



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2026 – 12:01 PM UTC

PDB ID : 4V8A / pdb_00004v8a
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

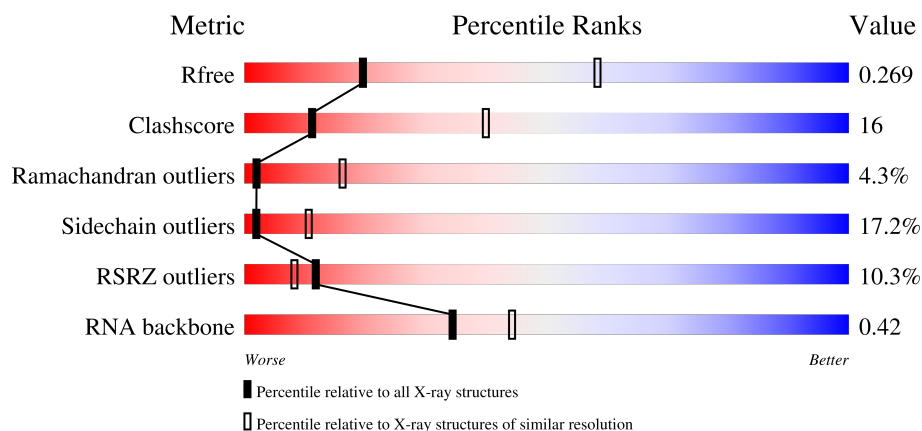
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	2915	4% 40% 44% 13% .
1	BA	2915	4% 50% 35% 12% .
2	AB	122	11% 30% 54% 14% .
2	BB	122	2% 56% 34% 9% .

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	-
52	T8B	BA	3001	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 279316 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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			

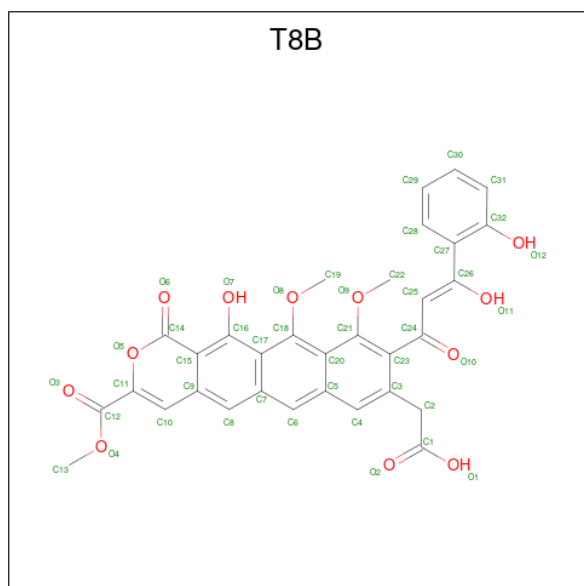
- Molecule 50 is a protein called 30S ribosomal protein S20.

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 (CCD ID: 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		

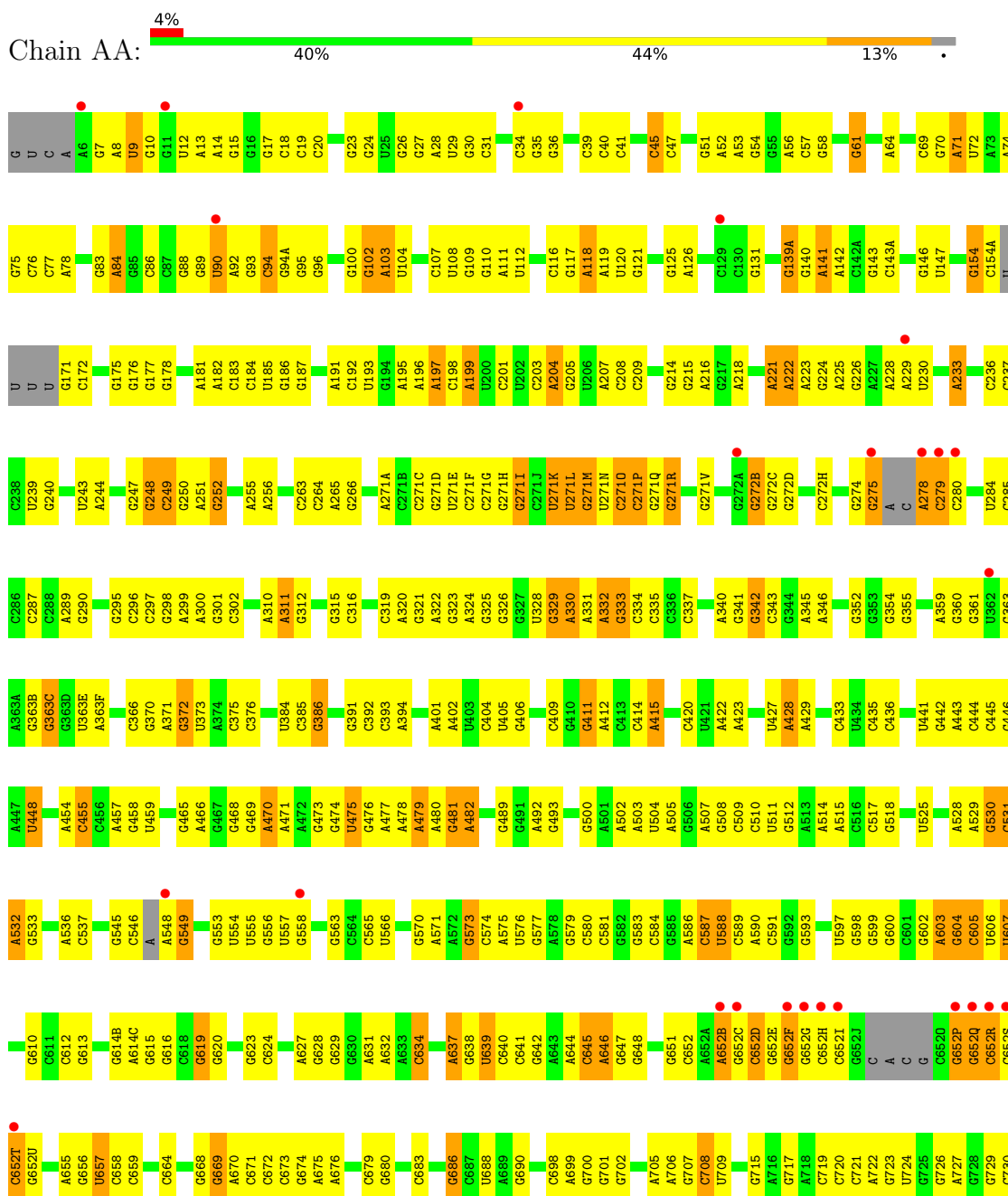
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

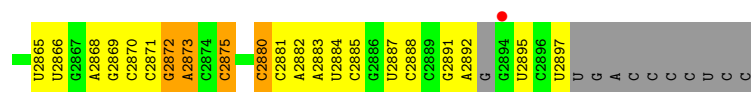
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S ribosomal RNA

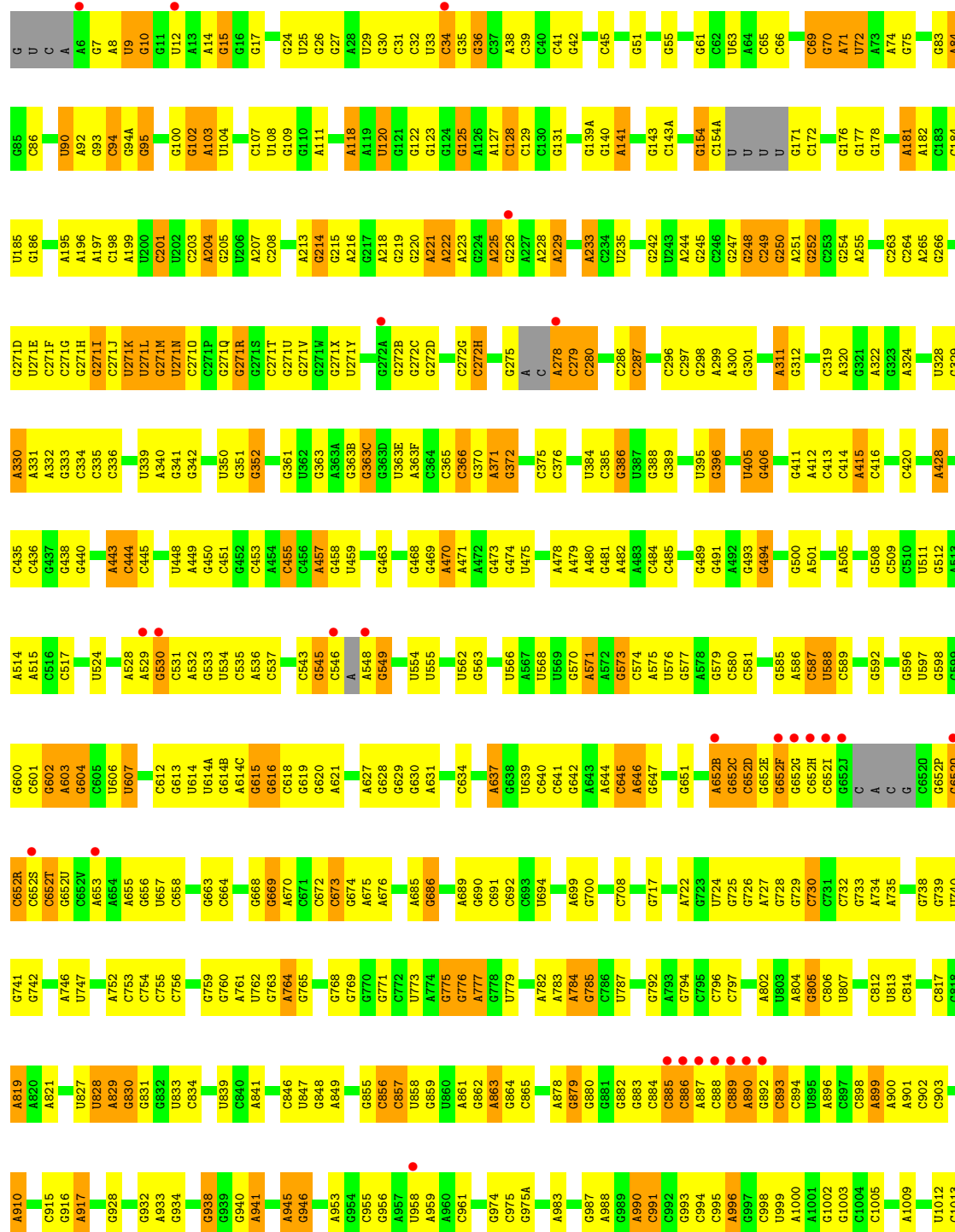




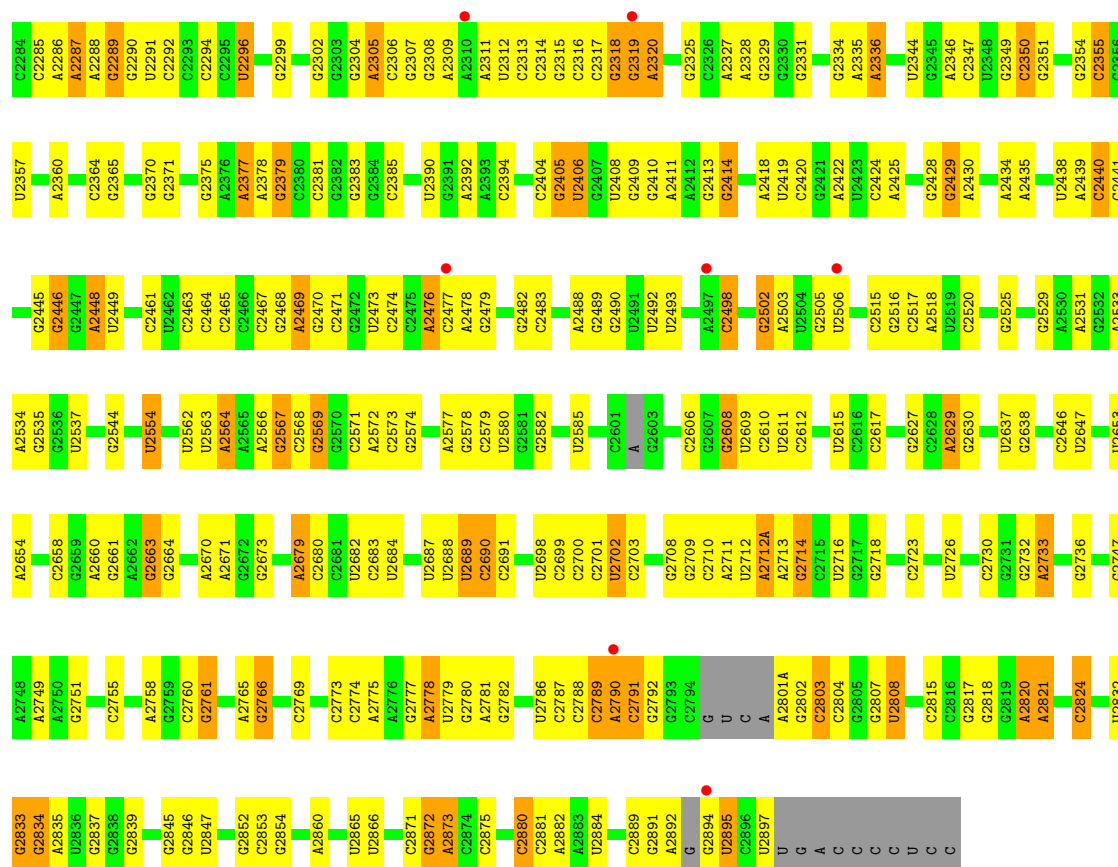
G2777	G2703	U2605	C2521	A2439	G2373	C2306	C2240	G2162	G2101	G2023	A1936
A2778	G2707	U2608	G2524	C2440	A2376	G2307	A2241	C2163	U2102	G2027	A1937
A2781	G2710	G2609	G2525	C2441	A2377	G2308	G2242	C2164	C2103	U2028	G1826
G2782	G2711	C2610	G2529	G2445	G2379	A2310	U2244	G2165	G2104	C1942	G1827
C2784	A2712	U2611	A2530	G2446	G2380	U2312	G2245	G2166	C2105	A1829	G1828
C2785	U2712A	C2612	A2531	G2447	C2381	U2313	G2246	U2167	A2030	U1946	A1835
U2786	A2713	U2615	G2535	A2448	G2382	C2314	A2247	A2169	G2032	C1947	U1833
C2787	U2712A	C2616	G2536	U2449	G2383	C2315	U2249	A2170	U2109	G1948	U1834
C2788	G2714	C2617	G2537	A2450	G2384	C2316	G2250	A2171	G2110	U1836	C1837
C2789	G2714	G2618	U2537	G2455	C2385	C2317	G2251	A2172	G2111	U1955	C1837
A2790	C2723	U2619	C2538	G2455	C2385	C2318	G2252	A2173	U2113	U1956	G1838
C2791	U2726	C2620	C2539	U2462	A2388	G2319	G2253	C2174	A2114	U1963	G1840
C2794	G2727	G2627	A2542	C2463	U2389	A2320	G2256	A2176	G2115	G1964	G1840
G	U2728	C2628	G2543	C2464	U2390	A2321	U2257	C2177	G2116	U1965	G1847
U	G2729	A2629	G2544	C2465	U2391	A2322	U2257	C2178	A2117	C1966	A1848
C	C2730	G2630	G2544	G2468	A2392	G2323	C2261	C2179	U2118	G1967	G1849
A	G2731	G2631	U2552	A2469	A2393	C2324	U2262	U2180	A2119	C2049	G1850
A2801A	G2732	U2632	G2553	C2470	A2394	G2325	U2263	G2181	G2120	C2051	A1853
G2802	A2733	A2639	U2554	C2471	C2395	G2326	C2264	C2184	U2122	G2052	A1854
C2803	G2735	G2640	G2558	G2472	G2396	A2327	C2264	C2185	G2123	A1970	A1876
C2804	G2736	U2641	C2559	C2473	G2397	A2328	A2269	G2186	G2124	A1971	A1877
U2808	G2737	G2645	U2562	C2474	G2400	G2329	A2269	G2187	G2125	A1972	G1878
G2811	A2738	C2646	G2563	C2475	C2403	G2330	U2272	C2188	A2126	G2055	G1882
A2812	U2740	U2647	U2564	A2476	C2404	U2332	A2273	U2189	G2127	A2057	G1883
C2814	G2741	G2655	A2565	C2477	C2405	A2333	A2274	G2190	U2130	A2060	A1884
C2815	C2742	U2656	G2566	G2481	U2406	G2334	A2275	G2191	G2131	A2061	A1986
C2816	G2743	G2657	G2567	C2482	G2407	A2335	A2276	G2192	U2132	A2062	G1987
G2817	U2744	C2658	C2568	G2483	U2408	G2337	G2277	G2193	G2133	G1980	G1888
G2818	C2745	U2659	U2572	C2484	G2409	G2338	A2278	A2198	C2136	A1981	G1889
G2819	A2746	A2660	C2573	G2485	A2410	G2339	A2279	A2199	A2135	C2065	G1891
A2820	G2747	C2661	G2574	C2487	C2411	C2342	G2280	A2200	G2137	C2066	A1890
A2821	U2748	A2662	C2575	G2488	G2414	U2344	G2281	C2201	C2138	U2068	G1991
G2822	G2749	G2663	C2576	G2489	G2415	G2345	G2282	U2203	G2139	G2069	G1892
A2823	U2750	G2673	G2577	C2490	C2416	A2346	C2284	G2205	G2140	A2071	C1992
G2831	C2752	C2680	G2578	G2494	U2419	U2347	A2285	G2206	G2141	G2070	C1993
U2832	G2755	C2683	G2582	G2495	C2420	U2348	A2286	G2207	C2142	U2074	G1899
G2833	U2756	U2684	U2583	C2498	G2421	U2350	A2287	A2208	U2144	U2075	A1900
G2834	A2757	U2685	U2584	C2499	U2422	G2351	G2288	U2218	C2145	G2076	G1906
A2835	G2758	G2686	G2585	G2502	C2424	G2354	U2291	G2223	G2146	C2078	G1998
G2838	G2759	U2687	A2587	G2503	A2425	C2355	C2292	G2224	G2147	U2079	C1999
G2839	U2760	U2688	G2588	U2504	C2426	C2356	C2293	A2225	G2148	A2082	A1913
G2845	G2761	U2689	A2590	G2505	G2428	U2357	G2294	C2226	U2150	G2083	U1915
G2846	A2764	C2690	C2591	U2506	G2429	C2358	C2295	A2227	G2151	C2084	U1916
U2847	G2765	A2693	G2592	C2507	A2430	U2359	U2296	G2228	G2152	G2085	U1917
G2848	C2766	G2694	U2593	U2514	U2431	A2360	A2298	C2229	G2153	A2014	A1927
U2849	C2767	C2695	C2594	G2515	A2432	G2361	G2299	U2233	G2154	G2094	A1928
A2850	C2768	U2696	G2595	G2516	A2433	G2362	G2300	G2234	G2155	G2095	U1929
G2854	C2769	G2697	A2600	G2517	A2434	C2363	C2301	G2235	G2156	U2096	G1930
G2855	U2770	U2698	C2601	U2518	A2435	G2364	G2302	C2236	A2158	C2097	U1931
C2856	C2771	C2699	A	U2519	G2436	C2365	G2303	G2237	G2159	U2098	C1934
	A2776	C2700	U2604	C2520	U2438	G2371	G2304	G2238	G2160	A2021	U2099
						G2372	A2305	G2239	C2161	G2100	U2022



