



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 12:22 AM EDT

PDB ID : 4V8D
Title : Structure analysis of ribosomal decoding (cognate tRNA-tyr complex).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

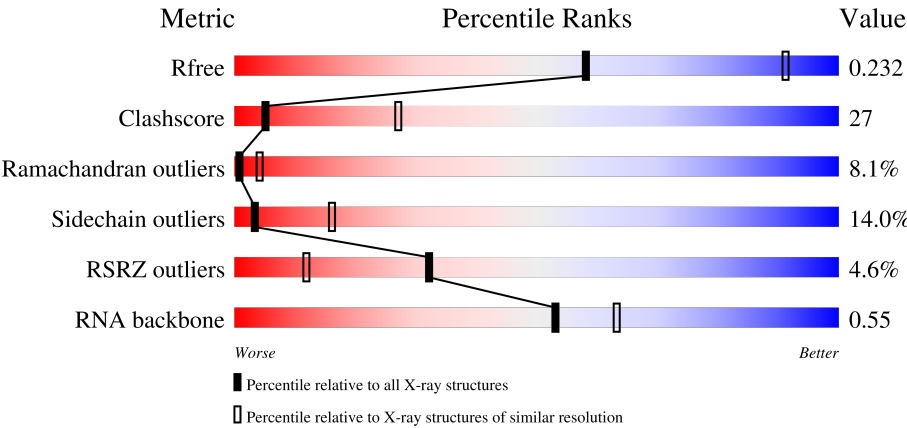
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	1506	<div> <div></div> <div>37%</div> <div>45%</div> <div>16%</div> </div>
1	CA	1506	<div> <div></div> <div>38%</div> <div>46%</div> <div>16%</div> </div>
2	AE	256	<div> <div>4%</div> <div>28%</div> <div>48%</div> <div>16%</div> <div>7%</div> </div>
2	CE	256	<div> <div>6%</div> <div>32%</div> <div>46%</div> <div>14%</div> <div>7%</div> </div>


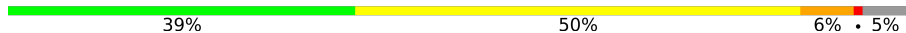



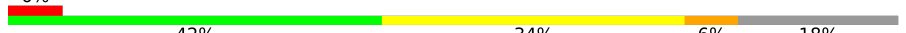
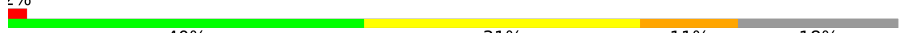




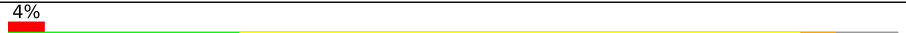





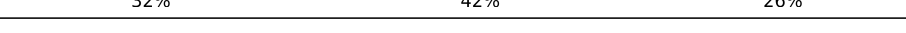


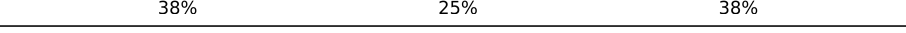




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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

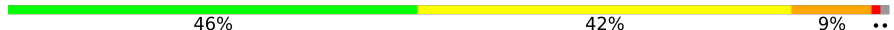


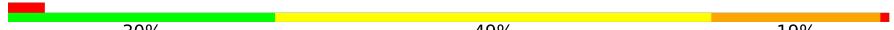

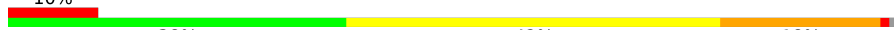




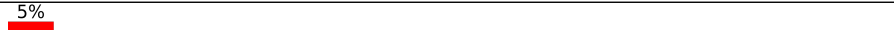

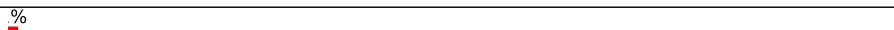
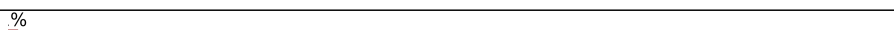




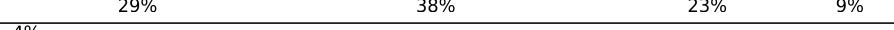

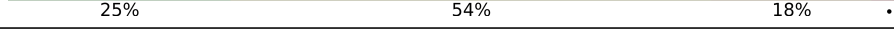



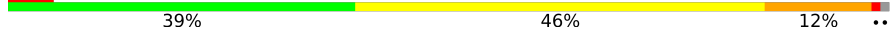
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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	85	
22	AD	85	
22	CB	85	
22	CD	85	
23	AC	77	
23	CC	77	
24	A1	16	
24	C1	16	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	

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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

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
55	MG	AA	1613	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1666	-	-	-	X
55	MG	AA	1683	-	-	-	X
55	MG	AA	1726	-	-	-	X
55	MG	AA	1728	-	-	-	X
55	MG	AA	1736	-	-	-	X
55	MG	AA	1750	-	-	-	X
55	MG	AA	1758	-	-	-	X
55	MG	AA	1768	-	-	-	X
55	MG	AA	1772	-	-	-	X
55	MG	AA	1775	-	-	-	X
55	MG	AA	1785	-	-	-	X
55	MG	AA	1791	-	-	-	X
55	MG	AA	1800	-	-	-	X
55	MG	AA	1804	-	-	-	X
55	MG	AA	1805	-	-	-	X
55	MG	AA	1806	-	-	-	X
55	MG	AA	1809	-	-	-	X
55	MG	AA	1815	-	-	-	X
55	MG	AA	1818	-	-	-	X
55	MG	AC	107	-	-	-	X
55	MG	BA	3041	-	-	-	X
55	MG	BA	3069	-	-	-	X
55	MG	BA	3078	-	-	-	X
55	MG	BA	3100	-	-	-	X
55	MG	BA	3122	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3137	-	-	-	X
55	MG	BA	3155	-	-	-	X
55	MG	BA	3171	-	-	-	X
55	MG	BA	3189	-	-	-	X
55	MG	BA	3192	-	-	-	X
55	MG	BA	3195	-	-	-	X
55	MG	BA	3209	-	-	-	X
55	MG	BA	3222	-	-	-	X
55	MG	BA	3245	-	-	-	X
55	MG	BA	3263	-	-	-	X
55	MG	BA	3266	-	-	-	X
55	MG	BA	3274	-	-	-	X
55	MG	BA	3300	-	-	-	X
55	MG	BA	3309	-	-	-	X
55	MG	BA	3323	-	-	-	X
55	MG	BA	3324	-	-	-	X
55	MG	BA	3333	-	-	-	X
55	MG	BA	3344	-	-	-	X
55	MG	BA	3353	-	-	-	X
55	MG	BA	3372	-	-	-	X
55	MG	BA	3373	-	-	-	X
55	MG	BA	3380	-	-	-	X
55	MG	BA	3382	-	-	-	X
55	MG	BA	3386	-	-	-	X
55	MG	BA	3391	-	-	-	X
55	MG	BA	3396	-	-	-	X
55	MG	BA	3406	-	-	-	X
55	MG	BA	3413	-	-	-	X
55	MG	BA	3421	-	-	-	X
55	MG	BA	3422	-	-	-	X
55	MG	BA	3426	-	-	-	X
55	MG	BA	3429	-	-	-	X
55	MG	BA	3433	-	-	-	X
55	MG	BA	3438	-	-	-	X
55	MG	BA	3440	-	-	-	X
55	MG	BA	3446	-	-	-	X
55	MG	BA	3451	-	-	-	X
55	MG	BA	3455	-	-	-	X
55	MG	BA	3456	-	-	-	X
55	MG	BA	3463	-	-	-	X
55	MG	BA	3472	-	-	-	X
55	MG	BA	3477	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3479	-	-	-	X
55	MG	BA	3487	-	-	-	X
55	MG	BA	3503	-	-	-	X
55	MG	BA	3504	-	-	-	X
55	MG	BA	3509	-	-	-	X
55	MG	BA	3510	-	-	-	X
55	MG	BA	3537	-	-	-	X
55	MG	BA	3540	-	-	-	X
55	MG	BA	3546	-	-	-	X
55	MG	BA	3550	-	-	-	X
55	MG	BB	203	-	-	-	X
55	MG	BB	208	-	-	-	X
55	MG	CA	1673	-	-	-	X
55	MG	CA	1678	-	-	-	X
55	MG	CA	1701	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1736	-	-	-	X
55	MG	CA	1740	-	-	-	X
55	MG	CA	1742	-	-	-	X
55	MG	CA	1759	-	-	-	X
55	MG	CA	1761	-	-	-	X
55	MG	CA	1762	-	-	-	X
55	MG	CA	1768	-	-	-	X
55	MG	CA	1773	-	-	-	X
55	MG	CA	1790	-	-	-	X
55	MG	CA	1804	-	-	-	X
55	MG	CA	1808	-	-	-	X
55	MG	CA	1812	-	-	-	X
55	MG	CA	1817	-	-	-	X
55	MG	CA	1819	-	-	-	X
55	MG	CB	103	-	-	-	X
55	MG	CK	201	-	-	-	X
55	MG	CR	101	-	-	-	X
55	MG	DA	3054	-	-	-	X
55	MG	DA	3085	-	-	-	X
55	MG	DA	3099	-	-	-	X
55	MG	DA	3100	-	-	-	X
55	MG	DA	3120	-	-	-	X
55	MG	DA	3172	-	-	-	X
55	MG	DA	3176	-	-	-	X
55	MG	DA	3207	-	-	-	X
55	MG	DA	3221	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3225	-	-	-	X
55	MG	DA	3227	-	-	-	X
55	MG	DA	3228	-	-	-	X
55	MG	DA	3238	-	-	-	X
55	MG	DA	3262	-	-	-	X
55	MG	DA	3279	-	-	-	X
55	MG	DA	3291	-	-	-	X
55	MG	DA	3330	-	-	-	X
55	MG	DA	3336	-	-	-	X
55	MG	DA	3342	-	-	-	X
55	MG	DA	3358	-	-	-	X
55	MG	DA	3365	-	-	-	X
55	MG	DA	3372	-	-	-	X
55	MG	DA	3382	-	-	-	X
55	MG	DA	3399	-	-	-	X
55	MG	DA	3409	-	-	-	X
55	MG	DA	3423	-	-	-	X
55	MG	DA	3425	-	-	-	X
55	MG	DA	3446	-	-	-	X
55	MG	DB	210	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299676 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	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
1	CA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CG	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	AH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CI	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	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CJ	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	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CK	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	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	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	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CN	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	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
14	CQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CR	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	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CW	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	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	AB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	AD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			
24	C1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			

- Molecule 25 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2912	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
25	DA	2907	Total 62607	C 27866	N 11712	O 20123	P 2906	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	INSERTION	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	166	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
26	DB	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
27	DD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
38	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
45	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
53	D7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
54	D8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	220	Total 220	Mg 220	1	0
55	AG	2	Total 2	Mg 2	0	0
55	AN	1	Total 1	Mg 1	0	0
55	AR	1	Total 1	Mg 1	0	0
55	AS	1	Total 1	Mg 1	0	0
55	AB	4	Total 4	Mg 4	0	0
55	AC	8	Total 8	Mg 8	0	0
55	AD	3	Total 3	Mg 3	0	0
55	A1	1	Total 1	Mg 1	0	0
55	BA	568	Total 568	Mg 568	2	0
55	BB	18	Total 18	Mg 18	0	0
55	BD	1	Total 1	Mg 1	0	0
55	BE	3	Total 3	Mg 3	0	0
55	BF	3	Total 3	Mg 3	0	0
55	BO	2	Total 2	Mg 2	0	0
55	B0	1	Total 1	Mg 1	0	0
55	B1	2	Total 2	Mg 2	0	0
55	B2	1	Total 1	Mg 1	0	0
55	B3	3	Total 3	Mg 3	0	0
55	BW	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B6	1	Total 1	Mg 1	0	0
55	B7	1	Total 1	Mg 1	0	0
55	CA	219	Total 219	Mg 219	0	0
55	CG	2	Total 2	Mg 2	0	0
55	CK	1	Total 1	Mg 1	0	0
55	CR	1	Total 1	Mg 1	0	0
55	CB	4	Total 4	Mg 4	0	0
55	CC	9	Total 9	Mg 9	0	0
55	CD	1	Total 1	Mg 1	0	0
55	DA	488	Total 488	Mg 488	0	0
55	DB	20	Total 20	Mg 20	0	0
55	DD	3	Total 3	Mg 3	0	0
55	DE	1	Total 1	Mg 1	0	0
55	DO	1	Total 1	Mg 1	0	0
55	D0	1	Total 1	Mg 1	0	0
55	D1	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	D5	2	Total 2	Mg 2	0	0
55	D7	1	Total 1	Mg 1	0	0
55	D8	1	Total 1	Mg 1	0	0

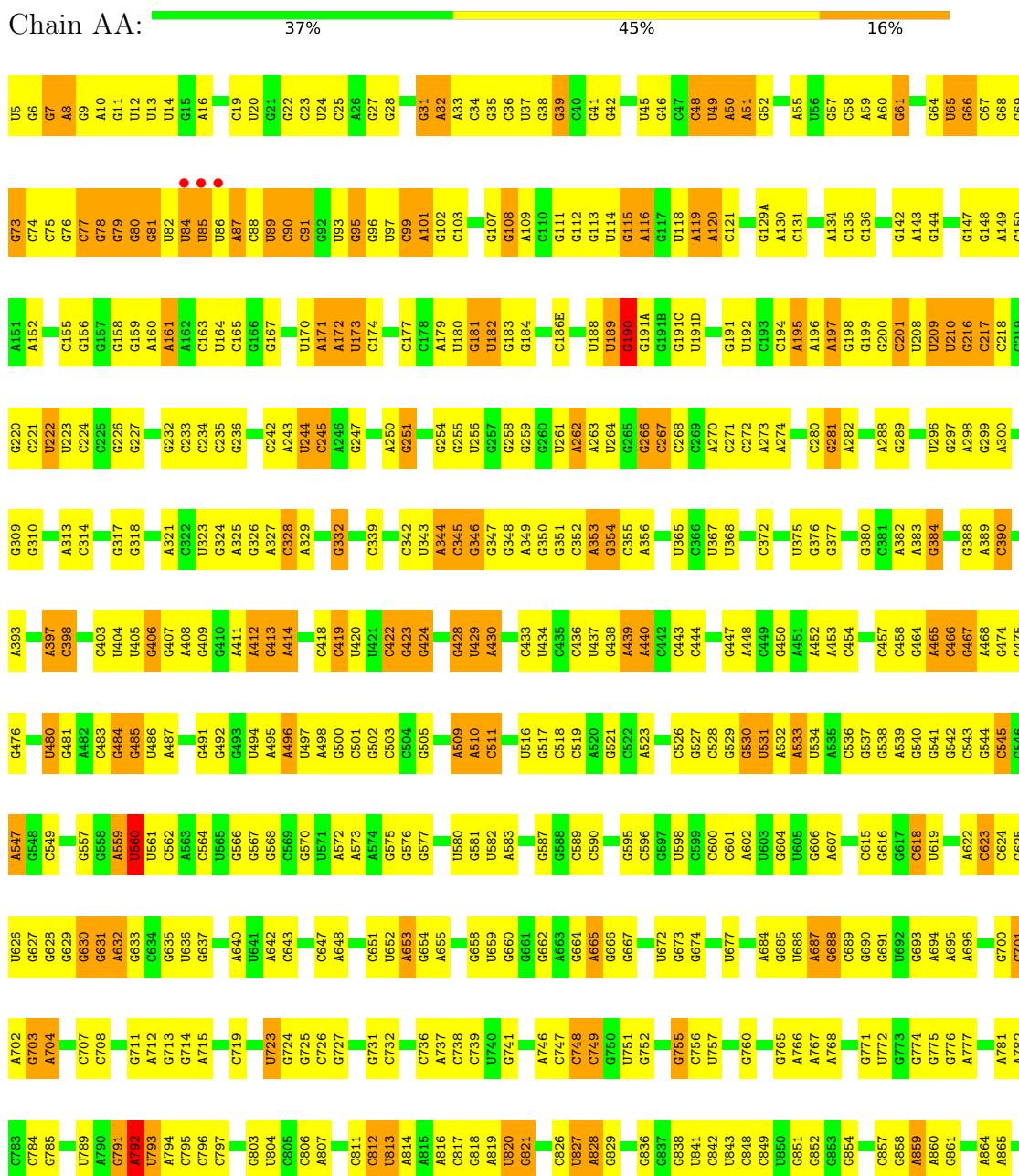
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

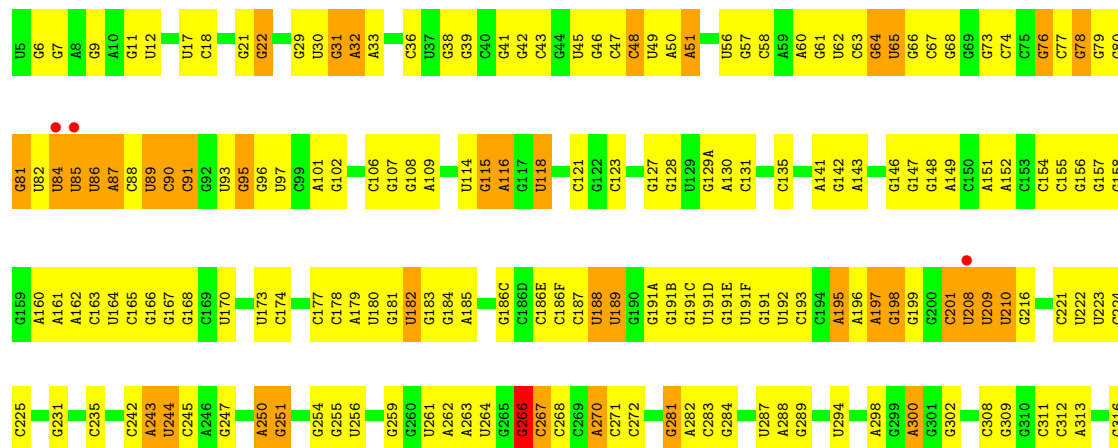
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

3 Residue-property plots

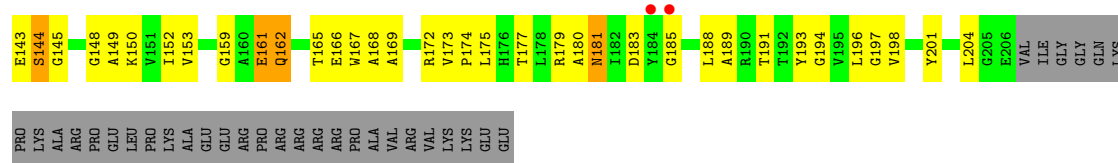
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

