



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 12:34 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

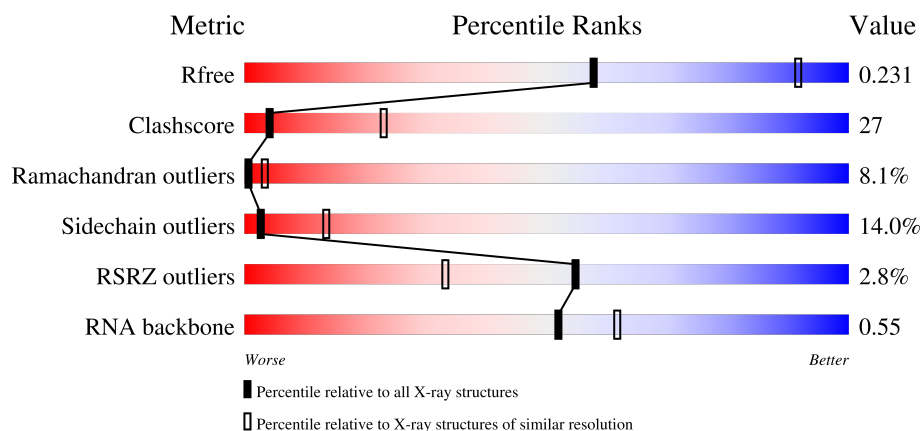
# 1 Overall quality at a glance

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.





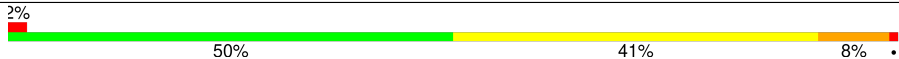
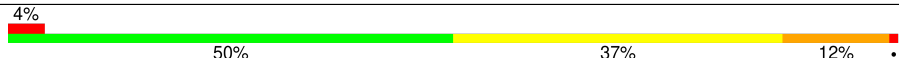
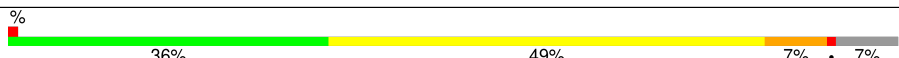
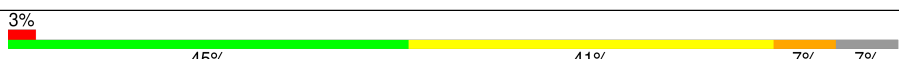
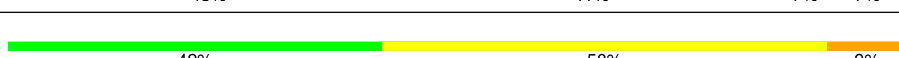
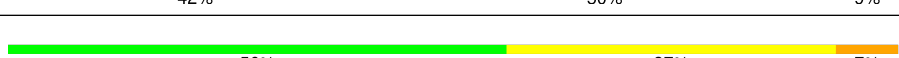


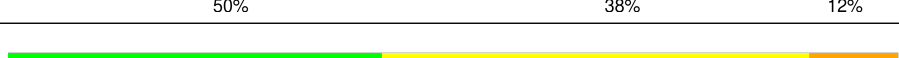




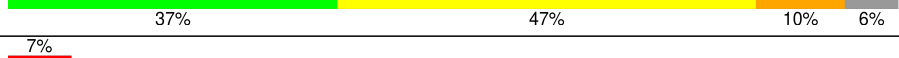
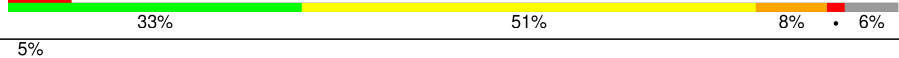
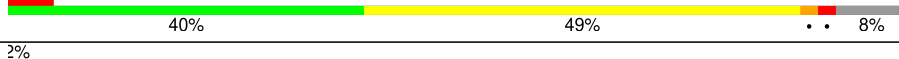

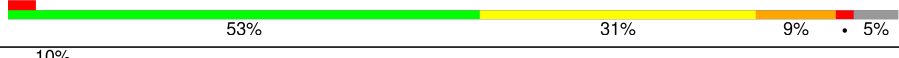

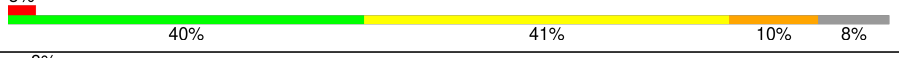
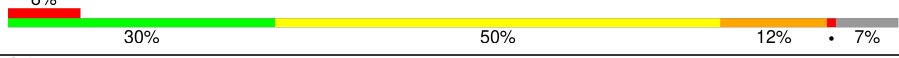
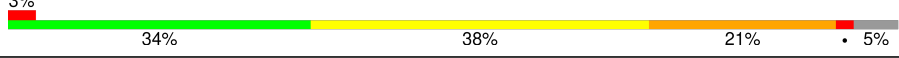

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	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>4%</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	

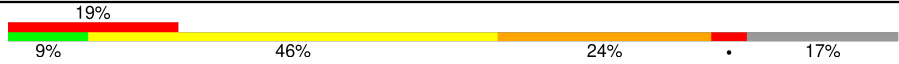


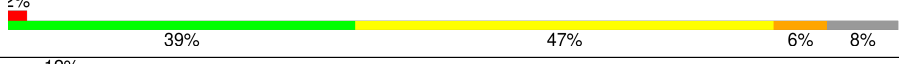
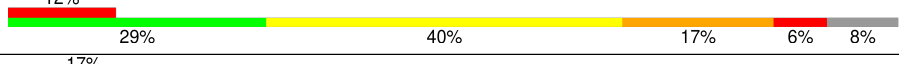
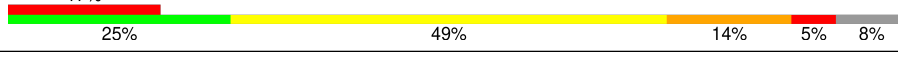
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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	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	1633	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1751	-	-	-	X
55	MG	AA	1757	-	-	-	X
55	MG	AA	1777	-	-	-	X
55	MG	AA	1804	-	-	-	X
55	MG	BA	3045	-	-	-	X
55	MG	BA	3126	-	-	-	X
55	MG	BA	3270	-	-	-	X
55	MG	BA	3373	-	-	-	X
55	MG	BA	3382	-	-	-	X
55	MG	BA	3424	-	-	-	X
55	MG	BA	3440	-	-	-	X
55	MG	BA	3472	-	-	-	X
55	MG	BA	3540	-	-	-	X
55	MG	CA	1675	-	-	-	X
55	MG	CA	1684	-	-	-	X
55	MG	CA	1716	-	-	-	X
55	MG	CA	1729	-	-	-	X
55	MG	CA	1733	-	-	-	X
55	MG	CA	1755	-	-	-	X
55	MG	CA	1776	-	-	-	X
55	MG	CA	1785	-	-	-	X
55	MG	CA	1806	-	-	-	X
55	MG	CA	1808	-	-	-	X
55	MG	DA	3114	-	-	-	X
55	MG	DA	3125	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3165	-	-	-	X
55	MG	DA	3239	-	-	-	X
55	MG	DA	3243	-	-	-	X
55	MG	DA	3270	-	-	-	X
55	MG	DA	3279	-	-	-	X
55	MG	DA	3310	-	-	-	X
55	MG	DA	3339	-	-	-	X
55	MG	DA	3366	-	-	-	X
55	MG	DA	3370	-	-	-	X
55	MG	DA	3371	-	-	-	X
55	MG	DA	3403	-	-	-	X
55	MG	DA	3406	-	-	-	X
55	MG	DA	3439	-	-	-	X
55	MG	DA	3458	-	-	-	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

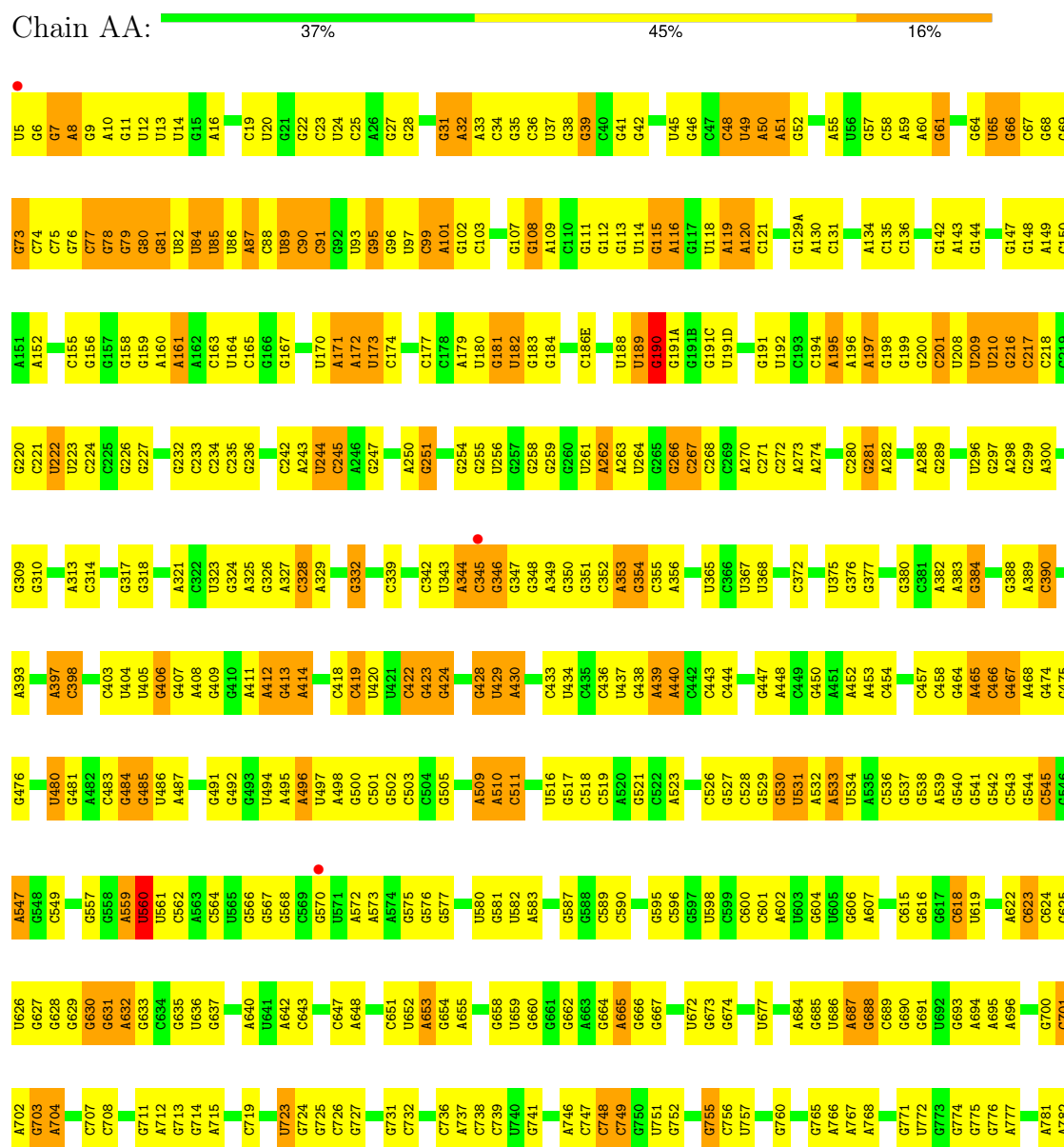
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

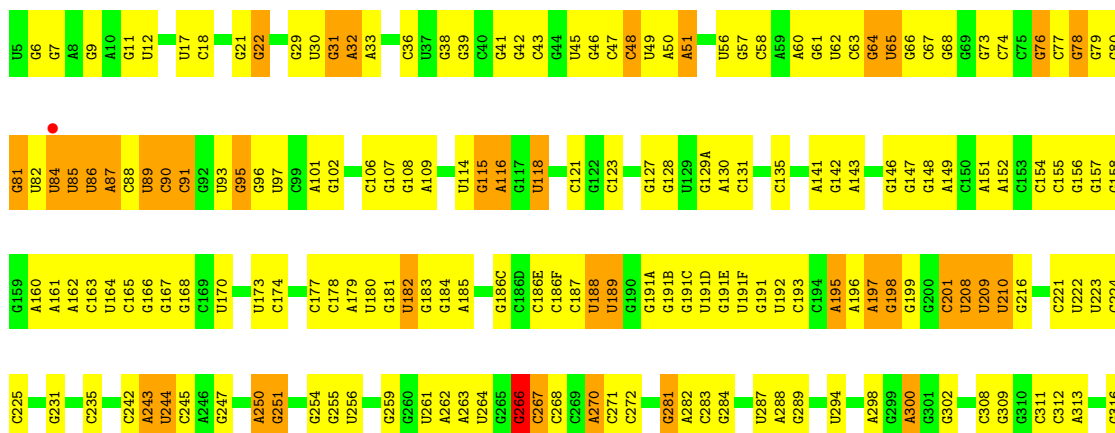
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

