



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:03 am GMT

PDB ID : 4V8A  
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*.  
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.  
Deposited on : 2011-12-05  
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

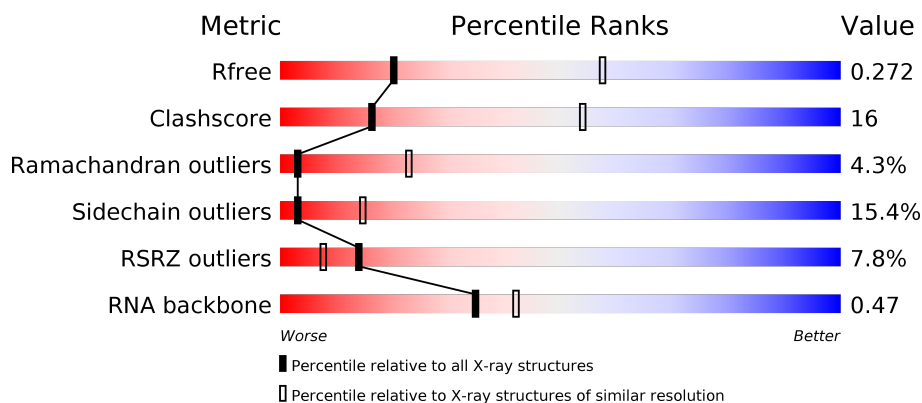
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.









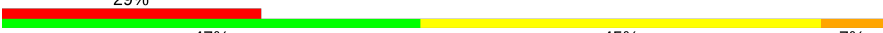







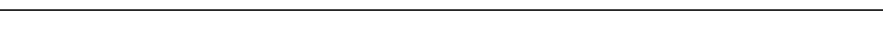




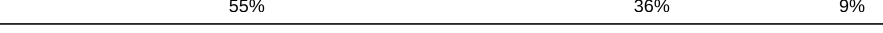





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	2915	<div> <div>4%</div> <div>37% 43% 15% ..</div> </div>
1	BA	2915	<div> <div>3%</div> <div>45% 34% 15% ..</div> </div>
2	AB	122	<div> <div>3%</div> <div>27% 52% 16% ..</div> </div>
2	BB	122	<div> <div></div> <div>49% 35% 13% ..</div> </div>




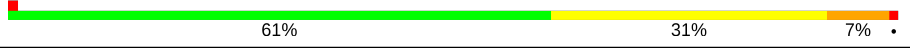






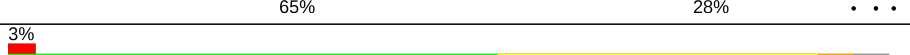
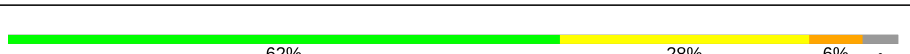





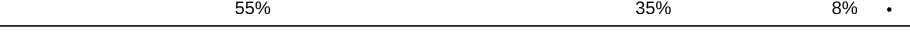
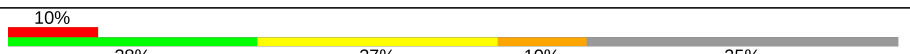





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Mol	Chain	Length	Quality of chain
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	205	
5	BF	205	
6	AG	182	
6	BG	182	
7	AH	180	
7	BH	180	
8	AI	148	
8	BI	148	
9	AN	140	
9	BN	140	
10	AO	122	
10	BO	122	
11	AP	150	
11	BP	150	
12	AQ	141	
12	BQ	141	
13	AR	118	
13	BR	118	
14	AS	112	
14	BS	112	
15	AT	146	

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Mol	Chain	Length	Quality of chain
15	BT	146	% 
16	AU	118	
16	BU	118	
17	AV	101	% 
17	BV	101	
18	AW	113	
18	BW	113	
19	AX	96	
19	BX	96	
20	AY	110	6% 
20	BY	110	% 
21	AZ	206	3% 
21	BZ	206	
22	A0	85	2% 
22	B0	85	
23	A1	98	3% 
23	B1	98	% 
24	A2	72	% 
24	B2	72	
25	A3	60	8% 
25	B3	60	
26	A4	71	10% 
26	B4	71	8% 
27	A5	60	
27	B5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1521	
31	DA	1521	
32	CB	256	
32	DB	256	
33	CC	239	
33	DC	239	
34	CD	209	
34	DD	209	
35	CE	162	
35	DE	162	
36	CF	101	
36	DF	101	
37	CG	156	
37	DG	156	
38	CH	138	
38	DH	138	
39	CI	128	
39	DI	128	
40	CJ	105	

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Mol	Chain	Length	Quality of chain
40	DJ	105	
41	CK	129	
41	DK	129	
42	CL	132	
42	DL	132	
43	CM	126	
43	DM	126	
44	CN	61	
44	DN	61	
45	CO	89	
45	DO	89	
46	CP	88	
46	DP	88	
47	CQ	105	
47	DQ	105	
48	CR	88	
48	DR	88	
49	CS	93	
49	DS	93	
50	CT	106	
50	DT	106	
51	CU	27	
51	DU	27	

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
52	T8B	AA	3001	-	-	X	X
52	T8B	BA	3001	-	-	X	X

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 279316 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			
1	BA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	272A	G	U	CONFLICT	GB AP008226.1
BA	272A	G	U	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			
2	BB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	120	G	A	CONFLICT	GB AP008226.1
BB	120	G	A	CONFLICT	GB AP008226.1

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
4	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			
5	BF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
6	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
7	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			
8	BI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
BI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
9	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
10	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			
11	BP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AS	110	Total	C	N	O	0	0	0
			865	544	172	149			
14	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
15	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
18	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
19	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
20	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
21	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
22	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
23	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				
25	B3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
26	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
27	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
28	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
30	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			
31	DA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
32	DB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
33	DC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	DD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
35	DE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			
36	DF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			
37	DG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
38	DH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			
39	DI	125	Total	C	N	O	0	0	0
			852	533	163	156			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	58	ARG	HIS	CONFLICT	UNP P80374
DI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	CJ	96	Total	C	N	O	0	0	0
			659	408	131	120			
40	DJ	96	Total	C	N	O	0	0	0
			659	408	131	120			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7
DJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			
41	DK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
42	DL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
43	DM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			
44	DN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
45	DO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
46	DP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
47	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			
48	DR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			
49	DS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			

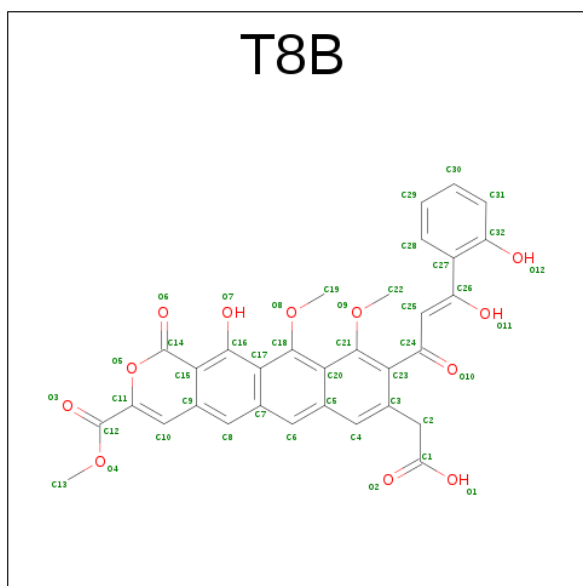
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			
50	DT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			

- Molecule 51 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is Thermorubin (three-letter code: T8B) (formula:  $C_{32}H_{24}O_{12}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	AA	1	Total	C	O	0	0
			44	32	12		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	BA	1	Total	C	O	0	0
			44	32	12		

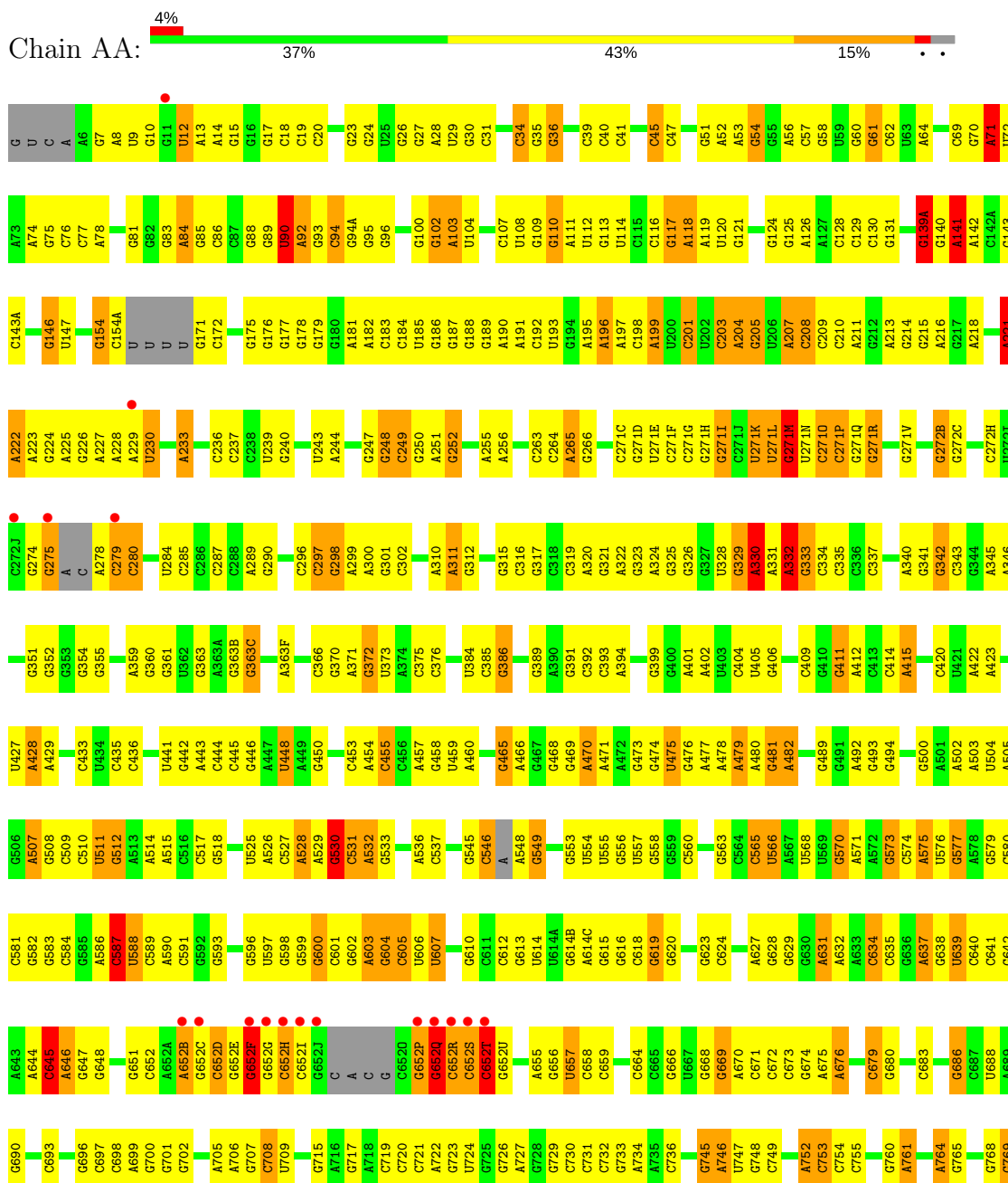
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	2	Total	Mg	0	0
			2	2		
53	BA	2	Total	Mg	0	0
			2	2		