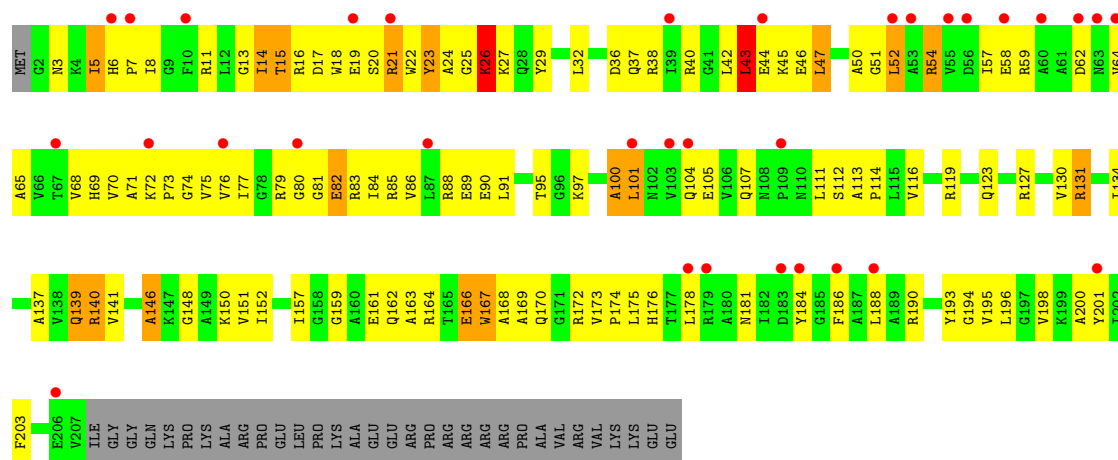




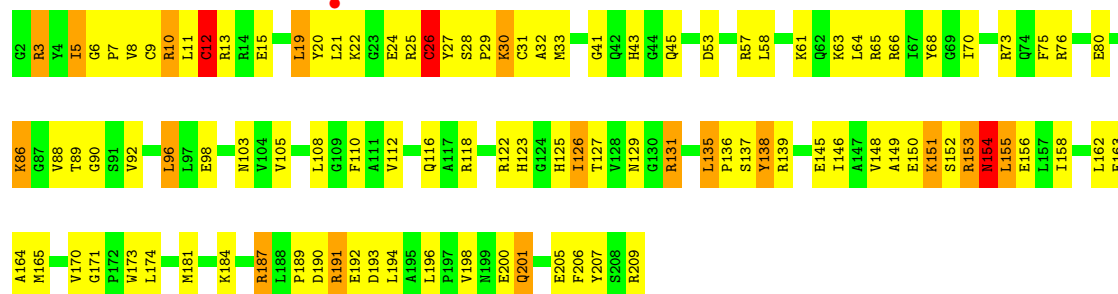




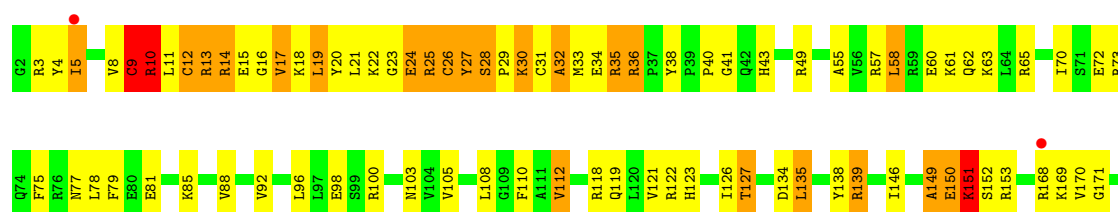
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

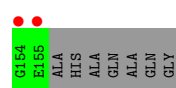
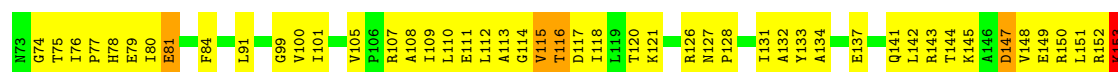


• Molecule 4: 30S RIBOSOMAL PROTEIN S4





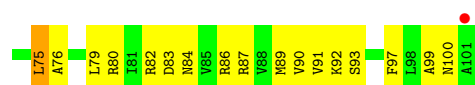
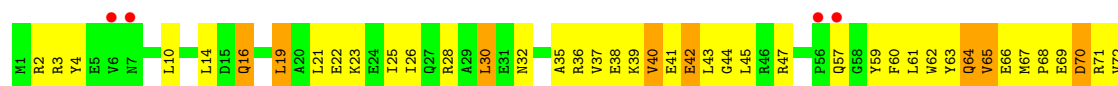
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



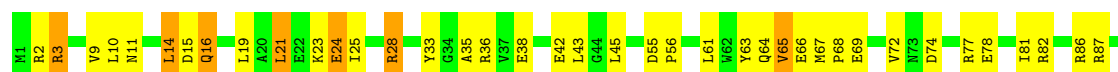
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



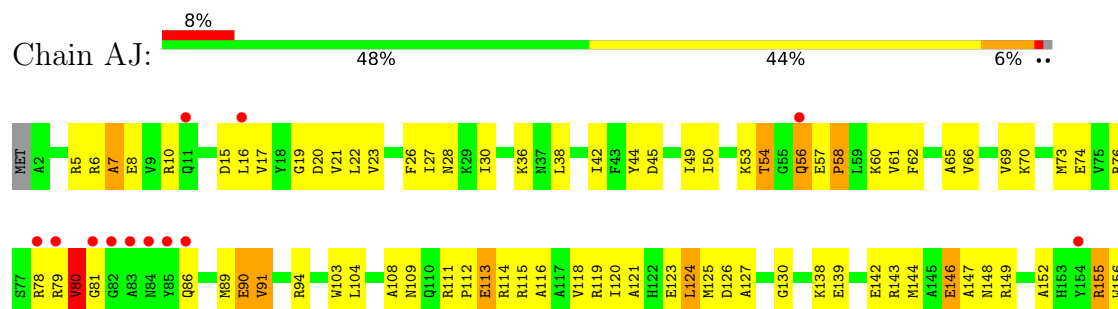
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



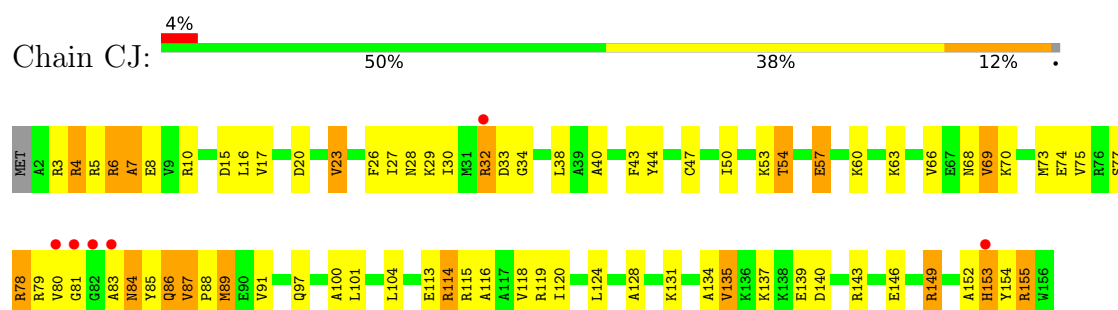
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



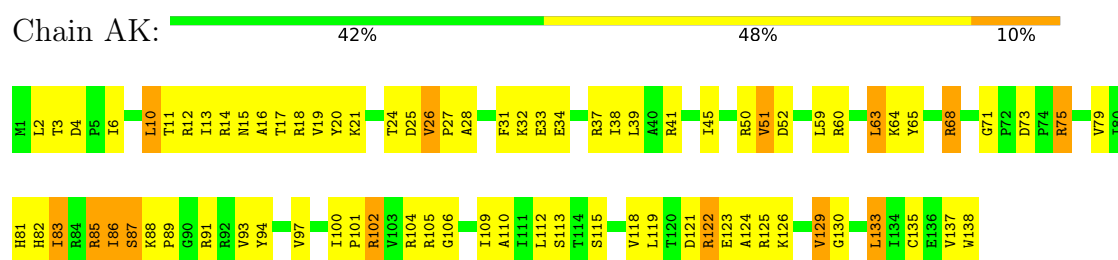
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



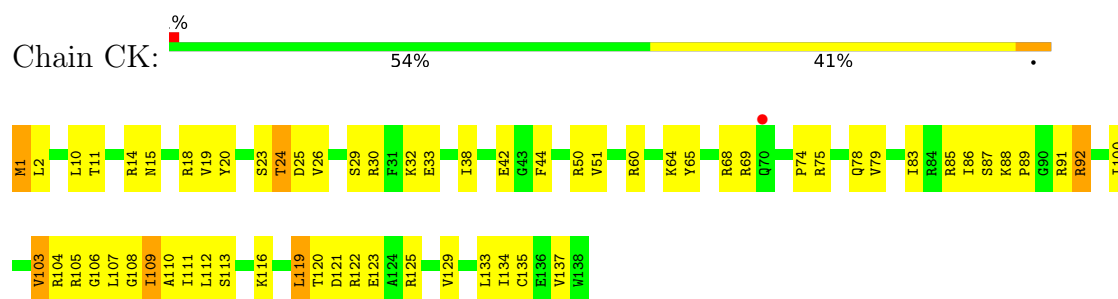
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



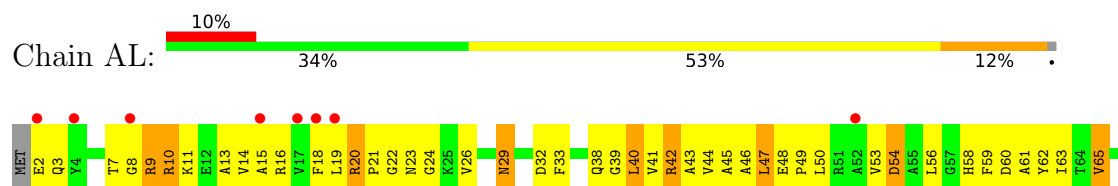
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

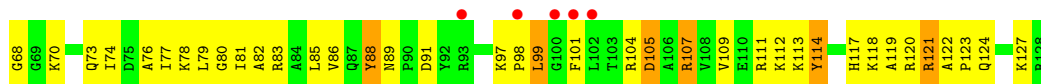


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

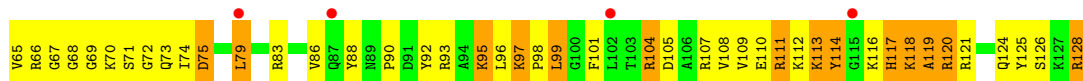


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

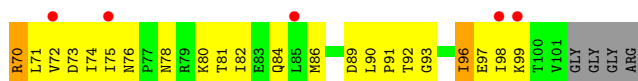
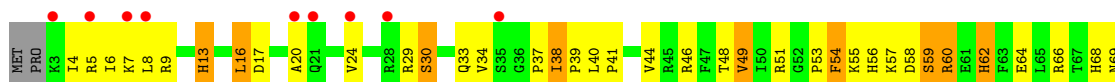




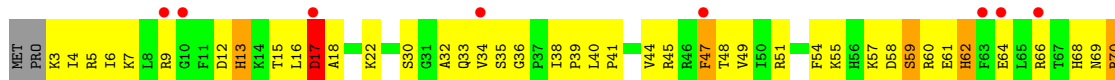
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



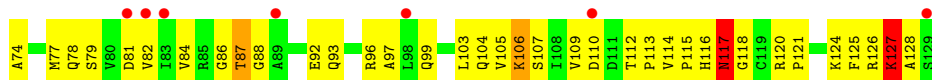
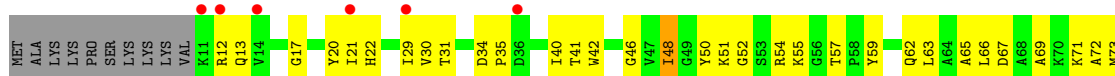
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

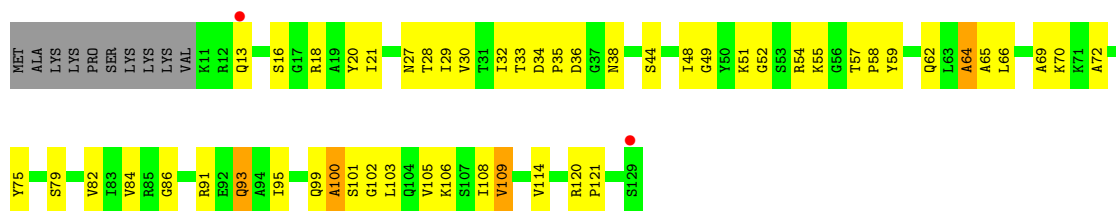


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

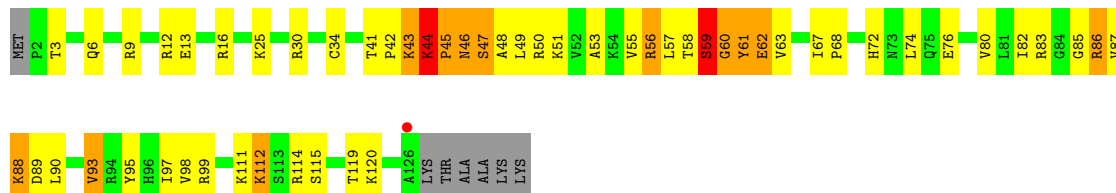


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

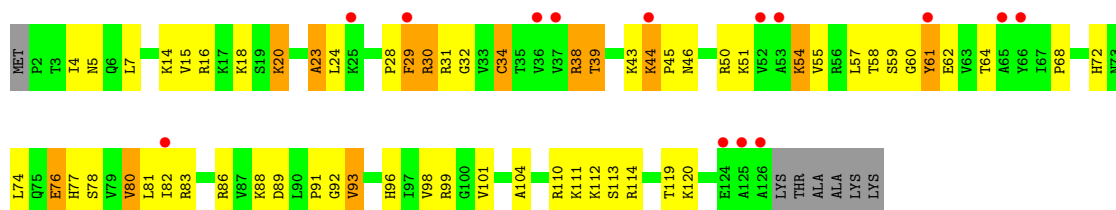




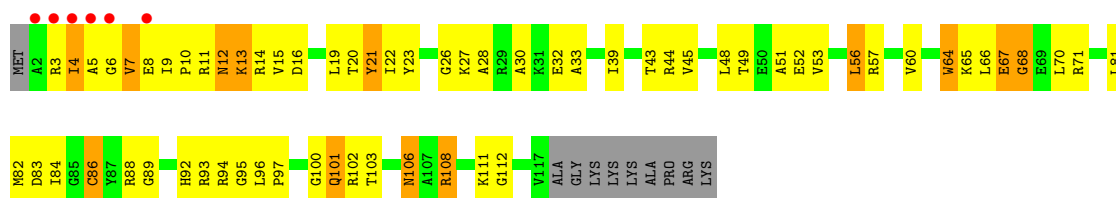
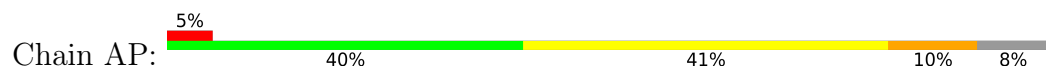
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



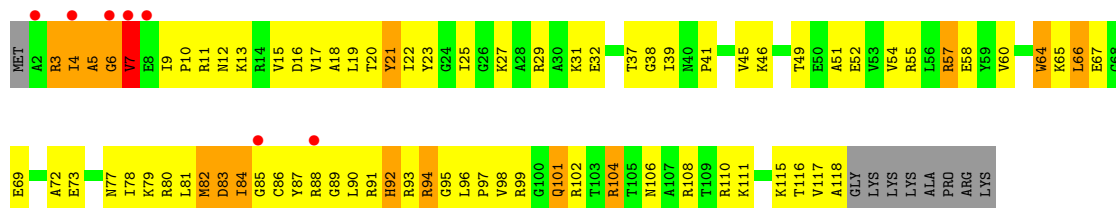
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



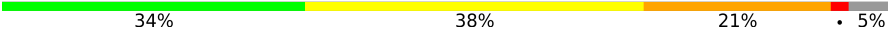
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

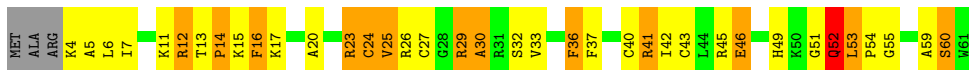


• Molecule 13: 30S RIBOSOMAL PROTEIN S13



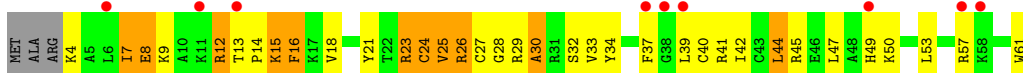
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:  34% 38% 21% 5%



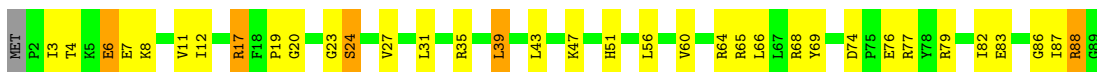
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:  15% 38% 39% 18% 5%



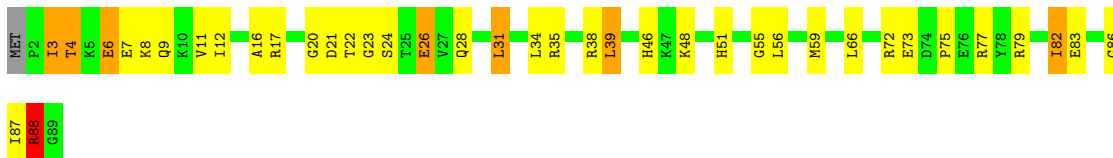
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:  60% 34% 6%



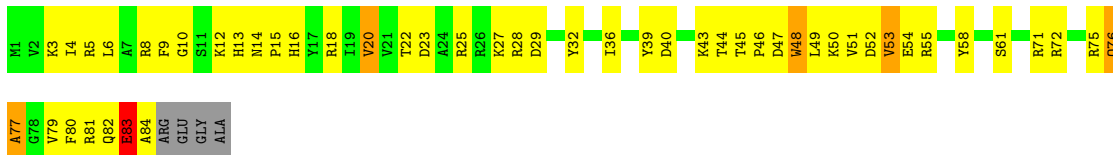
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:  55% 35% 8% 2%



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:  39% 50% 6% 5%



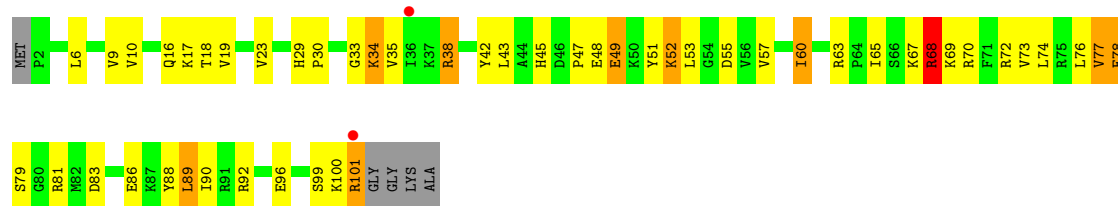
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:  2% 60% 31% 5% 5%

