



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:55 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

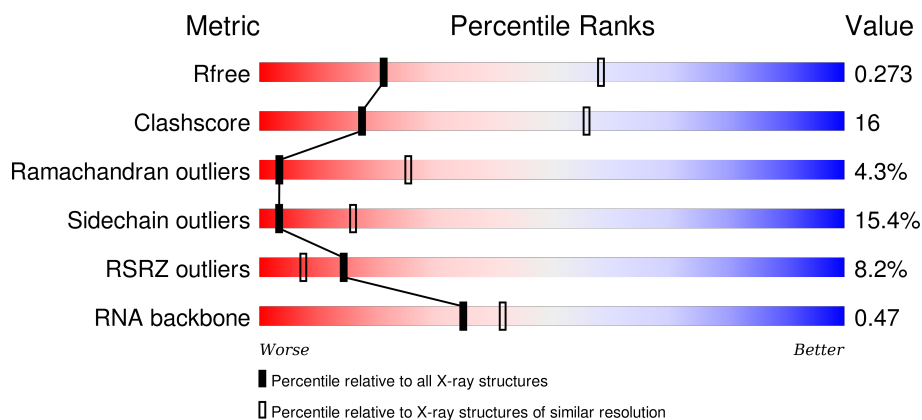
1 Overall quality at a glance

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.









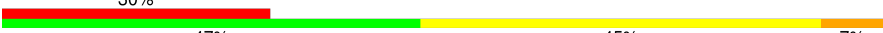


















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>36% 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>





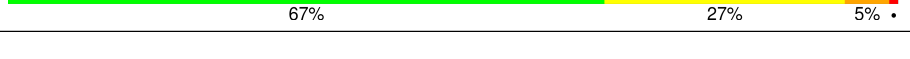
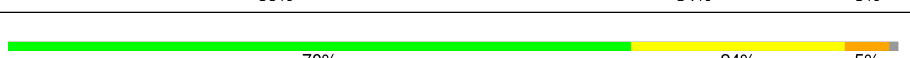


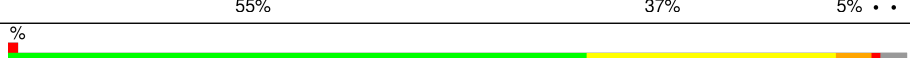
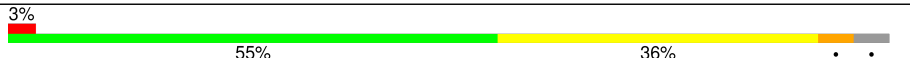
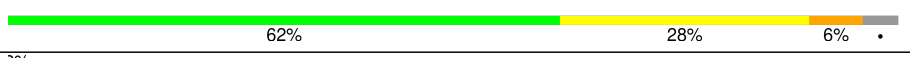

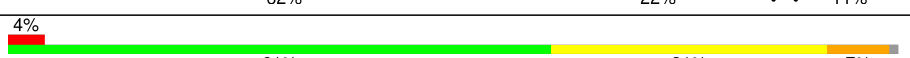

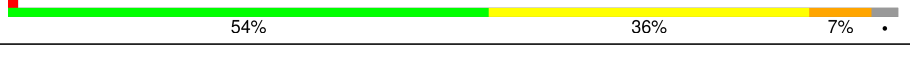


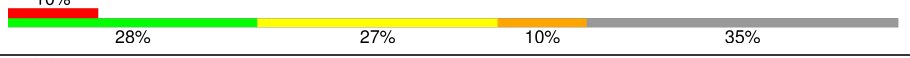
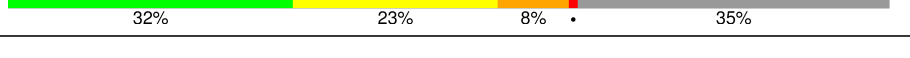




Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	
20	BY	110	
21	AZ	206	
21	BZ	206	
22	A0	85	
22	B0	85	
23	A1	98	
23	B1	98	
24	A2	72	
24	B2	72	
25	A3	60	
25	B3	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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 [i](#)

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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		0	0	0
			458	293	87	78				
25	B3	59	Total	C	N	O		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			

Continued on next page...

Continued from previous page...

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			

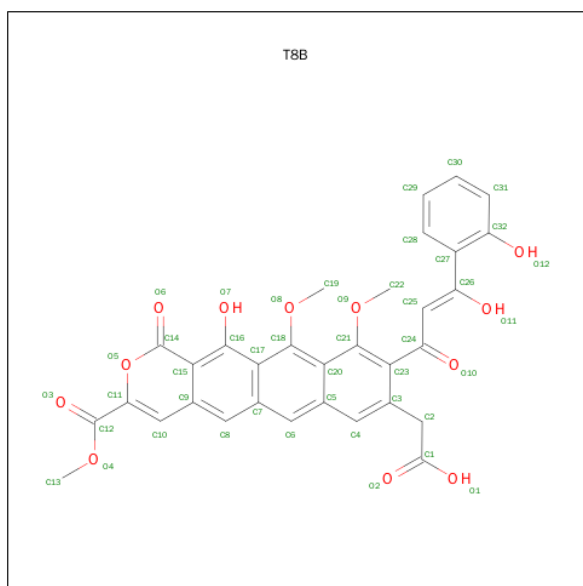
- Molecule 50 is a protein called 30S ribosomal protein S20.

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		

Continued on next page...

Continued from previous page...

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

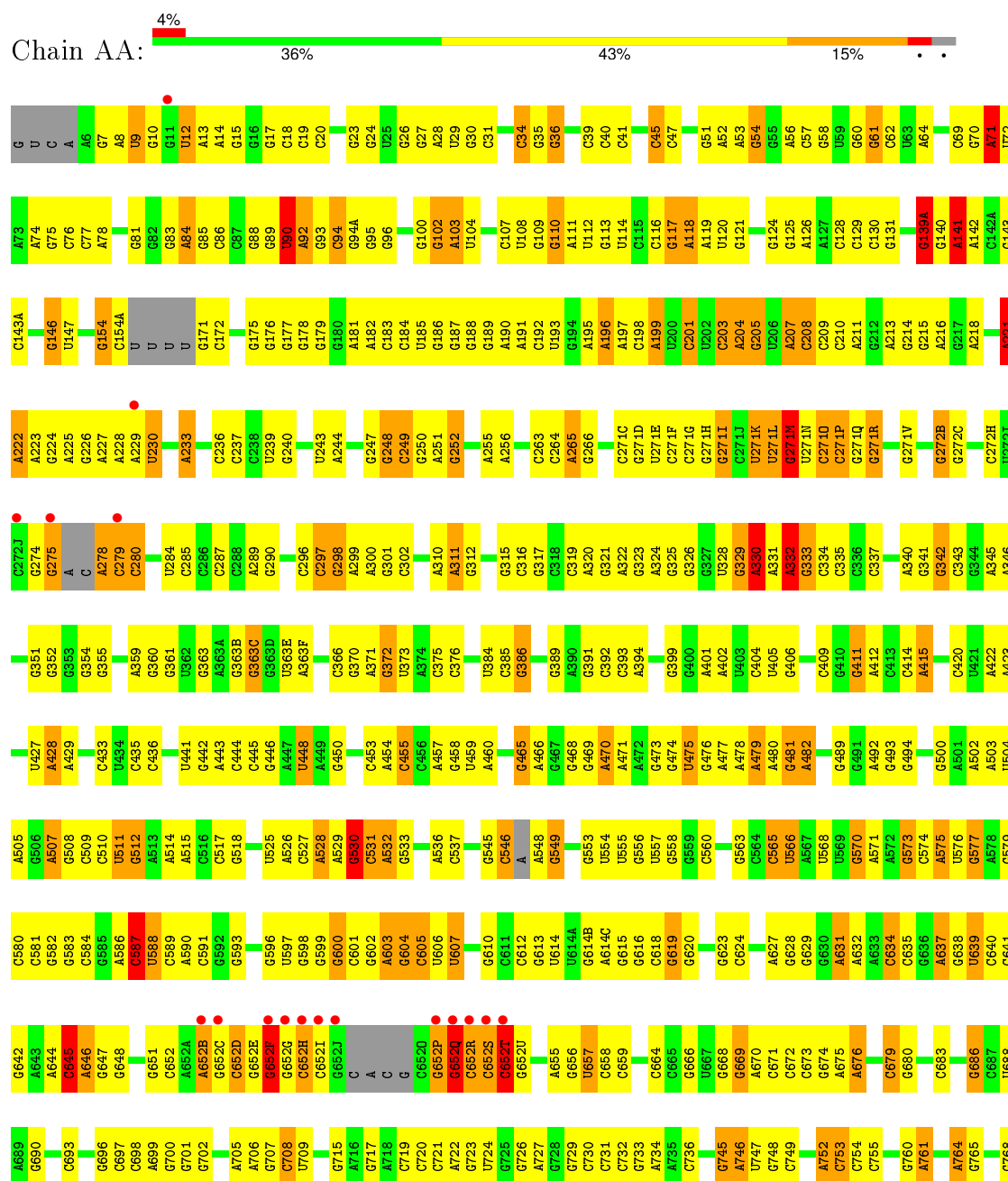
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

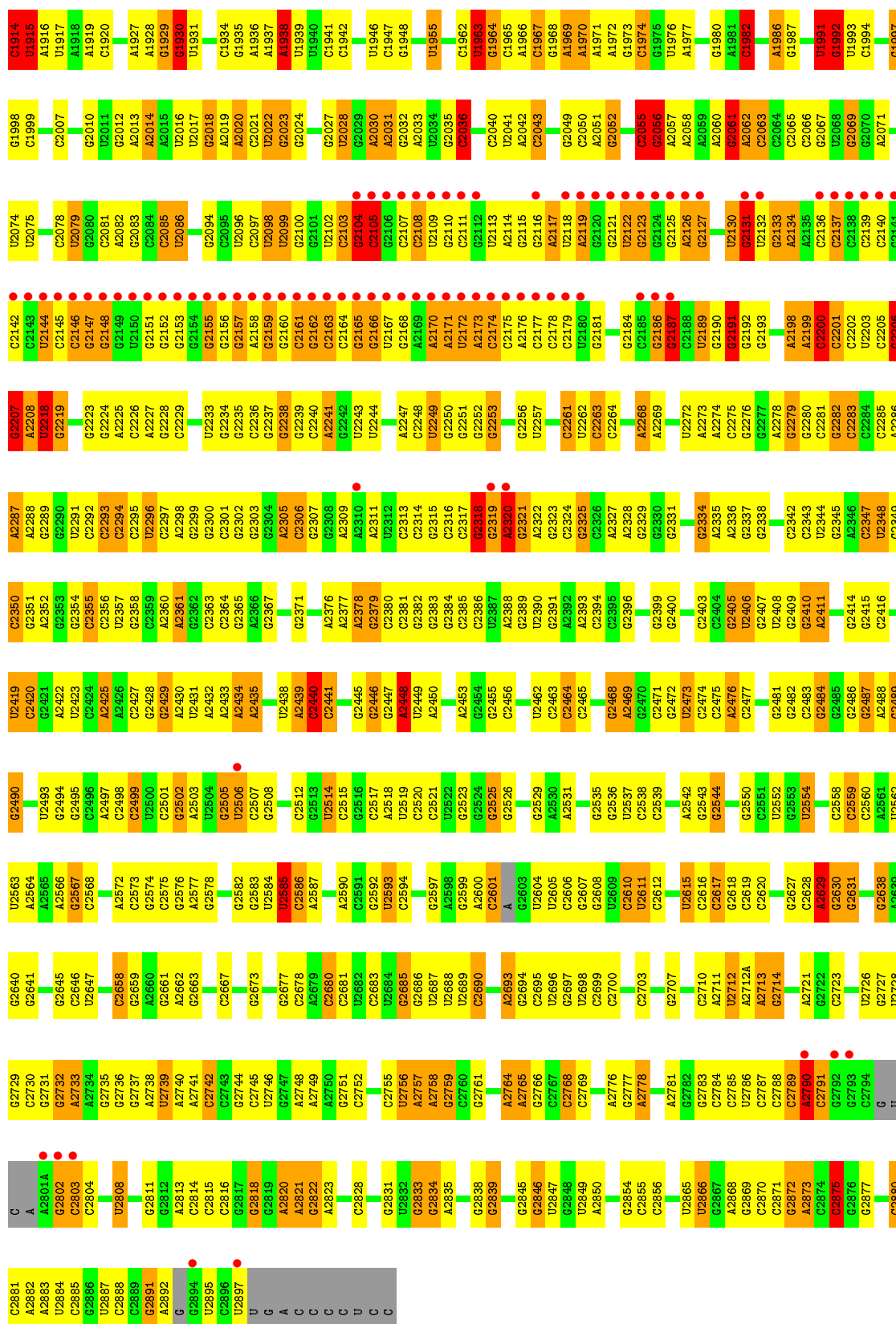
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