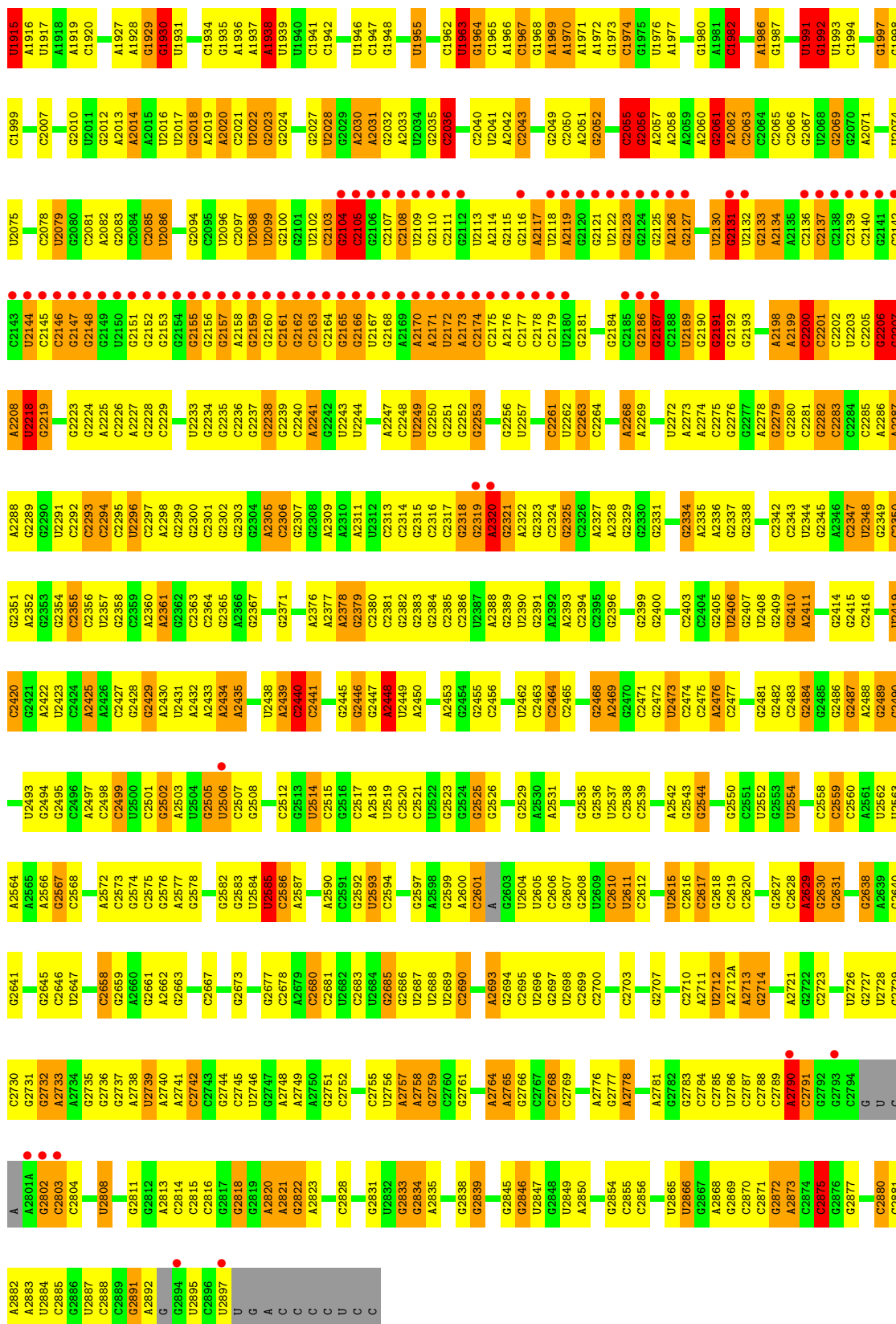
### 3 Residue-property plots

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

#### • Molecule 1: 23S ribosomal RNA

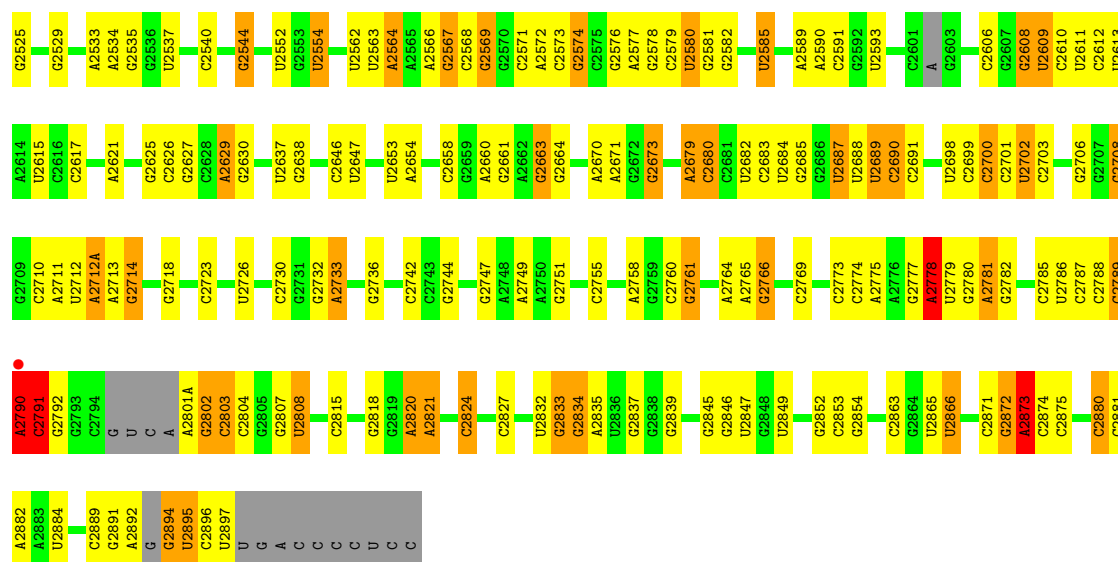




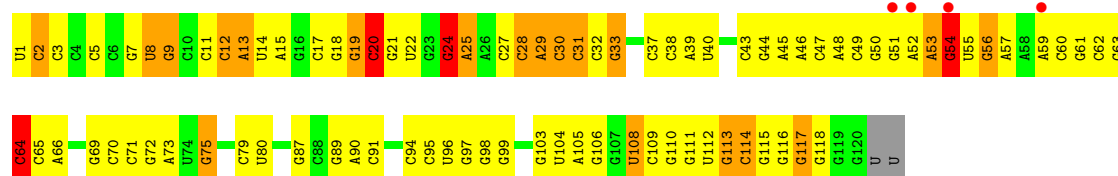


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C1166	U	U	U839	U839	G760	C678	A638	U566	A480	A390	C298	A244	C	A
G1169	A	U1019	G934	C840	G761	C679	G638	A567	A481	A84	G298	G245	A	A
G1170	A	A1020	U937	A841	G762	G680	C640	U568	A482	G396	A299	C246	G	G
G1171	A	A1021	U938	A842	G763	G681	C641	U569	A483	U405	A300	G247	A	A
G1173	G	G1022	G938	C846	G764	G682	G642	G570	C484	G406	G301	C248	U	U
A1174	A	U1023	U939	U847	G765	G683	G643	A571	C485	C409	A311	C249	U	U
A1175	G	G1024	G940	U848	G766	G684	A644	G573	A491	G410	G312	G250	G	G
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C1185	C	C1039	U955	A863	G778	G694	G652D	U584	G508	A429	G329	G271D	U	U
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C1193	U	C1048	U970	C881	G786	G702	A	C516	C516	A444	C337	U271L	U	U
A1194	U	G1049	C971	C882	G787	G703	G	C517	C517	C445	U339	U271M	U	U
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G1203	A	A	G978	C886	G791	G707	G652R	G602	C527	A449	G342	G271Q	U	U
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G1212	U	G	U988	C892	G796	G712	G652W	U607	A532	A454	U362	G271V	U	U
G1218	U	U	A989	C893	G797	G713	A654	G533	U534	C455	U363	G271W	U	U
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C1224	A	U	U993	C897	G801	G717	C658	U614A	C537	U459	G363C	G272B	U	U
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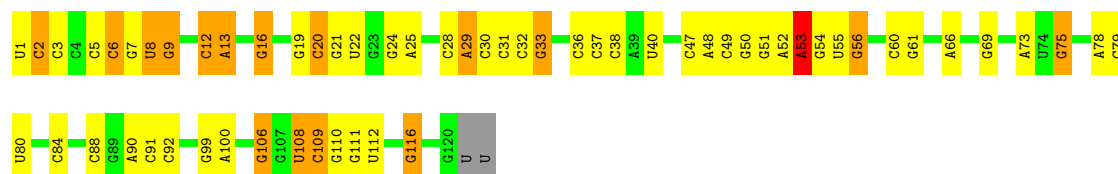
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	A2418	C2175	G2114		G2035	G1941	G1846	G1767	G1665	U1567		U1394	G1299
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	A2422	C2179	G2118		G2039	A1952	G1850	G1771	G1669	U1571		G1402	A1307
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A2503	C2424	A2274	G2121		C2044	G1955	G1853	C1774	G1672	U1579		G1405	G1310
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	A2430	A2277	G2126		G2049	G1960	G1858	G1783	G1677	A1584		C1408	
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	A2435	G2280	G2128		G2051	U1962	G1860	A1785	G1679	A1494			
		G2281	C2129		C2052	U1963	G1861	G1786	G1680	A1495			
	U2438	G2282	G2130		G2053	U1964	G1862	A1787	G1681	A1496			
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	G2516	C2284	G2131		G2055	U1966	G1864	G1789	G1683				
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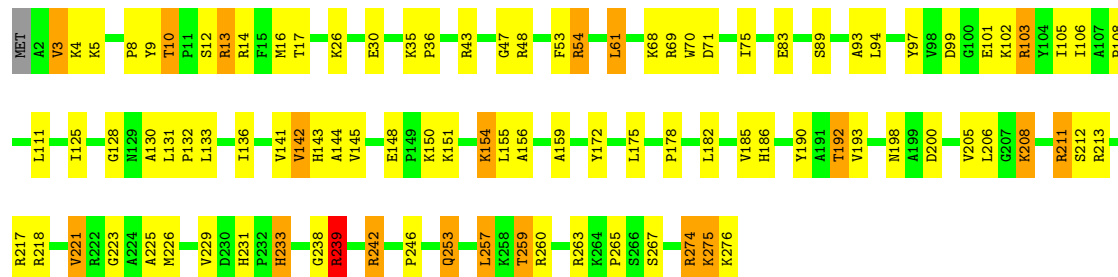
- Molecule 2: 5S ribosomal RNA



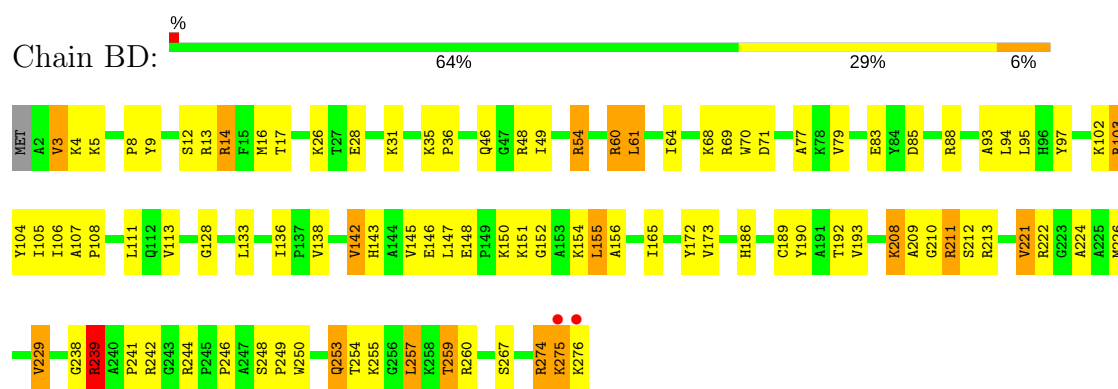
- Molecule 2: 5S ribosomal RNA



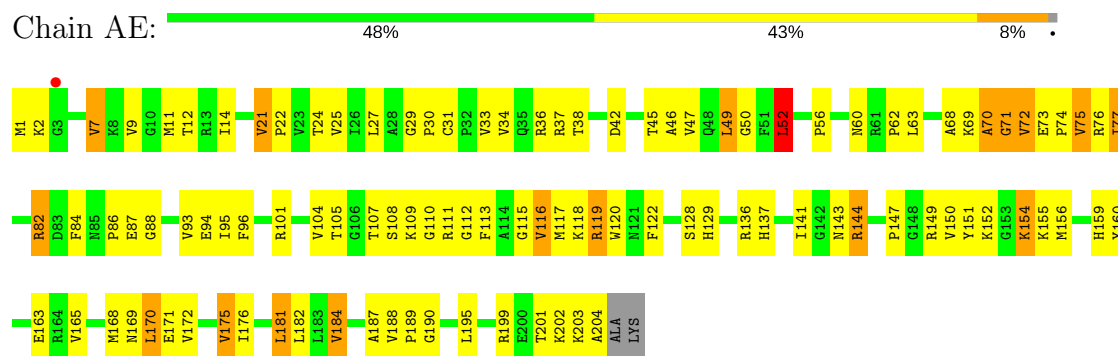
- Molecule 3: 50S ribosomal protein L2



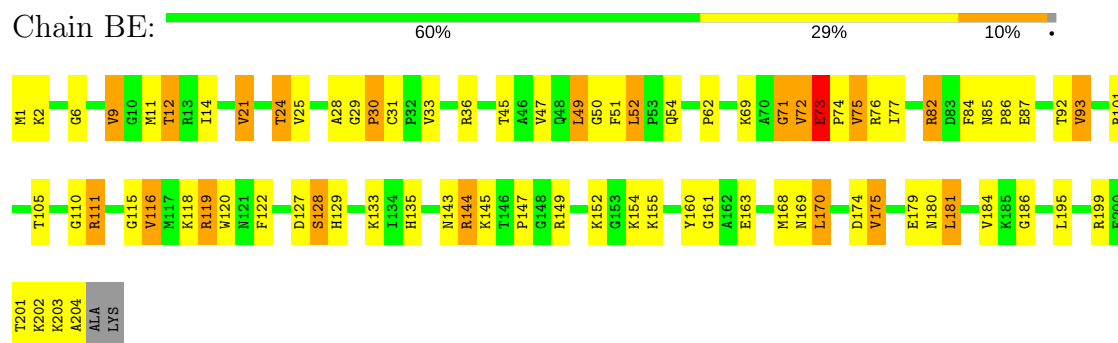
- Molecule 3: 50S ribosomal protein L2



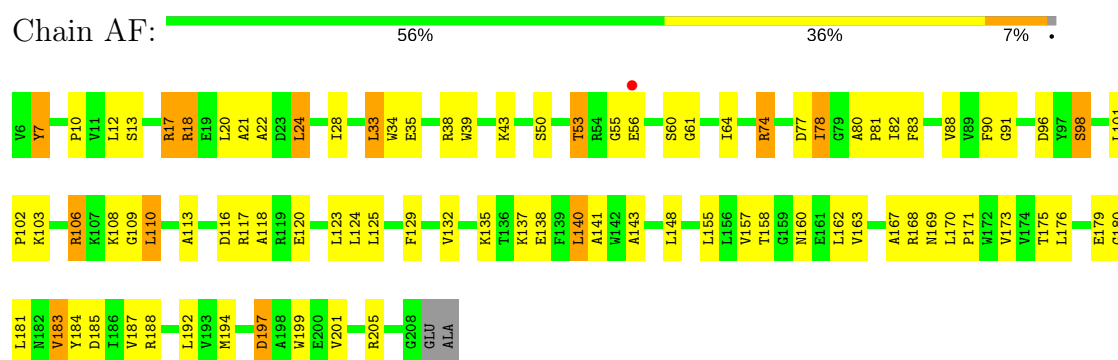
• Molecule 4: 50S ribosomal protein L3



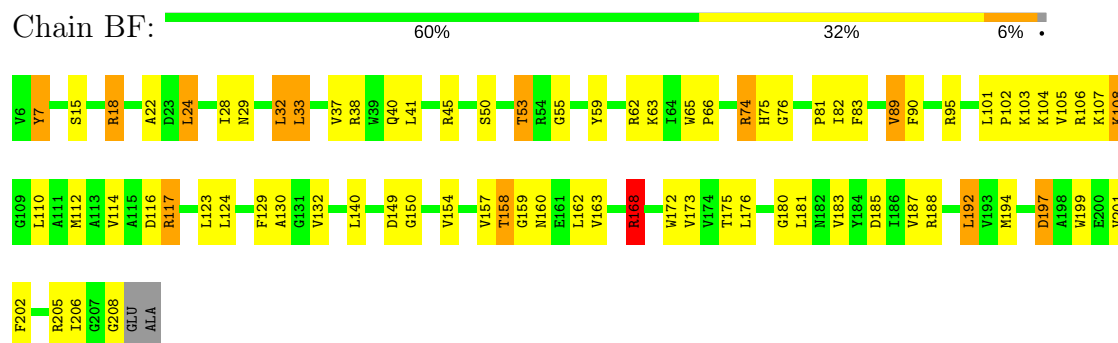
• Molecule 4: 50S ribosomal protein L3

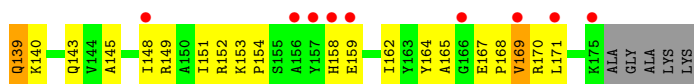


• Molecule 5: 50S ribosomal protein L4

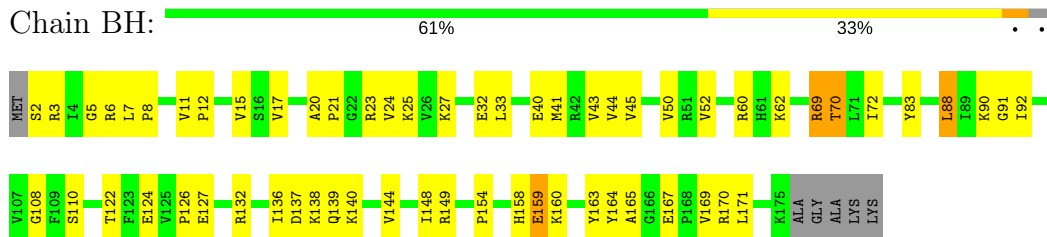


- Molecule 5: 50S ribosomal protein L4

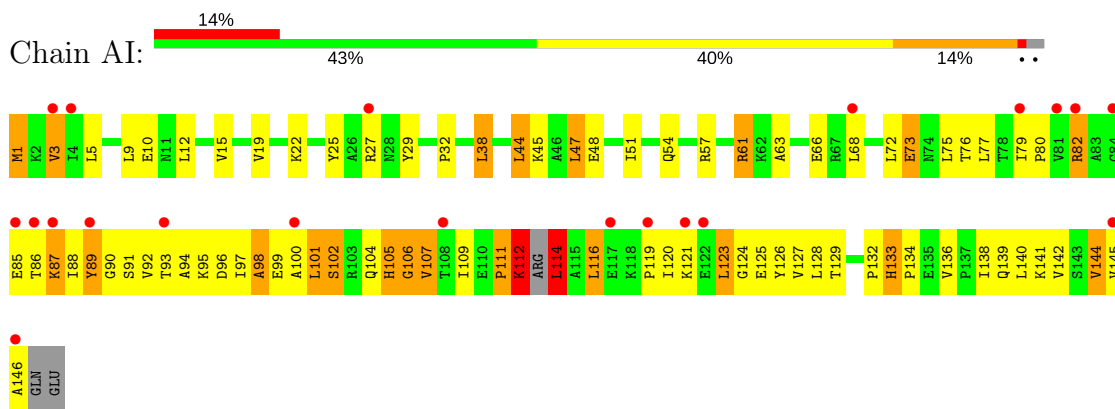




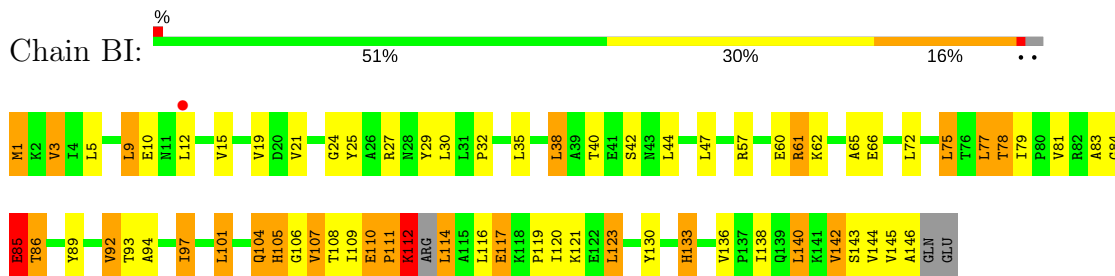
• Molecule 7: 50S ribosomal protein L6



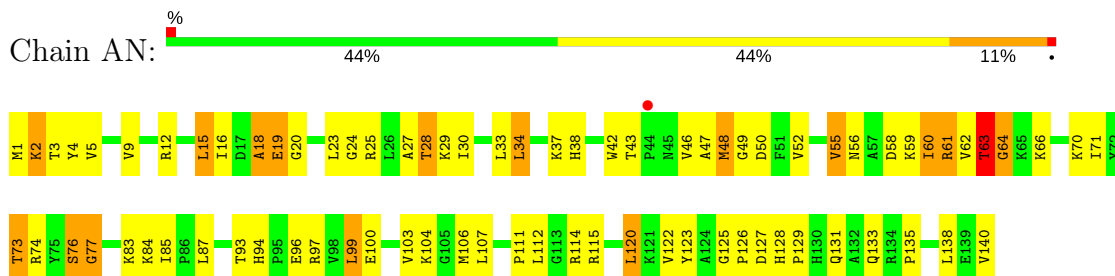
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

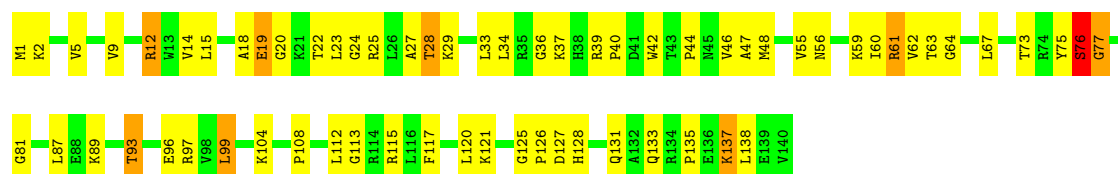


• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13





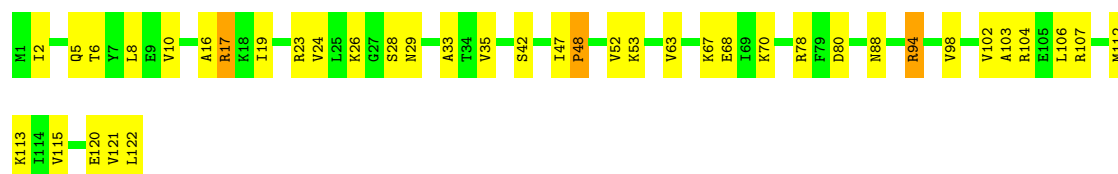
- Molecule 10: 50S ribosomal protein L14

Chain AO: 60% 37% .