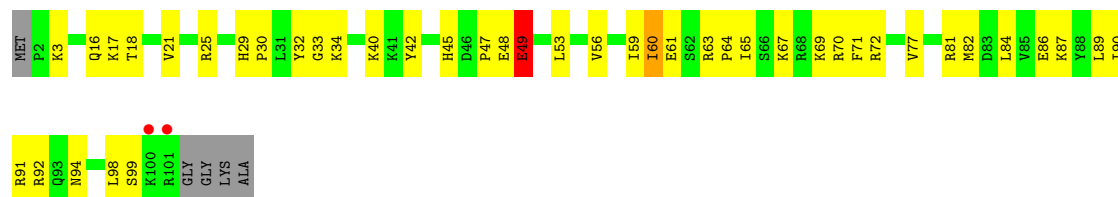


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

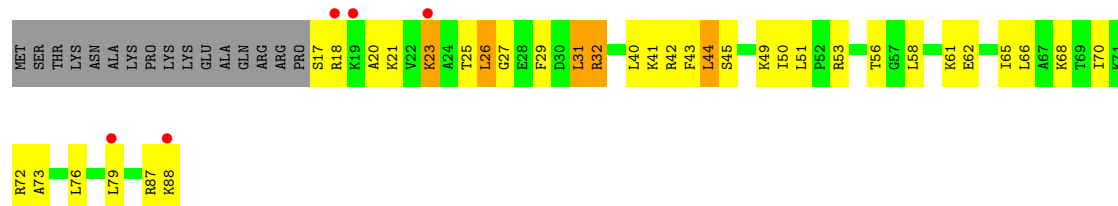
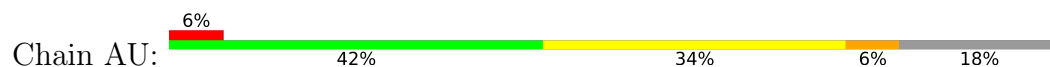
Chain AT:  2% 48% 38% 9% 5%



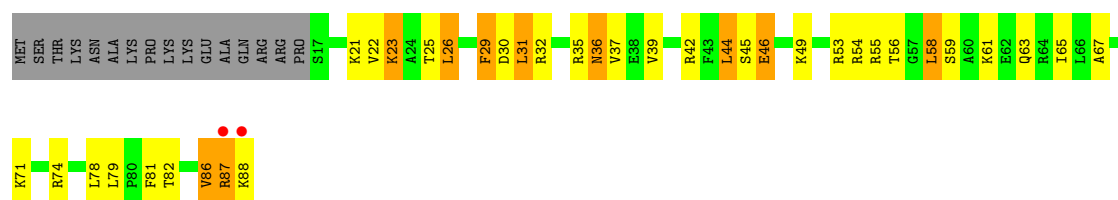
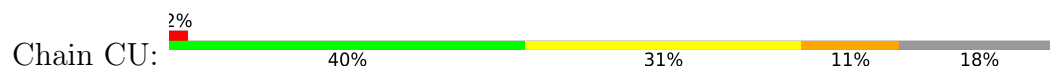
● Molecule 17: 30S RIBOSOMAL PROTEIN S17



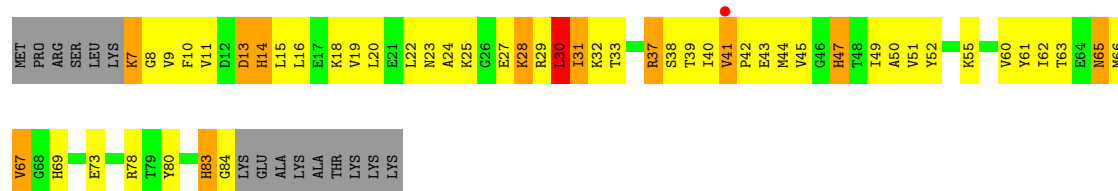
● Molecule 18: 30S RIBOSOMAL PROTEIN S18



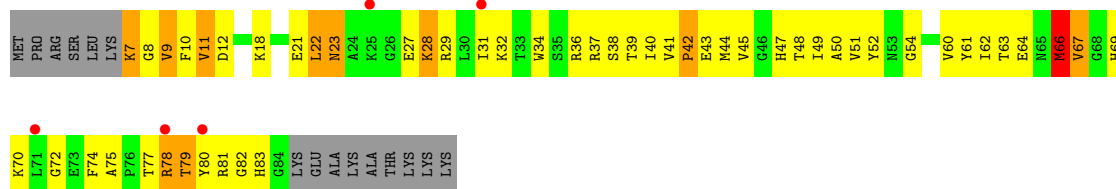
● Molecule 18: 30S RIBOSOMAL PROTEIN S18



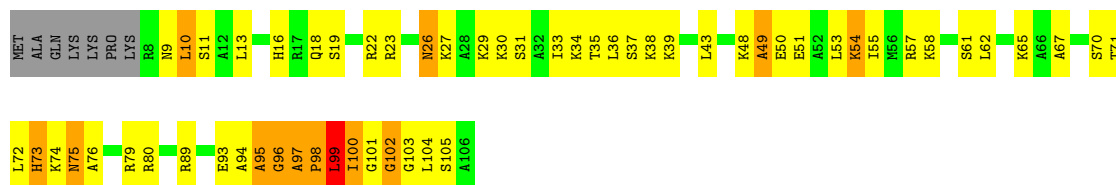
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



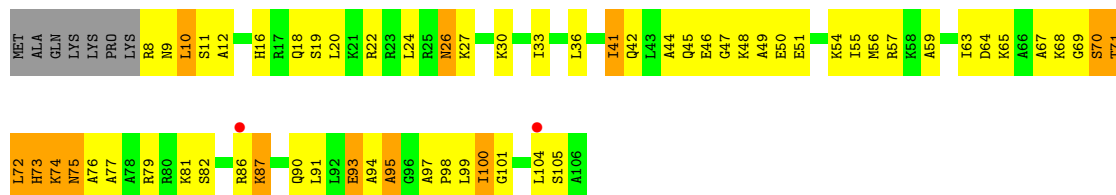
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



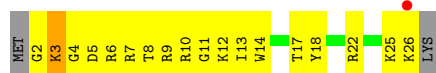
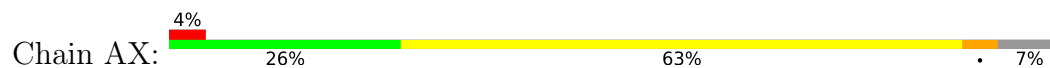
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



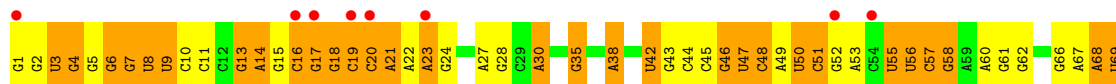
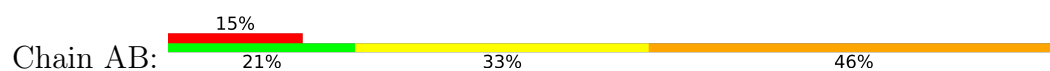
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

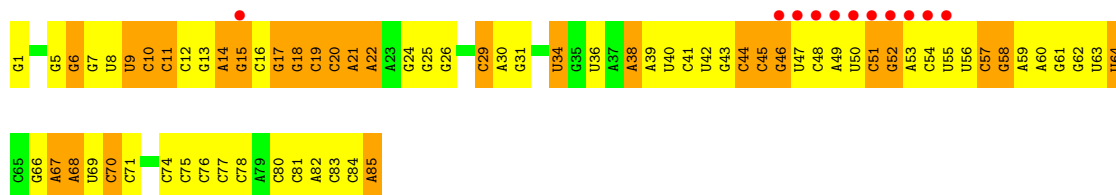
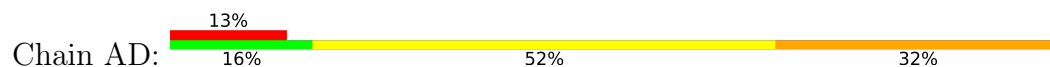


• Molecule 22: TRNA-TYR

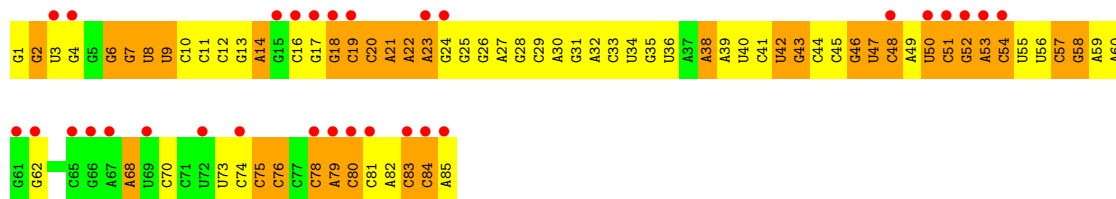
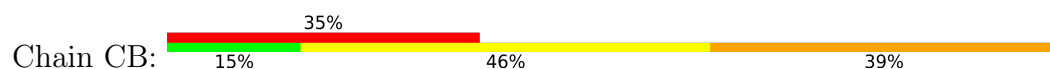




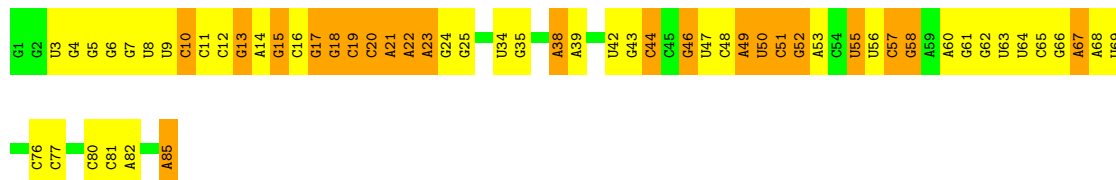
- Molecule 22: TRNA-TYR



- Molecule 22: TRNA-TYR



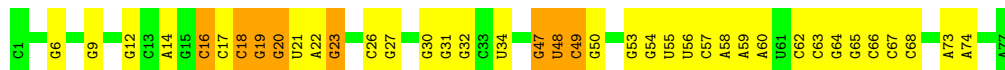
- Molecule 22: TRNA-TYR



- Molecule 23: TRNA-FMET



- Molecule 23: TRNA-FMET



- Molecule 24: MRNA

Chain A1: 



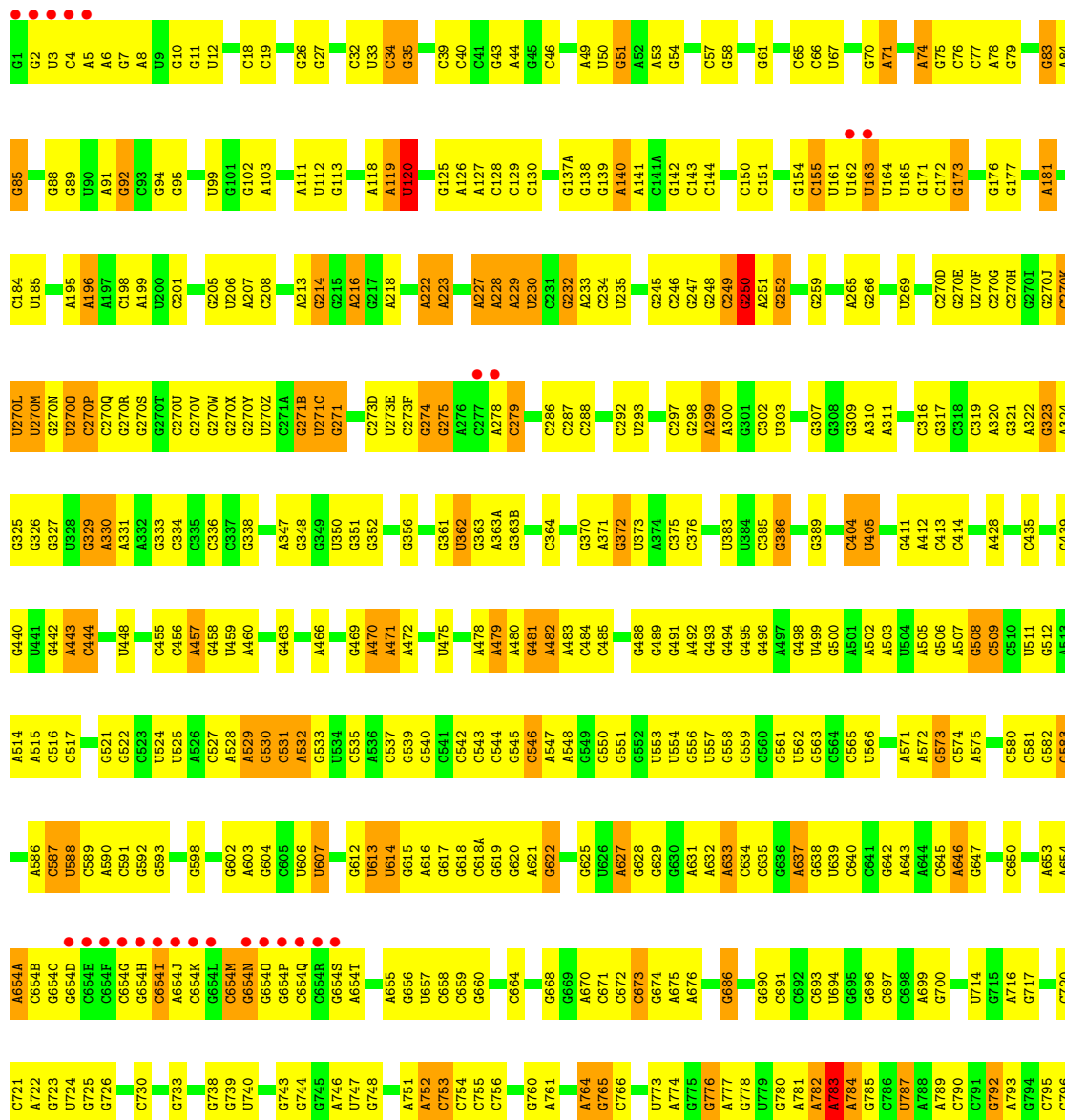
• Molecule 24: MRNA

Chain C1: 

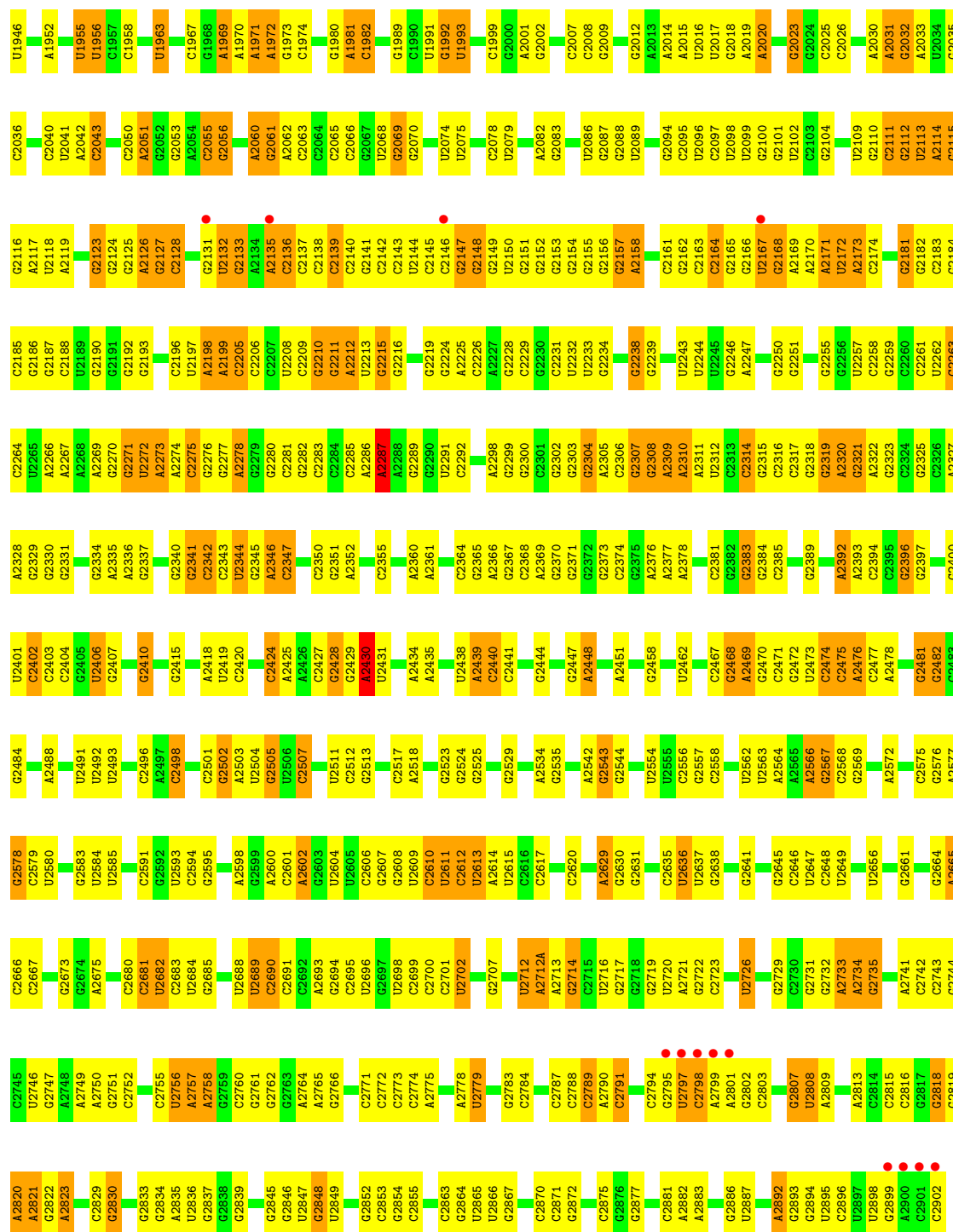


• Molecule 25: RNA (2912-MER)

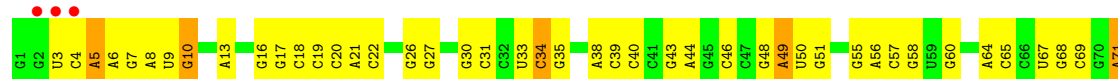
Chain BA: 



