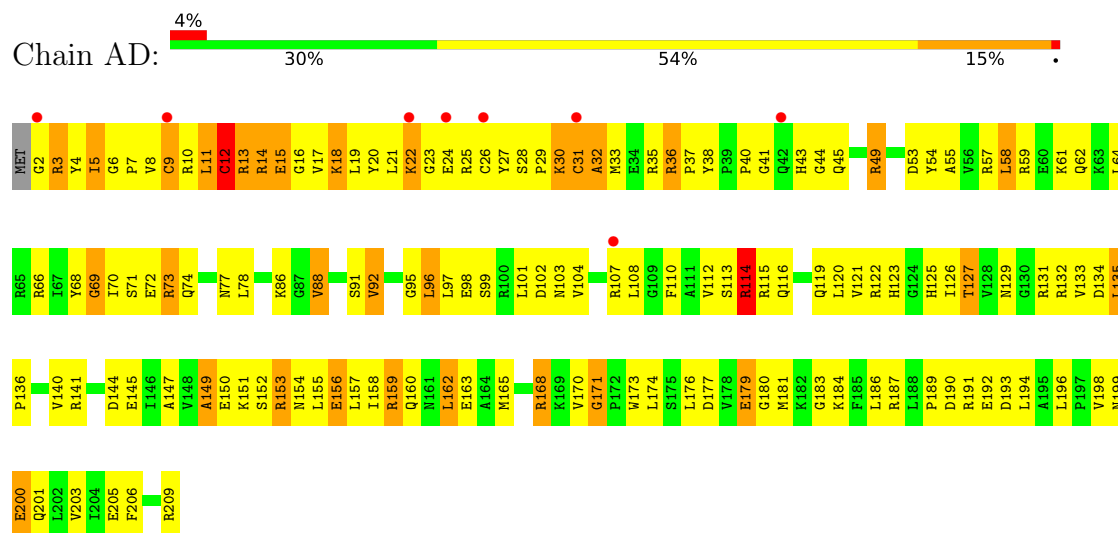
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



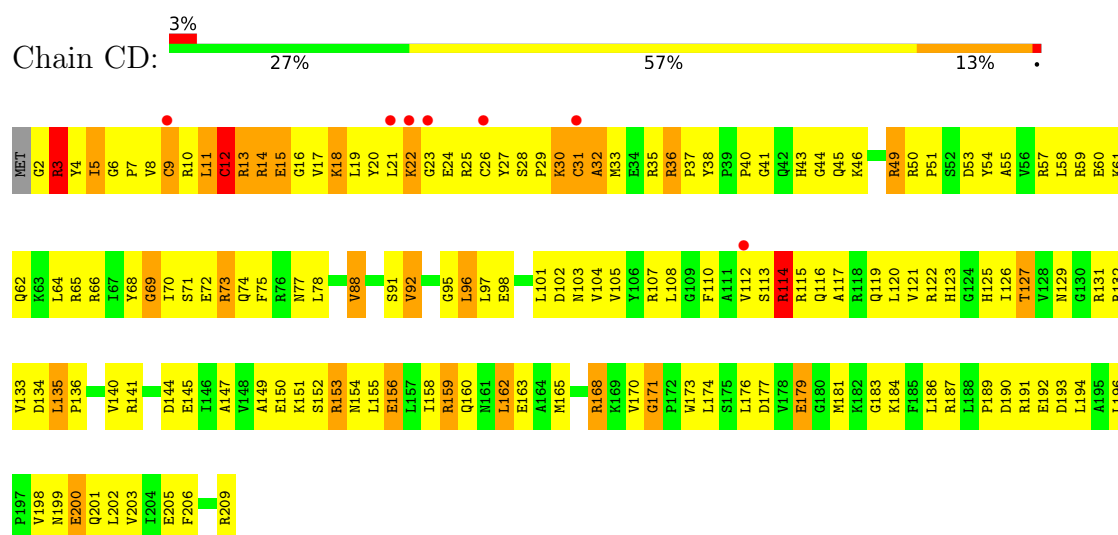
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



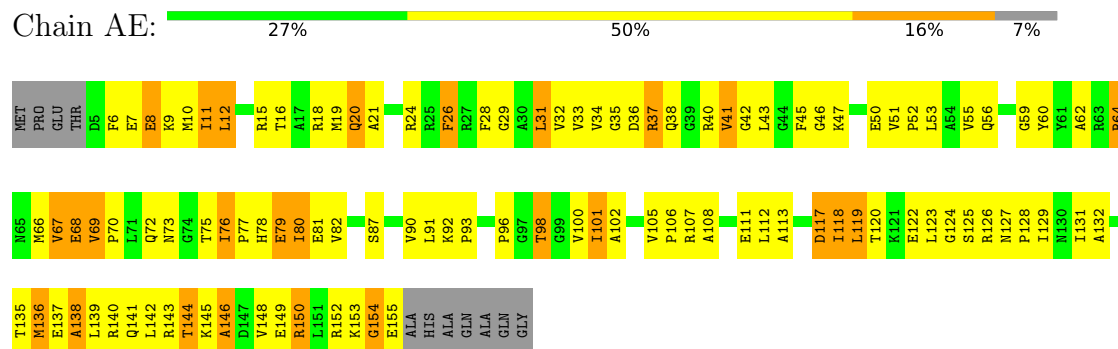
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

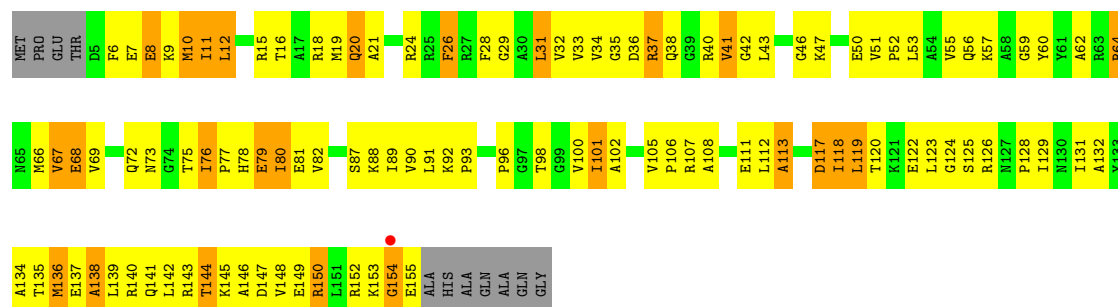


• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5





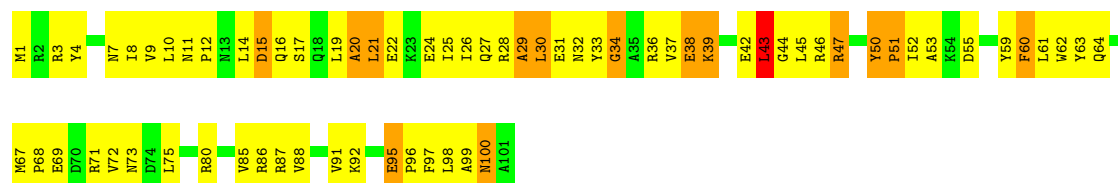
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 32% 57% 10% .



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF: 32% 53% 14% .



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

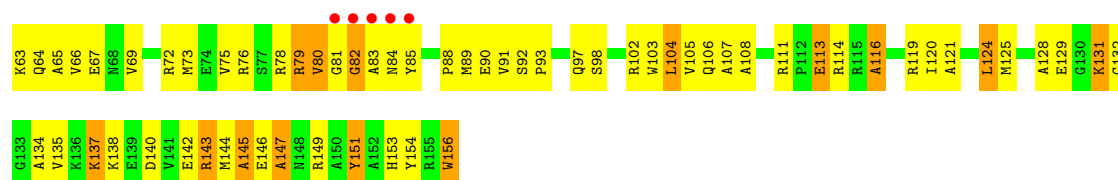
Chain AG: 3% 33% 53% 14% .



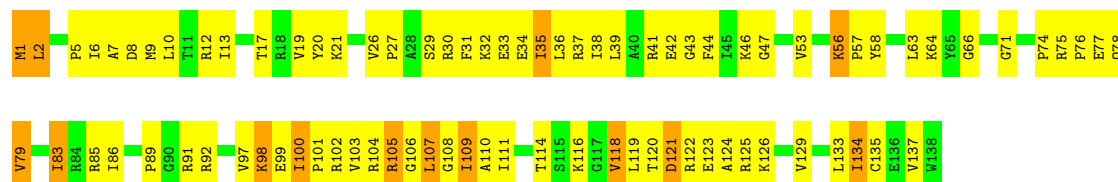
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG: 4% 32% 52% 15% .

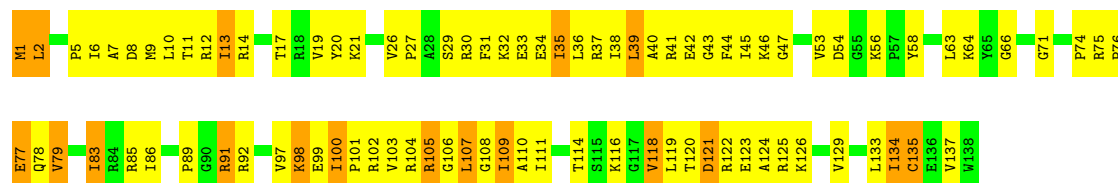




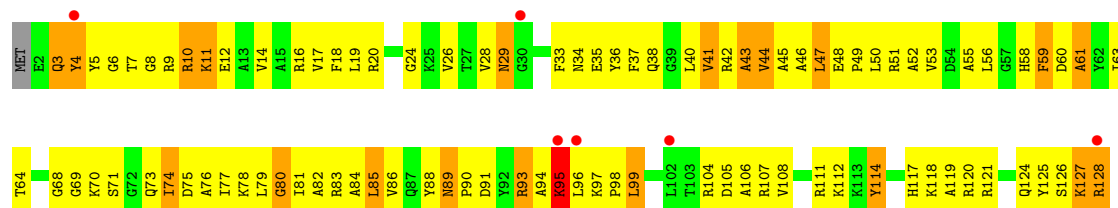
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



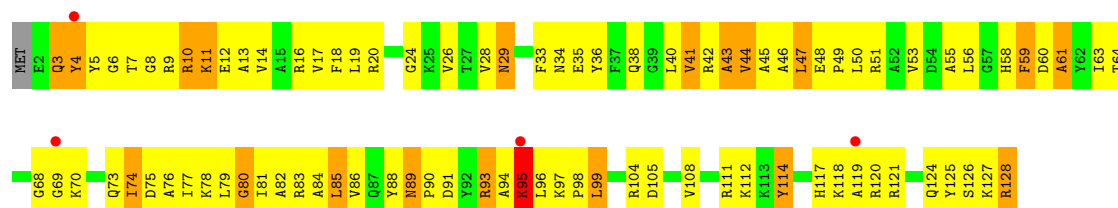
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



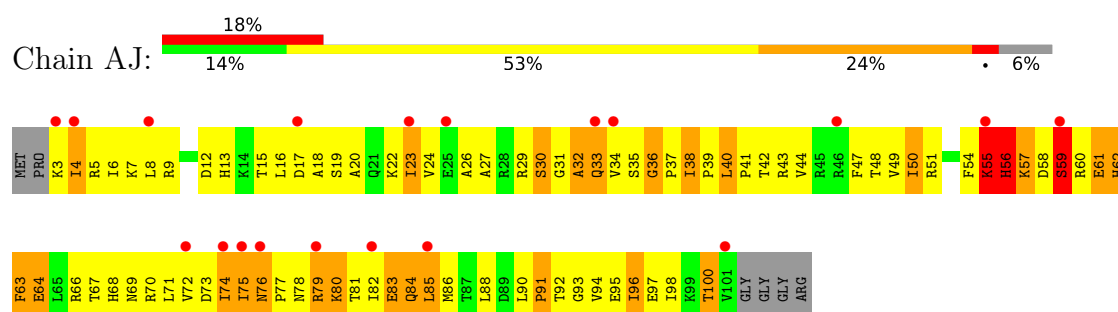
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



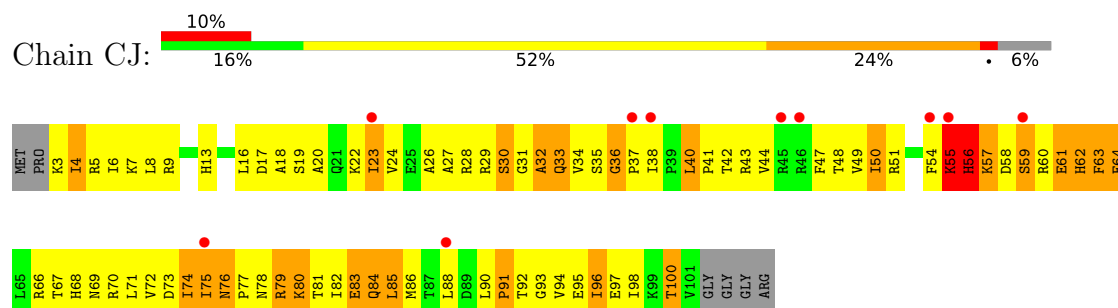
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



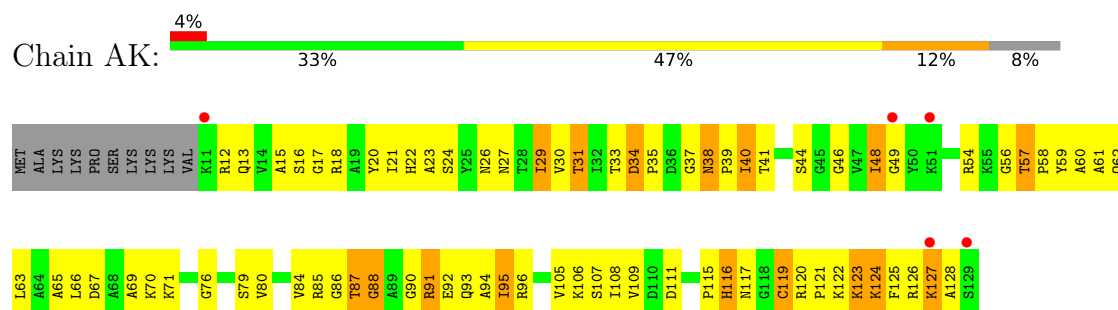
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



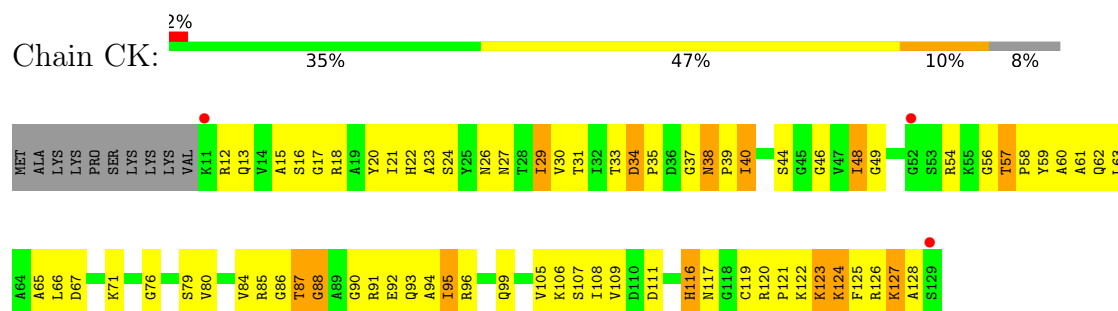
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



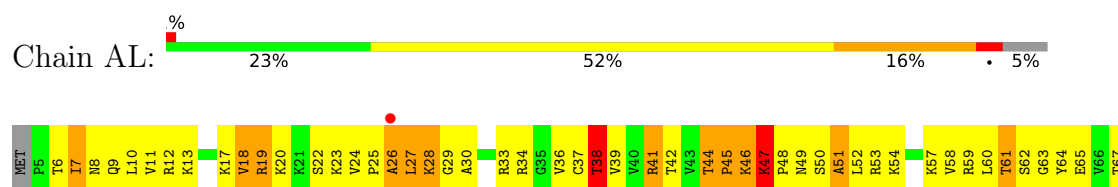
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

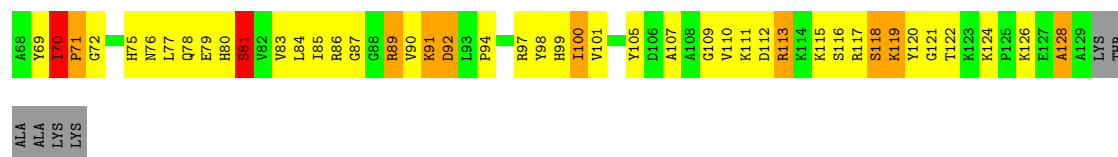


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

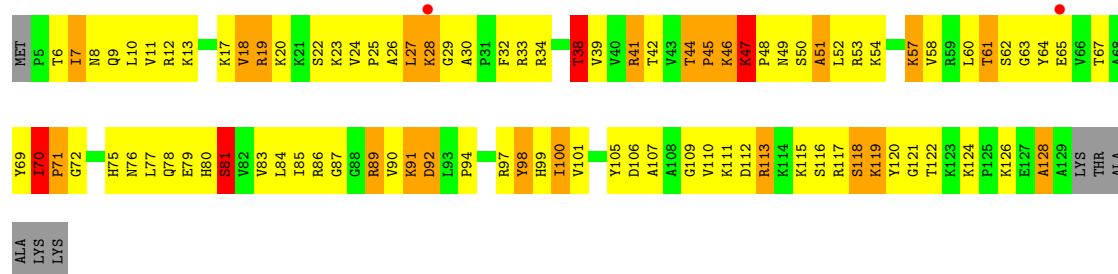


- Molecule 12: 30S RIBOSOMAL PROTEIN S12

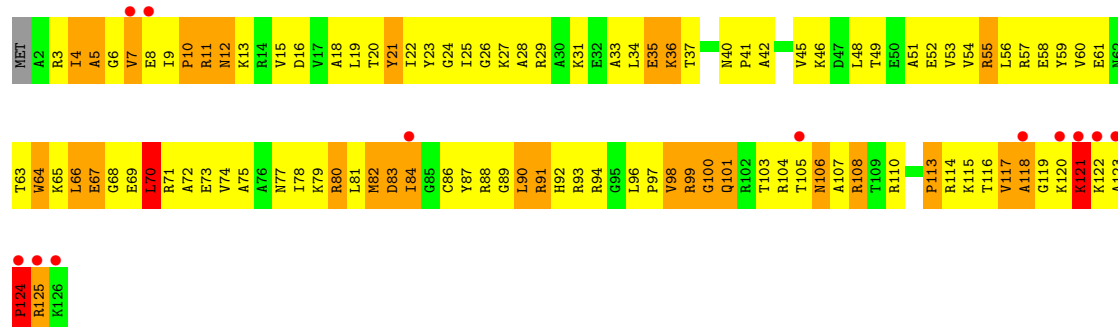
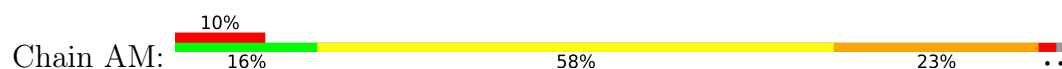




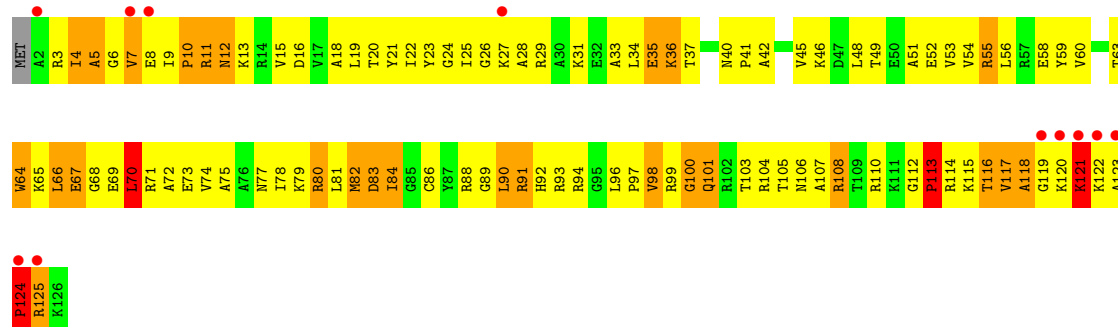
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