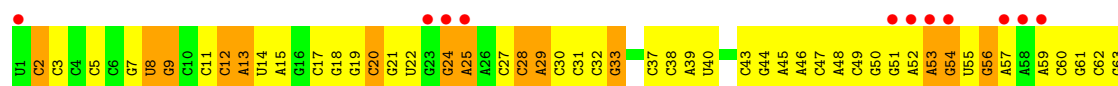
• Molecule 1: 23S ribosomal RNA



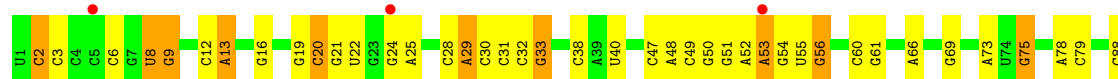




• Molecule 2: 5S ribosomal RNA

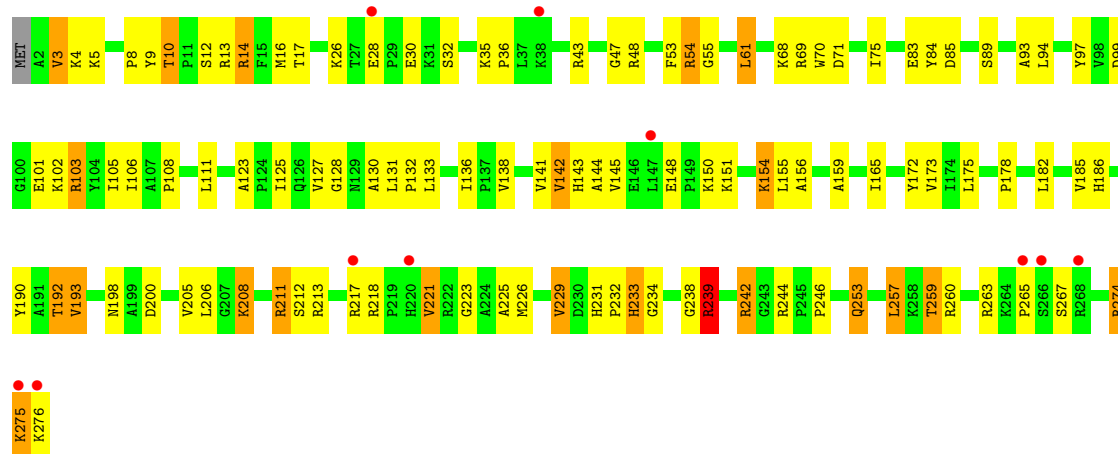


• Molecule 2: 5S ribosomal RNA

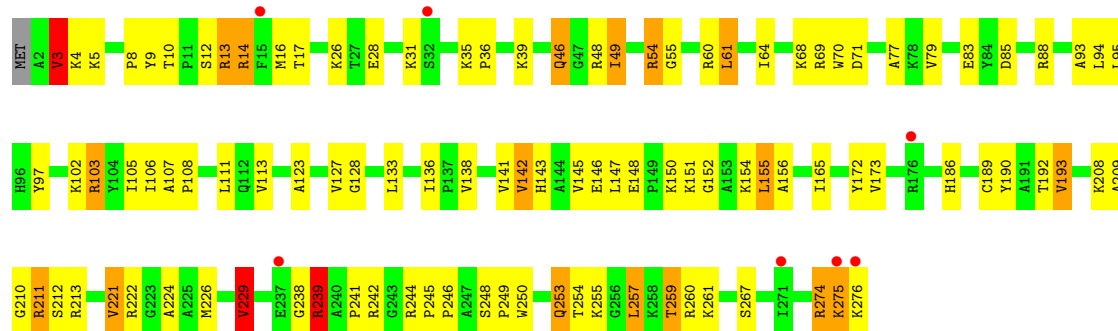


• Molecule 3: 50S ribosomal protein L2

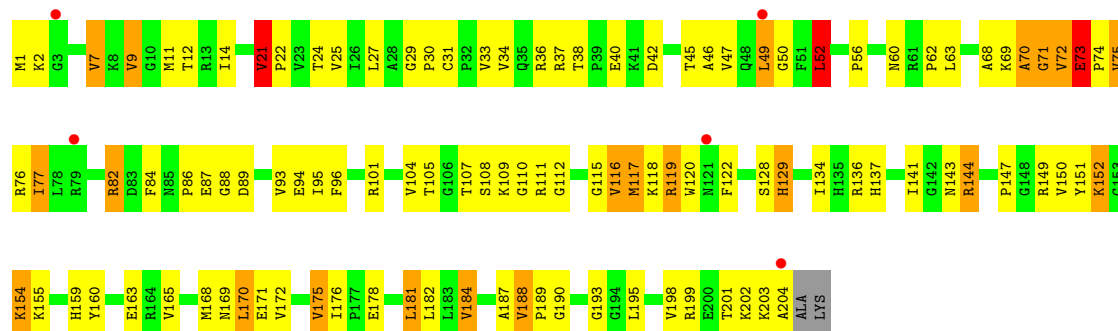




• Molecule 3: 50S ribosomal protein L2

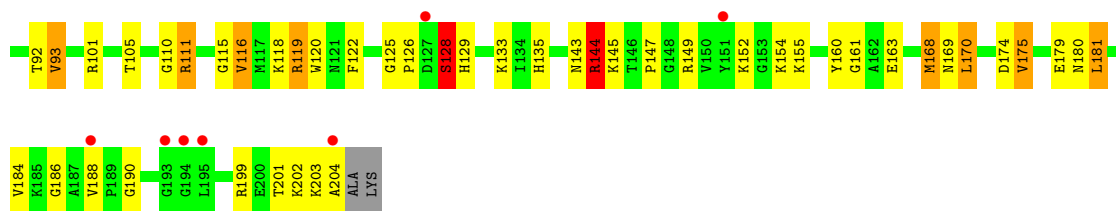


• Molecule 4: 50S ribosomal protein L3

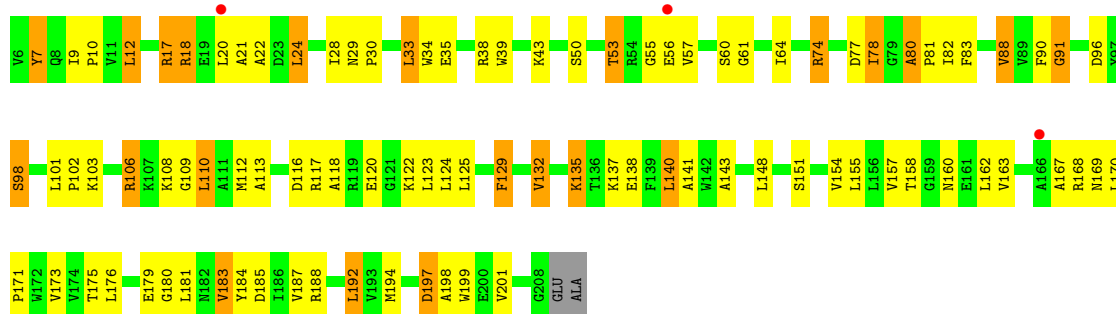


• Molecule 4: 50S ribosomal protein L3

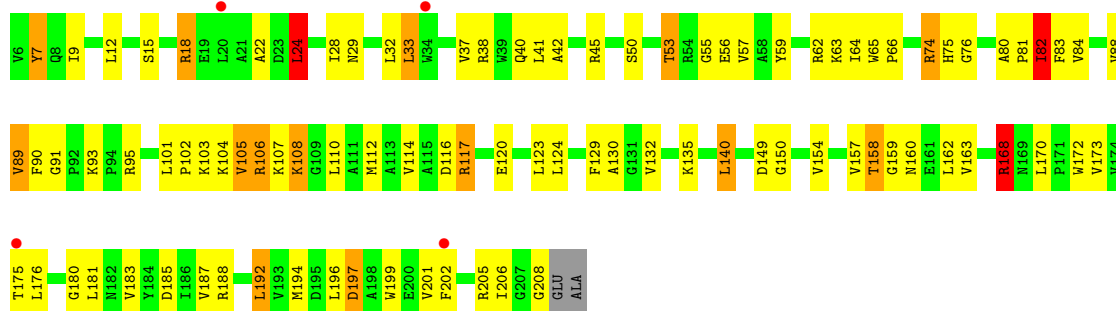




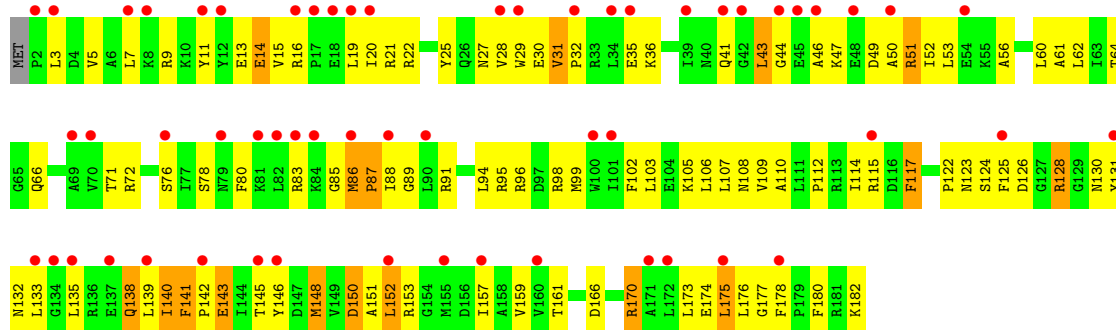
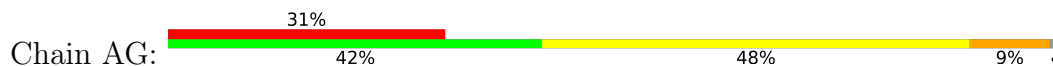
• Molecule 5: 50S ribosomal protein L4



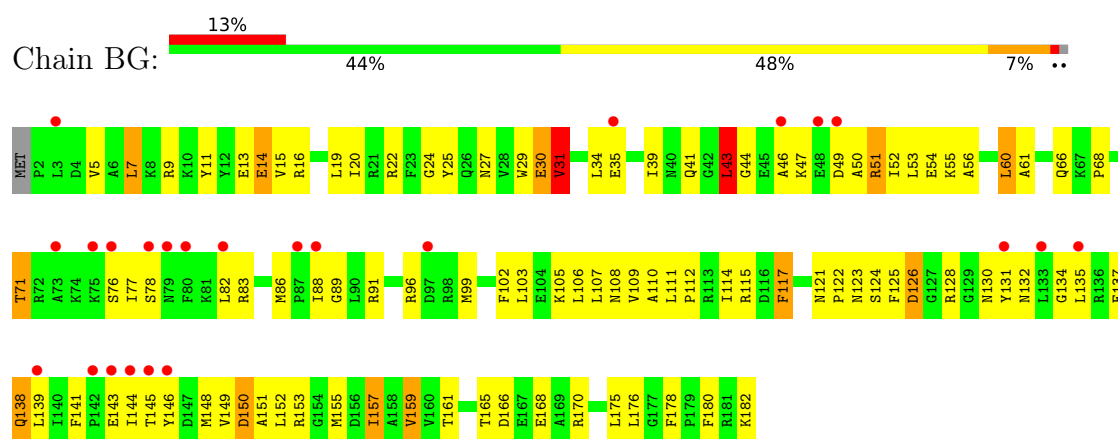
• Molecule 5: 50S ribosomal protein L4



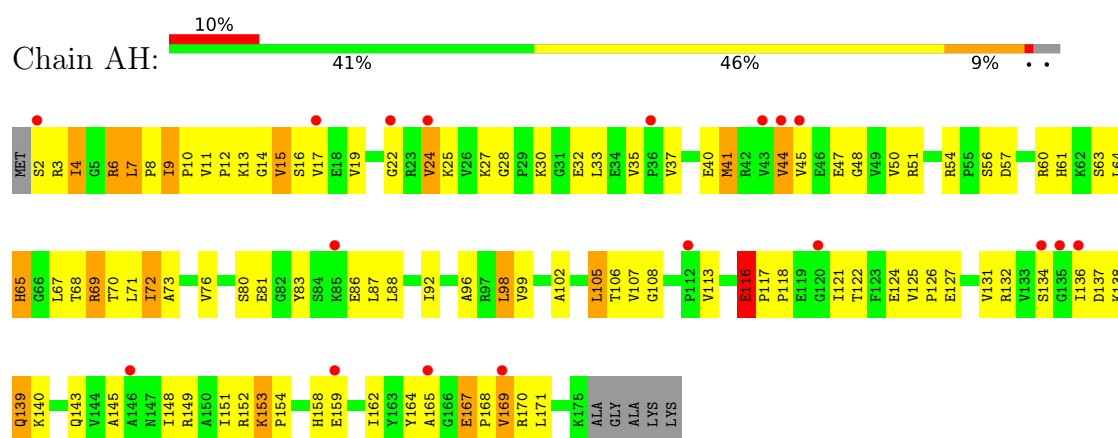
• Molecule 6: 50S ribosomal protein L5



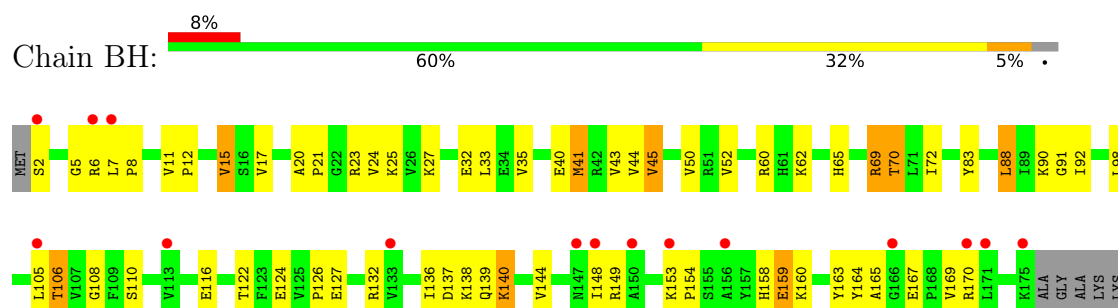
• Molecule 6: 50S ribosomal protein L5



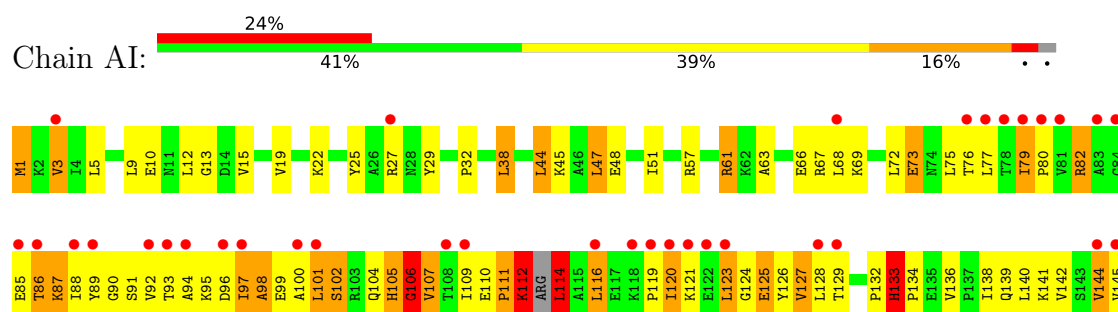
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