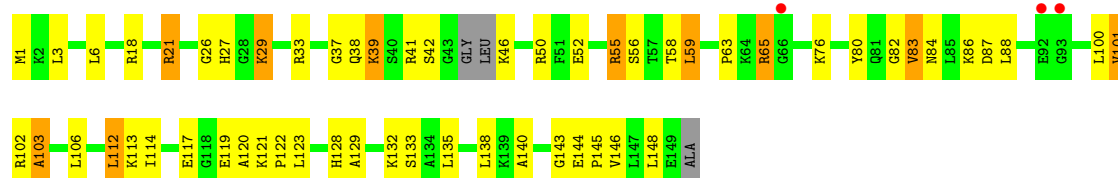
- Molecule 10: 50S ribosomal protein L14

Chain BO: 67% 30% .



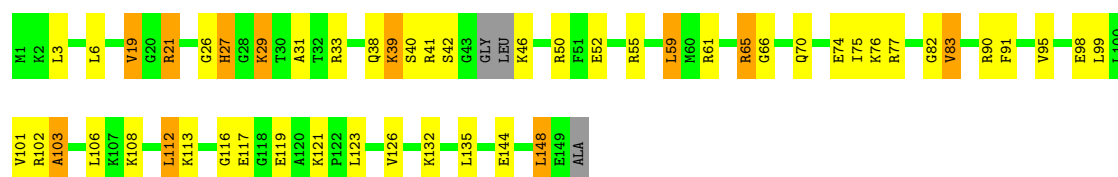
- Molecule 11: 50S ribosomal protein L15

Chain AP: 2% 60% 31% 7% .



- Molecule 11: 50S ribosomal protein L15

Chain BP: 64% 27% 9% .

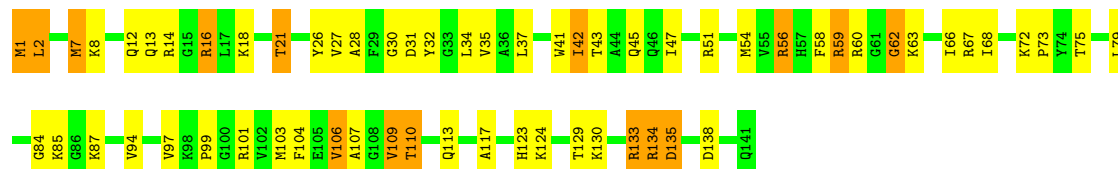


- Molecule 12: 50S ribosomal protein L16

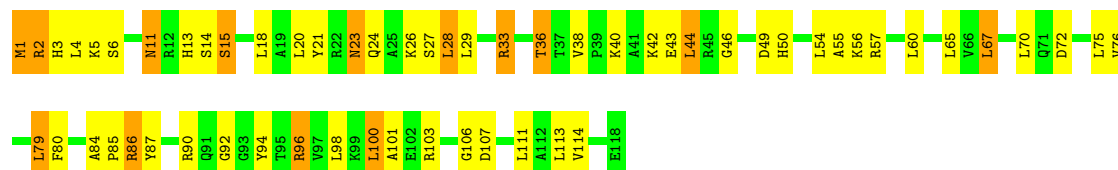
Chain AQ: 55% 36% 9% .



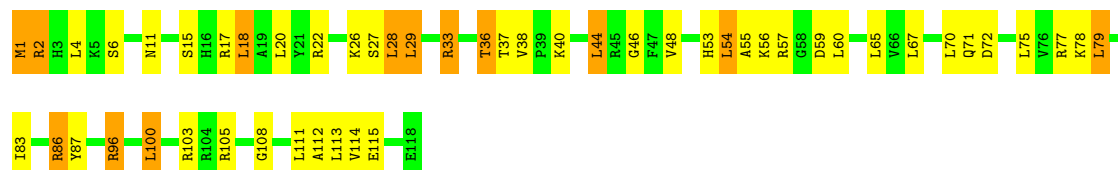
• Molecule 12: 50S ribosomal protein L16



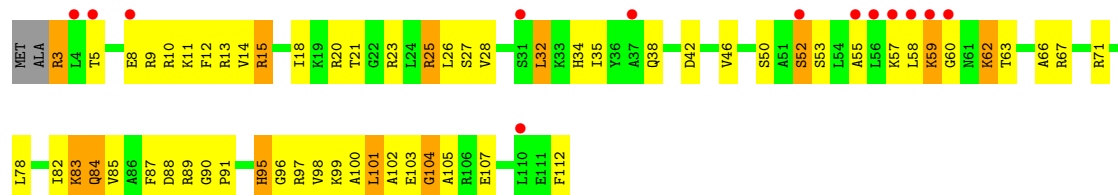
• Molecule 13: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L17

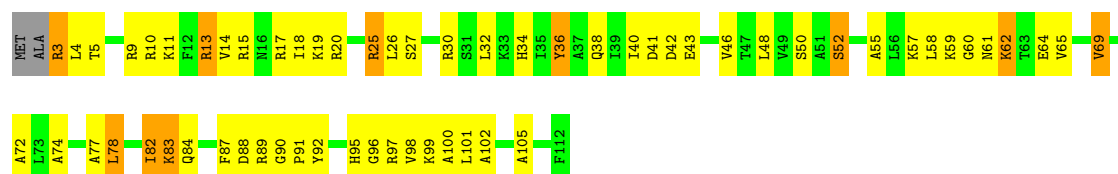


• Molecule 14: 50S ribosomal protein L18

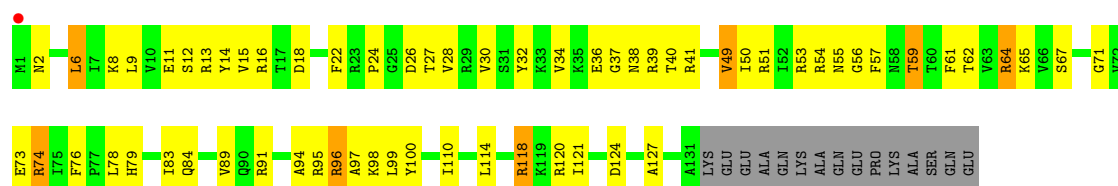


• Molecule 14: 50S ribosomal protein L18

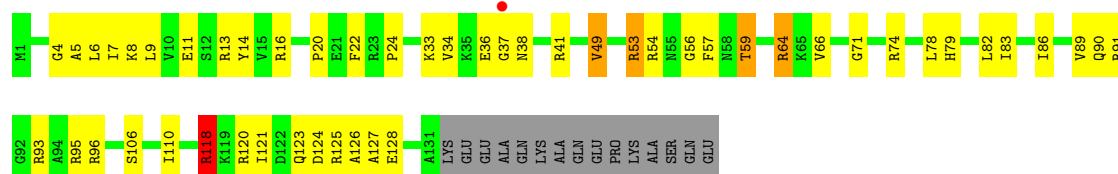




- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





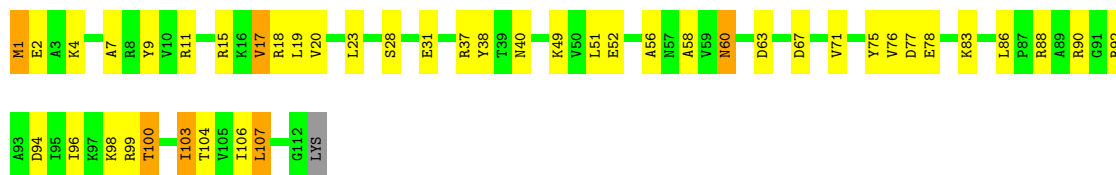
- Molecule 17: 50S ribosomal protein L21

Chain BV: 67% 27% 5% •



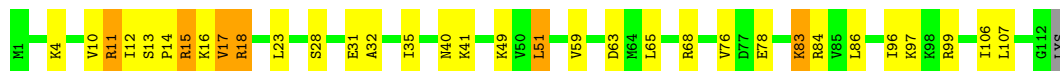
- Molecule 18: 50S ribosomal protein L22

Chain AW: 60% 34% 5% •



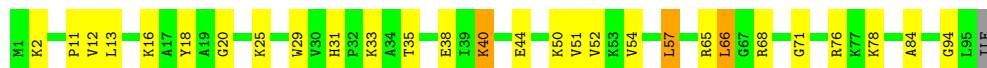
- Molecule 18: 50S ribosomal protein L22

Chain BW: 70% 24% 5% •



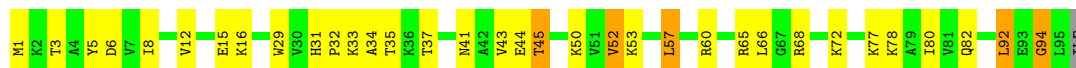
- Molecule 19: 50S ribosomal protein L23

Chain AX: 70% 26% 5% •



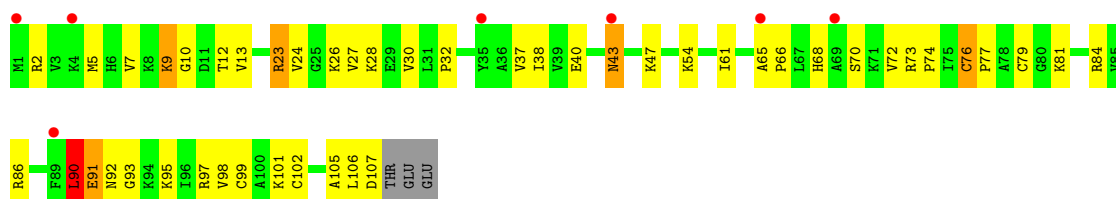
- Molecule 19: 50S ribosomal protein L23

Chain BX: 64% 30% 5% •

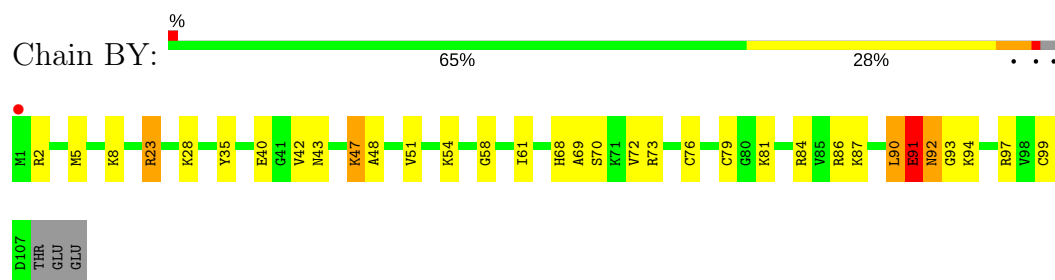


- Molecule 20: 50S ribosomal protein L24

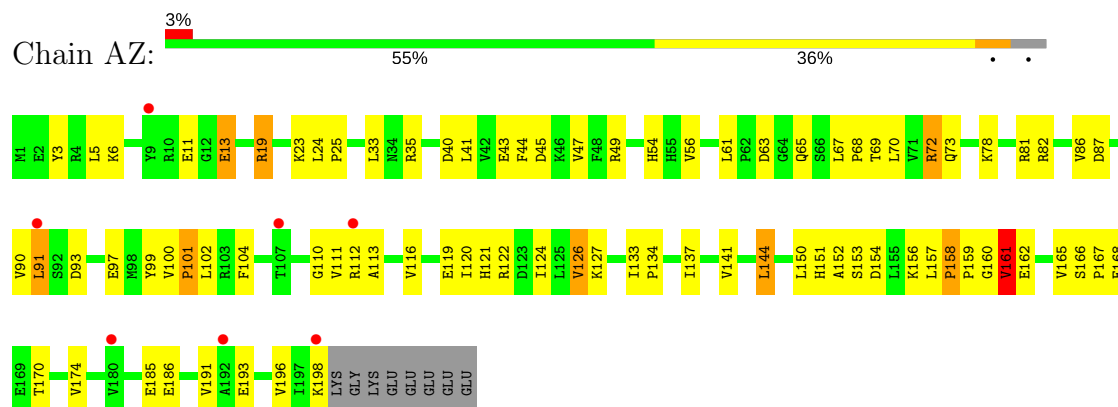
Chain AY: 6% 55% 37% 5% •



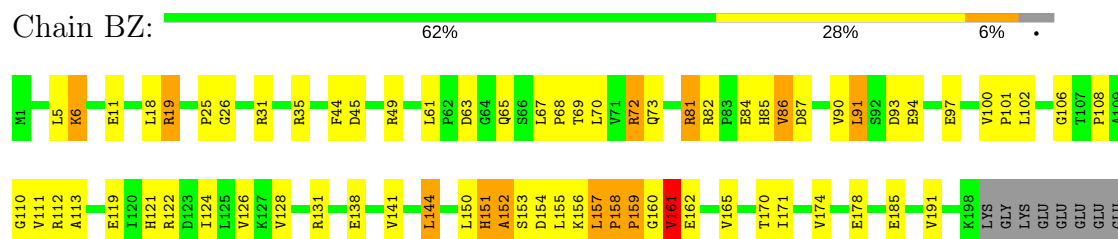
- Molecule 20: 50S ribosomal protein L24



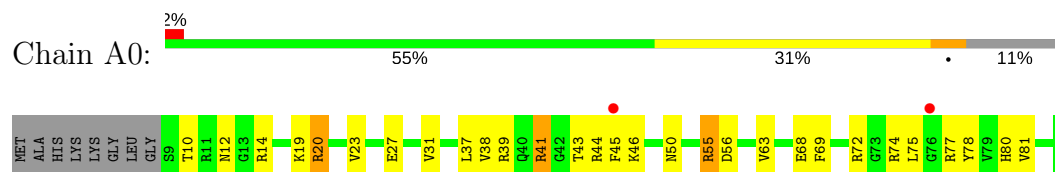
- Molecule 21: 50S ribosomal protein L25



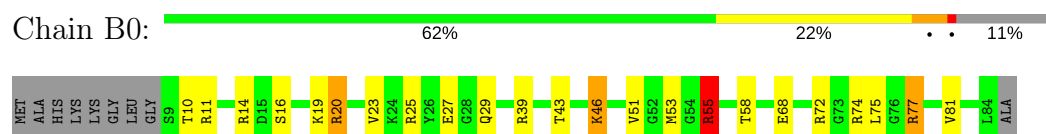
- Molecule 21: 50S ribosomal protein L25



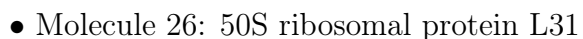
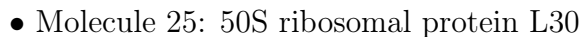
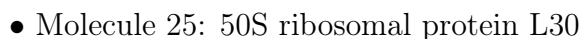
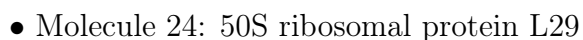
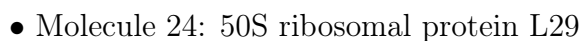
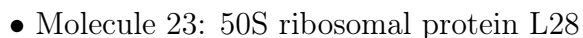
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