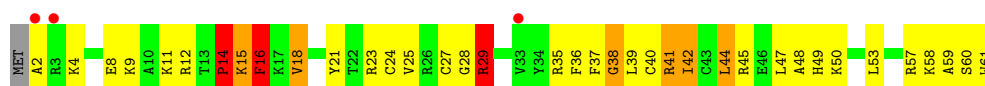


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

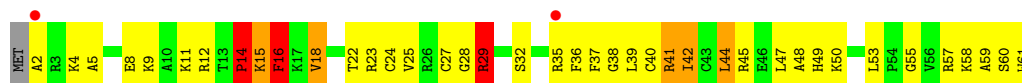


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

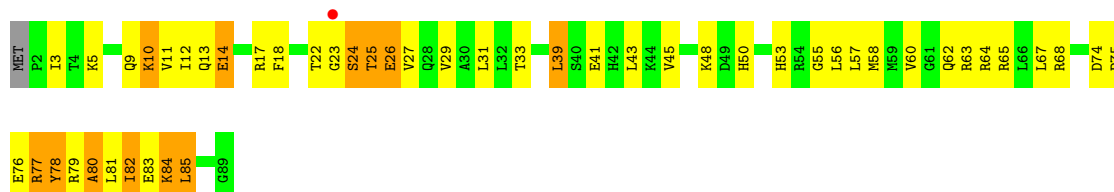




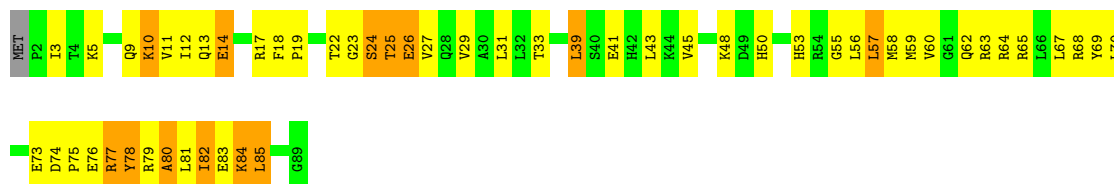
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



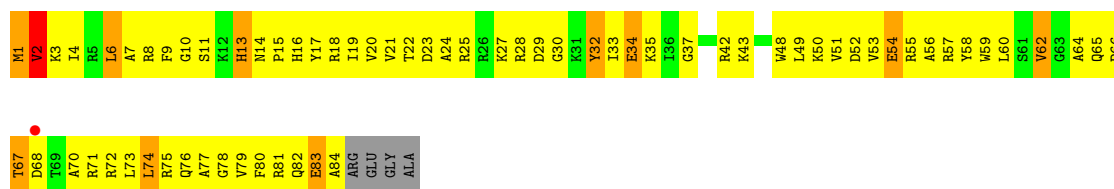
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



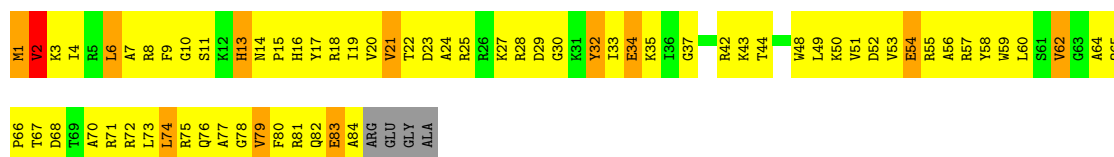
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

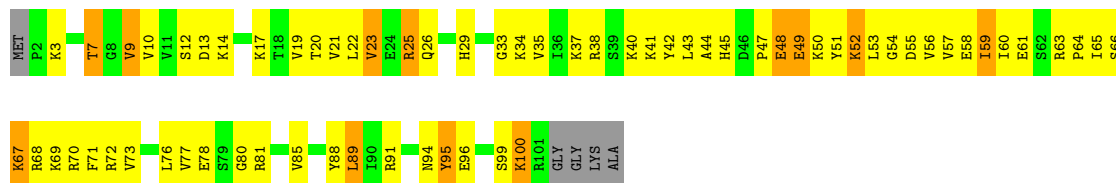


• Molecule 16: 30S RIBOSOMAL PROTEIN S16



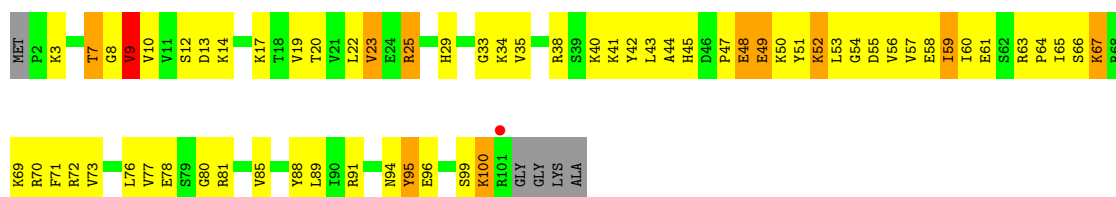
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:  31% 52% 11% 5%

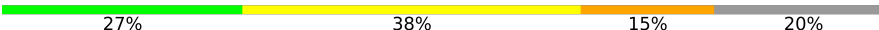


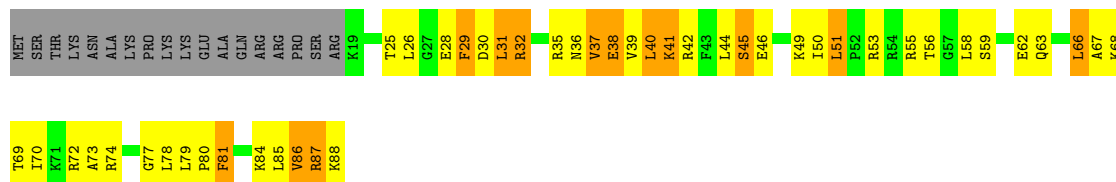
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:  % 34% 50% 10% 5%

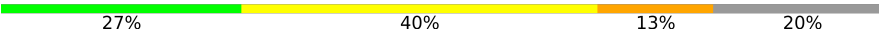


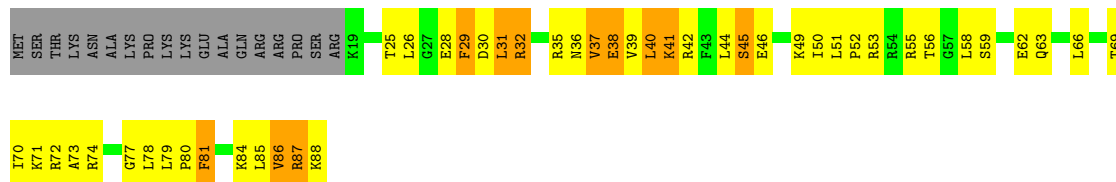
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:  27% 38% 15% 20%



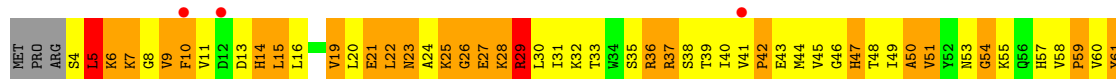
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:  27% 40% 13% 20%

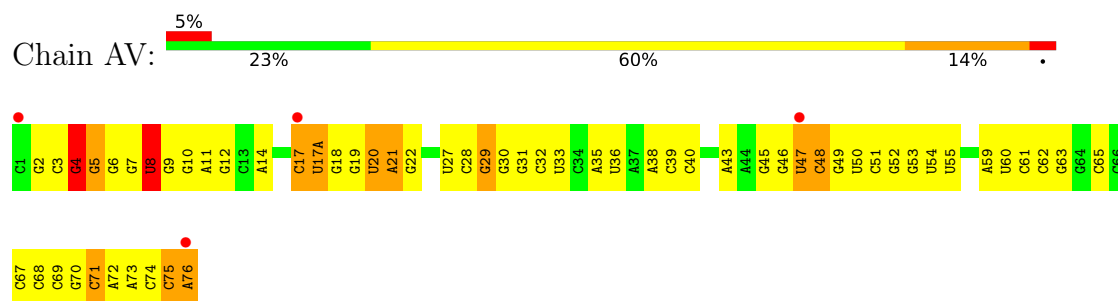


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

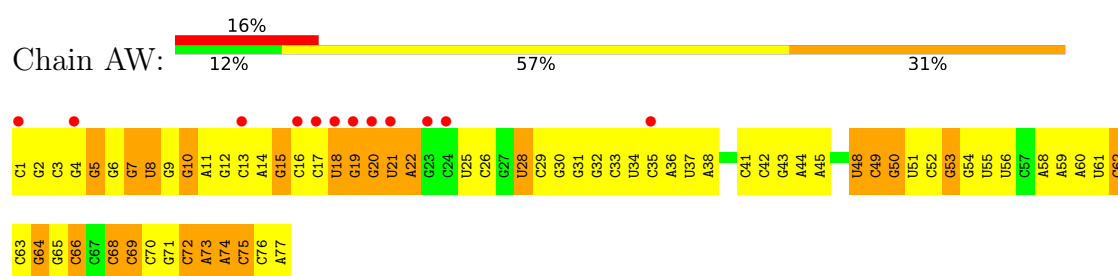
Chain AS:  8% 12% 41% 30% 15%



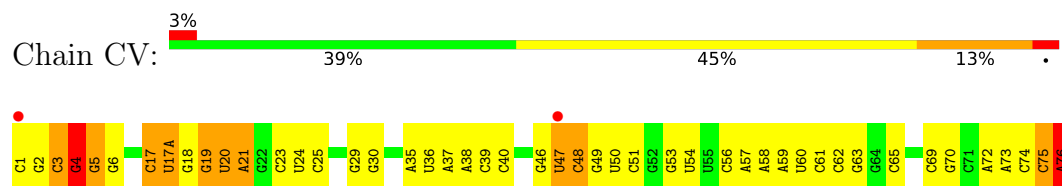
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



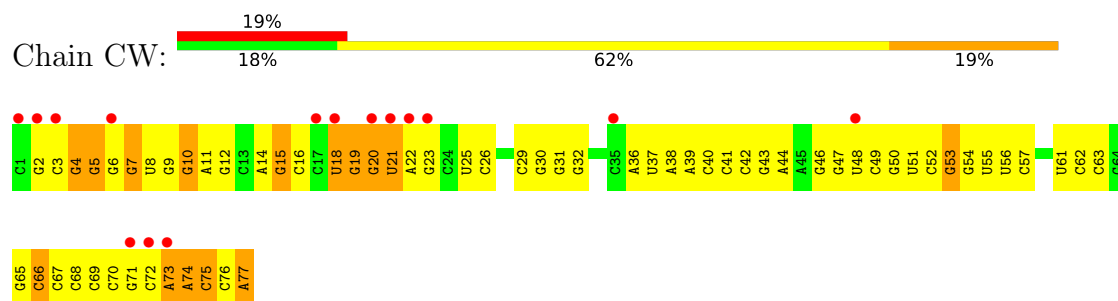
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



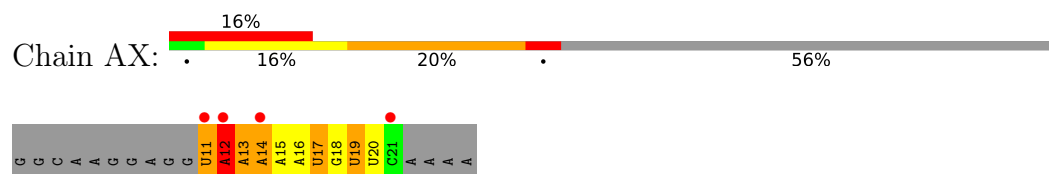
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 23: MRNA



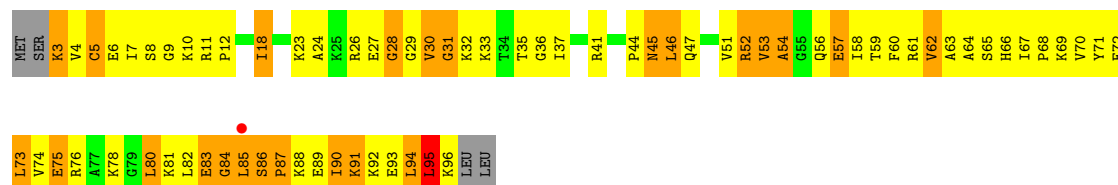
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G	Grey	No
C	Grey	No
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G	Grey	No
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G	Grey	No
A	Grey	No
G	Grey	No
U11	Red	Yes
A12	Orange	Yes
A13	Yellow-Orange	No
A14	Yellow	No
A15	Light Green	Yes
A16	Green	No
U17	Green	No
G18	Green	No
U19	Green	Yes
U20	Green	No
C21	Green	Yes
A	Grey	No
A	Grey	No
A	Grey	No
A	Grey	No

[illegible]

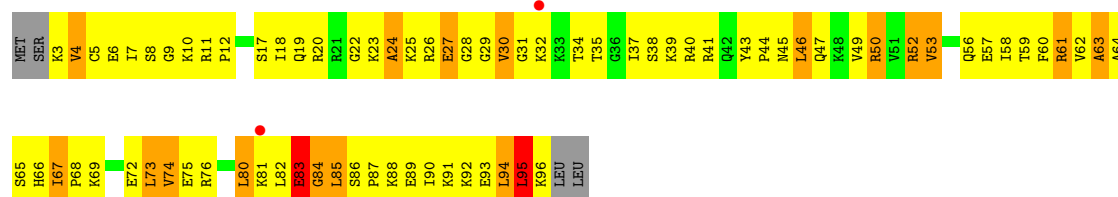
Chain CY:



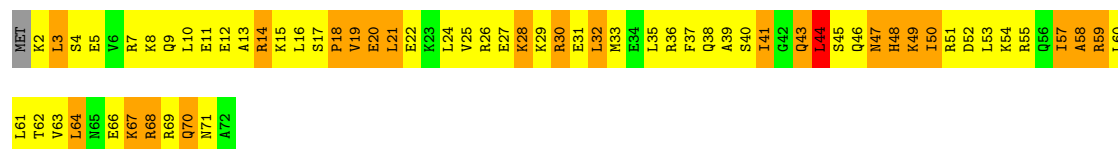
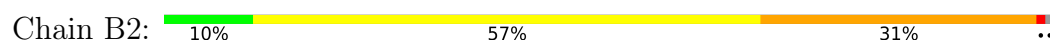
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



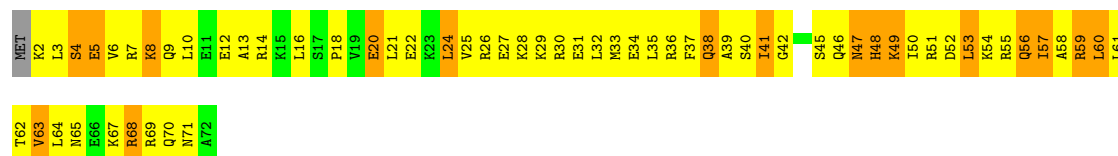
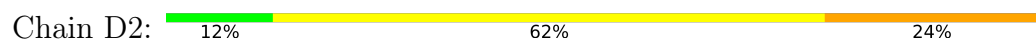
- Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

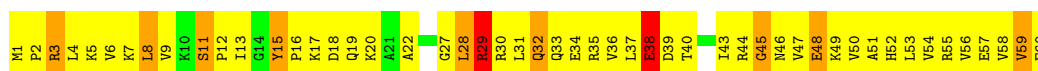


● Molecule 27: 50S RIBOSOMAL PROTEIN L29

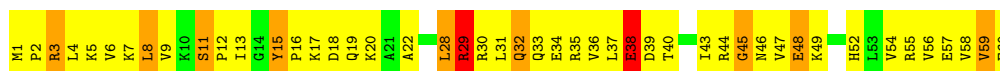


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

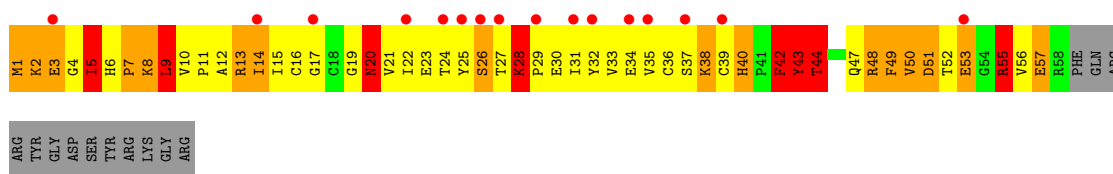




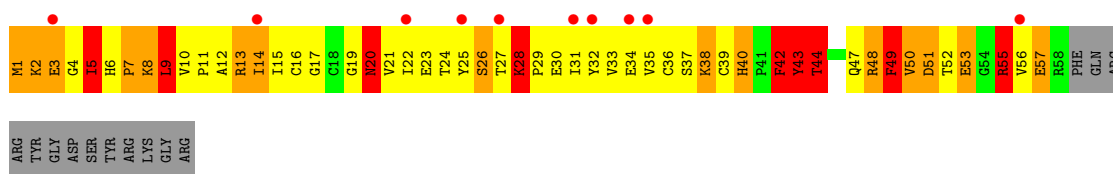
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

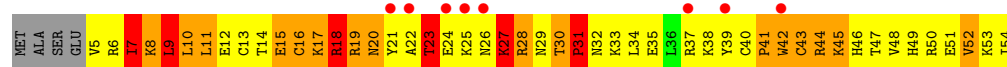


• Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6: 



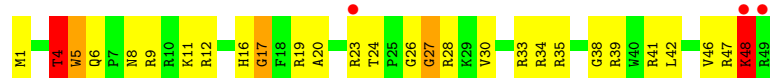
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7: 

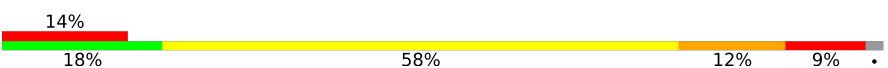


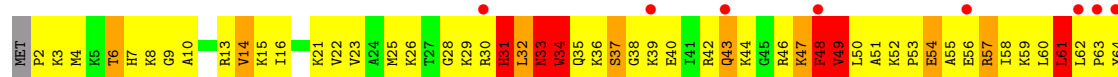
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7: 

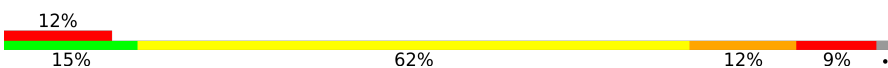


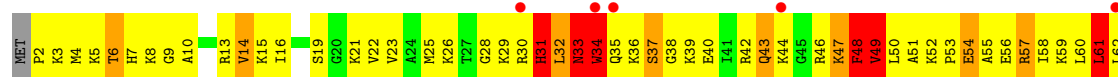
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8: 

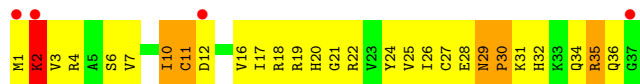


- Molecule 34: 50S RIBOSOMAL PROTEIN L36

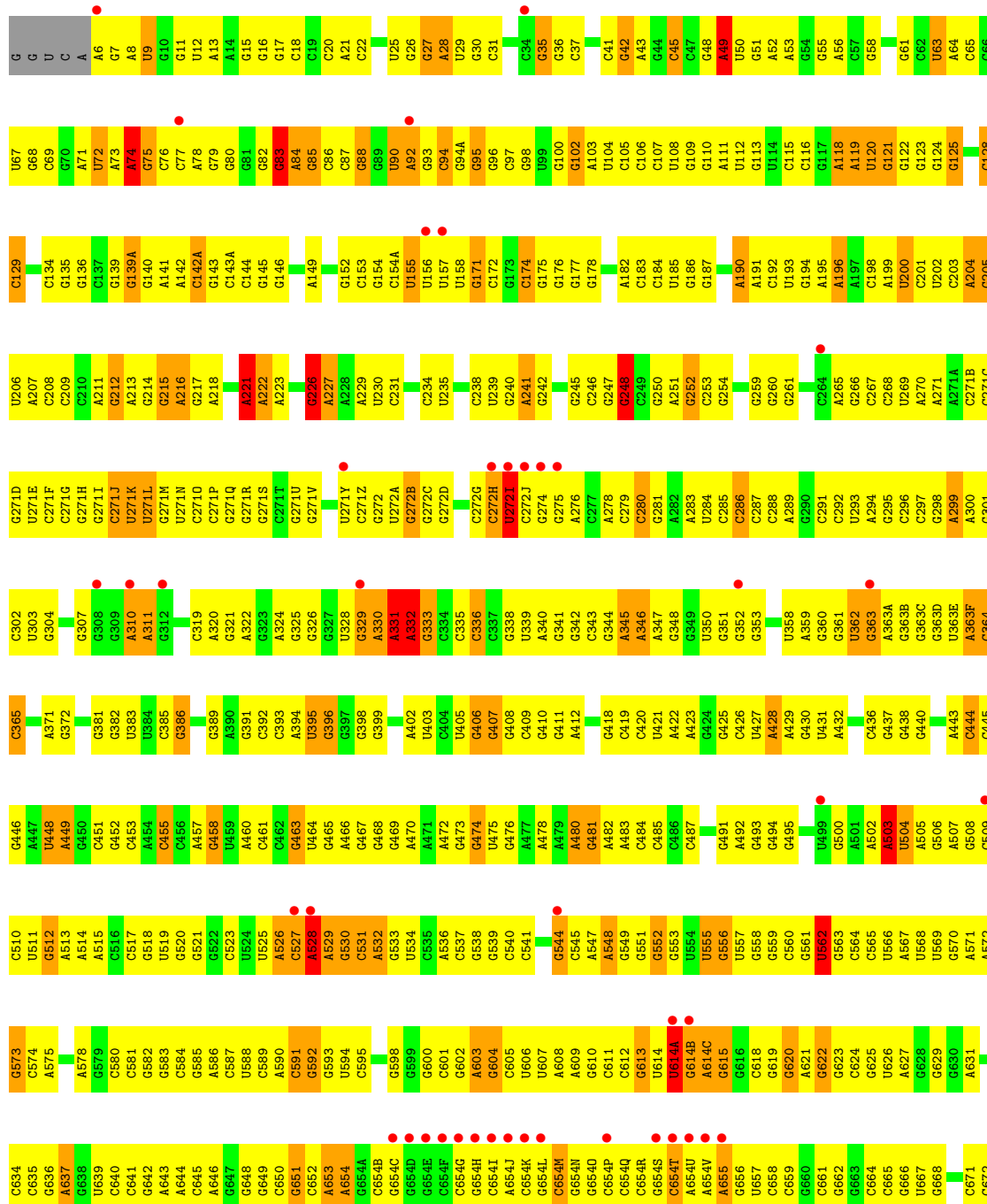
Chain B9: 