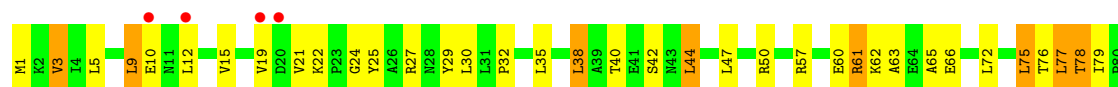


• Molecule 8: 50S ribosomal protein L9

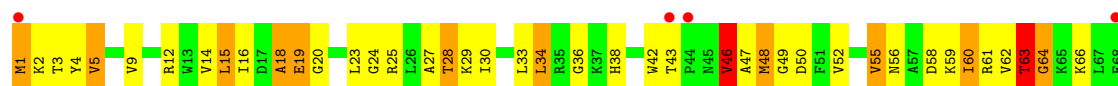




• Molecule 8: 50S ribosomal protein L9



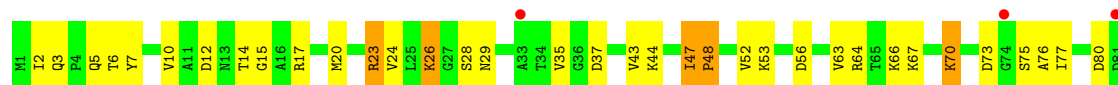
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

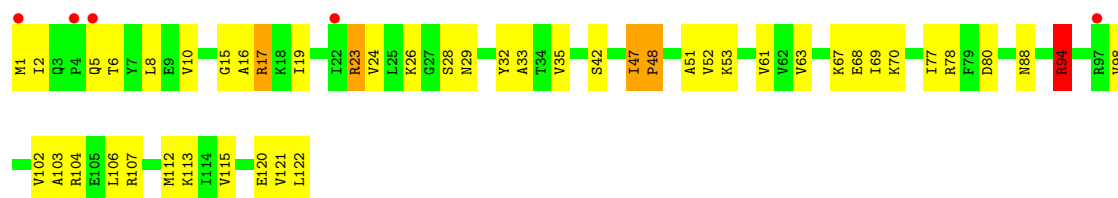


• Molecule 10: 50S ribosomal protein L14

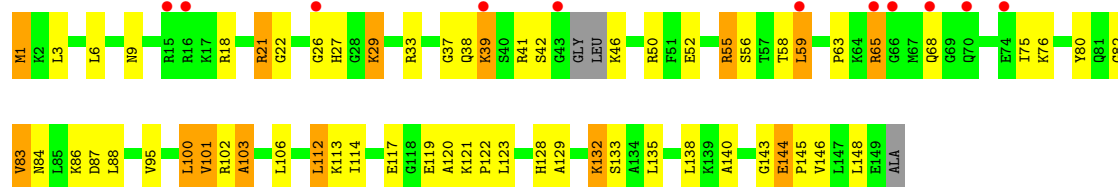


• Molecule 10: 50S ribosomal protein L14

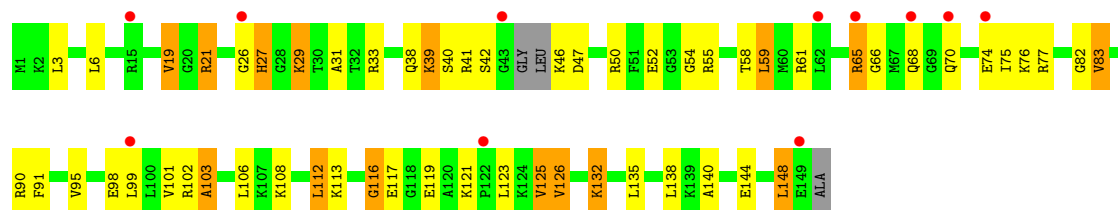




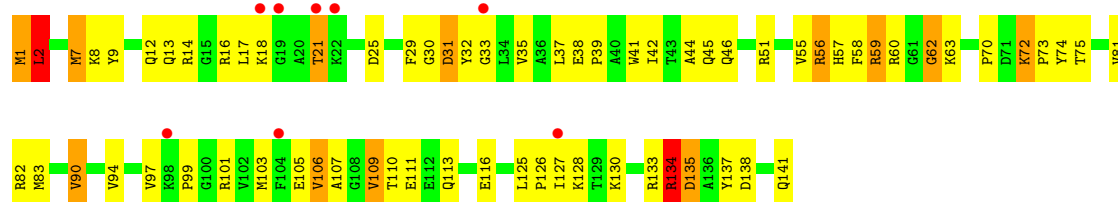
• Molecule 11: 50S ribosomal protein L15



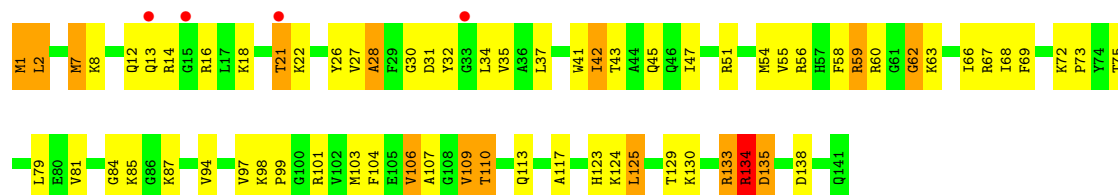
• Molecule 11: 50S ribosomal protein L15



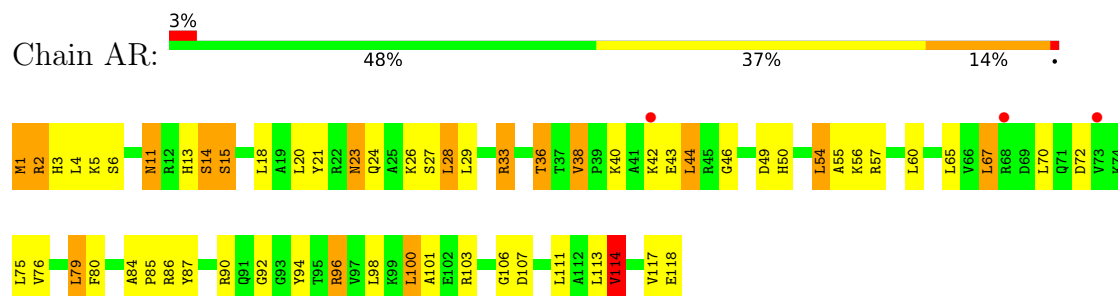
• Molecule 12: 50S ribosomal protein L16



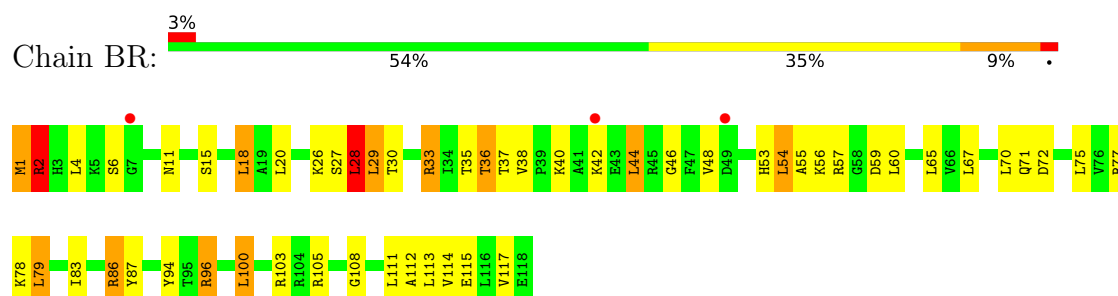
• Molecule 12: 50S ribosomal protein L16



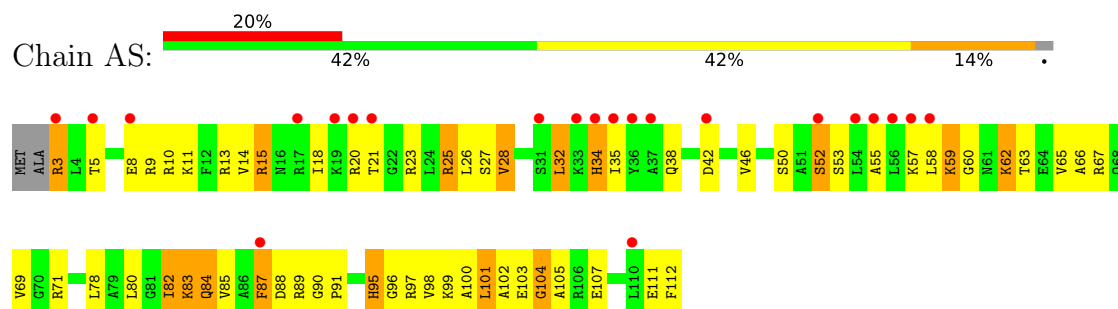
- Molecule 13: 50S ribosomal protein L17



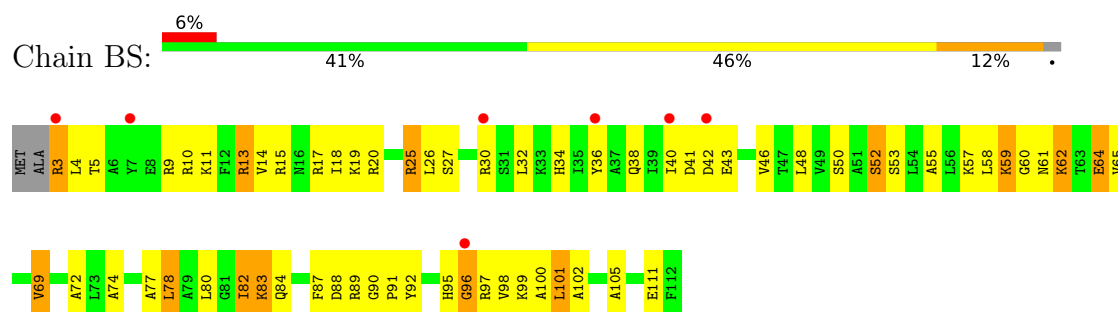
- Molecule 13: 50S ribosomal protein L17



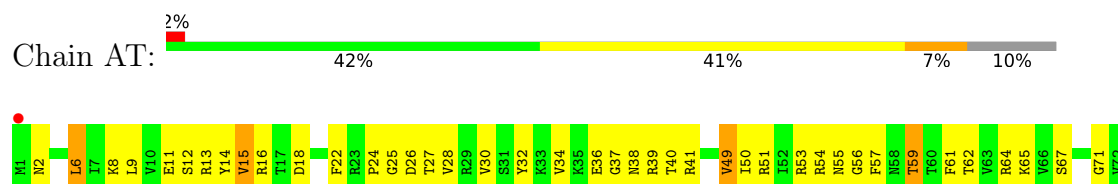
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19





• Molecule 15: 50S ribosomal protein L19



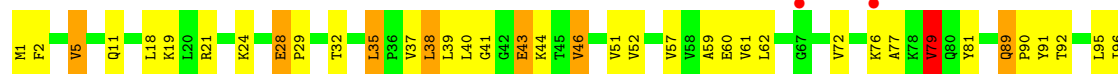
• Molecule 16: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L20

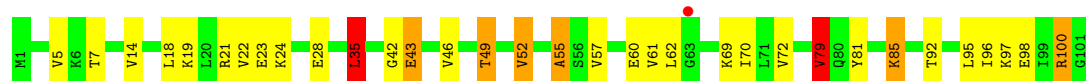


• Molecule 17: 50S ribosomal protein L21



• Molecule 17: 50S ribosomal protein L21

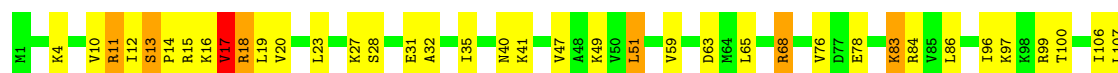




- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



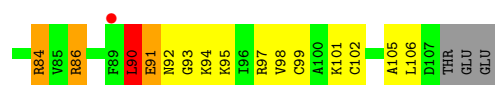
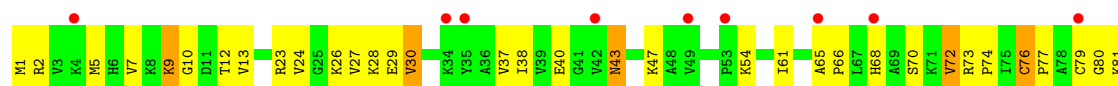
- Molecule 19: 50S ribosomal protein L23



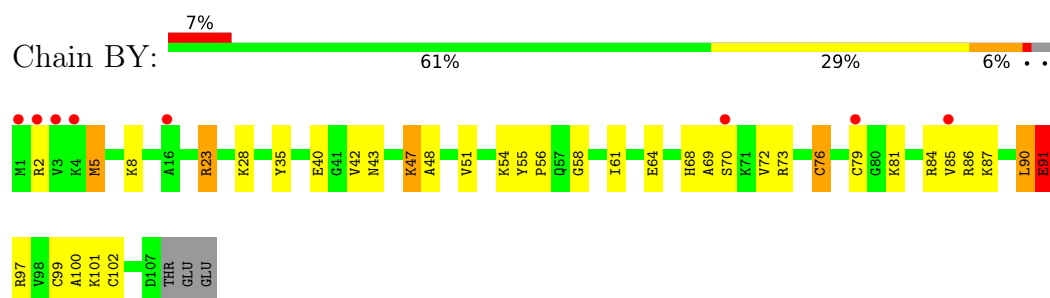
- Molecule 19: 50S ribosomal protein L23



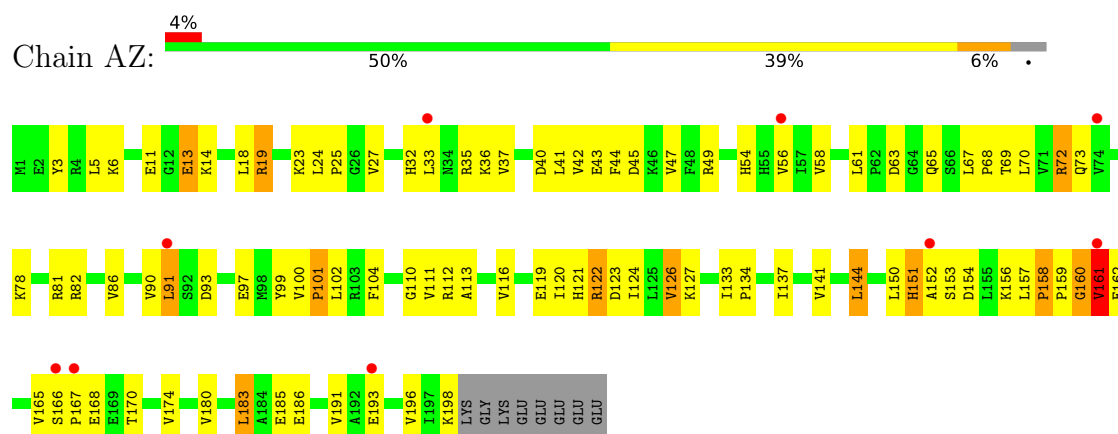
- Molecule 20: 50S ribosomal protein L24



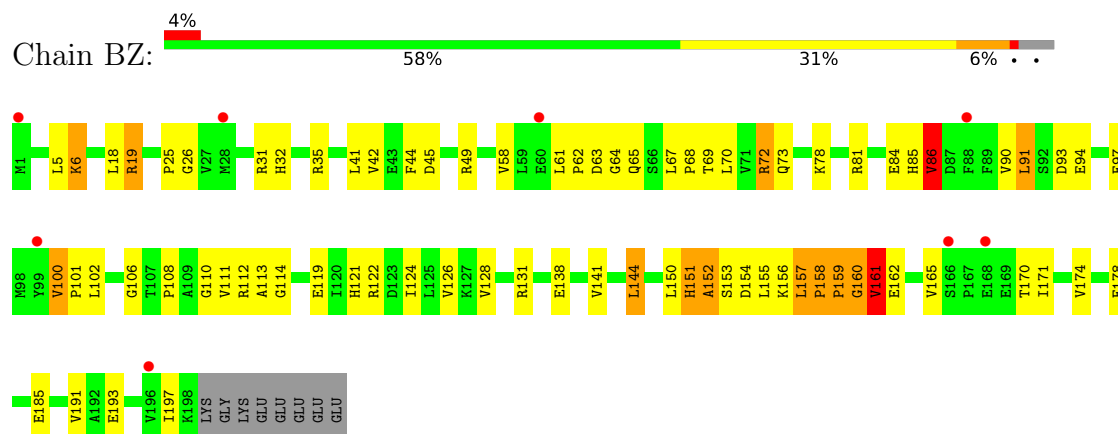
- Molecule 20: 50S ribosomal protein L24



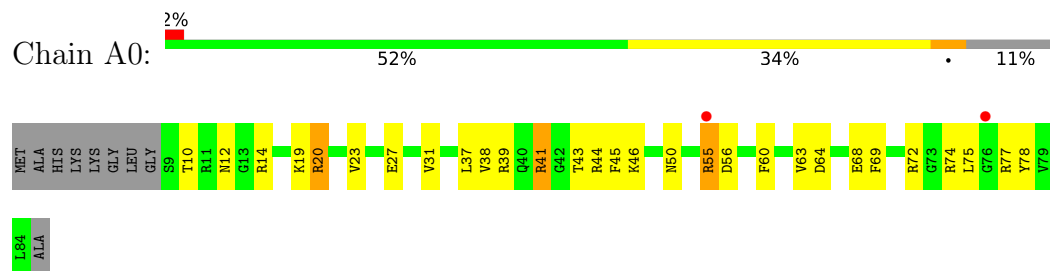
- Molecule 21: 50S ribosomal protein L25



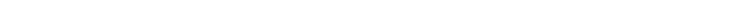
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27