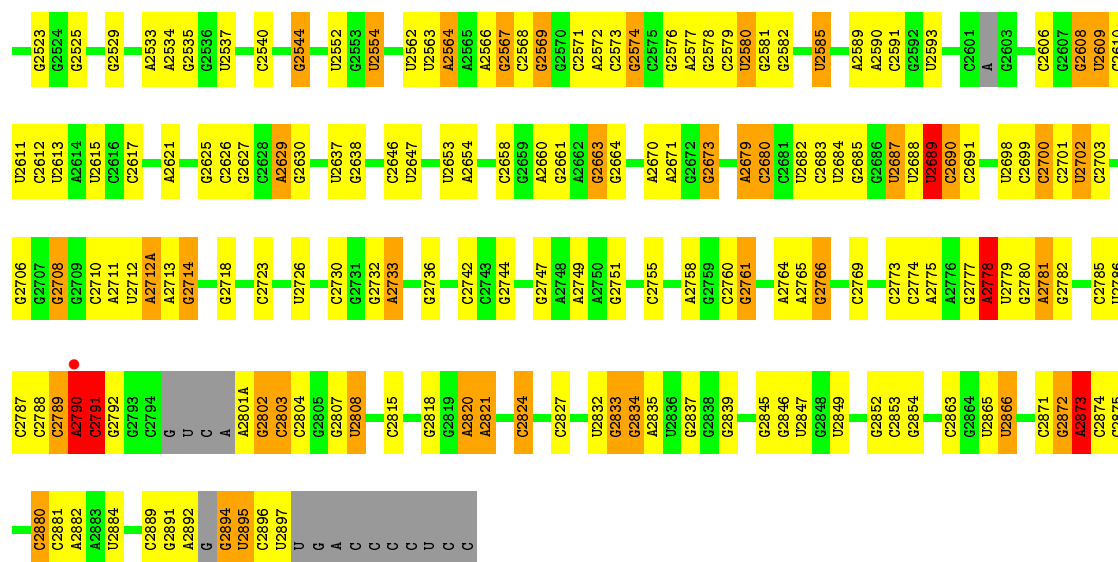


U1805	G1710	C1638	A1542	G1478	C1399	G1327	G1248	C1179	U	A1045	C975	C902	G836	G769
G1711	U1639	U1639	A1545	G1479	C1403	G1328	U1249	C1180	G	A1046	G975A	C903	C837	G770
C1712	C1640	C1640	A1546	G1480	C1404	U1329	G1250	G1183	G1107	G1047	C976	C904	C838	U773
G1720	C1644	C1644	C1547	U1481	U1405	G1330	G1252	G1184	C1109	A1048	G977	U905	U839	A774
G1721	G1645	G1645	C1548	U1482	U1406	G1332	A1253	G1185	C1109	C1049	A980	G906	C840	A775
U1818	C1646	C1646	C1549	G1483	C1407	C1333	A1253	G1186	G1111	A1050	G976	U907	A841	G775
A1819	G1647	G1647	A1558	G1485	C1408	G1334	G1256	G1187	A1112	C1051	C977	C908	C842	G776
U1820	C1648	C1648	G1559	A1486	C1409	U1335	U1257	U1188	G1113	G1052	C978	A909	A777	A777
G1823	G1651	G1651	G1560	G1487	G1410	A1336	C1258	A1189	G1114	C	A984	A910	G845	A778
G1823	A1652	A1652	C1564	U1489	C1411	G1337	G1259	G1190	G1115	G	C986	A911	G848	U779
G1826	G1653	G1653	C1565	U1490	A1412	G1338	G1260	G1191	C1116	G	G987	U913	A849	G780
C1827	A1654	A1654	A1572	G1491	G1413	G1339	C1261	G1192	G1120	A	A988	C914	C850	A781
G1828	A1655	A1655	G1568	G1492	G1416	U1340	A1265	G1193	G1121	G	G989	C915	G854	A783
A1829	C1656	C1656	G1569	C1493	C1417	U1341	A1266	U1198	G1122	U	A990	A916	G854	A784
C1833	C1657	C1657	A1570	A1494	G1418	G1343	U1267	U1199	G1123	G	C991	A917	G855	A785
U1833	G1660	G1660	A1571	A1495	A1419	U1344	A1273	U1205	G1124	U	C992	A918	C856	C786
U1834	C1661	C1661	A1572	U1496	U1420	G1344	A1274	U1206	G1125	A	G993	G919	C857	U787
G1835	G1662	G1662	C1575	U1497	G1421	C1350	C1270	C1201	G1125	G	C994	G920	U858	A788
C1837	C1663	C1663	U1576	C1501	G1422	C1351	U1271	C1202	U1130	C	C995	G921	C859	G792
G1838	A1664	A1664	C1577	C1502	G1423	C1351	A1272	G1203	G1131	U	A996	U922	U860	G793
A1839	G1665	G1665	U1578	G1503	A1427	A1354	U1273	A1204	A1132	A	G997	C923	A861	A794
G1840	C1666	C1666	A1579	C1504	G1428	G1355	A1278	G1206	U1133	U	U999	G928	A863	C795
C1844	G1667	G1667	A1580	C1505	G1429	U1357	A1278	G1206	G1136	A	A1001	G932	C864	C796
C1847	A1668	A1668	G1581	C1506	G1430	G1358	U1282	U1211	G1137	G	A1002	A933	A866	C797
A1848	C1669	C1669	C1582	C1507	U1431	A1359	G1283	A1213	G1138	C	G1003	G938	U868	A802
G1849	G1670	G1670	A1583	A1508	C1432	A1360	A1284	A1214	C1139	G	C1004	U938	U869	U803
G1850	U1671	U1671	A1584	C1509	U1433	G1364	G1285	G1215	C1140	C	C1005	A941	C870	A804
A1853	C1672	C1672	A1586	C1509A	A1434	A1365	A1286	G1216	U1142	C	C1007	G942	A870	G805
G1854	G1674	G1674	C1588	U1514	C1437	A1366	A1287	A1220	A1142A	A	C1008	U943	C873	C806
G1855	G1678	G1678	G1591	G1515	U1438	A1367	U1288	C1221	A1143	U	A1009	G944	C874	U807
C1858	C1684	C1684	G1593	C1516	A1439	G1368	U1292	C1221A	G1144	C	G	G946	C876	G808
G1863	G1685	G1685	G1594	U1518	G1441	C1370	C1293	G1222	A1148	U	U1012	G947	U877	C812
A1876	C1686	C1686	C1598	G1519	G1442	U1372	C1297	G1223	C1153	U	U1014	G948	A878	U813
A1877	U1688	U1688	U1602	U1523	A1445	A1373	G1298	A1226	G1154	U	G1015	C949	C879	C814
G1878	A1690	A1690	U1602	G1524	G1448	G1374	G1299	G1227	A1155	A	G1016	G950	C880	C815
C1882	C1691	C1691	C1607	G1526	A1449	C1375	U1300	G1228	A1156	C	G1017	C951	C881	C816
G1883	U1692	U1692	A1608	G1527	G1450	C1376	A1301	C1229	U1159	G	U1019	G952	C882	C817
A1884	C1693	C1693	A1609	A1528A	G1455	A1378	A1308	C1230	G1160	C	A1020	G954	C883	C818
A1889	G1694	G1694	A1610	G1529	G1459	G1381	G1309	C1231	G1161	G	C885	G954	C884	A819
A1890	C1695	C1695	C1611	C1530	A1460	G1382	G1310	G1232	G1162	U	C886	U958	C885	A820
C1891	G1696	G1696	G1612	G1530	G1461	C1383	U1312	G1236	U1165	C	G1025	C966	C886	A821
C1892	G1697	G1697	G1613	C1531	C1462	U1383	U1313	A1237	C1166	G	U1026	C967	C887	U822
A1899	A1698	A1698	A1614	C1532	C1463	A1384	C1314	G1238	U1167	C	A1027	C968	C888	G823
G1899	G1699	G1699	C1615	G	C1464	G1385	C1315	G1239	G1168	C	U1028	C969	C889	A824
C1892	U1700	U1700	U	U	C1464	C1386	U1316	U1240	G1168	U	U1033	C966	C890	C825
A1900	U1701	U1701	A	A	C1467	C1387	A1317	A1241	G1171	U	G	C966	C894	U826
G1906	G1702	G1702	G1618	C1537	G1470	A1393	G1318	A1242	G1171	C	U1033	C966	C894	U827
A1913	G1703	G1703	G1619	G1537	A1470	U1394	G1319	G1243	A1173	U	G1038	C967	C895	A828
	G1705	G1705	G1636	G1538	A1471	U1395	C1320	G1244	A1174	C	C1039	C968	C896	G830
	U1709	U1709	A1637	U1540	A1472	U1396	U1323	G1245	U1175	U	G1042	C970	C897	G831
				G1541	G1473			A1246	G1176	C	C1043	C971	C898	G832
								A1247	A1177	C	G1044	G974	A900	U833
									C1178	C			A901	C834
														A835

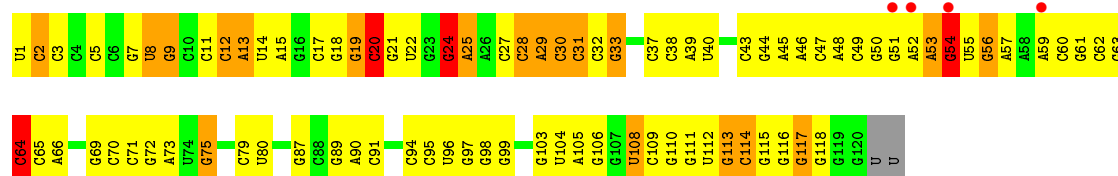


C1153	C1154	C1155	U1165	C1166	C1169	G1170	G1171	G1173	A1174	U1175	G1176	A1177	C1178	C1179	C1180	C1181	A1182	G1183	G1184	C1185	G1186	G1187	U1188	A1189	G1190	G1191	G1192	C1193	G1194	A1195	C1201	C1202	G1203	A1204	G1209	A1210	U1211	G1212	C1218	G1219	A1220	G1223	C1224	G1225	A1226	G1227		G1231	G1236	G1239			
U	C	C	U	U	A	A	A	A	G	G	U	G	C	G	A	U	A	U	G	C	C	A1106	C	U	G	G	G	G1107	U1108	C1109	A1110	A1111	G1112	U1113	G1114	G1115	C1116	G1125	A1126	U1129	U1130	G1131	C1135	G1136	G1139	A1140	G1141	U1142	U1143	G1149	C1150		
A917	G928	U932	G933	G934	U937	G938	G939	G940	A941	G944	A945	G946	G947	G948	C949	A953	G954	C955	G956	A957	U958	A959	A960	C961	C970	G974	G975	G976	G977	G978	A983	G987	U988	C991	G992	G993	C994	C995	A996	G997	A998	U999	A1000	A1001	G1002	G1003	C1004	C1005					
G831	G832	U833	C834	U839	C840	A841	C846	U847	G848	A849	G855	C856	C857	U858	G859	A861	G862	A863	G864	C865	A870	A878	A879	G880	G881	G882	G883	C884	C885	C886	A887	C888	C889	A890	G892	C893	C894	U895	C896	C897	C898	C899	A900	A901	C902	C903	U909	A910	A911	C912	C915	G916	
C756	U757	C758	G759	G760	A761	U762	G763	A764	G765	G768	G769	G770	G771	A772	G775	G776	A777	G778	A782	A783	A784	G785	C786	U787	A788	G792	A793	G794	G795	C796	G797	G798	A802	U803	A804	G805	C806	U807	C812	U813	C814	C817	G818	U819	A820	A821	U827	U828	C829				
G831	G832	U833	C834	U839	C840	A841	C846	U847	G848	A849	G855	C856	C857	U858	G859	A861	G862	A863	G864	C865	A870	A878	A879	G880	G881	G882	G883	C884	C885	C886	A887	C888	C889	A890	G892	C893	C894	U895	C896	C897	C898	C899	A900	A901	C902	C903	U909	A910	A911	C912	C915	G916	
A1009	U1012	C1013	U1019	A1020	A1021	G1022	G1023	G1024	G1025	U1026	A1027	A1028	U1033	G1037	C1038	G1039	C1040	C1041	G1042	G1043	G1044	A1045	A1046	G1047	C1049	A1050	C1051	C	A	G	G	A983	G987	U988	C991	G992	G993	C994	C995	A996	G997	A998	U999	A1000	A1001	G1002	G1003	C1004	C1005				
U	C	C	U	U	A	A	A	A	G	G	U	G	C	G	A	U	A	U	G	C	C	A1106	C	U	G	G	G	G1107	U1108	C1109	A1110	A1111	G1112	U1113	G1114	G1115	C1116	G1125	A1126	U1129	U1130	G1131	C1135	G1136	G1139	A1140	G1141	U1142	U1143	G1149	C1150		
G79	G83	A84	G85	G86	U89	A92	G93	C94	G94A	G95	G100	G102	A103	U104	C107	U108	G109	G110	A111	U114	C115	G116	U117	C118	A119	U120	G121	G122	G123	G124	G125	A126	G127	C128	G129	C130	G131	G136	G139A	G140	A142	C143	G143A	G151	G154	U154A	U	U					
U	U	C1172	G1176	G1177	G1178	G1179	G180	A181	C182	C183	C184	U185	A186	G187	G188	C192	A195	A196	C197	C198	A199	U200	U202	C201	G202	A203	G205	U206	A207	C208	G209	C210	A213	G214	G215	A216	G217	G218	G219	G220	A221	A222	A223	A225	C226	A227	A228	A229	A233	C234	U235	A236	U
G242	U243	G244	C246	G247	G248	G249	G250	A251	C252	G253	C254	A255	C263	G264	A265	G266	G271D	U271E	C271F	G271G	G271H	G271I	G271J	U271K	G271L	G271M	G271N	G271O	G271P	G271Q	G271R	G271S	G271T	G271U	G271V	G271W	G271X	G271Y	G272A	G272B	G272C	G272D	C272G	C272H	G275	C	A	A278	C279	C280	C286	C287	
C296	C297	A298	A299	A300	G301	A311	G312	C318	C319	A320	G321	C322	A323	A324	U328	G329	A330	A331	A332	G333	C334	C335	C336	C337	U338	A339	A340	G341	G342	U350	G351	G352	G361	U362	G363	A363A	G363B	G363C	U363D	U363E	A363F	C365	C366	G370	A371	C372	C375	C376	U384	C385			
G386	G389	A390	G396	U405	G406	C409	G410	G411	A412	C413	A414	A415	A416	C420	A428	C435	C436	G437	G438	G440	A443	C444	C445	A447	U448	G450	A451	G452	C453	A454	C455	C456	A457	G458	U459	A460	G463	U464	G465	G468	G469	A470	A471	C472	G473	G474	U475	U562					
A478	A479	A480	A481	A482	A483	A484	C485	G489	A491	A492	A493	G494	A505	G508	C509	U511	U512	A513	A514	A515	C516	C517	U524	U525	A526	A527	A528	A529	G530	C531	A532	G533	U534	C535	A536	C537	C543	G545	C546	A	A548	G549	U554	U555	G559	G562	A631						
G563	G564	U565	A567	U568	U569	G570	A571	A572	C573	A574	A575	U576	G577	G579	C580	C581	C584	G585	A586	C587	U588	C589	G592	G596	U597	G598	G599	G600	C601	G602	A603	A604	G605	U606	U607	C612	G613	U614	U614A	G614B	A614C	G615	G616	C618	G619	G620	A621	A627	G628	G629	G630	A631	
C634	A637	G638	U639	C640	C641	G642	A643	G644	G645	A646	G647	G648	G649	G650	G651	A652B	G652C	G652D	G652E	G652F	C652G	C652H	G652I	C	A	C	G	C652P	G652Q	G652R	C652S	G652T	G652U	G652V	A654	A655	G656	U657	C658	G659	G660	C661	G662	G663	G664	G668	G669	A670	G671	C672	C673	C674	
A675	A676	A677	C679	G680	G681	G682	G683	A685	G686	A689	G690	C691	G692	C693	U694	A699	G700	G708	G715	A716	G717	A722	G723	U724	G725	G726	A727	G728	G729	G730	G731	G732	G733	A734	A735	G738	G739	U740	G741	G742	A746	U747	G748	C749	A750	A751	A752	C753	C754	C755			

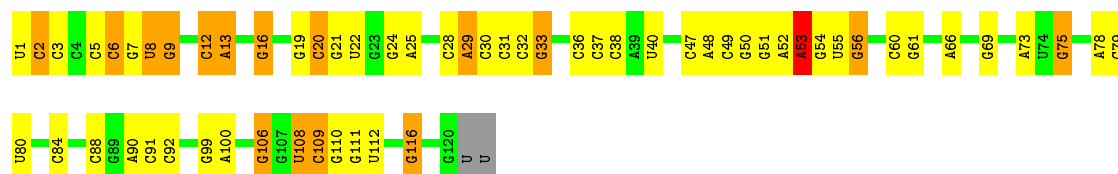
A2439	C2356	G2191	G2181	A2057	G1967	A1884	A1791	G1678	G1584	A1494	C1408	G1324	A1241
C2440	U2357	G2192	U2132	A2058	G1968	A1885	G1792	U1679	A1586	A1495	C1408	G1325	A1242
C2441	A2287	G2193	G2133	A2059	A1969	C1886	G1793	U1680	A1587	A1496	G1412	G1326	G1243
G2445	A2360	A2198	A2135	A2061	A1971	A1888	G1795	C1685	C1598	U1503	G1416	G1328	A1247
G2446	G2362	A2199	G2136	A2062	A1972	A1889	U1796	C1686	C1598	C1504	G1417	U1329	G1252
G2447	G2363	C2200	C2137	C2063	C1979	A1890	C1797	G1687	U1602	C1505	G1418	C1330	A1253
A2448	G2364	C2201	C2138		G1979	C1895	G1799	U1688	C1598	C1506	G1419	A1331	A1254
U2449	G2365	C2202	C2139	G2069	G1980	G1896	C1800	U1689	U1602	A1507	G1420	G1332	G1255
G2450	C2293	U2203	G2140	G2070	A1981	G1896	C1801	G1696	A1608	A1508	U1421	G1333	U1256
A2451	C2294	C2205	G2141	A2071	C1982	G1897	G1802	G1697	A1609	A1509	G1422		G1257
C2452	C2295	G2206	C2142		C1983	U1898	A1803	A1698	A1610	A1509B		G1337	C1258
	U2296	G2207	C2143	U2074	G1990	A1899	A1803	A1698	G1613	A1509A		G1338	
		A2208	U2144	U2075	G1990	A1900		G1699	G1613	A1509B		G1339	
C2461	G2299	G2218	C2145	U2076	U1991	A1901	C1806	A1701	A1614	G1510		U1340	A1262
U2462	A2376	G2219	C2146	A2077	G1992	A1902		A1701	A1614	G1510		U1341	U1263
C2463	A2377	G2220	C2147		G1992	A1903	A1810	G1702	G1617	U1514		U1342	G1264
C2464	G2302	G2221	G2148	U2079	U1993	G1903	G1811	G1711	G1622	U1515		A1342	A1265
C2465	G2303	G2222	G2149		G1997	G1906		C1711	G1622	C1516		G1343	G1266
C2466	G2304	G2223	U2150	U2086	G1998	G1907	G1814	C1712		C1516		G1344	U1267
C2467	A2305	G2224	G2151	G2087	G1999	G1908	A1815	G1719	C1625	U1517		A1349	A1268
G2468	G2306	G2225	G2152	G2087	G1999	G1908	G1816	U1720	G1626	U1518		C1350	A1269
A2469	G2307	A2225	G2153	G2088	C2007	C1913	G1817	U1720		G1519		C1351	C1270
G2470	G2308	G2226	G2154		C2008	C1914	U1818	A1722	G1633	G1529		U1357	G1271
C2471	A2309	A2227	G2155	G2093	C2009	U1915	A1819	U1739	A1634	C1530		A1357	A1272
G2472	G2310	G2228	G2156		G2012	U1916	U1820	U1740	G1635	C1532		G1358	U1273
U2473	A2311	C2229	G2157	U2096	G2013	U1917		G1746		G1532		A1360	A1274
C2474	U2312		A2158	C2097	A2013	A1918	G1823	G1753	G1647	U1541		G1364	A1275
C2475	C2313	G2235	G2159	U2098	C2014	A1919	G1824	C1754		G1541		G1365	A1278
A2476	A2314		G2160	U2099	A2015	G1928	A1825	A1755	C1648	A1542		A1366	G1279
C2477	G2315	G2238	G2161	A2101	A2016	G1929	U1834	G1756	G1649	A1542		A1367	U1282
A2478	C2316	G2239	C2162	G2107	U2016	G1930	G1835	U1757	G1650	A1542		G1368	G1283
C2479	C2317		G2163	U2102		U1931	G1827	G1758	G1651			G1370	A1286
G2480	G2480	A2247	C2164	C2103	A2020	U1926	U1828	G1759	G1652	A1545		U1372	C1289
G2481	U2406	C2248	G2165	C2105	C2021	A1927	A1829	C1754	G1653	C1546		A1373	C1290
U2482	G2407	U2249	G2166	C2106	U2022	A1928		A1754		C1547		U1378	C1292
C2483	U2408	G2250	G2167	G2107	G2023	G1929	U1834	G1756	A1654	C1548		A1379	C1293
G2489	G2409	G2251	U2167	C2107	G2024	G1930	U1835	U1757	G1655	U1570		G1380	U1294
G2410	G2410	G2252	G2168	C2108		U1931	G1835	G1757	G1656	A1570		U1394	C1295
A2411	A2411	G2253	A2169	U2109	U2028	G1935	G1836	G1758	C1657	A1570		A1395	
A2412	G2412		A2170	G2110	G2029	G1935	C1837	A1759	G1658	A1570		A1400	A1307
U2491	G2413	C2261	A2171	C2111	A2030	A1936	G1846	C1759	A1665	A1566		G1400	A1308
U2492	G2414	U2262	A2172	G2112	A2031	A1936	A1847	A1773	G1666	A1567		G1401	G1309
U2493		C2263	A2173	U2113	A2032	A1937	G1839	C1774	G1667	G1479		C1402	G1310
			C2174	U2114	G2033	A1938	G1840	A1762	G1668	G1480		G1403	G1311
	A2418		C2175	A2114	A2033	G1948		G1763	C1656	A1568		C1404	U1312
A2497	U2419	A2267	G2176	G2115	U2034	G1949	G1843	G1764	C1657	A1569		U1405	U1313
C2498	C2420	A2268	A2177	G2116	G2035	G1949			G1658	A1570		U1406	C1314
G2501	G2421		C2177	A2117	C2036	G1950	G1846	G1772	A1665	A1571		A1399	
G2502	U2422	G2271	C2178	U2118	G2037	U1951	A1847	C1774	G1665	A1571		A1395	
A2503	C2424	A2273	C2179	A2119	G2038	A1952	A1854	U1779	G1666	A1571		A1400	A1308
U2504	A2425	A2274	U2180	G2120	G2038	A1953	G1855	U1779	G1667	A1570		G1401	G1309
G2505	G2346	C2275	G2181	U2121	A2043	U1954	G1855	U1779	A1668	A1570		C1402	G1310
U2506	A2346	G2276	G2182	U2122	C2043	U1955	G1858	U1780	A1669	A1571		G1403	G1311
G2428	C2347	G2277	C2183	G2123	C2050	U1956	G1858	C1781	C1670	C1577		C1404	U1312
A2430	U2423	G2277	G2184	G2124	A2051	C1957	A1876	C1782	U1578	U1578		U1405	U1313
G2516	G2348	A2278	C2185	G2125	G1958	C1958	A1877	A1783	G1673	A1579		U1406	C1314
C2517	G2350	G2279	G2186	G2052	G1959	C1959	G1878	A1784	G1674	A1580		A1394	
U2518	G2351	G2280	G2187	G2053	G2053	U1963	G1878	A1785	C1675	A1581		A1395	
G2519	A2435	C2281	C2188	A2054	G2054	G1964	G1882	A1786	G1676	C1582		A1400	A1308
C2520	U2438	C2282	G2189	C2055	G2056	G1964	G1883			A1582		G1400	A1308
		C2283	G2190	U2130	G2056					A1583		G1401	G1309