● Molecule 34: 50S RIBOSOMAL PROTEIN L36

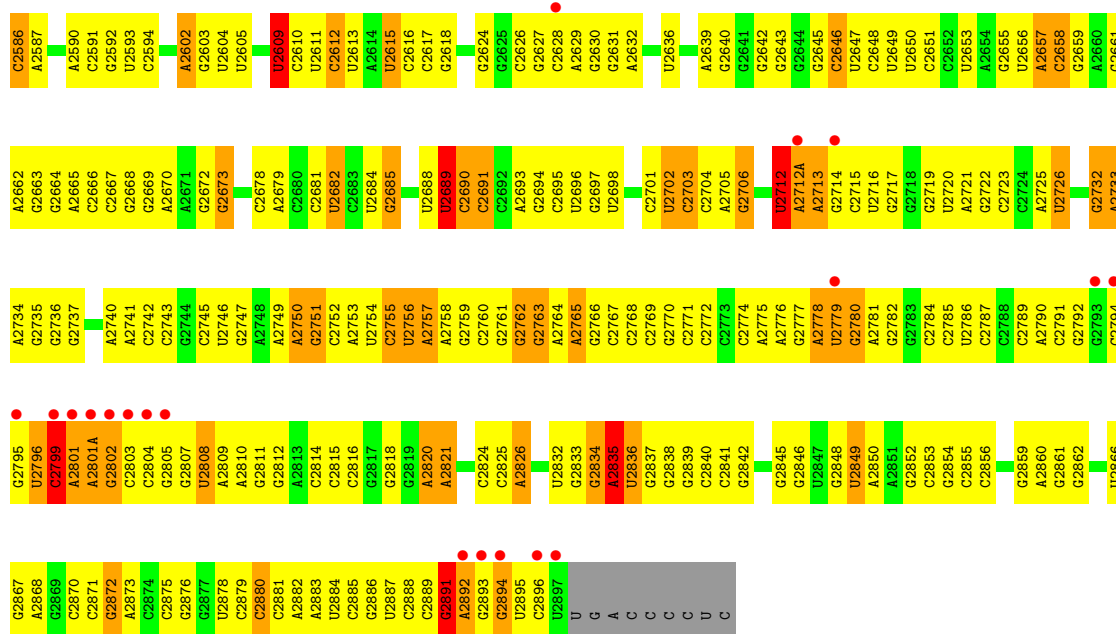


● Molecule 35: 23S RIBOSOMAL RNA

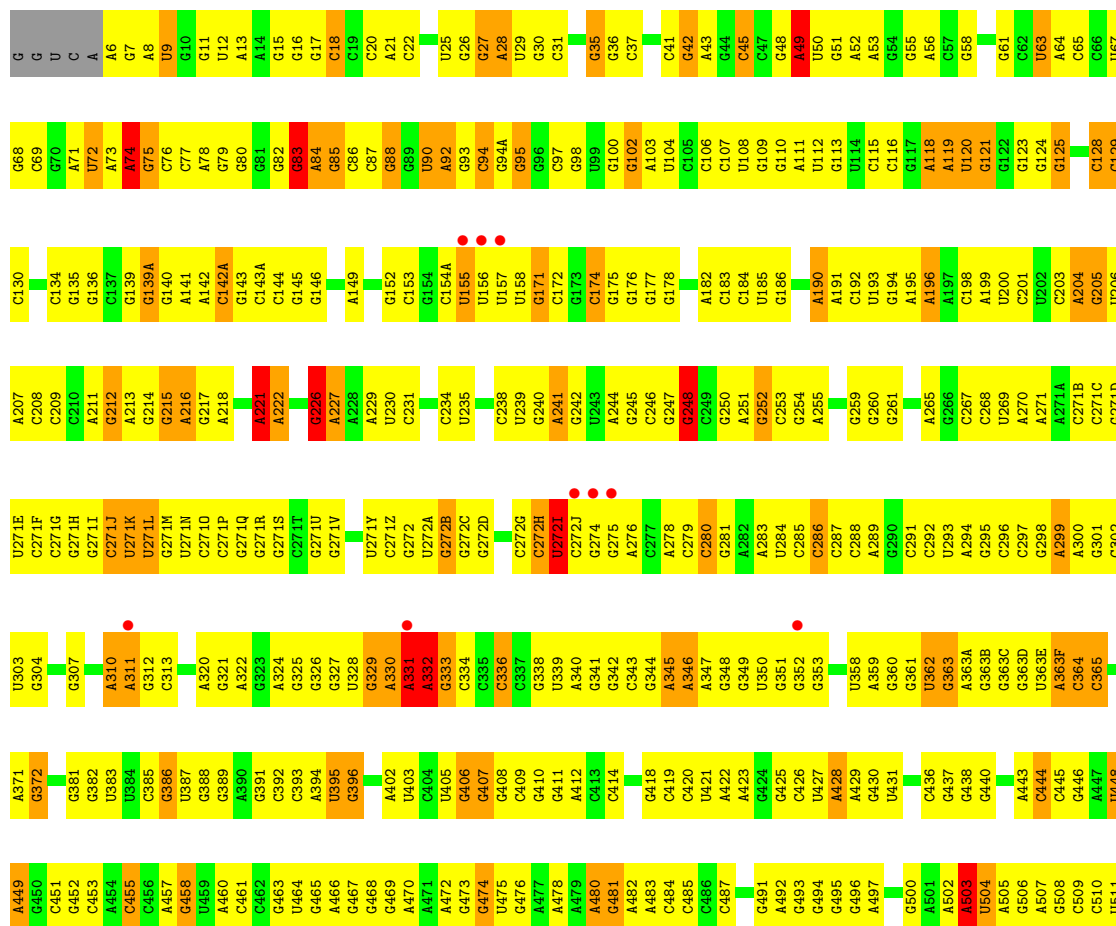


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A1528	G1459	C1386	A1322	A1253	A1189	A1126	G1062	C998	U937	U868	G805	G745	G674
A1529	A1528A	C1387	A1323	A1254	G1190	A1254	C1063	U999	G938	G869	C806	A746	A675
C1530	G1460	G1388	G1191	G1255	G1191	A1128	C1064	A1000	G939	A870	U807	U747	A676
C1531	G1461	G1389	G1324	G1256	G1192	G1192	A1001	G1001	G940	G808	G808	G748	A677
G1532	C1462	U1390	G1325	C1257	G1193	G1131	A1067	G1002	A941	G809	G809	G749	C678
G1533	C1463	U1391	U1326	C1258	G1196	A1132	G1068		G942	C876	U810	A750	C679
U1534	C1464	A1395	C1327	G1259	C1196	U1133	A1069	C1005	U943	U877	U811	A751	G680
A1535	G1465	U1396	G1328	G1260	C1197	U1135	A1070	C1006	G944	A878	C812	A752	G681
C1536	G1466	C1261	U1198	C1261	U1198	G1136	G1071	A945	A945	G879	U813	C753	G682
C1537	C1467	U1397	C1330	G1262	U1205	G1137	C1072	C1008	G946	G880	C814	C754	G683
A1472		U1263	A1331	U1263	G1203	G1138	A1073	A1009	G947	G881	C815	C755	G684
G1473		G1332	G1332	G1264	A1204	G1139	G1074	A1010	G948	G882	C816	C756	A685
G1474		G1333	G1333	A1265	U1205	G1140	C1075	G1011	C949	G883	C817	U757	G686
G1475		U1335	U1335	G1266	G1206	U1141	C1076	U1012	G950	C884	G818		C687
A1541		U1336	U1336	A1267	G1207	U1142	A1077	C1013	C951	G885		G758	U688
A1542		A1336	A1336	A1268	G1209	A1142A	U1078	U1014	G952	C886	A821	G759	U689
C1543		G1337	A1337	A1269	A1210	A1143	G1079	G1015	A953	A887	G823	G760	A690
A1544		U1405	G1338	C1270	U1211	G1144	C1080	G1016	G954	C888	G824	G761	
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A1546		C1407	U1341	A1272	G1213	C1146		U1019		A890	C826	G763	U694
		C1408	A1342	U1273	A1214	C1147	A1084	A1020	U958	A900	C827	G764	G695
C1551		G1343	G1343	A1274	G1215	A1148	A1088	A1021	A959	G892	U826	G765	G696
A1552		G1344	G1344	A1275	G1216	G1149	G1089	G1022	A960	C893	U827	C766	
A1553		G1345	G1345	A1276	C1217	C1150	U1090	U1023	A961	C894	U828	G767	A699
A1554		G1346	G1346	G1277	C1218	G1151	U1091	G1024	G962	U895	A829	G768	G700
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G1556		G1416	G1348	A1279	C1220	C1153	U1092	U1026	C964		G832	G770	G702
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G1561			C1353	U1288	C1224	C1158	U1097		C904	C904	G837	G775	G707
A1562		A1427	A1354	C1289	G1225	U1159	A1098	U1033	C970	U905	C838	G776	C708
G1563		C1428	G1355	A1290	A1226	G1160	G1099	G1034	C971	G906	U839	G777	U710
C1564		G1429	G1356	C1291	G1227	C1161	U1100	U1035	G972	U907	C840	G778	G709
G1565		C1430	U1357	U1292	G1228	G1162	U1101	G1036	G973	G908	A841	G779	G711
A1566		U1431	G1358		G1229	G1163	C1102	G1037	G974	A909	G842	G780	
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A1570		C1435	C1362	C1298	C1233	U1167	G1106	U1041	G977	U913	A784	A722	C721
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C1577		G1442		C1305	U1240	U1175	G1113	A1048	A984	G923	G855	G792	G728
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		C1376	C1376	A1308	G1243		C1116	G1051	C987	C926	U858	G795	G733
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A1586		G1448	A1379	A1246	A1246	G1183	G1120	C991	C992	G931	G862	G799	G740
A1587		G1380	G1380	C1314	U1247	G1184	C1121	A1057	C993	G932	A863	G801	U740
C1588		G1381	G1381	C1315	G1248	G1185	C1122	G1058	G993	A933	G864	G742	G742
C1589		C1382	G1382	U1316	U1249	G1186	G1123	G1059	G994	G934	C865	A802	G743
U1590		C1383	G1383	A1317	G1250	G1187	C1124	U1060	A996	C935	A866		

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G2521	A2453	C2386	G2315	G2239	G2168	G2104	U2034	U1964	A1900	A1821	G1759	A1664	A1595
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G2529	G2461	A2393	G2321	U2245	A2173	G2111	C2041	A1971	G1907	G1827	C1766	G1671	G1601
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A2531	G2463	C2395	G2323	A2247	C2175	G2113	A2042	A1973	G1909	G1829	U1768	C1675	A1603
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U2555	U2419	A2419	G2346	C2283	A2199	A2135	G2067	G2003	U1931	G1851	A1789	A1700	A1632
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U2563	C2424	C2351	G2352	A2288	G2204	C2140	C2073	G2009	A1936	G1856	C1796	C1711	A1637
A2564	A2425	A2352	G2353	G2289	G2206	G2141	U2074	G2010	A1937	G1857	C1797	C1712	U1638
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A2566	G2428	G2354	G2355	U2292	A2208	C2143	U2076	G2012	G1941	G1859	G1717	G1714	C1640
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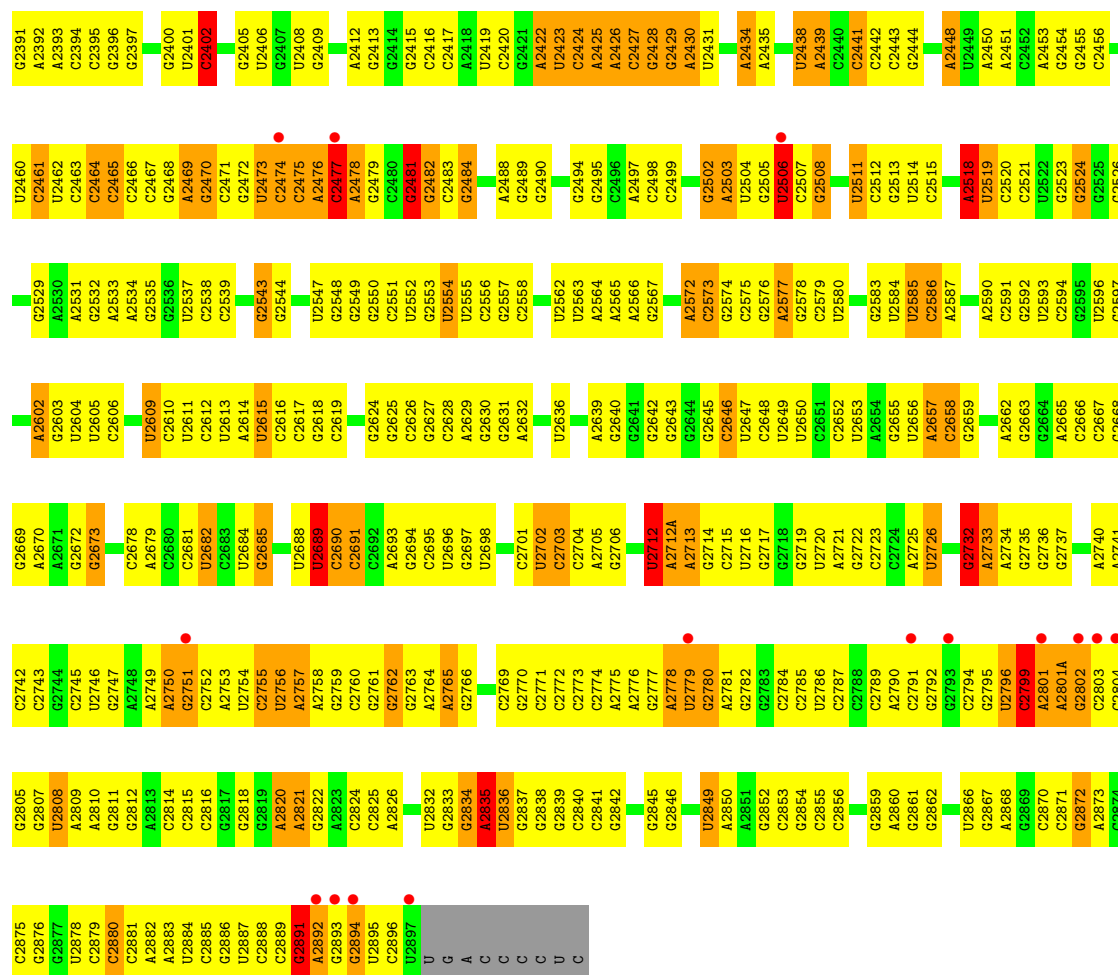


• Molecule 35: 23S RIBOSOMAL RNA

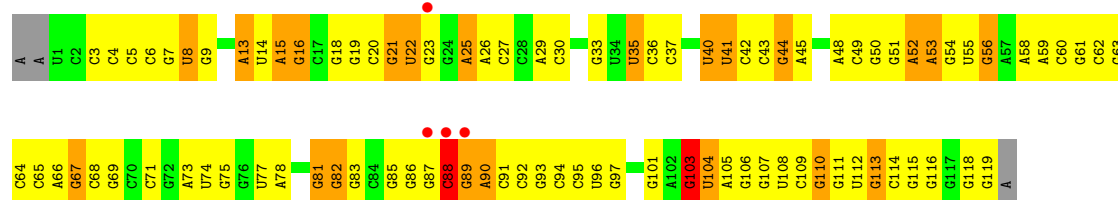


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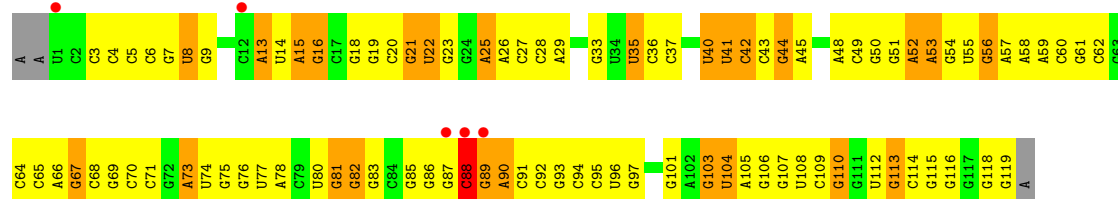
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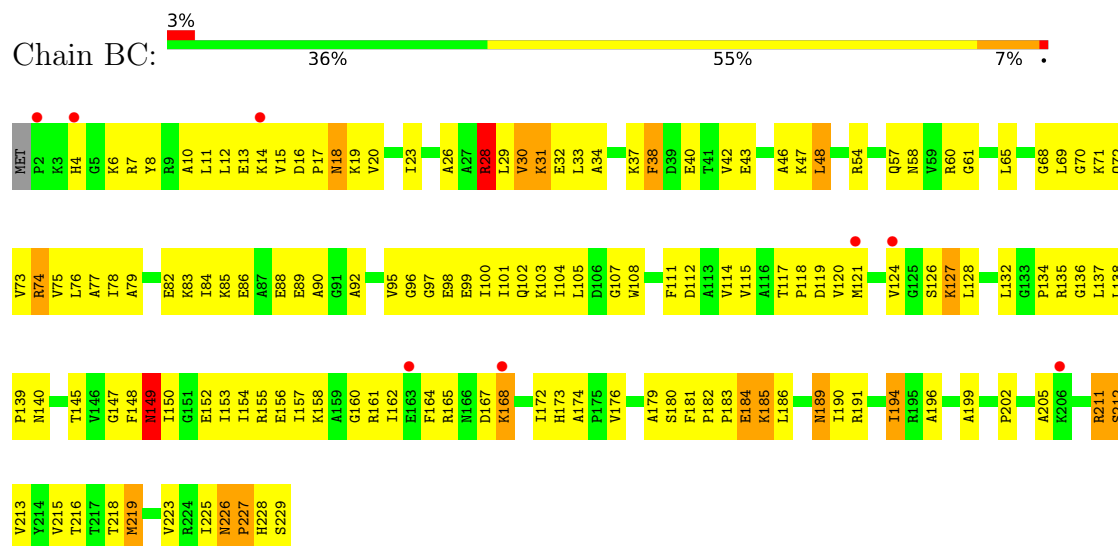
• Molecule 36: 5S RIBOSOMAL RNA



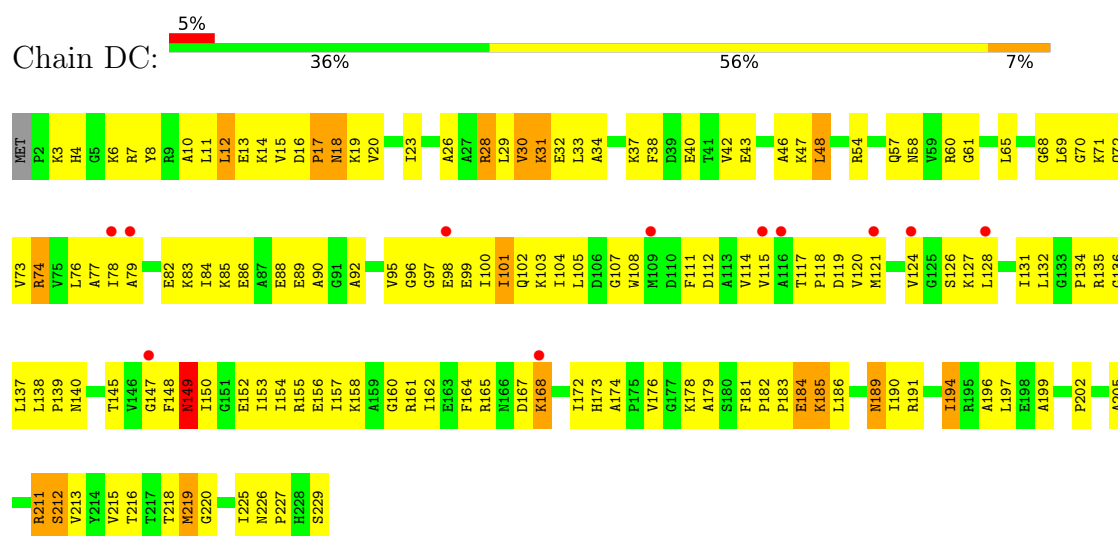
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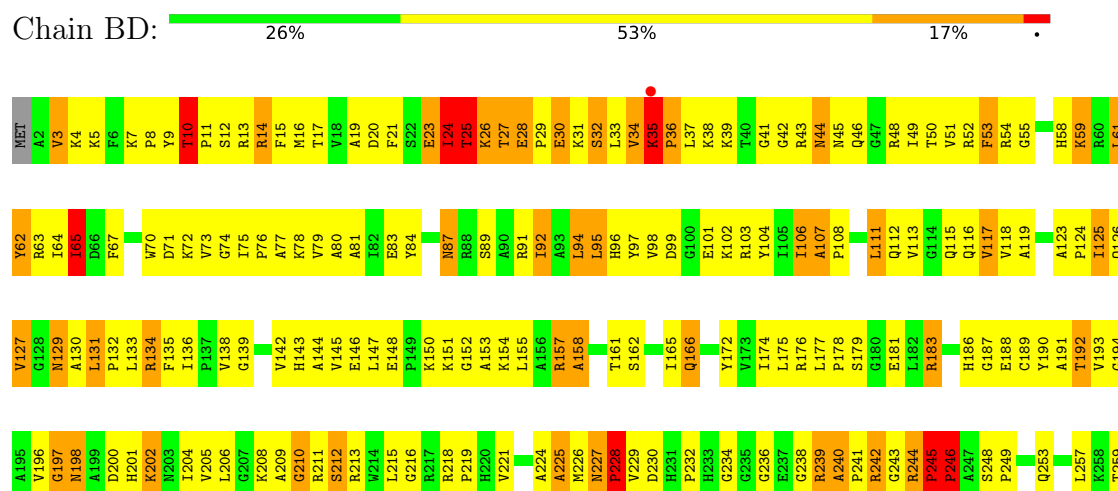
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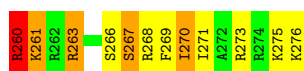