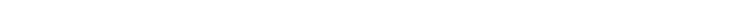


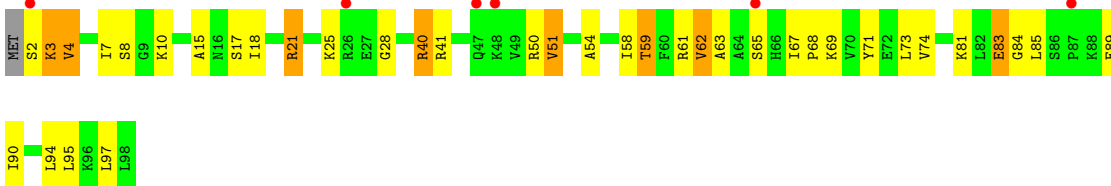
- Molecule 22: 50S ribosomal protein L27

Chain B0:  %

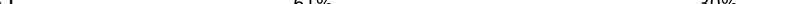


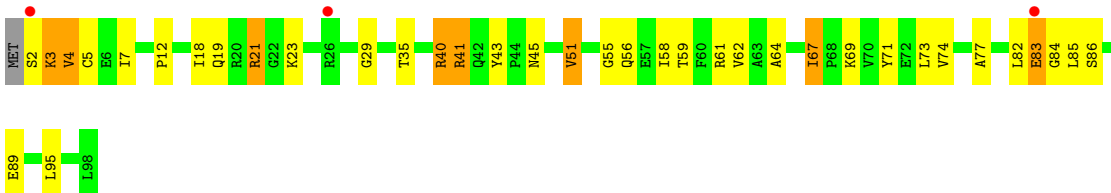
- Molecule 23: 50S ribosomal protein L28

Chain A1: 

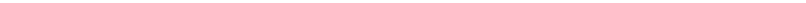


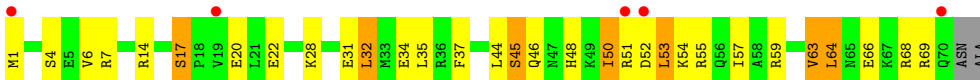
- Molecule 23: 50S ribosomal protein L28

Chain B1: 

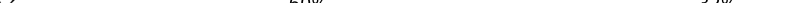


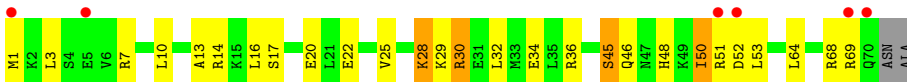
- Molecule 24: 50S ribosomal protein L29

Chain A2: 

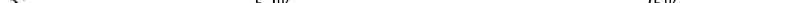


- Molecule 24: 50S ribosomal protein L29

Chain B2: 

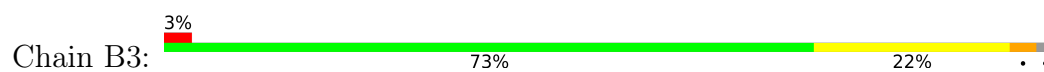


- Molecule 25: 50S ribosomal protein L30

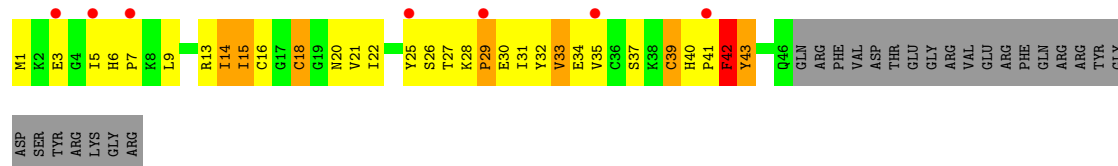
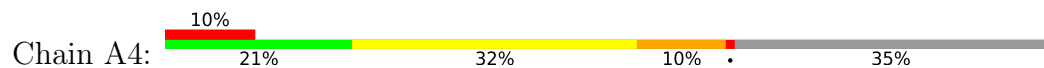
Chain A3: 



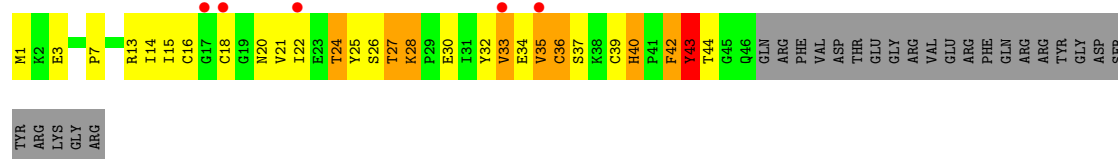
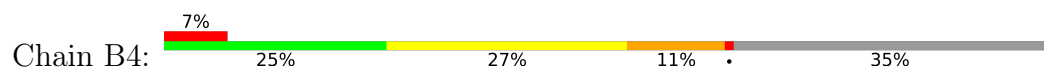
- Molecule 25: 50S ribosomal protein L30



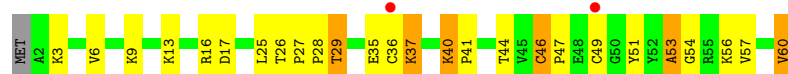
- Molecule 26: 50S ribosomal protein L31



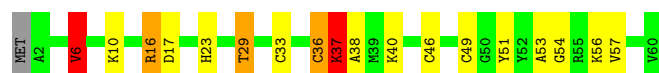
- Molecule 26: 50S ribosomal protein L31



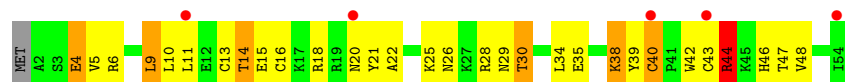
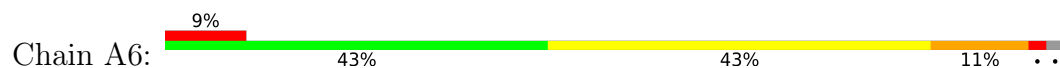
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

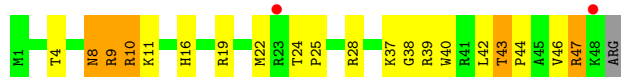




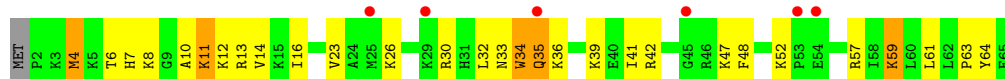
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



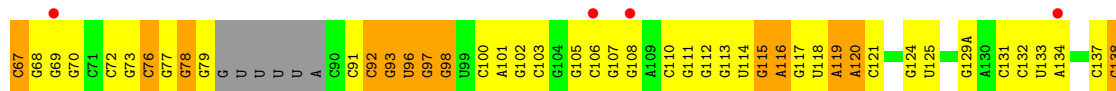
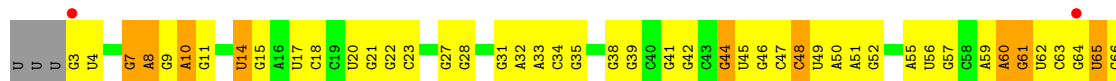
- Molecule 30: 50S ribosomal protein L35



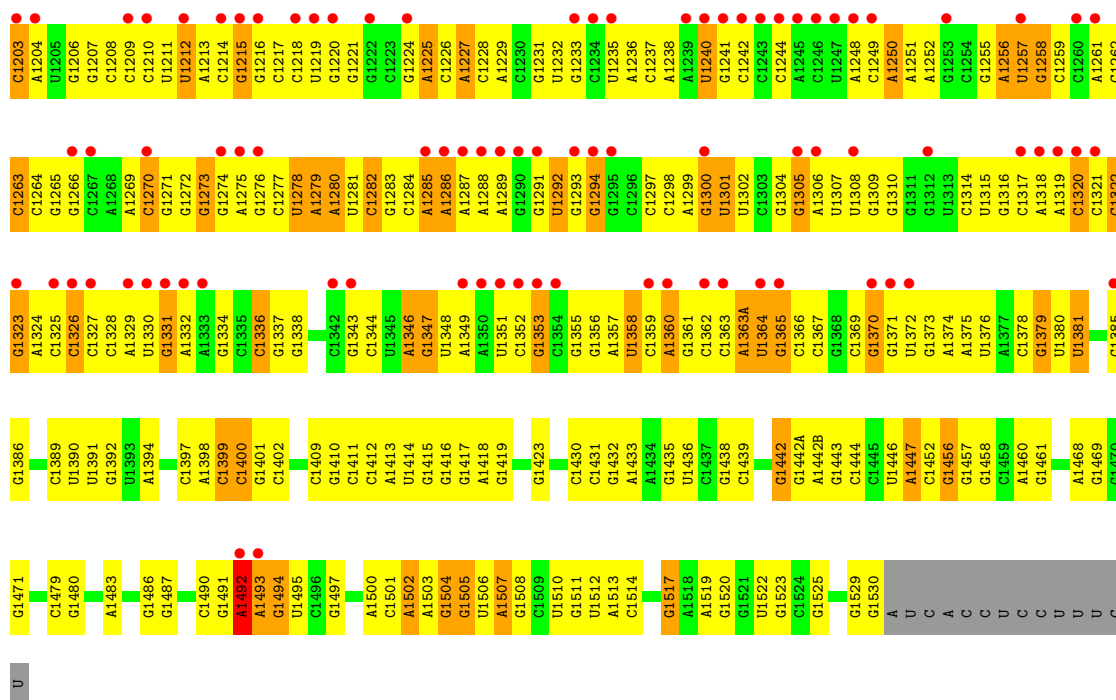
- Molecule 30: 50S ribosomal protein L35



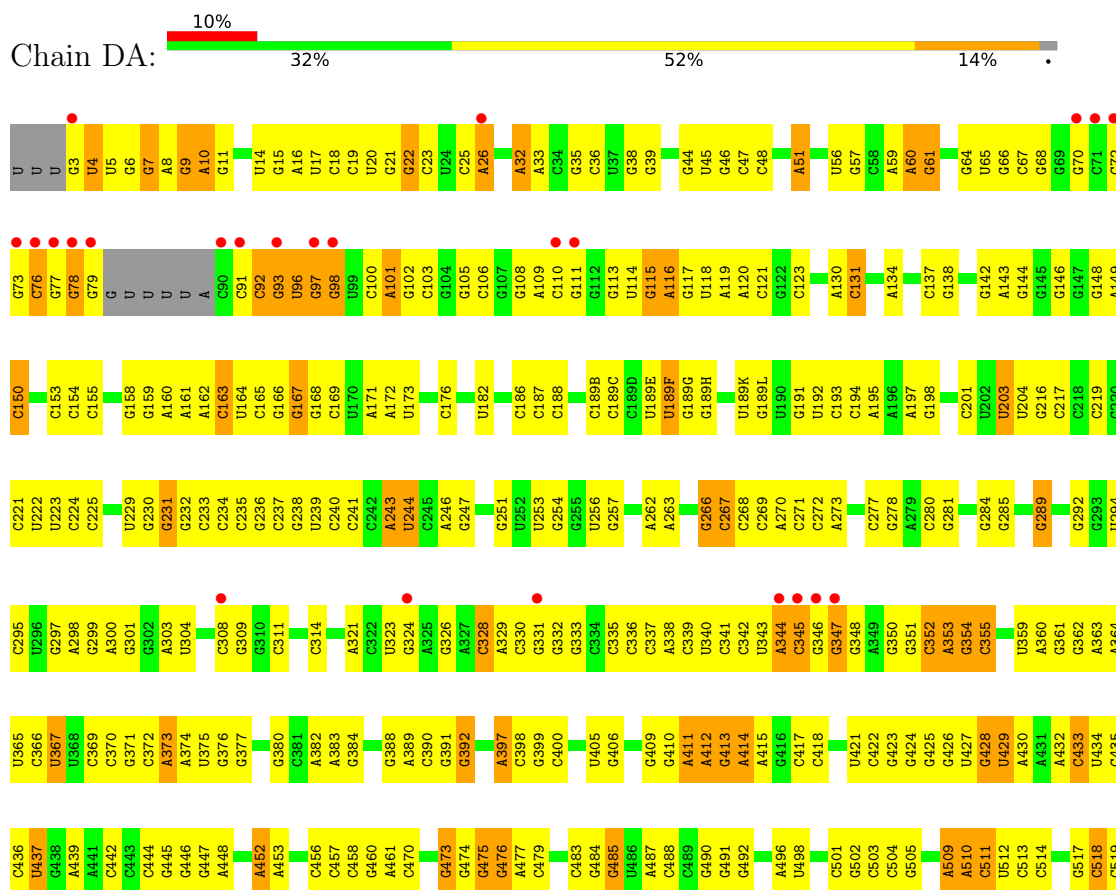
- Molecule 31: 16S ribosomal RNA

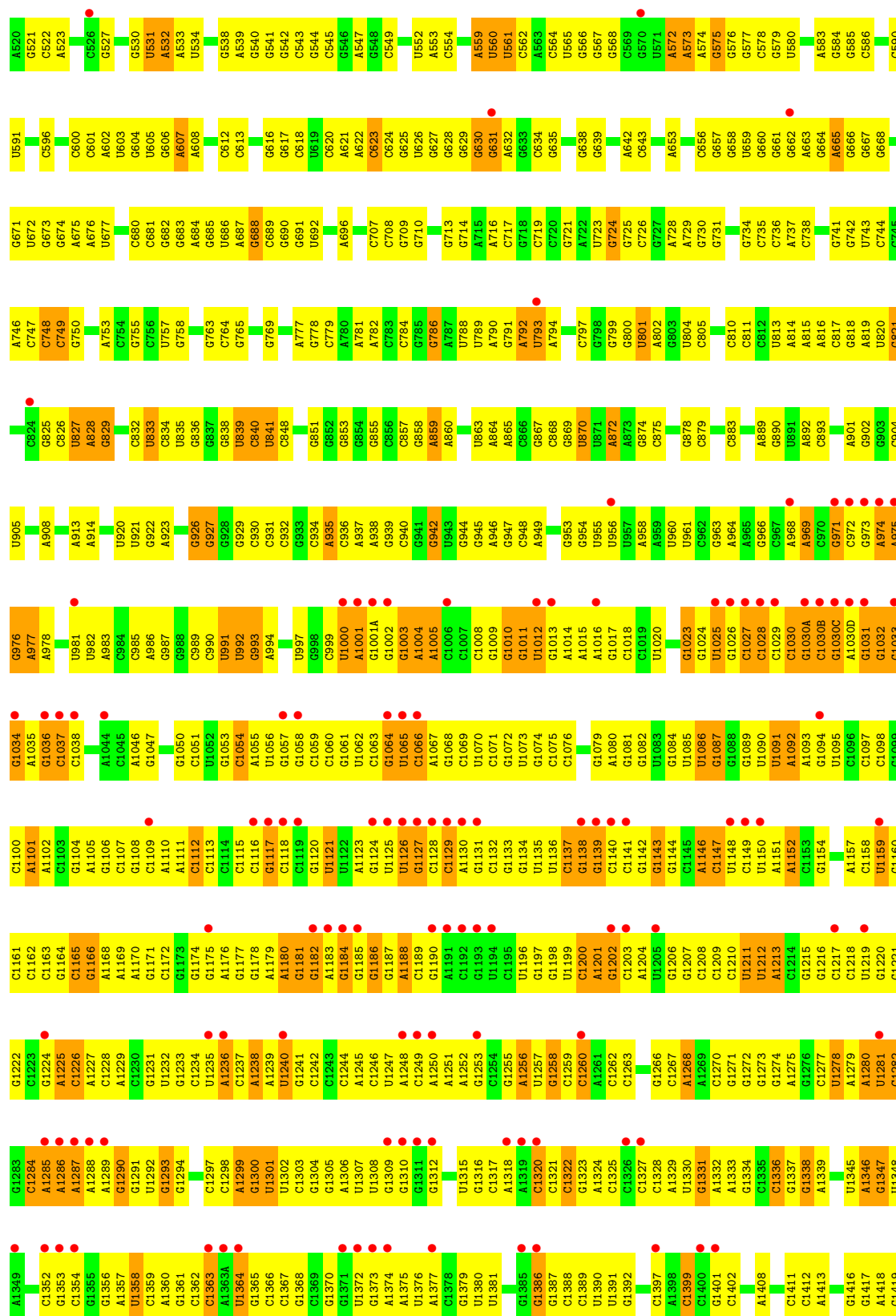


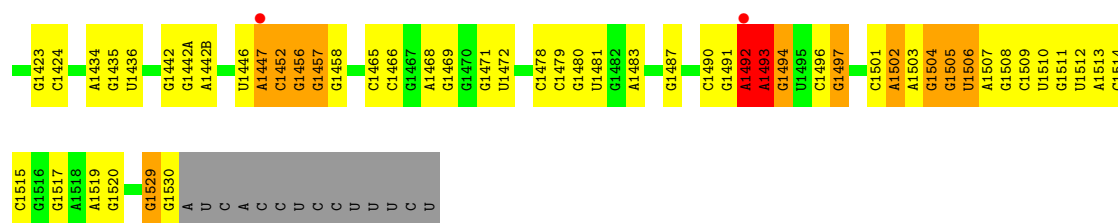




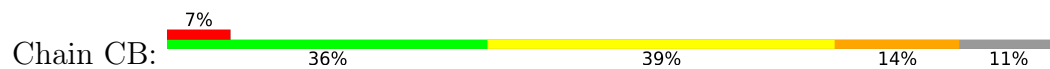
• Molecule 31: 16S ribosomal RNA



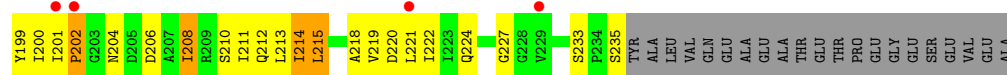
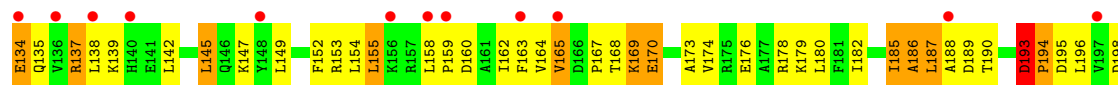
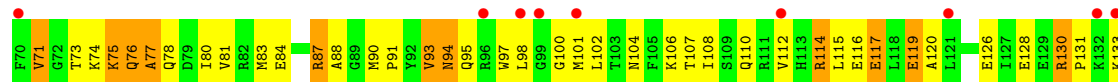
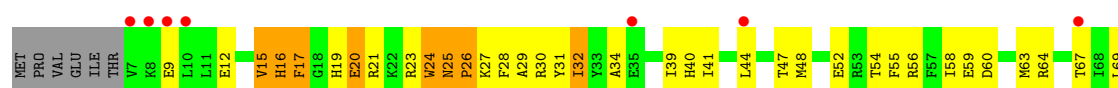