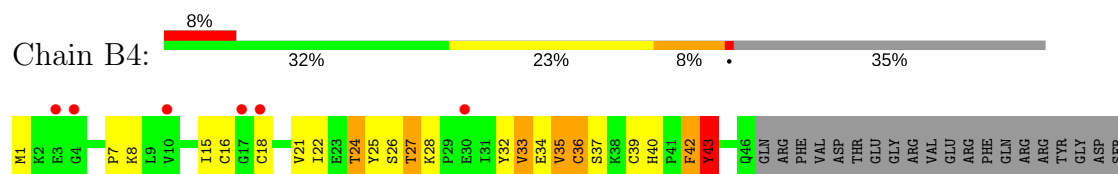


- Molecule 23: 50S ribosomal protein L28



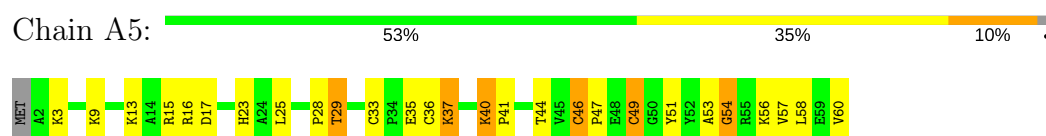
ASP  
SER  
TYR  
ARG  
LYS  
GLY  
ARG

- Molecule 26: 50S ribosomal protein L31

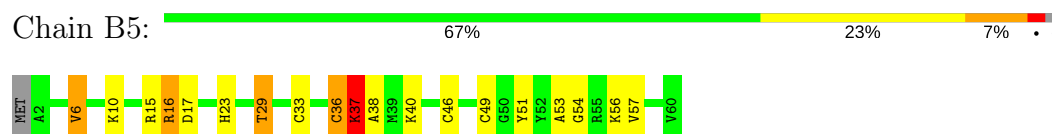


TYR  
ARG  
LYS  
GLY  
ARG

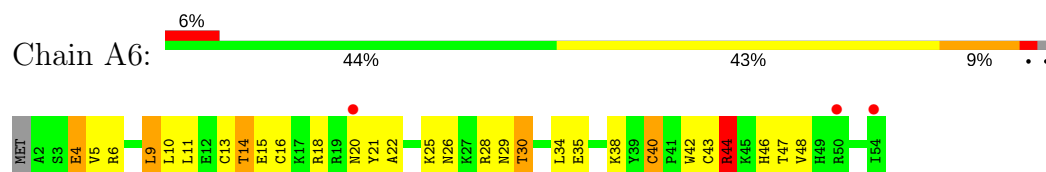
- Molecule 27: 50S ribosomal protein L32



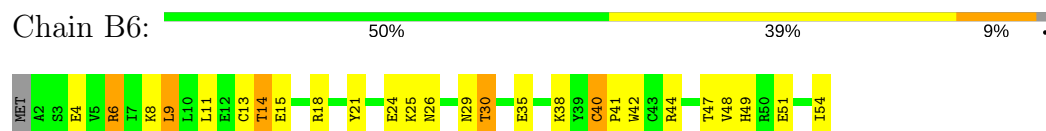
- Molecule 27: 50S ribosomal protein L32



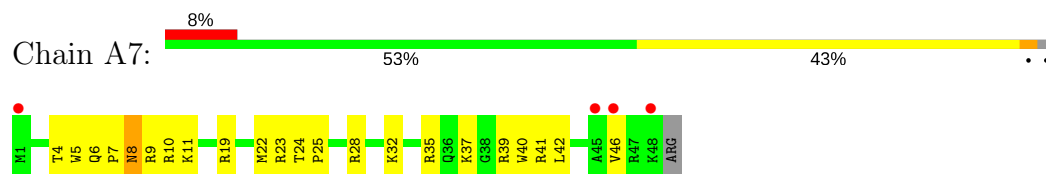
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

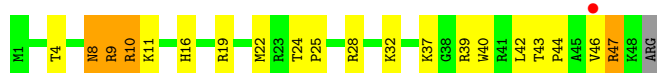


- Molecule 29: 50S ribosomal protein L34



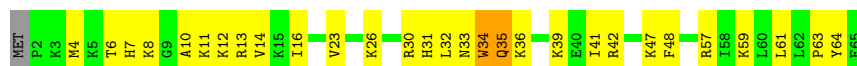
- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain A8: 54% 42%



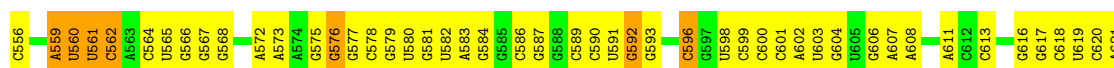
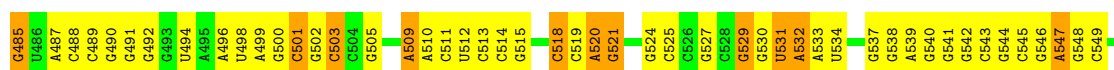
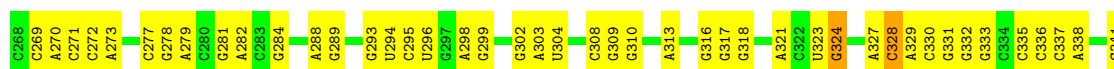
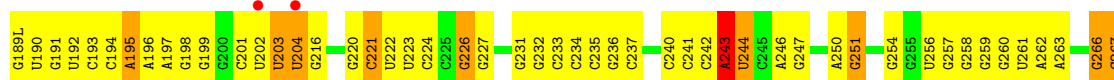
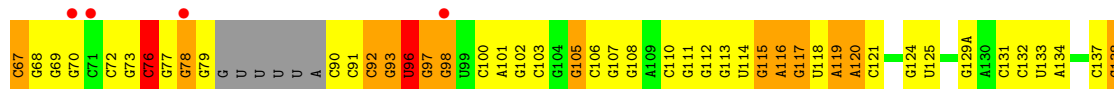
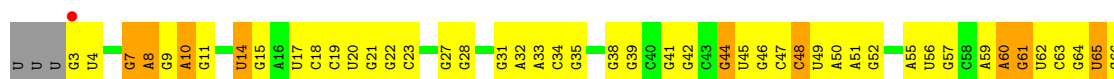
- Molecule 30: 50S ribosomal protein L35