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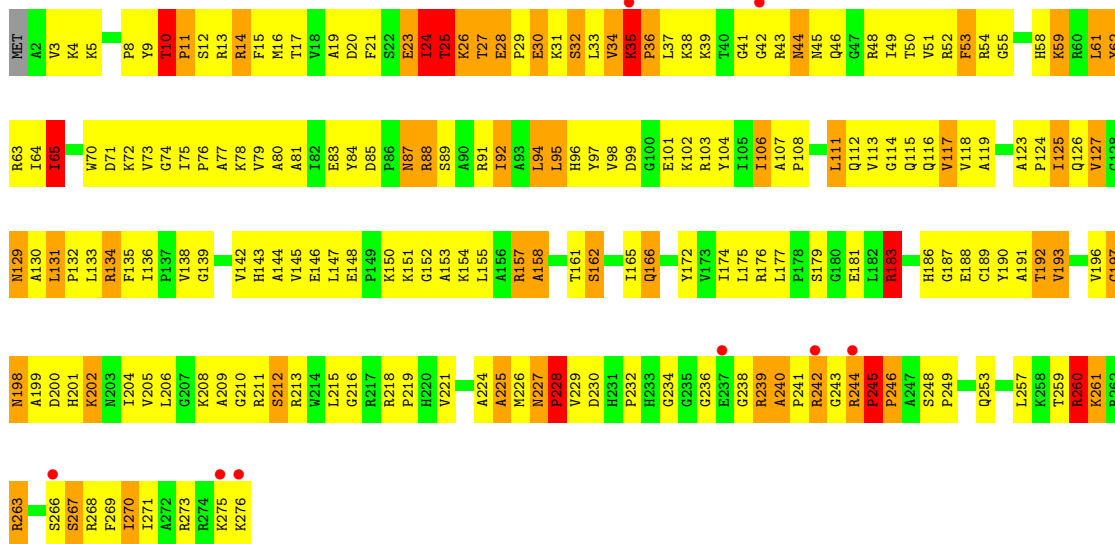


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

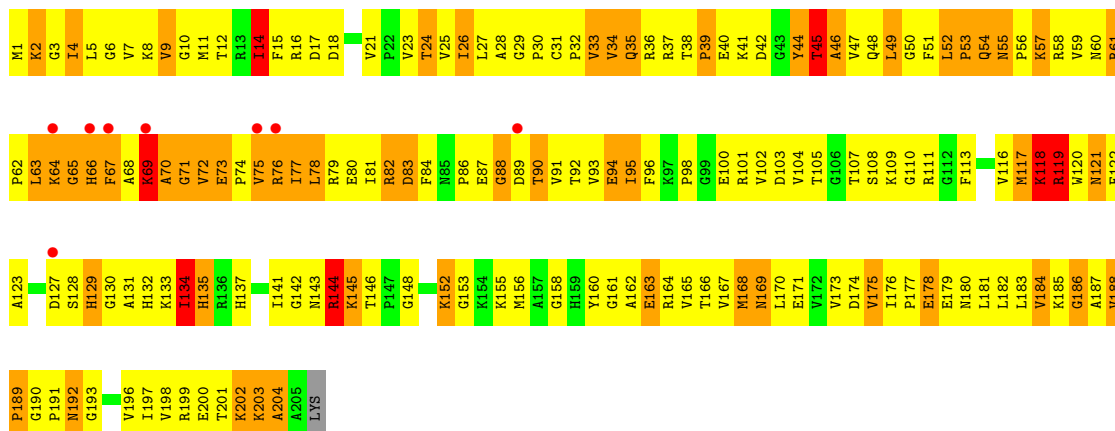
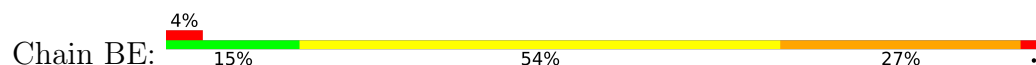




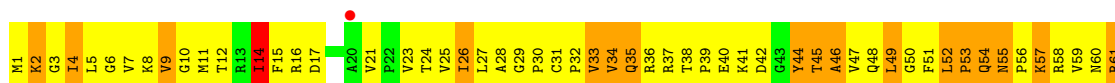
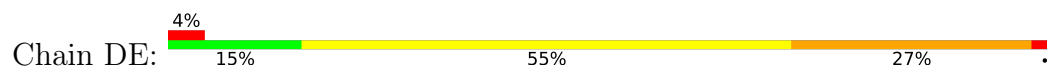
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

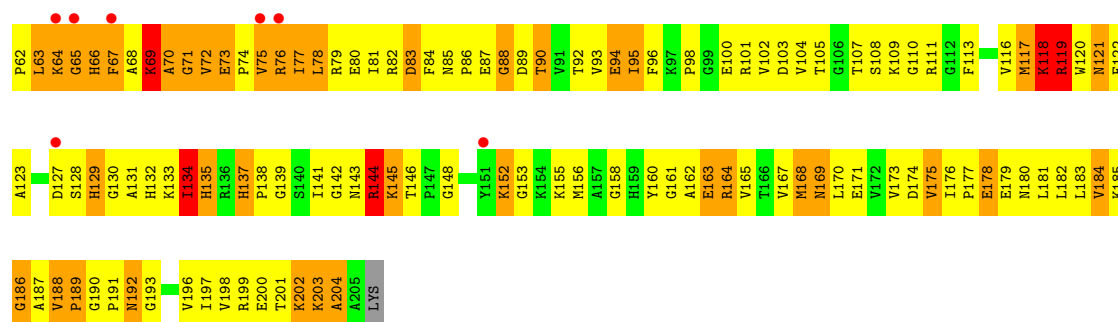


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

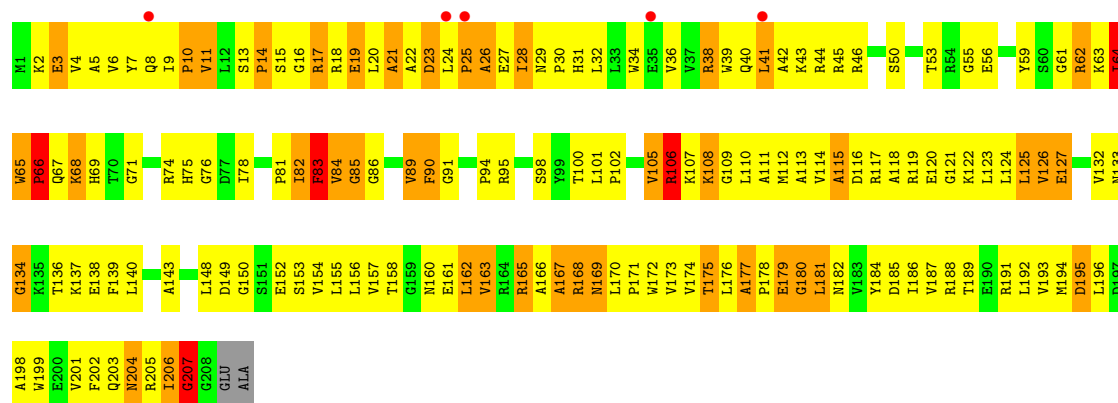


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

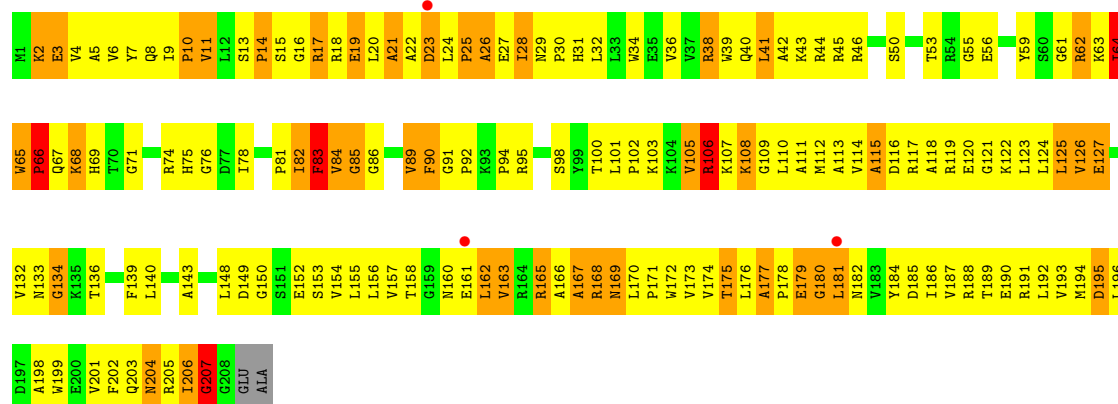




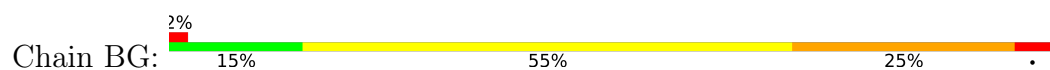
● Molecule 40: 50S RIBOSOMAL PROTEIN L4

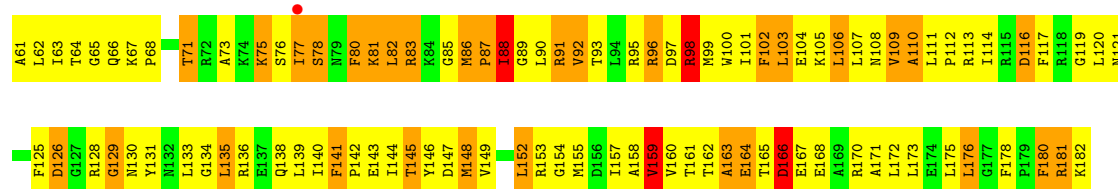


● Molecule 40: 50S RIBOSOMAL PROTEIN L4

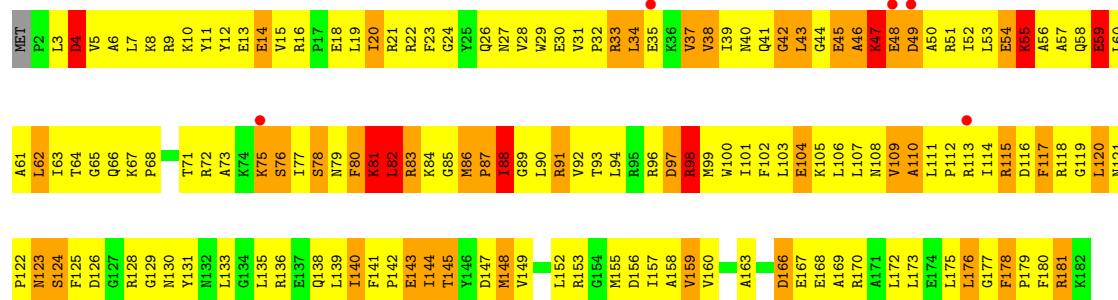
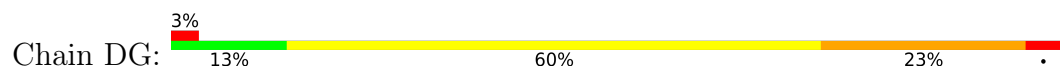


● Molecule 41: 50S RIBOSOMAL PROTEIN L5

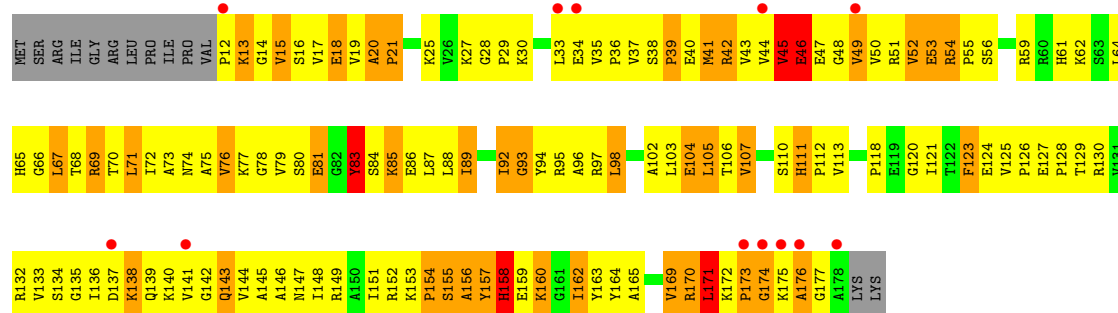
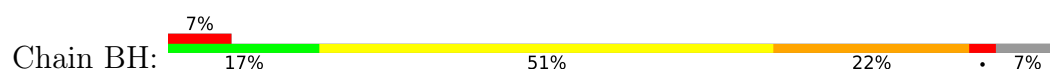




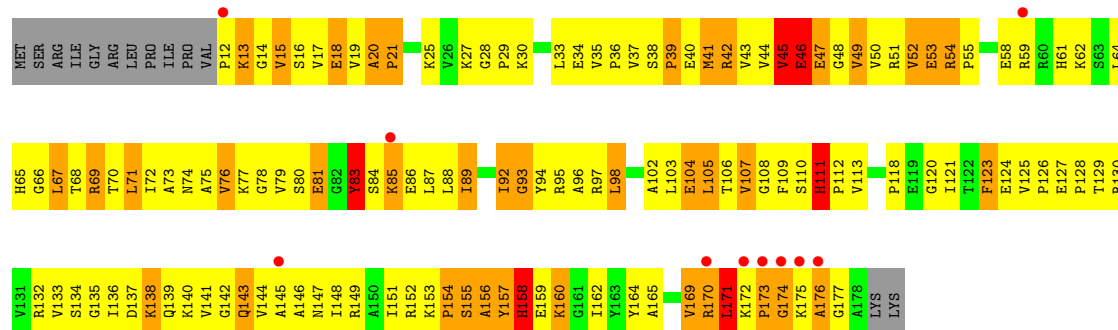
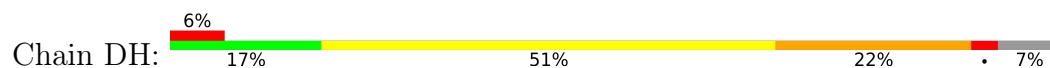
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 42: 50S RIBOSOMAL PROTEIN L6

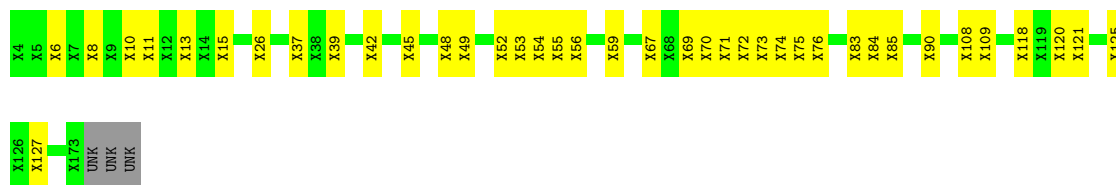


• Molecule 42: 50S RIBOSOMAL PROTEIN L6



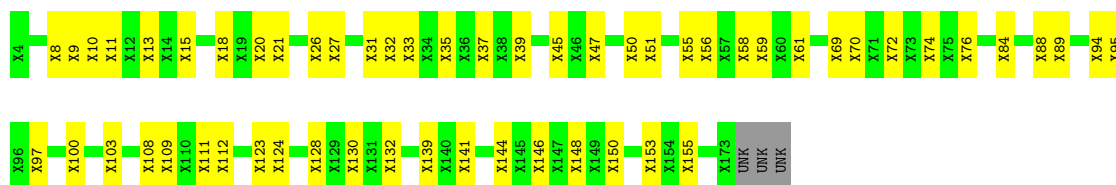
• Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain BJ:  76% 23% .

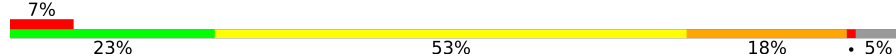


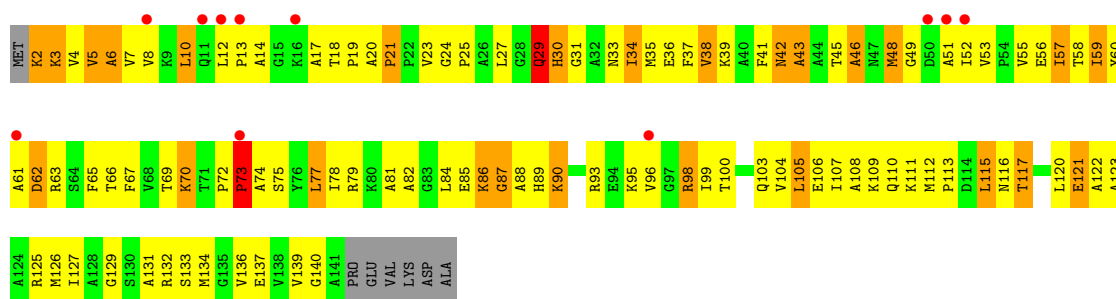
• Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain DJ:  66% 32% .