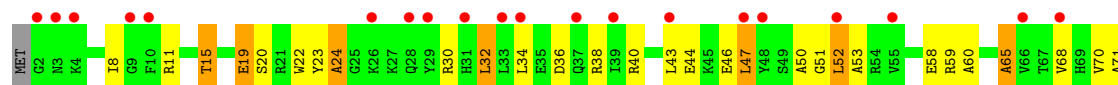
- Molecule 32: 30S ribosomal protein S2

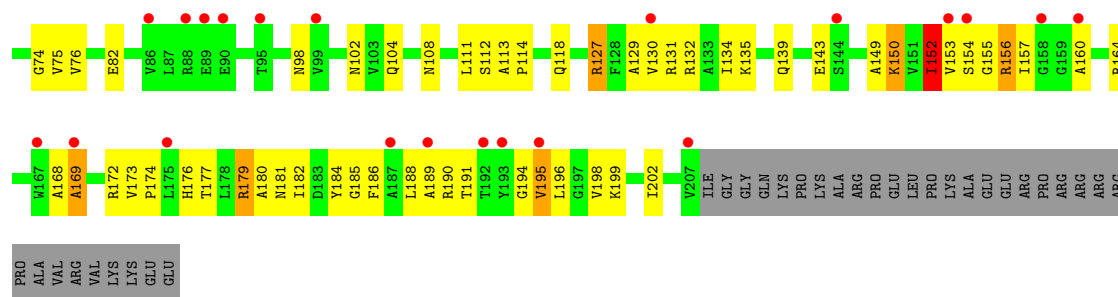


- Molecule 32: 30S ribosomal protein S2

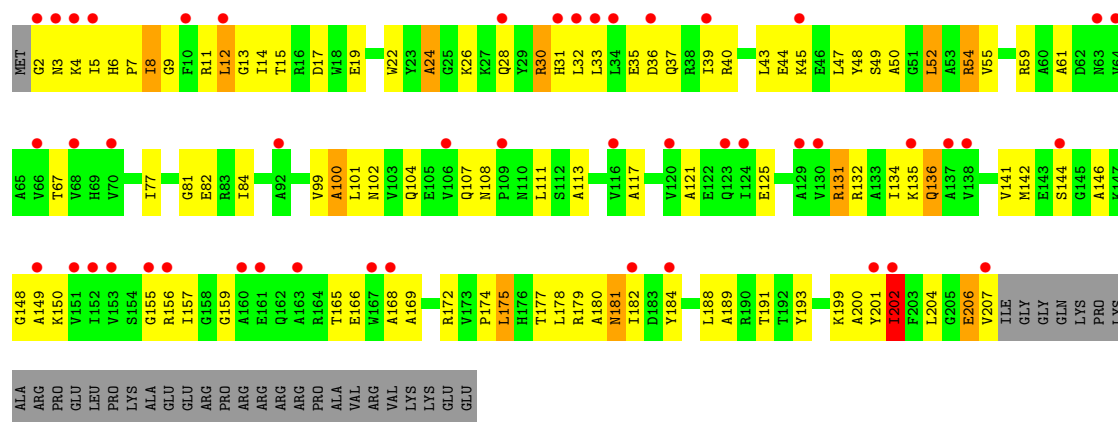


- Molecule 33: 30S ribosomal protein S3

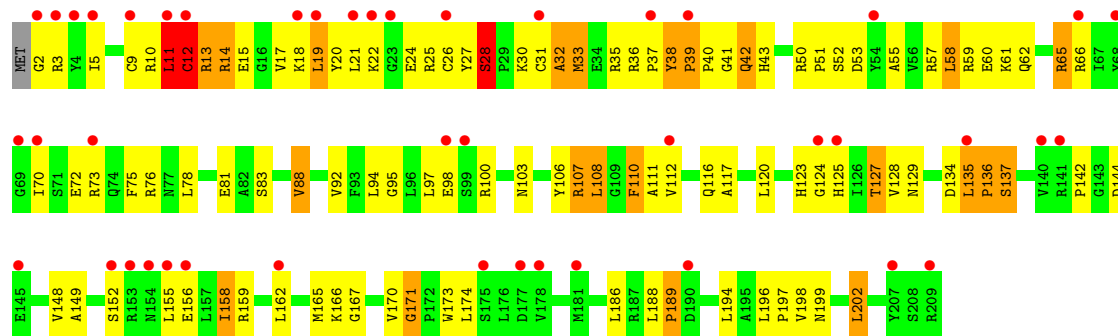




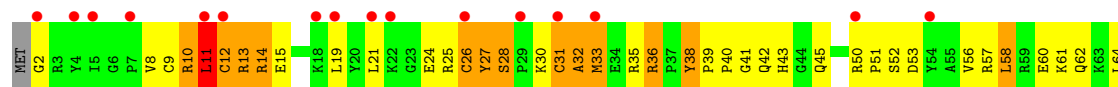
• Molecule 33: 30S ribosomal protein S3

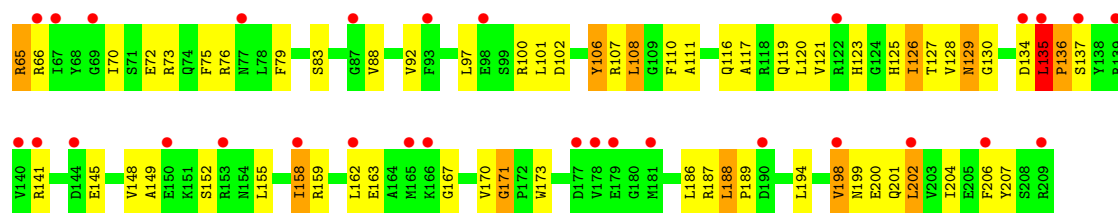


• Molecule 34: 30S ribosomal protein S4

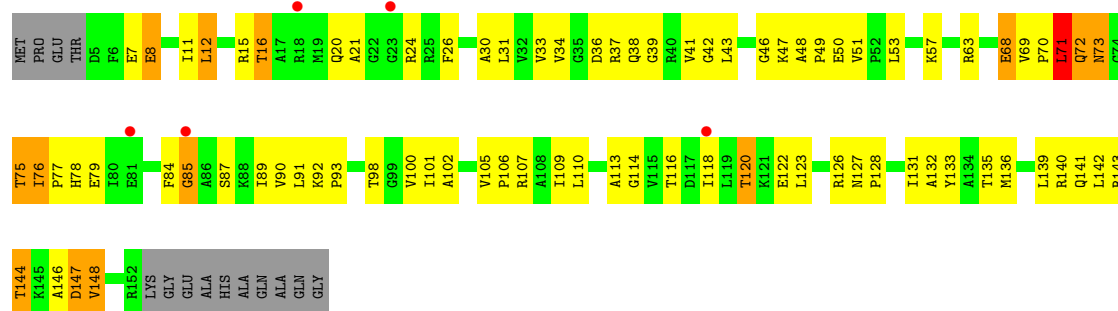


• Molecule 34: 30S ribosomal protein S4

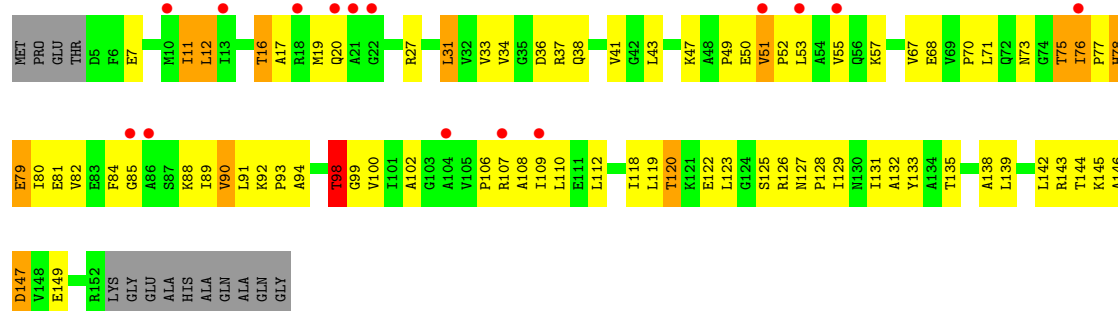




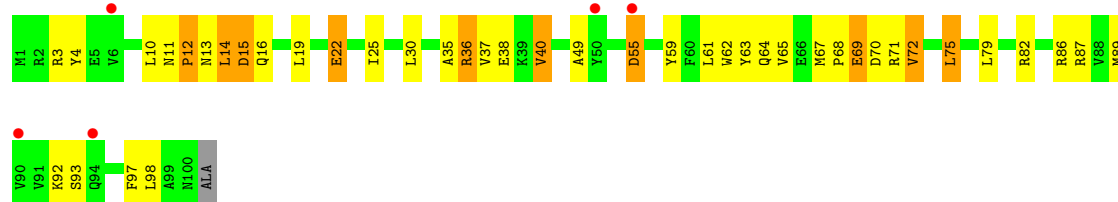
• Molecule 35: 30S ribosomal protein S5



• Molecule 35: 30S ribosomal protein S5

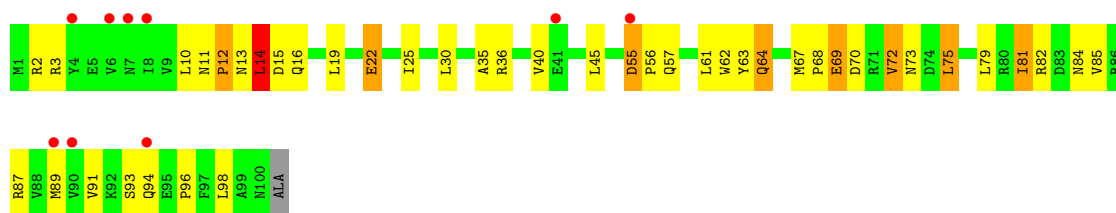


• Molecule 36: 30S ribosomal protein S6



• Molecule 36: 30S ribosomal protein S6

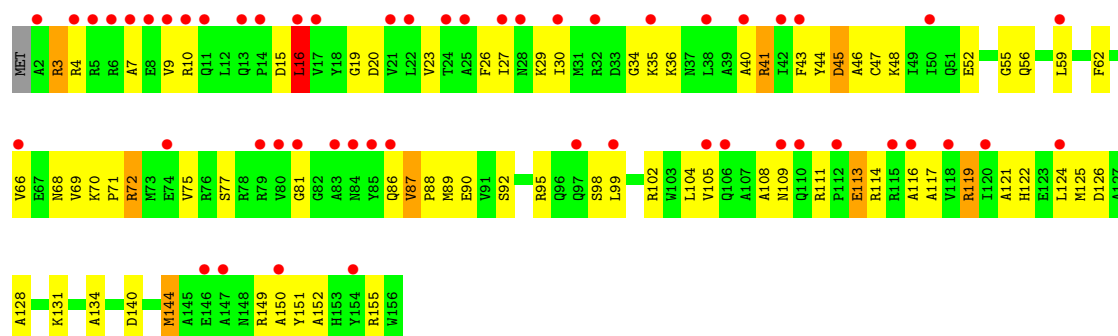




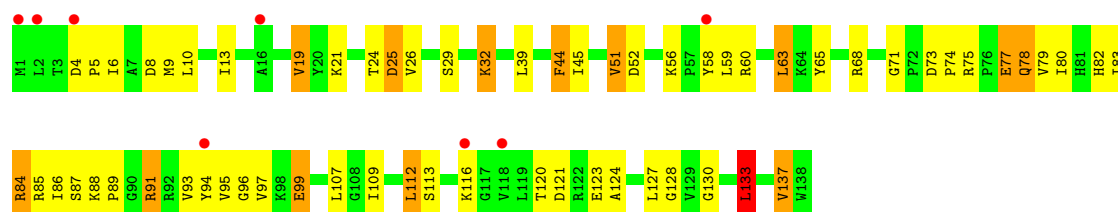
• Molecule 37: 30S ribosomal protein S7



• Molecule 37: 30S ribosomal protein S7

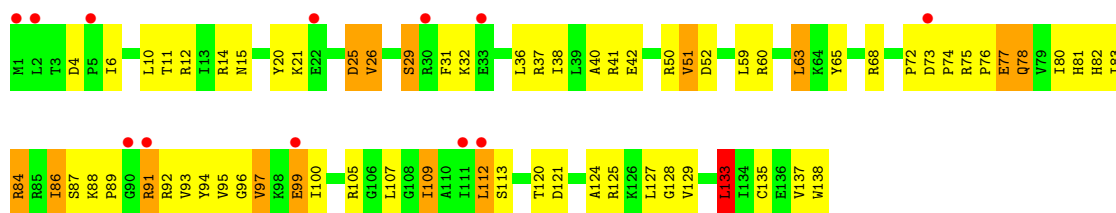


• Molecule 38: 30S ribosomal protein S8

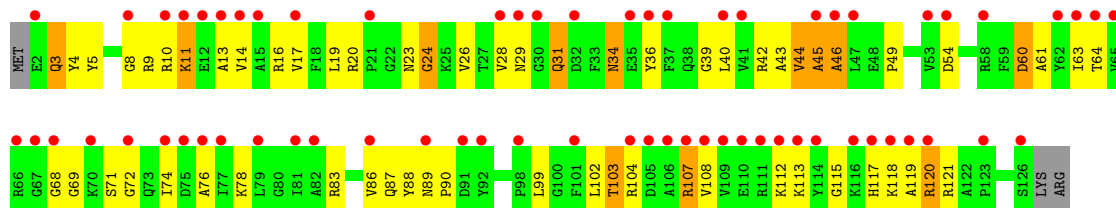


• Molecule 38: 30S ribosomal protein S8

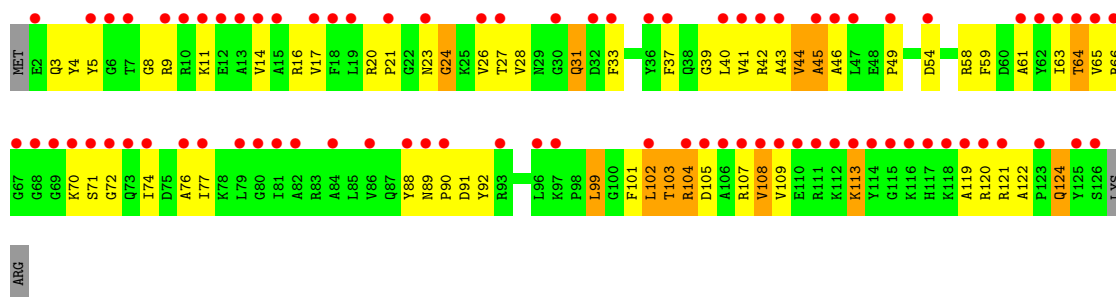




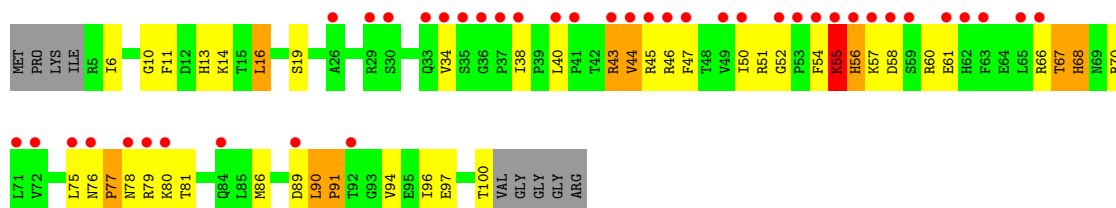
• Molecule 39: 30S ribosomal protein S9



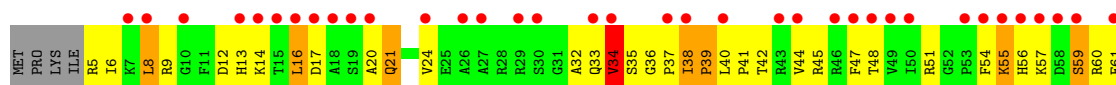
• Molecule 39: 30S ribosomal protein S9



• Molecule 40: 30S ribosomal protein S10

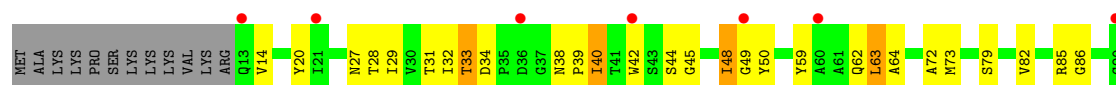


• Molecule 40: 30S ribosomal protein S10

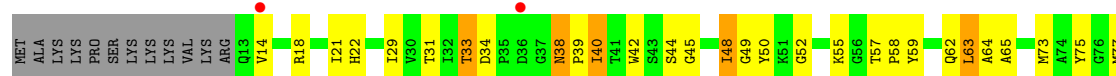




- Molecule 41: 30S ribosomal protein S11



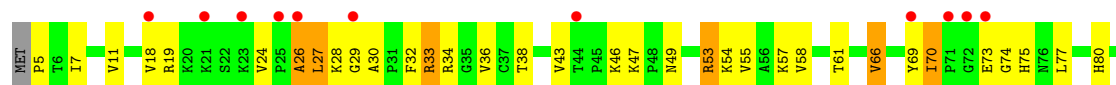
- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12