### 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.

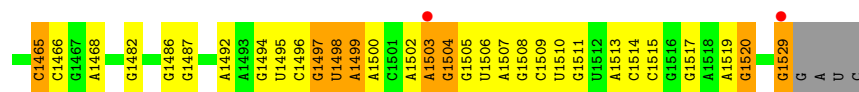
#### • Molecule 1: 16S ribosomal RNA



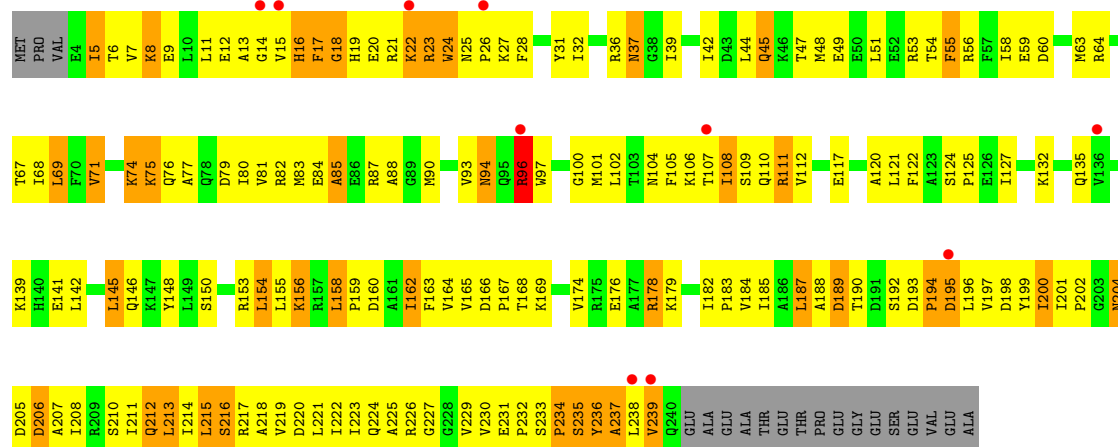




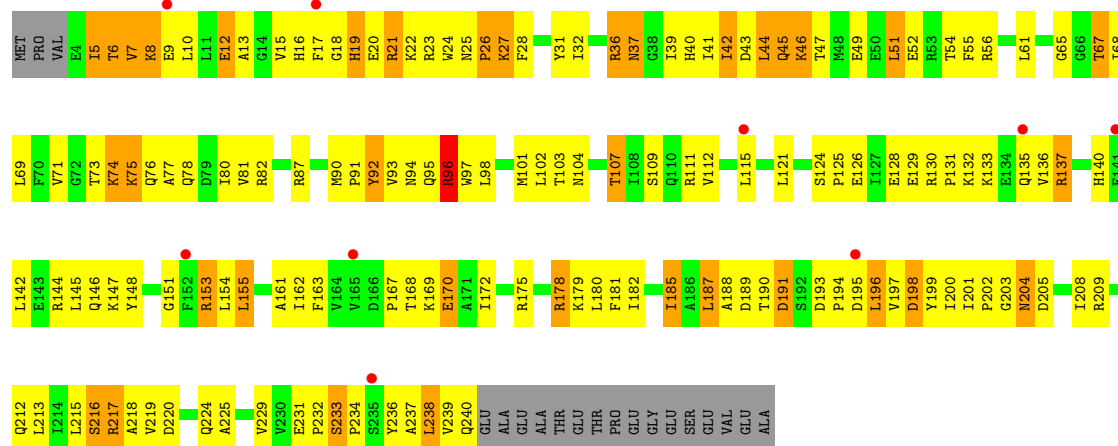




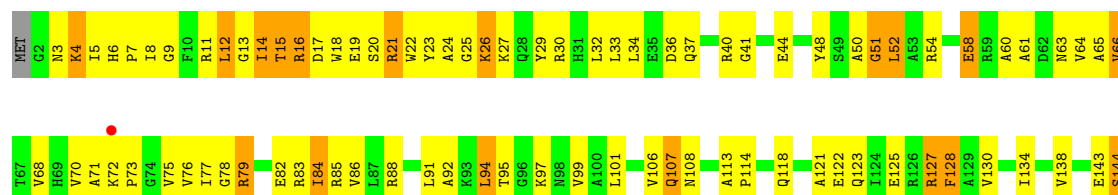
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

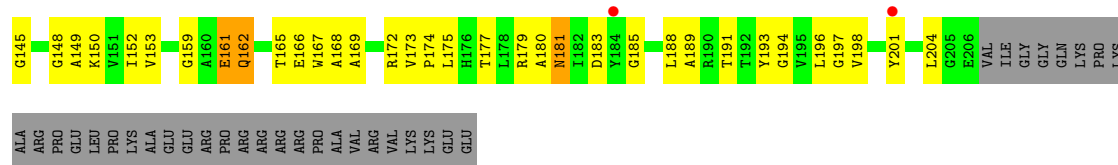


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

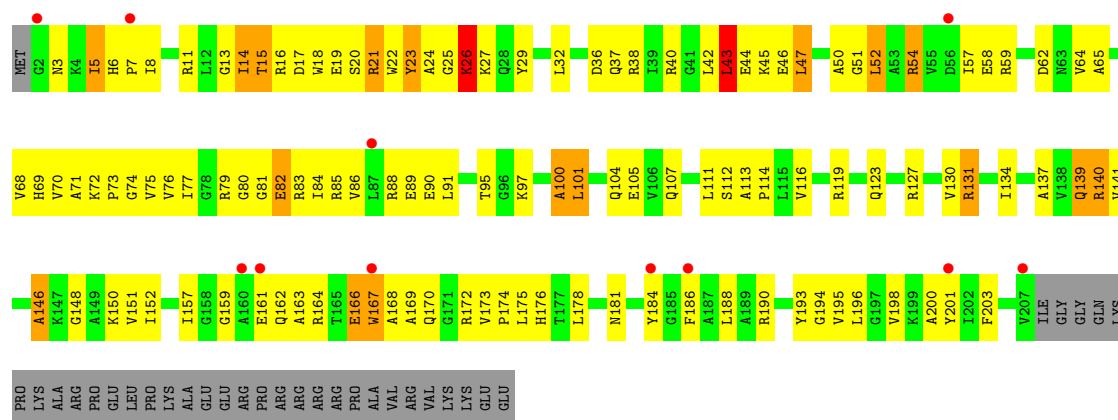


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

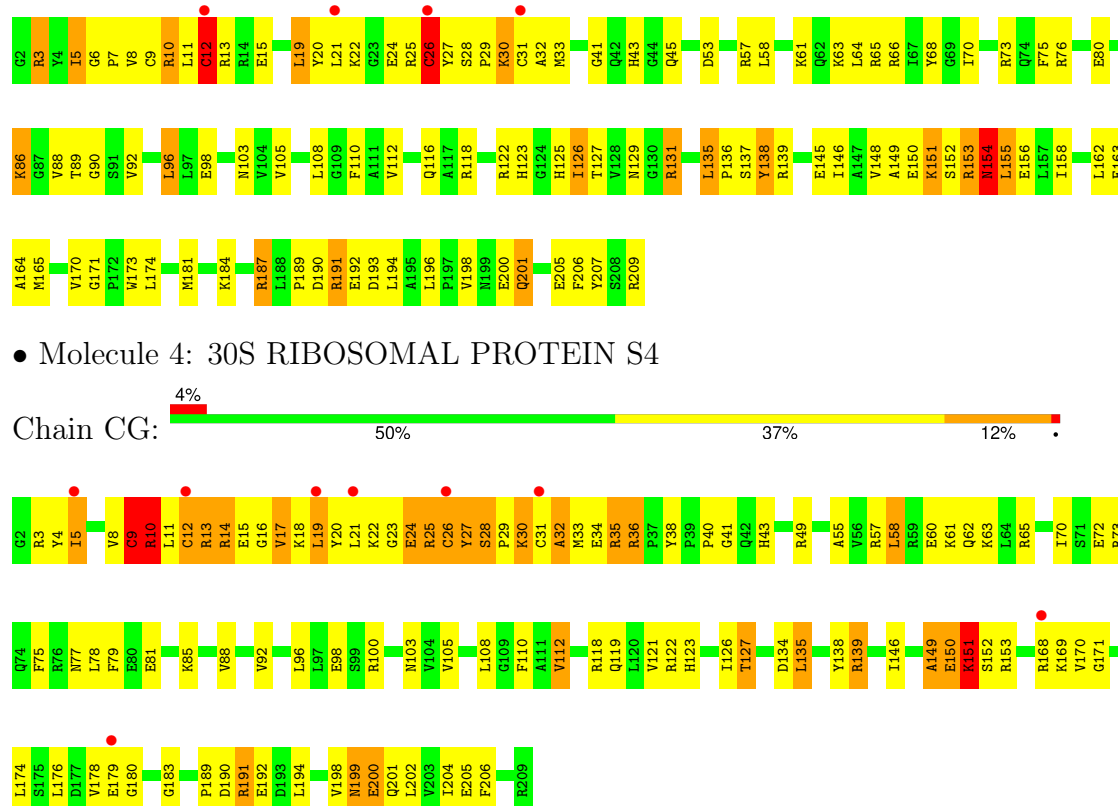




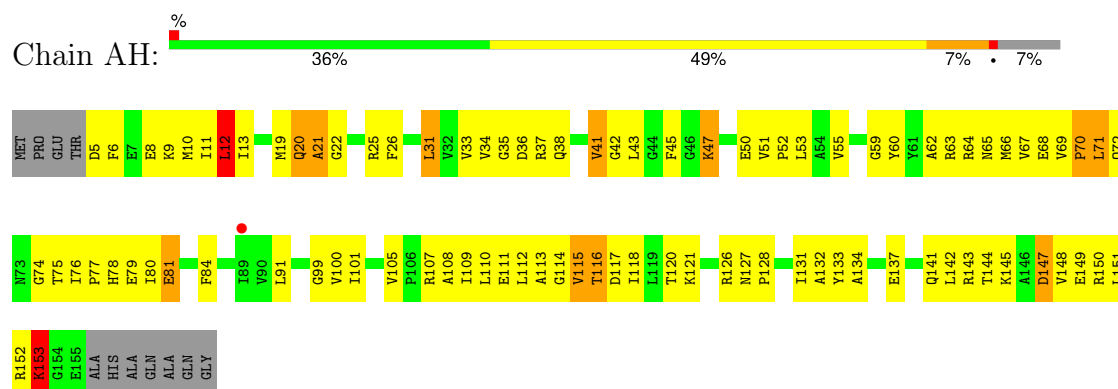
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



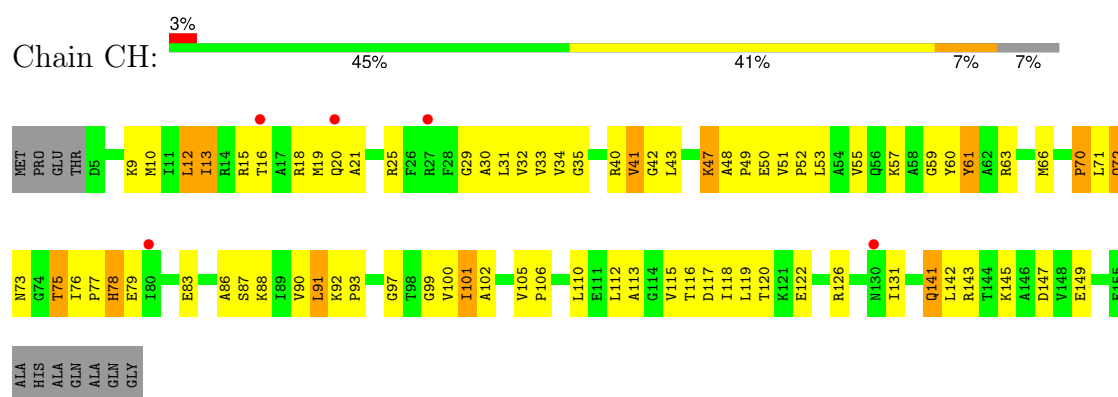
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



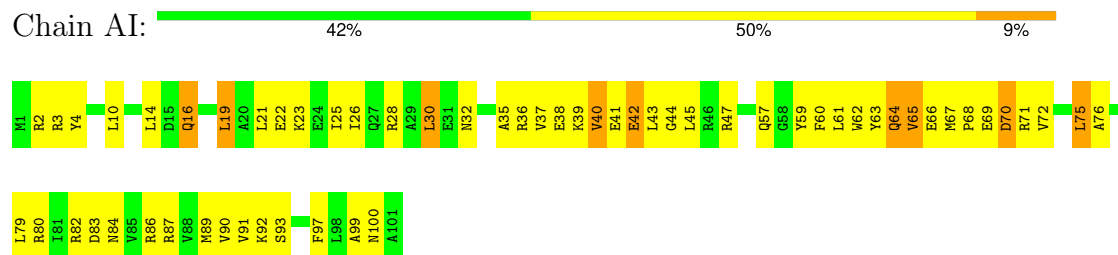
## • Molecule 5: 30S RIBOSOMAL PROTEIN S5



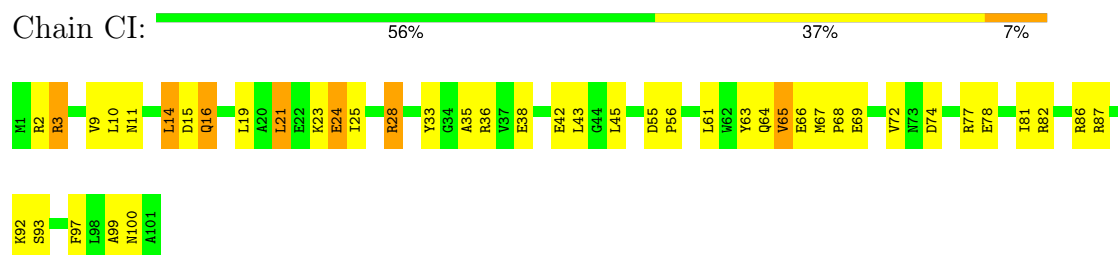
## • Molecule 5: 30S RIBOSOMAL PROTEIN S5



## • Molecule 6: 30S RIBOSOMAL PROTEIN S6

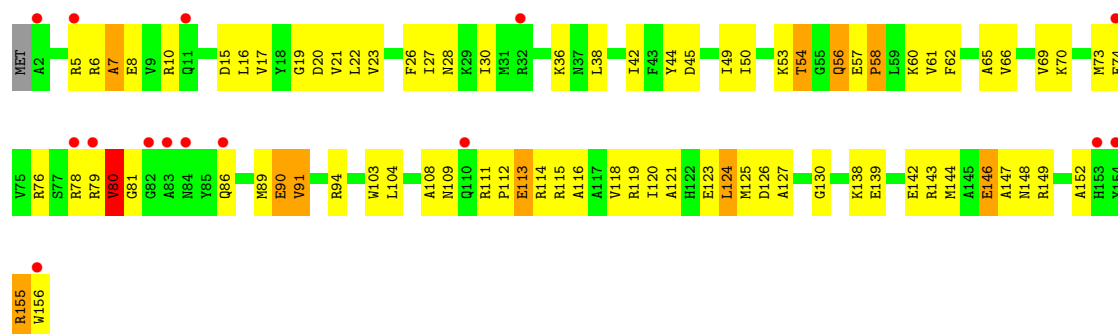


## • Molecule 6: 30S RIBOSOMAL PROTEIN S6

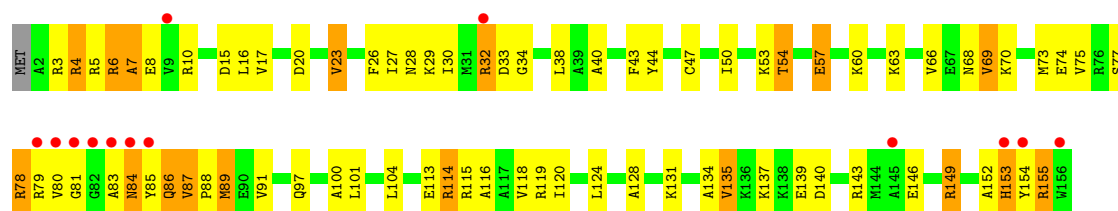


## • Molecule 7: 30S RIBOSOMAL PROTEIN S7

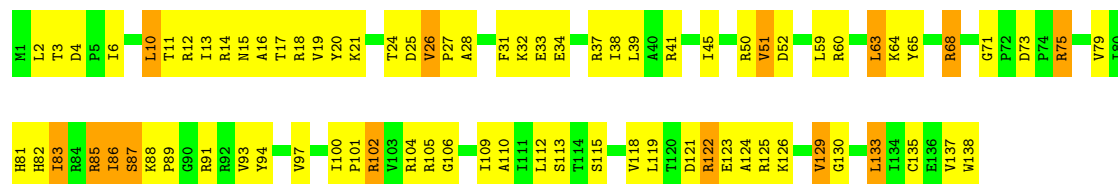




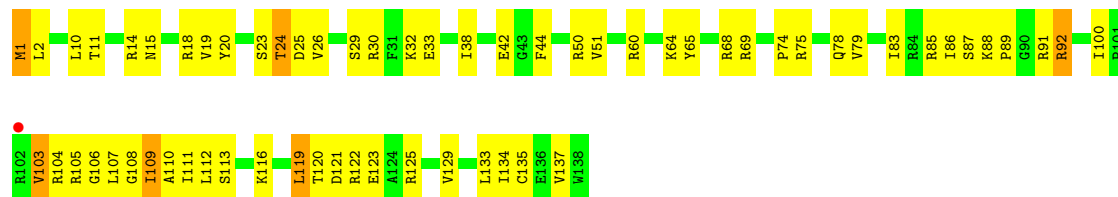
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