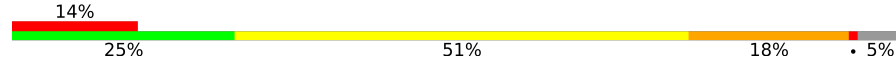


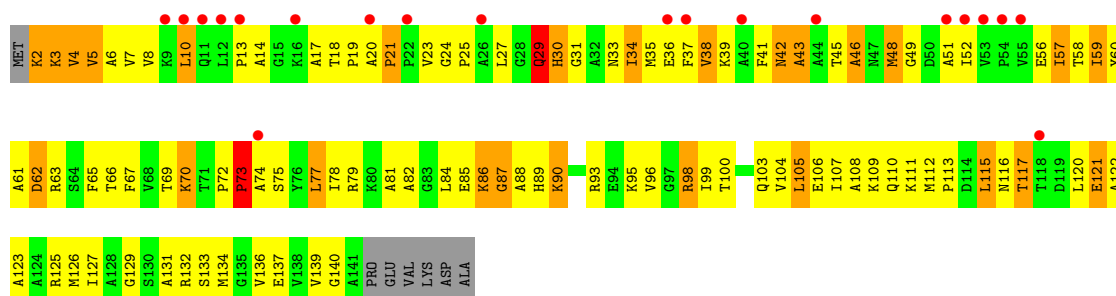
• Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK:  7% 23% 53% 18% . 5%



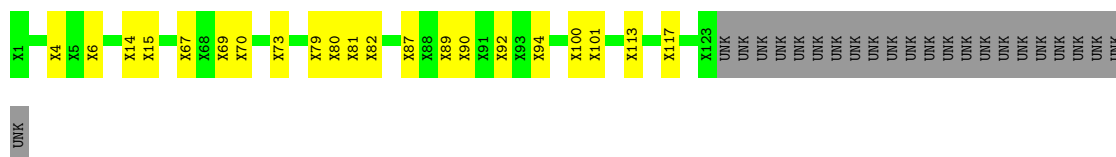
• Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain DK:  14% 25% 51% 18% . 5%



• Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BL:  65% 17% 18%



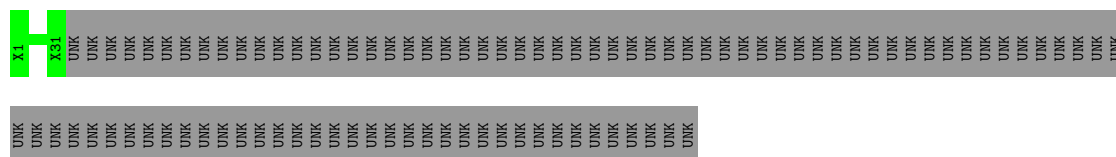
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BM:  23% . 75%



- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BL:  25% 75%



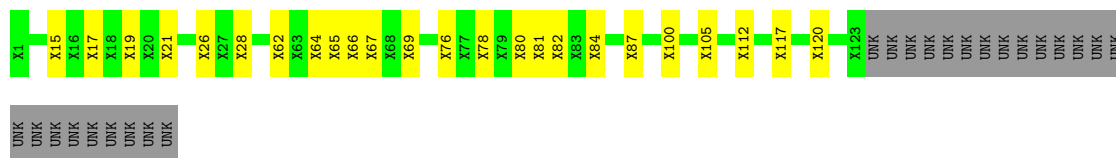
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BM:  21% . 76%



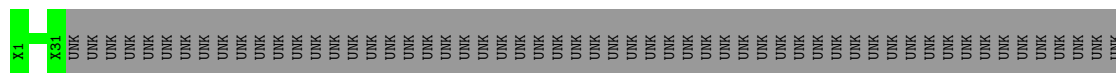
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DL:  62% 19% 18%

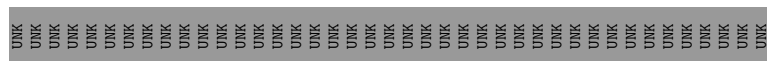
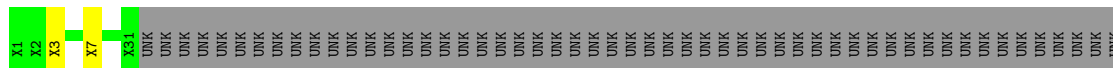


- Molecule 45: 50S RIBOSOMAL PROTEIN L12

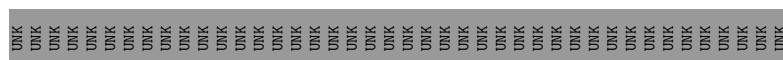
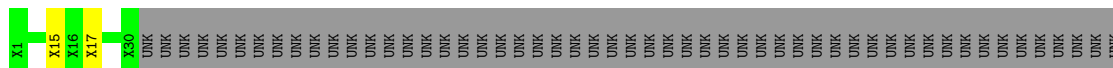
Chain DM:  25% 75%



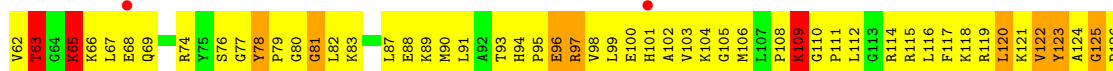
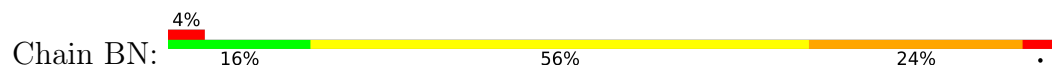
- Molecule 45: 50S RIBOSOMAL PROTEIN L12



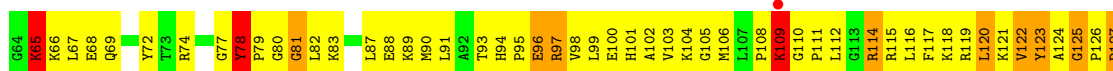
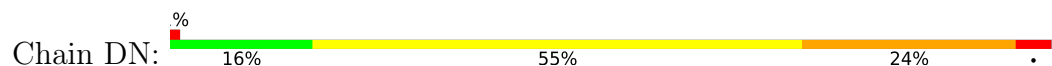
• Molecule 45: 50S RIBOSOMAL PROTEIN L12



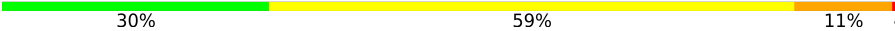
• Molecule 46: 50S RIBOSOMAL PROTEIN L13



- Molecule 46: 50S RIBOSOMAL PROTEIN L13



- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:  30% 59% 11% .



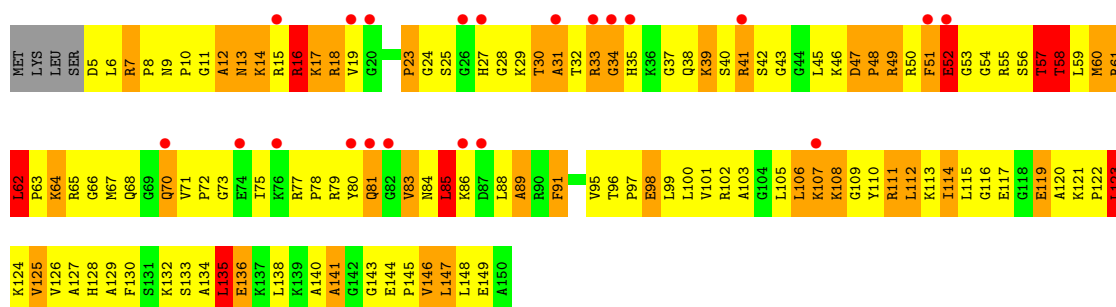
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO:  32% 54% 13% .



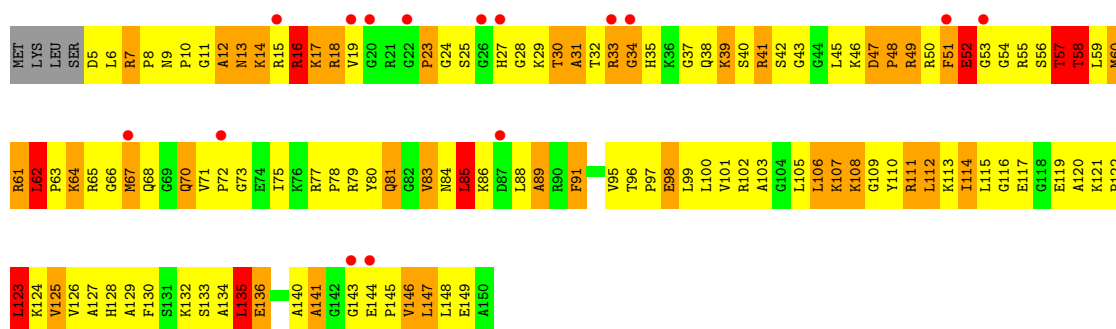
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:  14% 52% 25% .

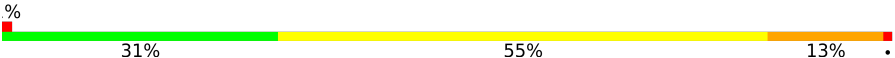


• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:  10% 51% 25% .



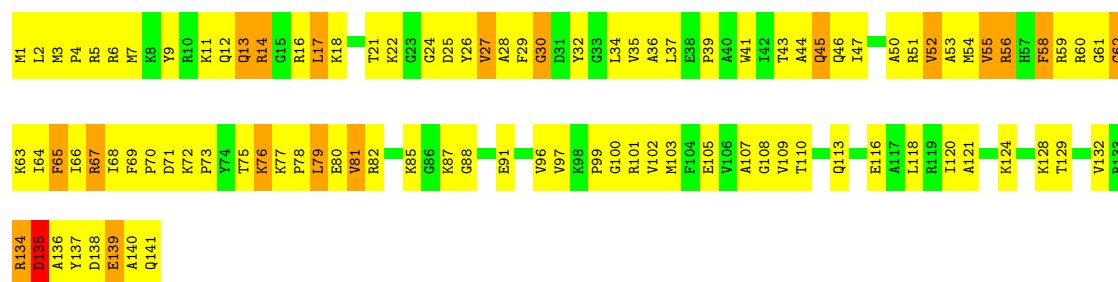
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:  31% 55% 13% .



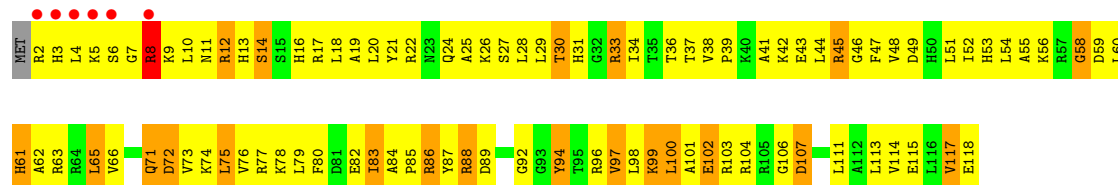
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ: 29% 57% 13% .



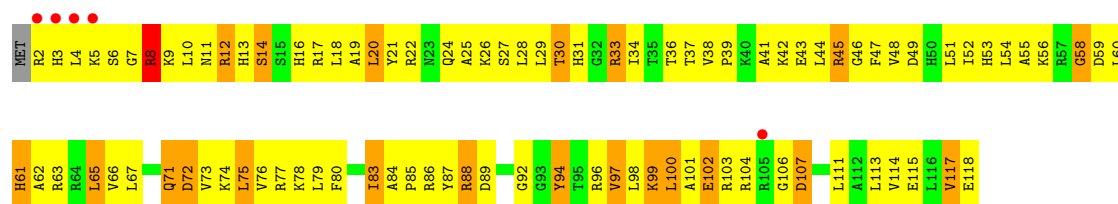
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR: 5% 19% 61% 18% ..



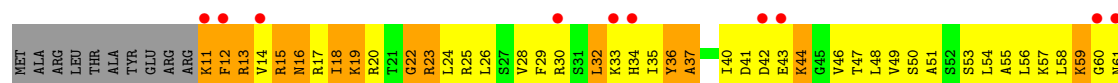
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR: 4% 19% 61% 18% ..



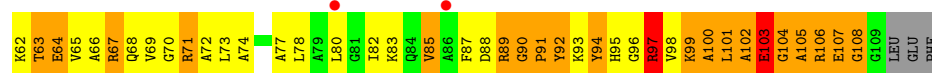
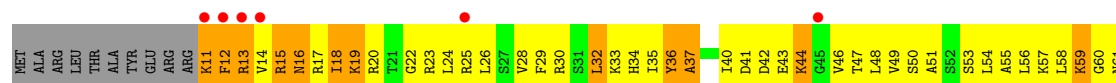
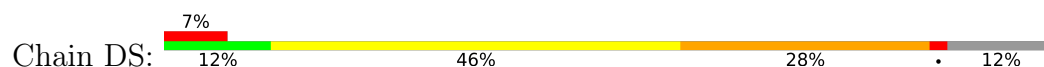
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS: 13% 12% 45% 29% . 12%

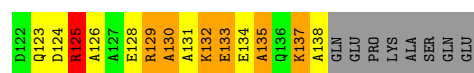
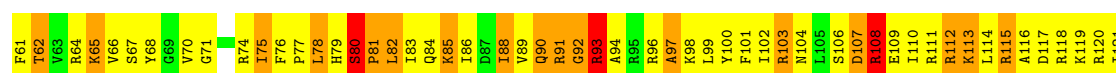
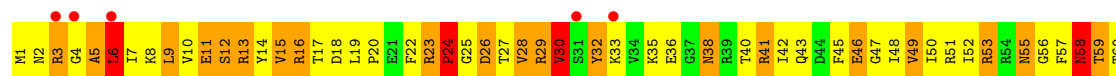
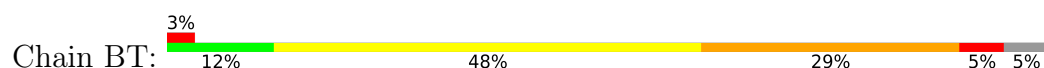




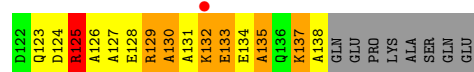
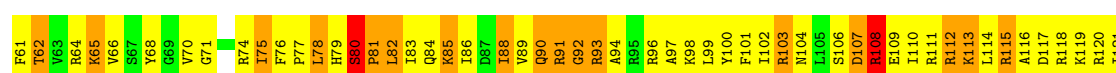
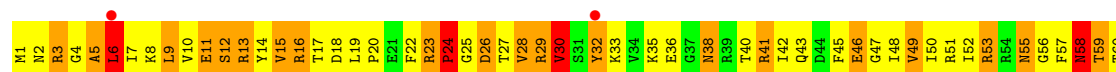
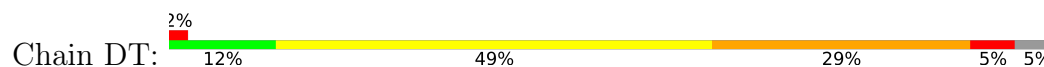
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



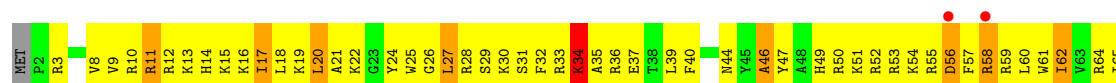
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

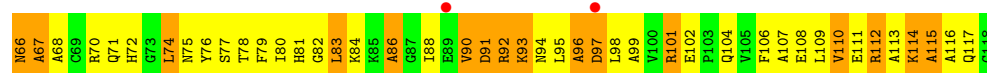


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

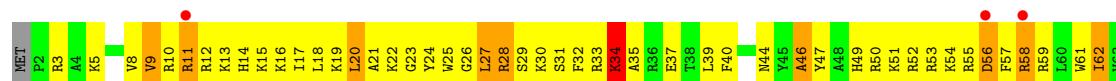


• Molecule 53: 50S RIBOSOMAL PROTEIN L20





● Molecule 53: 50S RIBOSOMAL PROTEIN L20



● Molecule 54: 50S RIBOSOMAL PROTEIN L21



● Molecule 54: 50S RIBOSOMAL PROTEIN L21

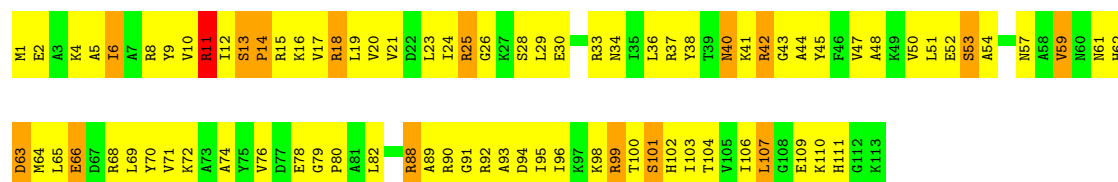


● Molecule 55: 50S RIBOSOMAL PROTEIN L22

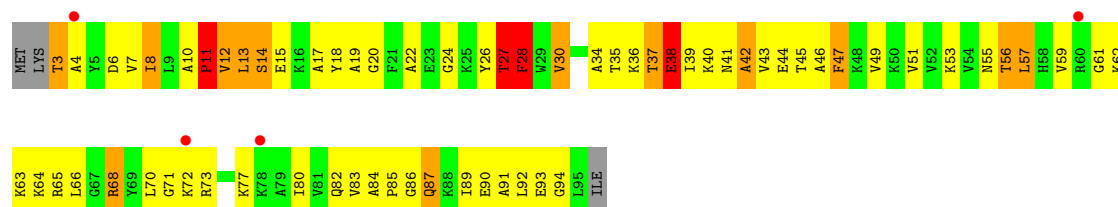


● Molecule 55: 50S RIBOSOMAL PROTEIN L22

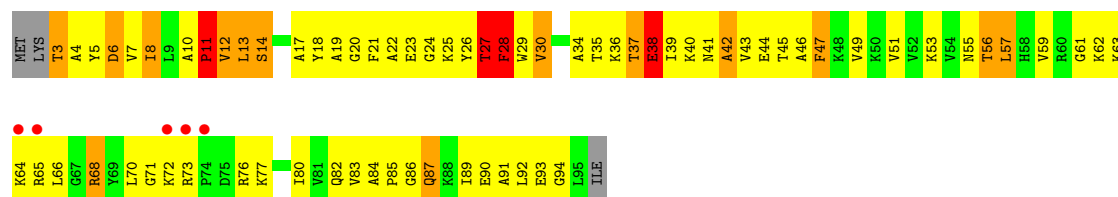




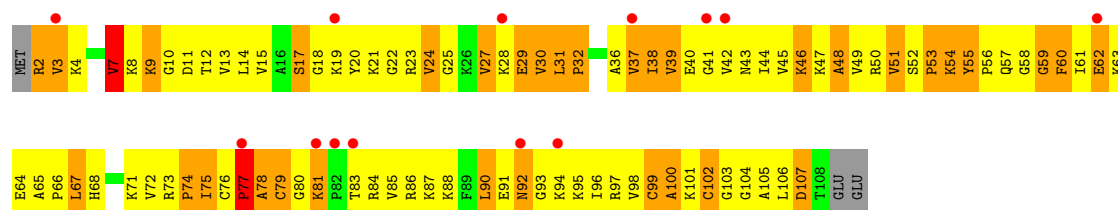
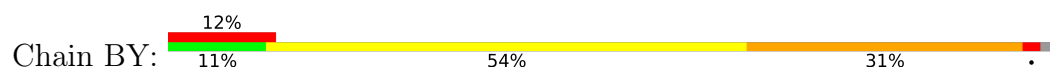
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



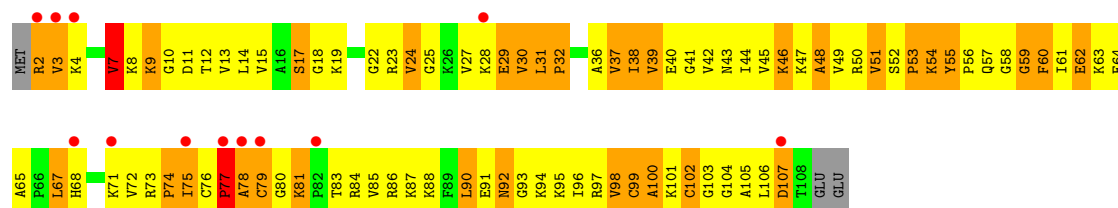
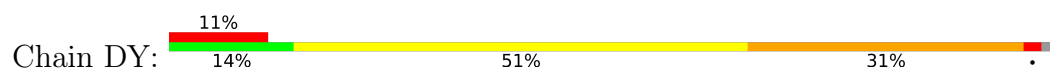
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