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A1847	G1769	C1658	A1567	A1495	A1412	A1331	C1251	A1174	C1100	U1033	A957	C879	A802
A1854	G1770	C1661	A1568	A1496	G1413	G1332	G1252	G1175	U1101	G1034	U958	C880	G805
A1858	G1771	C1662	A1569	U1497	G1416	U1340	A1253	A1177	C1102	G1042	A959	C882	C806
G1858	G1772	A1571	A1570	C1498	G1417	U1341	G1256	C1179	C1103	C1043	C961	C884	U807
U1864	A1776	A1668	C1575	G1500	G1418	G1348	C1261	C1180	U1105	G1044	C885	C886	U811
C1869	U1777	A1669	U1576	C1505	A1419	A1349	A1262	C1185	G1106	A1045	C887	C888	C812
C1870	U1778	C1577	C1578	A1506	G1421	U1352	U1263	C1186	G1107	A1046	C889	C890	C814
A1871	A1779	A1579	A1580	C1508	A1427	A1363	G1264	G1187	U1108	G1047	C891	C892	C817
A1872	A1780	A1676	A1581	C1509	C1428	A1364	A1265	U1188	C1109	A1048	C893	C894	G818
G1878	C1781	A1677	G1581	A1510	G1429	G1365	G1266	U1189	G1110	C1049	C895	C896	A819
A1884	A1782	A1678	A1582	G1512	C1430	G1366	A1269	A1189	U1111	A1050	C897	C898	A820
A1885	C1783	U1679	A1586	C1513	U1431	G1368	G1270	G1191	U1112	G1051	C899	C900	A821
C1886	A1784	G1680	A1587	U1514	A1434	A1369	A1272	G1195	C1121	A1054	C899	C901	U826
C1887	A1786	G1681	C1588	C1515	G1442	A1360	U1273	U1198	G1122	G1055	C897	C902	U827
G1888	C1790	C1686	C1589	U1516	G1443	C1363	A1278	C1201	G1125	G1056	C898	C903	U828
C1893	A1791	U1688	C1590	C1517	G1444	G1364	G1279	A1202	A1126	U1058	C899	C904	U829
C1894	G1792	C1591	G1592	G1518	A1444A	A1365	G1280	C1203	A1127	G1059	C899	C905	G830
G1899	U1793	A1690	G1593	U1520	C1445	G1368	A1284	G1204	A1128	U1060	C899	C906	G831
A1900	C1794	C1691	G1594	G1521	C1446	G1369	A1285	U1205	U1130	G1061	C899	C907	G832
A1901	G1795	U1692	G1595	G1522	G1447	C1370	A1286	G1206	G1131	G1062	C899	C908	U833
C1902	U1796	C1693	C1598	G1525	G1448	G1371	A1287	G1207	C1135	C1063	C899	C909	U834
C1903	C1797	C1694	C1599	G1526	A1449	G1372	U1288	C1208	U1136	U1065	C899	C910	U839
G1906	G1798	G1695	C1600	G1527	G1449A	A1373	C1290	C1209	G1137	U1066	C899	C911	C844
A1913	U1799	A1698	G1601	A1528	C1451	G1374	C1291	A1210	U1138	G1067	C899	C912	C846
C1914	C1800	G1702	G1606	A1529	C1458	A1379	U1292	U1211	G1139	A1069	C899	C913	U847
U1915	A1801	G1703	C1607	G1533	G1459	G1380	C1293	A1213	C1140	U1070	C899	C914	G848
A1916	C1804	G1704	A1608	U1534	A1460	G1381	C1298	A1214	U1141	G1071	C899	C915	A849
U1917	U1805	G1705	A1609	A1535	G1461	C1382	G1299	G1215	U1142	C1072	C899	C916	C850
A1918	A1810	U1706	A1610	C1537	C1464	A1384	A1301	C1218	A1143	G1073	C899	C917	U851
A1919	G1811	U1709	A1614	G1538	G1465	G1385	A1302	G1219	G1144	G1074	C899	C918	G852
C1920	A1812	C1710	C1617	U1540	G1466	C1386	G1303	A1220	C1145	C1075	C899	C919	G853
C1924	G1813	U1727	A1618	G1541	C1467	G1387	G1309	C1222	C1146	U1077	C899	C920	C856
C1925	A1816	A1728	U1621	G1542	A1469	G1388	G1310	G1228	C1147	U1078	C899	C921	C857
U1926	U1817	A1729	G1622	A1543	G1470	G1389	G1311	C1231	A1148	C1079	C899	C922	U858
A1927	U1818	U1730	G1623	C1544	A1471	U1394	U1312	C1230	G1151	A1080	C899	C923	U859
A1928	A1819	G1731	A1545	A1545A	A1472	A1395	U1313	C1152	C1152	U1082	C899	C924	U860
C1929	U1820	C1732	A1546	C1546	G1473	U1396	C1314	C1153	U1083	C1013	C899	C925	A861
G1930	A1821	G1733	C1640	C1547	G1474	U1397	C1315	G1235	A1084	G1015	C899	C926	G862
U1931	G1930	G1734	A1641	C1547	G1475	U1397	U1316	G1236	A1085	G1016	C899	C927	A863
A1932	A1825	C1735	G1642	C1548	C1476	G1400	A1317	G1237	A1086	U1019	C899	C928	G864
G1933	U1826	C1741	G1642	C1549	A1477	G1401	G1318	A1237	G1087	U1020	C899	C929	C865
A1936	A1829	G1742	C1648	U1550	G1478	A1402	G1319	G1238	A1088	A1021	C899	C930	A866
A1937	C1830	C1743	G1649	C1551	G1479	U1396	C1320	C1239	G1089	G1022	C899	C931	G867
C1938	G1831	U1754	G1651	A1546A	C1483	U1397	U1316	U1241	U1090	G1023	C899	C932	U868
A1939	C1832	C1755	A1652	C1547	G1484	U1406	U1323	A1242	G1091	G1024	C899	C933	A869
U1940	U1833	G1756	G1653	C1548	A1486	C1407	G1324	A1243	C1092	G1025	C899	C934	A870
G1945	U1834	U1762	A1654	C1549	G1487	C1408	C1327	G1244	U1094	U1026	C899	C935	G873
	G1835	A1763	A1655	G1550	C1489	C1409	G1328	U1249	A1096	A1028	C899	C936	
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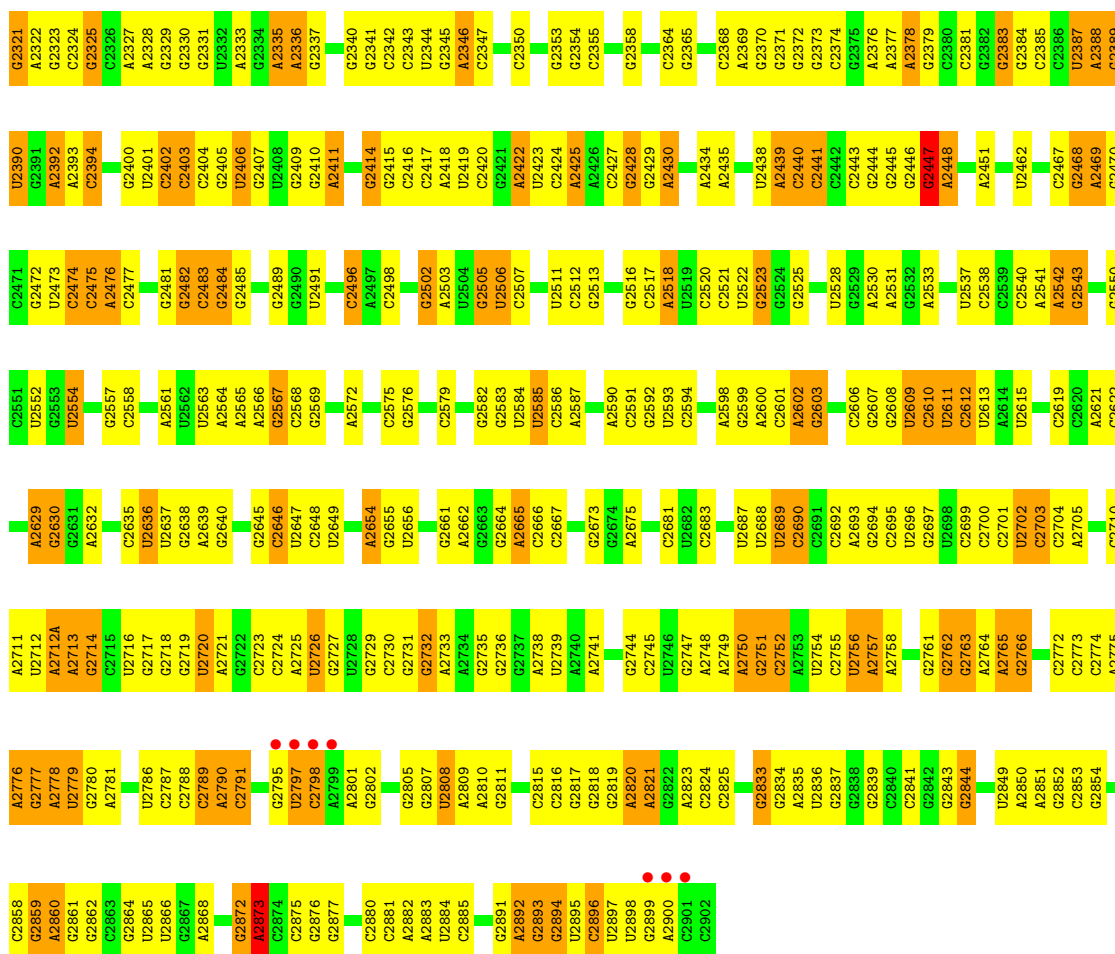


● Molecule 25: RNA (2912-MER)

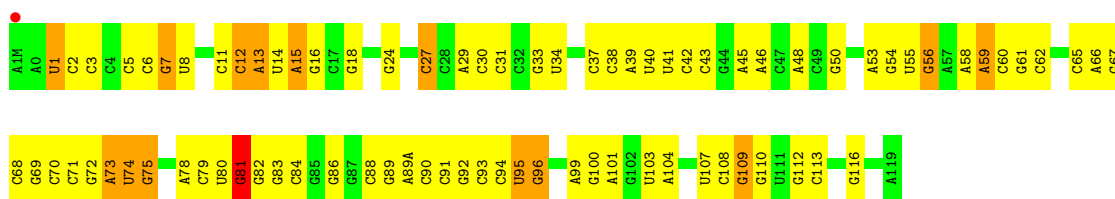


A1085	U1019	C951	C884	C817	A746	G666	G619	C537	U459	U358	A282	A241	C153	U72
A1086	A1020	G952	C885	G818	U747	U667	G620	C543	G463	G361	A283	G242	G154	A73
A1087	A1021	A953	C886	A819	G748	U668	A621	C543	G464	U362	U284	U244	C155	A74
A1088	G1022	G954	A887	A820		A668	G622		U464	U363	C285	G75	U	G75
G1089	U1023	C955	C888	A821	A751	G669	U626	A547	A465	G363	C287	G247	U	A78
U1090	G1024	G956	C889	A824	A752	G670	A627	A548	A466	A363A	C288	G248	U	G79
G1091	G1025	A957	A890	G825	G753	C671	G628	C549	G467	G363B	C289	C249	U	
U1092	U1026	U958	G892	C826	C754	C672		G550	G468	G363C	A289	G250	U	
A1093	A1027	A959	C893	U826	C755	C673	A631	U556	G469	G363D	C291	A251	G171	G83
U1094	A1028	C894	A894	U827	C756	G674	A632	U557	U363E	U363F	G290	A84	C172	A84
A1095	A1029	U961	U895	U828	C757	A675	A633	U558	A470	C364	C296	G252	G173	G85
U1096	G1030	G962	A896	G829	C758	A676	G634	G559	A478		C297		C174	
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A1098	U1035	U969	C898	G831	A761		G636	U561	A480		G299		G176	A91
U1099	G1036	C970	A899	G832	U762	G681	G637	U562	G481		G301	G259	G177	G92
C1100	G1037	C971	U900	U833	G763	G682	A637	U563	A482		C302	G260	G178	C93
U1101	U1038	G972	A901	A834	A764	G683	G638		A483		U303	A265		G94
	G1039	A973	C902	G839		G684	U639	A571		G386	G304	G266	A182	G95
C1104	C1040	G974	C903	A835	G768	A685	C640	A572	G491				C183	
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	U1042	G975	U905	C838	U773	G690	G642	A574	A493		G308	A270A	U185	U99
C1109	C1043	G976	G906	U839	A774		A643	C574	A390		G309	A270B	G101	G101
G1110	G1044	C977	U907	C844	G775	G699	A644	A575	G494		A310		G102	G102
A1111	A1045	G978	C908	G845	G776	A699	C645	U576	G495		A311		A103	A103
G1112	U1046	G979	A909	G846		G700	A646	G577	U499		A312	U270F	U104	U104
U1113	G1047	A980	A910	U847	U779	G701	G647		G500		G312	C270G	C105	C105
	C1048	A981	A911	G848	G780	G702		C580	A501			C270H	A197	C106
C1116	U1049	C982	C912	A849	A781	U703	C650	C581	A502		G315	G270I	C198	C107
G1117	A1050	A983	U913	C850	A782	G704	G651	U582	A503		C316	G270J	A199	U108
C1118	G1051	G984	C914	U851	A783	A705	C652	C583	U504		A320	C270K	U200	
G1119	C985	C985	C915	G854	A784	G706	A653		A505		G325	G270L	C201	A111
U1120	G986	G986	G916	G855	G785	G707	A654	U588	G506		G326	G270M		U112
C1121	G987	A987	A917	C856	G786	G708	A654A	C589	A507		A322	U270N	A204	
G1122	U988	A988	A918	U857	A787	U709	C654B	G592	G508		G323	U270O	C116	C116
	A1057	G989	G919	C857	A788	G710	G654C	G593	A514		G324	C270P	G117	G117
G1125	U1058	A990	G920	U858	A789	G711	G654D		C509		G325	G270Q	A118	A118
A1126	G1059	C991	G921	G859	C790	G715	C654E	G596	C510		G327	G270R	A119	A119
U1127	U1060	C992		U860	C791	A716	C654F	U597	G512		G328	G270S	U120	U120
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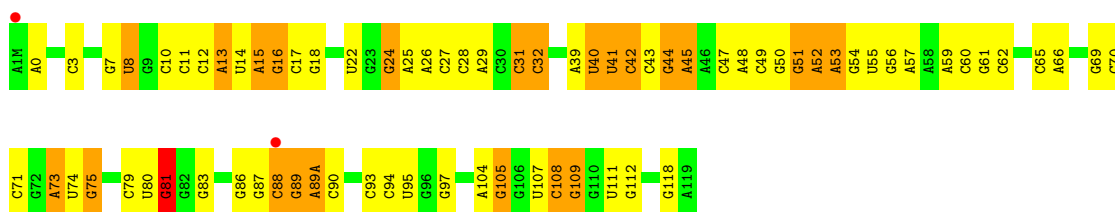
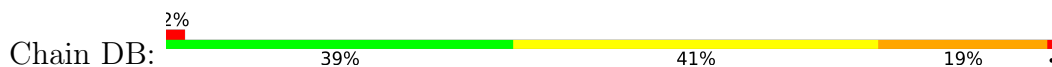
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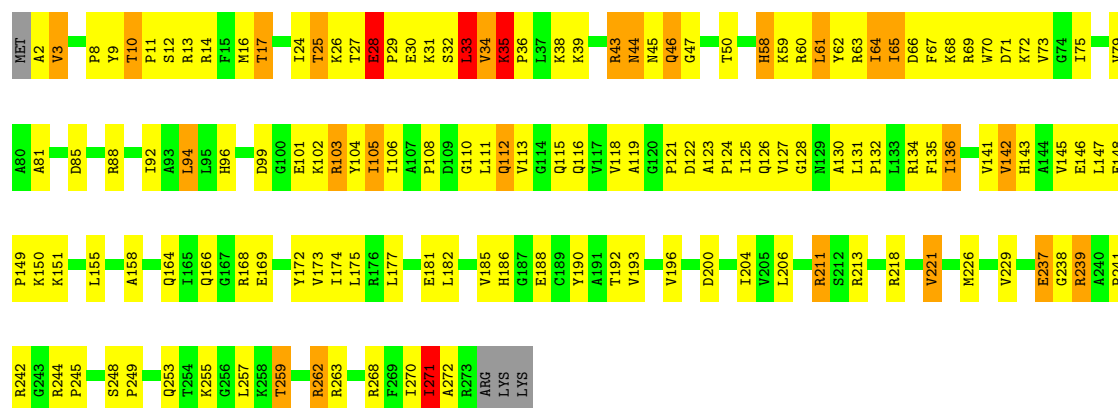


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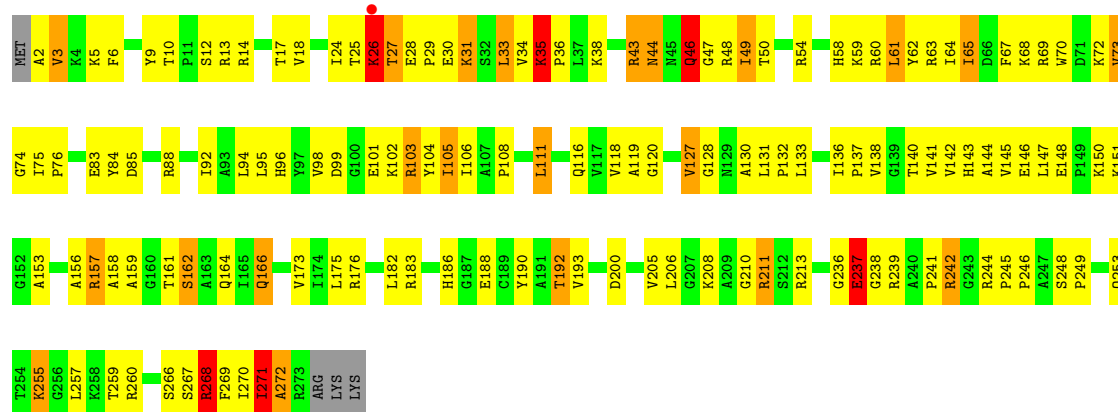
• Molecule 27: 50S ribosomal protein L2

Chain BD: 



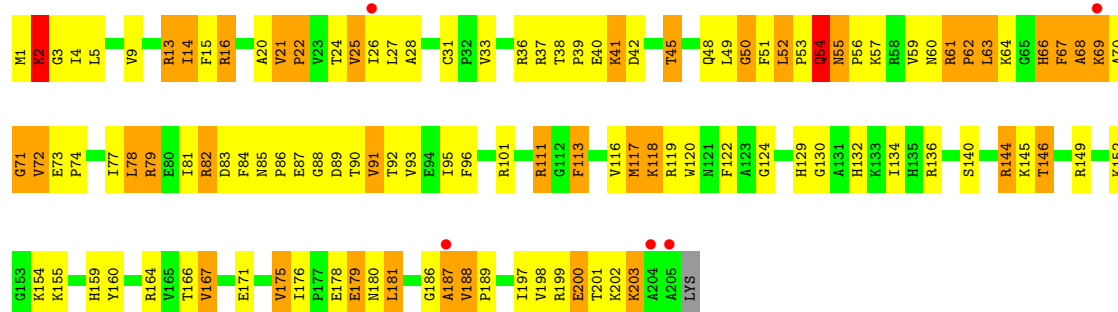
• Molecule 27: 50S ribosomal protein L2

Chain DD: 