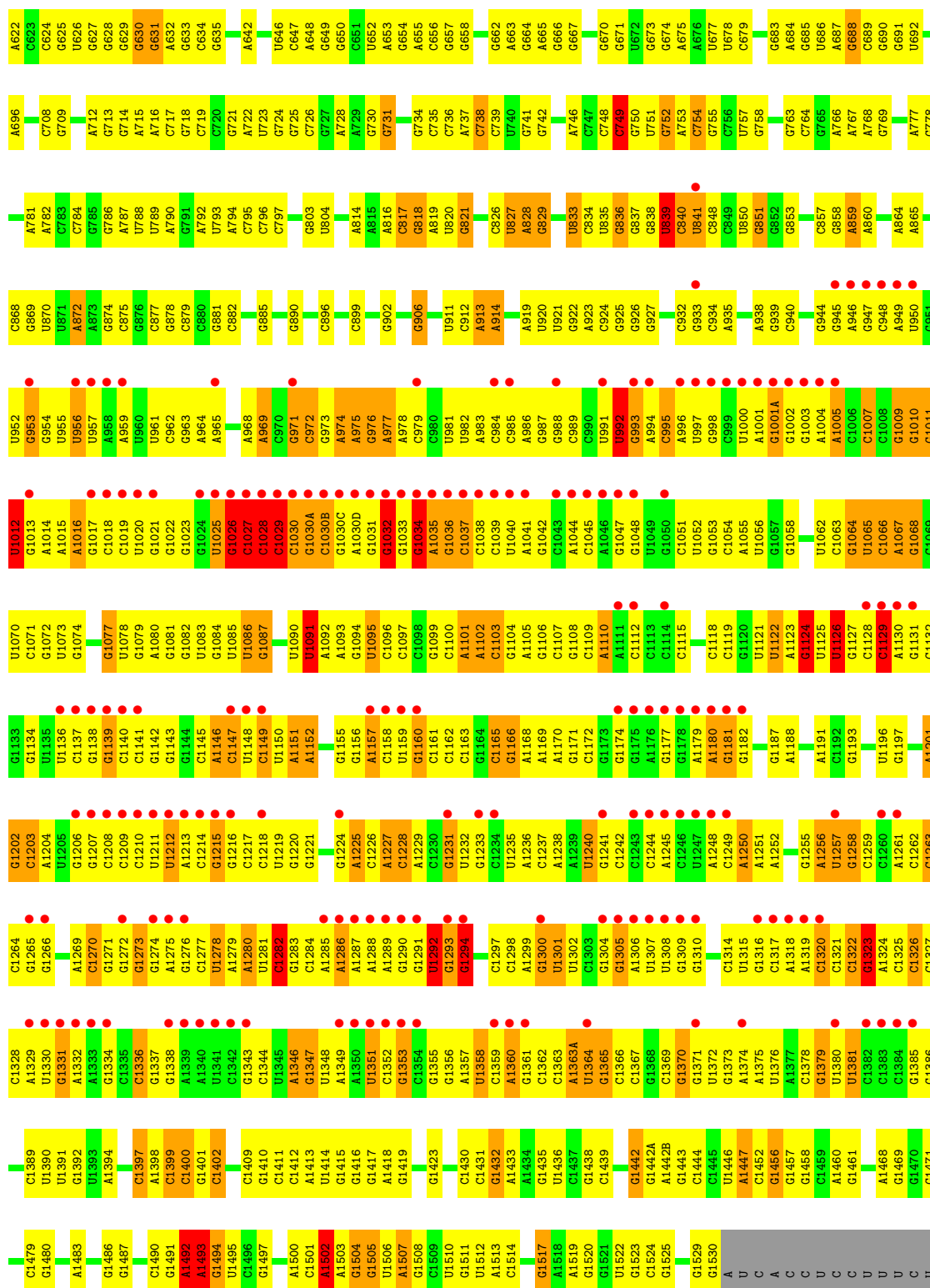
Chain B8: 66% 29%



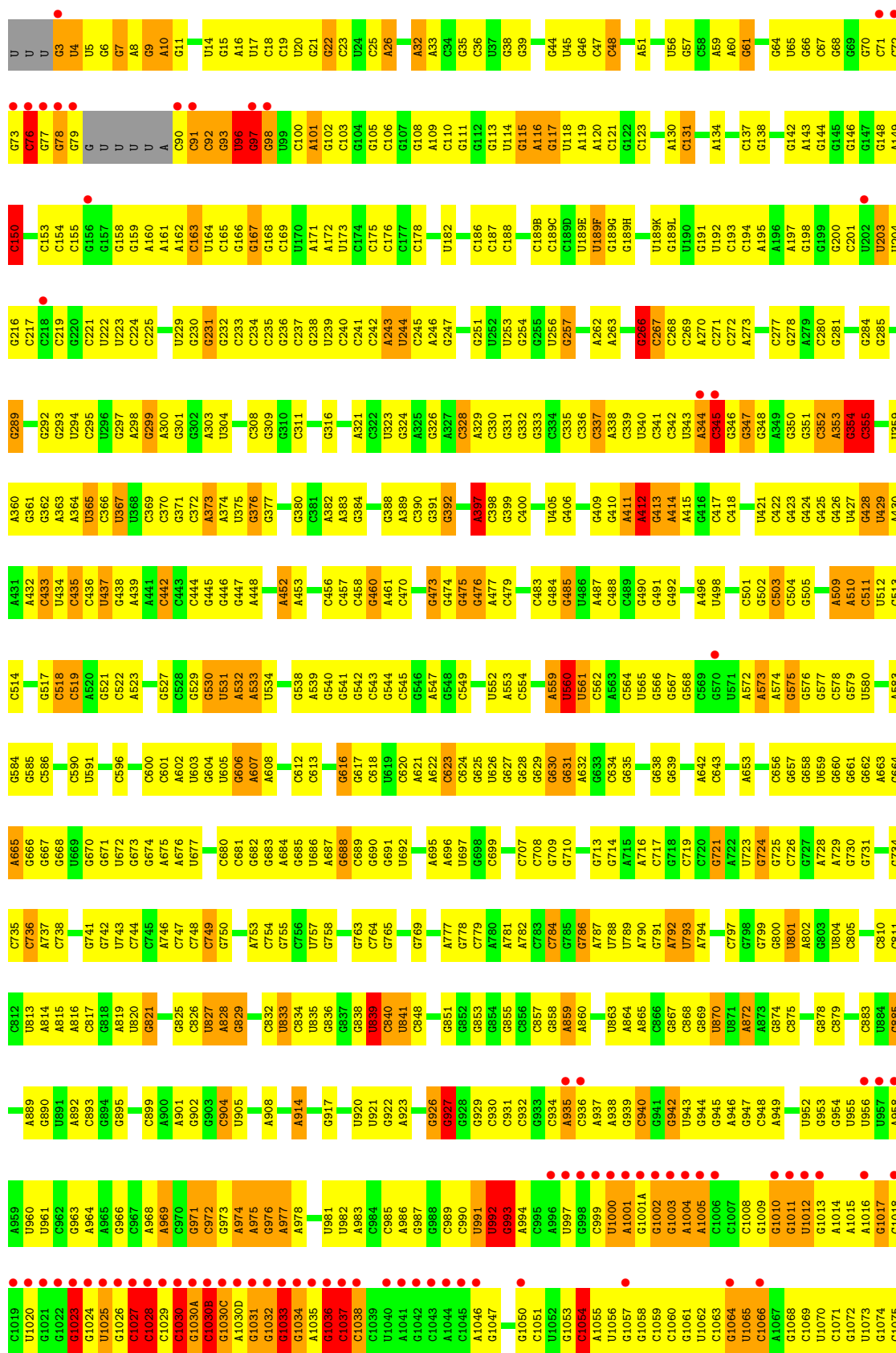
- Molecule 31: 16S ribosomal RNA

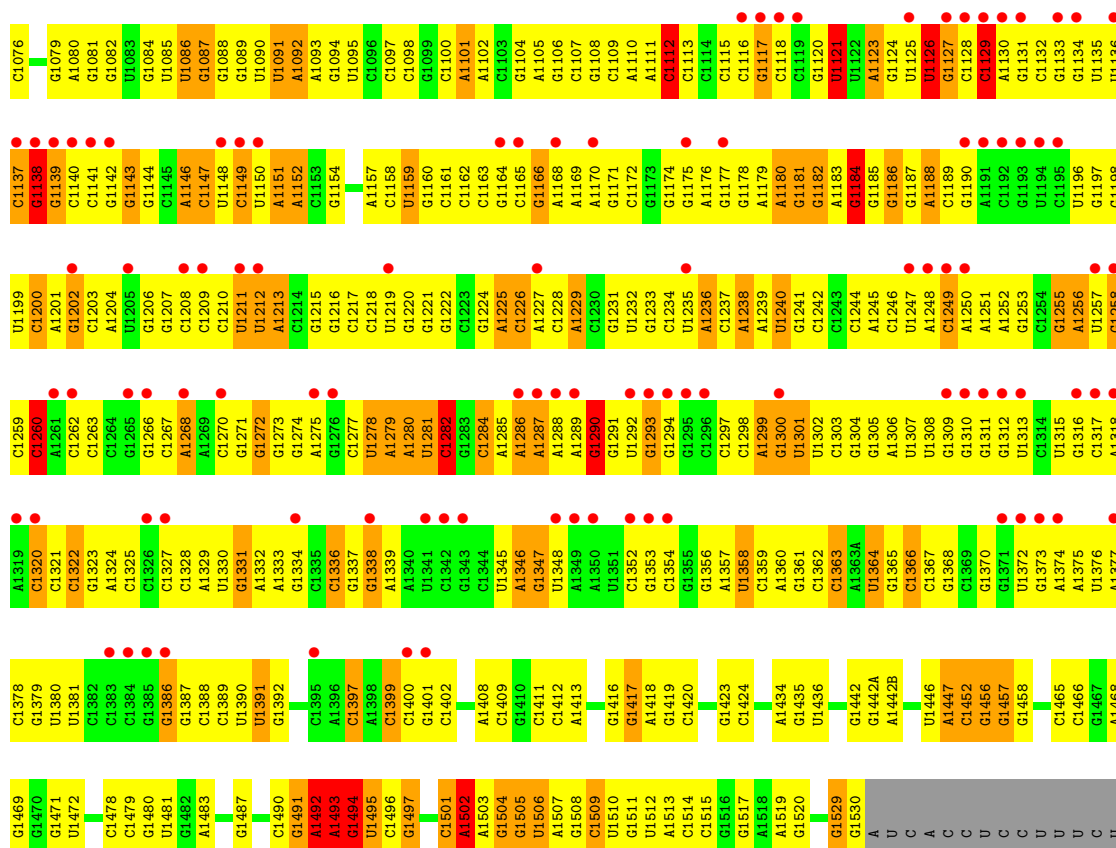
Chain CA: 13% 29% 54% 14%

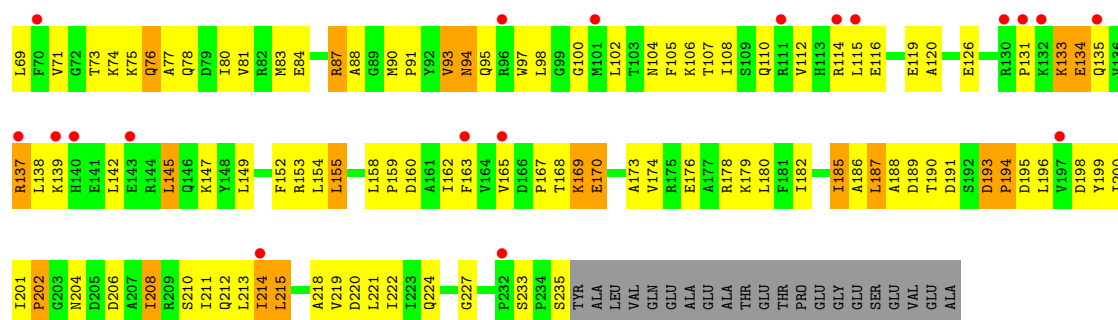




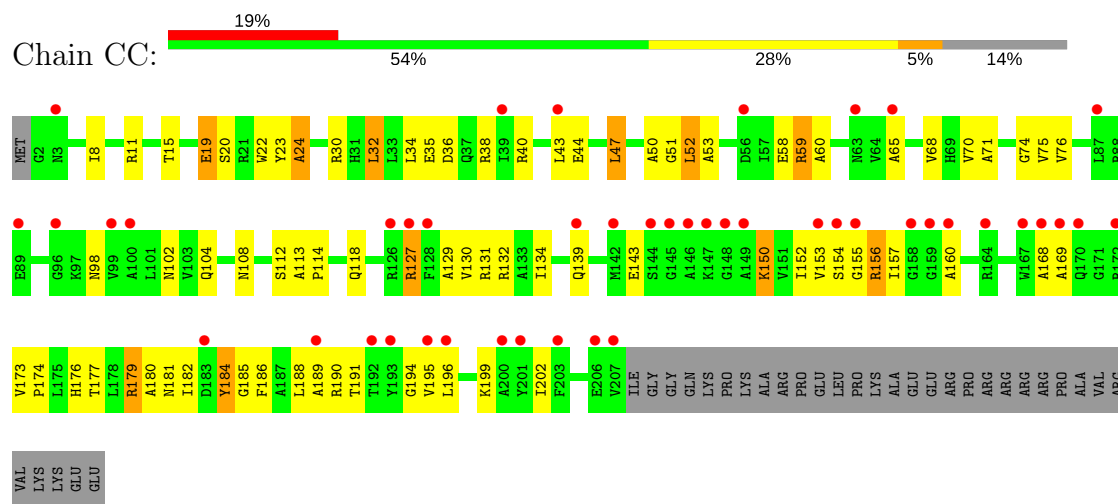
### • Molecule 31: 16S ribosomal RNA



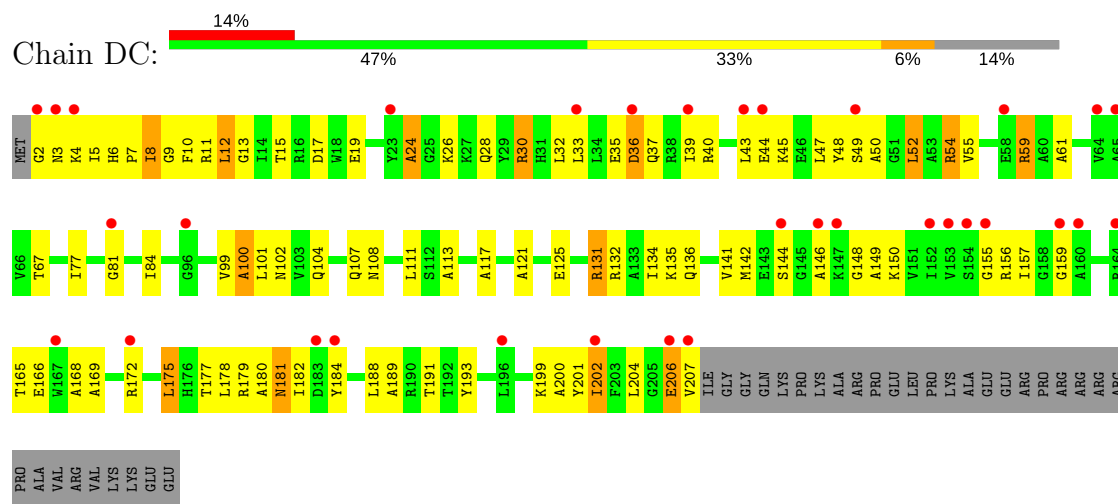




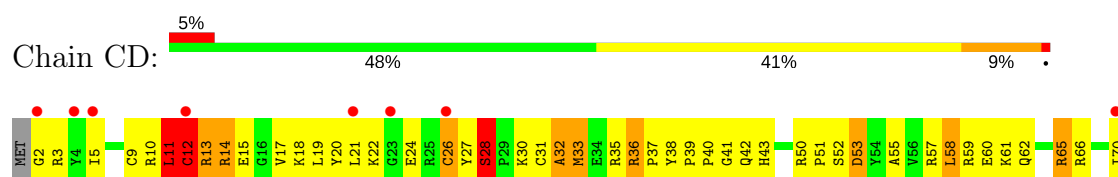
• Molecule 33: 30S ribosomal protein S3

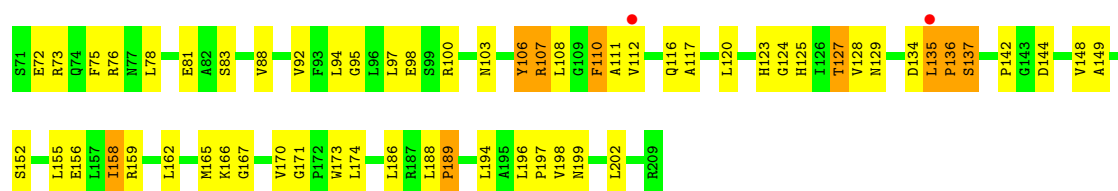


• Molecule 33: 30S ribosomal protein S3

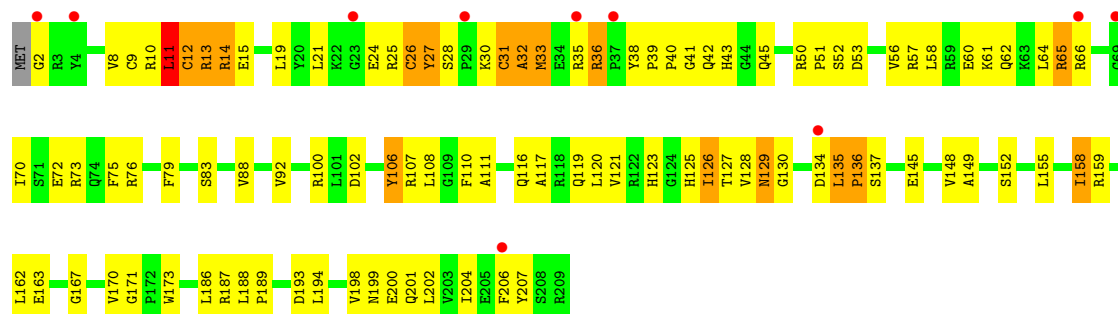


• Molecule 34: 30S ribosomal protein S4

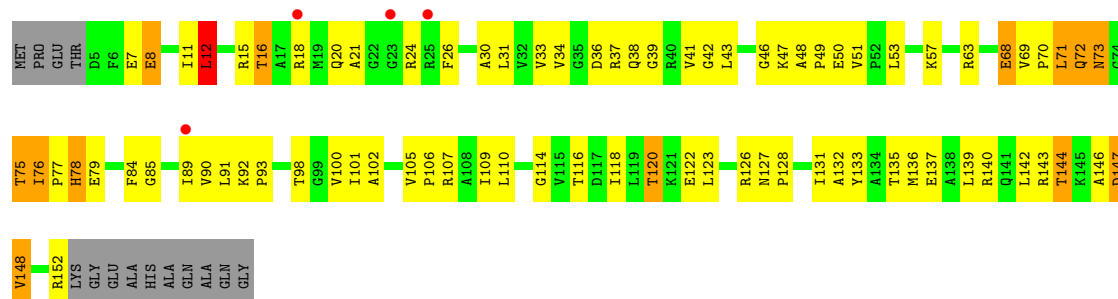
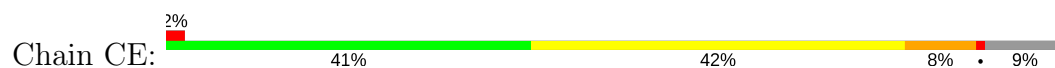




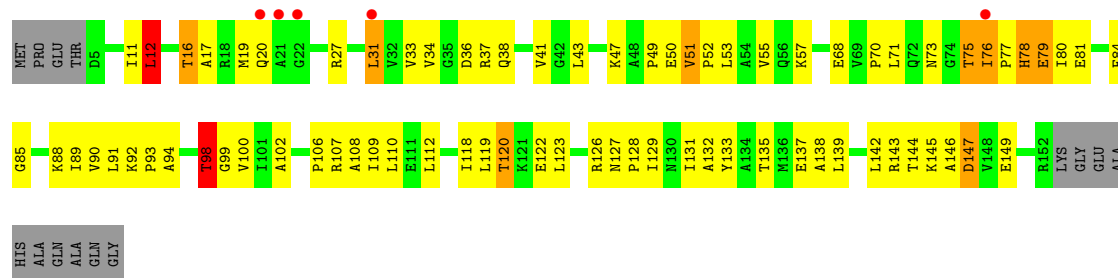
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5

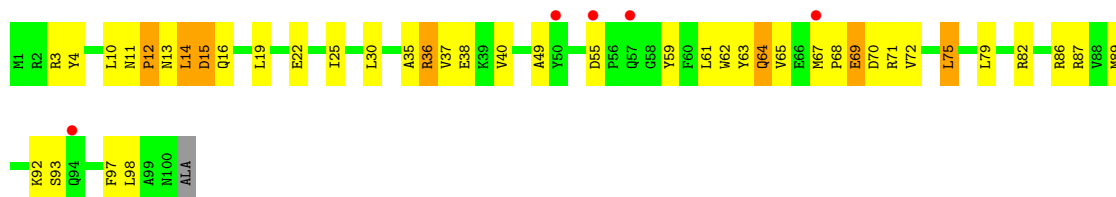


• Molecule 35: 30S ribosomal protein S5

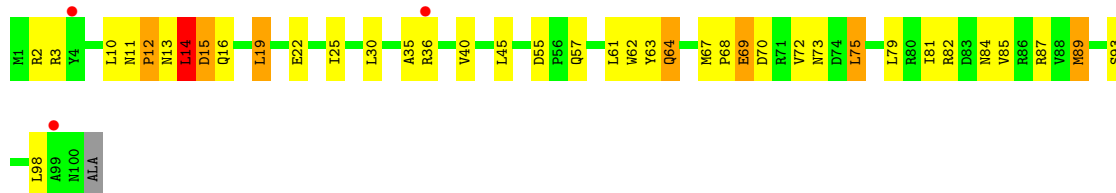


• Molecule 36: 30S ribosomal protein S6

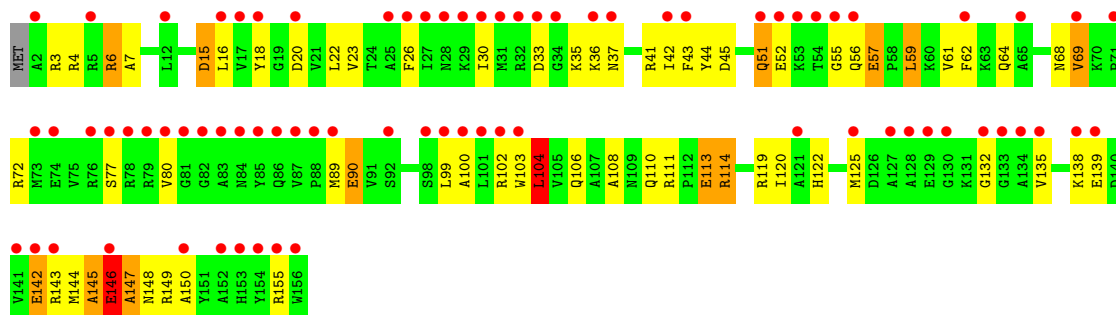




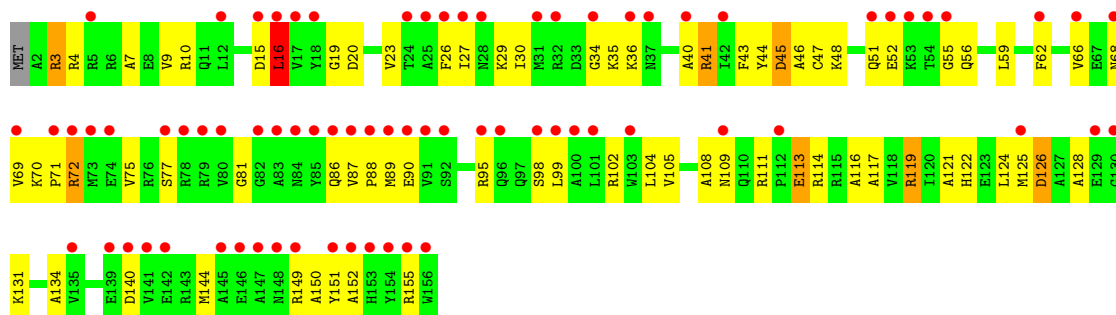
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

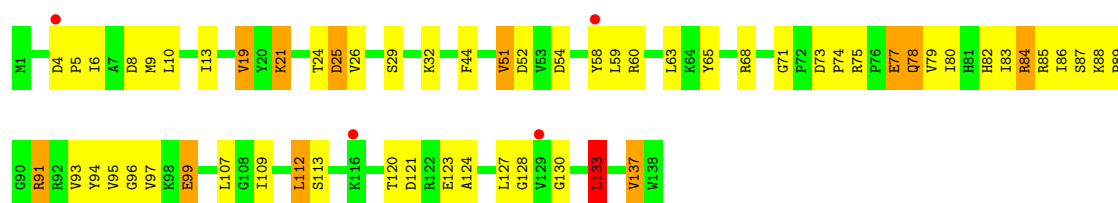


- Molecule 37: 30S ribosomal protein S7

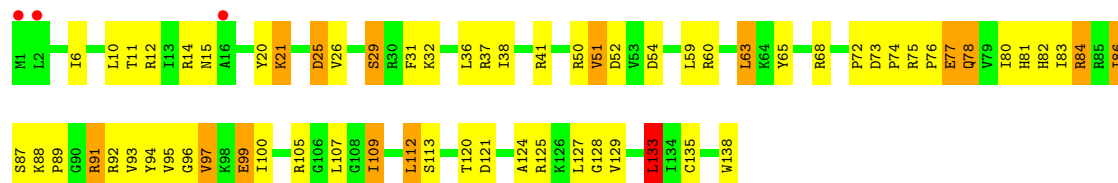


- Molecule 38: 30S ribosomal protein S8

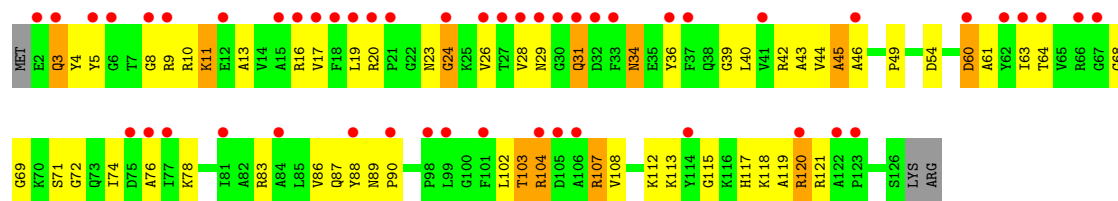
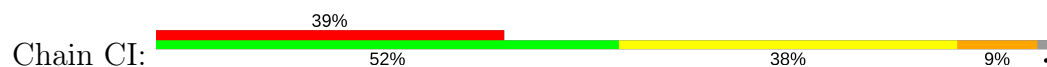