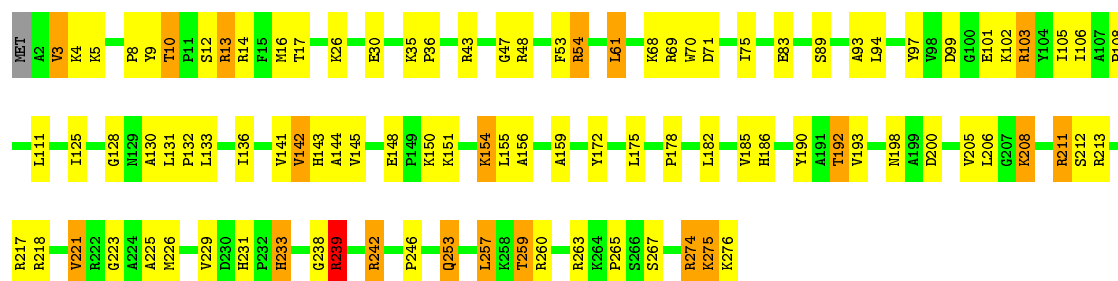
- Molecule 2: 5S ribosomal RNA



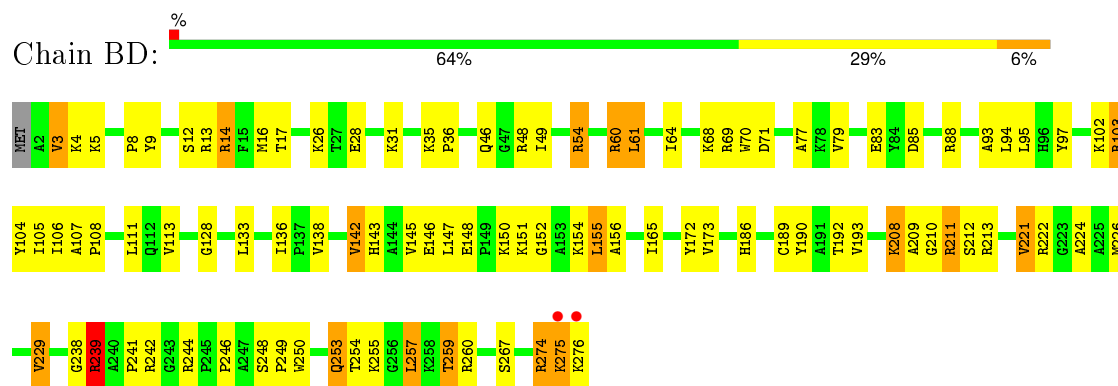
- Molecule 2: 5S ribosomal RNA



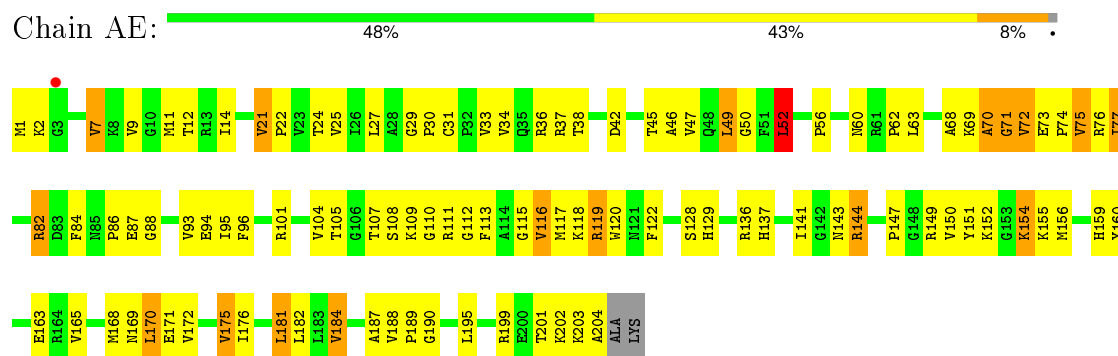
- Molecule 3: 50S ribosomal protein L2



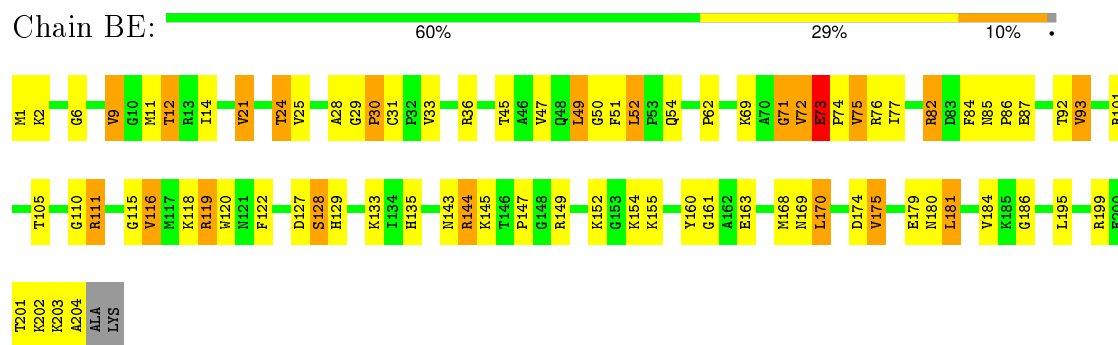
- Molecule 3: 50S ribosomal protein L2



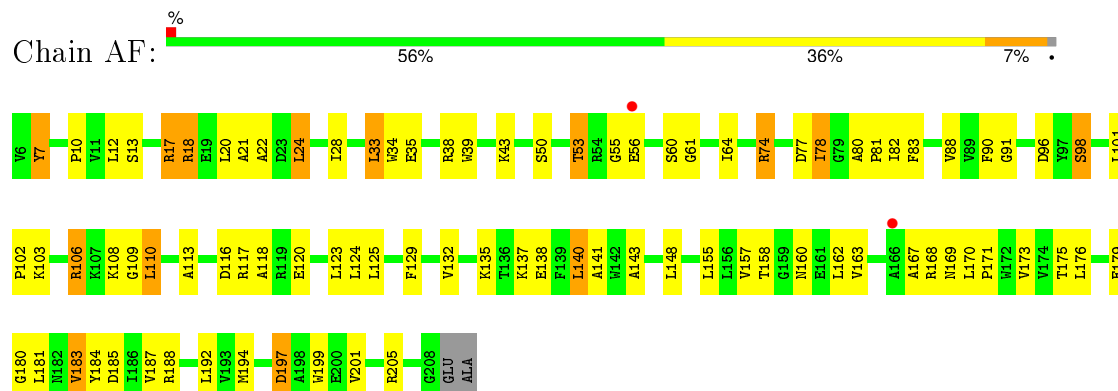
- Molecule 4: 50S ribosomal protein L3



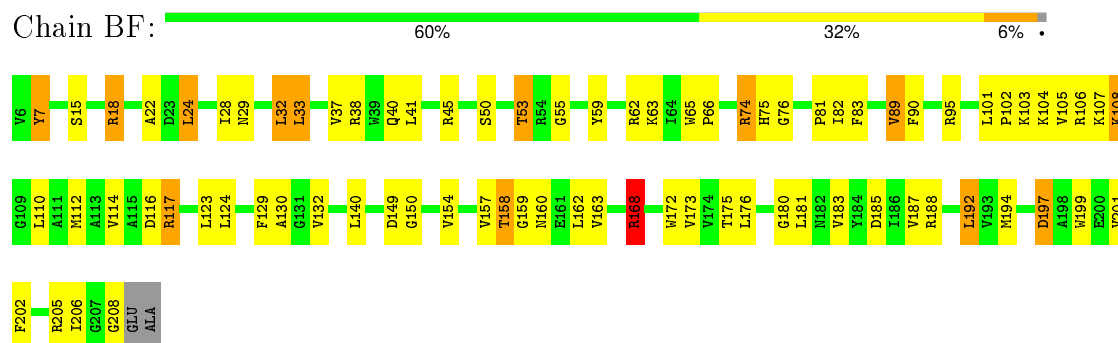
- Molecule 4: 50S ribosomal protein L3



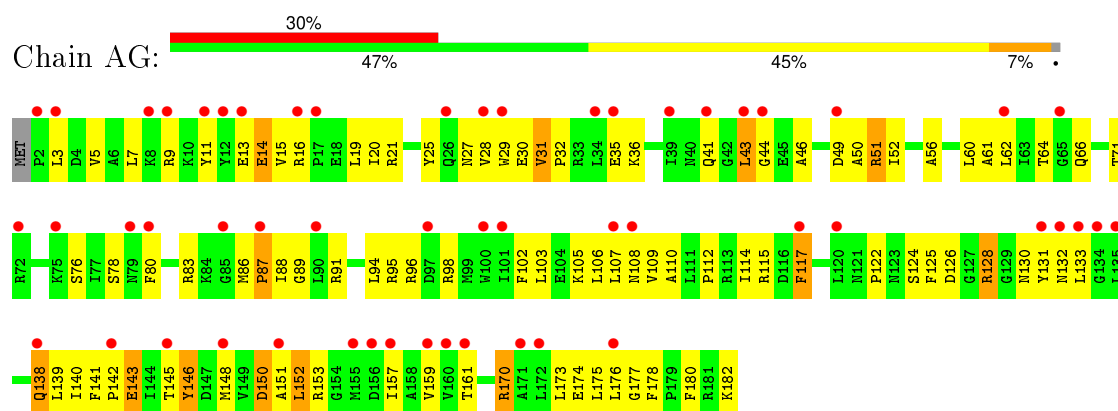
- Molecule 5: 50S ribosomal protein L4



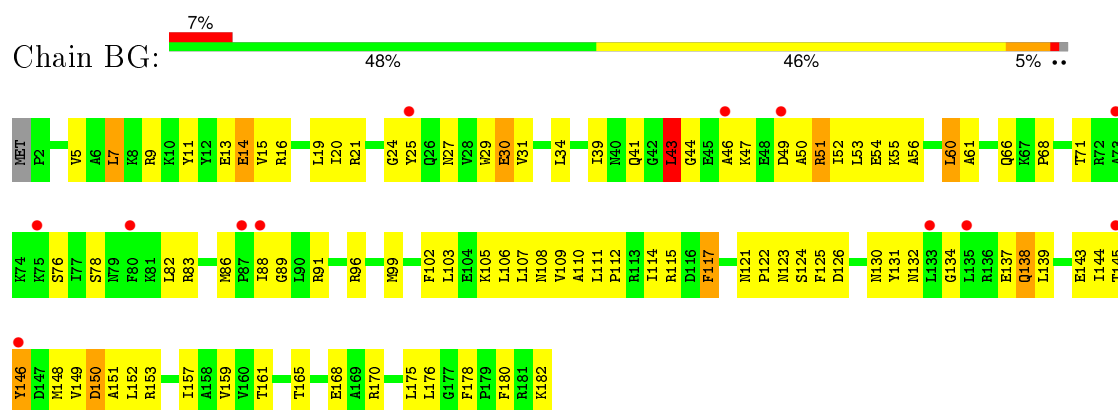
- Molecule 5: 50S ribosomal protein L4



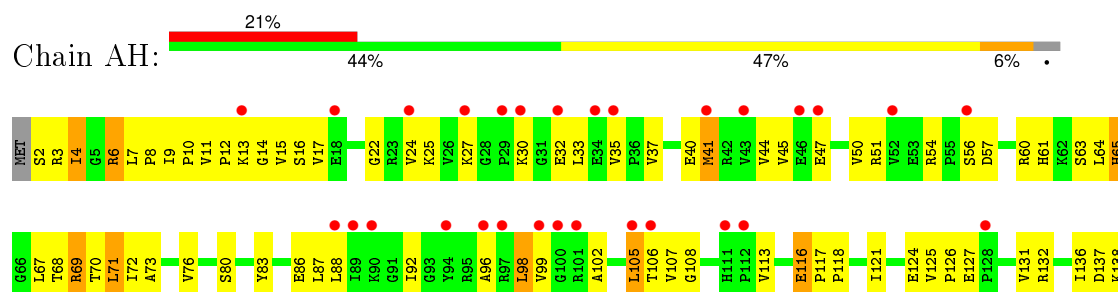
- Molecule 6: 50S ribosomal protein L5

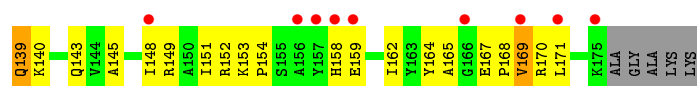


- Molecule 6: 50S ribosomal protein L5

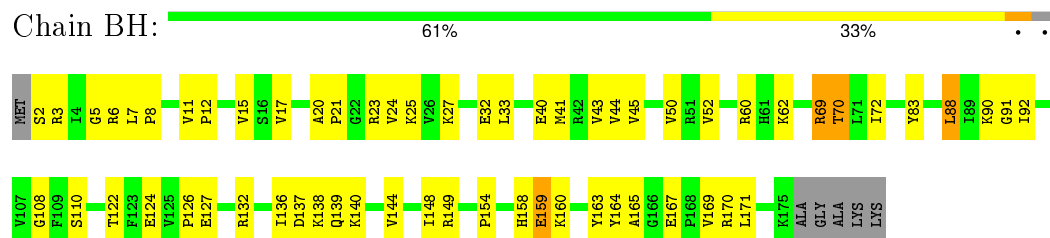


- Molecule 7: 50S ribosomal protein L6

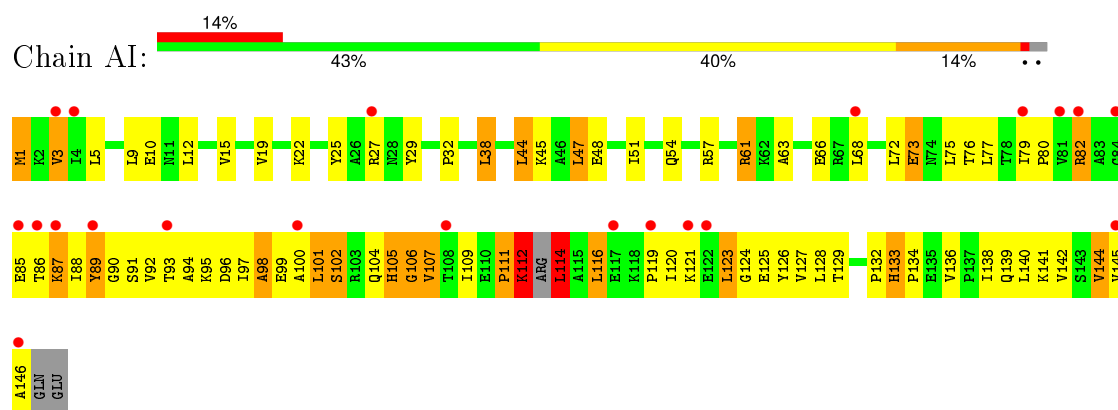




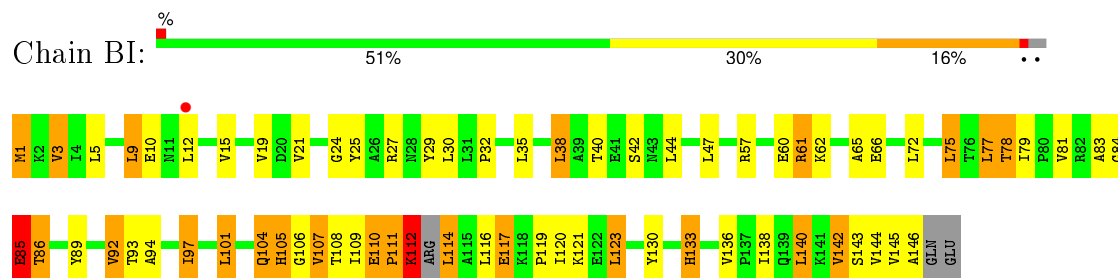
- Molecule 7: 50S ribosomal protein L6



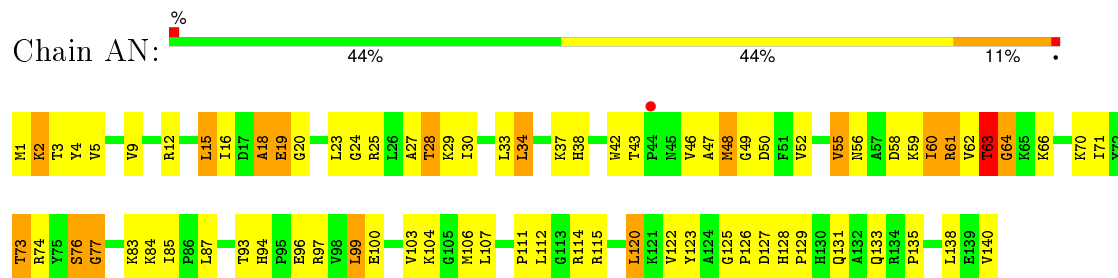
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9

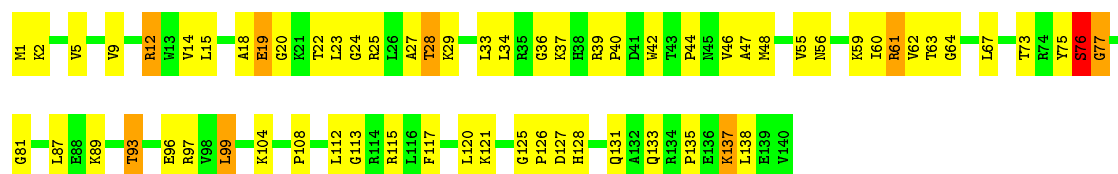


- Molecule 9: 50S ribosomal protein L13



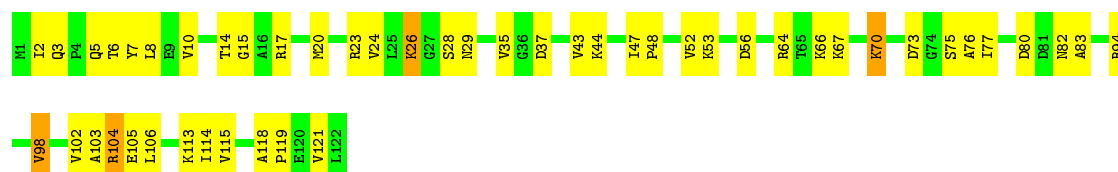
- Molecule 9: 50S ribosomal protein L13





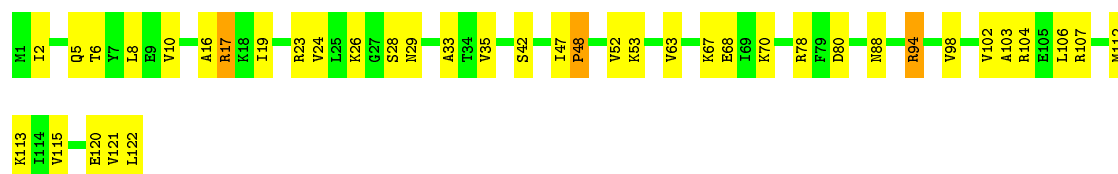
- Molecule 10: 50S ribosomal protein L14

Chain AO:

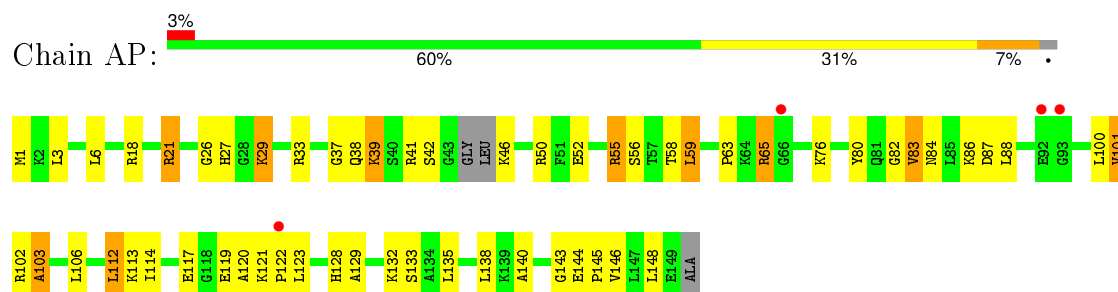


- Molecule 10: 50S ribosomal protein L14

Chain BO:

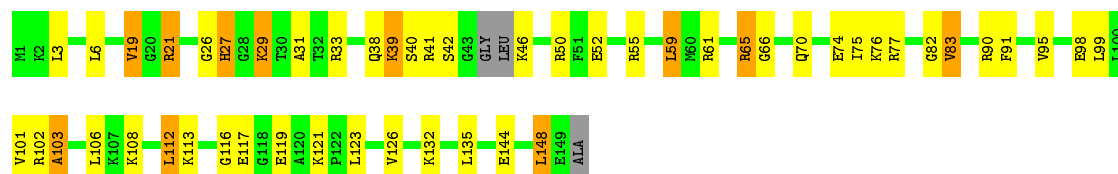


- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

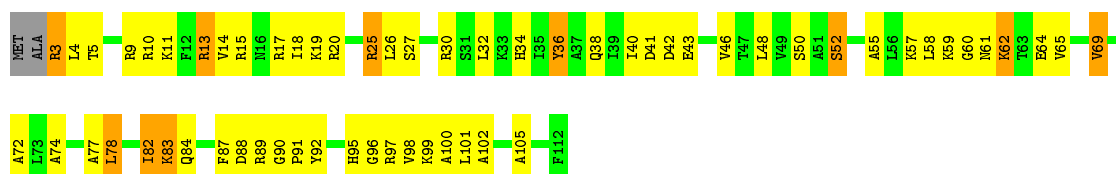
Chain BP:



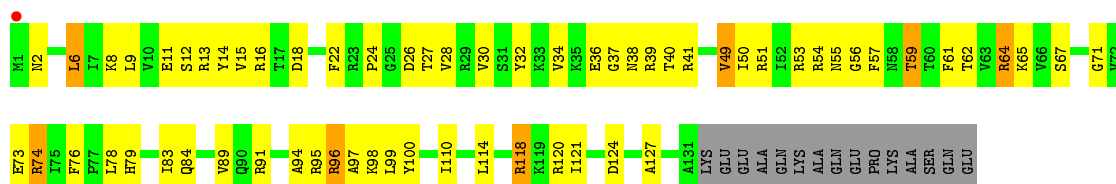
- Molecule 12: 50S ribosomal protein L16



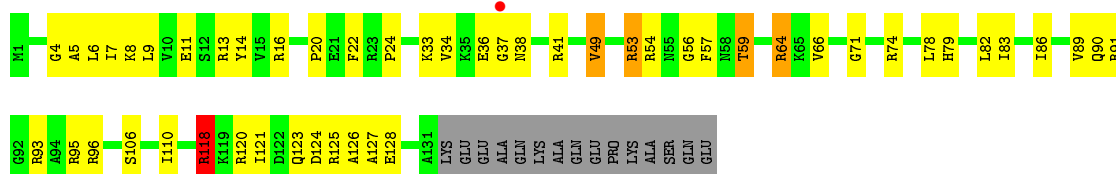




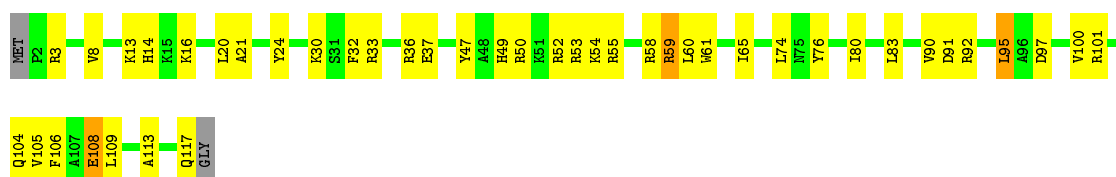
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



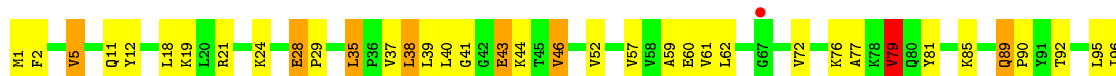
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





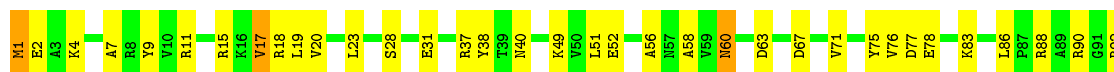
- Molecule 17: 50S ribosomal protein L21

Chain BV: 67% 27% 5% •



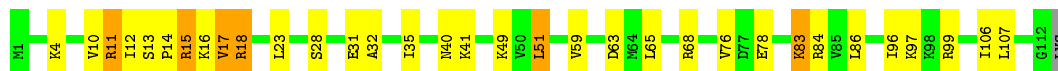
- Molecule 18: 50S ribosomal protein L22

Chain AW: 60% 34% 5% •



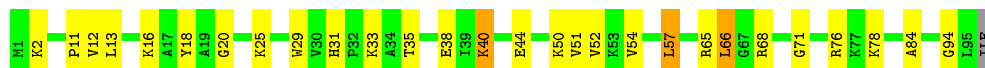
- Molecule 18: 50S ribosomal protein L22

Chain BW: 70% 24% 5% •



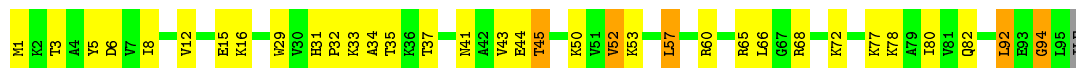
- Molecule 19: 50S ribosomal protein L23

Chain AX: 70% 26% 5% •



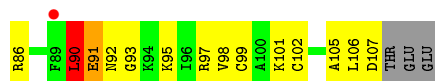
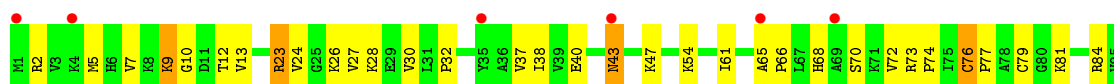
- Molecule 19: 50S ribosomal protein L23

Chain BX: 64% 30% 5% •

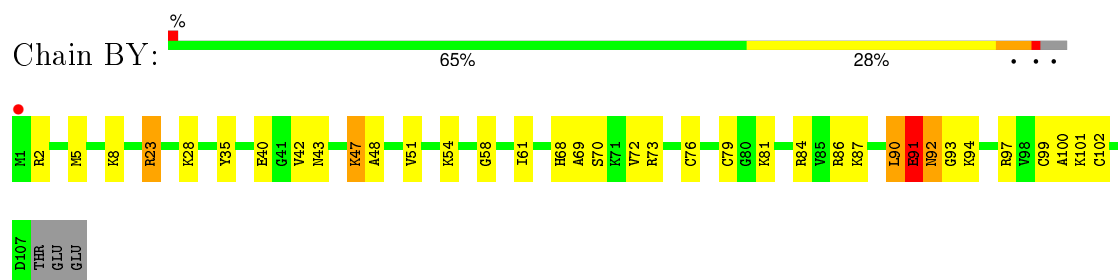


- Molecule 20: 50S ribosomal protein L24

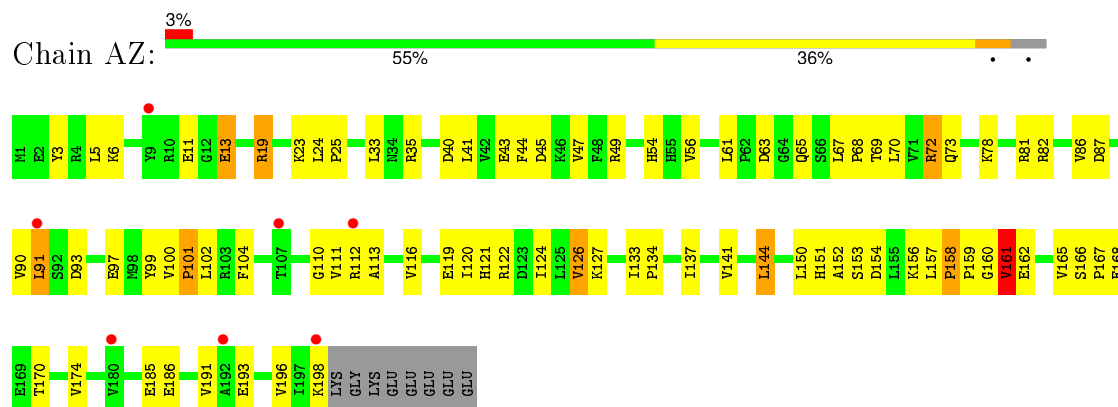
Chain AY: 6% 55% 37% 5% •



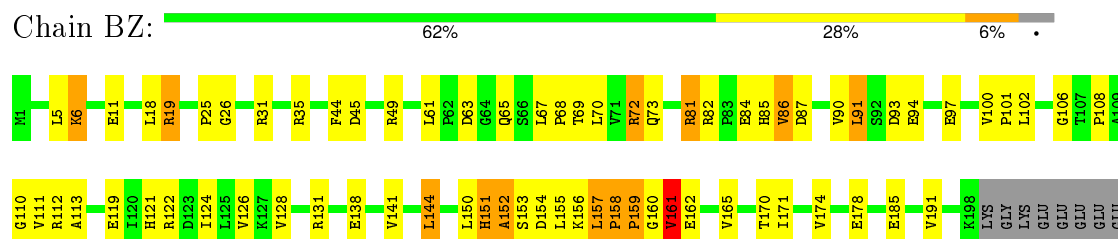
- Molecule 20: 50S ribosomal protein L24