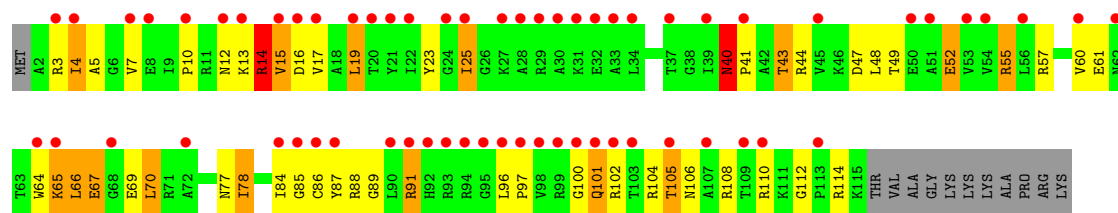


- Molecule 42: 30S ribosomal protein S12

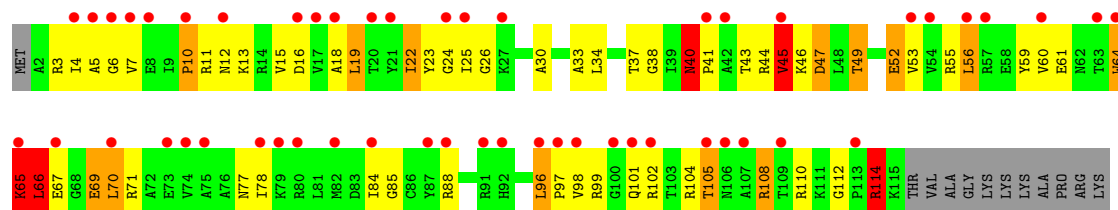
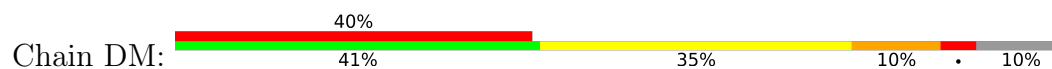


- Molecule 43: 30S ribosomal protein S13

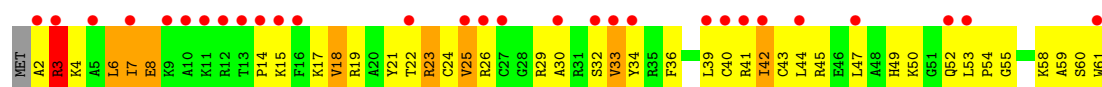




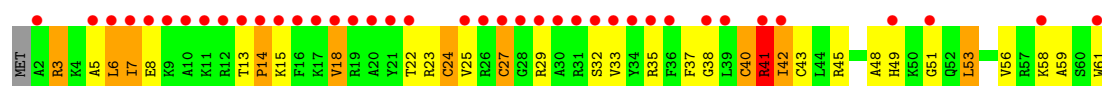
• Molecule 43: 30S ribosomal protein S13



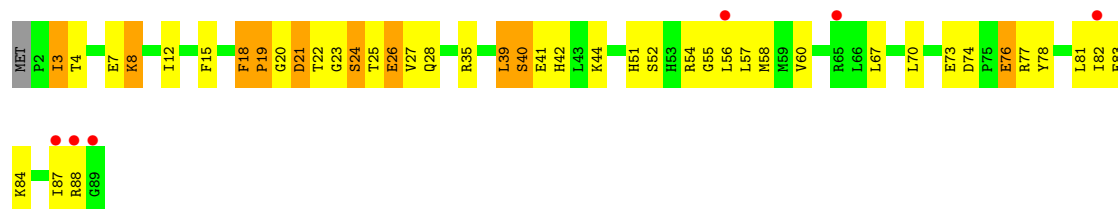
• Molecule 44: 30S ribosomal protein S14



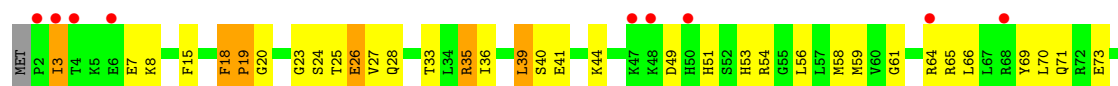
• Molecule 44: 30S ribosomal protein S14



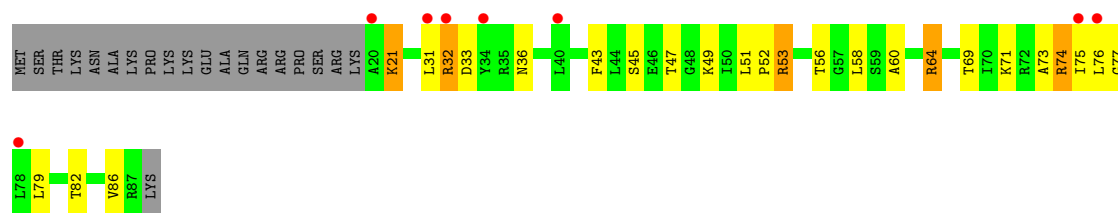
• Molecule 45: 30S ribosomal protein S15



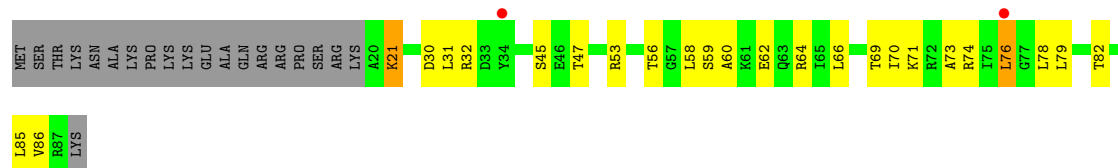
• Molecule 45: 30S ribosomal protein S15



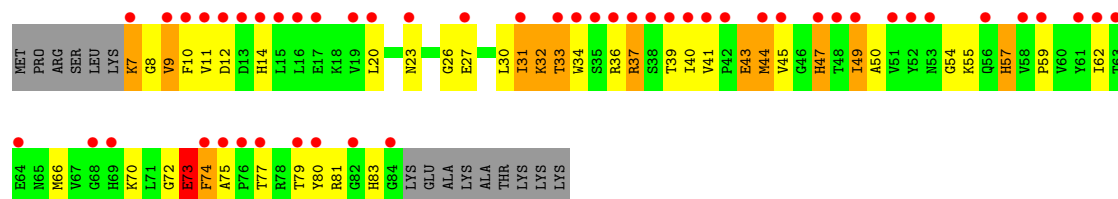




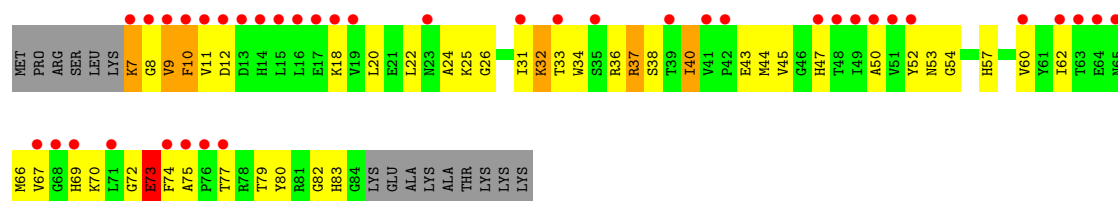
• Molecule 48: 30S ribosomal protein S18



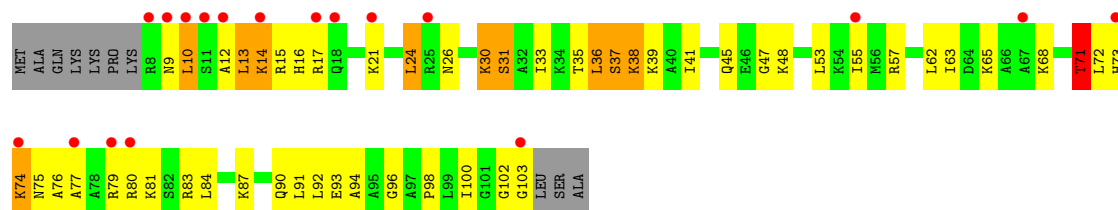
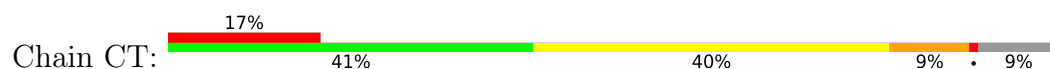
• Molecule 49: 30S ribosomal protein S19



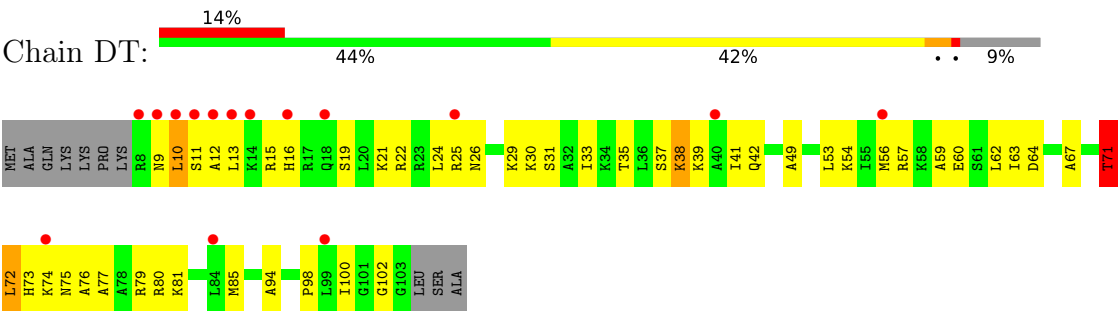
• Molecule 49: 30S ribosomal protein S19



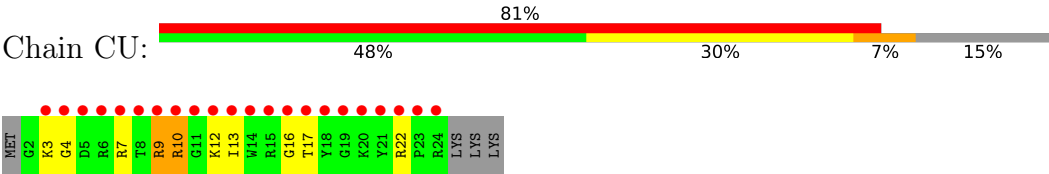
• Molecule 50: 30S ribosomal protein S20



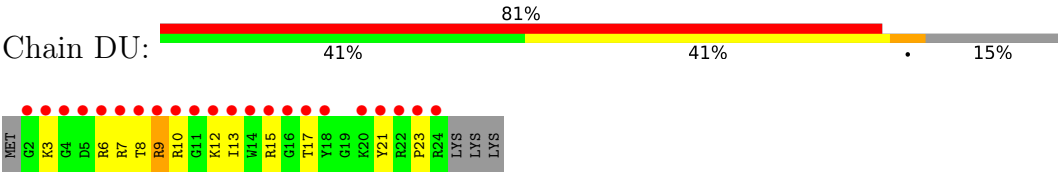
• Molecule 50: 30S ribosomal protein S20



● 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 49.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.8 (49.29-3.20)	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 0.226 , 0.269	Depositor DCC
R_{free} test set	63301 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.47	0/68203	0.51	1/106459 (0.0%)
1	BA	0.67	1/68203 (0.0%)	0.54	7/106459 (0.0%)
2	AB	0.49	0/2879	0.47	0/4492
2	BB	0.51	0/2879	0.51	0/4492
3	AD	0.69	0/2186	1.11	12/2944 (0.4%)
3	BD	0.86	0/2186	1.18	13/2944 (0.4%)
4	AE	0.69	0/1588	1.14	9/2145 (0.4%)
4	BE	0.93	0/1588	1.22	12/2145 (0.6%)
5	AF	0.63	0/1609	1.09	10/2177 (0.5%)
5	BF	0.91	1/1609 (0.1%)	1.15	13/2177 (0.6%)
6	AG	0.73	0/1393	1.09	5/1892 (0.3%)
6	BG	0.58	0/1393	1.03	7/1892 (0.4%)
7	AH	0.76	0/1343	1.11	11/1820 (0.6%)
7	BH	0.79	0/1343	1.05	3/1820 (0.2%)
8	AI	0.77	0/1061	1.21	12/1451 (0.8%)
8	BI	0.64	0/1061	1.17	8/1451 (0.6%)
9	AN	0.65	2/1139 (0.2%)	1.07	4/1538 (0.3%)
9	BN	1.00	0/1139	1.18	7/1538 (0.5%)
10	AO	0.63	0/933	1.15	5/1257 (0.4%)
10	BO	0.87	0/933	1.13	6/1257 (0.5%)
11	AP	0.60	0/1135	1.13	8/1510 (0.5%)
11	BP	0.85	1/1135 (0.1%)	1.18	11/1510 (0.7%)
12	AQ	0.65	0/1143	1.08	4/1527 (0.3%)
12	BQ	0.81	0/1143	1.13	9/1527 (0.6%)
13	AR	0.65	0/982	1.03	3/1312 (0.2%)
13	BR	0.97	0/982	1.06	2/1312 (0.2%)
14	AS	0.72	0/875	1.13	5/1168 (0.4%)
14	BS	0.72	0/875	1.10	6/1168 (0.5%)
15	AT	0.60	0/1077	1.06	7/1444 (0.5%)
15	BT	0.83	0/1077	1.06	0/1444
16	AU	0.68	0/977	1.06	2/1301 (0.2%)
16	BU	1.12	1/977 (0.1%)	1.16	6/1301 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AV	0.70	0/782	1.07	2/1049 (0.2%)
17	BV	0.91	0/782	1.07	4/1049 (0.4%)
18	AW	0.73	0/891	1.10	2/1197 (0.2%)
18	BW	1.09	0/891	1.14	5/1197 (0.4%)
19	AX	0.68	0/756	1.09	2/1016 (0.2%)
19	BX	0.88	0/756	1.04	2/1016 (0.2%)
20	AY	0.59	0/798	1.13	2/1073 (0.2%)
20	BY	0.80	0/798	1.20	6/1073 (0.6%)
21	AZ	0.67	0/1555	1.11	9/2118 (0.4%)
21	BZ	0.66	0/1555	1.09	7/2118 (0.3%)
22	A0	0.59	0/602	1.12	4/804 (0.5%)
22	B0	0.87	1/602 (0.2%)	1.02	1/804 (0.1%)
23	A1	0.60	0/752	0.99	0/1003
23	B1	0.81	0/752	1.04	2/1003 (0.2%)
24	A2	0.63	0/590	1.03	1/781 (0.1%)
24	B2	0.81	0/590	1.08	1/781 (0.1%)
25	A3	0.56	0/463	1.15	2/623 (0.3%)
25	B3	0.87	0/463	1.08	1/623 (0.2%)
26	A4	0.91	0/358	1.18	5/487 (1.0%)
26	B4	0.77	0/358	1.36	8/487 (1.6%)
27	A5	0.76	0/469	1.27	4/634 (0.6%)
27	B5	1.05	0/469	1.22	2/634 (0.3%)
28	A6	0.67	0/456	0.98	0/609
28	B6	0.78	0/456	0.99	2/609 (0.3%)
29	A7	0.78	0/426	1.08	0/561
29	B7	1.02	0/426	1.21	2/561 (0.4%)
30	A8	0.61	0/516	1.05	2/679 (0.3%)
30	B8	0.98	0/516	1.11	3/679 (0.4%)
31	CA	0.44	1/36054 (0.0%)	0.48	1/56272 (0.0%)
31	DA	0.43	1/36054 (0.0%)	0.47	2/56272 (0.0%)
32	CB	0.64	0/1811	1.12	9/2452 (0.4%)
32	DB	0.69	0/1811	1.18	14/2452 (0.6%)
33	CC	0.74	0/1474	1.04	6/2003 (0.3%)
33	DC	0.78	0/1474	1.05	6/2003 (0.3%)
34	CD	0.68	1/1550 (0.1%)	1.17	12/2106 (0.6%)
34	DD	0.77	4/1550 (0.3%)	1.23	17/2106 (0.8%)
35	CE	0.62	0/1121	1.07	1/1517 (0.1%)
35	DE	0.64	0/1121	1.09	3/1517 (0.2%)
36	CF	0.58	0/794	0.97	2/1082 (0.2%)
36	DF	0.58	0/794	0.96	1/1082 (0.1%)
37	CG	0.74	0/1186	1.07	6/1603 (0.4%)
37	DG	0.73	0/1186	1.07	4/1603 (0.2%)
38	CH	0.53	0/1065	1.06	5/1445 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DH	0.55	0/1065	1.03	2/1445 (0.1%)
39	CI	0.85	0/867	1.15	2/1180 (0.2%)
39	DI	0.82	0/867	1.10	4/1180 (0.3%)
40	CJ	0.88	1/672 (0.1%)	1.22	9/919 (1.0%)
40	DJ	0.86	0/672	1.16	5/919 (0.5%)
41	CK	0.57	0/843	1.08	1/1144 (0.1%)
41	DK	0.58	0/843	1.09	8/1144 (0.7%)
42	CL	0.58	0/925	0.99	1/1251 (0.1%)
42	DL	0.62	0/925	1.08	4/1251 (0.3%)
43	CM	0.95	0/811	1.19	9/1103 (0.8%)
43	DM	0.89	0/811	1.17	7/1103 (0.6%)
44	CN	0.72	0/487	1.03	1/649 (0.2%)
44	DN	0.72	0/487	1.12	3/649 (0.5%)
45	CO	0.58	0/735	0.98	2/981 (0.2%)
45	DO	0.54	0/735	0.96	2/981 (0.2%)
46	CP	0.62	0/667	1.00	2/905 (0.2%)
46	DP	0.52	0/667	0.99	2/905 (0.2%)
47	CQ	0.54	0/836	1.02	3/1117 (0.3%)
47	DQ	0.54	0/836	0.98	2/1117 (0.2%)
48	CR	0.55	0/519	0.99	0/699
48	DR	0.61	0/519	1.00	0/699
49	CS	0.97	1/558 (0.2%)	1.30	5/759 (0.7%)
49	DS	0.98	2/558 (0.4%)	1.28	6/759 (0.8%)
50	CT	0.55	0/710	1.19	2/940 (0.2%)
50	DT	0.55	0/710	1.05	2/940 (0.2%)
51	CU	0.78	0/203	1.02	0/266
51	DU	0.75	0/203	1.12	1/266 (0.4%)
All	All	0.60	18/303650 (0.0%)	0.72	463/454928 (0.1%)