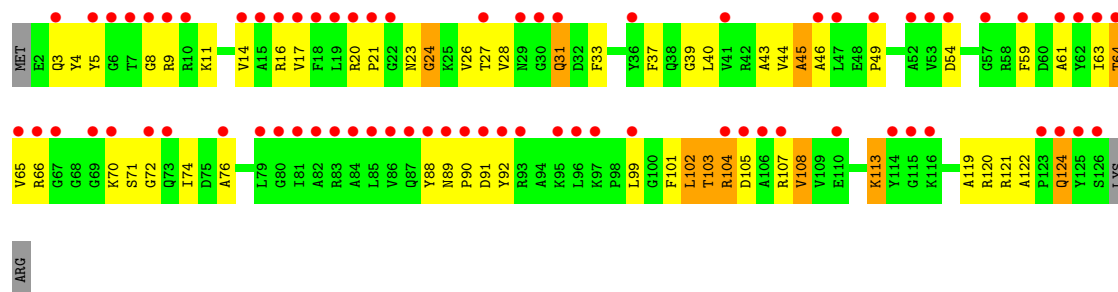
• Molecule 38: 30S ribosomal protein S8



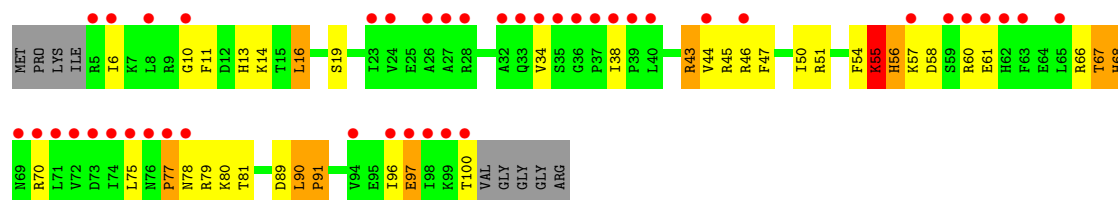
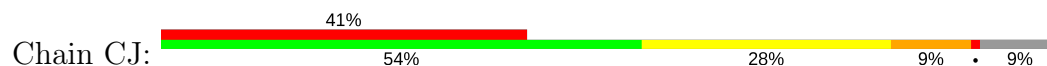
• Molecule 39: 30S ribosomal protein S9



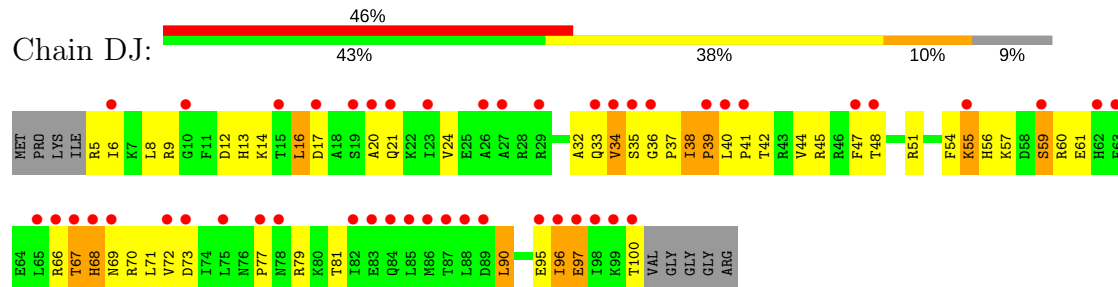
• Molecule 39: 30S ribosomal protein S9



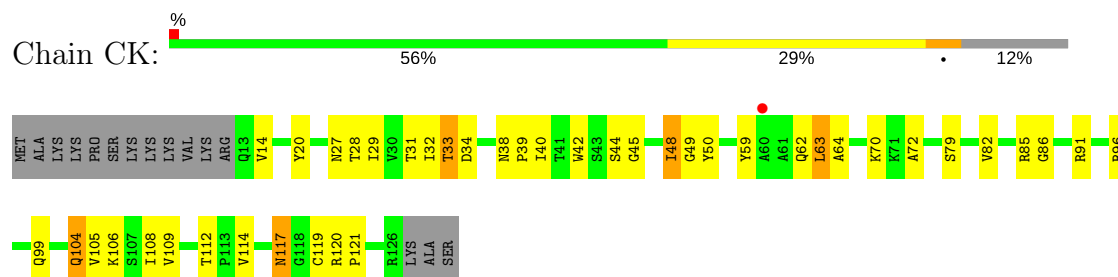
• Molecule 40: 30S ribosomal protein S10



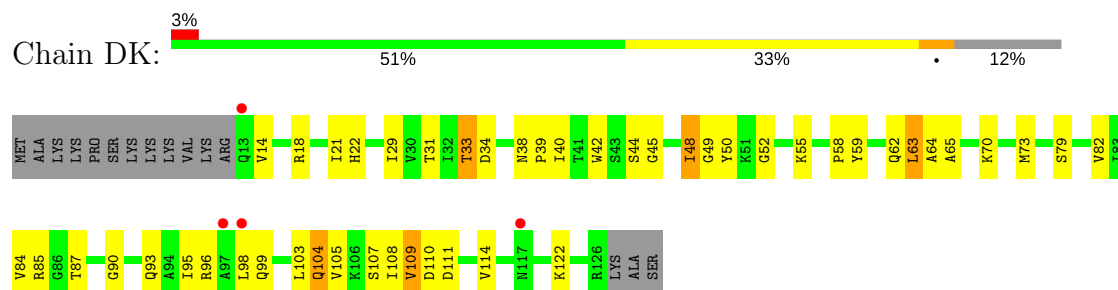
- Molecule 40: 30S ribosomal protein S10



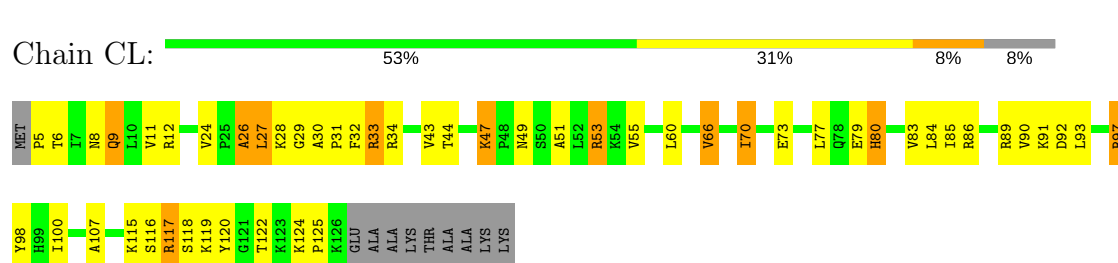
- Molecule 41: 30S ribosomal protein S11



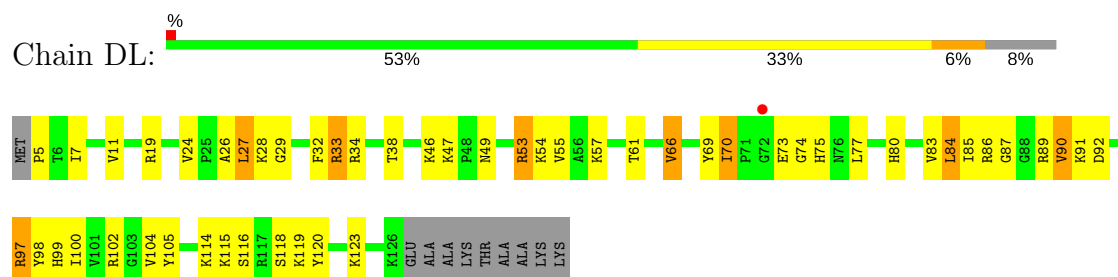
- Molecule 41: 30S ribosomal protein S11



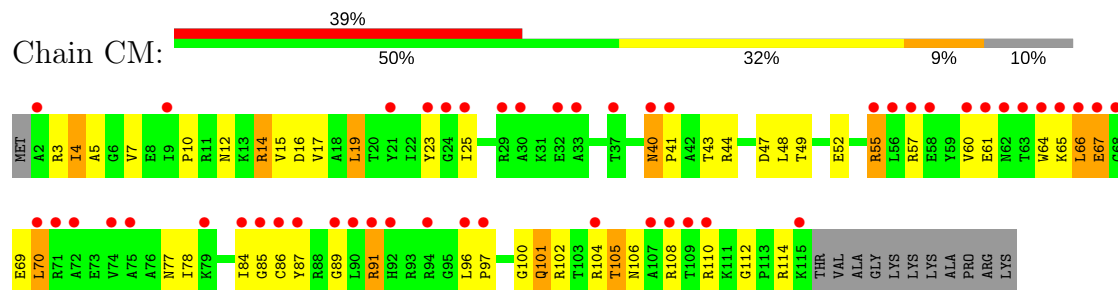
- Molecule 42: 30S ribosomal protein S12



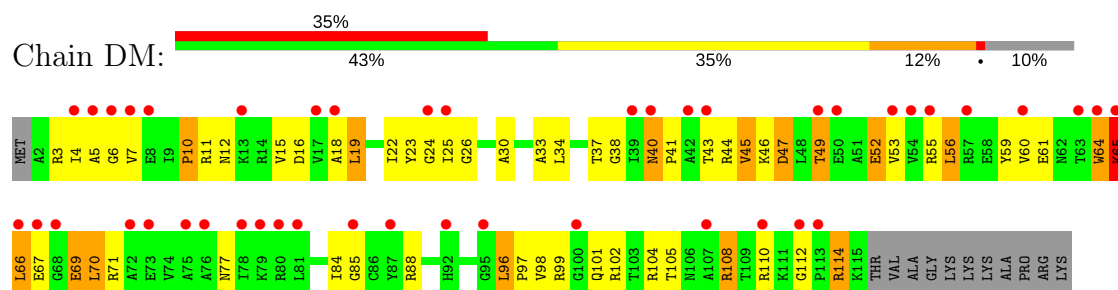
- Molecule 42: 30S ribosomal protein S12



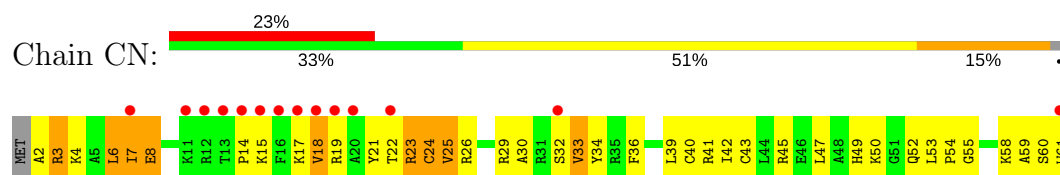
- Molecule 43: 30S ribosomal protein S13



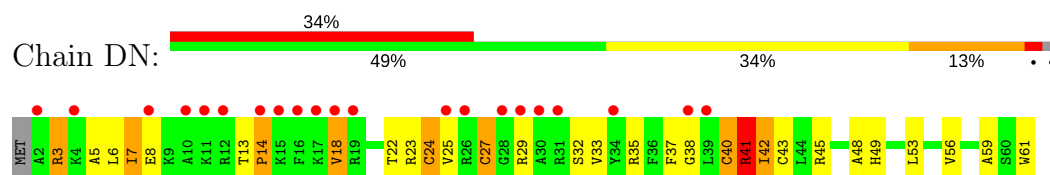
- Molecule 43: 30S ribosomal protein S13



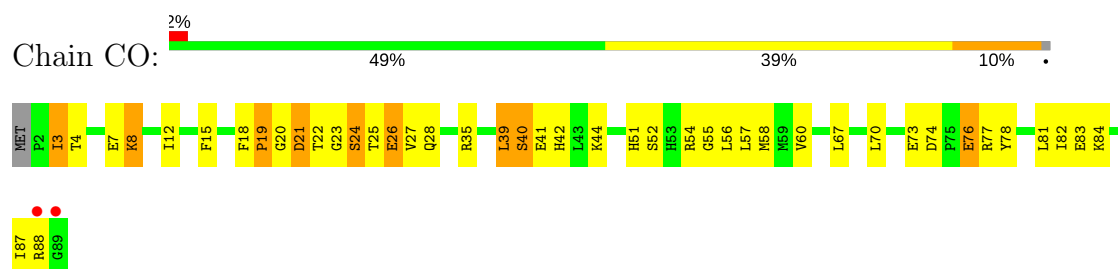
- Molecule 44: 30S ribosomal protein S14



- Molecule 44: 30S ribosomal protein S14

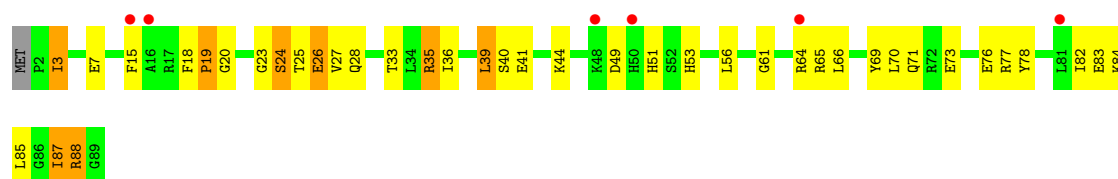


- Molecule 45: 30S ribosomal protein S15

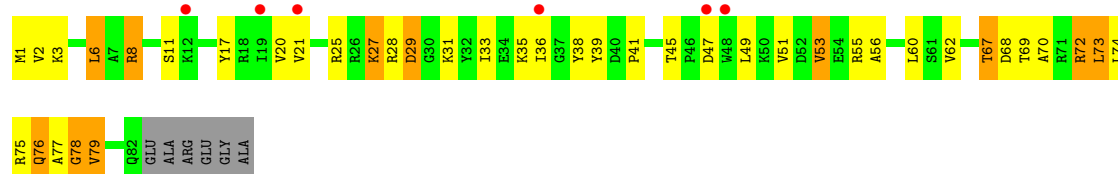


- Molecule 45: 30S ribosomal protein S15

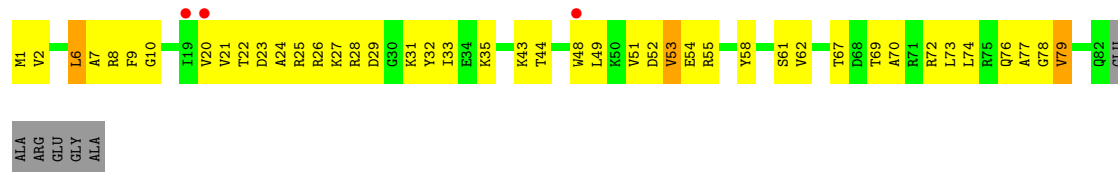




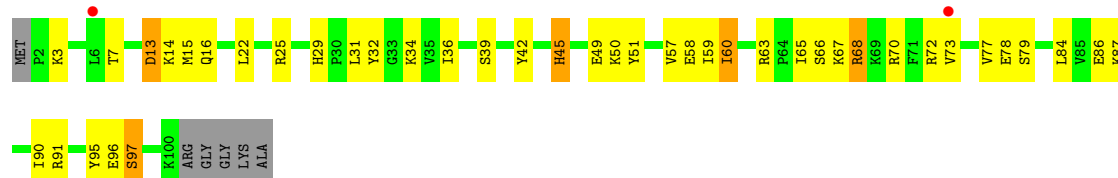
- Molecule 46: 30S ribosomal protein S16



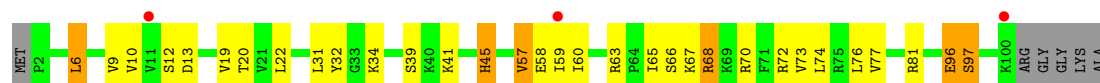
- Molecule 46: 30S ribosomal protein S16



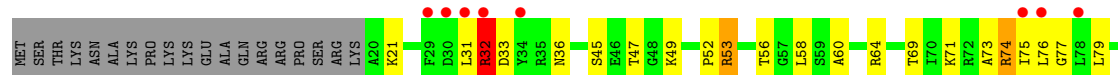
- Molecule 47: 30S ribosomal protein S17



- Molecule 47: 30S ribosomal protein S17

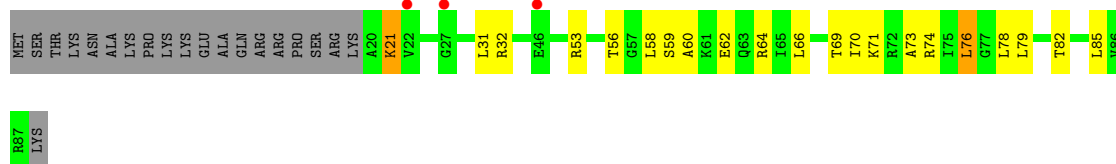


- Molecule 48: 30S ribosomal protein S18

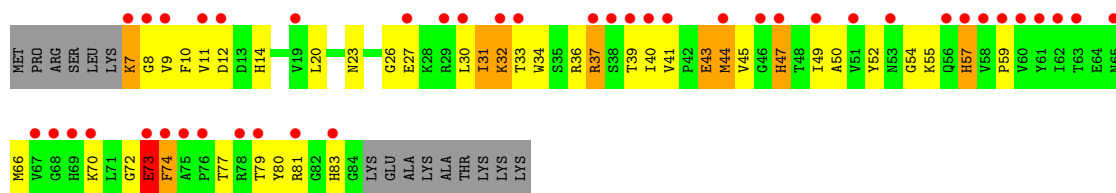




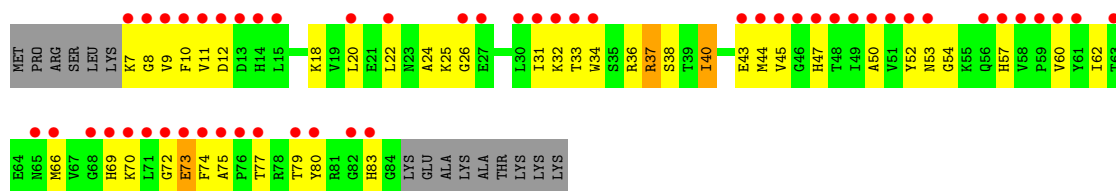
- Molecule 48: 30S ribosomal protein S18