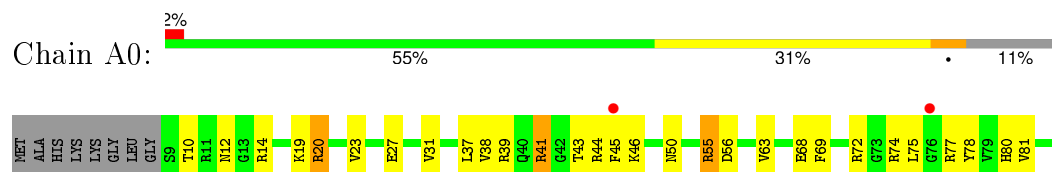
- Molecule 21: 50S ribosomal protein L25



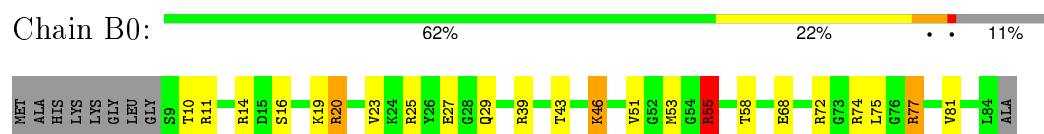
- Molecule 21: 50S ribosomal protein L25



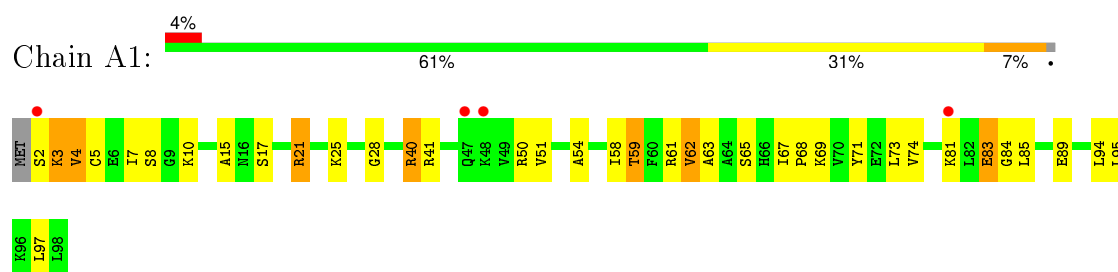
- Molecule 22: 50S ribosomal protein L27



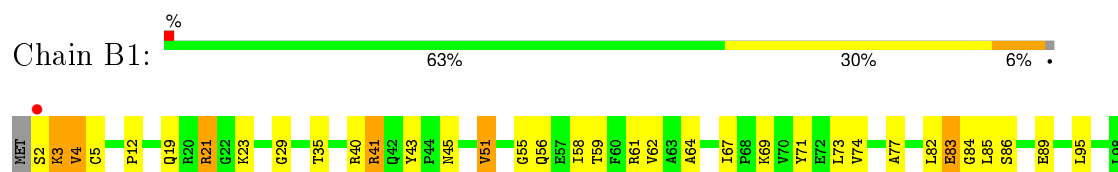
- Molecule 22: 50S ribosomal protein L27



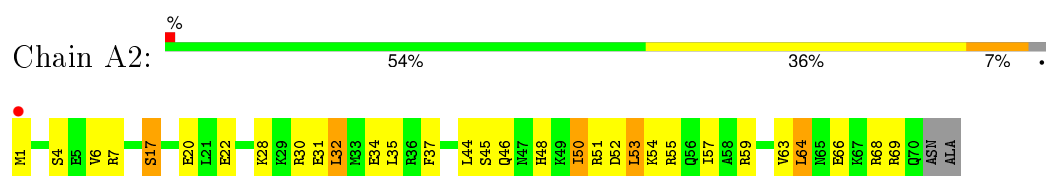
- Molecule 23: 50S ribosomal protein L28



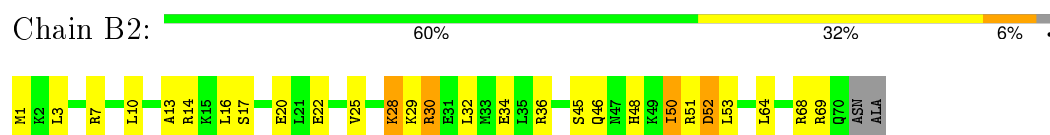
- Molecule 23: 50S ribosomal protein L28



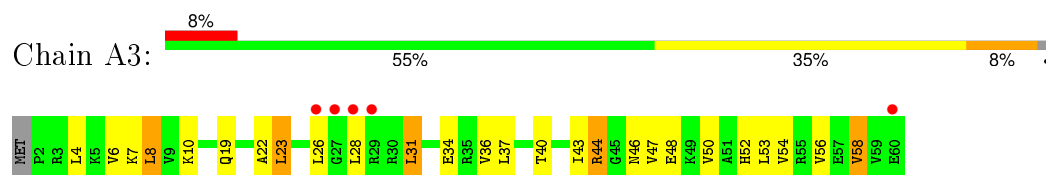
- Molecule 24: 50S ribosomal protein L29



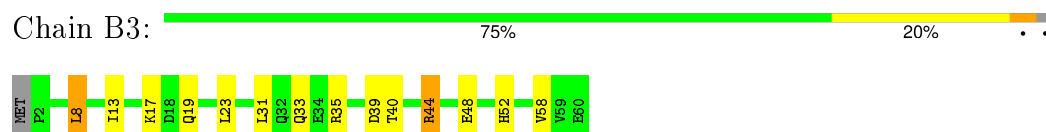
- Molecule 24: 50S ribosomal protein L29



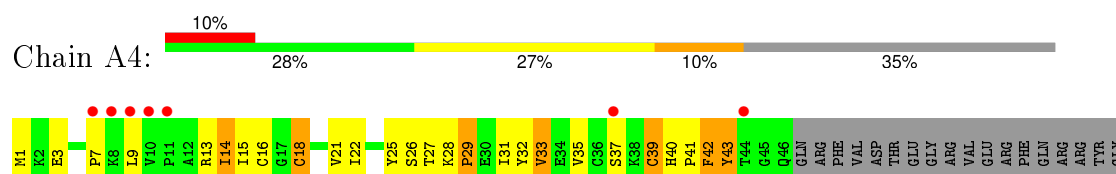
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

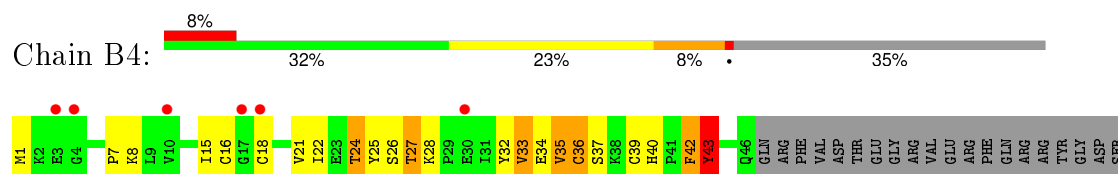


- Molecule 26: 50S ribosomal protein L31



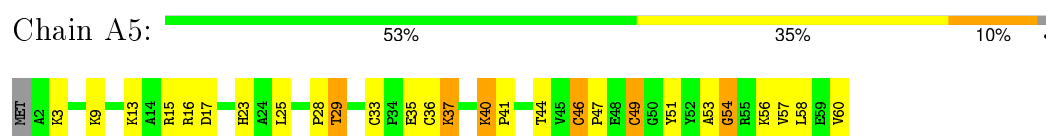
ASP
SER
TYR
ARG
LYS
GLY
ARG

- Molecule 26: 50S ribosomal protein L31

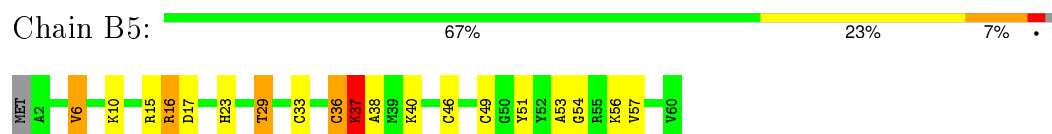


TYR
ARG
LYS
GLY
ARG

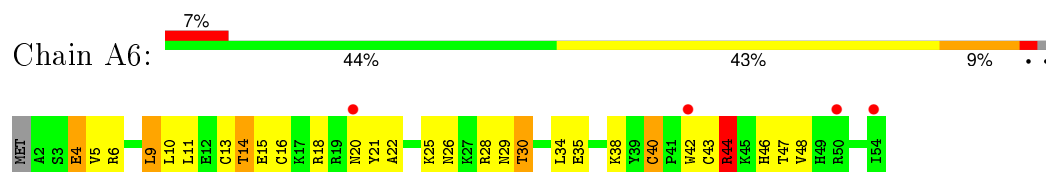
- Molecule 27: 50S ribosomal protein L32



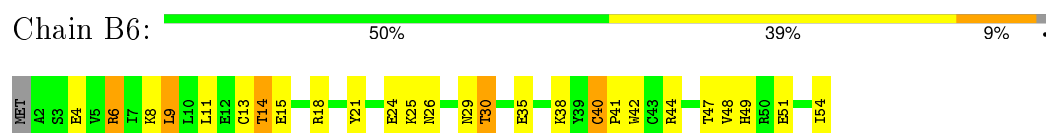
- Molecule 27: 50S ribosomal protein L32



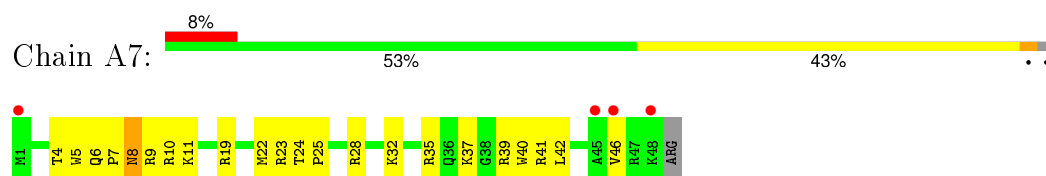
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



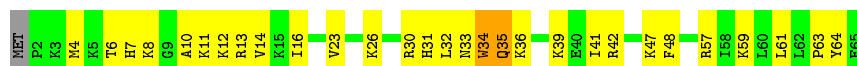
- Molecule 29: 50S ribosomal protein L34





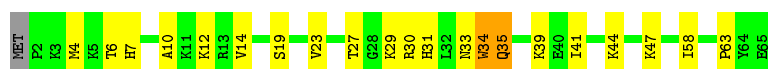
- Molecule 30: 50S ribosomal protein L35

Chain A8: 54% 42% ..



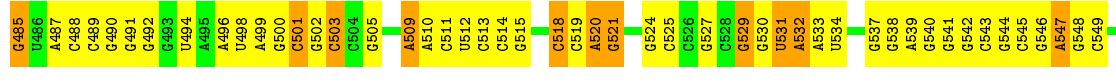
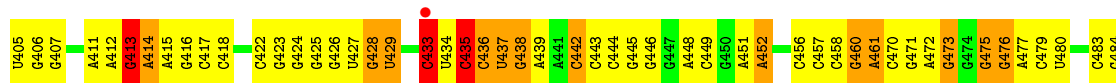
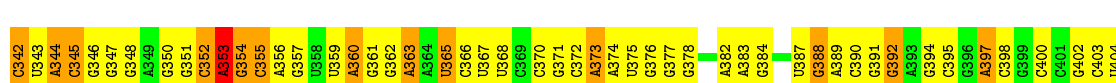
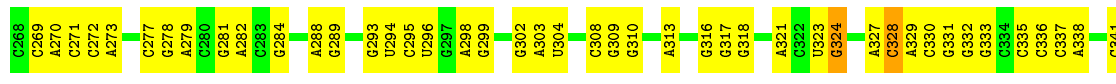
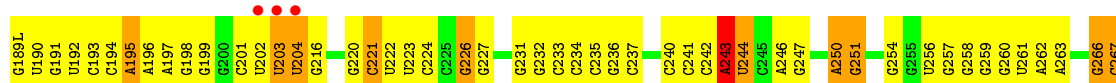
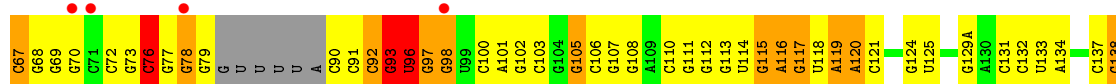
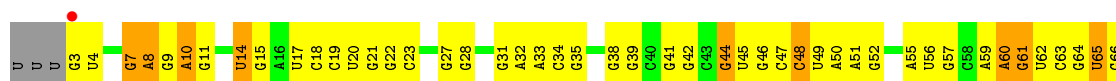
- Molecule 30: 50S ribosomal protein L35

Chain B8: 66% 29% ..



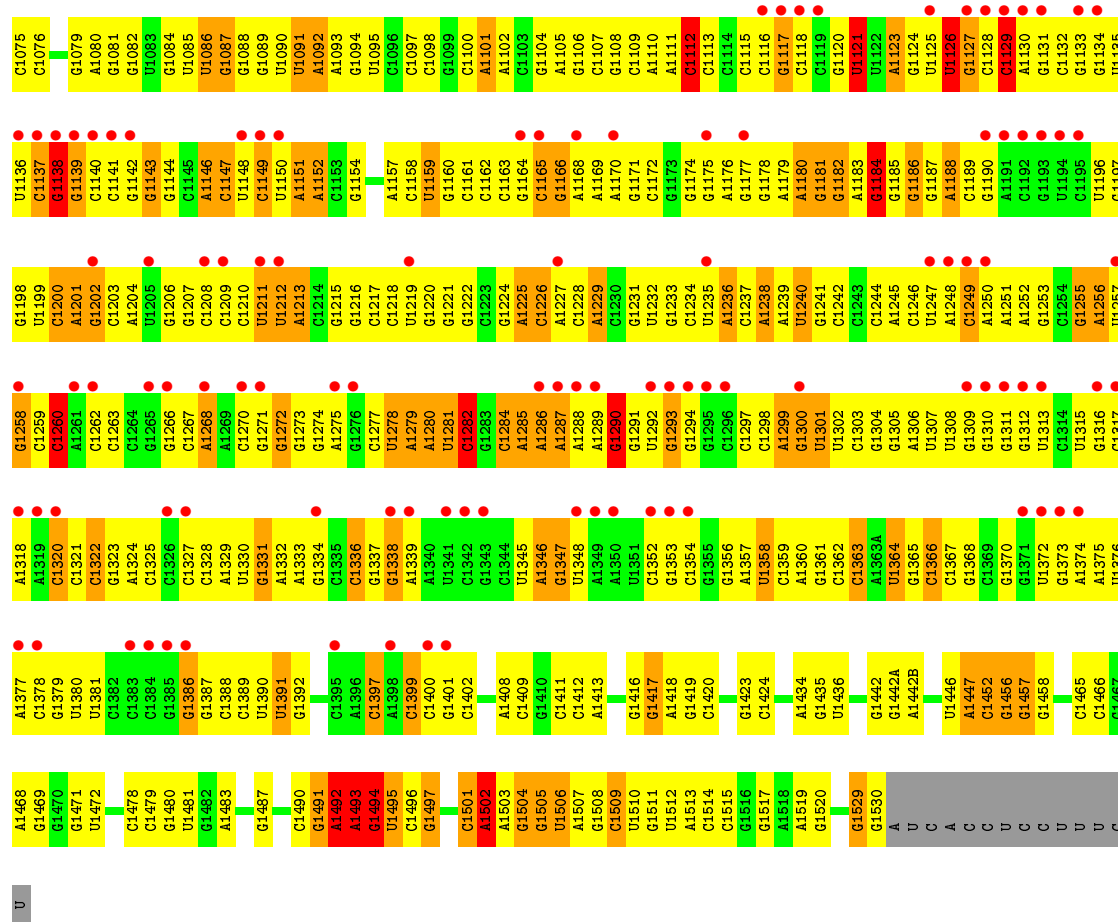
- Molecule 31: 16S ribosomal RNA

Chain CA: 13% 29% 53% 14% ..