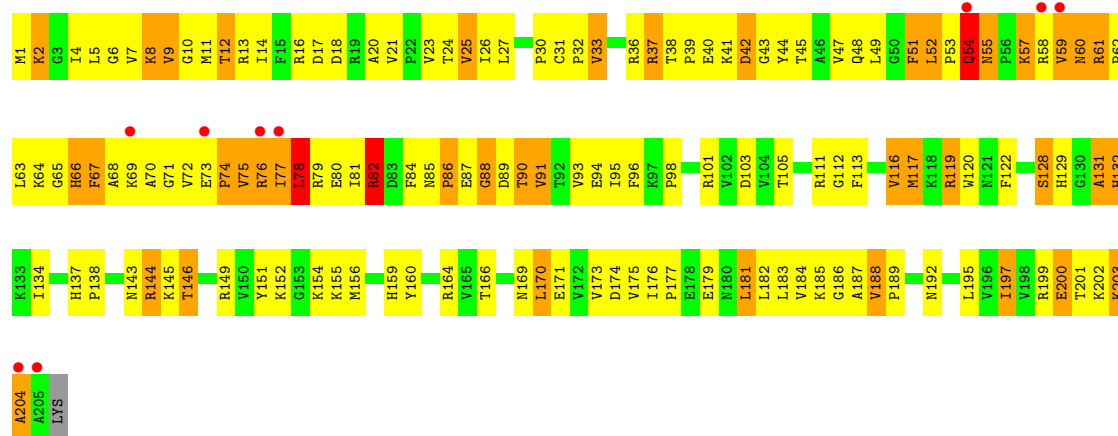
• Molecule 28: 50S ribosomal protein L3

Chain BE: 

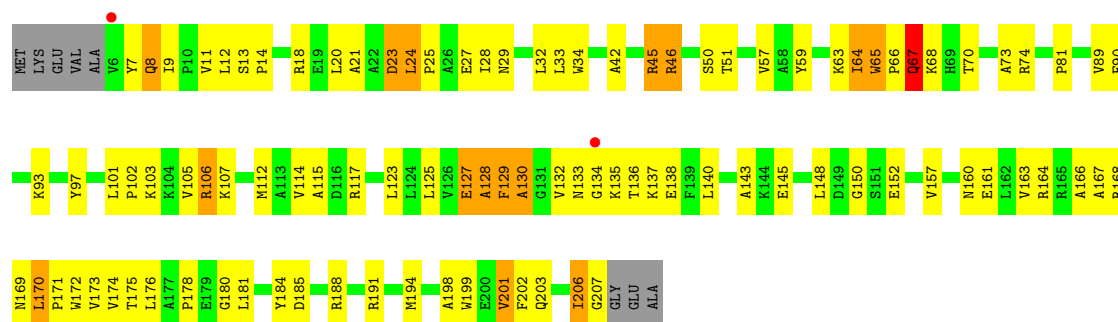


• Molecule 28: 50S ribosomal protein L3

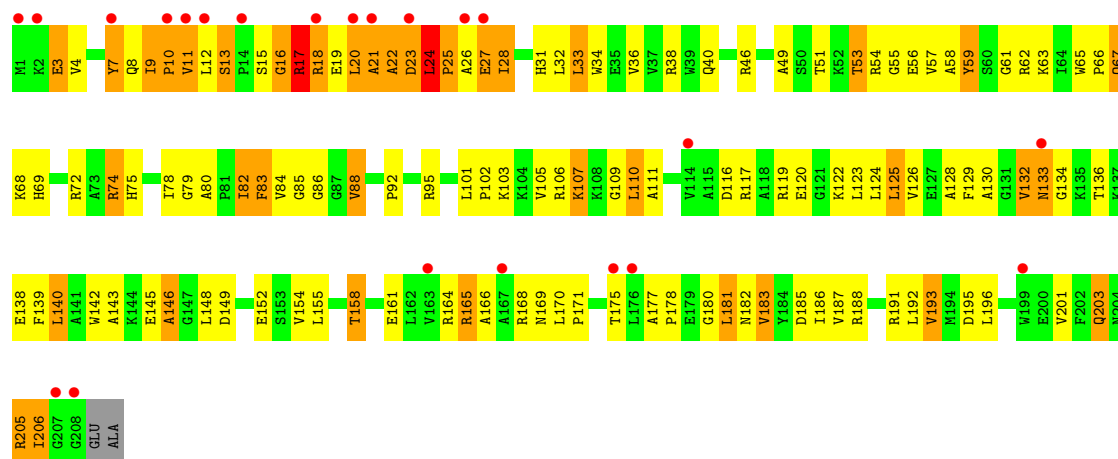
Chain DE: 



• Molecule 29: 50S ribosomal protein L4

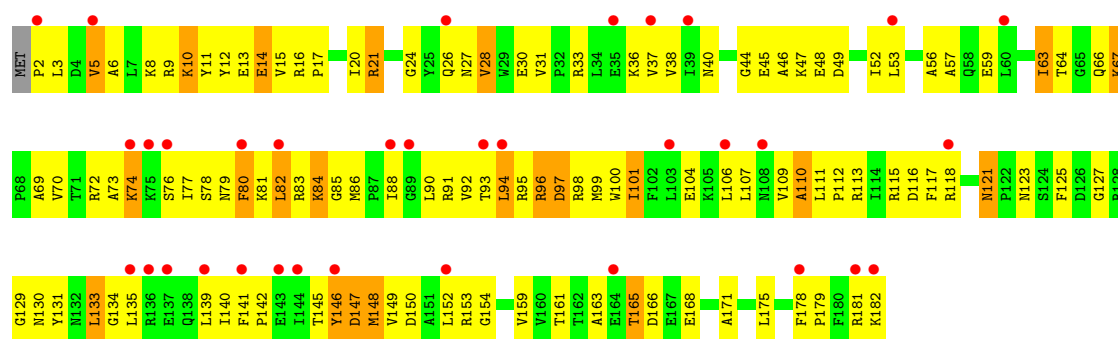


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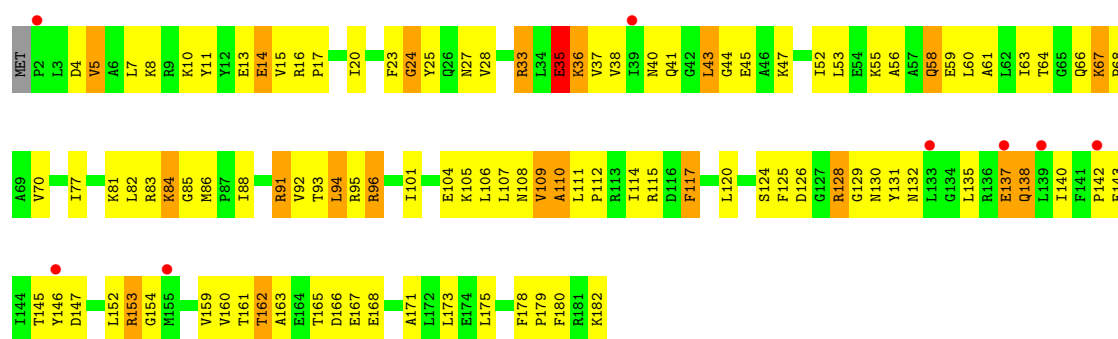
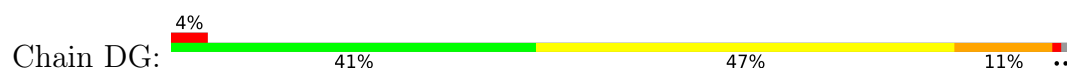


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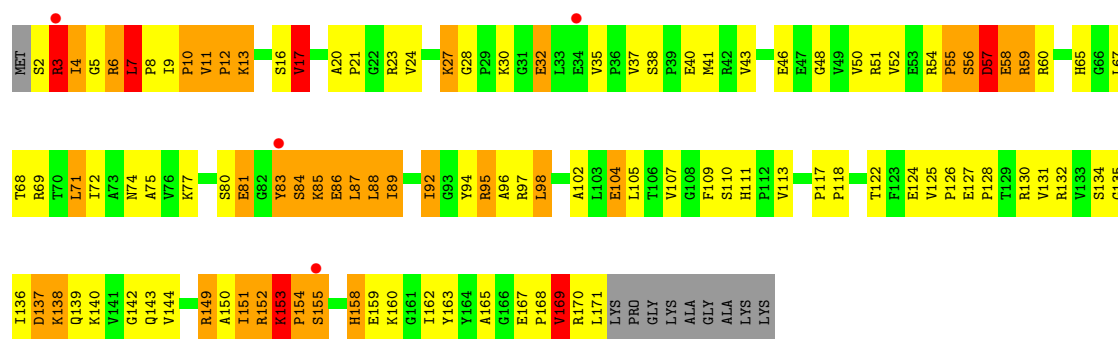




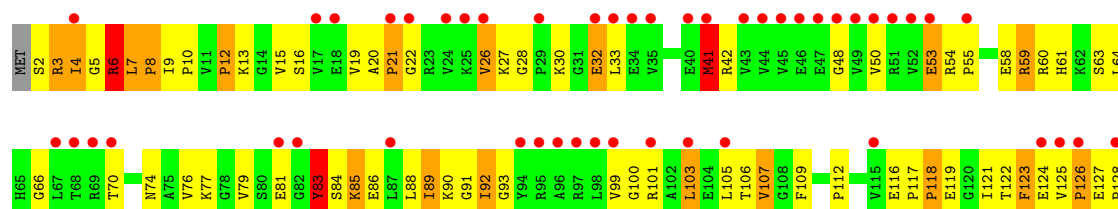
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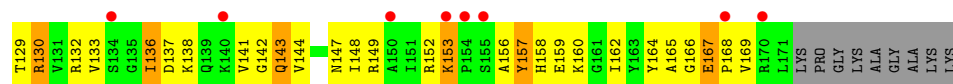


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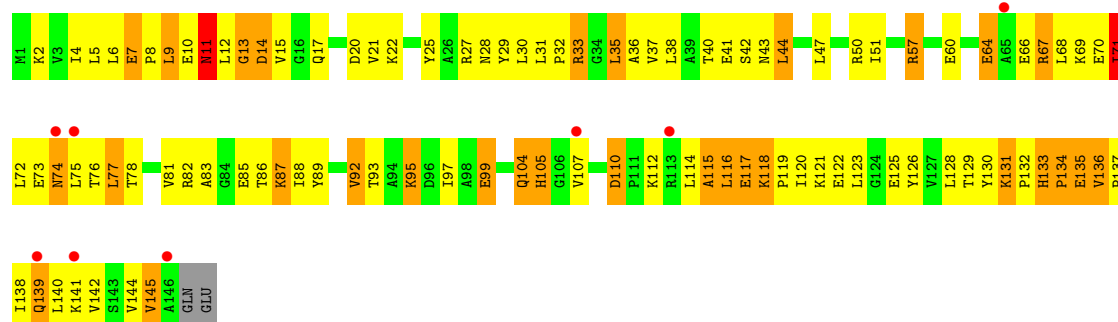


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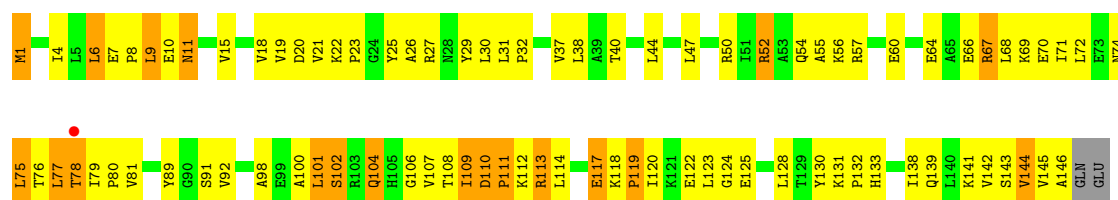




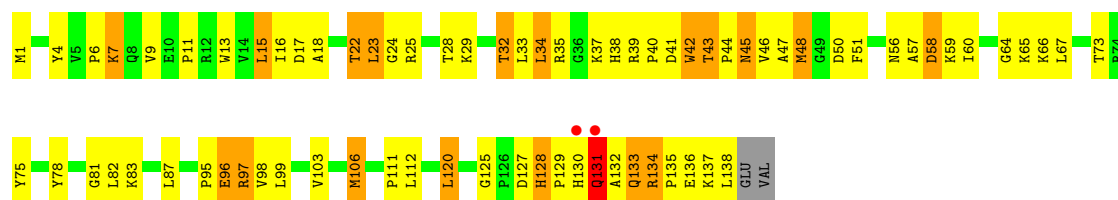
• Molecule 32: 50S ribosomal protein L9



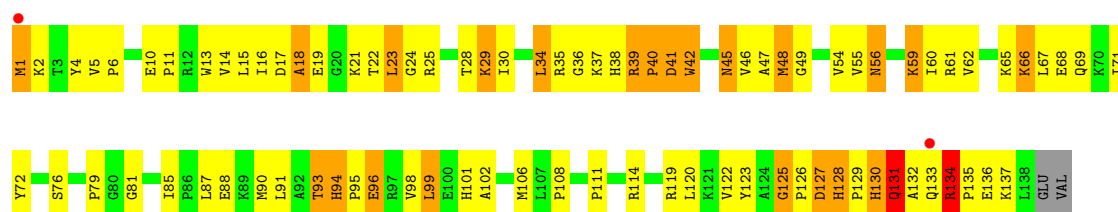
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13

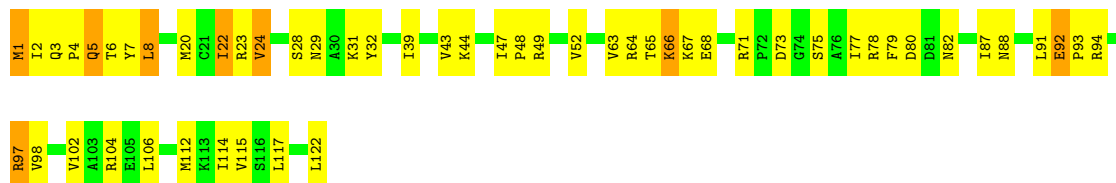


• Molecule 33: 50S ribosomal protein L13



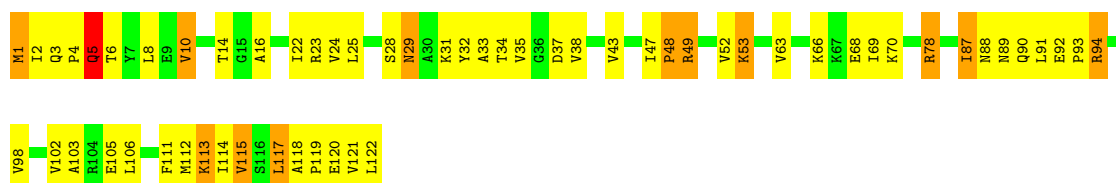
- Molecule 34: 50S ribosomal protein L14

Chain BN:  57% 37% 7%



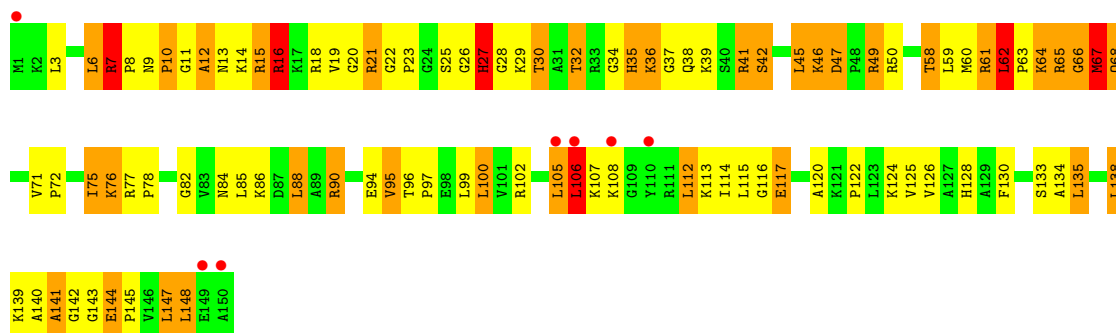
- Molecule 34: 50S ribosomal protein L14

Chain DN:  52% 38% 10%



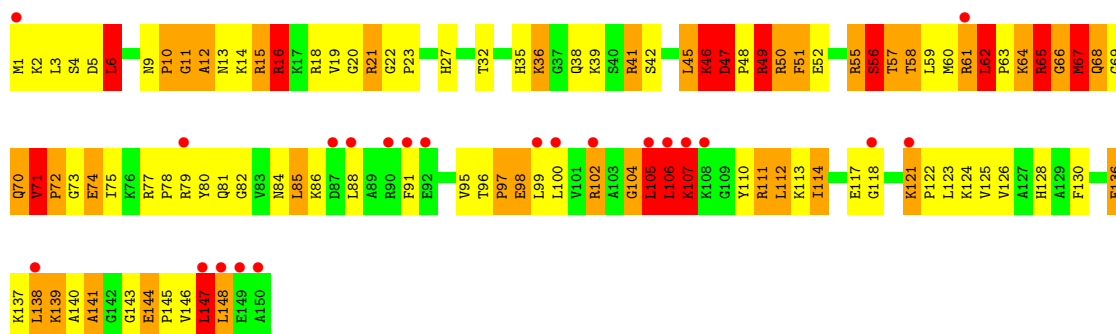
- Molecule 35: 50S ribosomal protein L15