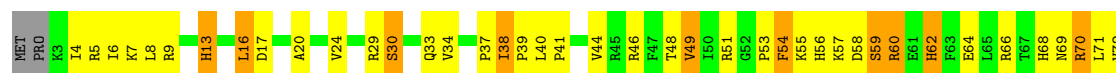




• Molecule 9: 30S RIBOSOMAL PROTEIN S9



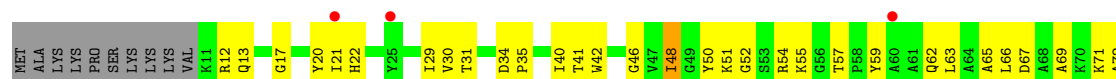
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

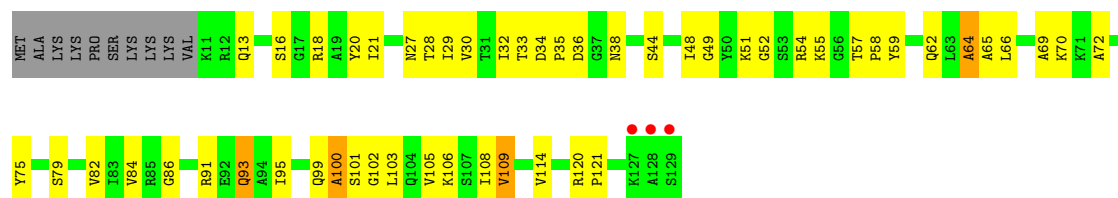


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

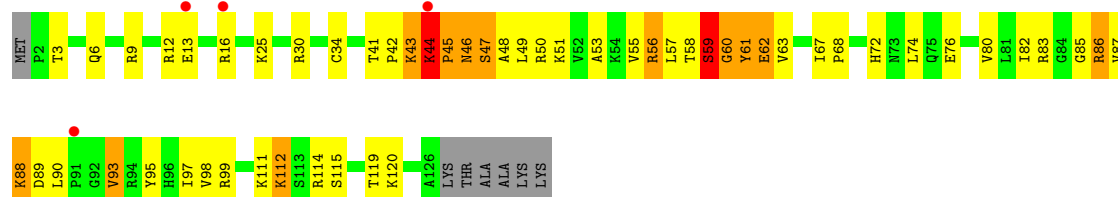


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

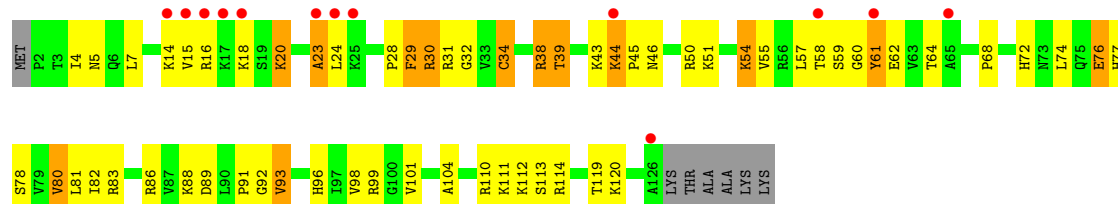




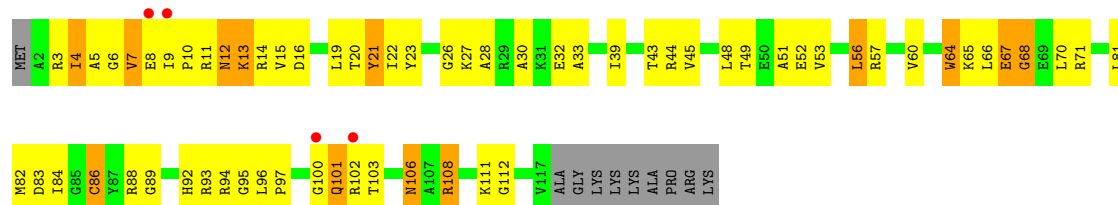
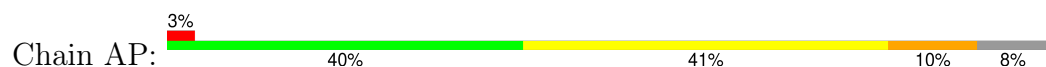
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



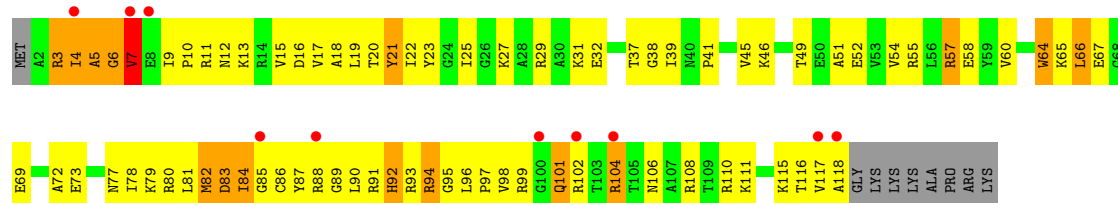
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



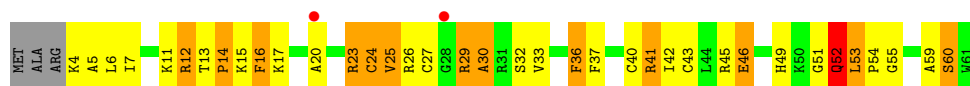
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



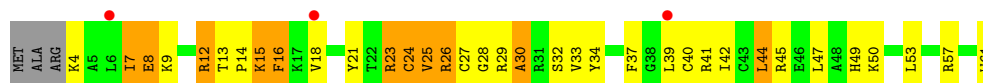
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



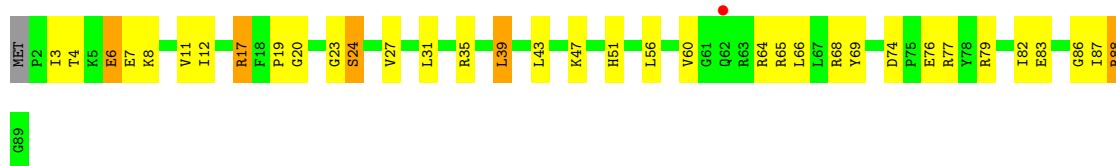
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



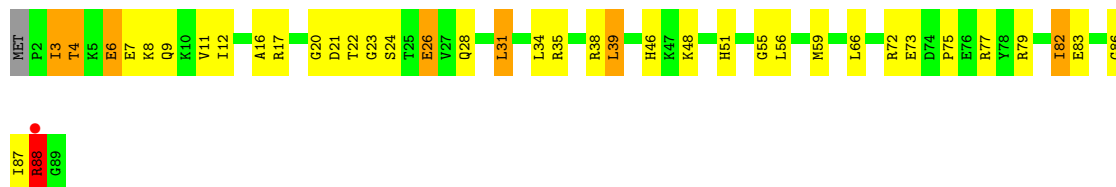
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 15: 30S RIBOSOMAL PROTEIN S15



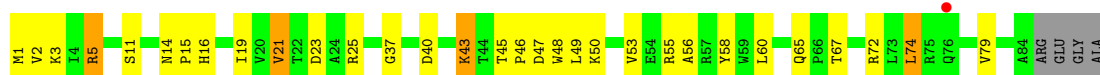
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



- Molecule 16: 30S RIBOSOMAL PROTEIN S16



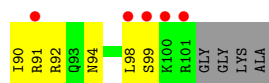




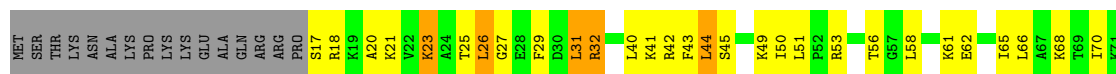
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



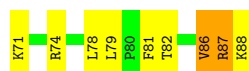
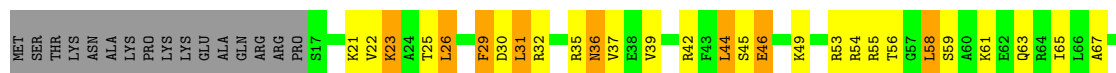
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

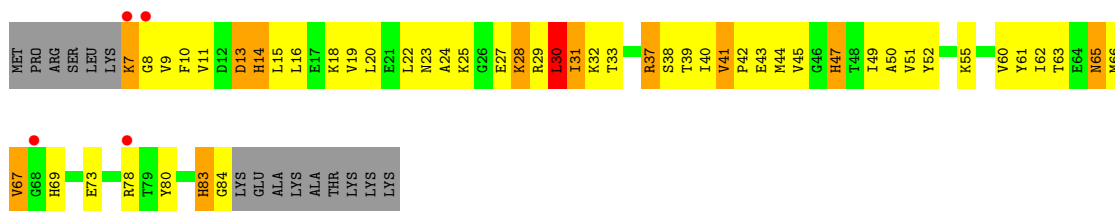


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

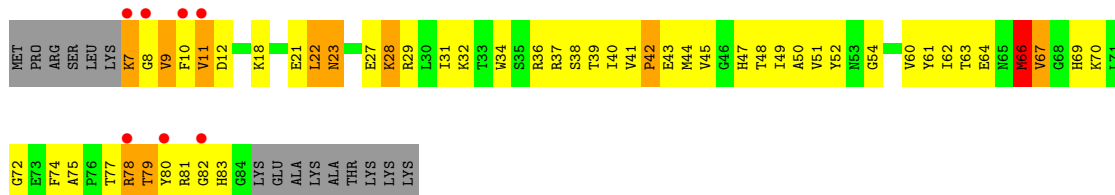


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

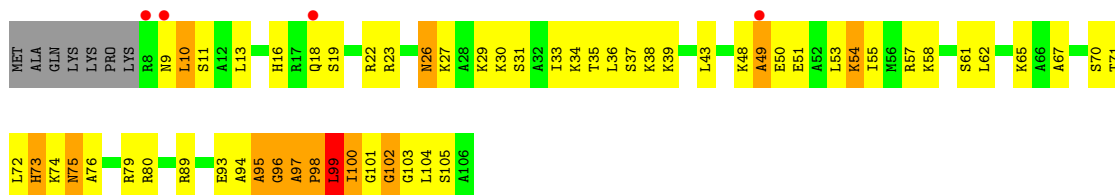
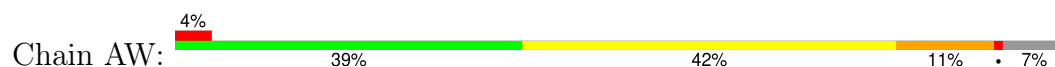




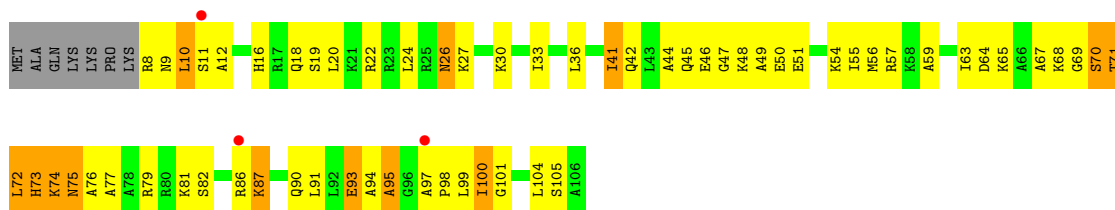
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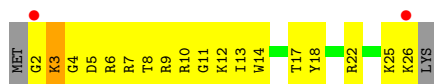
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

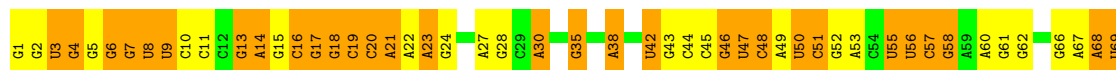
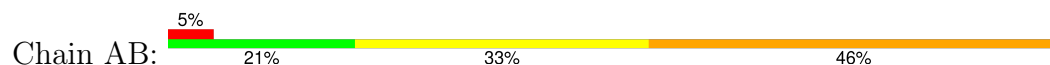


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

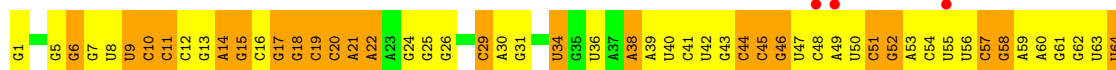
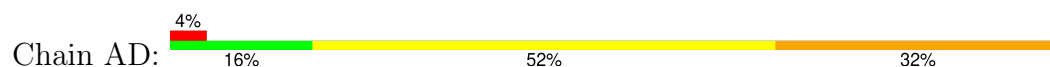




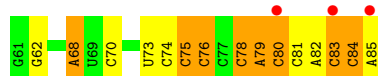
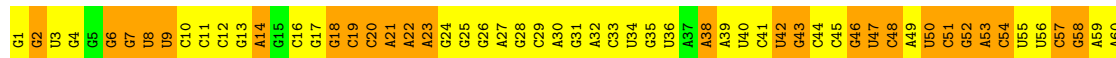
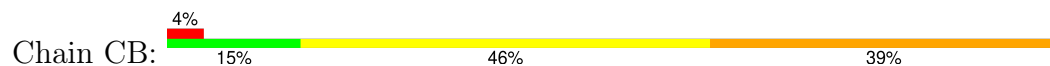
• Molecule 22: TRNA-TYR



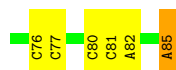
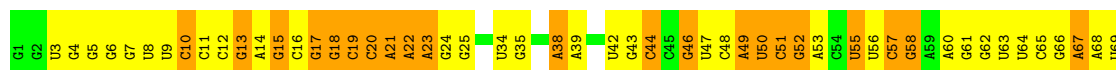
• Molecule 22: TRNA-TYR