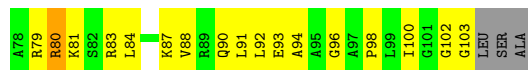
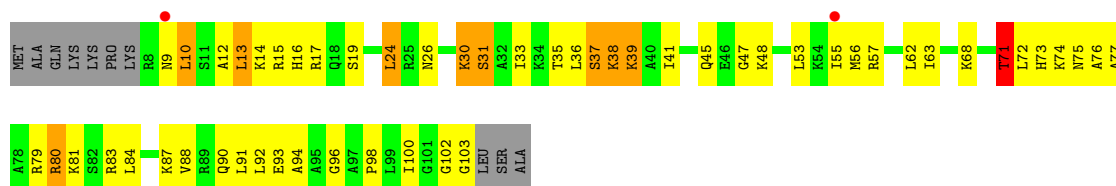
- Molecule 49: 30S ribosomal protein S19



- Molecule 49: 30S ribosomal protein S19

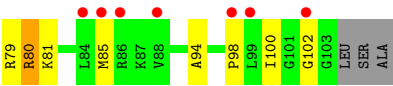


- Molecule 50: 30S ribosomal protein S20

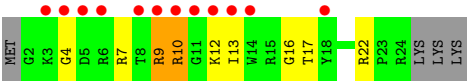
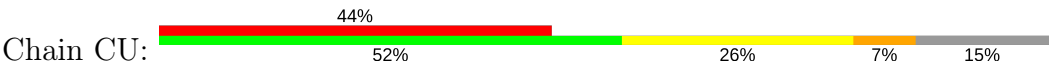


- Molecule 50: 30S ribosomal protein S20

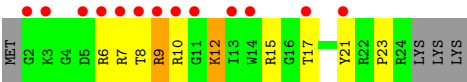




● Molecule 51: 30S ribosomal protein THX



● Molecule 51: 30S ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.273 0.227 , 0.272	Depositor DCC
$R_{free}$ test set	47270 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T8B

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	0.82	17/68203 (0.0%)	1.30	624/106459 (0.6%)
1	BA	1.20	70/68203 (0.1%)	1.37	800/106459 (0.8%)
2	AB	0.94	0/2879	1.25	21/4492 (0.5%)
2	BB	0.88	0/2879	1.26	21/4492 (0.5%)
3	AD	0.54	0/2186	0.75	2/2944 (0.1%)
3	BD	0.67	0/2186	0.81	4/2944 (0.1%)
4	AE	0.55	0/1588	0.76	0/2145
4	BE	0.72	0/1588	0.83	1/2145 (0.0%)
5	AF	0.51	0/1609	0.70	0/2177
5	BF	0.73	0/1609	0.77	0/2177
6	AG	0.61	0/1393	0.66	0/1892
6	BG	0.46	0/1393	0.64	0/1892
7	AH	0.58	0/1343	0.68	1/1820 (0.1%)
7	BH	0.59	0/1343	0.70	0/1820
8	AI	0.63	1/1061 (0.1%)	0.78	0/1451
8	BI	0.50	0/1061	0.74	0/1451
9	AN	0.52	0/1139	0.72	0/1538
9	BN	0.74	0/1139	0.78	0/1538
10	AO	0.50	0/933	0.72	1/1257 (0.1%)
10	BO	0.67	0/933	0.74	0/1257
11	AP	0.50	0/1135	0.75	1/1510 (0.1%)
11	BP	0.64	0/1135	0.81	2/1510 (0.1%)
12	AQ	0.53	0/1143	0.74	0/1527
12	BQ	0.64	0/1143	0.74	0/1527
13	AR	0.51	0/982	0.74	0/1312
13	BR	0.69	0/982	0.82	1/1312 (0.1%)
14	AS	0.64	0/875	0.79	0/1168
14	BS	0.53	0/875	0.79	1/1168 (0.1%)
15	AT	0.52	0/1077	0.73	0/1444
15	BT	0.61	0/1077	0.79	1/1444 (0.1%)
16	AU	0.56	0/977	0.69	0/1301
16	BU	0.88	1/977 (0.1%)	0.81	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AV	0.58	0/782	0.67	0/1049
17	BV	0.70	0/782	0.77	0/1049
18	AW	0.56	0/891	0.75	0/1197
18	BW	0.82	0/891	0.80	0/1197
19	AX	0.55	0/756	0.77	1/1016 (0.1%)
19	BX	0.66	0/756	0.76	1/1016 (0.1%)
20	AY	0.50	0/798	0.77	0/1073
20	BY	0.61	0/798	0.80	1/1073 (0.1%)
21	AZ	0.57	0/1555	0.68	0/2118
21	BZ	0.49	0/1555	0.71	0/2118
22	A0	0.50	0/602	0.69	0/804
22	B0	0.66	0/602	0.77	0/804
23	A1	0.51	0/752	0.72	0/1003
23	B1	0.62	0/752	0.76	0/1003
24	A2	0.59	0/590	0.68	0/781
24	B2	0.60	0/590	0.74	0/781
25	A3	0.45	0/463	0.69	0/623
25	B3	0.65	0/463	0.74	0/623
26	A4	0.65	0/358	0.74	0/487
26	B4	0.56	0/358	0.74	1/487 (0.2%)
27	A5	0.67	1/469 (0.2%)	0.83	2/634 (0.3%)
27	B5	0.79	0/469	0.88	0/634
28	A6	0.59	0/456	0.70	0/609
28	B6	0.68	0/456	0.74	0/609
29	A7	0.57	0/426	0.75	0/561
29	B7	0.78	0/426	0.84	0/561
30	A8	0.50	0/516	0.73	0/679
30	B8	0.70	0/516	0.82	0/679
31	CA	0.80	10/36054 (0.0%)	1.18	176/56272 (0.3%)
31	DA	0.77	7/36054 (0.0%)	1.19	211/56272 (0.4%)
32	CB	0.51	0/1811	0.69	0/2452
32	DB	0.56	0/1811	0.69	0/2452
33	CC	0.56	0/1474	0.65	0/2003
33	DC	0.58	0/1474	0.65	0/2003
34	CD	0.53	0/1550	0.72	3/2106 (0.1%)
34	DD	0.84	2/1550 (0.1%)	0.78	4/2106 (0.2%)
35	CE	0.49	0/1121	0.70	1/1517 (0.1%)
35	DE	0.52	0/1121	0.72	1/1517 (0.1%)
36	CF	0.49	0/794	0.64	0/1082
36	DF	0.49	0/794	0.67	1/1082 (0.1%)
37	CG	0.57	0/1186	0.65	0/1603
37	DG	0.56	0/1186	0.62	0/1603
38	CH	0.44	0/1065	0.67	0/1445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DH	0.44	0/1065	0.64	0/1445
39	CI	0.62	0/867	0.71	0/1180
39	DI	0.62	0/867	0.69	0/1180
40	CJ	0.60	0/672	0.74	1/919 (0.1%)
40	DJ	0.60	0/672	0.70	1/919 (0.1%)
41	CK	0.47	0/843	0.71	0/1144
41	DK	0.47	0/843	0.67	0/1144
42	CL	0.44	0/925	0.67	0/1251
42	DL	0.46	0/925	0.69	0/1251
43	CM	0.67	0/811	0.72	0/1103
43	DM	0.63	0/811	0.73	1/1103 (0.1%)
44	CN	0.60	0/487	0.68	0/649
44	DN	0.59	0/487	0.74	0/649
45	CO	0.49	0/735	0.64	0/981
45	DO	0.47	0/735	0.61	0/981
46	CP	0.51	0/667	0.70	0/905
46	DP	0.43	0/667	0.65	0/905
47	CQ	0.46	0/836	0.68	0/1117
47	DQ	0.47	0/836	0.66	0/1117
48	CR	0.43	0/519	0.64	0/699
48	DR	0.50	0/519	0.67	0/699
49	CS	0.69	0/558	0.88	1/759 (0.1%)
49	DS	0.76	1/558 (0.2%)	0.87	3/759 (0.4%)
50	CT	0.47	0/710	0.72	0/940
50	DT	0.42	0/710	0.68	0/940
51	CU	0.64	0/203	0.67	0/266
51	DU	0.59	0/203	0.70	0/266
All	All	0.86	110/303650 (0.0%)	1.16	1892/454928 (0.4%)

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
26	A4	0	1
34	CD	0	1
34	DD	0	1
42	CL	0	1
42	DL	0	1
All	All	0	5

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	DD	12	CYS	CB-SG	19.94	2.16	1.82
34	DD	26	CYS	CB-SG	15.79	2.09	1.82
31	DA	1492	A	C6-N6	-12.21	1.24	1.33
31	CA	1492	A	C2-N3	12.12	1.44	1.33
31	CA	1493	A	N9-C4	-11.96	1.30	1.37

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1492	A	C6-N1-C2	-28.45	101.53	118.60
31	DA	1492	A	C5-C6-N1	26.41	130.90	117.70
31	CA	1492	A	C8-N9-C4	-21.05	97.38	105.80
1	BA	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	BA	1332	G	N3-C4-C5	17.99	137.59	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A4	42	PHE	Peptide
34	CD	11	LEU	Peptide
42	CL	26	ALA	Peptide
34	DD	11	LEU	Peptide
42	DL	26	ALA	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	60900	0	30712	1406	0
1	BA	60900	0	30712	1060	0
2	AB	2574	0	1306	87	0
2	BB	2574	0	1306	35	0
3	AD	2136	0	2218	77	0
3	BD	2136	0	2218	81	0
4	AE	1555	0	1607	81	0
4	BE	1555	0	1607	54	0
5	AF	1576	0	1616	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	1576	0	1616	59	0
6	AG	1368	0	1324	70	0
6	BG	1368	0	1324	61	0
7	AH	1317	0	1376	66	0
7	BH	1317	0	1376	33	0
8	AI	1046	0	1067	55	2
8	BI	1046	0	1067	47	0
9	AN	1112	0	1180	60	0
9	BN	1112	0	1180	34	0
10	AO	923	0	981	28	0
10	BO	923	0	981	23	0
11	AP	1119	0	1186	38	0
11	BP	1119	0	1186	40	0
12	AQ	1122	0	1179	43	0
12	BQ	1122	0	1179	47	0
13	AR	968	0	1033	43	0
13	BR	968	0	1033	33	0
14	AS	865	0	905	62	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	48	0
15	BT	1063	0	1103	37	0
16	AU	959	0	1019	31	0
16	BU	959	0	1019	20	0
17	AV	771	0	830	22	0
17	BV	771	0	830	15	0
18	AW	881	0	935	25	0
18	BW	881	0	935	24	0
19	AX	742	0	799	22	0
19	BX	742	0	799	23	0
20	AY	785	0	832	36	0
20	BY	785	0	832	30	0
21	AZ	1522	0	1511	56	0
21	BZ	1522	0	1511	47	0
22	A0	594	0	604	27	0
22	B0	594	0	604	21	0
23	A1	745	0	804	26	0
23	B1	745	0	804	26	0
24	A2	588	0	643	31	0
24	B2	588	0	643	18	0
25	A3	458	0	503	22	0
25	B3	458	0	503	6	0
26	A4	349	0	340	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B4	349	0	340	16	0
27	A5	455	0	476	25	0
27	B5	455	0	476	18	0
28	A6	449	0	464	19	0
28	B6	449	0	466	17	0
29	A7	418	0	467	18	0
29	B7	418	0	467	14	0
30	A8	509	0	565	23	0
30	B8	509	0	565	20	0
31	CA	32208	0	16256	921	2
31	DA	32208	0	16254	923	0
32	CB	1777	0	1747	100	0
32	DB	1777	0	1747	95	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	58	0
34	CD	1520	0	1407	73	0
34	DD	1520	0	1406	85	0
35	CE	1105	0	1130	48	0
35	DE	1105	0	1130	54	0
36	CF	781	0	741	25	0
36	DF	781	0	741	29	0
37	CG	1167	0	1108	39	0
37	DG	1167	0	1108	46	0
38	CH	1045	0	1033	45	0
38	DH	1045	0	1033	53	0
39	CI	852	0	742	43	0
39	DI	852	0	742	52	0
40	CJ	659	0	552	31	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	24	0
41	DK	828	0	822	32	0
42	CL	909	0	927	43	0
42	DL	909	0	927	38	0
43	CM	801	0	743	33	0
43	DM	801	0	743	37	0
44	CN	478	0	498	33	0
44	DN	478	0	497	30	0
45	CO	724	0	749	32	0
45	DO	724	0	749	27	0
46	CP	651	0	638	33	0
46	DP	651	0	638	28	0
47	CQ	823	0	891	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DQ	823	0	891	22	0
48	CR	514	0	530	19	0
48	DR	514	0	530	17	0
49	CS	544	0	457	21	0
49	DS	544	0	457	26	0
50	CT	708	0	764	37	0
50	DT	708	0	764	26	0
51	CU	199	0	208	8	0
51	DU	199	0	208	6	0
52	AA	44	0	20	31	0
52	BA	44	0	20	23	0
53	AA	2	0	0	0	0
53	BA	2	0	0	0	0
All	All	279316	0	185722	7170	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 16.

The worst 5 of 7170 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)
52:AA:3001:T8B:C13	31:DA:1492:A:H5''	1.47	1.41
34:DD:26:CYS:SG	34:DD:26:CYS:CB	2.09	1.41
34:DD:12:CYS:SG	34:DD:12:CYS:CB	2.16	1.34
52:AA:3001:T8B:C22	52:AA:3001:T8B:H13	1.58	1.33
52:BA:3001:T8B:H13	52:BA:3001:T8B:C22	1.58	1.32

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)
8:AI:89:TYR:O	31:CA:357:G:O2'[2_654]	2.11	0.09
8:AI:91:SER:OG	31:CA:368:U:OP2[2_654]	2.12	0.08

## 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	
3	AD	273/276 (99%)	240 (88%)	27 (10%)	6 (2%)	8	41
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	12	51
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	4	28
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	4	28
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	6	38
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	4	28
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	2	16
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	7
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	3	20
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	4	28
8	AI	143/148 (97%)	103 (72%)	28 (20%)	12 (8%)	1	6
8	BI	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	1	9
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	1	11
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	3	23
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	4	29
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	29
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	2	16
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	4	28
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	5	33
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	5	33
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	3	23
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	20	64
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	6	34
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	6	34
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BT	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	22	65
16	AU	114/118 (97%)	104 (91%)	10 (9%)	0	100	100
16	BU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	AV	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	9	44
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	18	61
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	20	64
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	8	41
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	8	41
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	2	20
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	4	25
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	2	16
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	4	27
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	13	53
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	13	53
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	8	42
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	5	30
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	12	51
24	B2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	A3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	10	47
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	4
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	4
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	10	47
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	4	28
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	9	44
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	8	41
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	8	41
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	11	50
30	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CB	227/256 (89%)	171 (75%)	36 (16%)	20 (9%)	1	5
32	DB	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	1	11
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	2	17
33	DC	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	1	5
34	CD	206/209 (99%)	154 (75%)	40 (19%)	12 (6%)	2	15
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	4	28
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	1	8
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	4	28
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	31
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	24
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	11
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	3	25
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	12	51
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	4	26
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	6
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	1	11
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	1	4
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	11
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	4	27
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	6	35
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	3	23
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	3	23
43	CM	112/126 (89%)	84 (75%)	18 (16%)	10 (9%)	1	5
43	DM	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	0	3
44	CN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	5
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	17
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	28
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	7	40
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	1	5
46	DP	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	4	25
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	5	31
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	12	51
48	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	CS	76/93 (82%)	48 (63%)	17 (22%)	11 (14%)	0	1
49	DS	76/93 (82%)	54 (71%)	17 (22%)	5 (7%)	1	11
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	1	5
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	1	8
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	1	4
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	3	23

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	239	ARG
3	AD	275	LYS
5	AF	60	SER
6	AG	14	GLU
6	AG	78	SER