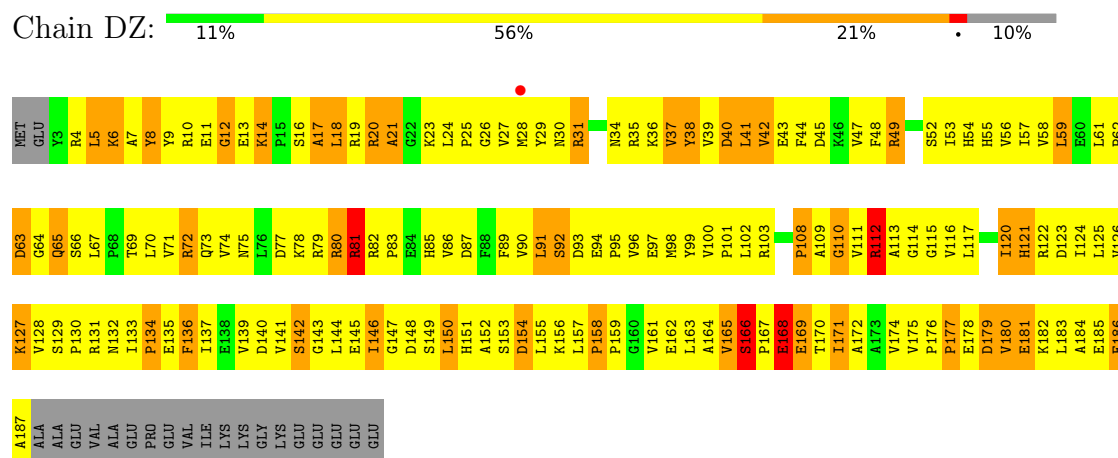
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• 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	291.84Å 270.36Å 402.36Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-3.60) 96.0 (50.00-3.60)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.260 0.224 , 0.223	Depositor DCC
R_{free} test set	40387 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	311552	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: ZN, 5MU, GDP, FUA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.50	0/36190	0.74	49/56486 (0.1%)
1	CA	0.50	0/36190	0.74	45/56486 (0.1%)
2	AB	0.63	1/1936 (0.1%)	1.09	14/2611 (0.5%)
2	CB	0.57	1/1936 (0.1%)	1.08	15/2611 (0.6%)
3	AC	0.72	1/1637 (0.1%)	1.03	9/2207 (0.4%)
3	CC	0.60	1/1637 (0.1%)	1.01	7/2207 (0.3%)
4	AD	0.55	0/1733	0.97	3/2318 (0.1%)
4	CD	0.49	0/1733	0.95	3/2318 (0.1%)
5	AE	0.76	1/1163 (0.1%)	1.11	9/1566 (0.6%)
5	CE	0.69	1/1163 (0.1%)	1.10	7/1566 (0.4%)
6	AF	0.55	0/856	1.00	6/1154 (0.5%)
6	CF	0.47	0/856	0.99	8/1154 (0.7%)
7	AG	0.58	0/1276	1.02	8/1709 (0.5%)
7	CG	0.51	0/1276	1.01	8/1709 (0.5%)
8	AH	0.66	0/1136	1.16	12/1527 (0.8%)
8	CH	0.58	0/1136	1.15	12/1527 (0.8%)
9	AI	0.58	0/1027	1.00	4/1373 (0.3%)
9	CI	0.47	0/1027	0.99	4/1373 (0.3%)
10	AJ	0.63	1/808 (0.1%)	1.02	2/1087 (0.2%)
10	CJ	0.52	1/808 (0.1%)	0.97	2/1087 (0.2%)
11	AK	0.69	0/900	1.04	4/1213 (0.3%)
11	CK	0.60	0/900	1.03	5/1213 (0.4%)
12	AL	0.68	1/987 (0.1%)	1.14	9/1322 (0.7%)
12	CL	0.63	1/987 (0.1%)	1.11	9/1322 (0.7%)
13	AM	0.56	1/999 (0.1%)	1.12	10/1338 (0.7%)
13	CM	0.51	1/999 (0.1%)	1.12	8/1338 (0.6%)
14	AN	0.63	0/501	1.02	1/664 (0.2%)
14	CN	0.56	0/501	1.00	0/664
15	AO	0.63	0/745	0.93	1/992 (0.1%)
15	CO	0.57	0/745	0.91	1/992 (0.1%)
16	AP	0.62	1/717 (0.1%)	0.98	1/965 (0.1%)
16	CP	0.57	1/717 (0.1%)	0.98	1/965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.65	1/837 (0.1%)	1.04	3/1119 (0.3%)
17	CQ	0.61	1/837 (0.1%)	1.04	4/1119 (0.4%)
18	AR	0.58	0/579	1.12	6/768 (0.8%)
18	CR	0.52	0/579	1.11	3/768 (0.4%)
19	AS	0.56	1/643 (0.2%)	0.96	4/867 (0.5%)
19	CS	0.53	1/643 (0.2%)	0.93	2/867 (0.2%)
20	AT	0.56	0/765	1.04	8/1007 (0.8%)
20	CT	0.50	0/765	1.04	8/1007 (0.8%)
21	AU	0.66	1/213 (0.5%)	0.96	0/279
21	CU	0.60	1/213 (0.5%)	0.94	0/279
22	AV	0.46	0/1810	0.73	0/2821
22	AW	0.45	0/1810	0.64	0/2821
22	CV	0.47	0/1810	0.69	1/2821 (0.0%)
22	CW	0.42	0/1810	0.60	1/2821 (0.0%)
23	AX	0.63	0/257	0.92	0/398
23	CX	0.59	0/257	0.83	0/398
24	AY	0.52	1/5313 (0.0%)	1.09	44/7195 (0.6%)
24	CY	0.53	2/5313 (0.0%)	1.08	40/7195 (0.6%)
25	B0	0.54	0/671	0.97	1/892 (0.1%)
25	D0	0.50	0/671	0.96	1/892 (0.1%)
26	B1	0.63	0/739	1.13	4/983 (0.4%)
26	D1	0.58	1/739 (0.1%)	1.06	2/983 (0.2%)
27	B2	0.42	0/600	1.03	6/793 (0.8%)
27	D2	0.43	0/600	0.91	1/793 (0.1%)
28	B3	0.59	1/473 (0.2%)	1.04	4/636 (0.6%)
28	D3	0.58	1/473 (0.2%)	1.02	4/636 (0.6%)
29	B4	0.86	0/461	1.41	9/623 (1.4%)
29	D4	0.91	0/461	1.41	10/623 (1.6%)
30	B5	0.55	0/473	1.11	5/639 (0.8%)
30	D5	0.58	0/473	1.11	4/639 (0.6%)
31	B6	0.75	0/440	1.46	11/586 (1.9%)
31	D6	0.74	0/440	1.42	5/586 (0.9%)
32	B7	0.62	1/427 (0.2%)	1.09	4/563 (0.7%)
32	D7	0.62	1/427 (0.2%)	1.10	4/563 (0.7%)
33	B8	0.67	1/516 (0.2%)	1.17	2/681 (0.3%)
33	D8	0.63	1/516 (0.2%)	1.16	2/681 (0.3%)
34	B9	0.59	0/310	1.01	0/407
34	D9	0.57	0/310	1.02	0/407
35	BA	0.48	1/69972 (0.0%)	0.73	88/109237 (0.1%)
35	DA	0.48	1/69972 (0.0%)	0.73	90/109237 (0.1%)
36	BB	0.42	0/2853	0.69	4/4451 (0.1%)
36	DB	0.43	0/2853	0.68	4/4451 (0.1%)
37	BC	0.44	0/1774	0.95	5/2391 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.42	0/1774	0.96	6/2391 (0.3%)
38	BD	0.67	0/2195	1.20	15/2955 (0.5%)
38	DD	0.64	0/2195	1.20	18/2955 (0.6%)
39	BE	0.61	1/1597 (0.1%)	1.14	16/2155 (0.7%)
39	DE	0.58	1/1597 (0.1%)	1.13	16/2155 (0.7%)
40	BF	0.50	1/1659 (0.1%)	1.10	16/2246 (0.7%)
40	DF	0.48	1/1659 (0.1%)	1.10	14/2246 (0.6%)
41	BG	0.55	1/1498 (0.1%)	1.20	17/2013 (0.8%)
41	DG	0.53	0/1498	1.13	18/2013 (0.9%)
42	BH	0.46	0/1293	1.08	6/1746 (0.3%)
42	DH	0.45	0/1293	1.07	6/1746 (0.3%)
44	BK	0.47	1/1045 (0.1%)	1.04	9/1418 (0.6%)
44	DK	0.49	1/1045 (0.1%)	1.05	9/1418 (0.6%)
46	BN	0.53	1/1132 (0.1%)	1.13	10/1527 (0.7%)
46	DN	0.50	1/1132 (0.1%)	1.13	10/1527 (0.7%)
47	BO	0.63	0/943	1.05	4/1269 (0.3%)
47	DO	0.61	0/943	1.05	6/1269 (0.5%)
48	BP	0.56	0/1131	1.33	14/1504 (0.9%)
48	DP	0.55	0/1131	1.30	13/1504 (0.9%)
49	BQ	0.62	0/1143	0.97	2/1527 (0.1%)
49	DQ	0.59	0/1143	0.97	1/1527 (0.1%)
50	BR	0.52	0/974	0.96	2/1302 (0.2%)
50	DR	0.50	0/974	0.96	3/1302 (0.2%)
51	BS	0.53	1/779 (0.1%)	1.05	7/1038 (0.7%)
51	DS	0.48	1/779 (0.1%)	1.06	6/1038 (0.6%)
52	BT	0.63	1/1156 (0.1%)	1.24	13/1544 (0.8%)
52	DT	0.62	1/1156 (0.1%)	1.23	13/1544 (0.8%)
53	BU	0.52	0/975	1.09	11/1297 (0.8%)
53	DU	0.49	0/975	1.08	11/1297 (0.8%)
54	BV	0.49	0/790	0.94	0/1057
54	DV	0.48	0/790	0.94	0/1057
55	BW	0.52	0/907	0.96	5/1216 (0.4%)
55	DW	0.50	0/907	0.97	5/1216 (0.4%)
56	BX	0.53	1/740 (0.1%)	1.02	6/995 (0.6%)
56	DX	0.52	1/740 (0.1%)	1.02	6/995 (0.6%)
57	BY	0.52	0/824	1.02	1/1100 (0.1%)
57	DY	0.53	0/824	1.01	1/1100 (0.1%)
58	BZ	0.61	1/1500 (0.1%)	1.08	8/2037 (0.4%)
58	DZ	0.56	1/1500 (0.1%)	1.07	6/2037 (0.3%)
All	All	0.51	49/333656 (0.0%)	0.84	1001/497270 (0.2%)

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	0	48
1	CA	0	43
22	AV	0	3
22	CV	0	1
23	AX	0	2
23	CX	0	1
35	BA	2	69
35	DA	2	58
36	BB	0	1
36	DB	0	1
37	BC	0	1
37	DC	0	1
44	BK	0	1
44	DK	0	1
46	DN	0	1
All	All	4	232

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	BS	108	GLY	C-N	-6.14	1.24	1.33
13	AM	125	ARG	C-N	-6.01	1.25	1.33
2	CB	240	GLN	C-N	-5.94	1.25	1.33
35	BA	272(I)	U	C1'-N1	5.89	1.57	1.48
33	B8	64	TYR	C-N	-5.87	1.25	1.33

The worst 5 of 1001 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	15.79	133.19	109.50
35	DA	1992	G	C2'-C3'-O3'	15.57	132.85	109.50
1	CA	575	G	C2'-C3'-O3'	14.20	130.80	109.50
1	AA	575	G	C2'-C3'-O3'	14.15	130.72	109.50
35	DA	1799	G	C2'-C3'-O3'	13.47	129.70	109.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1799	G	C3'
35	BA	1992	G	C3'

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Mol	Chain	Res	Type	Atom
35	DA	1799	G	C3'
35	DA	1992	G	C3'

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	112	G	Sidechain
1	AA	30	U	Sidechain
1	AA	39	G	Sidechain
1	AA	5	U	Sidechain

5.2 Too-close contacts [i](#)

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	32329	0	16318	1242	0
1	CA	32329	0	16318	1269	0
2	AB	1901	0	1951	267	0
2	CB	1901	0	1951	263	2
3	AC	1613	0	1677	221	0
3	CC	1613	0	1677	229	0
4	AD	1703	0	1763	190	0
4	CD	1703	0	1763	203	0
5	AE	1147	0	1207	137	0
5	CE	1147	0	1207	142	0
6	AF	843	0	857	84	0
6	CF	843	0	857	83	0
7	AG	1257	0	1296	108	0
7	CG	1257	0	1296	104	0
8	AH	1116	0	1177	101	0
8	CH	1116	0	1177	99	0
9	AI	1010	0	1035	146	0
9	CI	1010	0	1035	140	0
10	AJ	795	0	840	184	0
10	CJ	795	0	840	179	0
11	AK	885	0	904	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	80	0
12	AL	971	0	1057	136	0
12	CL	971	0	1057	133	0
13	AM	988	0	1059	161	0
13	CM	988	0	1059	158	0
14	AN	492	0	530	71	0
14	CN	492	0	530	71	0
15	AO	734	0	771	69	0
15	CO	734	0	771	66	0
16	AP	701	0	720	88	0
16	CP	701	0	720	90	0
17	AQ	824	0	891	61	0
17	CQ	824	0	891	57	0
18	AR	574	0	644	74	0
18	CR	574	0	644	73	0
19	AS	630	0	652	127	0
19	CS	630	0	652	124	0
20	AT	763	0	861	102	0
20	CT	763	0	861	98	0
21	AU	209	0	221	19	0
21	CU	209	0	221	22	0
22	AV	1640	0	836	72	0
22	AW	1640	0	836	82	0
22	CV	1640	0	836	47	0
22	CW	1640	0	836	71	0
23	AX	230	0	119	26	0
23	CX	230	0	119	21	0
24	AY	5215	0	5287	850	0
24	CY	5215	0	5287	796	0
25	B0	662	0	688	87	0
25	D0	662	0	688	89	0
26	B1	732	0	808	136	0
26	D1	732	0	808	133	0
27	B2	598	0	653	114	0
27	D2	598	0	653	118	0
28	B3	468	0	523	63	0
28	D3	468	0	523	57	0
29	B4	451	0	448	102	0
29	D4	451	0	449	106	0
30	B5	459	0	480	111	0
30	D5	459	0	480	114	0
31	B6	433	0	461	177	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	D6	433	0	461	180	0
32	B7	419	0	467	41	0
32	D7	419	0	467	42	0
33	B8	508	0	576	110	0
33	D8	508	0	576	112	0
34	B9	307	0	335	40	0
34	D9	307	0	335	42	0
35	BA	62474	0	31497	2709	0
35	DA	62474	0	31497	2748	0
36	BB	2551	0	1295	127	0
36	DB	2551	0	1295	137	0
37	BC	1742	0	1798	180	0
37	DC	1742	0	1798	178	2
38	BD	2145	0	2234	318	0
38	DD	2145	0	2234	319	0
39	BE	1564	0	1629	303	0
39	DE	1564	0	1629	306	0
40	BF	1624	0	1677	274	0
40	DF	1624	0	1677	276	0
41	BG	1474	0	1534	298	0
41	DG	1474	0	1534	287	0
42	BH	1269	0	1337	241	0
42	DH	1269	0	1337	227	0
43	BJ	851	0	191	28	0
43	DJ	851	0	195	44	0
44	BK	1026	0	1066	163	0
44	DK	1026	0	1066	158	0
45	BL	506	0	111	14	0
45	BM	151	0	33	1	0
45	Bl	151	0	32	0	0
45	Bm	146	0	32	3	0
45	DL	506	0	115	16	0
45	DM	151	0	32	0	0
45	DI	151	0	32	1	0
45	Dm	146	0	31	1	0
46	BN	1105	0	1180	207	0
46	DN	1105	0	1180	208	0
47	BO	933	0	996	116	0
47	DO	933	0	996	114	0
48	BP	1114	0	1187	307	0
48	DP	1114	0	1187	308	0
49	BQ	1122	0	1179	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	DQ	1122	0	1179	158	0
50	BR	960	0	1021	173	0
50	DR	960	0	1021	168	0
51	BS	771	0	832	182	0
51	DS	771	0	832	175	0
52	BT	1142	0	1202	259	0
52	DT	1142	0	1202	253	0
53	BU	958	0	1015	188	0
53	DU	958	0	1015	189	0
54	BV	779	0	852	145	0
54	DV	779	0	852	147	0
55	BW	896	0	953	105	0
55	DW	896	0	953	98	0
56	BX	726	0	778	89	0
56	DX	726	0	778	92	0
57	BY	811	0	901	178	0
57	DY	811	0	901	176	0
58	BZ	1468	0	1492	247	0
58	DZ	1468	0	1492	291	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AY	1	0	0	0	0
60	CY	1	0	0	0	0
61	AY	37	0	47	13	0
61	CY	37	0	47	22	0
62	AY	28	0	12	8	0
62	CY	28	0	12	8	0
All	All	311552	0	214129	23348	2

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 45.

The worst 5 of 23348 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)
42:DH:157:TYR:CE1	42:DH:171:LEU:HD22	1.61	1.35
42:BH:157:TYR:CE1	42:BH:171:LEU:HD22	1.62	1.32
42:DH:157:TYR:HE1	42:DH:171:LEU:CD2	1.50	1.24
42:BH:157:TYR:HE1	42:BH:171:LEU:CD2	1.50	1.24
40:DF:3:GLU:HA	40:DF:24:LEU:HG	1.24	1.20

All (2) 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	37:DC:28:ARG:NH2[2_646]	1.56	0.64
2:CB:65:GLY:O	37:DC:28:ARG:CZ[2_646]	1.87	0.33

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	233/256 (91%)	139 (60%)	53 (23%)	41 (18%)	0	1
2	CB	233/256 (91%)	140 (60%)	51 (22%)	42 (18%)	0	1
3	AC	205/239 (86%)	133 (65%)	50 (24%)	22 (11%)	0	5
3	CC	205/239 (86%)	132 (64%)	52 (25%)	21 (10%)	0	5
4	AD	206/209 (99%)	134 (65%)	50 (24%)	22 (11%)	0	5
4	CD	206/209 (99%)	134 (65%)	51 (25%)	21 (10%)	0	5
5	AE	149/162 (92%)	119 (80%)	21 (14%)	9 (6%)	1	13
5	CE	149/162 (92%)	117 (78%)	24 (16%)	8 (5%)	1	14
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	10
6	CF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	10
7	AG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	12
7	CG	153/156 (98%)	110 (72%)	32 (21%)	11 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	136/138 (99%)	103 (76%)	30 (22%)	3 (2%)	5	30
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	3	26
9	AI	121/128 (94%)	81 (67%)	26 (22%)	14 (12%)	0	4
9	CI	121/128 (94%)	82 (68%)	27 (22%)	12 (10%)	0	6
10	AJ	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	2
10	CJ	97/105 (92%)	61 (63%)	20 (21%)	16 (16%)	0	2
11	AK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	1	15
11	CK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	1	15
12	AL	123/132 (93%)	82 (67%)	23 (19%)	18 (15%)	0	3
12	CL	123/132 (93%)	82 (67%)	22 (18%)	19 (15%)	0	2
13	AM	123/126 (98%)	77 (63%)	25 (20%)	21 (17%)	0	2
13	CM	123/126 (98%)	77 (63%)	26 (21%)	20 (16%)	0	2
14	AN	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	11
14	CN	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	0	7
15	AO	86/89 (97%)	55 (64%)	23 (27%)	8 (9%)	0	6
15	CO	86/89 (97%)	53 (62%)	24 (28%)	9 (10%)	0	5
16	AP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	0	7
16	CP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	0	7
17	AQ	98/105 (93%)	78 (80%)	15 (15%)	5 (5%)	1	15
17	CQ	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	2	19
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	9
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	9
19	AS	77/93 (83%)	43 (56%)	14 (18%)	20 (26%)	0	0
19	CS	77/93 (83%)	43 (56%)	15 (20%)	19 (25%)	0	0
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0	2
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	2
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	3
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
24	AY	663/691 (96%)	435 (66%)	137 (21%)	91 (14%)	0	3
24	CY	663/691 (96%)	449 (68%)	134 (20%)	80 (12%)	0	4
25	B0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	1	16
26	B1	92/98 (94%)	64 (70%)	15 (16%)	13 (14%)	0	3
26	D1	92/98 (94%)	67 (73%)	13 (14%)	12 (13%)	0	3
27	B2	69/72 (96%)	35 (51%)	18 (26%)	16 (23%)	0	0
27	D2	69/72 (96%)	29 (42%)	31 (45%)	9 (13%)	0	3
28	B3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	0	7
28	D3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	0	7
29	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
29	D4	56/71 (79%)	28 (50%)	13 (23%)	15 (27%)	0	0
30	B5	57/60 (95%)	37 (65%)	9 (16%)	11 (19%)	0	1
30	D5	57/60 (95%)	38 (67%)	7 (12%)	12 (21%)	0	1
31	B6	48/54 (89%)	21 (44%)	12 (25%)	15 (31%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	5	31
32	D7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	5	31
33	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	1
33	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	1
34	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	3
34	D9	35/37 (95%)	21 (60%)	8 (23%)	6 (17%)	0	2
37	BC	226/229 (99%)	163 (72%)	51 (23%)	12 (5%)	1	14
37	DC	226/229 (99%)	163 (72%)	50 (22%)	13 (6%)	1	13
38	BD	273/276 (99%)	189 (69%)	50 (18%)	34 (12%)	0	4
38	DD	273/276 (99%)	188 (69%)	50 (18%)	35 (13%)	0	3
39	BE	203/206 (98%)	122 (60%)	45 (22%)	36 (18%)	0	1
39	DE	203/206 (98%)	124 (61%)	44 (22%)	35 (17%)	0	2
40	BF	206/210 (98%)	132 (64%)	44 (21%)	30 (15%)	0	3
40	DF	206/210 (98%)	133 (65%)	42 (20%)	31 (15%)	0	2
41	BG	177/182 (97%)	110 (62%)	43 (24%)	24 (14%)	0	3
41	DG	177/182 (97%)	115 (65%)	36 (20%)	26 (15%)	0	2
42	BH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0
42	DH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	8
44	DK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	8
46	BN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	2
46	DN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	2
47	BO	120/122 (98%)	91 (76%)	19 (16%)	10 (8%)	0	8
47	DO	120/122 (98%)	93 (78%)	17 (14%)	10 (8%)	0	8
48	BP	144/150 (96%)	72 (50%)	45 (31%)	27 (19%)	0	1
48	DP	144/150 (96%)	72 (50%)	44 (31%)	28 (19%)	0	1
49	BQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	1	16
49	DQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	1	16
50	BR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	4
50	DR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	4
51	BS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
51	DS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
52	BT	136/146 (93%)	76 (56%)	32 (24%)	28 (21%)	0	1
52	DT	136/146 (93%)	75 (55%)	32 (24%)	29 (21%)	0	1
53	BU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	5
53	DU	115/118 (98%)	67 (58%)	35 (30%)	13 (11%)	0	4
54	BV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	1
54	DV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	1
55	BW	111/113 (98%)	80 (72%)	21 (19%)	10 (9%)	0	6
55	DW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	8
56	BX	91/96 (95%)	56 (62%)	26 (29%)	9 (10%)	0	6
56	DX	91/96 (95%)	57 (63%)	25 (28%)	9 (10%)	0	6
57	BY	105/110 (96%)	42 (40%)	36 (34%)	27 (26%)	0	0
57	DY	105/110 (96%)	43 (41%)	36 (34%)	26 (25%)	0	0
58	BZ	183/206 (89%)	108 (59%)	42 (23%)	33 (18%)	0	1
58	DZ	183/206 (89%)	114 (62%)	37 (20%)	32 (18%)	0	1
All	All	13200/13966 (94%)	8607 (65%)	2874 (22%)	1719 (13%)	0	3

5 of 1719 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	20	GLU
2	AB	95	GLN