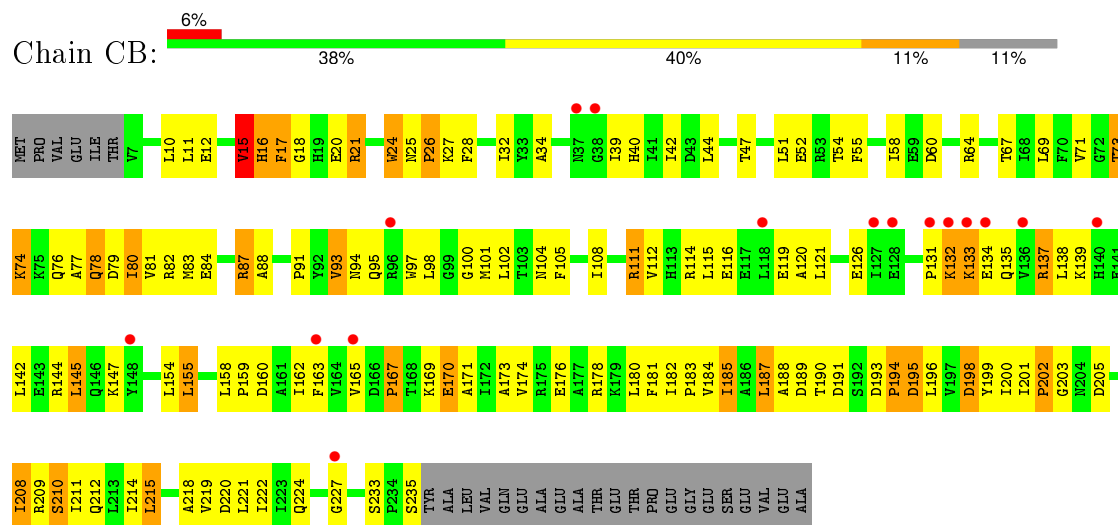




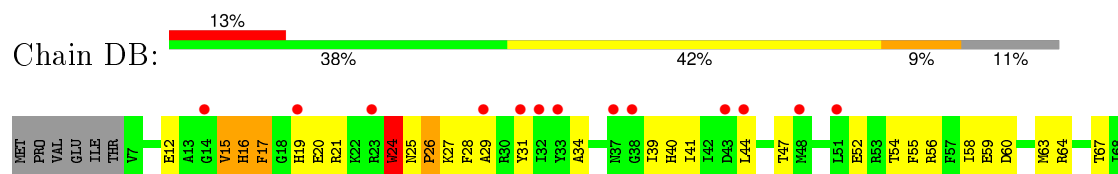


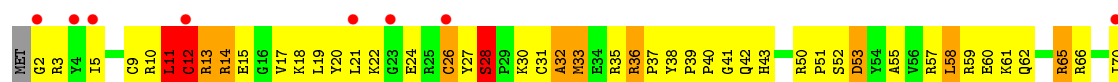


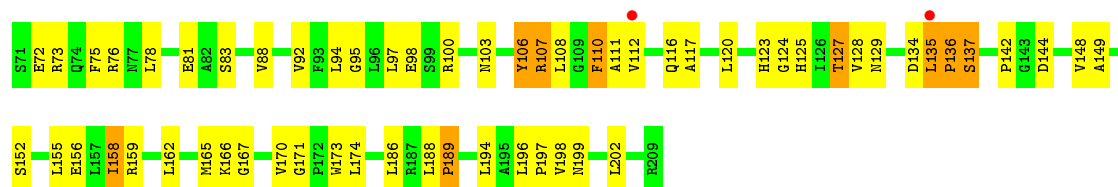
- Molecule 32: 30S ribosomal protein S2



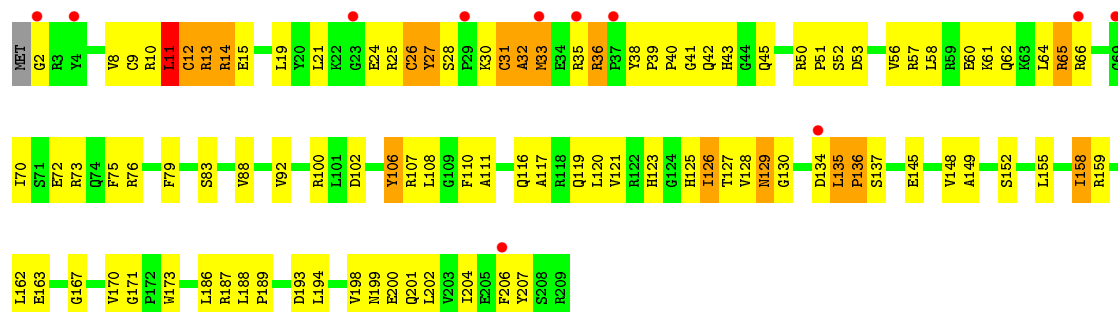
- Molecule 32: 30S ribosomal protein S2



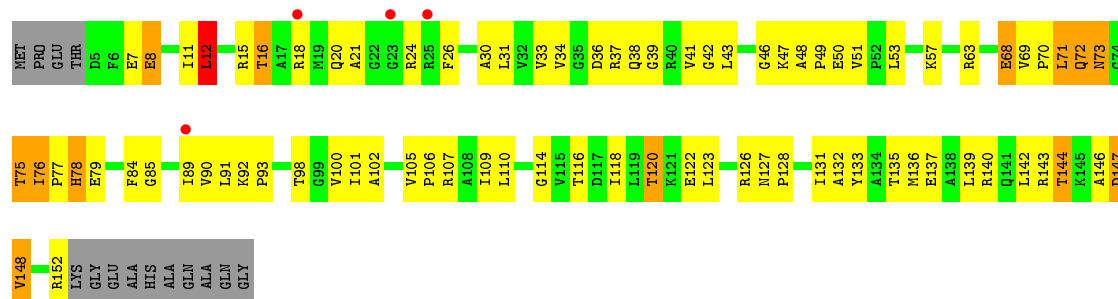
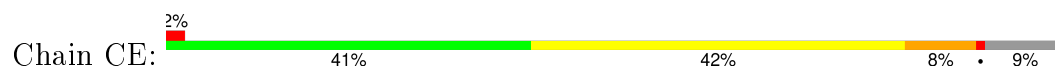




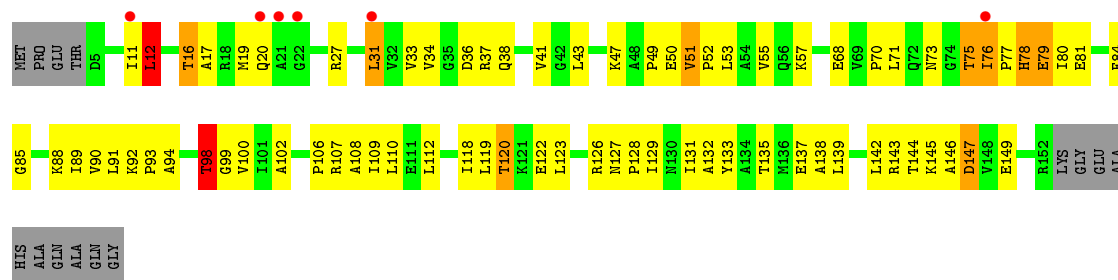
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5

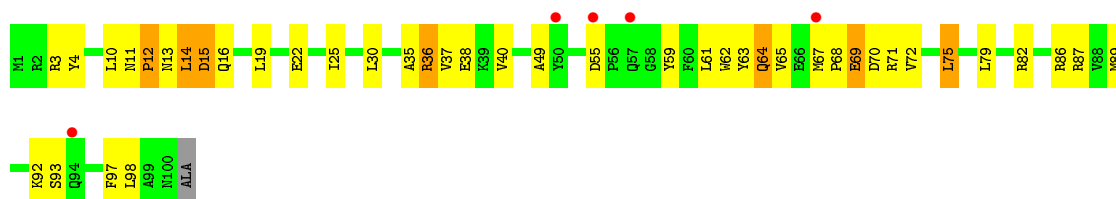


• Molecule 35: 30S ribosomal protein S5

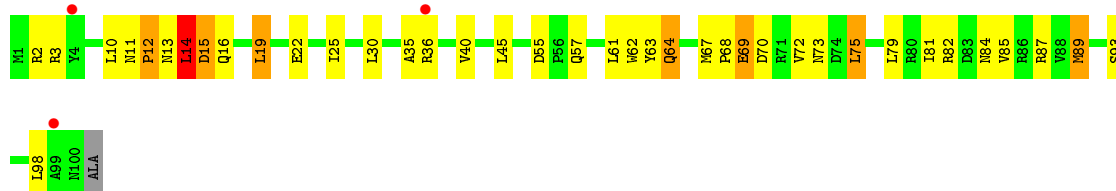


• Molecule 36: 30S ribosomal protein S6

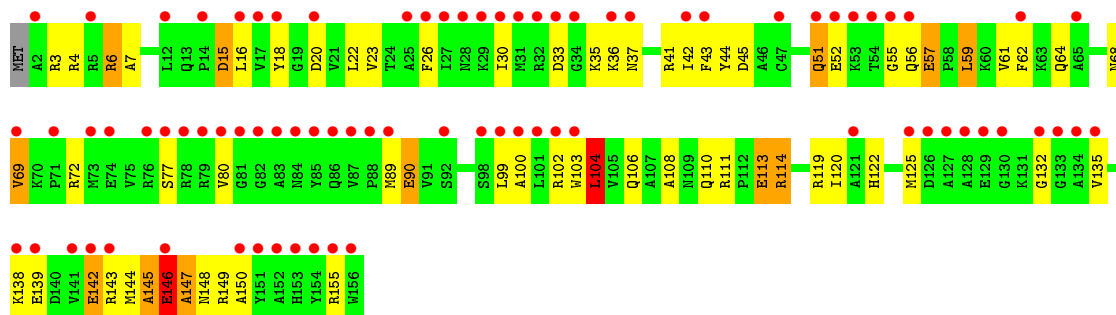




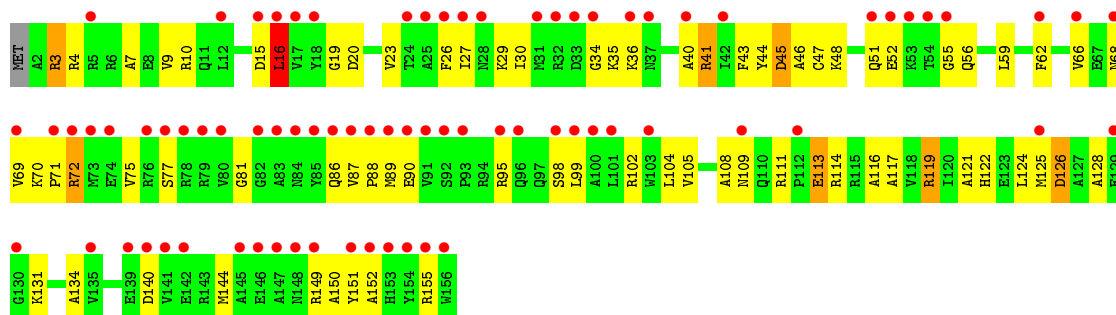
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

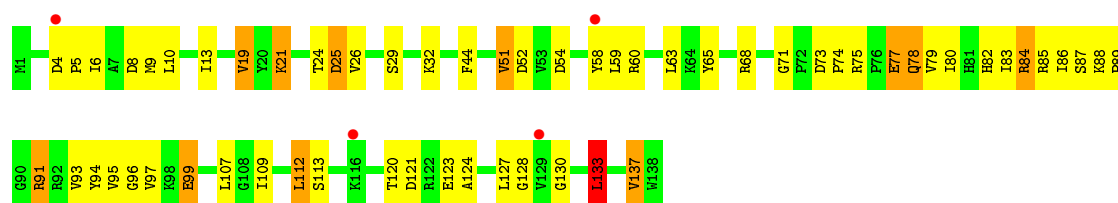


- Molecule 37: 30S ribosomal protein S7

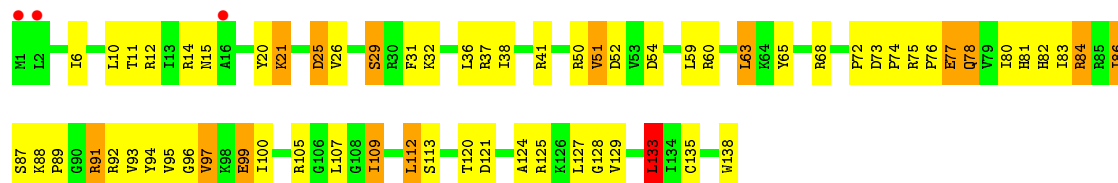


- Molecule 38: 30S ribosomal protein S8

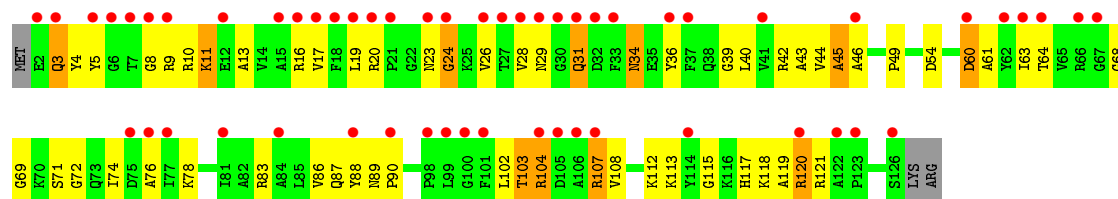
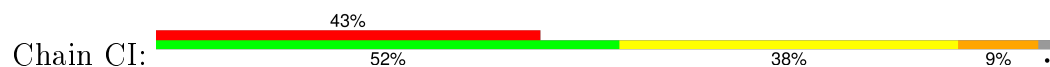




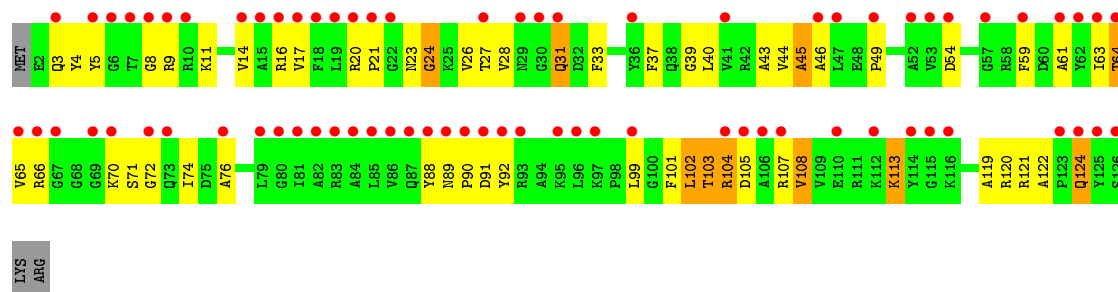
• Molecule 38: 30S ribosomal protein S8



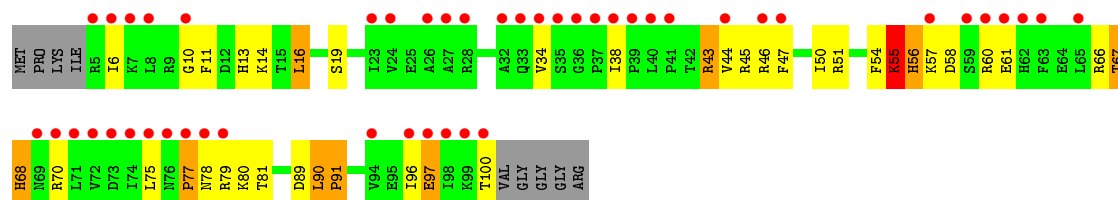
• Molecule 39: 30S ribosomal protein S9



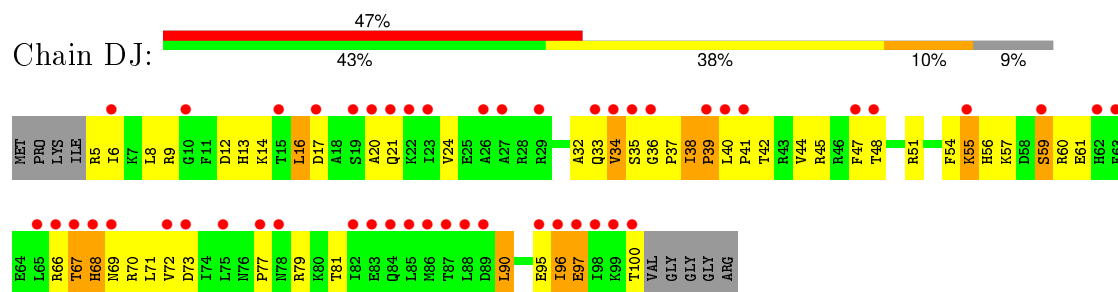
• Molecule 39: 30S ribosomal protein S9



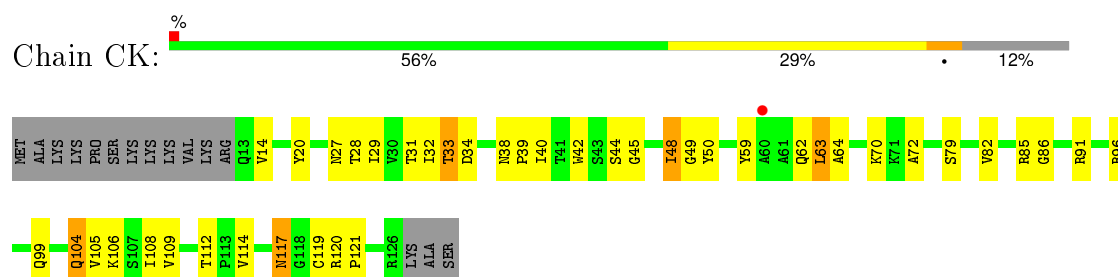
• Molecule 40: 30S ribosomal protein S10