Chain BO:  5% 35% 37% 24%

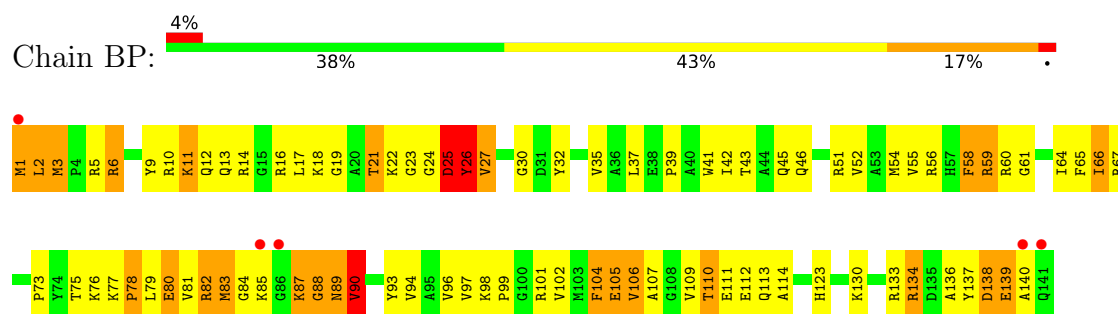


- Molecule 35: 50S ribosomal protein L15

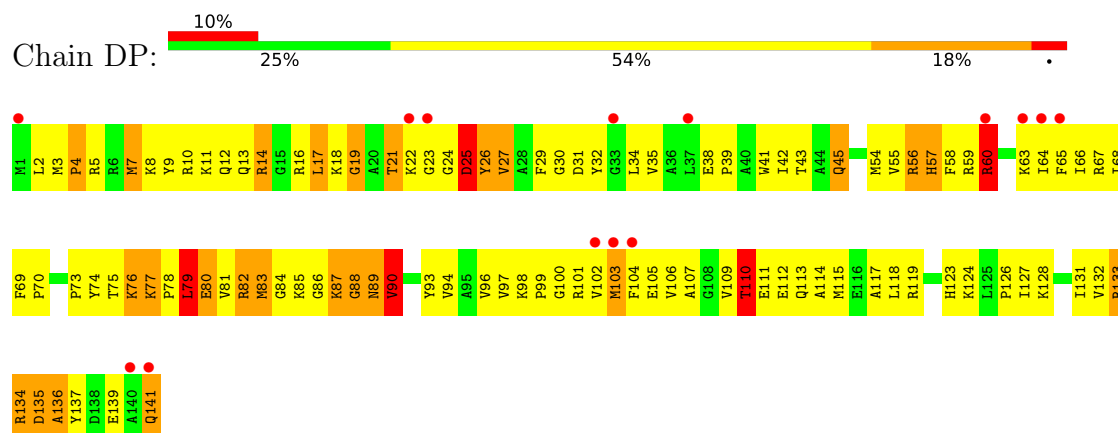
Chain DO:  15% 29% 38% 23% 9%



- Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17

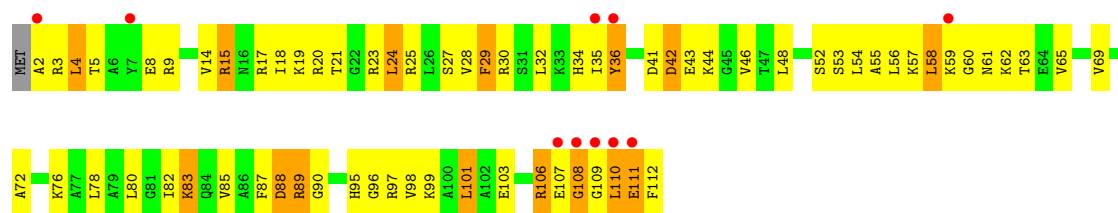


• Molecule 37: 50S ribosomal protein L17

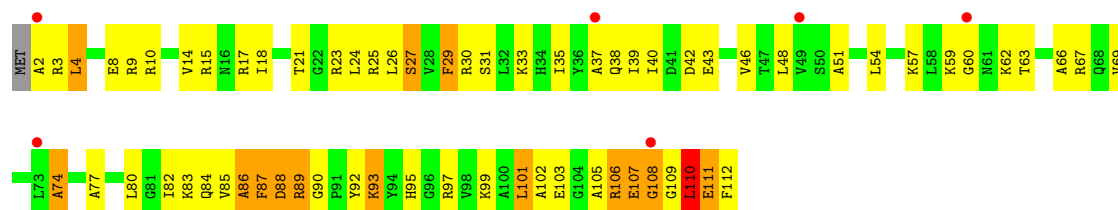


• Molecule 38: 50S ribosomal protein L18

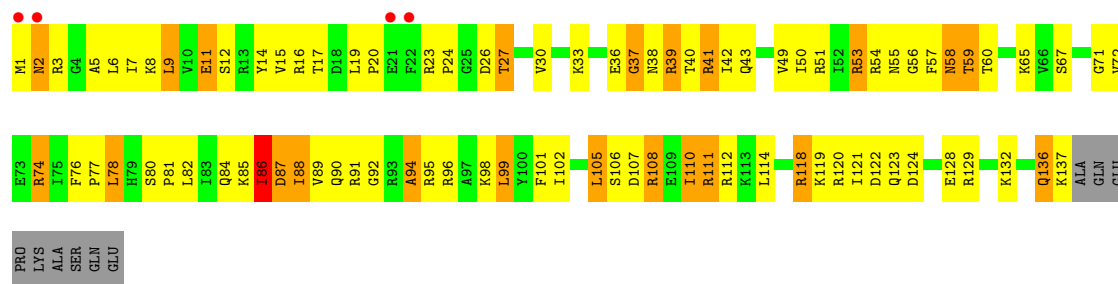




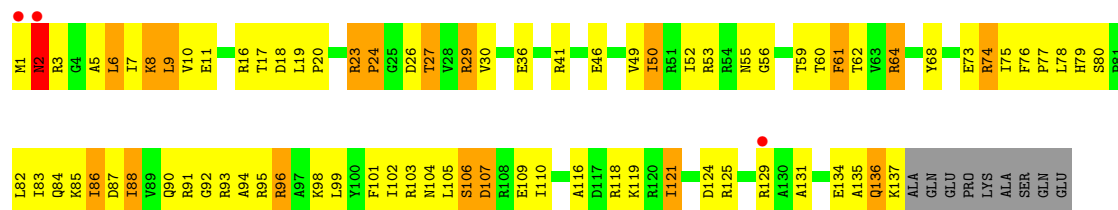
• Molecule 38: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L19

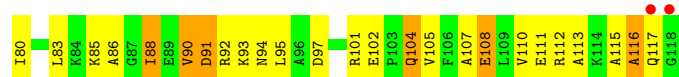


• Molecule 39: 50S ribosomal protein L19

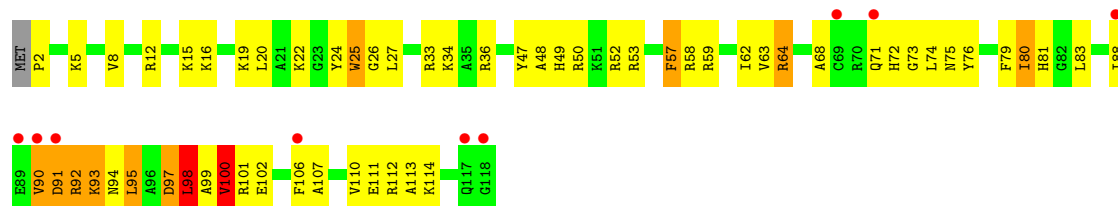


• Molecule 40: 50S ribosomal protein L20

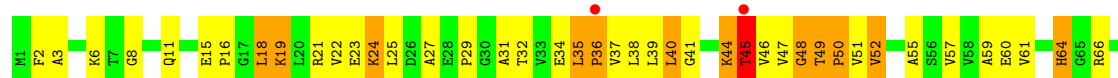




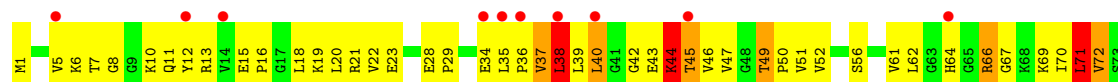
- Molecule 40: 50S ribosomal protein L20



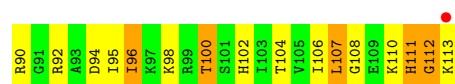
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

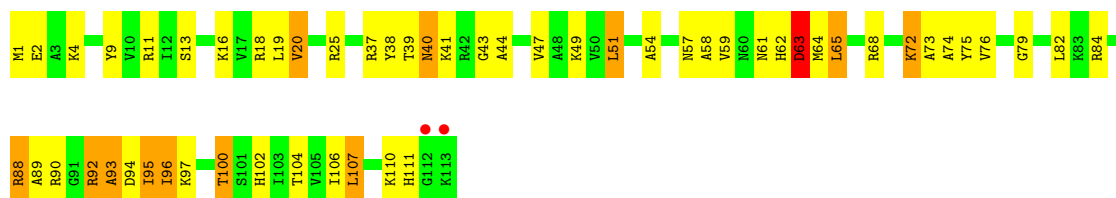


- Molecule 42: 50S ribosomal protein L22

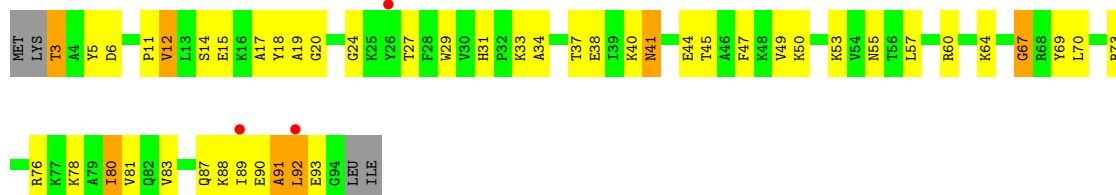


- Molecule 42: 50S ribosomal protein L22

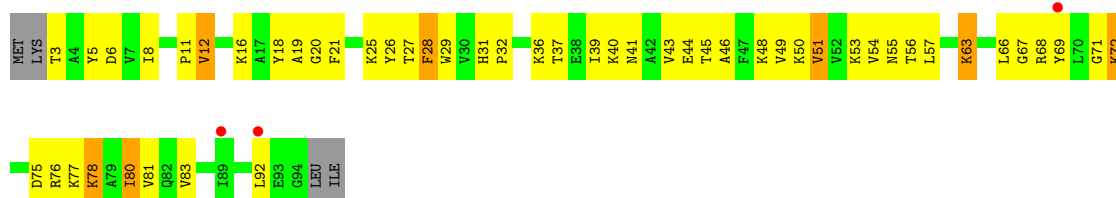
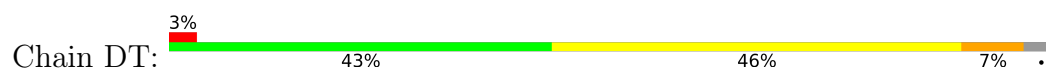




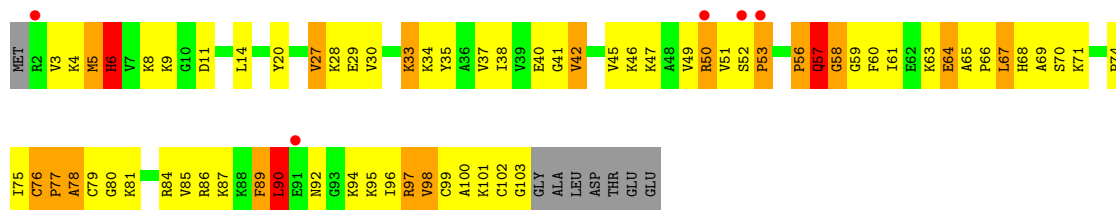
• Molecule 43: 50S ribosomal protein L23



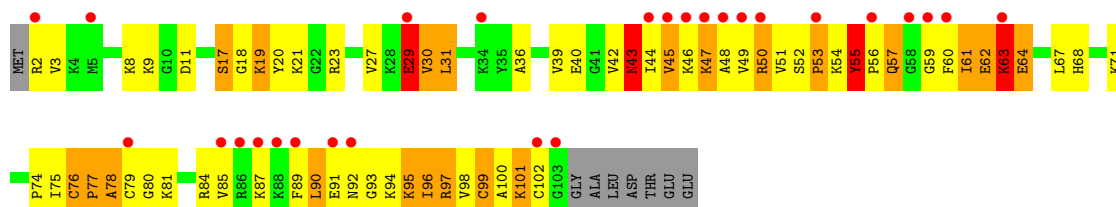
• Molecule 43: 50S ribosomal protein L23



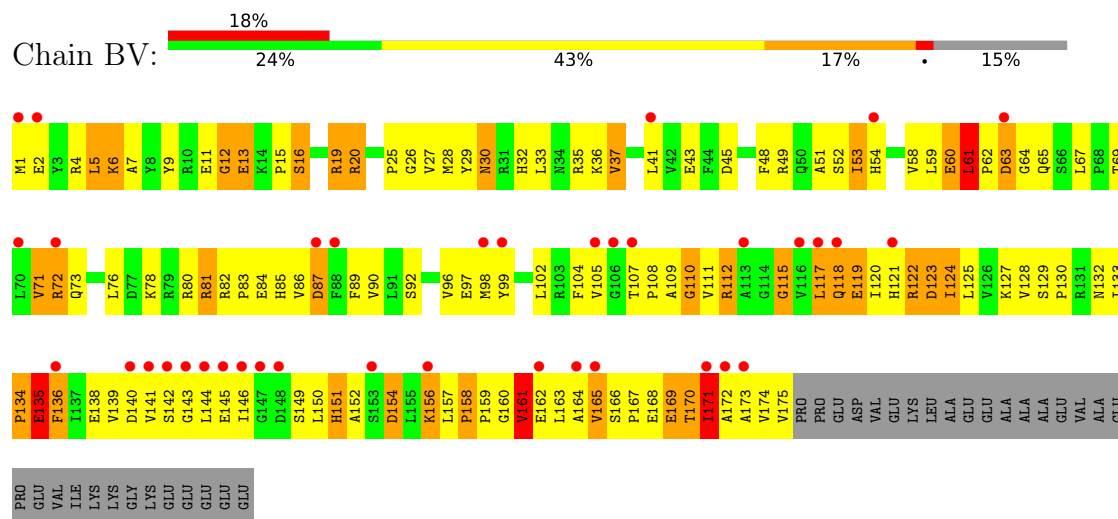
• Molecule 44: 50S ribosomal protein L24



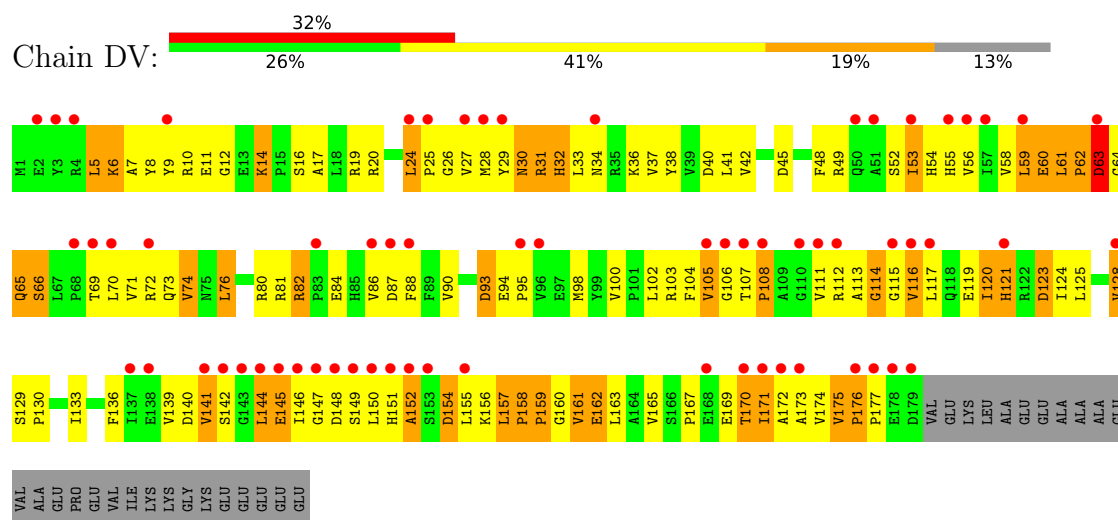
• Molecule 44: 50S ribosomal protein L24



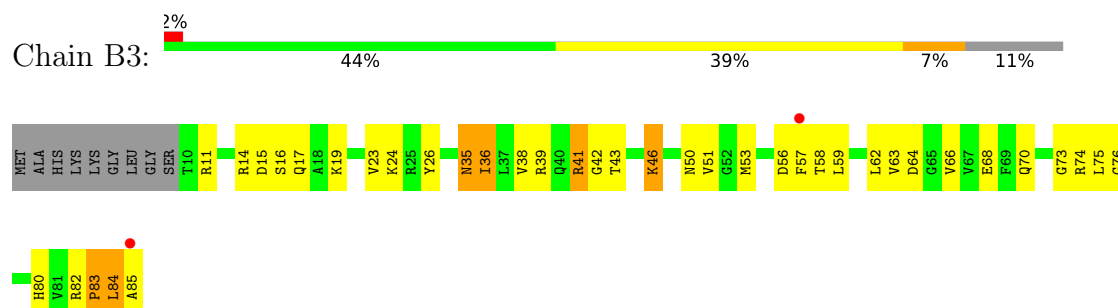
- Molecule 45: 50S ribosomal protein L25



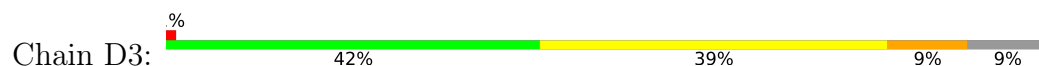
- Molecule 45: 50S ribosomal protein L25

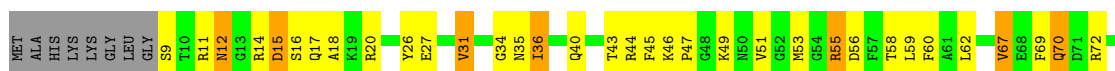


- Molecule 46: 50S ribosomal protein L27

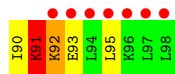
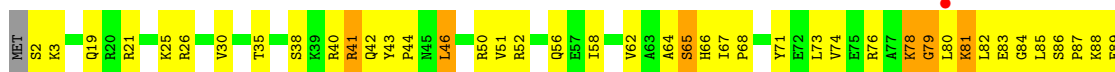


- Molecule 46: 50S ribosomal protein L27

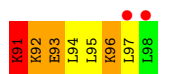
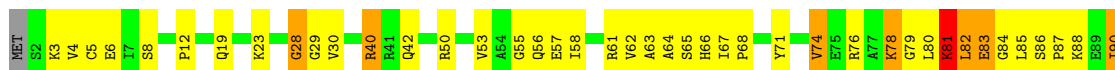




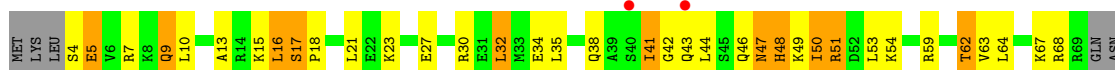
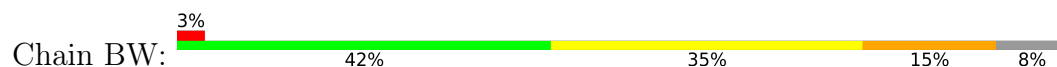
- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

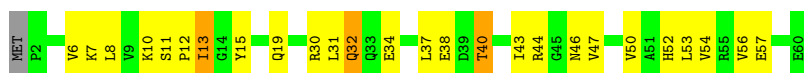


- Molecule 48: 50S ribosomal protein L29

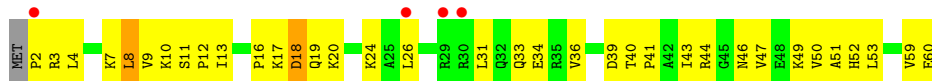


- Molecule 49: 50S ribosomal protein L30

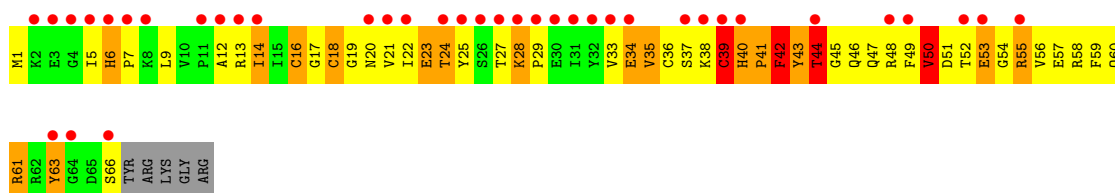
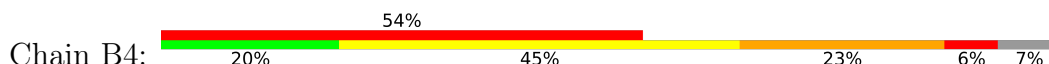