### 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	
3	AD	215/218 (99%)	185 (86%)	30 (14%)	4	18
3	BD	215/218 (99%)	189 (88%)	26 (12%)	6	26
4	AE	163/166 (98%)	139 (85%)	24 (15%)	3	16
4	BE	163/166 (98%)	134 (82%)	29 (18%)	2	10
5	AF	158/162 (98%)	133 (84%)	25 (16%)	3	14
5	BF	158/162 (98%)	138 (87%)	20 (13%)	5	23
6	AG	128/156 (82%)	110 (86%)	18 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BG	128/156 (82%)	114 (89%)	14 (11%)	7	30
7	AH	141/148 (95%)	125 (89%)	16 (11%)	7	29
7	BH	141/148 (95%)	124 (88%)	17 (12%)	6	26
8	AI	102/124 (82%)	76 (74%)	26 (26%)	0	2
8	BI	102/124 (82%)	76 (74%)	26 (26%)	0	2
9	AN	117/119 (98%)	94 (80%)	23 (20%)	1	8
9	BN	117/119 (98%)	91 (78%)	26 (22%)	1	5
10	AO	98/100 (98%)	89 (91%)	9 (9%)	11	38
10	BO	98/100 (98%)	89 (91%)	9 (9%)	11	38
11	AP	113/116 (97%)	96 (85%)	17 (15%)	3	16
11	BP	113/116 (97%)	97 (86%)	16 (14%)	4	18
12	AQ	111/111 (100%)	94 (85%)	17 (15%)	3	15
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	15
13	AR	101/101 (100%)	80 (79%)	21 (21%)	1	6
13	BR	101/101 (100%)	79 (78%)	22 (22%)	1	6
14	AS	84/88 (96%)	67 (80%)	17 (20%)	1	7
14	BS	84/88 (96%)	72 (86%)	12 (14%)	4	18
15	AT	110/127 (87%)	99 (90%)	11 (10%)	9	35
15	BT	110/127 (87%)	100 (91%)	10 (9%)	11	39
16	AU	93/94 (99%)	83 (89%)	10 (11%)	7	31
16	BU	93/94 (99%)	77 (83%)	16 (17%)	2	11
17	AV	80/82 (98%)	63 (79%)	17 (21%)	1	6
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	6
18	AW	89/92 (97%)	75 (84%)	14 (16%)	3	14
18	BW	89/92 (97%)	78 (88%)	11 (12%)	5	24
19	AX	75/78 (96%)	67 (89%)	8 (11%)	8	31
19	BX	75/78 (96%)	66 (88%)	9 (12%)	6	26
20	AY	80/91 (88%)	70 (88%)	10 (12%)	5	24
20	BY	80/91 (88%)	72 (90%)	8 (10%)	9	35
21	AZ	159/179 (89%)	139 (87%)	20 (13%)	5	24
21	BZ	159/179 (89%)	137 (86%)	22 (14%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A0	59/67 (88%)	52 (88%)	7 (12%)	6	26
22	B0	59/67 (88%)	52 (88%)	7 (12%)	6	26
23	A1	78/83 (94%)	68 (87%)	10 (13%)	5	23
23	B1	78/83 (94%)	70 (90%)	8 (10%)	8	33
24	A2	65/67 (97%)	56 (86%)	9 (14%)	4	19
24	B2	65/67 (97%)	57 (88%)	8 (12%)	5	25
25	A3	49/52 (94%)	43 (88%)	6 (12%)	6	25
25	B3	49/52 (94%)	43 (88%)	6 (12%)	6	25
26	A4	39/63 (62%)	32 (82%)	7 (18%)	2	10
26	B4	39/63 (62%)	30 (77%)	9 (23%)	1	4
27	A5	50/52 (96%)	43 (86%)	7 (14%)	4	18
27	B5	50/52 (96%)	43 (86%)	7 (14%)	4	18
28	A6	50/52 (96%)	40 (80%)	10 (20%)	1	7
28	B6	50/52 (96%)	41 (82%)	9 (18%)	2	10
29	A7	41/42 (98%)	35 (85%)	6 (15%)	3	17
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	5
30	A8	52/55 (94%)	45 (86%)	7 (14%)	4	20
30	B8	52/55 (94%)	47 (90%)	5 (10%)	10	37
32	CB	177/220 (80%)	141 (80%)	36 (20%)	1	7
32	DB	177/220 (80%)	142 (80%)	35 (20%)	1	8
33	CC	114/188 (61%)	95 (83%)	19 (17%)	2	12
33	DC	114/188 (61%)	96 (84%)	18 (16%)	3	14
34	CD	139/181 (77%)	117 (84%)	22 (16%)	3	14
34	DD	139/181 (77%)	120 (86%)	19 (14%)	4	19
35	CE	108/123 (88%)	86 (80%)	22 (20%)	1	7
35	DE	108/123 (88%)	88 (82%)	20 (18%)	2	9
36	CF	77/90 (86%)	65 (84%)	12 (16%)	3	14
36	DF	77/90 (86%)	65 (84%)	12 (16%)	3	14
37	CG	104/127 (82%)	86 (83%)	18 (17%)	2	11
37	DG	104/127 (82%)	88 (85%)	16 (15%)	3	15
38	CH	103/119 (87%)	85 (82%)	18 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DH	103/119 (87%)	84 (82%)	19 (18%)	2	9
39	CI	62/99 (63%)	53 (86%)	9 (14%)	4	17
39	DI	62/99 (63%)	54 (87%)	8 (13%)	5	22
40	CJ	52/92 (56%)	42 (81%)	10 (19%)	1	9
40	DJ	52/92 (56%)	41 (79%)	11 (21%)	1	6
41	CK	81/99 (82%)	69 (85%)	12 (15%)	3	16
41	DK	81/99 (82%)	71 (88%)	10 (12%)	5	25
42	CL	92/109 (84%)	81 (88%)	11 (12%)	6	26
42	DL	92/109 (84%)	83 (90%)	9 (10%)	9	36
43	CM	63/101 (62%)	49 (78%)	14 (22%)	1	5
43	DM	63/101 (62%)	49 (78%)	14 (22%)	1	5
44	CN	46/50 (92%)	35 (76%)	11 (24%)	1	3
44	DN	46/50 (92%)	33 (72%)	13 (28%)	0	1
45	CO	77/80 (96%)	65 (84%)	12 (16%)	3	14
45	DO	77/80 (96%)	66 (86%)	11 (14%)	4	18
46	CP	63/74 (85%)	49 (78%)	14 (22%)	1	5
46	DP	63/74 (85%)	53 (84%)	10 (16%)	3	13
47	CQ	94/97 (97%)	90 (96%)	4 (4%)	33	71
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	8	32
48	CR	49/77 (64%)	44 (90%)	5 (10%)	8	34
48	DR	49/77 (64%)	46 (94%)	3 (6%)	22	61
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	36 (86%)	6 (14%)	4	18
50	CT	65/82 (79%)	53 (82%)	12 (18%)	2	9
50	DT	65/82 (79%)	57 (88%)	8 (12%)	5	25
51	CU	18/22 (82%)	16 (89%)	2 (11%)	7	30
51	DU	18/22 (82%)	14 (78%)	4 (22%)	1	5
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	3	15

5 of 1333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	BR	6	SER

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Mol	Chain	Res	Type
24	B2	34	GLU
40	DJ	72	VAL
13	BR	96	ARG
17	BV	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
13	BR	13	HIS
35	CE	78	HIS
43	DM	106	ASN
19	BX	31	HIS
30	B8	35	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2817/2915 (96%)	581 (20%)	0
1	BA	2817/2915 (96%)	586 (20%)	0
2	AB	119/122 (97%)	25 (21%)	0
2	BB	119/122 (97%)	21 (17%)	0
31	CA	1496/1521 (98%)	339 (22%)	0
31	DA	1496/1521 (98%)	341 (22%)	0
All	All	8864/9116 (97%)	1893 (21%)	0

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	14	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
52	T8B	AA	3001	53	40,48,48	0.99	2 (5%)	51,71,71	1.29	7 (13%)
52	T8B	BA	3001	53	40,48,48	0.99	2 (5%)	51,71,71	1.30	8 (15%)

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
52	T8B	AA	3001	53	-	0/22/26/26	0/5/5/5
52	T8B	BA	3001	53	-	0/22/26/26	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AA	3001	T8B	C25-C24	2.26	1.50	1.43
52	BA	3001	T8B	C25-C24	2.28	1.50	1.43
52	BA	3001	T8B	O11-C26	2.88	1.38	1.32
52	AA	3001	T8B	O11-C26	2.89	1.38	1.32

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C21-C23-C24	-3.73	120.19	125.09
52	AA	3001	T8B	C21-C23-C24	-3.72	120.21	125.09
52	AA	3001	T8B	C2-C3-C4	-2.88	118.75	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C2-C3-C4	-2.87	118.76	122.17
52	BA	3001	T8B	O4-C12-C11	-2.19	108.73	112.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	AA	3001	T8B	31	0
52	BA	3001	T8B	23	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	2827/2915 (96%)	0.02	117 (4%) 38 25	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	0.08	73 (2%) 56 41	27, 56, 110, 126	0
2	AB	120/122 (98%)	0.02	4 (3%) 47 31	68, 95, 108, 111	0
2	BB	120/122 (98%)	-0.25	0 100 100	46, 80, 95, 103	0
3	AD	275/276 (99%)	-0.15	0 100 100	45, 67, 83, 103	0
3	BD	275/276 (99%)	-0.16	2 (0%) 87 80	36, 59, 78, 103	0
4	AE	204/206 (99%)	-0.10	1 (0%) 90 85	47, 72, 87, 98	0
4	BE	204/206 (99%)	-0.18	0 100 100	33, 60, 81, 96	0
5	AF	203/205 (99%)	-0.34	1 (0%) 90 85	44, 77, 95, 112	0
5	BF	203/205 (99%)	-0.23	0 100 100	27, 64, 90, 110	0
6	AG	181/182 (99%)	1.35	52 (28%) 1 1	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.10	9 (4%) 30 17	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.90	36 (20%) 1 1	80, 93, 101, 108	0
7	BH	174/180 (96%)	-0.16	0 100 100	63, 78, 91, 98	0
8	AI	145/148 (97%)	0.59	21 (14%) 3 1	72, 104, 116, 123	0
8	BI	145/148 (97%)	-0.10	1 (0%) 87 80	68, 90, 98, 100	0
9	AN	140/140 (100%)	-0.09	1 (0%) 87 80	59, 73, 90, 94	0
9	BN	140/140 (100%)	-0.19	0 100 100	38, 57, 82, 85	0
10	AO	122/122 (100%)	-0.33	0 100 100	56, 73, 85, 91	0
10	BO	122/122 (100%)	-0.22	0 100 100	43, 64, 82, 89	0
11	AP	147/150 (98%)	-0.01	3 (2%) 65 50	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.17	0 100 100	28, 68, 91, 100	0
12	AQ	141/141 (100%)	-0.04	1 (0%) 87 80	60, 78, 91, 97	0
12	BQ	141/141 (100%)	-0.09	0 100 100	44, 65, 78, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AR	118/118 (100%)	-0.19	0 100 100	47, 66, 78, 88	0
13	BR	118/118 (100%)	-0.20	0 100 100	35, 53, 69, 86	0
14	AS	110/112 (98%)	0.53	13 (11%) 5 3	74, 91, 102, 109	0
14	BS	110/112 (98%)	-0.13	0 100 100	58, 79, 93, 100	0
15	AT	131/146 (89%)	-0.22	1 (0%) 86 77	66, 76, 99, 109	0
15	BT	131/146 (89%)	-0.27	1 (0%) 86 77	55, 68, 91, 102	0
16	AU	116/118 (98%)	-0.05	0 100 100	53, 70, 84, 89	0
16	BU	116/118 (98%)	-0.15	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.19	1 (0%) 82 72	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.31	0 100 100	31, 61, 81, 95	0
18	AW	112/113 (99%)	-0.24	0 100 100	50, 59, 80, 104	0
18	BW	112/113 (99%)	-0.31	0 100 100	36, 45, 75, 106	0
19	AX	95/96 (98%)	-0.08	0 100 100	54, 71, 89, 93	0
19	BX	95/96 (98%)	-0.18	0 100 100	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.15	7 (6%) 20 11	71, 81, 94, 105	0
20	BY	107/110 (97%)	-0.24	1 (0%) 84 75	56, 71, 89, 103	0
21	AZ	198/206 (96%)	0.01	7 (3%) 44 29	80, 92, 103, 108	0
21	BZ	198/206 (96%)	-0.36	0 100 100	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.24	2 (2%) 56 41	59, 74, 84, 89	0
22	B0	76/85 (89%)	-0.24	0 100 100	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.12	3 (3%) 49 33	54, 71, 94, 99	0
23	B1	97/98 (98%)	-0.08	1 (1%) 82 72	42, 65, 91, 95	0
24	A2	70/72 (97%)	-0.06	1 (1%) 75 63	65, 81, 92, 101	0
24	B2	70/72 (97%)	-0.13	0 100 100	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.44	5 (8%) 11 7	63, 74, 92, 101	0
25	B3	59/60 (98%)	-0.16	0 100 100	43, 56, 84, 94	0
26	A4	46/71 (64%)	0.55	7 (15%) 2 1	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.27	6 (13%) 4 2	98, 107, 113, 118	0
27	A5	59/60 (98%)	-0.35	0 100 100	46, 64, 78, 91	0
27	B5	59/60 (98%)	-0.19	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.15	3 (5%) 24 14	62, 77, 87, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	B6	53/54 (98%)	-0.10	0 100 100	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.14	4 (8%) 12 7	43, 54, 79, 99	0
29	B7	48/49 (97%)	-0.00	1 (2%) 64 49	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.12	0 100 100	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.12	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.56	191 (12%) 4 3	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.51	178 (11%) 5 3	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.11	14 (6%) 22 12	93, 103, 111, 117	0
32	DB	229/256 (89%)	0.65	32 (13%) 3 2	95, 105, 112, 115	0
33	CC	206/239 (86%)	1.00	45 (21%) 1 1	92, 106, 112, 115	0
33	DC	206/239 (86%)	0.88	33 (16%) 2 1	97, 108, 115, 120	0
34	CD	208/209 (99%)	0.03	10 (4%) 31 19	85, 98, 108, 114	0
34	DD	208/209 (99%)	0.02	10 (4%) 31 19	87, 97, 107, 123	0
35	CE	148/162 (91%)	-0.14	4 (2%) 55 40	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.10	5 (3%) 46 30	84, 96, 104, 110	0
36	CF	100/101 (99%)	-0.07	5 (5%) 30 17	80, 92, 101, 107	0
36	DF	100/101 (99%)	-0.15	3 (3%) 51 35	84, 93, 103, 110	0
37	CG	155/156 (99%)	2.13	76 (49%) 0 0	99, 109, 115, 120	0
37	DG	155/156 (99%)	2.07	74 (47%) 0 0	97, 109, 115, 119	0
38	CH	138/138 (100%)	0.05	4 (2%) 52 37	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.09	3 (2%) 62 48	86, 96, 102, 106	0
39	CI	125/128 (97%)	1.89	50 (40%) 0 0	97, 111, 117, 120	0
39	DI	125/128 (97%)	2.78	73 (58%) 0 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	2.14	43 (44%) 0 0	100, 109, 115, 117	0
40	DJ	96/105 (91%)	1.93	48 (50%) 0 0	97, 110, 115, 119	0
41	CK	114/129 (88%)	-0.12	1 (0%) 84 75	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.23	4 (3%) 44 29	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.23	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.15	1 (0%) 86 77	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.13	49 (42%) 0 0	102, 111, 118, 126	0
43	DM	114/126 (90%)	1.75	44 (38%) 0 0	101, 109, 115, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	CN	60/61 (98%)	1.18	14 (23%) 1 1	99, 108, 116, 118	0
44	DN	60/61 (98%)	1.58	21 (35%) 0 0	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.01	2 (2%) 61 46	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.18	6 (6%) 18 10	81, 93, 103, 107	0
46	CP	82/88 (93%)	0.61	6 (7%) 16 9	88, 96, 106, 112	0
46	DP	82/88 (93%)	0.42	3 (3%) 42 27	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.04	2 (2%) 65 50	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.17	3 (3%) 51 35	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.14	8 (11%) 5 3	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.20	3 (4%) 35 22	85, 93, 104, 106	0
49	CS	78/93 (83%)	2.61	43 (55%) 0 0	107, 111, 117, 123	0
49	DS	78/93 (83%)	2.85	52 (66%) 0 0	91, 112, 117, 119	0
50	CT	96/106 (90%)	0.18	2 (2%) 64 49	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.69	10 (10%) 7 4	82, 92, 100, 101	0
51	CU	23/27 (85%)	2.86	12 (52%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	2.64	13 (56%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.25	1586 (7%) 14 8	27, 84, 115, 128	0

The worst 5 of 1586 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	CI	30	GLY	12.5
49	CS	40	ILE	12.4
43	CM	85	GLY	12.0
31	CA	1353	G	11.0
31	CA	1286	A	10.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
52	T8B	BA	3001	44/44	0.89	0.34	4.94	20,20,20,20	0
52	T8B	AA	3001	44/44	0.85	0.28	2.12	20,20,20,20	0
53	MG	BA	3002	1/1	0.85	0.15	-	30,30,30,30	0
53	MG	AA	3002	1/1	0.95	0.20	-	30,30,30,30	0
53	MG	BA	3003	1/1	0.94	0.16	-	30,30,30,30	0
53	MG	AA	3003	1/1	0.98	0.17	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.