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%)	183 (91%)	19 (9%)	8	32
2	CB	202/220 (92%)	183 (91%)	19 (9%)	8	32
3	AC	160/188 (85%)	144 (90%)	16 (10%)	7	30
3	CC	160/188 (85%)	144 (90%)	16 (10%)	7	30
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	30
4	CD	180/181 (99%)	163 (91%)	17 (9%)	8	32
5	AE	115/123 (94%)	99 (86%)	16 (14%)	3	19
5	CE	115/123 (94%)	98 (85%)	17 (15%)	3	17
6	AF	90/90 (100%)	83 (92%)	7 (8%)	11	38
6	CF	90/90 (100%)	84 (93%)	6 (7%)	15	42
7	AG	126/127 (99%)	116 (92%)	10 (8%)	11	37
7	CG	126/127 (99%)	115 (91%)	11 (9%)	9	34
8	AH	119/119 (100%)	113 (95%)	6 (5%)	22	49
8	CH	119/119 (100%)	111 (93%)	8 (7%)	15	42
9	AI	98/99 (99%)	90 (92%)	8 (8%)	10	36
9	CI	98/99 (99%)	90 (92%)	8 (8%)	10	36
10	AJ	88/92 (96%)	74 (84%)	14 (16%)	2	15
10	CJ	88/92 (96%)	75 (85%)	13 (15%)	3	17
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	33
11	CK	90/99 (91%)	83 (92%)	7 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	32
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	28
13	AM	99/101 (98%)	89 (90%)	10 (10%)	7	30
13	CM	99/101 (98%)	89 (90%)	10 (10%)	7	30
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	19
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	AO	79/80 (99%)	73 (92%)	6 (8%)	12	39
15	CO	79/80 (99%)	72 (91%)	7 (9%)	9	33
16	AP	72/74 (97%)	66 (92%)	6 (8%)	10	35
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	31
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	32
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	32
18	AR	61/77 (79%)	58 (95%)	3 (5%)	22	49
18	CR	61/77 (79%)	58 (95%)	3 (5%)	22	49
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	21
19	CS	69/80 (86%)	60 (87%)	9 (13%)	4	21
20	AT	76/82 (93%)	67 (88%)	9 (12%)	5	24
20	CT	76/82 (93%)	67 (88%)	9 (12%)	5	24
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	563/582 (97%)	480 (85%)	83 (15%)	3	17
24	CY	563/582 (97%)	490 (87%)	73 (13%)	4	21
25	B0	66/67 (98%)	57 (86%)	9 (14%)	3	20
25	D0	66/67 (98%)	57 (86%)	9 (14%)	3	20
26	B1	78/83 (94%)	64 (82%)	14 (18%)	2	11
26	D1	78/83 (94%)	70 (90%)	8 (10%)	7	30
27	B2	66/67 (98%)	60 (91%)	6 (9%)	9	33
27	D2	66/67 (98%)	57 (86%)	9 (14%)	3	20
28	B3	51/52 (98%)	46 (90%)	5 (10%)	7	31
28	D3	51/52 (98%)	46 (90%)	5 (10%)	7	31
29	B4	51/63 (81%)	37 (72%)	14 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D4	51/63 (81%)	37 (72%)	14 (28%)	0	3
30	B5	51/52 (98%)	48 (94%)	3 (6%)	18	45
30	D5	51/52 (98%)	48 (94%)	3 (6%)	18	45
31	B6	49/52 (94%)	37 (76%)	12 (24%)	1	4
31	D6	49/52 (94%)	37 (76%)	12 (24%)	1	4
32	B7	41/42 (98%)	38 (93%)	3 (7%)	13	40
32	D7	41/42 (98%)	38 (93%)	3 (7%)	13	40
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	13
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	13
34	B9	34/34 (100%)	31 (91%)	3 (9%)	9	33
34	D9	34/34 (100%)	30 (88%)	4 (12%)	5	24
37	BC	180/181 (99%)	166 (92%)	14 (8%)	11	38
37	DC	180/181 (99%)	166 (92%)	14 (8%)	11	38
38	BD	217/218 (100%)	182 (84%)	35 (16%)	2	15
38	DD	217/218 (100%)	182 (84%)	35 (16%)	2	15
39	BE	165/166 (99%)	134 (81%)	31 (19%)	1	10
39	DE	165/166 (99%)	136 (82%)	29 (18%)	2	12
40	BF	165/166 (99%)	153 (93%)	12 (7%)	13	40
40	DF	165/166 (99%)	153 (93%)	12 (7%)	13	40
41	BG	155/156 (99%)	130 (84%)	25 (16%)	2	15
41	DG	155/156 (99%)	127 (82%)	28 (18%)	2	11
42	BH	136/148 (92%)	122 (90%)	14 (10%)	7	30
42	DH	136/148 (92%)	122 (90%)	14 (10%)	7	30
44	BK	104/111 (94%)	88 (85%)	16 (15%)	2	16
44	DK	104/111 (94%)	88 (85%)	16 (15%)	2	16
46	BN	117/119 (98%)	100 (86%)	17 (14%)	3	18
46	DN	117/119 (98%)	100 (86%)	17 (14%)	3	18
47	BO	100/100 (100%)	92 (92%)	8 (8%)	11	37
47	DO	100/100 (100%)	91 (91%)	9 (9%)	9	33
48	BP	112/116 (97%)	92 (82%)	20 (18%)	2	11
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	16
49	DQ	111/111 (100%)	95 (86%)	16 (14%)	3	18
50	BR	100/101 (99%)	86 (86%)	14 (14%)	3	19
50	DR	100/101 (99%)	86 (86%)	14 (14%)	3	19
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	19
51	DS	77/88 (88%)	66 (86%)	11 (14%)	3	19
52	BT	120/127 (94%)	98 (82%)	22 (18%)	2	11
52	DT	120/127 (94%)	99 (82%)	21 (18%)	2	12
53	BU	92/94 (98%)	85 (92%)	7 (8%)	12	39
53	DU	92/94 (98%)	85 (92%)	7 (8%)	12	39
54	BV	82/82 (100%)	70 (85%)	12 (15%)	3	18
54	DV	82/82 (100%)	70 (85%)	12 (15%)	3	18
55	BW	91/92 (99%)	84 (92%)	7 (8%)	12	38
55	DW	91/92 (99%)	84 (92%)	7 (8%)	12	38
56	BX	74/78 (95%)	62 (84%)	12 (16%)	2	15
56	DX	74/78 (95%)	62 (84%)	12 (16%)	2	15
57	BY	87/91 (96%)	73 (84%)	14 (16%)	2	15
57	DY	87/91 (96%)	73 (84%)	14 (16%)	2	15
58	BZ	162/179 (90%)	128 (79%)	34 (21%)	1	7
58	DZ	162/179 (90%)	143 (88%)	19 (12%)	5	25
All	All	11080/11566 (96%)	9716 (88%)	1364 (12%)	4	23

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	CY	377	VAL
41	DG	120	LEU
24	CY	630	GLN
24	CY	357	ARG
37	DC	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 364 such sidechains are listed below:

Mol	Chain	Res	Type
15	CO	37	ASN
38	DD	116	GLN
20	CT	42	GLN
25	D0	12	ASN
39	DE	180	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	272 (18%)	43 (2%)
1	CA	1503/1522 (98%)	268 (17%)	43 (2%)
22	AV	76/77 (98%)	15 (19%)	0
22	AW	76/77 (98%)	25 (32%)	1 (1%)
22	CV	76/77 (98%)	14 (18%)	0
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AX	11/25 (44%)	4 (36%)	1 (9%)
23	CX	11/25 (44%)	4 (36%)	1 (9%)
35	BA	2900/2915 (99%)	600 (20%)	71 (2%)
35	DA	2900/2915 (99%)	596 (20%)	71 (2%)
36	BB	118/122 (96%)	25 (21%)	0
36	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9476 (98%)	1867 (19%)	232 (2%)

5 of 1867 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2891	G
35	DA	2689	U
1	CA	992	U
35	DA	2481	G
35	DA	1819	A

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

4 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	$\# Z > 2$
22	5MU	AV	54	22	18,21,23	0.39	0	25,30,35	0.51	0
22	5MU	CW	55	22	18,21,23	0.31	0	25,30,35	0.51	0
22	5MU	AW	55	22	18,21,23	0.28	0	25,30,35	0.51	0
22	5MU	CV	54	22	18,21,23	0.29	0	25,30,35	0.48	0

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
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2
22	5MU	CW	55	22	-	0/7/25/26	0/2/2/2
22	5MU	AW	55	22	-	0/7/25/26	0/2/2/2
22	5MU	CV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0
22	CW	55	5MU	2	0
22	AW	55	5MU	1	0
22	CV	54	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 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	FUA	CY	702	-	39,40,40	1.71	7 (17%)	50,64,64	1.56	10 (20%)
61	FUA	AY	702	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)
62	GDP	CY	703	60	29,30,30	1.08	1 (3%)	45,47,47	1.86	10 (22%)
62	GDP	AY	703	60	29,30,30	1.06	1 (3%)	45,47,47	1.72	9 (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	FUA	CY	702	-	-	8/16/92/92	0/4/4/4
61	FUA	AY	702	-	-	7/16/92/92	0/4/4/4
62	GDP	CY	703	60	-	3/16/32/32	0/3/3/3
62	GDP	AY	703	60	-	2/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	FUA	C23-C22	-4.55	1.39	1.51
61	AY	702	FUA	C23-C22	-4.43	1.39	1.51
61	AY	702	FUA	C23-C24	-4.35	1.39	1.53
61	CY	702	FUA	C23-C24	-4.35	1.39	1.53
61	AY	702	FUA	C29-C22	4.24	1.53	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CY	703	GDP	C2-N3-C4	5.50	121.78	112.30
61	AY	702	FUA	C24-C23-C22	5.35	124.11	112.72
62	AY	703	GDP	C2-N3-C4	5.33	121.48	112.30
62	CY	703	GDP	C5-C4-N3	-4.91	120.58	128.39
62	AY	703	GDP	C5-C4-N3	-4.78	120.78	128.39

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	702	FUA	C13-C17-C22-C23
61	AY	702	FUA	C13-C17-C22-C29
61	CY	702	FUA	C13-C17-C22-C23
61	CY	702	FUA	C13-C17-C22-C29
62	AY	703	GDP	C5'-O5'-PA-O3A

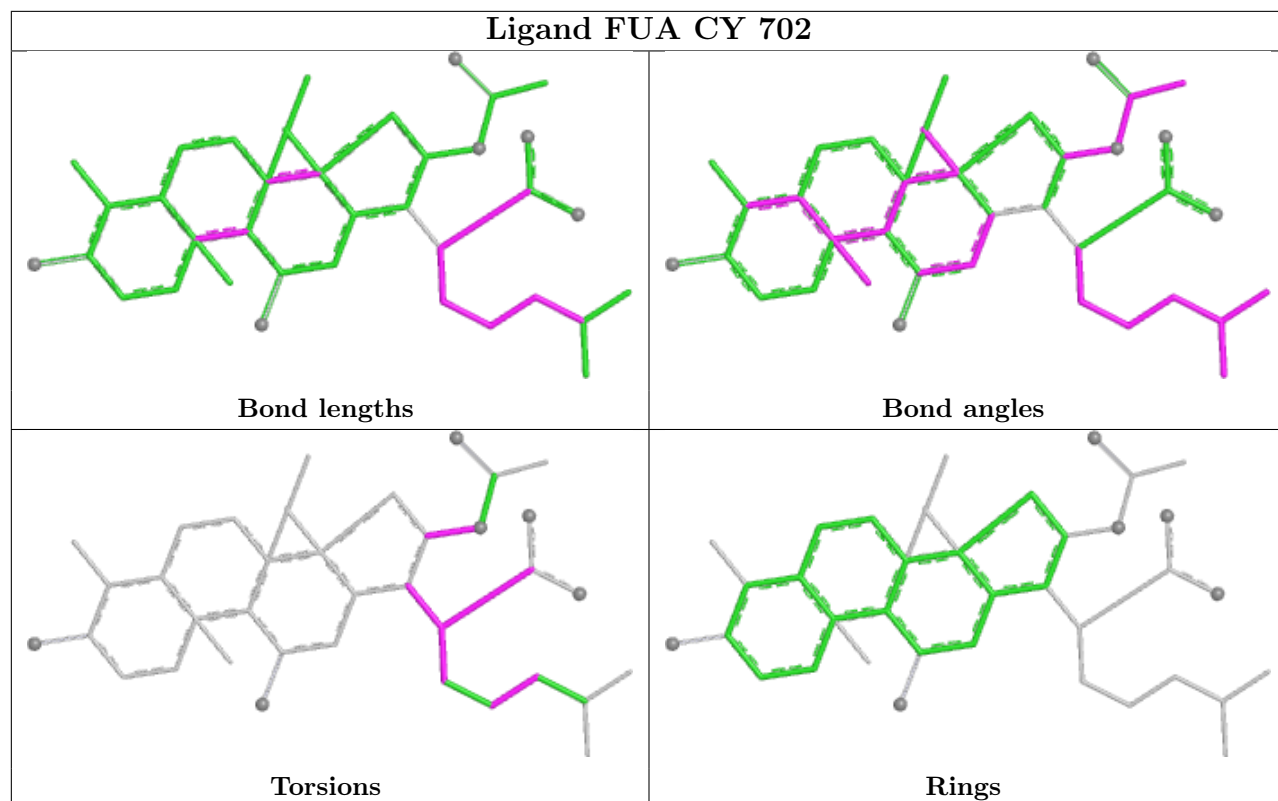
There are no ring outliers.

4 monomers are involved in 51 short contacts:

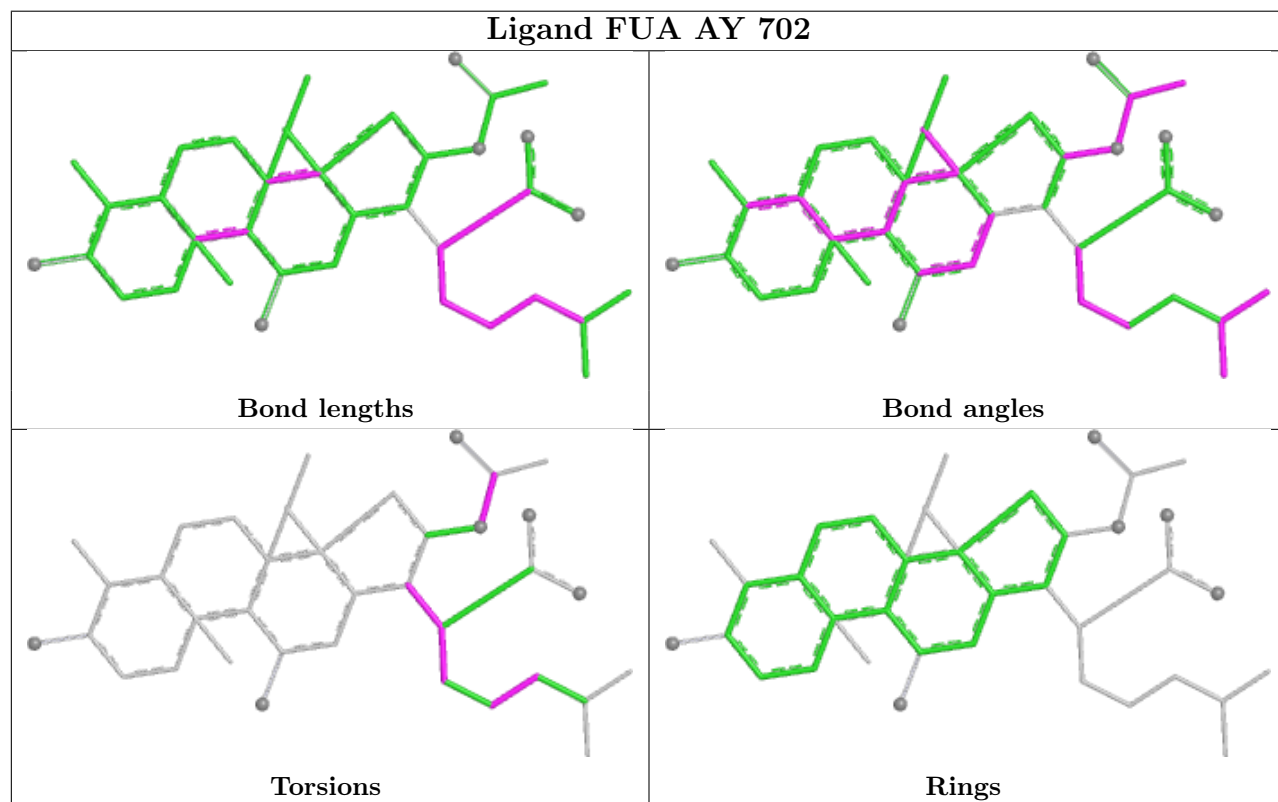
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CY	702	FUA	22	0
61	AY	702	FUA	13	0
62	CY	703	GDP	8	0
62	AY	703	GDP	8	0

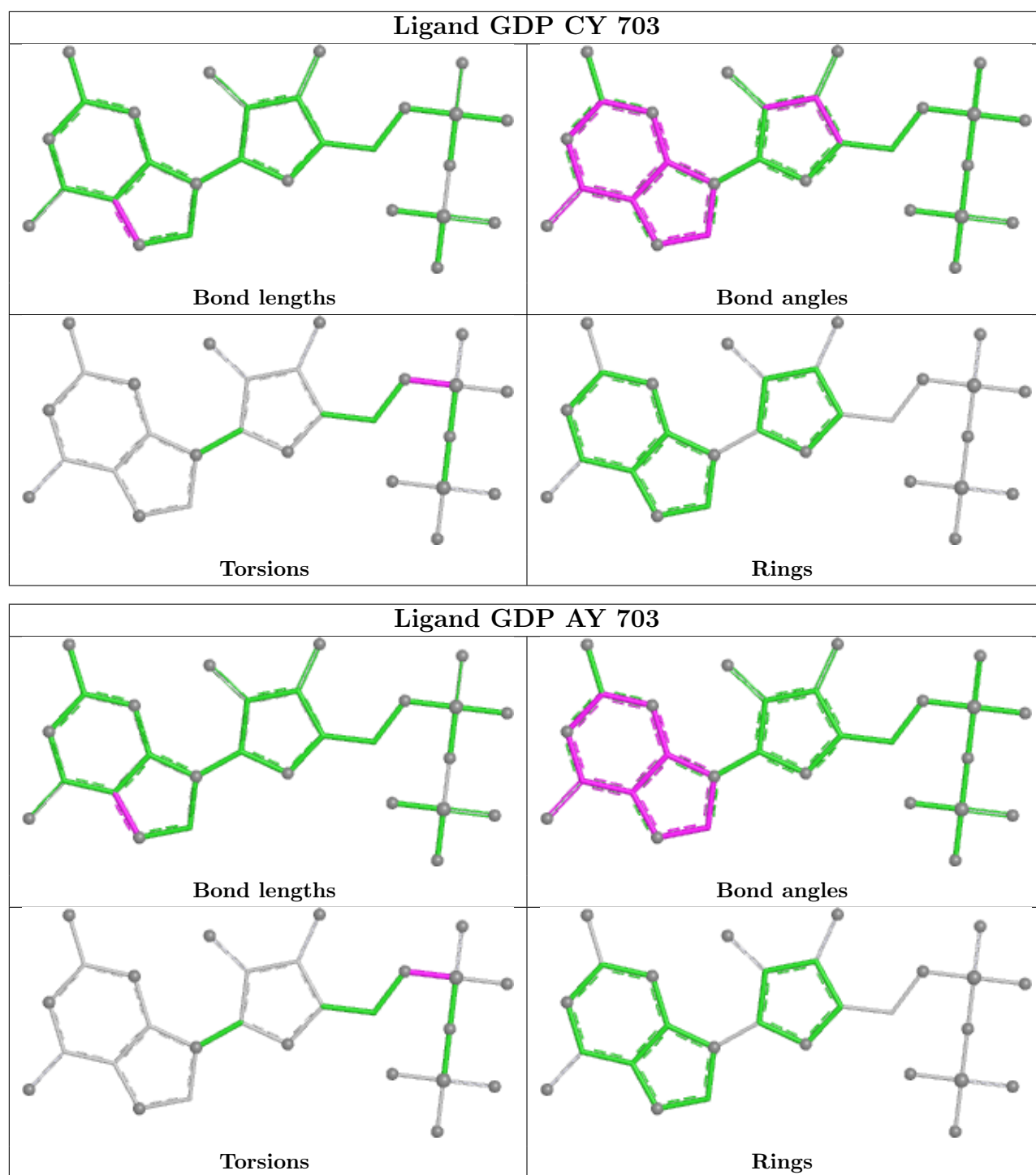
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FUA CY 702



Ligand FUA AY 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	CI	2
9	AI	2
45	DL	1
45	BL	1
41	BG	1
41	DG	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DL	30:UNK	C	52:UNK	N	38.40
1	BL	30:UNK	C	52:UNK	N	36.36
1	BG	112:PRO	C	113:ARG	N	3.27
1	DG	112:PRO	C	113:ARG	N	3.05
1	CI	53:VAL	C	54:ASP	N	2.98