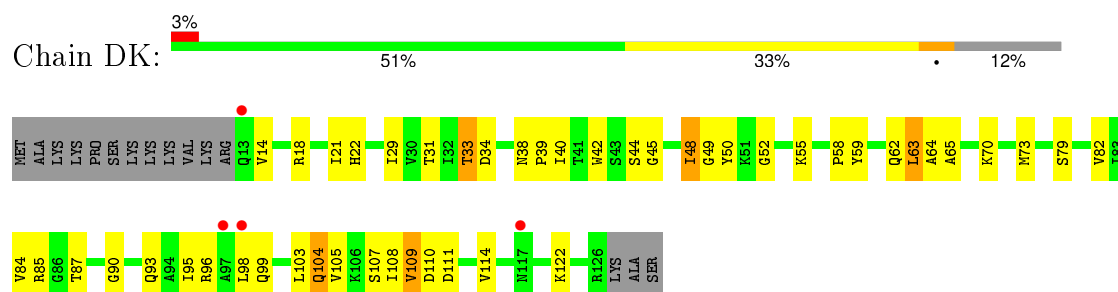
- Molecule 40: 30S ribosomal protein S10



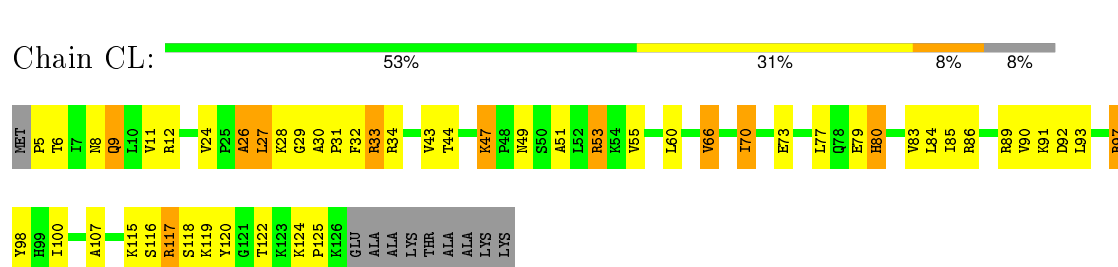
- Molecule 41: 30S ribosomal protein S11



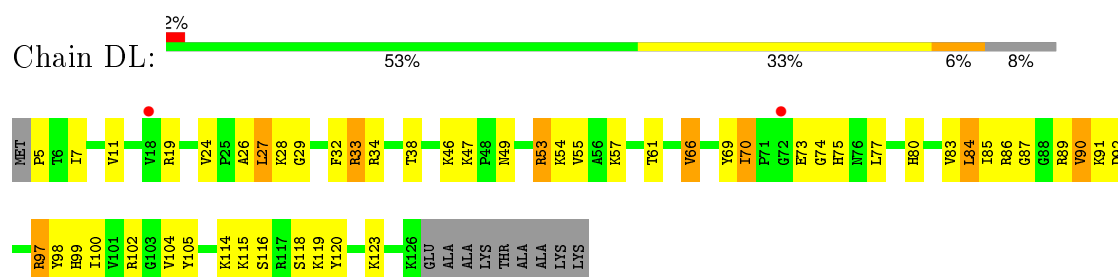
- Molecule 41: 30S ribosomal protein S11



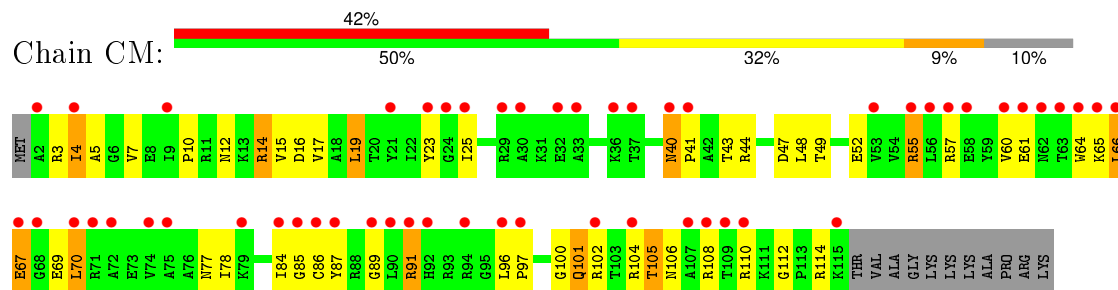
- Molecule 42: 30S ribosomal protein S12



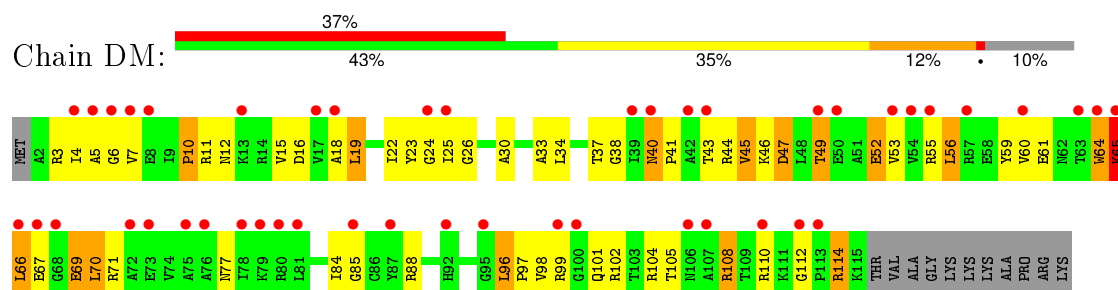
- Molecule 42: 30S ribosomal protein S12



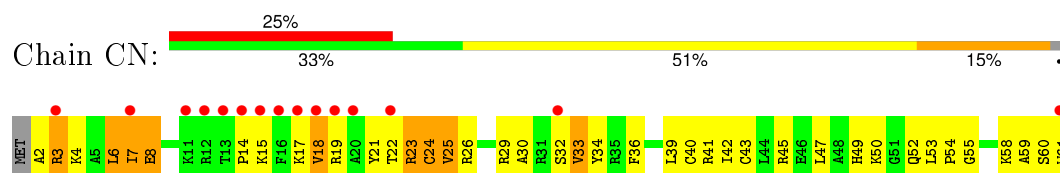
- Molecule 43: 30S ribosomal protein S13



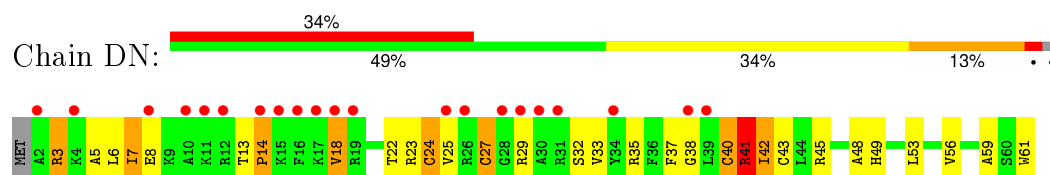
- Molecule 43: 30S ribosomal protein S13



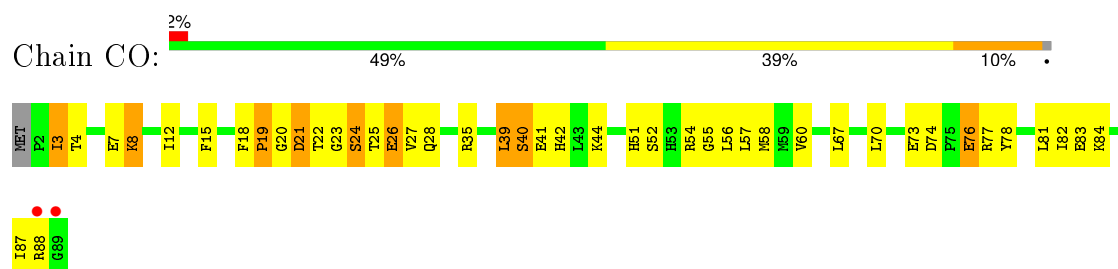
- Molecule 44: 30S ribosomal protein S14



- Molecule 44: 30S ribosomal protein S14

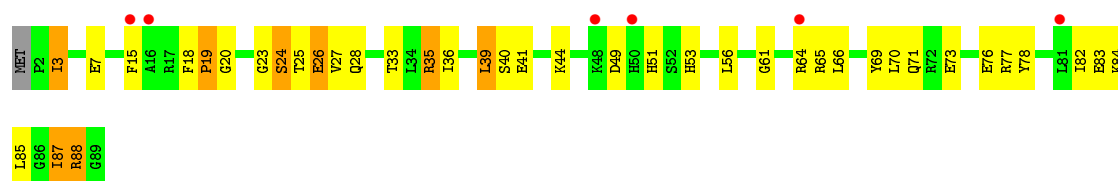


- Molecule 45: 30S ribosomal protein S15

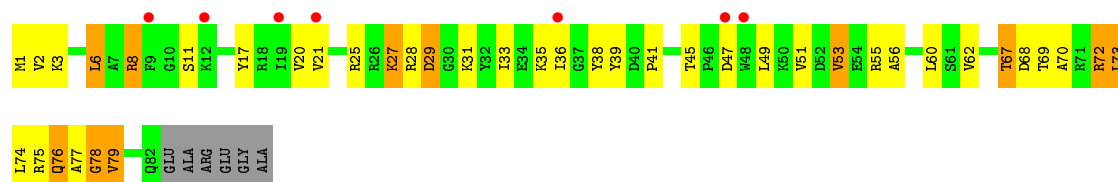


- Molecule 45: 30S ribosomal protein S15

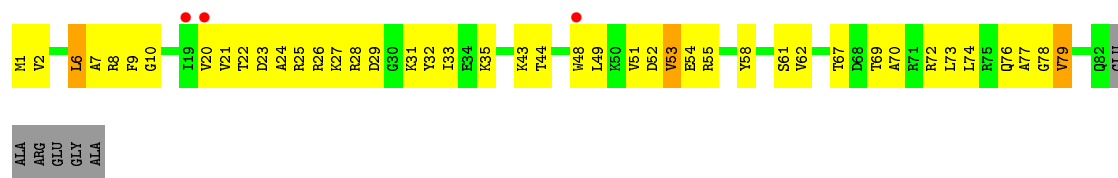




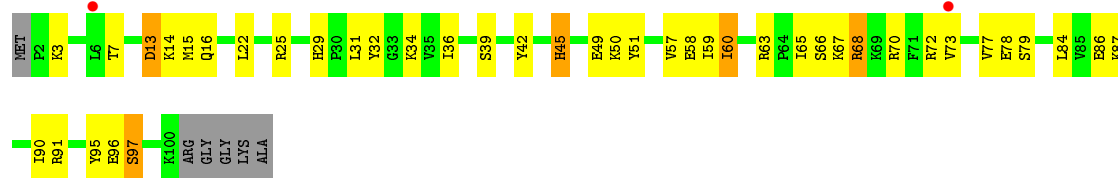
- Molecule 46: 30S ribosomal protein S16



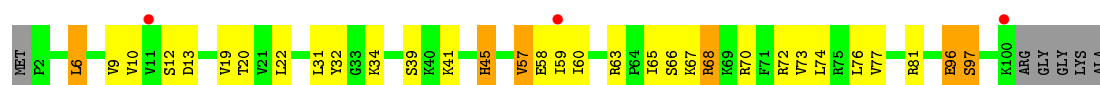
- Molecule 46: 30S ribosomal protein S16



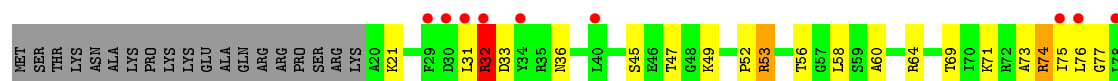
- Molecule 47: 30S ribosomal protein S17



- Molecule 47: 30S ribosomal protein S17

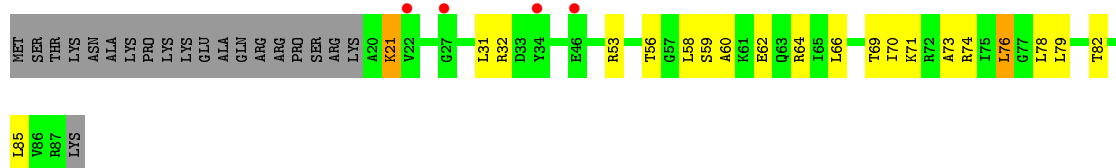


- Molecule 48: 30S ribosomal protein S18

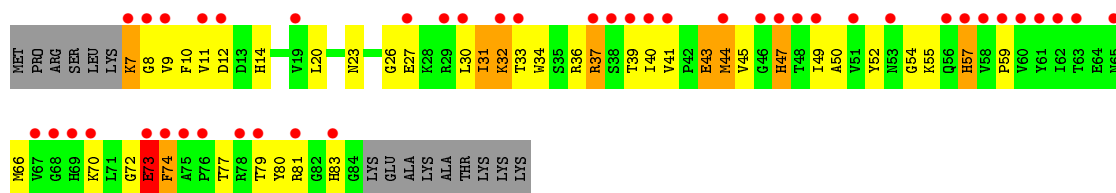




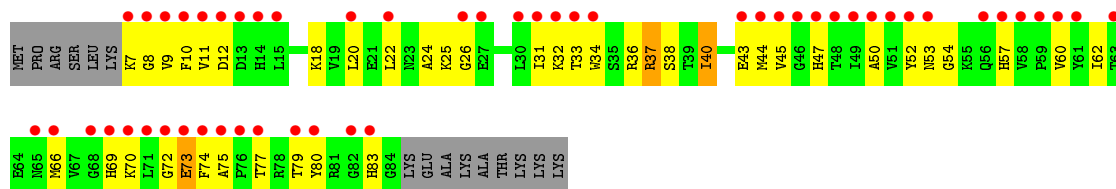
- Molecule 48: 30S ribosomal protein S18



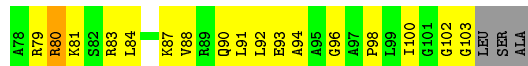
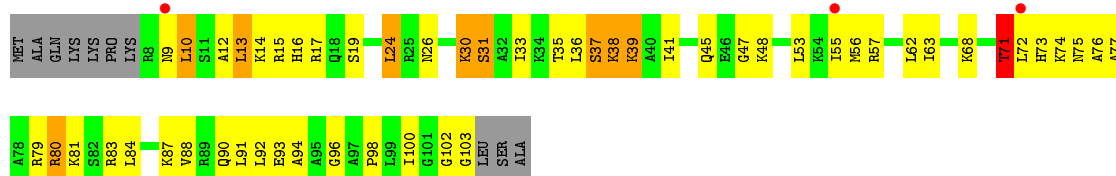
- Molecule 49: 30S ribosomal protein S19



- Molecule 49: 30S ribosomal protein S19

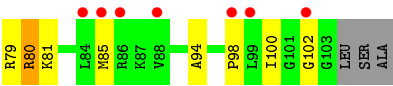


- Molecule 50: 30S ribosomal protein S20

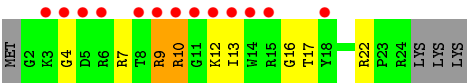


- Molecule 50: 30S ribosomal protein S20

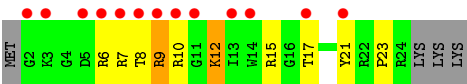




● Molecule 51: 30S ribosomal protein THX



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.273 0.229 , 0.273	Depositor DCC
R_{free} test set	47287 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1261811 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:H13	52:AA:3001:T8B:C22	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	45
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	13	55
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	4	31
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	4	31
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	7	41
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	4	31
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	2	18
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	8
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	3	22
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	4	31
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	10
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	1	13
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	3	25
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	5	32
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	5	32
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	2	18
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	4	31
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	6	36
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	6	36
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	3	25
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	21	67
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	6	37
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	6	37
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	5	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BT	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	24	69
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	48
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	19	65
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	21	67
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	8	45
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	8	45
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	3	22
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	4	28
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	2	18
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	4	30
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	14	57
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	14	57
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	9	46
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	5	33
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	13	55
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%)	11	51
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	5
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	5
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	11	51
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	4	31
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	9	48
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	8	45
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	8	45
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	12	54
30	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

Continued on next page...