• Molecule 22: TRNA-TYR



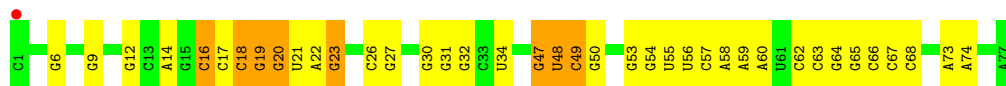
• Molecule 22: TRNA-TYR



• Molecule 23: TRNA-FMET



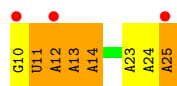
- Molecule 23: TRNA-FMET



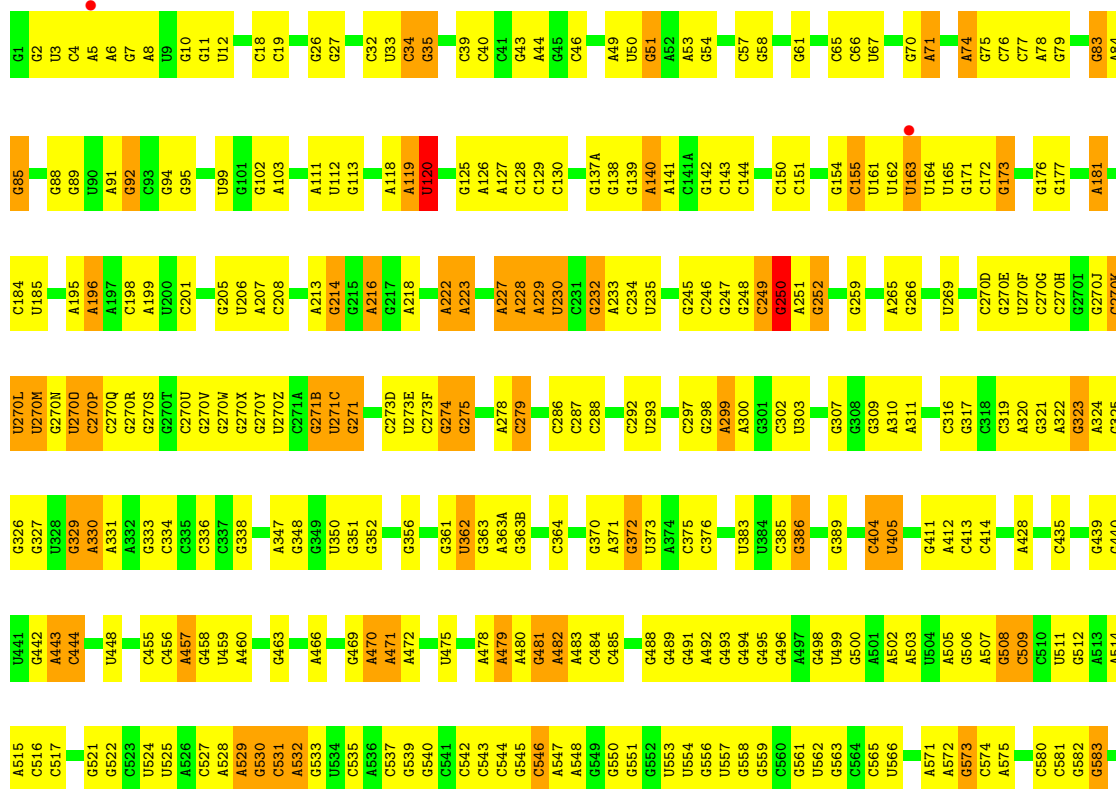
- Molecule 24: MRNA



- Molecule 24: MRNA



- Molecule 25: RNA (2912-MER)

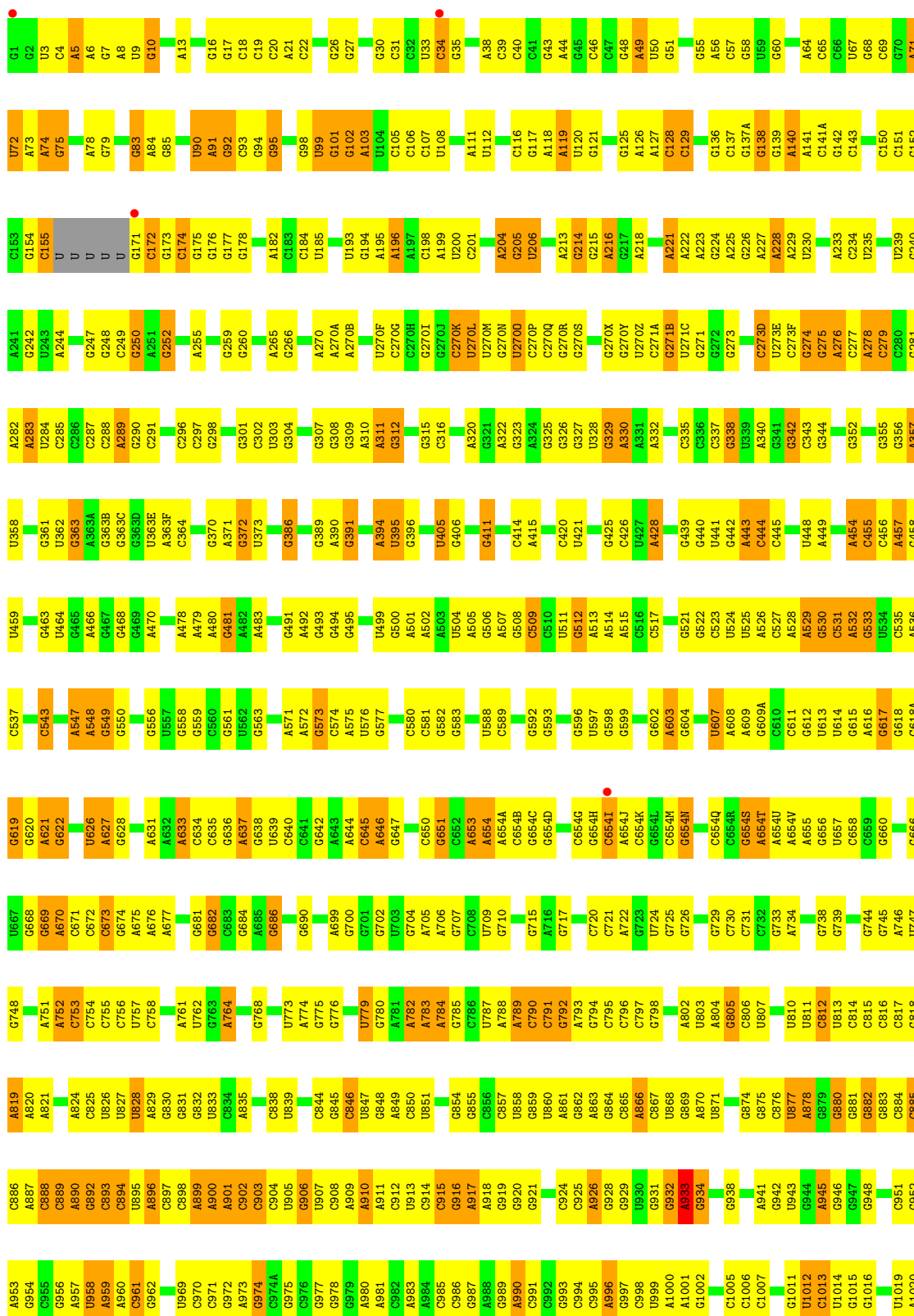


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C2403	C2404	G2405	A2406	G2407	G2410	G2415	A2418	U2419	C2420	C2424	A2425	A2426	C2427	G2428	G2429	A2430	U2431	A2434	A2435	U2438	A2439	C2440	C2441	G2444	G2447	A2448	A2451	G2458	U2462	C2467	G2468	A2469	G2470	C2471	G2472	U2473	C2474	C2475	A2477	C2478	G2481	G2482	G2483	G2484	G2485	G2486	G2487																						
G2330	G2331	G2334	A2335	A2336	G2337	G2340	G2341	C2342	C2343	U2344	G2345	A2346	C2347	C2350	G2351	A2352	C2355	A2360	A2361	C2364	G2365	C2366	C2367	C2368	A2369	G2370	G2371	G2372	G2373	C2374	G2375	A2376	A2377	A2378	C2381	G2382	G2383	G2384	C2385	G2389	A2392	A2393	C2394	G2395	G2396	G2400	C2402																						
A2266	A2267	A2268	A2269	U2270	U2271	A2272	A2273	C2275	G2276	A2277	G2278	G2279	G2280	C2281	G2282	C2283	G2284	C2285	A2286	A2287	A2288	G2289	G2290	G2291	C2292	A2298	G2299	G2300	G2301	G2302	G2303	G2304	A2305	C2306	G2307	G2308	A2309	A2310	A2311	G2312	G2313	C2314	G2315	C2316	G2317	G2318	G2319	A2320	G2321	A2322	C2323	G2324	G2325	G2326	A2327	A2328	G2329												
G2187	C2188	U2189	G2190	A2191	G2192	G2193	C2196	U2197	A2198	A2199	G2200	C2201	G2202	A2203	G2204	G2205	G2206	G2207	U2208	C2209	G2210	G2211	A2212	G2213	G2214	G2215	A2216	G2219	G2220	A2221	G2222	A2223	G2224	A2225	C2226	A2227	G2228	G2229	G2230	C2231	G2232	U2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	U2244	G2245	G2246	A2247	G2250	G2251	G2255	G2256	G2257	C2258	G2259	G2260	C2261	G2262	C2263	G2264	U2265
U2118	A2119	G2123	A2124	G2125	A2126	G2127	G2128	G2131	U2132	G2133	A2134	A2135	C2136	G2137	C2138	G2139	C2140	C2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	C2149	U2150	G2151	C2152	G2153	C2154	G2155	G2156	G2157	A2158	C2161	G2162	C2163	G2164	G2165	G2166	U2167	G2168	A2169	U2170	A2171	U2172	C2173	G2174	G2181	G2182	C2183	G2184	C2185	G2186														
C2040	U2041	C2042	C2043	C2050	A2051	G2052	G2053	G2054	C2055	G2056	A2060	G2061	A2062	C2063	C2064	G2065	C2066	G2067	U2068	G2069	G2070	U2074	U2075	C2078	U2079	A2082	G2083	U2086	G2087	G2088	U2089	G2090	G2091	A2092	A2093	A2094	C2095	U2096	C2097	U2098	U2099	G2100	G2101	U2102	C2103	G2104	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	A2117														
A1952	U1955	U1956	C1957	C1958	G1958	U1963	U1967	C1968	A1969	A1970	A1971	A1972	C1973	C1974	G1980	A1981	C1982	G1983	C1984	G1989	C1990	U1991	G1992	U1993	C1999	G2000	A2001	G2002	C2007	C2008	G2009	G2010	A2011	A2012	A2013	A2014	U2015	U2016	U2017	G2018	A2019	A2020	G2023	G2024	C2025	C2026	A2030	A2031	G2032	A2033	U2034	G2035	C2036																
G1769	G1770	A1847	U1854	A1773	G1776	U1777	U1778	U1779	A1870	A1871	G1872	U1783	A1784	A1785	C1857	G1888	U1889	G1792	U1893	U1794	C1795	U1796	C1797	U1902	G1903	C1800	A1801	A1802	A1803	U1805	A1810	G1811	A1812	G1813	G1816	G1817	U1818	A1819	U1820	A1821	A1825	A1829	G1830	C1831	U1832	U1833	U1834	G1835	G1839	G1763	G1764																		
G1661	C1662	A1847	A1854	A1773	G1776	U1777	U1778	U1779	A1870	A1871	G1872	U1783	A1784	A1785	C1857	G1888	U1889	G1792	U1893	U1794	C1795	U1796	C1797	U1902	G1903	C1800	A1801	A1802	A1803	U1805	A1810	G1811	A1812	G1813	G1816	G1817	U1818	A1819	U1820	A1821	A1825	A1829	G1830	C1831	U1832	U1833	U1834	G1835	G1839	G1763	G1764																		

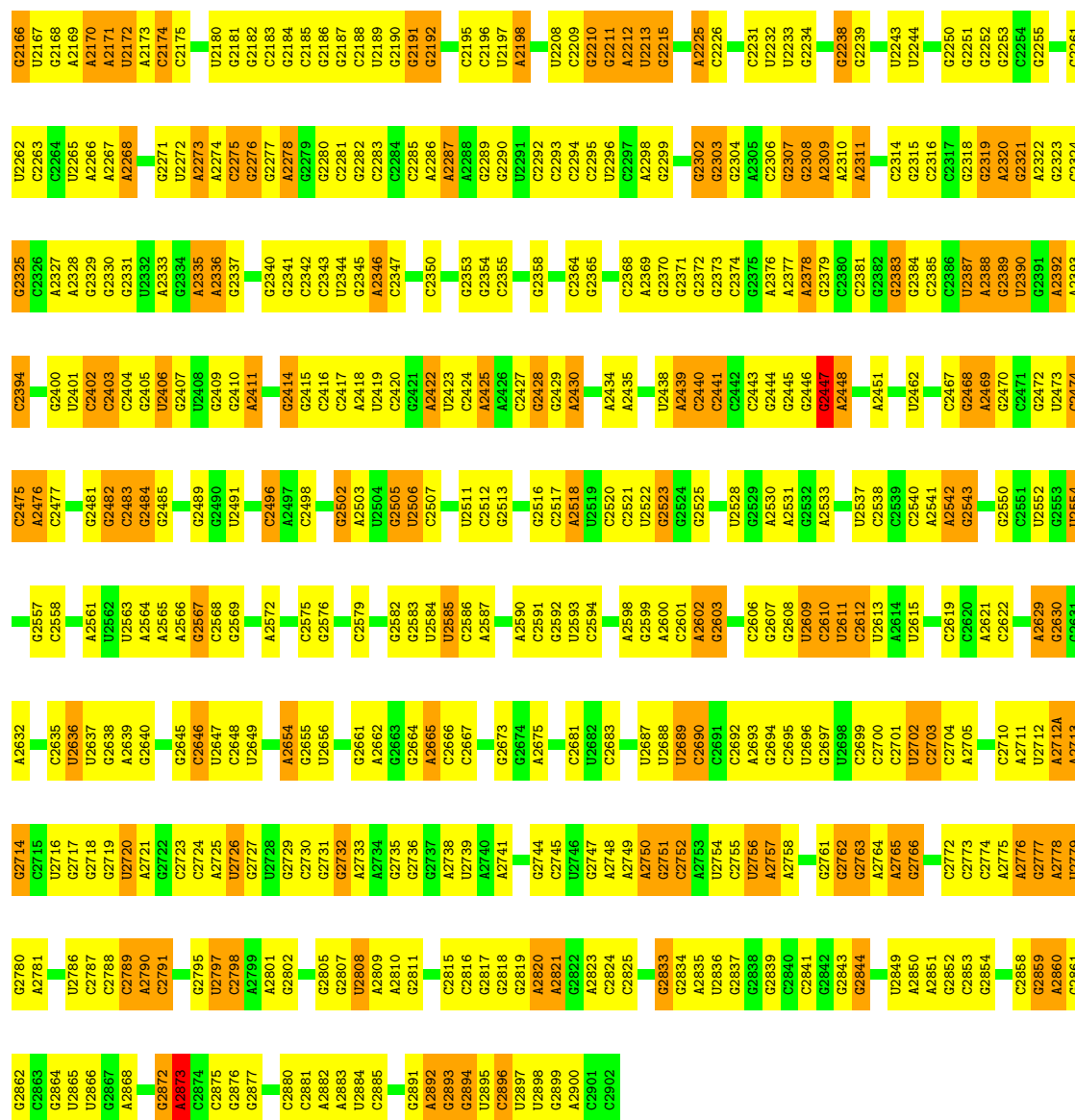
● Molecule 25: RNA (2912-MER)