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 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	DD	12	CYS	CB-SG	10.58	2.16	1.81
34	DD	26	CYS	CB-SG	8.44	2.09	1.81
49	DS	7	LYS	CB-CG	7.21	1.74	1.52
34	DD	26	CYS	CA-C	6.78	1.61	1.52
34	DD	12	CYS	CA-CB	6.12	1.62	1.53

The worst 5 of 463 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DD	12	CYS	N-CA-C	-16.29	91.56	111.11
49	DS	8	GLY	N-CA-C	14.76	140.87	115.62
34	CD	12	CYS	N-CA-C	-12.93	97.19	111.28
49	CS	8	GLY	N-CA-C	12.66	143.18	113.18
1	BA	1915	U	C4'-C3'-C2'	-11.10	91.50	102.60

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	1412	0
1	BA	60900	0	30712	1079	0
2	AB	2574	0	1306	86	0
2	BB	2574	0	1306	36	0
3	AD	2136	0	2218	79	0
3	BD	2136	0	2218	84	0
4	AE	1555	0	1607	82	0
4	BE	1555	0	1607	56	0
5	AF	1576	0	1616	61	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	62	0
6	AG	1368	0	1324	76	0
6	BG	1368	0	1324	66	0
7	AH	1317	0	1376	69	0
7	BH	1317	0	1376	36	0
8	AI	1046	0	1067	57	2
8	BI	1046	0	1067	49	0
9	AN	1112	0	1180	64	0
9	BN	1112	0	1180	38	0
10	AO	923	0	981	30	0
10	BO	923	0	981	24	0
11	AP	1119	0	1186	40	0
11	BP	1119	0	1186	41	0
12	AQ	1122	0	1179	47	0
12	BQ	1122	0	1179	49	0
13	AR	968	0	1033	47	0
13	BR	968	0	1033	36	0
14	AS	865	0	905	61	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	51	0
15	BT	1063	0	1103	38	0
16	AU	959	0	1019	33	0
16	BU	959	0	1019	21	0
17	AV	771	0	830	23	0
17	BV	771	0	830	15	0
18	AW	881	0	935	26	0
18	BW	881	0	935	25	0
19	AX	742	0	799	22	0
19	BX	742	0	799	24	0
20	AY	785	0	832	36	0
20	BY	785	0	832	28	0
21	AZ	1522	0	1511	57	0
21	BZ	1522	0	1511	50	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	27	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	24	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	17	0
27	A5	455	0	476	24	0
27	B5	455	0	476	18	0
28	A6	449	0	464	20	0
28	B6	449	0	466	17	0
29	A7	418	0	467	19	0
29	B7	418	0	467	16	0
30	A8	509	0	565	27	0
30	B8	509	0	565	19	0
31	CA	32208	0	16256	920	2
31	DA	32208	0	16254	926	0
32	CB	1777	0	1747	103	0
32	DB	1777	0	1747	98	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	59	0
34	CD	1520	0	1407	75	0
34	DD	1520	0	1406	88	0
35	CE	1105	0	1130	51	0
35	DE	1105	0	1130	55	0
36	CF	781	0	741	25	0
36	DF	781	0	741	30	0
37	CG	1167	0	1108	40	0
37	DG	1167	0	1108	48	0
38	CH	1045	0	1033	46	0
38	DH	1045	0	1033	55	0
39	CI	852	0	742	43	0
39	DI	852	0	742	53	0
40	CJ	659	0	552	30	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	26	0
41	DK	828	0	822	34	0
42	CL	909	0	927	43	0
42	DL	909	0	927	40	0
43	CM	801	0	743	34	0
43	DM	801	0	743	39	0
44	CN	478	0	498	33	0
44	DN	478	0	497	31	0
45	CO	724	0	749	32	0
45	DO	724	0	749	29	0
46	CP	651	0	638	36	0
46	DP	651	0	638	31	0
47	CQ	823	0	891	34	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	20	0
48	CR	514	0	530	20	0
48	DR	514	0	530	19	0
49	CS	544	0	457	21	0
49	DS	544	0	457	27	0
50	CT	708	0	764	37	0
50	DT	708	0	764	30	0
51	CU	199	0	208	9	0
51	DU	199	0	208	7	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	7318	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 7318 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%)	5	29
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	8	37
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	3	20
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	3	20
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	4	27
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	3	20
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	1	11
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	5
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	2	14
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	3	20
8	AI	143/148 (97%)	103 (72%)	28 (20%)	12 (8%)	0	4
8	BI	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	1	6
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	1	8
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	2	16
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	21
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	3	21
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	1	11
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	3	20
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	3	24
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	3	24
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	2	16
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14	47
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	4	25
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	4	25
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	3	22

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%)	16	50
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%)	6	31
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	45
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	14	47
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	5	29
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	5	29
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	2	14
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	2	18
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	1	11
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	2	19
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	9	39
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	9	39
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	5	31
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	3	21
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	8	37
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%)	6	34
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	0	3
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	0	3
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	6	34
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	20
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	6	31
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	5	29
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	5	29
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	7	36
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%)	0	3
32	DB	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	1	7
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	1	12
33	DC	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	0	3
34	CD	206/209 (99%)	154 (75%)	40 (19%)	12 (6%)	1	10
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	3	20
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	1	5
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	3	20
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	3	22
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	2	17
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	8
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	2	18
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	8	37
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	2	18
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	4
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	1	8
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	0	3
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	8
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	2	19
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	4	25
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	2	16
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	2	16
43	CM	112/126 (89%)	84 (75%)	18 (16%)	10 (9%)	0	3
43	DM	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	0	2
44	CN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	0	3
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	12
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	20
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	5	29
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	0	3
46	DP	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	2	18
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	1	12

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%)	3	22
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	8	37
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	7
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	0	3
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	1	6
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0	3
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	2	16

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%)	179 (83%)	36 (17%)	2	11
3	BD	215/218 (99%)	185 (86%)	30 (14%)	3	17
4	AE	163/166 (98%)	134 (82%)	29 (18%)	2	10
4	BE	163/166 (98%)	132 (81%)	31 (19%)	1	9
5	AF	158/162 (98%)	130 (82%)	28 (18%)	2	10
5	BF	158/162 (98%)	131 (83%)	27 (17%)	2	11
6	AG	128/156 (82%)	106 (83%)	22 (17%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BG	128/156 (82%)	109 (85%)	19 (15%)	3	15
7	AH	141/148 (95%)	118 (84%)	23 (16%)	2	12
7	BH	141/148 (95%)	122 (86%)	19 (14%)	4	19
8	AI	102/124 (82%)	75 (74%)	27 (26%)	0	3
8	BI	102/124 (82%)	76 (74%)	26 (26%)	0	3
9	AN	117/119 (98%)	91 (78%)	26 (22%)	1	5
9	BN	117/119 (98%)	90 (77%)	27 (23%)	1	5
10	AO	98/100 (98%)	86 (88%)	12 (12%)	5	22
10	BO	98/100 (98%)	86 (88%)	12 (12%)	5	22
11	AP	113/116 (97%)	91 (80%)	22 (20%)	1	8
11	BP	113/116 (97%)	95 (84%)	18 (16%)	2	13
12	AQ	111/111 (100%)	91 (82%)	20 (18%)	2	9
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	14
13	AR	101/101 (100%)	78 (77%)	23 (23%)	1	5
13	BR	101/101 (100%)	78 (77%)	23 (23%)	1	5
14	AS	84/88 (96%)	64 (76%)	20 (24%)	1	4
14	BS	84/88 (96%)	70 (83%)	14 (17%)	2	11
15	AT	110/127 (87%)	98 (89%)	12 (11%)	6	26
15	BT	110/127 (87%)	97 (88%)	13 (12%)	5	23
16	AU	93/94 (99%)	82 (88%)	11 (12%)	5	23
16	BU	93/94 (99%)	77 (83%)	16 (17%)	2	10
17	AV	80/82 (98%)	65 (81%)	15 (19%)	1	9
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	6
18	AW	89/92 (97%)	73 (82%)	16 (18%)	2	9
18	BW	89/92 (97%)	75 (84%)	14 (16%)	2	13
19	AX	75/78 (96%)	65 (87%)	10 (13%)	4	19
19	BX	75/78 (96%)	65 (87%)	10 (13%)	4	19
20	AY	80/91 (88%)	67 (84%)	13 (16%)	2	12
20	BY	80/91 (88%)	68 (85%)	12 (15%)	3	15
21	AZ	159/179 (89%)	132 (83%)	27 (17%)	2	11
21	BZ	159/179 (89%)	136 (86%)	23 (14%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A0	59/67 (88%)	52 (88%)	7 (12%)	5	23
22	B0	59/67 (88%)	52 (88%)	7 (12%)	5	23
23	A1	78/83 (94%)	66 (85%)	12 (15%)	2	14
23	B1	78/83 (94%)	69 (88%)	9 (12%)	5	24
24	A2	65/67 (97%)	55 (85%)	10 (15%)	2	14
24	B2	65/67 (97%)	58 (89%)	7 (11%)	6	27
25	A3	49/52 (94%)	40 (82%)	9 (18%)	1	9
25	B3	49/52 (94%)	43 (88%)	6 (12%)	5	22
26	A4	39/63 (62%)	29 (74%)	10 (26%)	0	3
26	B4	39/63 (62%)	27 (69%)	12 (31%)	0	1
27	A5	50/52 (96%)	44 (88%)	6 (12%)	5	23
27	B5	50/52 (96%)	44 (88%)	6 (12%)	5	23
28	A6	50/52 (96%)	39 (78%)	11 (22%)	1	6
28	B6	50/52 (96%)	42 (84%)	8 (16%)	2	13
29	A7	41/42 (98%)	34 (83%)	7 (17%)	2	11
29	B7	41/42 (98%)	33 (80%)	8 (20%)	1	8
30	A8	52/55 (94%)	45 (86%)	7 (14%)	4	19
30	B8	52/55 (94%)	47 (90%)	5 (10%)	8	32
32	CB	177/220 (80%)	135 (76%)	42 (24%)	1	4
32	DB	177/220 (80%)	139 (78%)	38 (22%)	1	6
33	CC	114/188 (61%)	90 (79%)	24 (21%)	1	6
33	DC	114/188 (61%)	98 (86%)	16 (14%)	3	17
34	CD	139/181 (77%)	117 (84%)	22 (16%)	2	13
34	DD	139/181 (77%)	117 (84%)	22 (16%)	2	13
35	CE	108/123 (88%)	89 (82%)	19 (18%)	2	10
35	DE	108/123 (88%)	87 (81%)	21 (19%)	1	8
36	CF	77/90 (86%)	63 (82%)	14 (18%)	2	9
36	DF	77/90 (86%)	62 (80%)	15 (20%)	1	8
37	CG	104/127 (82%)	87 (84%)	17 (16%)	2	12
37	DG	104/127 (82%)	90 (86%)	14 (14%)	4	19
38	CH	103/119 (87%)	86 (84%)	17 (16%)	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%)	1	9
39	CI	62/99 (63%)	52 (84%)	10 (16%)	2	13
39	DI	62/99 (63%)	51 (82%)	11 (18%)	2	10
40	CJ	52/92 (56%)	41 (79%)	11 (21%)	1	6
40	DJ	52/92 (56%)	39 (75%)	13 (25%)	0	3
41	CK	81/99 (82%)	70 (86%)	11 (14%)	3	18
41	DK	81/99 (82%)	70 (86%)	11 (14%)	3	18
42	CL	92/109 (84%)	78 (85%)	14 (15%)	3	14
42	DL	92/109 (84%)	80 (87%)	12 (13%)	4	20
43	CM	63/101 (62%)	47 (75%)	16 (25%)	0	3
43	DM	63/101 (62%)	46 (73%)	17 (27%)	0	2
44	CN	46/50 (92%)	34 (74%)	12 (26%)	0	3
44	DN	46/50 (92%)	31 (67%)	15 (33%)	0	1
45	CO	77/80 (96%)	65 (84%)	12 (16%)	2	13
45	DO	77/80 (96%)	66 (86%)	11 (14%)	3	16
46	CP	63/74 (85%)	48 (76%)	15 (24%)	1	4
46	DP	63/74 (85%)	50 (79%)	13 (21%)	1	7
47	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	43
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	6	27
48	CR	49/77 (64%)	42 (86%)	7 (14%)	3	16
48	DR	49/77 (64%)	45 (92%)	4 (8%)	10	39
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	33 (79%)	9 (21%)	1	6
50	CT	65/82 (79%)	53 (82%)	12 (18%)	1	9
50	DT	65/82 (79%)	56 (86%)	9 (14%)	3	18
51	CU	18/22 (82%)	16 (89%)	2 (11%)	6	25
51	DU	18/22 (82%)	15 (83%)	3 (17%)	2	11
All	All	8652/9990 (87%)	7161 (83%)	1491 (17%)	2	10

5 of 1491 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	CB	133	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	CO	83	GLU
33	CC	32	LEU
32	CB	126	GLU
37	CG	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
36	CF	57	GLN
32	DB	94	ASN
49	DS	83	HIS
37	CG	109	ASN
43	CM	106	ASN

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%)	590 (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%)	1897 (21%)	177 (1%)

5 of 1897 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	2689	U
31	CA	1165	C
31	CA	60	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	428	G
31	DA	60	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 oligosaccharides 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	BA	3001	53	48,48,48	1.00	2 (4%)	63,71,71	1.28	9 (14%)
52	T8B	AA	3001	53	48,48,48	1.01	2 (4%)	63,71,71	1.28	9 (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	BA	3001	53	-	0/26/26/26	0/5/5/5
52	T8B	AA	3001	53	-	0/26/26/26	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	O11-C26	3.13	1.38	1.31
52	BA	3001	T8B	O11-C26	3.12	1.38	1.31
52	BA	3001	T8B	C25-C24	2.27	1.50	1.43
52	AA	3001	T8B	C25-C24	2.25	1.50	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C21-C23-C24	-4.27	120.19	125.09
52	AA	3001	T8B	C21-C23-C24	-4.25	120.21	125.09
52	BA	3001	T8B	O5-C14-O6	3.22	120.29	116.45
52	AA	3001	T8B	O5-C14-O6	3.22	120.29	116.45
52	BA	3001	T8B	O11-C26-C25	2.94	124.96	121.09

There are no chirality outliers.