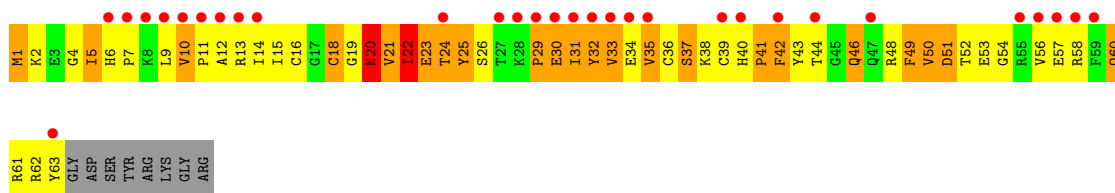
- Molecule 49: 50S ribosomal protein L30



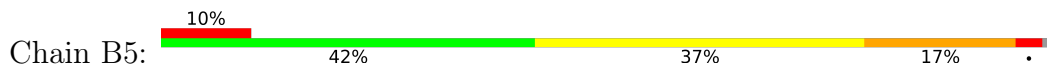
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



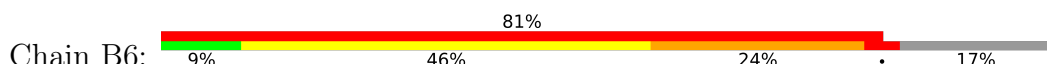
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32

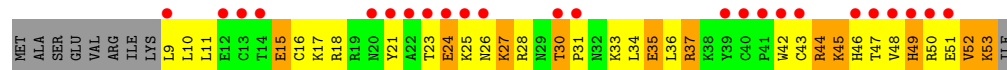
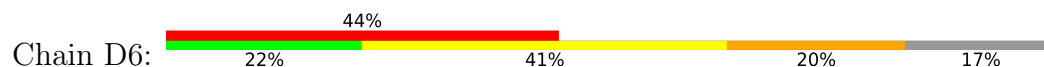


- Molecule 52: 50S ribosomal protein L33

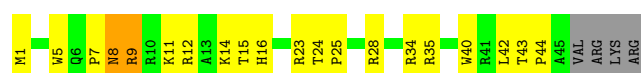




- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



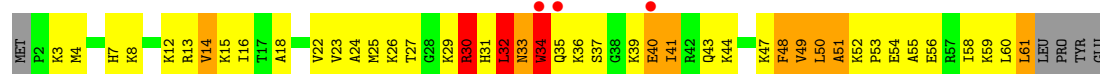
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.67Å 451.75Å 625.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.06 – 3.00 257.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.06-3.00) 93.5 (257.02-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, R_{free}	0.203 , 0.235 0.204 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299676	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, MG, MIA

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	0.28	0/36139	0.67	20/56406 (0.0%)
1	CA	0.28	0/36142	0.66	20/56410 (0.0%)
2	AE	0.22	0/1959	0.42	0/2642
2	CE	0.22	0/1959	0.42	0/2642
3	AF	0.22	0/1629	0.42	0/2195
3	CF	0.21	0/1636	0.40	0/2205
4	AG	0.29	1/1733 (0.1%)	0.44	0/2318
4	CG	0.27	0/1733	0.47	0/2318
5	AH	0.24	0/1171	0.44	0/1576
5	CH	0.24	0/1171	0.44	0/1576
6	AI	0.24	0/856	0.42	0/1154
6	CI	0.24	0/856	0.42	0/1154
7	AJ	0.22	0/1276	0.40	0/1709
7	CJ	0.22	0/1276	0.38	0/1709
8	AK	0.23	0/1136	0.44	0/1527
8	CK	0.22	0/1136	0.42	0/1527
9	AL	0.23	0/1029	0.41	0/1379
9	CL	0.22	0/1029	0.42	0/1379
10	AM	0.22	0/814	0.42	0/1095
10	CM	0.21	0/814	0.43	0/1095
11	AN	0.24	0/900	0.44	0/1213
11	CN	0.24	0/900	0.43	0/1213
12	AO	0.26	0/991	0.49	0/1327
12	CO	0.25	0/991	0.49	0/1327
13	AP	0.22	0/938	0.45	0/1258
13	CP	0.20	0/943	0.41	0/1265
14	AQ	0.27	0/485	0.47	0/643
14	CQ	0.23	0/485	0.43	0/643
15	AR	0.24	0/745	0.43	0/992
15	CR	0.23	0/745	0.39	0/992
16	AS	0.22	0/721	0.44	0/970
16	CS	0.23	0/721	0.42	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/847	0.43	0/1131
17	CT	0.24	0/847	0.42	0/1131
18	AU	0.25	0/596	0.45	0/790
18	CU	0.24	0/596	0.44	0/790
19	AV	0.23	0/638	0.45	0/860
19	CV	0.22	0/638	0.43	0/860
20	AW	0.22	0/765	0.42	0/1007
20	CW	0.23	0/765	0.45	0/1007
21	AX	0.22	0/221	0.41	0/288
21	CX	0.21	0/221	0.40	0/288
22	AB	0.28	0/1992	0.60	0/3099
22	AD	0.21	0/1992	0.50	0/3099
22	CB	0.26	0/1992	0.57	0/3099
22	CD	0.20	0/1992	0.49	0/3099
23	AC	0.25	0/1835	0.59	1/2859 (0.0%)
23	CC	0.24	0/1835	0.57	0/2859
24	A1	0.33	0/389	0.64	0/604
24	C1	0.38	0/389	0.65	0/604
25	BA	0.37	0/70233	0.75	52/109643 (0.0%)
25	DA	0.33	1/70122 (0.0%)	0.70	54/109469 (0.0%)
26	BB	0.33	0/2928	0.80	11/4568 (0.2%)
26	DB	0.29	0/2928	0.74	4/4568 (0.1%)
27	BD	0.32	0/2165	0.58	1/2919 (0.0%)
27	DD	0.29	0/2165	0.52	0/2919
28	BE	0.29	0/1601	0.55	0/2160
28	DE	0.27	0/1601	0.52	0/2160
29	BF	0.28	0/1620	0.50	0/2194
29	DF	0.26	0/1662	0.52	0/2249
30	BG	0.24	0/1499	0.43	0/2016
30	DG	0.21	0/1499	0.42	0/2016
31	BH	0.25	0/1332	0.50	0/1802
31	DH	0.21	0/1332	0.44	0/1802
32	BK	0.24	0/1151	0.49	0/1558
32	DK	0.23	0/1151	0.51	0/1558
33	BM	0.26	0/1131	0.49	0/1525
33	DM	0.23	0/1131	0.44	0/1525
34	BN	0.27	0/943	0.46	0/1269
34	DN	0.26	0/943	0.46	0/1269
35	BO	0.28	0/1162	0.58	0/1544
35	DO	0.24	0/1162	0.45	0/1544
36	BP	0.27	0/1143	0.46	0/1527
36	DP	0.24	0/1143	0.41	0/1527
37	B0	0.26	0/982	0.48	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	D0	0.25	0/974	0.45	0/1302
38	BQ	0.26	0/892	0.50	0/1187
38	DQ	0.23	0/892	0.46	0/1187
39	BR	0.28	0/1155	0.49	0/1542
39	DR	0.25	0/1155	0.44	0/1542
40	B1	0.28	0/982	0.49	0/1306
40	D1	0.24	0/982	0.44	0/1306
41	B2	0.26	0/790	0.48	0/1057
41	D2	0.27	0/790	0.51	0/1057
42	BS	0.27	0/911	0.47	0/1220
42	DS	0.26	0/911	0.44	0/1220
43	BT	0.31	0/739	0.49	0/993
43	DT	0.28	0/739	0.46	0/993
44	BU	0.29	0/798	0.52	0/1064
44	DU	0.26	0/798	0.48	0/1064
45	BV	0.23	0/1427	0.48	1/1935 (0.1%)
45	DV	0.22	0/1460	0.43	0/1982
46	B3	0.28	0/615	0.46	0/819
46	D3	0.26	0/621	0.44	0/827
47	BZ	0.27	0/770	0.50	0/1022
47	DZ	0.26	0/770	0.50	0/1022
48	BW	0.28	0/560	0.52	0/741
48	DW	0.25	0/560	0.45	0/741
49	BX	0.25	0/474	0.42	0/635
49	DX	0.22	0/474	0.41	0/635
50	B4	0.22	0/545	0.49	0/733
50	D4	0.23	0/527	0.51	0/709
51	B5	0.25	0/473	0.51	0/639
51	D5	0.24	0/473	0.54	0/639
52	B6	0.26	0/396	0.46	0/529
52	D6	0.23	0/396	0.51	0/529
53	B7	0.31	0/399	0.44	0/526
53	D7	0.26	0/399	0.44	0/526
54	B8	0.33	0/486	0.55	0/638
54	D8	0.33	0/486	0.67	0/638
All	All	0.30	2/324157 (0.0%)	0.65	164/485451 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
31	BH	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	2873	A	N7-C5	-5.99	1.35	1.39
4	AG	12	CYS	CB-SG	5.09	1.90	1.82

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	2311	A	N1-C2-N3	12.09	135.35	129.30
25	DA	2311	A	N1-C6-N6	10.02	124.61	118.60
25	BA	673	C	C2-N3-C4	-10.01	114.89	119.90
26	BB	95	U	C5-C4-O4	9.25	131.45	125.90
25	DA	673	C	C2-N3-C4	-9.13	115.33	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	BH	153	LYS	Peptide

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	32284	0	16296	1132	1
1	CA	32287	0	16295	1151	1
2	AE	1924	0	1975	160	0
2	CE	1924	0	1975	155	0
3	AF	1605	0	1668	115	0
3	CF	1612	0	1677	117	0
4	AG	1703	0	1763	116	0
4	CG	1703	0	1763	116	0
5	AH	1155	0	1213	75	0
5	CH	1155	0	1213	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AI	843	0	857	52	0
6	CI	843	0	857	41	0
7	AJ	1257	0	1296	66	0
7	CJ	1257	0	1296	73	0
8	AK	1116	0	1177	76	0
8	CK	1116	0	1177	48	0
9	AL	1010	0	1037	80	0
9	CL	1010	0	1037	112	0
10	AM	801	0	849	76	0
10	CM	801	0	849	83	0
11	AN	885	0	904	58	0
11	CN	885	0	904	38	0
12	AO	975	0	1062	96	0
12	CO	975	0	1062	66	0
13	AP	928	0	987	76	0
13	CP	933	0	992	81	0
14	AQ	476	0	511	42	0
14	CQ	476	0	511	39	0
15	AR	734	0	771	33	0
15	CR	734	0	771	32	0
16	AS	705	0	725	57	0
16	CS	705	0	725	23	0
17	AT	834	0	904	43	0
17	CT	834	0	904	39	0
18	AU	591	0	662	27	0
18	CU	591	0	662	37	0
19	AV	624	0	636	52	0
19	CV	624	0	636	67	0
20	AW	763	0	861	63	0
20	CW	763	0	861	58	0
21	AX	217	0	234	18	0
21	CX	217	0	234	20	0
22	AB	1814	0	932	112	0
22	AD	1814	0	932	110	0
22	CB	1814	0	932	111	0
22	CD	1814	0	932	99	0
23	AC	1643	0	837	41	0
23	CC	1643	0	837	38	0
24	A1	346	0	174	19	0
24	C1	346	0	174	17	0
25	BA	62707	0	31614	1935	0
25	DA	62607	0	31565	2087	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BB	2617	0	1328	89	0
26	DB	2617	0	1328	108	0
27	BD	2115	0	2195	197	0
27	DD	2115	0	2195	189	0
28	BE	1568	0	1634	146	0
28	DE	1568	0	1634	183	0
29	BF	1585	0	1632	111	0
29	DF	1627	0	1680	162	0
30	BG	1474	0	1535	129	0
30	DG	1474	0	1535	101	0
31	BH	1307	0	1382	147	0
31	DH	1307	0	1382	101	1
32	BK	1136	0	1223	102	0
32	DK	1136	0	1223	79	0
33	BM	1104	0	1180	75	0
33	DM	1104	0	1180	82	0
34	BN	933	0	996	51	0
34	DN	933	0	996	55	0
35	BO	1145	0	1228	176	0
35	DO	1145	0	1228	299	0
36	BP	1122	0	1179	140	0
36	DP	1122	0	1179	166	0
37	B0	968	0	1033	75	0
37	D0	960	0	1021	66	0
38	BQ	882	0	943	84	0
38	DQ	882	0	943	79	0
39	BR	1141	0	1202	98	0
39	DR	1141	0	1202	94	0
40	B1	964	0	1022	74	0
40	D1	964	0	1022	84	0
41	B2	779	0	852	72	0
41	D2	779	0	852	114	0
42	BS	900	0	964	41	0
42	DS	900	0	964	52	0
43	BT	725	0	778	48	0
43	DT	725	0	778	50	0
44	BU	785	0	878	99	0
44	DU	785	0	878	91	0
45	BV	1397	0	1430	138	0
45	DV	1428	0	1454	125	0
46	B3	607	0	628	41	0
46	D3	613	0	633	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BZ	763	0	848	50	0
47	DZ	763	0	848	48	0
48	BW	558	0	610	38	0
48	DW	558	0	610	43	0
49	BX	469	0	518	21	0
49	DX	469	0	518	24	0
50	B4	533	0	522	128	0
50	D4	515	0	510	71	0
51	B5	459	0	480	92	0
51	D5	459	0	476	39	0
52	B6	389	0	404	80	0
52	D6	389	0	404	51	0
53	B7	391	0	432	17	0
53	D7	391	0	432	25	0
54	B8	480	0	549	116	0
54	D8	480	0	549	81	0
55	A1	1	0	0	0	0
55	AA	220	0	0	0	0
55	AB	4	0	0	0	0
55	AC	8	0	0	0	0
55	AD	3	0	0	0	0
55	AG	2	0	0	0	0
55	AN	1	0	0	0	0
55	AR	1	0	0	0	0
55	AS	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	2	0	0	0	0
55	B2	1	0	0	0	0
55	B3	3	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B7	1	0	0	0	0
55	BA	568	0	0	0	0
55	BB	18	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BW	1	0	0	0	0
55	CA	219	0	0	0	0
55	CB	4	0	0	0	0
55	CC	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CK	1	0	0	0	0
55	CR	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	1	0	0	0	0
55	D3	1	0	0	0	0
55	D5	2	0	0	0	0
55	D7	1	0	0	0	0
55	D8	1	0	0	0	0
55	DA	488	0	0	0	0
55	DB	20	0	0	0	0
55	DD	3	0	0	0	0
55	DE	1	0	0	0	0
55	DO	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299676	0	200977	13379	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 27.

The worst 5 of 13379 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)
35:DO:46:LYS:HD3	35:DO:51:PHE:CD1	1.38	1.55
54:B8:34:TRP:CB	54:B8:35:GLN:HB2	1.34	1.55
50:B4:37:SER:HB3	50:B4:42:PHE:CD1	1.40	1.52
35:DO:71:VAL:HG13	35:DO:72:PRO:CD	1.44	1.47
35:BO:19:VAL:HG23	35:BO:27:HIS:CB	1.45	1.46

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)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.97	0.23
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.19	0.01

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	AE	235/256 (92%)	170 (72%)	44 (19%)	21 (9%)	1	3
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	0	2
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	2	13
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	1	7
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	3	17
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	1	5
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	3	20
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	12	45
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	4	24
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	4	21
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	3	17
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	1	9
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	6	31
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	1	5
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	1	5
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	4	23
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	12
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	2	15
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	3	20
12	AO	123/132 (93%)	104 (85%)	7 (6%)	12 (10%)	0	2
12	CO	123/132 (93%)	96 (78%)	21 (17%)	6 (5%)	2	13
13	AP	114/126 (90%)	76 (67%)	26 (23%)	12 (10%)	0	2
13	CP	115/126 (91%)	83 (72%)	18 (16%)	14 (12%)	0	1
14	AQ	56/61 (92%)	37 (66%)	7 (12%)	12 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CQ	56/61 (92%)	39 (70%)	9 (16%)	8 (14%)	0	1
15	AR	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	14
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	6	30
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	1	8
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	8
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	4	23
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	1	10
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	2	15
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	0	2
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	3
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	4
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	0	3
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	3
21	CX	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	1
27	BD	270/276 (98%)	227 (84%)	30 (11%)	13 (5%)	2	13
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	15
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
28	DE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	BF	200/210 (95%)	177 (88%)	14 (7%)	9 (4%)	2	14
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	0	2
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	1	5
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	1	8
31	BH	168/180 (93%)	113 (67%)	20 (12%)	35 (21%)	0	0
31	DH	168/180 (93%)	108 (64%)	36 (21%)	24 (14%)	0	1
32	BK	144/148 (97%)	90 (62%)	39 (27%)	15 (10%)	0	2
32	DK	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	1	6
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	1	9
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	2
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	39
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BO	148/150 (99%)	99 (67%)	29 (20%)	20 (14%)	0	1
35	DO	148/150 (99%)	92 (62%)	25 (17%)	31 (21%)	0	0
36	BP	139/141 (99%)	102 (73%)	19 (14%)	18 (13%)	0	1
36	DP	139/141 (99%)	92 (66%)	31 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	97 (84%)	11 (10%)	8 (7%)	1	6
37	D0	115/118 (98%)	95 (83%)	15 (13%)	5 (4%)	2	15
38	BQ	109/112 (97%)	85 (78%)	17 (16%)	7 (6%)	1	7
38	DQ	109/112 (97%)	73 (67%)	26 (24%)	10 (9%)	1	3
39	BR	135/146 (92%)	105 (78%)	21 (16%)	9 (7%)	1	6
39	DR	135/146 (92%)	108 (80%)	18 (13%)	9 (7%)	1	6
40	B1	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	2	15
40	D1	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	2	12
41	B2	99/101 (98%)	81 (82%)	12 (12%)	6 (6%)	1	8
41	D2	99/101 (98%)	68 (69%)	17 (17%)	14 (14%)	0	1
42	BS	111/113 (98%)	92 (83%)	13 (12%)	6 (5%)	2	11
42	DS	111/113 (98%)	92 (83%)	15 (14%)	4 (4%)	3	19
43	BT	90/96 (94%)	81 (90%)	5 (6%)	4 (4%)	2	15
43	DT	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	2	10
44	BU	100/110 (91%)	65 (65%)	21 (21%)	14 (14%)	0	1
44	DU	100/110 (91%)	62 (62%)	19 (19%)	19 (19%)	0	0
45	BV	173/206 (84%)	112 (65%)	32 (18%)	29 (17%)	0	0
45	DV	177/206 (86%)	109 (62%)	39 (22%)	29 (16%)	0	1
46	B3	74/85 (87%)	65 (88%)	6 (8%)	3 (4%)	3	16
46	D3	75/85 (88%)	64 (85%)	8 (11%)	3 (4%)	3	17
47	BZ	95/98 (97%)	79 (83%)	12 (13%)	4 (4%)	3	16
47	DZ	95/98 (97%)	76 (80%)	11 (12%)	8 (8%)	1	4
48	BW	64/72 (89%)	53 (83%)	6 (9%)	5 (8%)	1	4
48	DW	64/72 (89%)	54 (84%)	6 (9%)	4 (6%)	1	7
49	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	37
49	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	2	11
50	B4	64/71 (90%)	36 (56%)	12 (19%)	16 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	61/71 (86%)	22 (36%)	22 (36%)	17 (28%)	0	0
51	B5	57/60 (95%)	44 (77%)	6 (10%)	7 (12%)	0	1
51	D5	57/60 (95%)	46 (81%)	8 (14%)	3 (5%)	2	11
52	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
52	D6	43/54 (80%)	26 (60%)	8 (19%)	9 (21%)	0	0
53	B7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	D7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
54	B8	58/65 (89%)	42 (72%)	8 (14%)	8 (14%)	0	1
54	D8	58/65 (89%)	37 (64%)	13 (22%)	8 (14%)	0	1
All	All	11319/12052 (94%)	8735 (77%)	1671 (15%)	913 (8%)	1	4