Chain DA:  40% 45% 16%



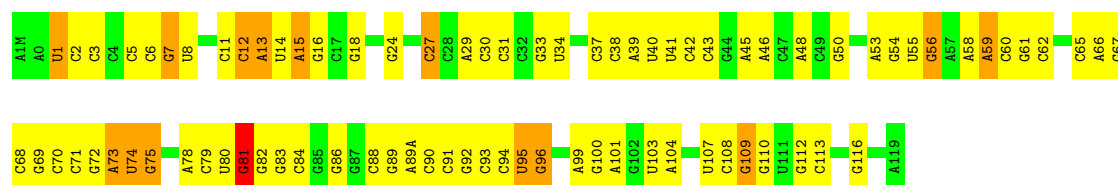






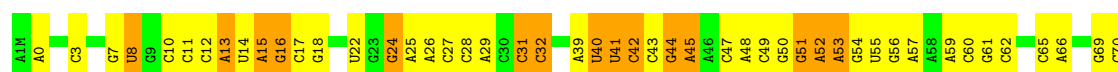
• Molecule 26: 5S RIBOSOMAL RNA

Chain BB: 33% 55% 11%



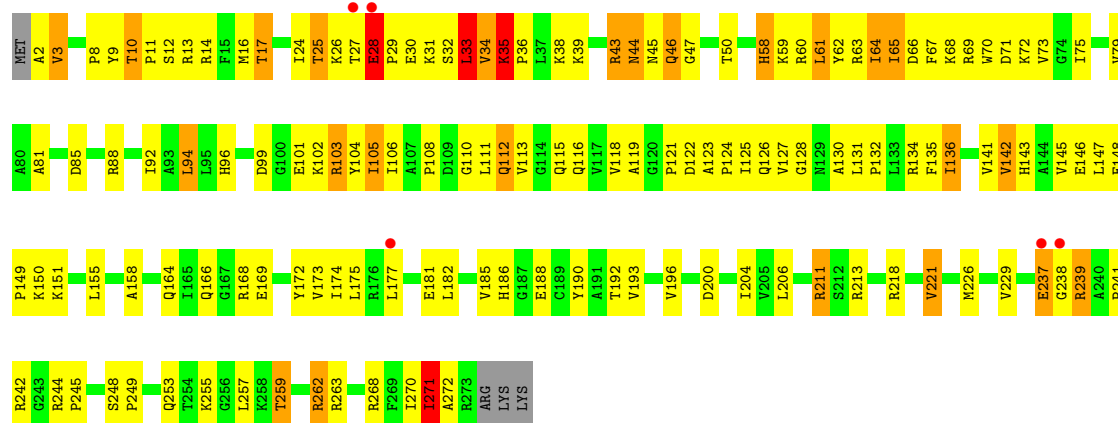
• Molecule 26: 5S RIBOSOMAL RNA

Chain DB: 39% 41% 19%

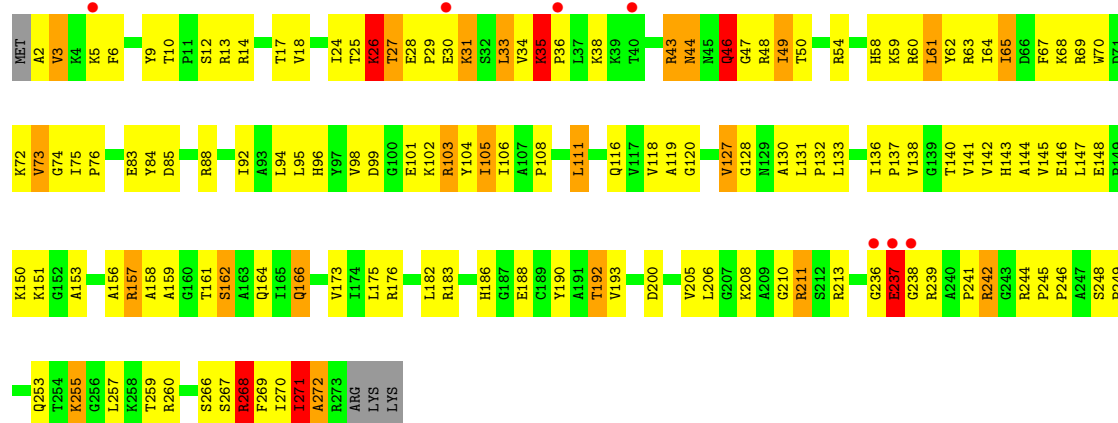




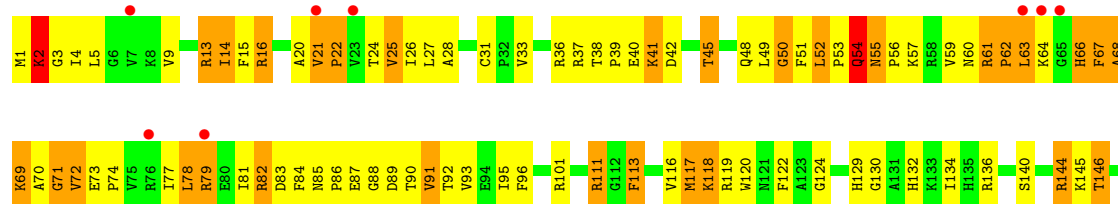
• Molecule 27: 50S ribosomal protein L2



• Molecule 27: 50S ribosomal protein L2

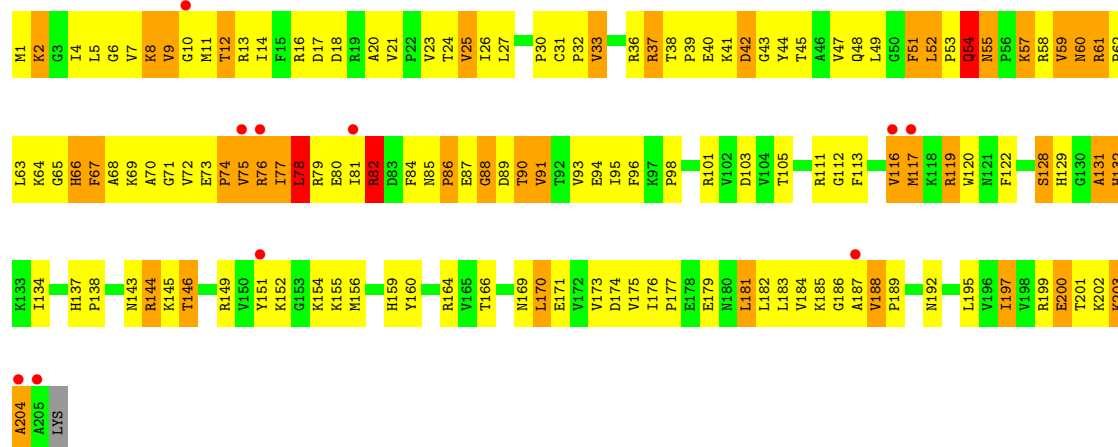


• Molecule 28: 50S ribosomal protein L3

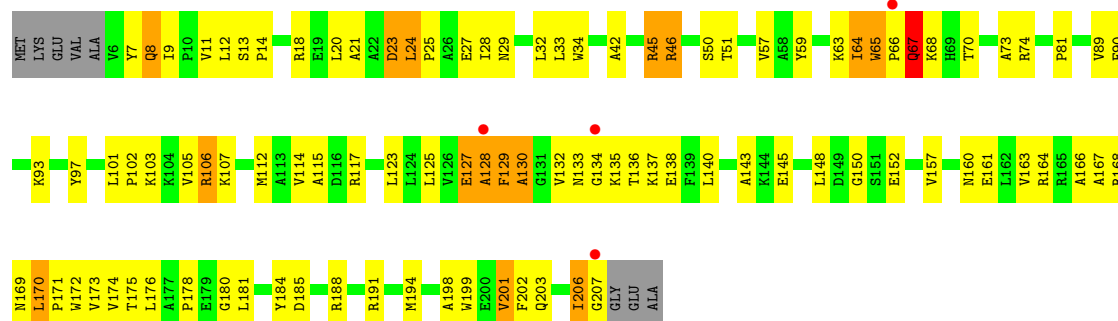




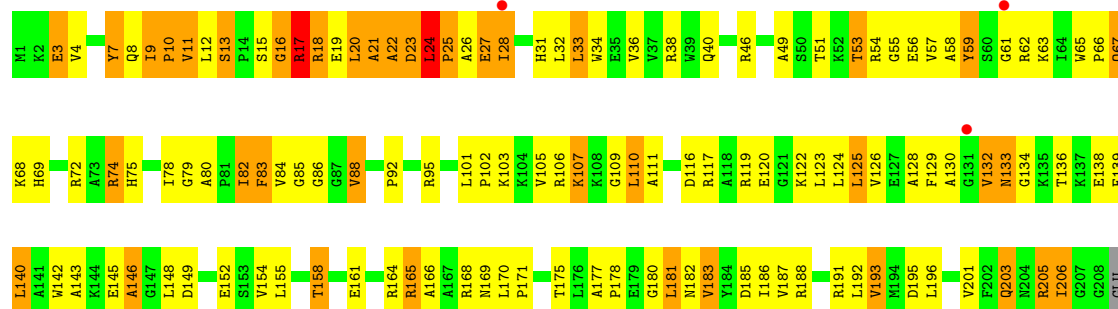
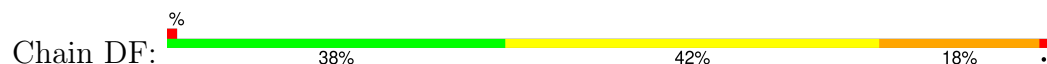
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

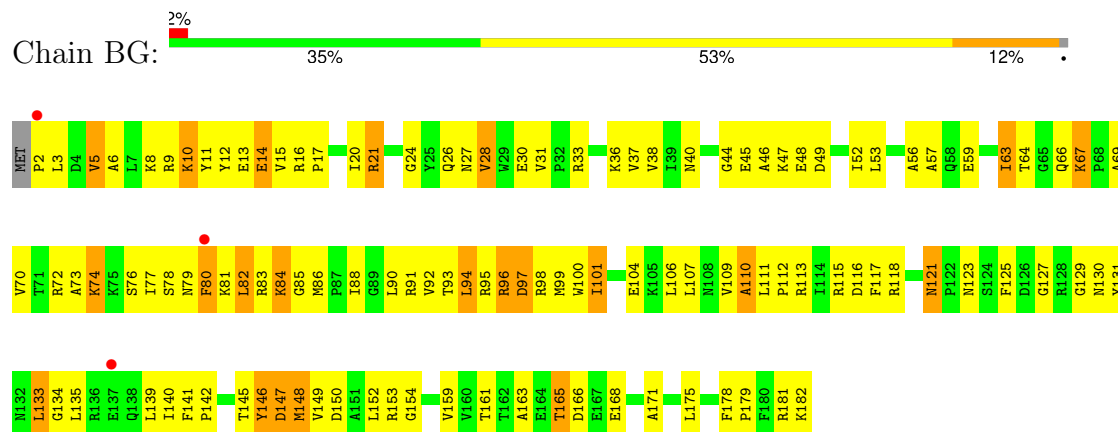


• Molecule 29: 50S ribosomal protein L4

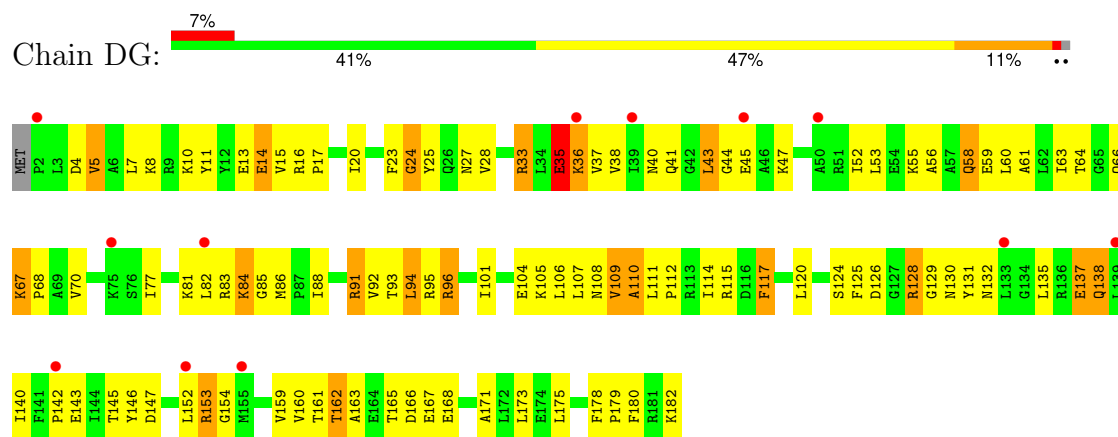


ALA

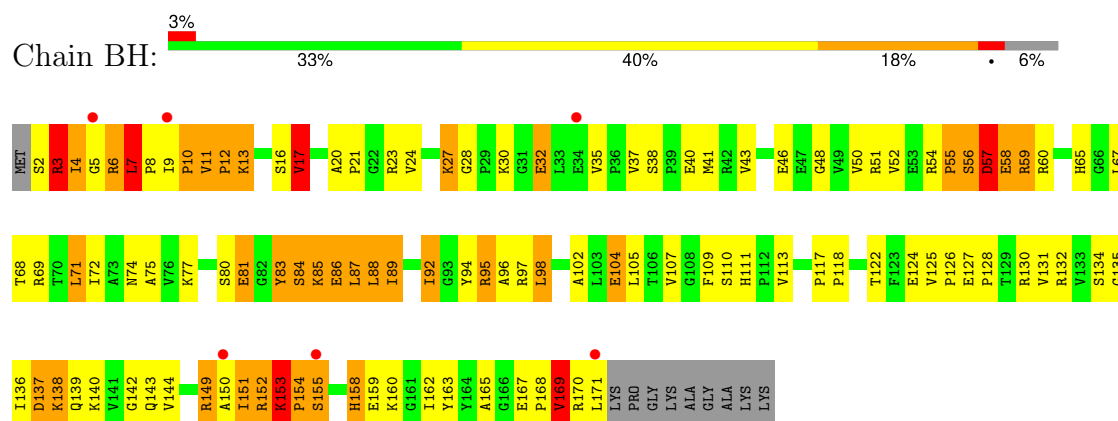
- Molecule 30: 50S ribosomal protein L5



- Molecule 30: 50S ribosomal protein L5

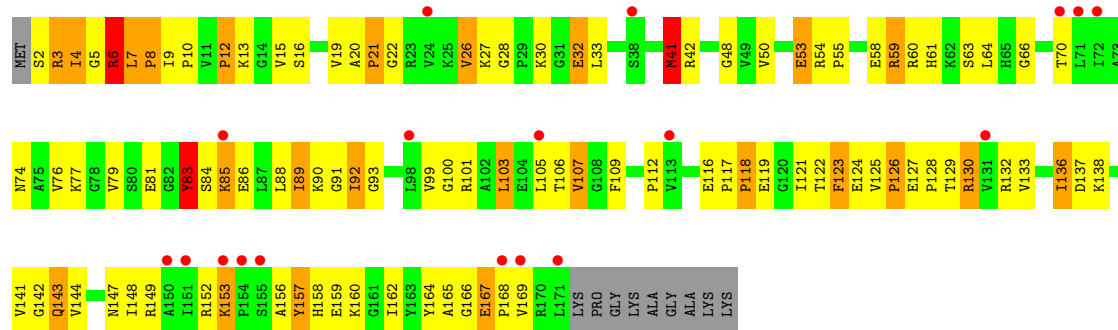


- Molecule 31: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L6

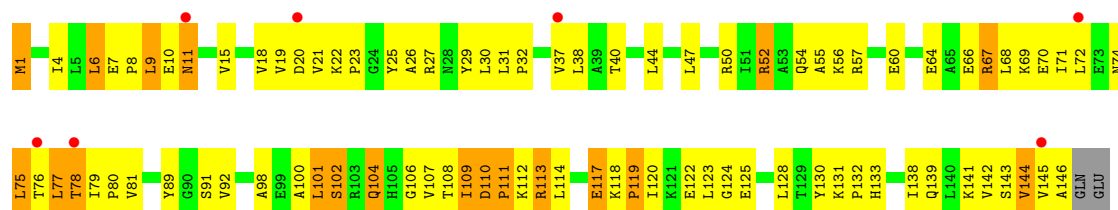
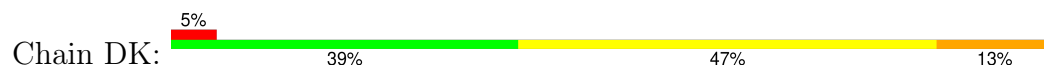