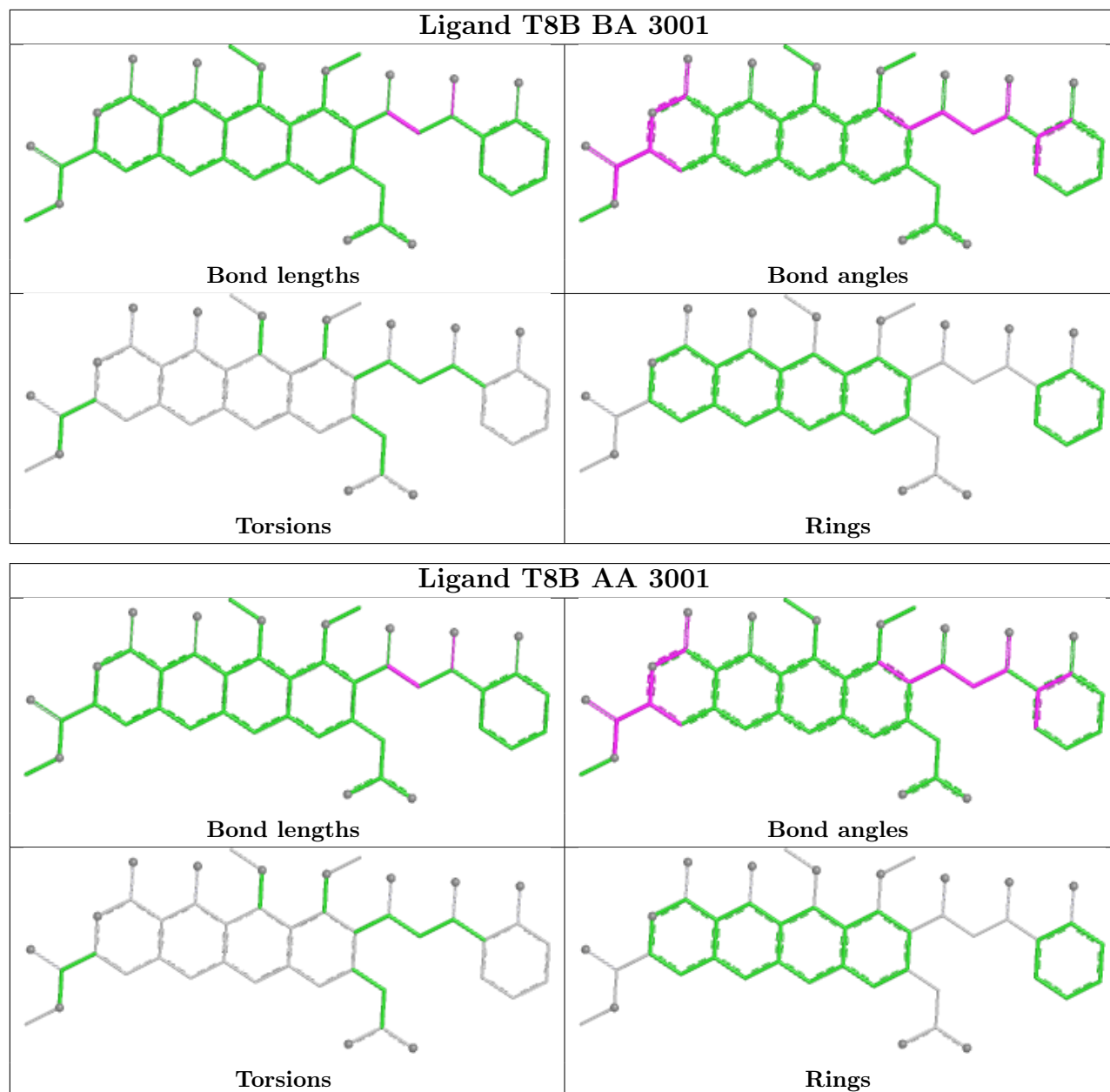
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 54 short contacts:

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

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



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%)	0.09	120 (4%)	40	25	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	-0.00	104 (3%)	45	28	27, 56, 110, 126	0
2	AB	120/122 (98%)	0.86	13 (10%)	11	7	68, 95, 108, 111	0
2	BB	120/122 (98%)	0.21	3 (2%)	58	39	46, 80, 95, 103	0
3	AD	275/276 (99%)	0.34	10 (3%)	46	28	45, 67, 82, 103	0
3	BD	275/276 (99%)	0.35	7 (2%)	58	39	36, 59, 78, 103	0
4	AE	204/206 (99%)	0.22	5 (2%)	58	39	47, 72, 87, 98	0
4	BE	204/206 (99%)	0.36	7 (3%)	48	30	33, 60, 81, 96	0
5	AF	203/205 (99%)	0.27	3 (1%)	72	52	44, 77, 95, 112	0
5	BF	203/205 (99%)	0.33	4 (1%)	65	45	26, 64, 90, 110	0
6	AG	181/182 (99%)	1.65	57 (31%)	1	1	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.85	24 (13%)	7	6	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.99	18 (10%)	12	8	80, 93, 101, 108	0
7	BH	174/180 (96%)	0.79	15 (8%)	16	11	63, 78, 91, 98	0
8	AI	145/148 (97%)	1.46	36 (24%)	2	2	72, 104, 116, 123	0
8	BI	145/148 (97%)	0.44	4 (2%)	55	35	68, 90, 98, 100	0
9	AN	140/140 (100%)	0.34	5 (3%)	46	28	58, 73, 90, 94	0
9	BN	140/140 (100%)	0.47	6 (4%)	40	24	38, 57, 82, 85	0
10	AO	122/122 (100%)	0.29	3 (2%)	58	39	56, 73, 85, 91	0
10	BO	122/122 (100%)	0.41	5 (4%)	41	25	43, 63, 82, 89	0
11	AP	147/150 (98%)	0.65	11 (7%)	20	13	47, 81, 96, 105	0
11	BP	147/150 (98%)	0.61	11 (7%)	20	13	28, 68, 91, 100	0
12	AQ	141/141 (100%)	0.53	8 (5%)	29	19	60, 78, 91, 97	0
12	BQ	141/141 (100%)	0.34	4 (2%)	55	35	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%)	0.37	3 (2%) 58 39	47, 66, 78, 88	0
13	BR	118/118 (100%)	0.31	3 (2%) 58 39	35, 53, 69, 86	0
14	AS	110/112 (98%)	1.33	22 (20%) 3 2	74, 91, 102, 109	0
14	BS	110/112 (98%)	0.68	7 (6%) 25 16	58, 79, 93, 100	0
15	AT	131/146 (89%)	0.37	3 (2%) 61 41	66, 76, 99, 109	0
15	BT	131/146 (89%)	0.53	8 (6%) 27 17	55, 68, 91, 102	0
16	AU	116/118 (98%)	0.26	2 (1%) 69 49	53, 70, 84, 89	0
16	BU	116/118 (98%)	0.19	1 (0%) 81 64	34, 50, 70, 84	0
17	AV	101/101 (100%)	0.24	2 (1%) 65 45	48, 79, 93, 103	0
17	BV	101/101 (100%)	0.19	1 (0%) 79 63	31, 61, 81, 95	0
18	AW	112/113 (99%)	0.15	2 (1%) 67 48	50, 59, 80, 104	0
18	BW	112/113 (99%)	0.21	1 (0%) 81 64	36, 45, 75, 106	0
19	AX	95/96 (98%)	0.67	7 (7%) 20 13	54, 71, 89, 93	0
19	BX	95/96 (98%)	0.47	3 (3%) 50 31	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.78	10 (9%) 14 9	71, 81, 94, 105	0
20	BY	107/110 (97%)	0.75	8 (7%) 20 13	56, 71, 89, 103	0
21	AZ	198/206 (96%)	0.69	9 (4%) 38 24	80, 92, 103, 108	0
21	BZ	198/206 (96%)	0.49	8 (4%) 42 26	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.46	2 (2%) 57 37	59, 74, 84, 89	0
22	B0	76/85 (89%)	0.34	1 (1%) 75 55	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.69	6 (6%) 26 17	54, 71, 94, 99	0
23	B1	97/98 (98%)	0.45	3 (3%) 51 32	42, 65, 91, 95	0
24	A2	70/72 (97%)	0.63	5 (7%) 22 14	65, 81, 92, 101	0
24	B2	70/72 (97%)	0.62	6 (8%) 16 11	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.76	6 (10%) 12 8	63, 74, 92, 101	0
25	B3	59/60 (98%)	0.50	2 (3%) 48 30	43, 56, 84, 94	0
26	A4	46/71 (64%)	1.17	7 (15%) 5 4	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.93	5 (10%) 10 7	98, 107, 113, 118	0
27	A5	59/60 (98%)	0.25	2 (3%) 48 30	46, 64, 78, 91	0
27	B5	59/60 (98%)	0.33	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.52	5 (9%) 14 9	62, 76, 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%)	0.37	1 (1%) 66 46	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.41	5 (10%) 11 8	43, 54, 79, 99	0
29	B7	48/49 (97%)	0.31	2 (4%) 40 25	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.81	6 (9%) 14 9	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.58	3 (4%) 36 23	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.85	188 (12%) 8 6	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.80	147 (9%) 13 9	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.82	18 (7%) 18 12	93, 103, 111, 117	0
32	DB	229/256 (89%)	1.10	32 (13%) 6 5	95, 105, 112, 115	0
33	CC	206/239 (86%)	1.29	41 (19%) 3 2	92, 106, 112, 115	0
33	DC	206/239 (86%)	1.35	48 (23%) 2 2	97, 108, 115, 120	0
34	CD	208/209 (99%)	1.39	44 (21%) 2 2	85, 98, 108, 114	0
34	DD	208/209 (99%)	1.29	46 (22%) 2 2	87, 97, 107, 123	0
35	CE	148/162 (91%)	0.51	5 (3%) 48 30	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.77	15 (10%) 12 8	84, 96, 104, 110	0
36	CF	100/101 (99%)	0.60	5 (5%) 34 22	80, 92, 101, 107	0
36	DF	100/101 (99%)	0.73	9 (9%) 15 10	84, 93, 103, 110	0
37	CG	155/156 (99%)	2.07	71 (45%) 0 1	99, 109, 115, 120	0
37	DG	155/156 (99%)	1.72	53 (34%) 1 1	97, 109, 115, 119	0
38	CH	138/138 (100%)	0.68	8 (5%) 29 18	82, 94, 101, 104	0
38	DH	138/138 (100%)	0.90	12 (8%) 16 11	86, 96, 102, 106	0
39	CI	125/128 (97%)	2.24	65 (52%) 0 1	97, 111, 117, 120	0
39	DI	125/128 (97%)	2.73	82 (65%) 0 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	2.03	41 (42%) 0 1	100, 109, 115, 117	0
40	DJ	96/105 (91%)	2.18	50 (52%) 0 1	97, 110, 115, 119	0
41	CK	114/129 (88%)	0.79	9 (7%) 18 12	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.63	8 (7%) 22 14	75, 95, 103, 107	0
42	CL	122/132 (92%)	0.94	13 (10%) 11 7	72, 85, 96, 100	0
42	DL	122/132 (92%)	0.95	15 (12%) 8 6	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.35	62 (54%) 0 0	102, 111, 118, 126	0
43	DM	114/126 (90%)	2.03	51 (44%) 0 1	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%)	2.22	29 (48%) 0 1	99, 108, 116, 118	0
44	DN	60/61 (98%)	2.80	39 (65%) 0 0	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.62	6 (6%) 23 15	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.80	9 (10%) 12 8	81, 93, 103, 107	0
46	CP	82/88 (93%)	1.20	14 (17%) 4 3	88, 96, 106, 112	0
46	DP	82/88 (93%)	1.41	21 (25%) 1 2	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.72	7 (7%) 22 14	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.81	7 (7%) 22 14	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.79	8 (11%) 9 6	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.56	2 (2%) 53 35	85, 93, 104, 106	0
49	CS	78/93 (83%)	2.53	50 (64%) 0 0	107, 111, 117, 123	0
49	DS	78/93 (83%)	2.07	39 (50%) 0 1	91, 112, 117, 119	0
50	CT	96/106 (90%)	1.05	18 (18%) 3 2	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.99	15 (15%) 5 4	82, 92, 100, 101	0
51	CU	23/27 (85%)	4.94	22 (95%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	3.82	22 (95%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.63	2096 (10%) 12 8	26, 84, 115, 128	0

The worst 5 of 2096 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CA	1286	A	9.7
51	CU	14	TRP	9.2
49	CS	40	ILE	8.8
39	DI	126	SER	8.4
31	CA	1353	G	8.3

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](#)

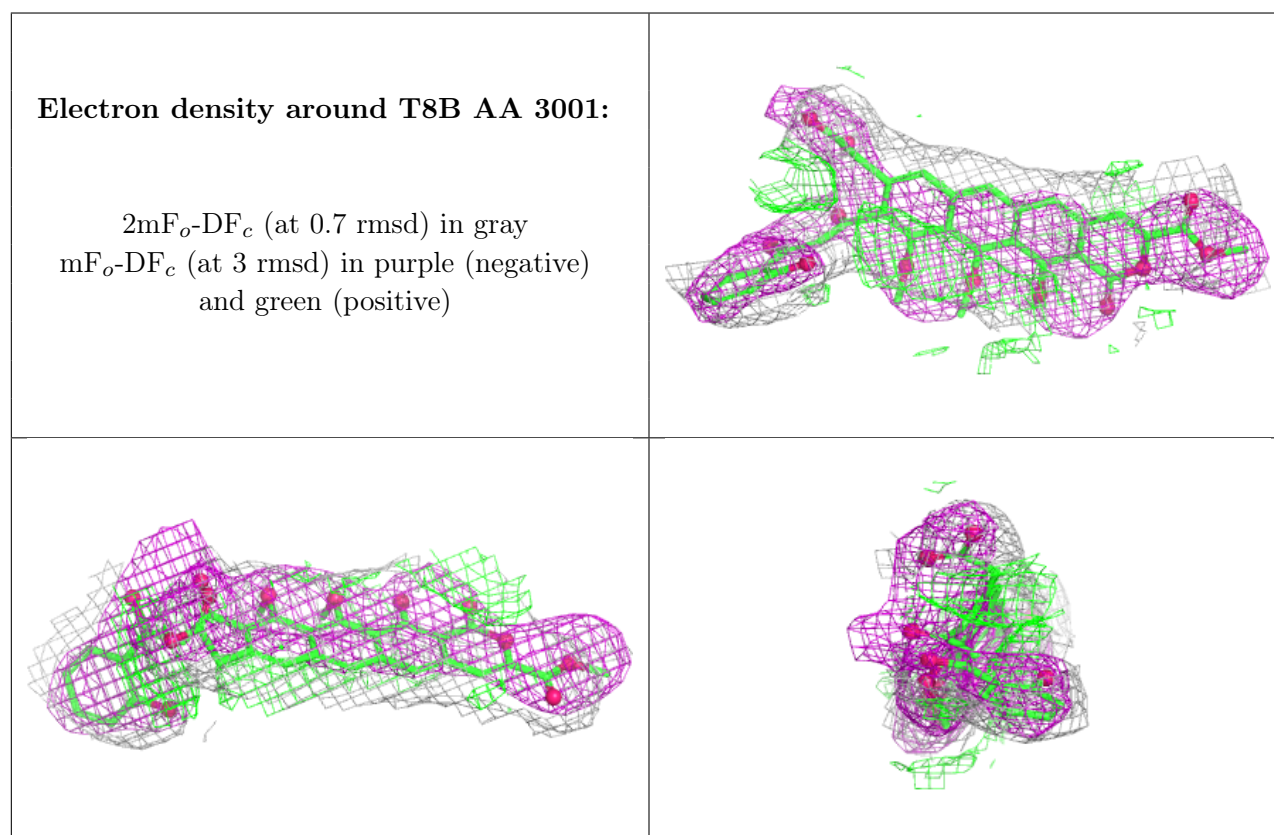
There are no oligosaccharides in this entry.

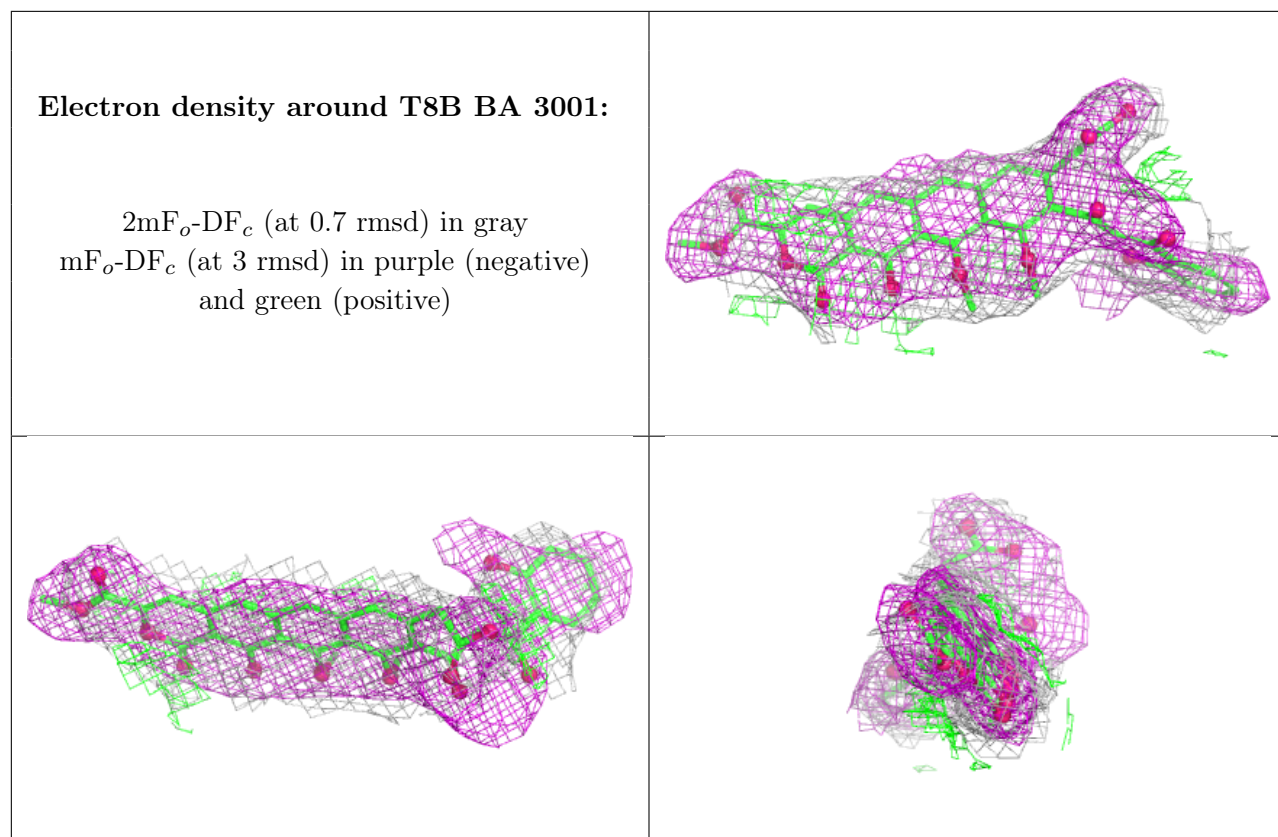
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	T8B	AA	3001	44/44	0.74	0.15	20,20,20,20	0
53	MG	BA	3002	1/1	0.78	0.13	30,30,30,30	0
52	T8B	BA	3001	44/44	0.79	0.13	20,20,20,20	0
53	MG	AA	3002	1/1	0.90	0.16	30,30,30,30	0
53	MG	AA	3003	1/1	0.97	0.15	30,30,30,30	0
53	MG	BA	3003	1/1	0.97	0.20	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.