Continued from previous page...

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	12
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	2	19
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	17
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	5	31
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	1	9
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	5	31
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	34
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	27
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	13
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	4	28
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	13	55
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	4	29
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	7
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	1	13
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	1	5
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	2	13
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	4	30
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	6	39
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	3	26
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	3	26
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	6
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	19
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	31
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	8	44
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	28
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	2	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	5	34
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	13	55
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	12
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	1	6
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	1	9
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	1	5
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	3	25

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	20
3	BD	215/218 (99%)	189 (88%)	26 (12%)	6	28
4	AE	163/166 (98%)	139 (85%)	24 (15%)	4	18
4	BE	163/166 (98%)	134 (82%)	29 (18%)	2	11
5	AF	158/162 (98%)	133 (84%)	25 (16%)	3	15
5	BF	158/162 (98%)	138 (87%)	20 (13%)	5	25
6	AG	128/156 (82%)	110 (86%)	18 (14%)	4	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BG	128/156 (82%)	114 (89%)	14 (11%)	8	33
7	AH	141/148 (95%)	125 (89%)	16 (11%)	7	31
7	BH	141/148 (95%)	124 (88%)	17 (12%)	6	28
8	AI	102/124 (82%)	76 (74%)	26 (26%)	1	2
8	BI	102/124 (82%)	76 (74%)	26 (26%)	1	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	41
10	BO	98/100 (98%)	89 (91%)	9 (9%)	11	41
11	AP	113/116 (97%)	96 (85%)	17 (15%)	3	17
11	BP	113/116 (97%)	97 (86%)	16 (14%)	4	19
12	AQ	111/111 (100%)	94 (85%)	17 (15%)	3	17
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	17
13	AR	101/101 (100%)	80 (79%)	21 (21%)	1	7
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	19
15	AT	110/127 (87%)	99 (90%)	11 (10%)	9	37
15	BT	110/127 (87%)	100 (91%)	10 (9%)	12	42
16	AU	93/94 (99%)	83 (89%)	10 (11%)	8	33
16	BU	93/94 (99%)	77 (83%)	16 (17%)	2	12
17	AV	80/82 (98%)	63 (79%)	17 (21%)	1	7
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	AW	89/92 (97%)	75 (84%)	14 (16%)	3	15
18	BW	89/92 (97%)	78 (88%)	11 (12%)	6	27
19	AX	75/78 (96%)	67 (89%)	8 (11%)	8	34
19	BX	75/78 (96%)	66 (88%)	9 (12%)	6	28
20	AY	80/91 (88%)	70 (88%)	10 (12%)	6	26
20	BY	80/91 (88%)	72 (90%)	8 (10%)	9	37
21	AZ	159/179 (89%)	139 (87%)	20 (13%)	5	26
21	BZ	159/179 (89%)	137 (86%)	22 (14%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A0	59/67 (88%)	52 (88%)	7 (12%)	6	28
22	B0	59/67 (88%)	52 (88%)	7 (12%)	6	28
23	A1	78/83 (94%)	68 (87%)	10 (13%)	5	25
23	B1	78/83 (94%)	70 (90%)	8 (10%)	9	36
24	A2	65/67 (97%)	56 (86%)	9 (14%)	4	21
24	B2	65/67 (97%)	57 (88%)	8 (12%)	6	27
25	A3	49/52 (94%)	43 (88%)	6 (12%)	6	27
25	B3	49/52 (94%)	43 (88%)	6 (12%)	6	27
26	A4	39/63 (62%)	32 (82%)	7 (18%)	2	11
26	B4	39/63 (62%)	30 (77%)	9 (23%)	1	4
27	A5	50/52 (96%)	43 (86%)	7 (14%)	4	20
27	B5	50/52 (96%)	43 (86%)	7 (14%)	4	20
28	A6	50/52 (96%)	40 (80%)	10 (20%)	1	8
28	B6	50/52 (96%)	41 (82%)	9 (18%)	2	11
29	A7	41/42 (98%)	35 (85%)	6 (15%)	4	19
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
30	A8	52/55 (94%)	45 (86%)	7 (14%)	5	22
30	B8	52/55 (94%)	47 (90%)	5 (10%)	10	39
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%)	3	13
33	DC	114/188 (61%)	96 (84%)	18 (16%)	3	15
34	CD	139/181 (77%)	117 (84%)	22 (16%)	3	15
34	DD	139/181 (77%)	120 (86%)	19 (14%)	4	21
35	CE	108/123 (88%)	86 (80%)	22 (20%)	1	7
35	DE	108/123 (88%)	88 (82%)	20 (18%)	2	10
36	CF	77/90 (86%)	65 (84%)	12 (16%)	3	15
36	DF	77/90 (86%)	65 (84%)	12 (16%)	3	15
37	CG	104/127 (82%)	86 (83%)	18 (17%)	2	12
37	DG	104/127 (82%)	88 (85%)	16 (15%)	3	16
38	CH	103/119 (87%)	85 (82%)	18 (18%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DH	103/119 (87%)	84 (82%)	19 (18%)	2	10
39	CI	62/99 (63%)	53 (86%)	9 (14%)	4	19
39	DI	62/99 (63%)	54 (87%)	8 (13%)	5	24
40	CJ	52/92 (56%)	42 (81%)	10 (19%)	2	10
40	DJ	52/92 (56%)	41 (79%)	11 (21%)	1	7
41	CK	81/99 (82%)	69 (85%)	12 (15%)	4	18
41	DK	81/99 (82%)	71 (88%)	10 (12%)	6	27
42	CL	92/109 (84%)	81 (88%)	11 (12%)	6	28
42	DL	92/109 (84%)	83 (90%)	9 (10%)	10	38
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	15
45	DO	77/80 (96%)	66 (86%)	11 (14%)	4	19
46	CP	63/74 (85%)	49 (78%)	14 (22%)	1	5
46	DP	63/74 (85%)	53 (84%)	10 (16%)	3	14
47	CQ	94/97 (97%)	90 (96%)	4 (4%)	35	75
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	8	34
48	CR	49/77 (64%)	44 (90%)	5 (10%)	9	36
48	DR	49/77 (64%)	46 (94%)	3 (6%)	23	64
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	36 (86%)	6 (14%)	4	19
50	CT	65/82 (79%)	53 (82%)	12 (18%)	2	10
50	DT	65/82 (79%)	57 (88%)	8 (12%)	6	27
51	CU	18/22 (82%)	16 (89%)	2 (11%)	8	32
51	DU	18/22 (82%)	14 (78%)	4 (22%)	1	5
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	3	16

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

Mol	Chain	Res	Type
13	BR	6	SER

Continued on next page...

Continued from previous page...

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	2819/2915 (96%)	581 (20%)	59 (2%)
1	BA	2819/2915 (96%)	586 (20%)	60 (2%)
2	AB	119/122 (97%)	25 (21%)	0
2	BB	119/122 (97%)	21 (17%)	0
31	CA	1496/1521 (98%)	339 (22%)	31 (2%)
31	DA	1496/1521 (98%)	341 (22%)	27 (1%)
All	All	8868/9116 (97%)	1893 (21%)	177 (1%)

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

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	1047	G
1	BA	1819	A
31	DA	560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1106	A
1	BA	1301	A

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

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%)	57,71,71	1.25	8 (14%)
52	T8B	BA	3001	53	40,48,48	0.99	2 (5%)	57,71,71	1.26	8 (14%)

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	2.31	1.50	1.43
52	BA	3001	T8B	C25-C24	2.33	1.50	1.43
52	BA	3001	T8B	O11-C26	2.85	1.38	1.32
52	AA	3001	T8B	O11-C26	2.86	1.38	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C21-C23-C24	-3.49	120.19	125.04
52	AA	3001	T8B	C21-C23-C24	-3.47	120.21	125.04
52	AA	3001	T8B	C2-C3-C4	-2.74	118.75	122.13
52	BA	3001	T8B	C2-C3-C4	-2.74	118.76	122.13
52	BA	3001	T8B	O4-C12-C11	-2.16	108.73	112.47

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2827/2915 (96%)	0.05	121 (4%) 39 25	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	0.10	77 (2%) 58 44	27, 56, 110, 126	0
2	AB	120/122 (98%)	0.05	4 (3%) 50 35	68, 95, 108, 111	0
2	BB	120/122 (98%)	-0.23	0 100 100	46, 80, 95, 103	0
3	AD	275/276 (99%)	-0.13	0 100 100	45, 67, 83, 103	0
3	BD	275/276 (99%)	-0.14	2 (0%) 89 83	36, 59, 78, 103	0
4	AE	204/206 (99%)	-0.07	1 (0%) 91 87	47, 72, 87, 98	0
4	BE	204/206 (99%)	-0.16	0 100 100	33, 60, 81, 96	0
5	AF	203/205 (99%)	-0.33	2 (0%) 84 75	44, 77, 95, 112	0
5	BF	203/205 (99%)	-0.21	0 100 100	27, 64, 90, 110	0
6	AG	181/182 (99%)	1.40	54 (29%) 1 0	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.13	12 (6%) 22 12	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.95	38 (21%) 1 1	80, 93, 101, 108	0
7	BH	174/180 (96%)	-0.14	0 100 100	63, 78, 91, 98	0
8	AI	145/148 (97%)	0.62	21 (14%) 3 2	72, 104, 116, 123	0
8	BI	145/148 (97%)	-0.08	1 (0%) 89 83	68, 90, 98, 100	0
9	AN	140/140 (100%)	-0.07	1 (0%) 89 83	59, 73, 90, 94	0
9	BN	140/140 (100%)	-0.17	0 100 100	38, 57, 82, 85	0
10	AO	122/122 (100%)	-0.31	0 100 100	56, 73, 85, 91	0
10	BO	122/122 (100%)	-0.20	0 100 100	43, 64, 82, 89	0
11	AP	147/150 (98%)	0.02	4 (2%) 58 44	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.15	0 100 100	28, 68, 91, 100	0
12	AQ	141/141 (100%)	-0.01	1 (0%) 89 83	60, 78, 91, 97	0
12	BQ	141/141 (100%)	-0.07	0 100 100	44, 65, 78, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AR	118/118 (100%)	-0.17	0 100 100	47, 66, 78, 88	0
13	BR	118/118 (100%)	-0.18	0 100 100	35, 53, 69, 86	0
14	AS	110/112 (98%)	0.57	13 (11%) 6 4	74, 91, 102, 109	0
14	BS	110/112 (98%)	-0.11	0 100 100	58, 79, 93, 100	0
15	AT	131/146 (89%)	-0.20	1 (0%) 87 80	66, 76, 99, 109	0
15	BT	131/146 (89%)	-0.25	1 (0%) 87 80	55, 68, 91, 102	0
16	AU	116/118 (98%)	-0.02	0 100 100	53, 70, 84, 89	0
16	BU	116/118 (98%)	-0.13	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.17	1 (0%) 84 75	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.30	0 100 100	31, 61, 81, 95	0
18	AW	112/113 (99%)	-0.22	0 100 100	50, 59, 80, 104	0
18	BW	112/113 (99%)	-0.29	0 100 100	36, 45, 75, 106	0
19	AX	95/96 (98%)	-0.06	0 100 100	54, 71, 89, 93	0
19	BX	95/96 (98%)	-0.16	0 100 100	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.17	7 (6%) 22 12	71, 81, 94, 105	0
20	BY	107/110 (97%)	-0.22	1 (0%) 85 78	56, 71, 89, 103	0
21	AZ	198/206 (96%)	0.03	7 (3%) 48 32	80, 92, 103, 108	0
21	BZ	198/206 (96%)	-0.34	0 100 100	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.27	2 (2%) 59 45	59, 74, 84, 89	0
22	B0	76/85 (89%)	-0.22	0 100 100	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.15	4 (4%) 41 27	54, 71, 94, 99	0
23	B1	97/98 (98%)	-0.06	1 (1%) 84 75	42, 65, 91, 95	0
24	A2	70/72 (97%)	-0.04	1 (1%) 78 65	65, 81, 92, 101	0
24	B2	70/72 (97%)	-0.11	0 100 100	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.48	5 (8%) 13 7	63, 74, 92, 101	0
25	B3	59/60 (98%)	-0.14	0 100 100	43, 56, 84, 94	0
26	A4	46/71 (64%)	0.59	7 (15%) 3 2	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.30	6 (13%) 5 3	98, 107, 113, 118	0
27	A5	59/60 (98%)	-0.33	0 100 100	46, 64, 78, 91	0
27	B5	59/60 (98%)	-0.17	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.18	4 (7%) 17 9	62, 77, 87, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	53/54 (98%)	-0.07	0 100 100	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.17	4 (8%) 14 7	43, 54, 79, 99	0
29	B7	48/49 (97%)	0.02	1 (2%) 67 52	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.15	0 100 100	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.15	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.61	200 (13%) 4 2	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.55	184 (12%) 5 3	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.14	16 (6%) 19 11	93, 103, 111, 117	0
32	DB	229/256 (89%)	0.69	33 (14%) 3 2	95, 105, 112, 115	0
33	CC	206/239 (86%)	1.05	48 (23%) 1 1	92, 106, 112, 115	0
33	DC	206/239 (86%)	0.92	36 (17%) 2 1	97, 108, 115, 120	0
34	CD	208/209 (99%)	0.06	10 (4%) 34 21	85, 98, 108, 114	0
34	DD	208/209 (99%)	0.05	11 (5%) 30 17	87, 97, 107, 123	0
35	CE	148/162 (91%)	-0.12	4 (2%) 58 44	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.13	6 (4%) 41 27	84, 96, 104, 110	0
36	CF	100/101 (99%)	-0.04	5 (5%) 32 19	80, 92, 101, 107	0
36	DF	100/101 (99%)	-0.12	3 (3%) 54 39	84, 93, 103, 110	0
37	CG	155/156 (99%)	2.20	80 (51%) 0 0	99, 109, 115, 120	0
37	DG	155/156 (99%)	2.15	77 (49%) 0 0	97, 109, 115, 119	0
38	CH	138/138 (100%)	0.08	4 (2%) 55 41	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.06	3 (2%) 65 50	86, 96, 102, 106	0
39	CI	125/128 (97%)	1.97	55 (44%) 0 0	97, 111, 117, 120	0
39	DI	125/128 (97%)	2.88	74 (59%) 0 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	2.22	47 (48%) 0 0	100, 109, 115, 117	0
40	DJ	96/105 (91%)	2.00	49 (51%) 0 0	97, 110, 115, 119	0
41	CK	114/129 (88%)	-0.10	1 (0%) 85 78	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.25	4 (3%) 48 32	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.21	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.12	2 (1%) 74 62	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.21	53 (46%) 0 0	102, 111, 118, 126	0
43	DM	114/126 (90%)	1.81	46 (40%) 0 0	101, 109, 115, 117	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CN	60/61 (98%)	1.23	15 (25%) 1 1	99, 108, 116, 118	0
44	DN	60/61 (98%)	1.64	21 (35%) 0 0	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.04	2 (2%) 64 49	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.21	6 (6%) 20 11	81, 93, 103, 107	0
46	CP	82/88 (93%)	0.65	7 (8%) 13 7	88, 96, 106, 112	0
46	DP	82/88 (93%)	0.46	3 (3%) 45 30	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.07	2 (2%) 68 54	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.20	3 (3%) 54 39	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.17	9 (13%) 4 3	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.23	4 (5%) 26 14	85, 93, 104, 106	0
49	CS	78/93 (83%)	2.70	44 (56%) 0 0	107, 111, 117, 123	0
49	DS	78/93 (83%)	2.94	52 (66%) 0 0	91, 112, 117, 119	0
50	CT	96/106 (90%)	0.21	3 (3%) 52 38	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.73	12 (12%) 5 3	82, 92, 100, 101	0
51	CU	23/27 (85%)	2.97	13 (56%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	2.74	13 (56%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.29	1665 (8%) 14 7	27, 84, 115, 128	0

The worst 5 of 1665 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	CI	30	GLY	12.8
49	CS	40	ILE	12.6
43	CM	85	GLY	12.3
31	CA	1353	G	11.3
31	CA	1286	A	11.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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.