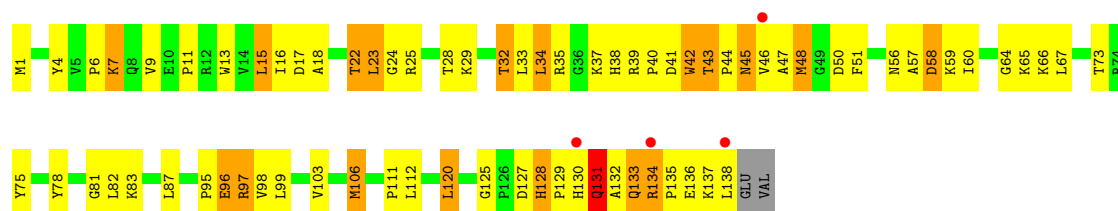
• Molecule 32: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L9

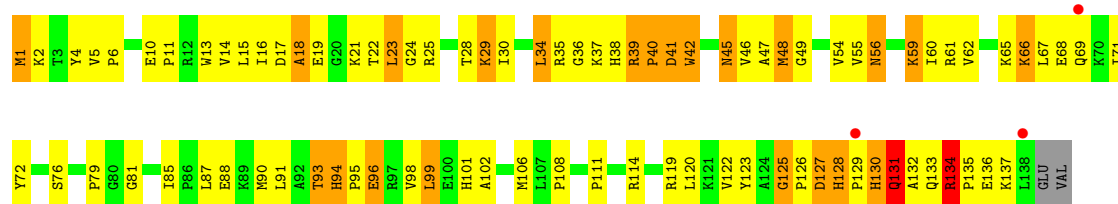


• Molecule 33: 50S ribosomal protein L13



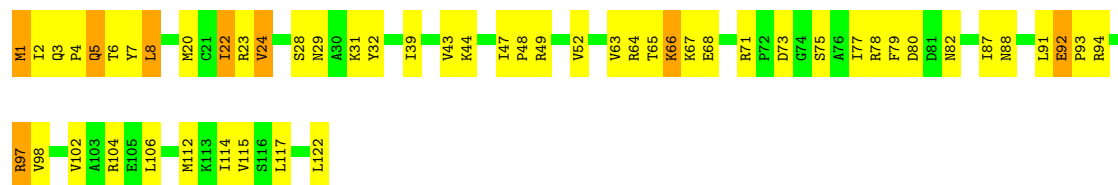
• Molecule 33: 50S ribosomal protein L13





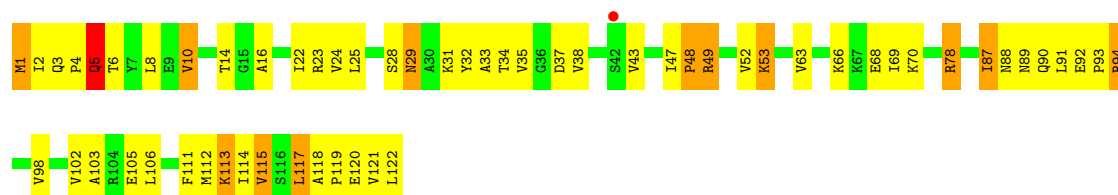
• Molecule 34: 50S ribosomal protein L14

Chain BN: 57% 37% 7%



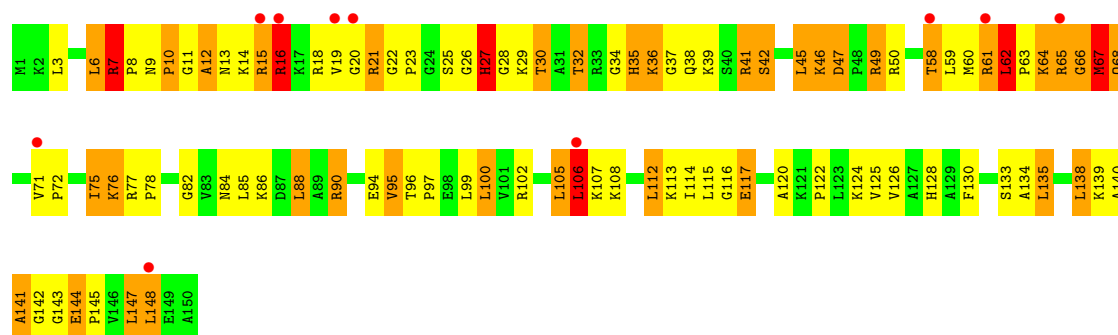
• Molecule 34: 50S ribosomal protein L14

Chain DN: 52% 38% 10%



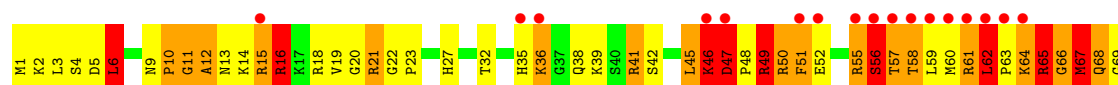
• Molecule 35: 50S ribosomal protein L15

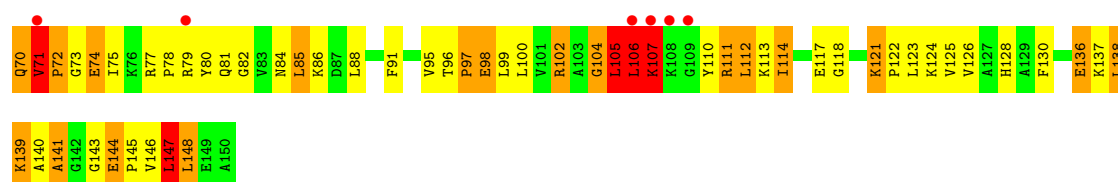
Chain BO: 35% 37% 24%



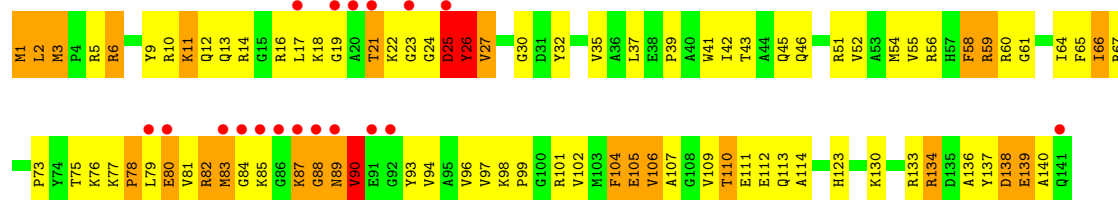
• Molecule 35: 50S ribosomal protein L15

Chain DO: 29% 38% 23% 9%

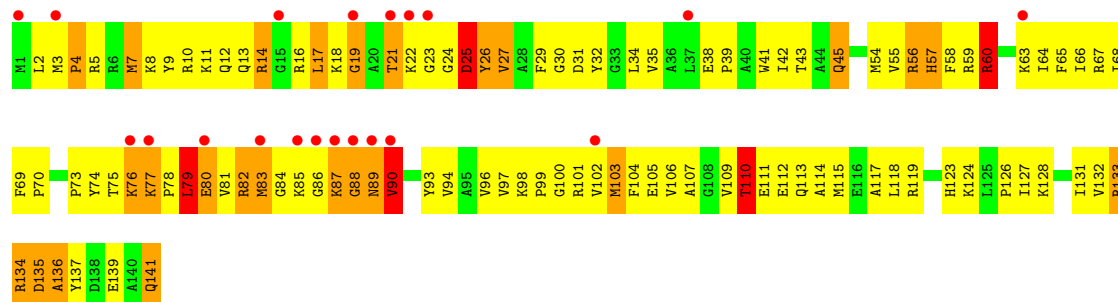




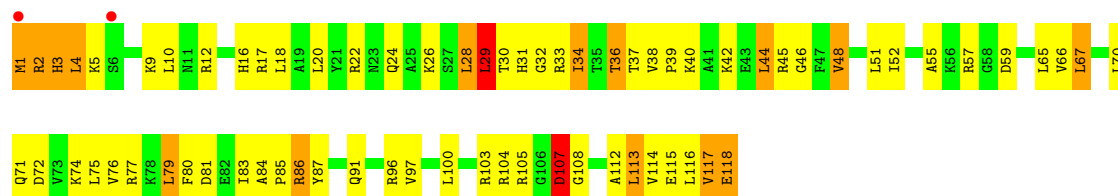
• Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17

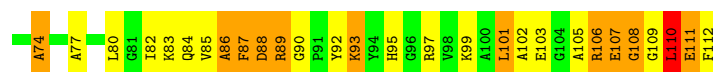




- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



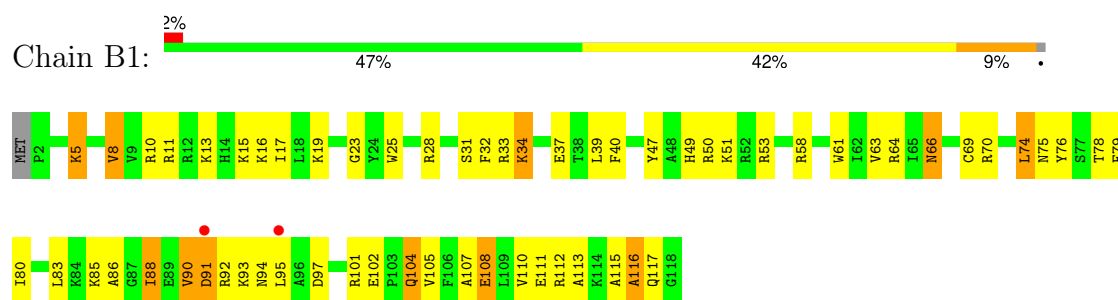
PRO  
LYS  
ALA  
SER  
GLN  
GLU

- Molecule 39: 50S ribosomal protein L19

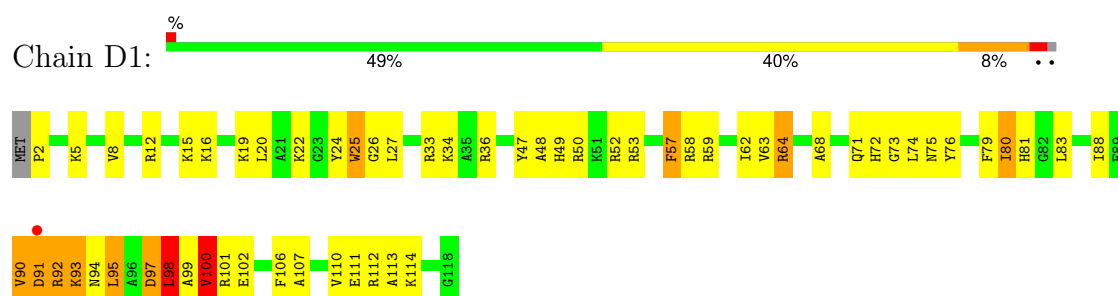




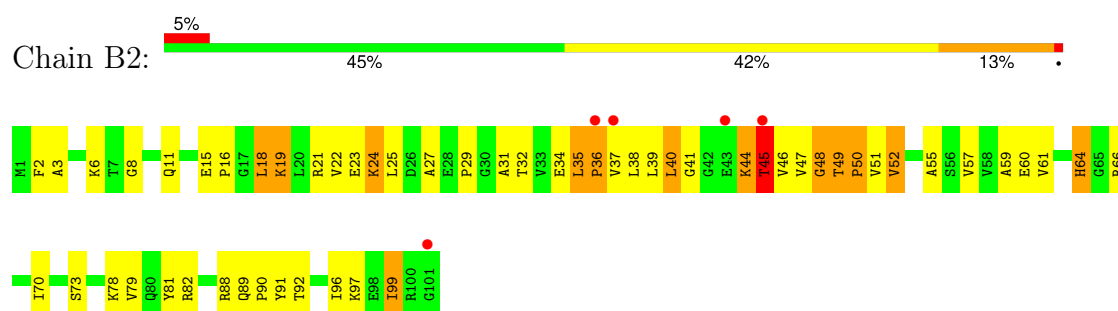
- Molecule 40: 50S ribosomal protein L20



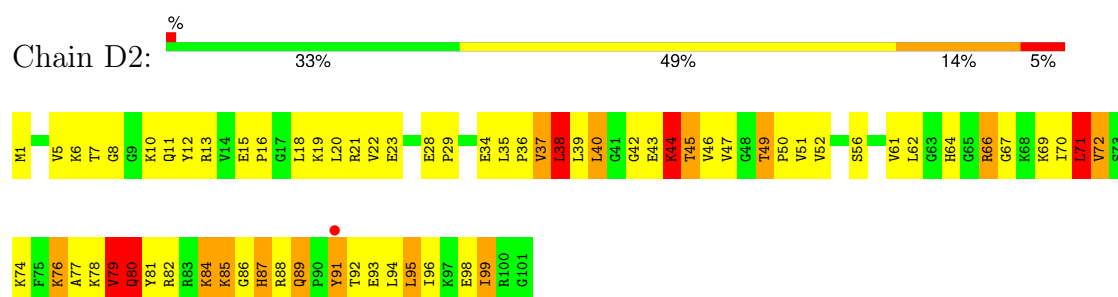
- Molecule 40: 50S ribosomal protein L20