5 of 913 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	195	ASP
2	AE	236	TYR
2	AE	237	ALA
3	AF	4	LYS
3	AF	12	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	165 (80%)	40 (20%)	1	7
2	CE	205/220 (93%)	180 (88%)	25 (12%)	5	21
3	AF	159/188 (85%)	141 (89%)	18 (11%)	6	24
3	CF	160/188 (85%)	143 (89%)	17 (11%)	6	26
4	AG	180/180 (100%)	160 (89%)	20 (11%)	6	25
4	CG	180/180 (100%)	160 (89%)	20 (11%)	6	25
5	AH	116/123 (94%)	97 (84%)	19 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CH	116/123 (94%)	102 (88%)	14 (12%)	5	21
6	AI	90/90 (100%)	80 (89%)	10 (11%)	6	25
6	CI	90/90 (100%)	81 (90%)	9 (10%)	7	29
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	2	12
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	11
8	AK	119/119 (100%)	106 (89%)	13 (11%)	6	25
8	CK	119/119 (100%)	111 (93%)	8 (7%)	16	49
9	AL	98/99 (99%)	86 (88%)	12 (12%)	5	21
9	CL	98/99 (99%)	81 (83%)	17 (17%)	2	10
10	AM	89/92 (97%)	79 (89%)	10 (11%)	6	24
10	CM	89/92 (97%)	78 (88%)	11 (12%)	4	20
11	AN	90/99 (91%)	79 (88%)	11 (12%)	5	21
11	CN	90/99 (91%)	85 (94%)	5 (6%)	21	56
12	AO	104/109 (95%)	95 (91%)	9 (9%)	10	37
12	CO	104/109 (95%)	94 (90%)	10 (10%)	8	32
13	AP	94/101 (93%)	87 (93%)	7 (7%)	13	44
13	CP	94/101 (93%)	83 (88%)	11 (12%)	5	22
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	4	20
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	11	39
15	AR	79/80 (99%)	73 (92%)	6 (8%)	13	43
15	CR	79/80 (99%)	67 (85%)	12 (15%)	3	14
16	AS	72/74 (97%)	68 (94%)	4 (6%)	21	56
16	CS	72/74 (97%)	64 (89%)	8 (11%)	6	25
17	AT	95/97 (98%)	85 (90%)	10 (10%)	7	27
17	CT	95/97 (98%)	92 (97%)	3 (3%)	39	74
18	AU	63/77 (82%)	57 (90%)	6 (10%)	8	32
18	CU	63/77 (82%)	51 (81%)	12 (19%)	1	8
19	AV	67/80 (84%)	55 (82%)	12 (18%)	2	9
19	CV	67/80 (84%)	58 (87%)	9 (13%)	4	17
20	AW	76/82 (93%)	68 (90%)	8 (10%)	7	27
20	CW	76/82 (93%)	66 (87%)	10 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	178 (83%)	36 (17%)	2	11
27	DD	214/218 (98%)	181 (85%)	33 (15%)	2	13
28	BE	165/166 (99%)	135 (82%)	30 (18%)	1	9
28	DE	165/166 (99%)	139 (84%)	26 (16%)	2	12
29	BF	161/166 (97%)	141 (88%)	20 (12%)	4	20
29	DF	165/166 (99%)	140 (85%)	25 (15%)	3	14
30	BG	155/156 (99%)	135 (87%)	20 (13%)	4	19
30	DG	155/156 (99%)	139 (90%)	16 (10%)	7	28
31	BH	142/148 (96%)	122 (86%)	20 (14%)	3	16
31	DH	142/148 (96%)	124 (87%)	18 (13%)	4	19
32	BK	122/124 (98%)	101 (83%)	21 (17%)	2	10
32	DK	122/124 (98%)	106 (87%)	16 (13%)	4	18
33	BM	117/119 (98%)	98 (84%)	19 (16%)	2	12
33	DM	117/119 (98%)	97 (83%)	20 (17%)	2	10
34	BN	100/100 (100%)	92 (92%)	8 (8%)	12	40
34	DN	100/100 (100%)	87 (87%)	13 (13%)	4	19
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	1
36	BP	111/111 (100%)	94 (85%)	17 (15%)	2	13
36	DP	111/111 (100%)	89 (80%)	22 (20%)	1	7
37	B0	101/101 (100%)	85 (84%)	16 (16%)	2	12
37	D0	100/101 (99%)	82 (82%)	18 (18%)	1	9
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	2	12
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	9	34
39	BR	120/127 (94%)	99 (82%)	21 (18%)	2	10
39	DR	120/127 (94%)	102 (85%)	18 (15%)	3	14
40	B1	93/94 (99%)	85 (91%)	8 (9%)	10	37
40	D1	93/94 (99%)	82 (88%)	11 (12%)	5	22
41	B2	82/82 (100%)	70 (85%)	12 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	D2	82/82 (100%)	69 (84%)	13 (16%)	2	12
42	BS	92/92 (100%)	79 (86%)	13 (14%)	3	16
42	DS	92/92 (100%)	76 (83%)	16 (17%)	2	10
43	BT	74/78 (95%)	65 (88%)	9 (12%)	5	21
43	DT	74/78 (95%)	63 (85%)	11 (15%)	3	14
44	BU	85/91 (93%)	72 (85%)	13 (15%)	2	13
44	DU	85/91 (93%)	67 (79%)	18 (21%)	1	5
45	BV	154/179 (86%)	126 (82%)	28 (18%)	1	9
45	DV	158/179 (88%)	138 (87%)	20 (13%)	4	19
46	B3	61/67 (91%)	57 (93%)	4 (7%)	16	49
46	D3	62/67 (92%)	55 (89%)	7 (11%)	6	24
47	BZ	82/83 (99%)	69 (84%)	13 (16%)	2	12
47	DZ	82/83 (99%)	68 (83%)	14 (17%)	2	10
48	BW	62/67 (92%)	51 (82%)	11 (18%)	2	9
48	DW	62/67 (92%)	51 (82%)	11 (18%)	2	9
49	BX	51/52 (98%)	46 (90%)	5 (10%)	8	30
49	DX	51/52 (98%)	48 (94%)	3 (6%)	19	54
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	11
50	D4	57/63 (90%)	46 (81%)	11 (19%)	1	8
51	B5	51/52 (98%)	42 (82%)	9 (18%)	2	10
51	D5	51/52 (98%)	41 (80%)	10 (20%)	1	7
52	B6	44/52 (85%)	34 (77%)	10 (23%)	1	4
52	D6	44/52 (85%)	40 (91%)	4 (9%)	9	34
53	B7	38/42 (90%)	33 (87%)	5 (13%)	4	18
53	D7	38/42 (90%)	33 (87%)	5 (13%)	4	18
54	B8	50/55 (91%)	37 (74%)	13 (26%)	0	2
54	D8	50/55 (91%)	41 (82%)	9 (18%)	1	9
All	All	9565/9996 (96%)	8229 (86%)	1336 (14%)	3	16

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	DD	192	THR

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Mol	Chain	Res	Type
37	D0	105	ARG
28	DE	144	ARG
27	DD	166	GLN
33	DM	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
37	D0	11	ASN
39	DR	43	GLN
45	DV	75	ASN
37	B0	61	HIS
37	B0	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1501/1506 (99%)	295 (19%)	43 (2%)
1	CA	1501/1506 (99%)	296 (19%)	49 (3%)
22	AB	83/85 (97%)	38 (45%)	8 (9%)
22	AD	83/85 (97%)	26 (31%)	5 (6%)
22	CB	83/85 (97%)	38 (45%)	9 (10%)
22	CD	83/85 (97%)	25 (30%)	4 (4%)
23	AC	76/77 (98%)	11 (14%)	1 (1%)
23	CC	76/77 (98%)	13 (17%)	3 (3%)
24	A1	15/16 (93%)	6 (40%)	2 (13%)
24	C1	15/16 (93%)	6 (40%)	3 (20%)
25	BA	2911/2912 (99%)	542 (18%)	51 (1%)
25	DA	2905/2912 (99%)	569 (19%)	53 (1%)
26	BB	121/122 (99%)	17 (14%)	0
26	DB	121/122 (99%)	27 (22%)	1 (0%)
All	All	9574/9606 (99%)	1909 (19%)	232 (2%)

5 of 1909 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U

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Mol	Chain	Res	Type
1	AA	32	A

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	115	G
25	DA	2447	G
1	CA	1053	G
25	DA	2402	C
25	DA	1379	A

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

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	MIA	AD	38	22	24,31,32	1.89	2 (8%)	26,44,47	2.74	10 (38%)
22	MIA	CD	38	22	24,31,32	1.91	2 (8%)	26,44,47	2.79	10 (38%)
22	MIA	AB	38	22	24,31,32	1.83	2 (8%)	26,44,47	2.35	10 (38%)
22	MIA	CB	38	22	24,31,32	1.96	2 (8%)	26,44,47	2.38	9 (34%)

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	MIA	AD	38	22	-	8/11/33/34	0/3/3/3
22	MIA	CD	38	22	-	7/11/33/34	0/3/3/3
22	MIA	AB	38	22	-	4/11/33/34	0/3/3/3
22	MIA	CB	38	22	-	4/11/33/34	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CB	38	MIA	C6-N6	6.56	1.46	1.34
22	CB	38	MIA	C13-C14	6.35	1.50	1.32
22	CD	38	MIA	C6-N6	6.28	1.46	1.34
22	AD	38	MIA	C6-N6	6.19	1.45	1.34
22	CD	38	MIA	C13-C14	6.12	1.49	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	38	MIA	C11-S10-C2	10.19	109.88	102.27
22	AD	38	MIA	C11-S10-C2	9.70	109.51	102.27
22	CB	38	MIA	C11-S10-C2	7.57	107.92	102.27
22	AB	38	MIA	C11-S10-C2	5.97	106.72	102.27
22	AB	38	MIA	C12-C13-C14	-5.85	115.77	127.14

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AB	38	MIA	N1-C2-S10-C11
22	AB	38	MIA	N3-C2-S10-C11
22	AB	38	MIA	C12-C13-C14-C15
22	AB	38	MIA	C12-C13-C14-C16
22	AD	38	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AD	38	MIA	3	0
22	CD	38	MIA	4	0
22	AB	38	MIA	1	0
22	CB	38	MIA	3	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1608 ligands modelled in this entry, 1608 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1502/1506 (99%)	-0.36	5 (0%) 94 84	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.28	13 (0%) 84 63	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.24	11 (4%) 32 12	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.57	15 (6%) 20 6	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.29	7 (3%) 45 19	88, 113, 149, 158	0
3	CF	206/239 (86%)	1.03	33 (16%) 1 1	101, 135, 165, 180	0
4	AG	208/208 (100%)	-0.32	1 (0%) 91 75	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.24	3 (1%) 75 49	75, 95, 123, 135	0
5	AH	151/162 (93%)	0.01	2 (1%) 77 51	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.19	2 (1%) 77 51	84, 106, 131, 167	0
6	AI	101/101 (100%)	0.44	5 (4%) 28 10	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.07	0 100 100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.40	12 (7%) 13 4	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.05	6 (3%) 39 15	100, 119, 147, 158	0
8	AK	138/138 (100%)	-0.28	0 100 100	81, 103, 117, 132	0
8	CK	138/138 (100%)	0.02	1 (0%) 87 69	81, 108, 125, 136	0
9	AL	127/128 (99%)	0.51	13 (10%) 6 2	83, 138, 159, 166	0
9	CL	127/128 (99%)	0.09	6 (4%) 31 11	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.77	14 (14%) 2 1	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.83	12 (12%) 4 1	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.77	13 (10%) 5 2	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.21	2 (1%) 70 41	74, 99, 133, 164	0
12	AO	125/132 (94%)	-0.22	1 (0%) 86 65	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.62	14 (11%) 5 1	63, 91, 126, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.23	6 (5%) 27 10	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.19	7 (5%) 21 7	91, 145, 161, 169	0
14	AQ	58/61 (95%)	-0.15	0 100 100	87, 103, 120, 127	0
14	CQ	58/61 (95%)	1.17	9 (15%) 2 1	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.14	0 100 100	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.06	0 100 100	67, 96, 124, 136	0
16	AS	84/88 (95%)	-0.36	0 100 100	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.32	2 (2%) 59 30	76, 91, 118, 157	0
17	AT	100/105 (95%)	-0.35	2 (2%) 65 36	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.03	2 (2%) 65 36	75, 100, 126, 144	0
18	AU	72/88 (81%)	0.56	5 (6%) 16 5	77, 97, 135, 164	0
18	CU	72/88 (81%)	0.17	2 (2%) 53 25	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.12	1 (1%) 77 51	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.55	5 (6%) 19 6	128, 152, 178, 186	0
20	AW	99/106 (93%)	-0.17	0 100 100	96, 121, 148, 153	0
20	CW	99/106 (93%)	0.21	2 (2%) 65 36	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.21	1 (4%) 38 15	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.78	2 (8%) 12 4	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.73	13 (15%) 2 1	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.30	11 (13%) 3 1	70, 147, 206, 218	0
22	CB	84/85 (98%)	1.60	30 (35%) 0 0	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.64	0 100 100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.42	0 100 100	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.59	0 100 100	79, 104, 143, 165	0
24	A1	16/16 (100%)	-0.21	0 100 100	66, 97, 168, 177	0
24	C1	16/16 (100%)	-0.18	0 100 100	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.04	42 (1%) 75 49	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.18	66 (2%) 60 31	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.27	1 (0%) 86 65	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.46	2 (1%) 72 44	78, 110, 139, 198	0
27	BD	272/276 (98%)	0.03	0 100 100	39, 59, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	-0.08	1 (0%) 92 79	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.11	5 (2%) 59 30	44, 77, 125, 150	0
28	DE	205/206 (99%)	0.07	9 (4%) 34 13	56, 92, 144, 157	0
29	BF	202/210 (96%)	0.08	2 (0%) 82 59	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.84	22 (10%) 6 2	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.94	34 (18%) 1 0	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.37	8 (4%) 34 13	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.13	4 (2%) 59 30	71, 105, 126, 151	0
31	DH	170/180 (94%)	1.56	56 (32%) 0 0	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.46	8 (5%) 25 9	72, 120, 141, 153	0
32	DK	146/148 (98%)	-0.20	1 (0%) 87 69	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.08	2 (1%) 75 49	58, 79, 115, 136	0
33	DM	138/140 (98%)	0.12	2 (1%) 75 49	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.07	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	0.04	0 100 100	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.32	7 (4%) 31 11	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.85	22 (14%) 2 1	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.17	5 (3%) 44 18	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.43	14 (9%) 7 2	58, 100, 130, 154	0
37	B0	118/118 (100%)	0.01	0 100 100	53, 74, 96, 106	0
37	D0	117/118 (99%)	0.03	1 (0%) 84 63	62, 81, 100, 117	0
38	BQ	111/112 (99%)	0.73	10 (9%) 9 3	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.24	6 (5%) 25 9	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.15	4 (2%) 51 23	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.07	3 (2%) 62 33	73, 94, 154, 184	0
40	B1	117/118 (99%)	0.00	2 (1%) 70 41	50, 70, 98, 140	0
40	D1	117/118 (99%)	0.49	9 (7%) 13 4	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.08	3 (2%) 50 22	46, 91, 116, 128	0
41	D2	101/101 (100%)	0.97	14 (13%) 2 1	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.04	1 (0%) 84 63	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.16	2 (1%) 68 40	61, 75, 109, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.35	3 (3%) 46 20	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.22	3 (3%) 46 20	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.48	5 (4%) 29 11	70, 94, 144, 165	0
44	DU	102/110 (92%)	1.47	27 (26%) 0 0	78, 111, 162, 172	0
45	BV	175/206 (84%)	1.29	37 (21%) 1 0	79, 120, 189, 194	0
45	DV	179/206 (86%)	1.88	65 (36%) 0 0	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.16	2 (2%) 56 27	51, 72, 92, 125	0
46	D3	77/85 (90%)	-0.04	1 (1%) 77 51	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.44	8 (8%) 11 3	48, 71, 115, 155	0
47	DZ	97/98 (98%)	-0.07	2 (2%) 63 34	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.35	2 (3%) 50 22	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.40	2 (3%) 50 22	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.03	0 100 100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.58	4 (6%) 17 5	76, 103, 136, 159	0
50	B4	66/71 (92%)	2.42	38 (57%) 0 0	112, 153, 176, 181	0
50	D4	63/71 (88%)	1.98	30 (47%) 0 0	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.38	6 (10%) 6 2	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.82	8 (13%) 3 1	61, 84, 169, 188	0
52	B6	45/54 (83%)	5.94	44 (97%) 0 0	117, 148, 164, 173	0
52	D6	45/54 (83%)	2.59	24 (53%) 0 0	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.03	0 100 100	38, 48, 68, 85	0
53	D7	45/49 (91%)	0.00	0 100 100	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.35	2 (3%) 46 20	51, 68, 88, 115	0
54	D8	60/65 (92%)	0.34	3 (5%) 28 10	64, 80, 106, 132	0
All	All	21100/21658 (97%)	0.13	975 (4%) 32 12	38, 95, 177, 247	0

The worst 5 of 975 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	654(J)	A	19.6
29	DF	1	MET	18.4
25	DA	654(L)	G	15.7
25	BA	654(J)	A	14.8
25	DA	654(K)	C	14.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MIA	AD	38	29/30	0.92	0.18	98,122,141,145	0
22	MIA	CB	38	29/30	0.94	0.19	63,95,112,126	0
22	MIA	CD	38	29/30	0.94	0.21	101,121,146,154	0
22	MIA	AB	38	29/30	0.96	0.18	65,78,90,93	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.