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	1504/1522 (98%)	0.18	68 (4%) 38 21	23, 62, 148, 220	0
1	CA	1504/1522 (98%)	0.15	39 (2%) 57 33	26, 65, 148, 220	0
2	AB	235/256 (91%)	0.34	6 (2%) 57 33	40, 81, 147, 159	0
2	CB	235/256 (91%)	0.24	6 (2%) 57 33	43, 82, 147, 158	0
3	AC	207/239 (86%)	0.37	4 (1%) 66 39	31, 72, 113, 118	0
3	CC	207/239 (86%)	0.21	3 (1%) 73 46	33, 75, 115, 121	0
4	AD	208/209 (99%)	0.31	8 (3%) 44 25	46, 79, 115, 124	0
4	CD	208/209 (99%)	0.27	7 (3%) 48 27	48, 80, 116, 125	0
5	AE	151/162 (93%)	-0.26	0 100 100	25, 50, 90, 112	0
5	CE	151/162 (93%)	-0.18	1 (0%) 84 61	27, 52, 91, 112	0
6	AF	101/101 (100%)	0.23	0 100 100	55, 85, 110, 118	0
6	CF	101/101 (100%)	0.03	0 100 100	60, 87, 111, 118	0
7	AG	155/156 (99%)	0.21	5 (3%) 50 29	51, 79, 109, 136	0
7	CG	155/156 (99%)	0.14	6 (3%) 43 24	55, 81, 111, 136	0
8	AH	138/138 (100%)	-0.11	0 100 100	32, 54, 75, 82	0
8	CH	138/138 (100%)	-0.14	0 100 100	35, 56, 76, 83	0
9	AI	127/128 (99%)	0.61	6 (4%) 36 20	50, 83, 114, 120	0
9	CI	127/128 (99%)	0.40	4 (3%) 51 29	53, 86, 114, 120	0
10	AJ	99/105 (94%)	1.19	19 (19%) 3 3	47, 100, 155, 159	0
10	CJ	99/105 (94%)	0.81	10 (10%) 12 10	50, 102, 156, 159	0
11	AK	119/129 (92%)	0.06	5 (4%) 40 22	42, 59, 100, 123	0
11	CK	119/129 (92%)	0.01	3 (2%) 58 34	44, 60, 102, 124	0
12	AL	125/132 (94%)	0.03	1 (0%) 82 58	38, 57, 87, 127	0
12	CL	125/132 (94%)	0.05	2 (1%) 70 43	39, 58, 88, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.80	12 (9%) 13 10	68, 111, 139, 171	0
13	CM	125/126 (99%)	0.63	11 (8%) 15 11	70, 112, 139, 172	0
14	AN	60/61 (98%)	0.43	3 (5%) 34 19	39, 59, 92, 97	0
14	CN	60/61 (98%)	0.30	2 (3%) 49 28	44, 61, 93, 98	0
15	AO	88/89 (98%)	-0.05	1 (1%) 78 52	35, 61, 91, 100	0
15	CO	88/89 (98%)	-0.07	0 100 100	38, 61, 94, 100	0
16	AP	84/88 (95%)	0.15	1 (1%) 76 50	54, 73, 96, 131	0
16	CP	84/88 (95%)	0.11	0 100 100	57, 74, 98, 132	0
17	AQ	100/105 (95%)	-0.08	0 100 100	43, 64, 89, 98	0
17	CQ	100/105 (95%)	-0.01	1 (1%) 79 54	46, 66, 90, 97	0
18	AR	70/88 (79%)	0.02	0 100 100	42, 69, 94, 108	0
18	CR	70/88 (79%)	-0.04	0 100 100	45, 70, 95, 109	0
19	AS	79/93 (84%)	0.92	7 (8%) 15 11	77, 106, 144, 149	0
19	CS	79/93 (84%)	0.67	2 (2%) 58 34	78, 107, 144, 150	0
20	AT	99/106 (93%)	0.39	6 (6%) 27 16	63, 84, 126, 129	0
20	CT	99/106 (93%)	0.33	4 (4%) 42 24	64, 85, 127, 129	0
21	AU	25/27 (92%)	1.19	5 (20%) 3 3	63, 82, 118, 122	0
21	CU	25/27 (92%)	0.90	1 (4%) 42 24	66, 86, 120, 123	0
22	AV	76/77 (98%)	-0.00	4 (5%) 32 19	32, 67, 110, 127	0
22	AW	76/77 (98%)	1.13	12 (15%) 5 5	71, 168, 192, 201	0
22	CV	76/77 (98%)	0.17	2 (2%) 57 33	47, 84, 121, 151	0
22	CW	76/77 (98%)	1.35	15 (19%) 3 3	78, 176, 200, 210	0
23	AX	11/25 (44%)	1.11	4 (36%) 1 1	28, 94, 149, 166	0
23	CX	11/25 (44%)	1.50	5 (45%) 0 1	45, 106, 156, 168	0
24	AY	667/691 (96%)	0.07	12 (1%) 67 40	61, 99, 140, 150	0
24	CY	667/691 (96%)	0.27	17 (2%) 58 34	73, 108, 148, 161	0
25	B0	84/85 (98%)	0.72	7 (8%) 17 12	67, 82, 140, 163	0
25	D0	84/85 (98%)	0.75	7 (8%) 17 12	69, 84, 141, 163	0
26	B1	94/98 (95%)	0.04	1 (1%) 78 52	41, 70, 118, 128	0
26	D1	94/98 (95%)	0.22	2 (2%) 63 37	53, 80, 123, 131	0
27	B2	71/72 (98%)	0.27	0 100 100	77, 116, 150, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.20	0 100 100	95, 119, 146, 163	0
28	B3	60/60 (100%)	0.30	0 100 100	63, 88, 114, 135	0
28	D3	60/60 (100%)	0.37	0 100 100	64, 89, 114, 134	0
29	B4	58/71 (81%)	1.33	16 (27%) 1 2	76, 135, 220, 222	0
29	D4	58/71 (81%)	1.09	10 (17%) 4 4	77, 137, 220, 222	0
30	B5	59/60 (98%)	0.83	11 (18%) 3 4	52, 80, 153, 172	0
30	D5	59/60 (98%)	0.91	11 (18%) 3 4	52, 80, 153, 172	0
31	B6	50/54 (92%)	0.99	8 (16%) 5 5	56, 89, 107, 117	0
31	D6	50/54 (92%)	0.81	8 (16%) 5 5	56, 90, 108, 117	0
32	B7	49/49 (100%)	0.41	3 (6%) 27 16	47, 64, 119, 132	0
32	D7	49/49 (100%)	0.26	3 (6%) 27 16	47, 64, 120, 132	0
33	B8	64/65 (98%)	0.93	9 (14%) 6 6	63, 75, 105, 125	0
33	D8	64/65 (98%)	0.88	8 (12%) 8 7	65, 76, 105, 126	0
34	B9	37/37 (100%)	0.15	1 (2%) 56 32	60, 71, 85, 89	0
34	D9	37/37 (100%)	0.52	4 (10%) 11 9	60, 73, 87, 91	0
35	BA	2901/2915 (99%)	0.37	93 (3%) 50 29	30, 76, 162, 221	0
35	DA	2901/2915 (99%)	0.32	74 (2%) 57 33	29, 77, 162, 221	0
36	BB	119/122 (97%)	0.78	4 (3%) 48 27	65, 106, 138, 183	0
36	DB	119/122 (97%)	0.59	5 (4%) 40 22	66, 108, 138, 183	0
37	BC	228/229 (99%)	0.35	8 (3%) 47 27	42, 97, 147, 160	0
37	DC	228/229 (99%)	0.38	11 (4%) 35 20	43, 98, 148, 162	0
38	BD	275/276 (99%)	-0.00	1 (0%) 88 70	31, 52, 82, 101	0
38	DD	275/276 (99%)	-0.01	8 (2%) 53 30	32, 52, 82, 101	0
39	BE	205/206 (99%)	0.42	8 (3%) 43 24	44, 77, 128, 135	0
39	DE	205/206 (99%)	0.40	8 (3%) 43 24	44, 77, 128, 134	0
40	BF	208/210 (99%)	0.47	5 (2%) 59 34	53, 110, 166, 177	0
40	DF	208/210 (99%)	0.45	3 (1%) 73 46	53, 111, 166, 176	0
41	BG	181/182 (99%)	0.26	4 (2%) 62 36	63, 95, 131, 143	0
41	DG	181/182 (99%)	0.30	5 (2%) 55 31	86, 110, 137, 151	0
42	BH	167/180 (92%)	0.63	12 (7%) 21 14	81, 117, 143, 159	0
42	DH	167/180 (92%)	0.55	10 (5%) 27 17	81, 118, 143, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BJ	0/173	-	-	-	-
43	DJ	0/173	-	-	-	-
44	BK	140/147 (95%)	0.89	11 (7%) 18 13	162, 180, 186, 188	0
44	DK	140/147 (95%)	0.92	20 (14%) 6 6	162, 180, 186, 187	0
45	BL	0/125	-	-	-	-
45	BM	0/125	-	-	-	-
45	Bl	0/125	-	-	-	-
45	Bm	0/125	-	-	-	-
45	DL	0/125	-	-	-	-
45	DM	0/125	-	-	-	-
45	Dl	0/125	-	-	-	-
45	Dm	0/125	-	-	-	-
46	BN	139/140 (99%)	0.42	6 (4%) 40 22	60, 91, 132, 137	0
46	DN	139/140 (99%)	0.42	2 (1%) 73 46	61, 91, 132, 137	0
47	BO	122/122 (100%)	-0.22	0 100 100	35, 60, 73, 86	0
47	DO	122/122 (100%)	-0.11	0 100 100	36, 61, 73, 88	0
48	BP	146/150 (97%)	1.02	21 (14%) 6 6	46, 111, 137, 157	0
48	DP	146/150 (97%)	0.79	15 (10%) 12 10	50, 113, 137, 157	0
49	BQ	141/141 (100%)	0.12	1 (0%) 84 61	45, 65, 88, 119	0
49	DQ	141/141 (100%)	0.15	0 100 100	45, 66, 89, 120	0
50	BR	117/118 (99%)	0.33	6 (5%) 33 19	49, 81, 101, 128	0
50	DR	117/118 (99%)	0.44	5 (4%) 40 22	53, 82, 101, 128	0
51	BS	99/112 (88%)	1.04	15 (15%) 5 5	82, 116, 140, 144	0
51	DS	99/112 (88%)	0.87	8 (8%) 18 12	83, 117, 141, 145	0
52	BT	138/146 (94%)	0.32	5 (3%) 46 26	55, 83, 149, 176	0
52	DT	138/146 (94%)	0.41	3 (2%) 62 36	57, 84, 149, 177	0
53	BU	117/118 (99%)	0.38	4 (3%) 48 27	62, 80, 114, 135	0
53	DU	117/118 (99%)	0.47	5 (4%) 40 22	62, 81, 115, 134	0
54	BV	101/101 (100%)	0.74	5 (4%) 34 19	59, 116, 133, 141	0
54	DV	101/101 (100%)	0.67	3 (2%) 52 30	61, 116, 134, 140	0
55	BW	113/113 (100%)	0.21	1 (0%) 81 56	61, 79, 119, 158	0
55	DW	113/113 (100%)	0.15	0 100 100	63, 80, 120, 159	0
56	BX	93/96 (96%)	0.61	4 (4%) 40 22	76, 91, 110, 114	0
56	DX	93/96 (96%)	0.51	5 (5%) 31 18	76, 92, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	107/110 (97%)	1.00	13 (12%) 8 7	78, 127, 149, 155	0
57	DY	107/110 (97%)	0.99	12 (11%) 10 8	78, 127, 149, 155	0
58	BZ	185/206 (89%)	0.31	3 (1%) 70 43	47, 90, 135, 143	0
58	DZ	185/206 (89%)	0.47	1 (0%) 87 66	68, 99, 138, 146	0
All	All	22794/24788 (91%)	0.33	872 (3%) 44 25	23, 82, 154, 222	0

The worst 5 of 872 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	1036	G	9.3
1	CA	1036	G	9.0
24	AY	116	PRO	8.3
14	AN	2	ALA	8.0
35	BA	1541	G	7.7

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
22	5MU	AW	55	20/22	0.64	0.13	161,165,168,168	0
22	5MU	CW	55	20/22	0.73	0.11	178,179,186,186	0
22	5MU	CV	54	20/22	0.91	0.09	89,92,95,96	0
22	5MU	AV	54	20/22	0.91	0.09	82,84,86,86	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

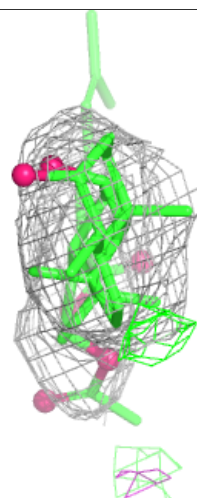
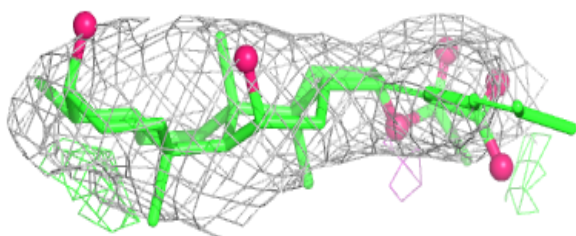
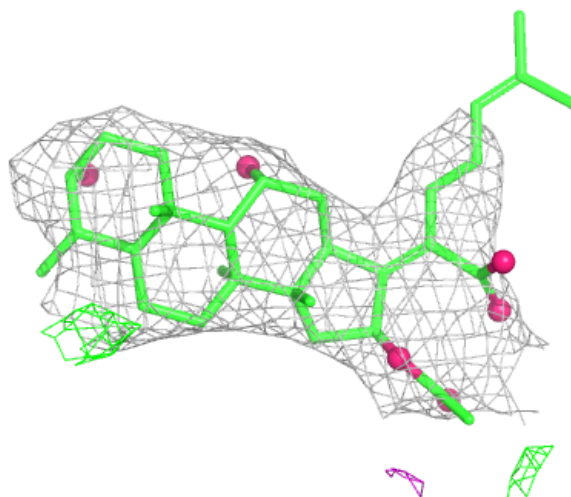
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	FUA	CY	702	37/37	0.82	0.17	102,104,107,109	0
59	ZN	B4	101	1/1	0.83	0.07	122,122,122,122	0
61	FUA	AY	702	37/37	0.87	0.17	98,102,110,111	0
59	ZN	D4	101	1/1	0.88	0.09	164,164,164,164	0
62	GDP	CY	703	28/28	0.93	0.09	81,87,94,95	0
62	GDP	AY	703	28/28	0.95	0.07	78,82,83,84	0
60	MG	AY	701	1/1	0.95	0.13	30,30,30,30	0
60	MG	CY	701	1/1	0.98	0.08	39,39,39,39	0
59	ZN	CD	301	1/1	0.99	0.13	49,49,49,49	0
59	ZN	AN	101	1/1	1.00	0.01	35,35,35,35	0
59	ZN	CN	101	1/1	1.00	0.01	66,66,66,66	0
59	ZN	AD	301	1/1	1.00	0.12	32,32,32,32	0
59	ZN	D9	101	1/1	1.00	0.02	86,86,86,86	0
59	ZN	B9	101	1/1	1.00	0.01	62,62,62,62	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.

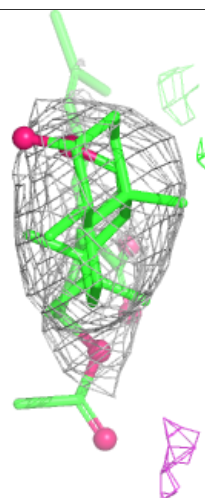
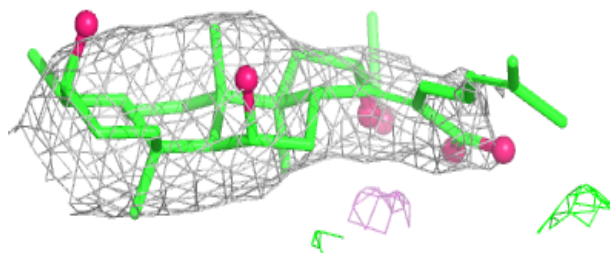
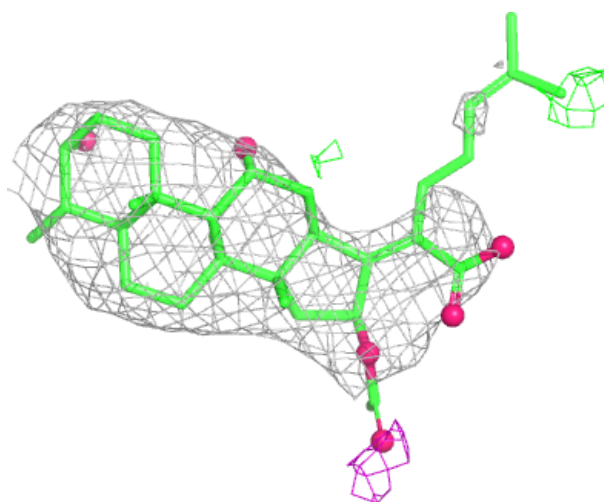
Electron density around FUA CY 702:

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



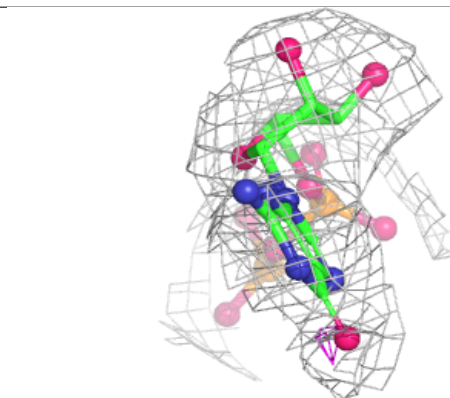
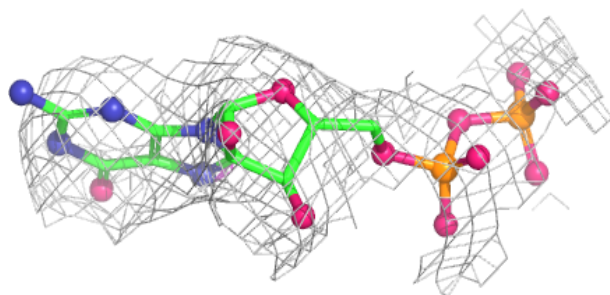
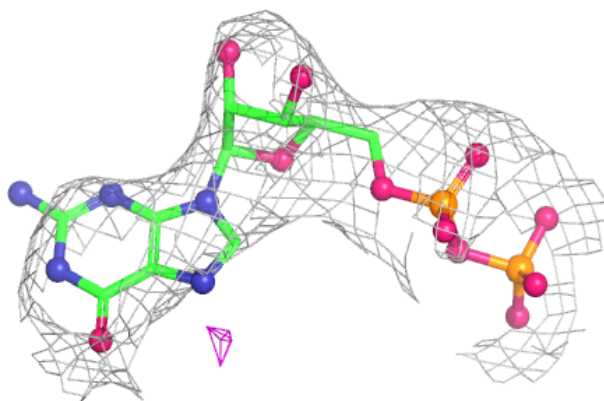
Electron density around FUA AY 702:

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

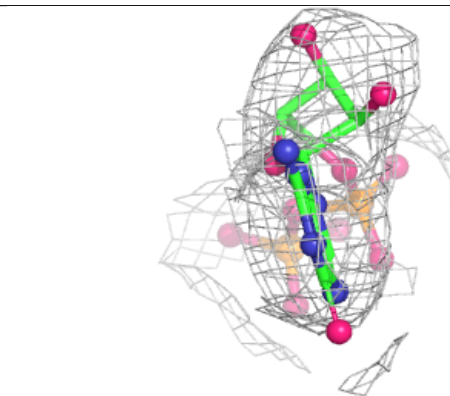
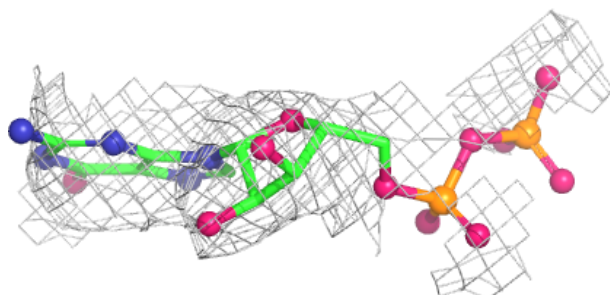
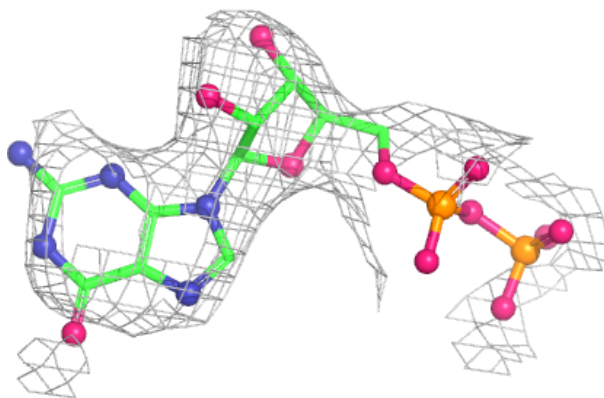


Electron density around GDP CY 703:

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

**Electron density around GDP AY 703:**

$2mF_o-DF_c$ (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.