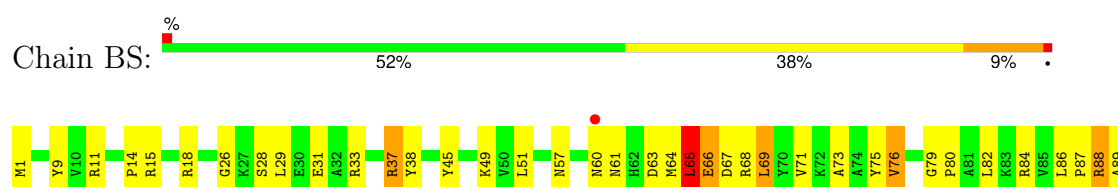
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

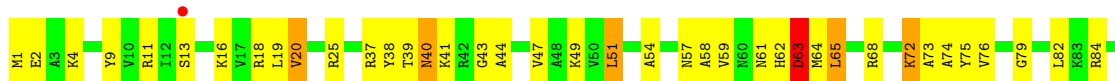


- Molecule 42: 50S ribosomal protein L22

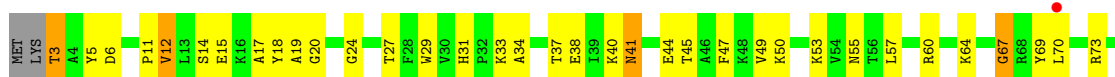




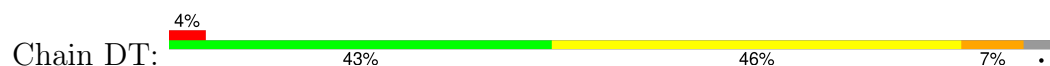
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23

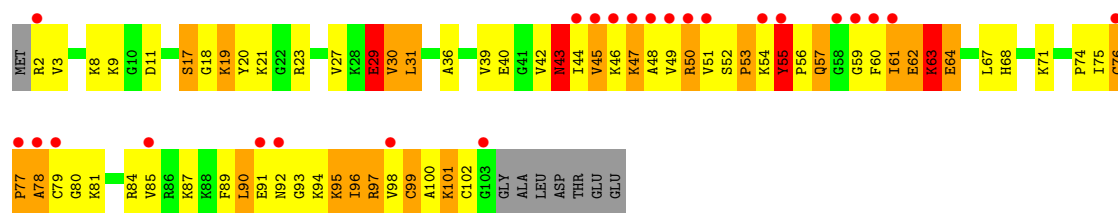


- Molecule 44: 50S ribosomal protein L24

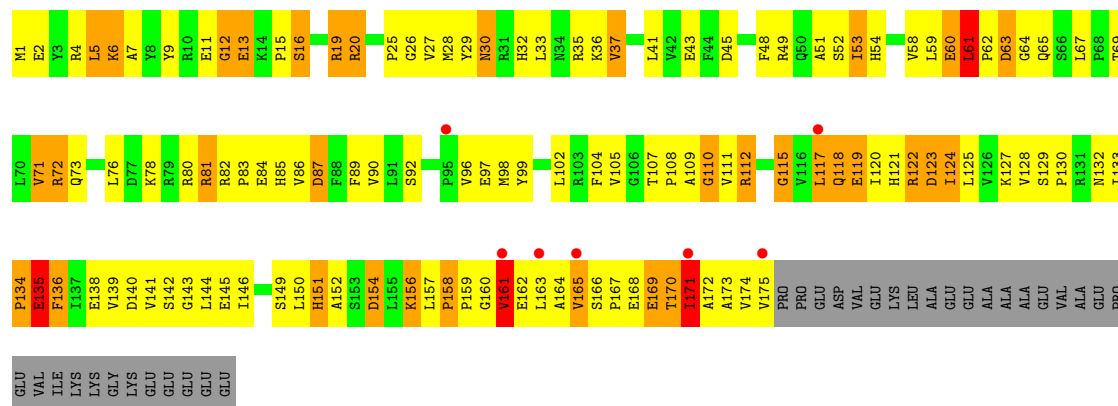
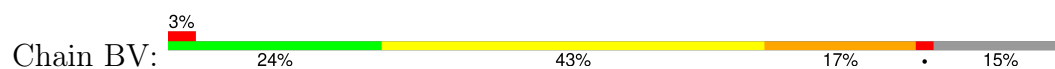


- Molecule 44: 50S ribosomal protein L24

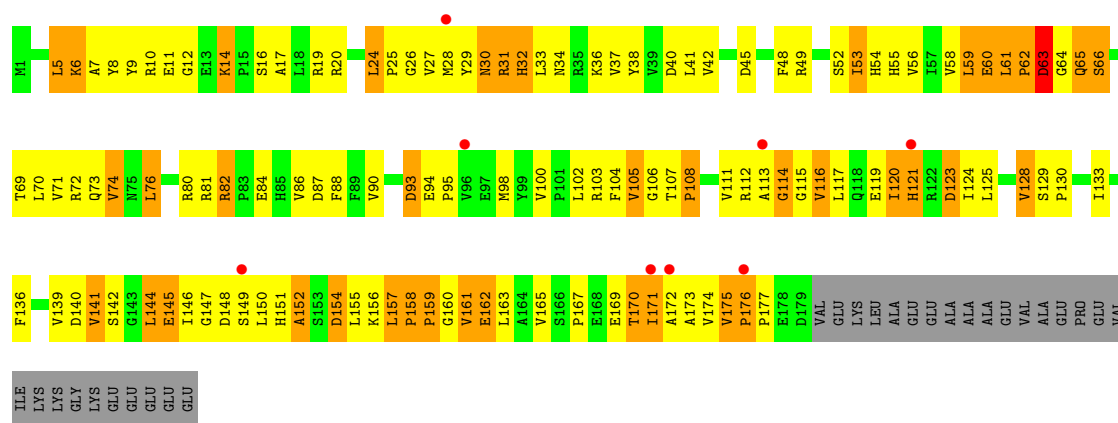




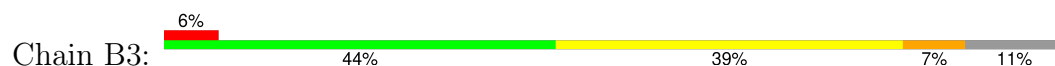
- Molecule 45: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L25

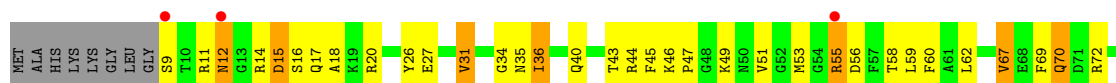
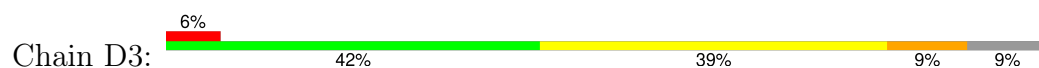


- Molecule 46: 50S ribosomal protein L27

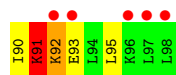




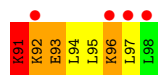
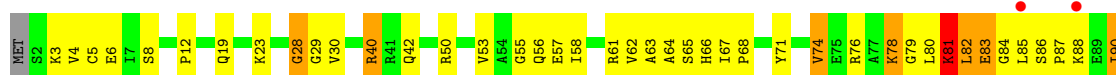
• Molecule 46: 50S ribosomal protein L27



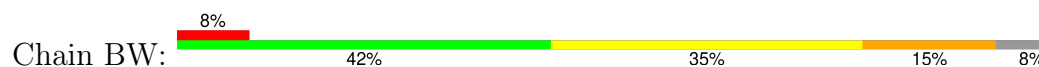
• Molecule 47: 50S ribosomal protein L28



• Molecule 47: 50S ribosomal protein L28

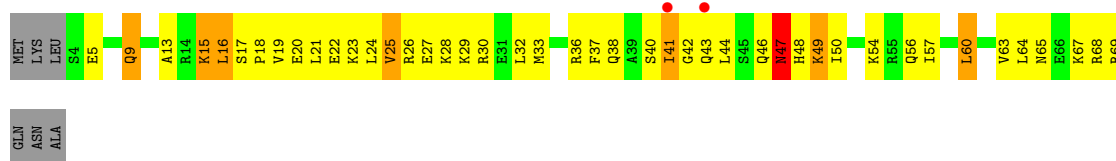


• Molecule 48: 50S ribosomal protein L29



• Molecule 48: 50S ribosomal protein L29





- Molecule 49: 50S ribosomal protein L30

Chain BX: 55% 38% 5%



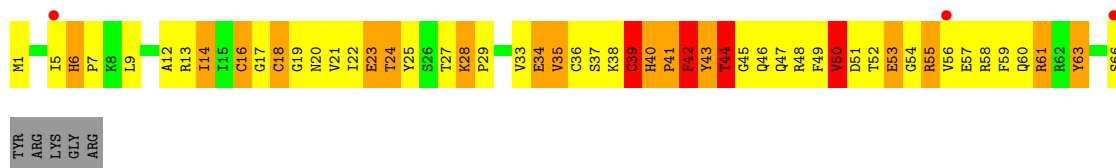
- Molecule 49: 50S ribosomal protein L30

Chain DX: 2% 40% 55%



- Molecule 50: 50S ribosomal protein L31

Chain B4: 4% 20% 45% 23% 6% 7%



- Molecule 50: 50S ribosomal protein L31

Chain D4: 8% 13% 42% 31% 11%

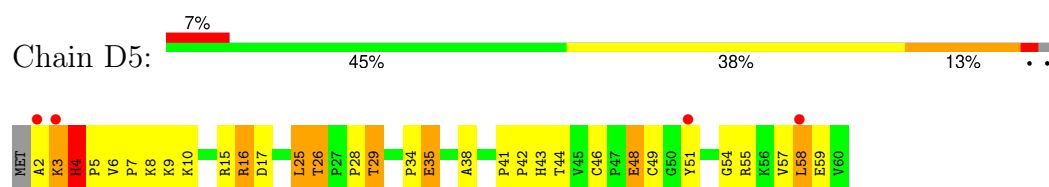


- Molecule 51: 50S ribosomal protein L32

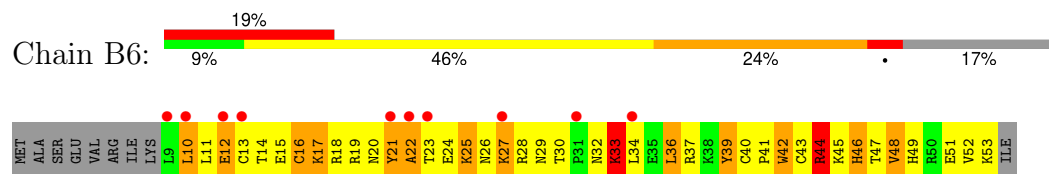
Chain B5: 7% 42% 37% 17%



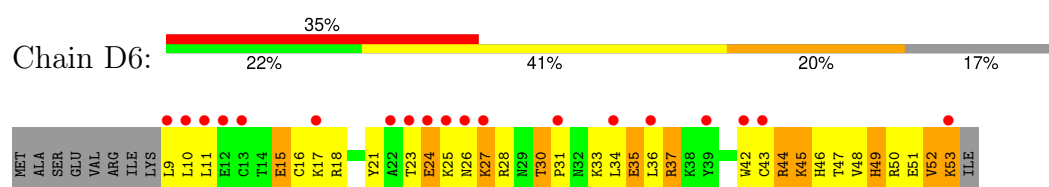
- Molecule 51: 50S ribosomal protein L32



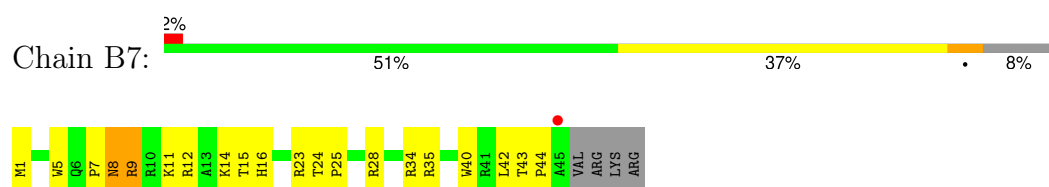
- Molecule 52: 50S ribosomal protein L33



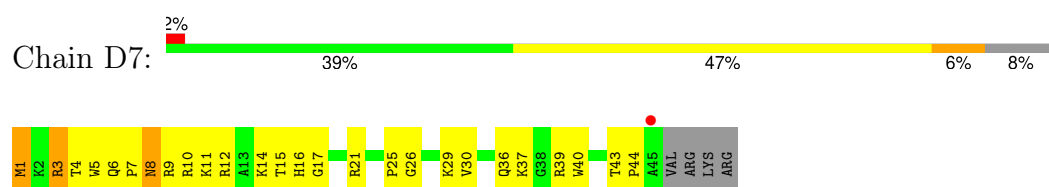
- Molecule 52: 50S ribosomal protein L33



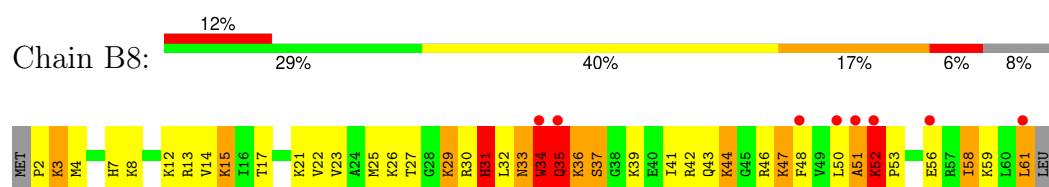
- Molecule 53: 50S ribosomal protein L34



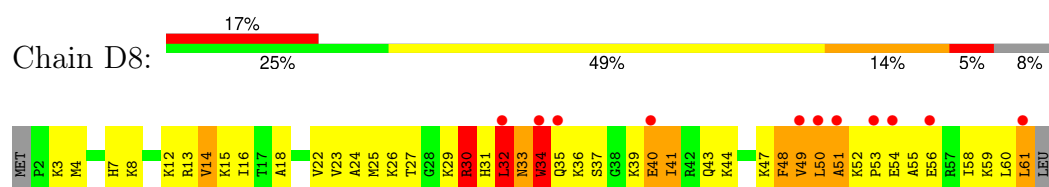
- Molecule 53: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	210.67Å 451.75Å 625.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.06 – 3.00 154.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.06-3.00) 93.5 (154.06-3.00)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, $R_{free}$	0.203 , 0.235 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 76.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	299676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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%)	0	2
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	0	1
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	2	10
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	1	6
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	2	14
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	1	4
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	3	17
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	10	39
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	3	20
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	3	18
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	2	14
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	1	7
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	5	27
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	1	4
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	1	4
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	3	19
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	1	9
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	2	13
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	3	17
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	10
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	11
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	5	26
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	1	7
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	7
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	3	19
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	1	8
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	2	13
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	0	2
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	0	2
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	3
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	0	2
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	0	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	11
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	12
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	1
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	12
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	0	1
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	1	4
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	1	7
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	5
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	1	7
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	2
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	33
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	18

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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	1
37	B0	116/118 (98%)	97 (84%)	11 (10%)	8 (7%)	1	5
37	D0	115/118 (98%)	95 (83%)	15 (13%)	5 (4%)	2	13
38	BQ	109/112 (97%)	85 (78%)	17 (16%)	7 (6%)	1	6
38	DQ	109/112 (97%)	73 (67%)	26 (24%)	10 (9%)	0	2
39	BR	135/146 (92%)	105 (78%)	21 (16%)	9 (7%)	1	5
39	DR	135/146 (92%)	108 (80%)	18 (13%)	9 (7%)	1	5
40	B1	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	2	13
40	D1	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	1	9
41	B2	99/101 (98%)	81 (82%)	12 (12%)	6 (6%)	1	7
41	D2	99/101 (98%)	68 (69%)	17 (17%)	14 (14%)	0	1
42	BS	111/113 (98%)	92 (83%)	13 (12%)	6 (5%)	1	9
42	DS	111/113 (98%)	92 (83%)	15 (14%)	4 (4%)	3	16
43	BT	90/96 (94%)	81 (90%)	5 (6%)	4 (4%)	2	12
43	DT	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	1	8
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	0
46	B3	74/85 (87%)	65 (88%)	6 (8%)	3 (4%)	2	13
46	D3	75/85 (88%)	64 (85%)	8 (11%)	3 (4%)	2	14
47	BZ	95/98 (97%)	79 (83%)	12 (13%)	4 (4%)	2	13
47	DZ	95/98 (97%)	76 (80%)	11 (12%)	8 (8%)	0	3
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	6
49	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	7	32
49	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	1	9
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%)	1	9
52	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	0
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	3

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	6
2	CE	205/220 (93%)	180 (88%)	25 (12%)	4	18
3	AF	159/188 (85%)	141 (89%)	18 (11%)	4	21
3	CF	160/188 (85%)	143 (89%)	17 (11%)	5	23
4	AG	180/180 (100%)	160 (89%)	20 (11%)	5	21
4	CG	180/180 (100%)	160 (89%)	20 (11%)	5	21
5	AH	116/123 (94%)	97 (84%)	19 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CH	116/123 (94%)	102 (88%)	14 (12%)	4	18
6	AI	90/90 (100%)	80 (89%)	10 (11%)	5	21
6	CI	90/90 (100%)	81 (90%)	9 (10%)	6	25
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	2	10
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	9
8	AK	119/119 (100%)	106 (89%)	13 (11%)	5	22
8	CK	119/119 (100%)	111 (93%)	8 (7%)	13	43
9	AL	98/99 (99%)	86 (88%)	12 (12%)	4	18
9	CL	98/99 (99%)	81 (83%)	17 (17%)	1	8
10	AM	89/92 (97%)	79 (89%)	10 (11%)	5	21
10	CM	89/92 (97%)	78 (88%)	11 (12%)	4	17
11	AN	90/99 (91%)	79 (88%)	11 (12%)	4	18
11	CN	90/99 (91%)	85 (94%)	5 (6%)	17	49
12	AO	104/109 (95%)	95 (91%)	9 (9%)	8	32
12	CO	104/109 (95%)	94 (90%)	10 (10%)	7	27
13	AP	94/101 (93%)	87 (93%)	7 (7%)	11	38
13	CP	94/101 (93%)	83 (88%)	11 (12%)	4	19
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	3	17
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	9	34
15	AR	79/80 (99%)	73 (92%)	6 (8%)	11	37
15	CR	79/80 (99%)	67 (85%)	12 (15%)	2	11
16	AS	72/74 (97%)	68 (94%)	4 (6%)	17	49
16	CS	72/74 (97%)	64 (89%)	8 (11%)	5	21
17	AT	95/97 (98%)	85 (90%)	10 (10%)	5	23
17	CT	95/97 (98%)	92 (97%)	3 (3%)	34	67
18	AU	63/77 (82%)	57 (90%)	6 (10%)	7	28
18	CU	63/77 (82%)	51 (81%)	12 (19%)	1	7
19	AV	67/80 (84%)	55 (82%)	12 (18%)	1	8
19	CV	67/80 (84%)	58 (87%)	9 (13%)	3	15
20	AW	76/82 (93%)	68 (90%)	8 (10%)	5	23
20	CW	76/82 (93%)	66 (87%)	10 (13%)	3	15

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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%)	1	9
27	DD	214/218 (98%)	181 (85%)	33 (15%)	2	11
28	BE	165/166 (99%)	135 (82%)	30 (18%)	1	7
28	DE	165/166 (99%)	139 (84%)	26 (16%)	2	10
29	BF	161/166 (97%)	141 (88%)	20 (12%)	4	17
29	DF	165/166 (99%)	140 (85%)	25 (15%)	2	11
30	BG	155/156 (99%)	135 (87%)	20 (13%)	3	16
30	DG	155/156 (99%)	139 (90%)	16 (10%)	6	24
31	BH	142/148 (96%)	122 (86%)	20 (14%)	3	13
31	DH	142/148 (96%)	124 (87%)	18 (13%)	3	17
32	BK	122/124 (98%)	101 (83%)	21 (17%)	1	8
32	DK	122/124 (98%)	106 (87%)	16 (13%)	3	15
33	BM	117/119 (98%)	98 (84%)	19 (16%)	2	10
33	DM	117/119 (98%)	97 (83%)	20 (17%)	1	8
34	BN	100/100 (100%)	92 (92%)	8 (8%)	10	35
34	DN	100/100 (100%)	87 (87%)	13 (13%)	3	16
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	1
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	1
36	BP	111/111 (100%)	94 (85%)	17 (15%)	2	11
36	DP	111/111 (100%)	89 (80%)	22 (20%)	1	6
37	B0	101/101 (100%)	85 (84%)	16 (16%)	2	10
37	D0	100/101 (99%)	82 (82%)	18 (18%)	1	7
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	2	10
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	7	29
39	BR	120/127 (94%)	99 (82%)	21 (18%)	1	8
39	DR	120/127 (94%)	102 (85%)	18 (15%)	2	12
40	B1	93/94 (99%)	85 (91%)	8 (9%)	8	32
40	D1	93/94 (99%)	82 (88%)	11 (12%)	4	19
41	B2	82/82 (100%)	70 (85%)	12 (15%)	2	12

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

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	2.09	3 (12%)	22,44,47	2.76	8 (36%)
22	MIA	CB	38	22	24,31,32	2.13	3 (12%)	22,44,47	2.38	8 (36%)
22	MIA	CD	38	22	24,31,32	2.12	3 (12%)	22,44,47	2.83	8 (36%)
22	MIA	AB	38	22	24,31,32	2.04	3 (12%)	22,44,47	2.38	7 (31%)

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	CB	38	22	-	4/11/33/34	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



The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CB	38	MIA	C6-N6	7.39	1.46	1.34
22	CD	38	MIA	C6-N6	7.08	1.46	1.34
22	AD	38	MIA	C6-N6	6.98	1.45	1.34
22	AB	38	MIA	C6-N6	6.85	1.45	1.34
22	CB	38	MIA	C13-C14	6.08	1.50	1.32

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	38	MIA	C11-S10-C2	10.16	109.88	102.25
22	AD	38	MIA	C11-S10-C2	9.68	109.51	102.25
22	CB	38	MIA	C11-S10-C2	7.56	107.92	102.25
22	AB	38	MIA	C12-C13-C14	-6.26	115.77	127.01
22	AB	38	MIA	C11-S10-C2	5.96	106.72	102.25

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	CB	38	MIA	3	0
22	CD	38	MIA	4	0
22	AB	38	MIA	1	0

## 5.5 Carbohydrates

There are no oligosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1502/1506 (99%)	-0.29	3 (0%) 92 84	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.25	9 (0%) 85 71	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.31	10 (4%) 41 24	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.49	9 (3%) 44 26	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.34	3 (1%) 71 50	88, 113, 149, 158	0
3	CF	206/239 (86%)	0.51	11 (5%) 33 19	101, 135, 165, 180	0
4	AG	208/208 (100%)	0.25	4 (1%) 66 44	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.25	8 (3%) 44 26	75, 95, 123, 135	0
5	AH	151/162 (93%)	-0.01	1 (0%) 84 68	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.33	5 (3%) 49 29	84, 106, 131, 167	0
6	AI	101/101 (100%)	-0.26	0 100 100	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.39	0 100 100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.42	15 (9%) 15 8	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.52	13 (8%) 18 10	100, 119, 147, 158	0
8	AK	138/138 (100%)	0.09	0 100 100	81, 103, 117, 132	0
8	CK	138/138 (100%)	-0.06	1 (0%) 84 68	81, 108, 125, 136	0
9	AL	127/128 (99%)	0.40	3 (2%) 59 37	83, 138, 159, 166	0
9	CL	127/128 (99%)	0.46	8 (6%) 27 15	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.51	0 100 100	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.56	7 (7%) 23 13	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.35	6 (5%) 35 20	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.23	3 (2%) 58 36	74, 99, 133, 164	0
12	AO	125/132 (94%)	0.06	4 (3%) 50 30	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.42	13 (10%) 13 7	63, 91, 126, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	116/126 (92%)	0.31	4 (3%)	48	28	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.59	10 (8%)	18	10	91, 145, 161, 169	0
14	AQ	58/61 (95%)	0.42	2 (3%)	48	28	87, 103, 120, 127	0
14	CQ	58/61 (95%)	0.81	3 (5%)	34	19	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.02	1 (1%)	77	58	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.03	1 (1%)	77	58	67, 96, 124, 136	0
16	AS	84/88 (95%)	0.37	4 (4%)	36	21	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.11	1 (1%)	76	56	76, 91, 118, 157	0
17	AT	100/105 (95%)	0.39	7 (7%)	24	13	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.38	6 (6%)	29	16	75, 100, 126, 144	0
18	AU	72/88 (81%)	-0.12	0	100	100	77, 97, 135, 164	0
18	CU	72/88 (81%)	-0.31	0	100	100	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.33	4 (5%)	34	19	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.74	7 (8%)	17	9	128, 152, 178, 186	0
20	AW	99/106 (93%)	0.40	4 (4%)	43	25	96, 121, 148, 153	0
20	CW	99/106 (93%)	0.29	3 (3%)	52	31	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.57	2 (8%)	20	11	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.86	3 (12%)	10	6	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.32	4 (4%)	36	21	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.15	3 (3%)	46	27	70, 147, 206, 218	0
22	CB	84/85 (98%)	0.46	3 (3%)	46	27	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.00	0	100	100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.17	1 (1%)	74	54	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.14	1 (1%)	74	54	79, 104, 143, 165	0
24	A1	16/16 (100%)	0.62	3 (18%)	4	3	66, 97, 168, 177	0
24	C1	16/16 (100%)	0.70	3 (18%)	4	3	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.62	10 (0%)	90	81	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.41	12 (0%)	89	77	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.55	0	100	100	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.24	2 (1%)	70	49	78, 110, 139, 198	0
27	BD	272/276 (98%)	-0.11	5 (1%)	67	45	39, 59, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	272/276 (98%)	-0.08	7 (2%) 57 35	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.31	13 (6%) 27 15	44, 77, 125, 150	0
28	DE	205/206 (99%)	0.24	10 (4%) 36 20	56, 92, 144, 157	0
29	BF	202/210 (96%)	-0.24	4 (1%) 64 43	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.08	3 (1%) 73 52	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.12	3 (1%) 69 47	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.52	12 (6%) 26 14	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.15	6 (3%) 47 28	71, 105, 126, 151	0
31	DH	170/180 (94%)	0.95	18 (10%) 13 7	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.29	4 (2%) 56 34	72, 120, 141, 153	0
32	DK	146/148 (98%)	0.27	7 (4%) 36 21	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.20	4 (2%) 54 32	58, 79, 115, 136	0
33	DM	138/140 (98%)	0.35	3 (2%) 62 40	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.22	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	0.18	1 (0%) 82 66	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.31	10 (6%) 25 14	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.79	23 (15%) 6 4	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.52	18 (12%) 9 5	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.88	20 (14%) 7 4	58, 100, 130, 154	0
37	B0	118/118 (100%)	-0.18	2 (1%) 69 47	53, 74, 96, 106	0
37	D0	117/118 (99%)	-0.11	2 (1%) 69 47	62, 81, 100, 117	0
38	BQ	111/112 (99%)	-0.13	3 (2%) 56 34	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.09	3 (2%) 56 34	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.32	5 (3%) 46 27	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.34	6 (4%) 39 23	73, 94, 154, 184	0
40	B1	117/118 (99%)	-0.12	2 (1%) 69 47	50, 70, 98, 140	0
40	D1	117/118 (99%)	-0.06	1 (0%) 81 63	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.26	5 (4%) 35 20	46, 91, 116, 128	0
41	D2	101/101 (100%)	0.17	1 (0%) 79 60	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.25	1 (0%) 81 63	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.03	3 (2%) 56 34	61, 75, 109, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BT	92/96 (95%)	-0.04	2 (2%) 62 40	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.18	4 (4%) 40 23	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.54	10 (9%) 14 8	70, 94, 144, 165	0
44	DU	102/110 (92%)	1.26	24 (23%) 2 2	78, 111, 162, 172	0
45	BV	175/206 (84%)	0.57	7 (4%) 43 25	79, 120, 189, 194	0
45	DV	179/206 (86%)	0.66	8 (4%) 39 22	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.05	5 (6%) 26 14	51, 72, 92, 125	0
46	D3	77/85 (90%)	0.40	5 (6%) 26 15	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.29	7 (7%) 23 13	48, 71, 115, 155	0
47	DZ	97/98 (98%)	0.42	6 (6%) 28 15	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.11	6 (9%) 16 9	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.07	2 (3%) 52 31	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.21	0 100 100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.04	1 (1%) 69 47	76, 103, 136, 159	0
50	B4	66/71 (92%)	0.41	3 (4%) 39 22	112, 153, 176, 181	0
50	D4	63/71 (88%)	0.58	6 (9%) 15 9	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.56	4 (6%) 25 14	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.39	4 (6%) 25 14	61, 84, 169, 188	0
52	B6	45/54 (83%)	1.39	10 (22%) 3 2	117, 148, 164, 173	0
52	D6	45/54 (83%)	1.89	19 (42%) 1 1	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.45	1 (2%) 62 40	38, 48, 68, 85	0
53	D7	45/49 (91%)	-0.08	1 (2%) 62 40	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.35	8 (13%) 8 5	51, 68, 88, 115	0
54	D8	60/65 (92%)	1.12	11 (18%) 4 3	64, 80, 106, 132	0
All	All	21100/21658 (97%)	-0.03	599 (2%) 55 33	38, 95, 177, 247	0

The worst 5 of 599 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	B5	2	ALA	9.6
7	CJ	81	GLY	9.4
51	D5	2	ALA	9.2
31	DH	150	ALA	8.1
9	CL	115	GLY	7.9

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MIA	CD	38	29/30	0.90	0.14	101,121,146,154	0
22	MIA	CB	38	29/30	0.91	0.12	63,95,112,126	0
22	MIA	AD	38	29/30	0.93	0.12	98,122,141,145	0
22	MIA	AB	38	29/30	0.95	0.10	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.