



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:00 am GMT

PDB ID : 4V6D  
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting  
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.  
Deposited on : 2009-06-27  
Resolution : 3.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

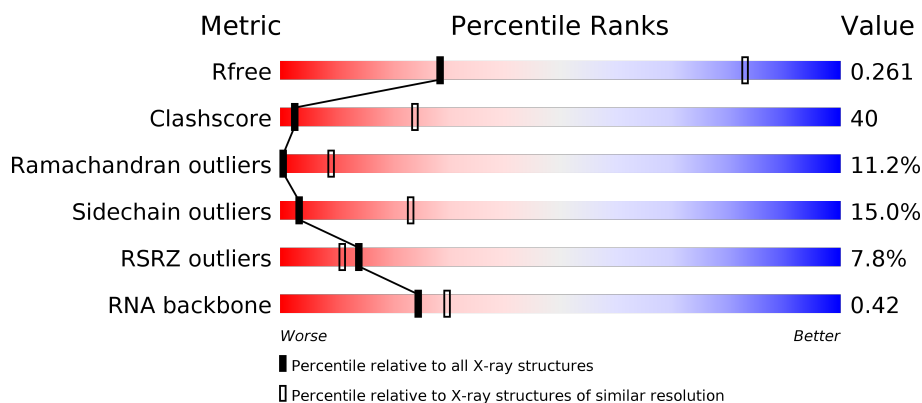
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1010 (4.10-3.54)
Clashscore	112137	1038 (4.08-3.56)
Ramachandran outliers	110173	1062 (4.10-3.54)
Sidechain outliers	110143	1055 (4.10-3.54)
RSRZ outliers	101464	1025 (4.10-3.54)
RNA backbone	2435	1016 (4.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	AB	241	<div> <div>44%</div> <div> <div>17%</div> <div>55%</div> <div>15%</div> <div>•</div> <div>10%</div> </div> </div>
1	CB	241	<div> <div>20%</div> <div> <div>20%</div> <div>56%</div> <div>13%</div> <div>•</div> <div>10%</div> </div> </div>
2	AC	233	<div> <div>2%</div> <div> <div>33%</div> <div>44%</div> <div>10%</div> <div>•</div> <div>12%</div> </div> </div>
2	CC	233	<div> <div>2%</div> <div> <div>32%</div> <div>45%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>

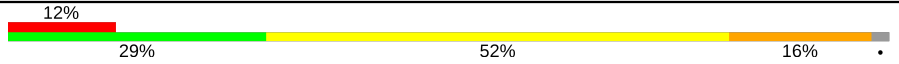
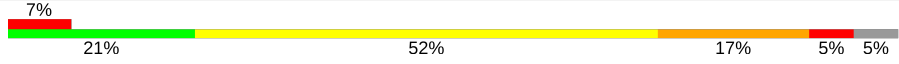
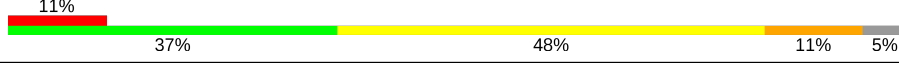
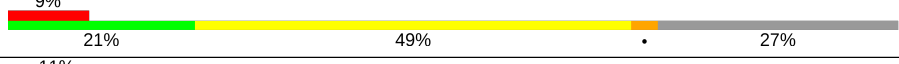
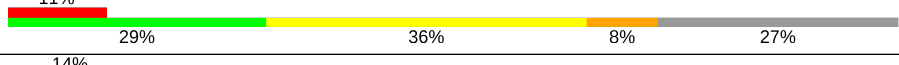
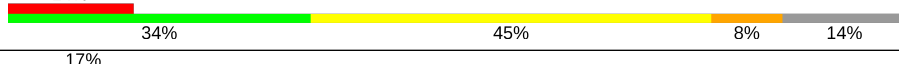
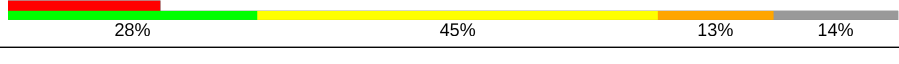


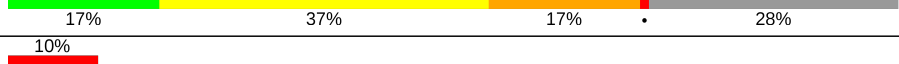

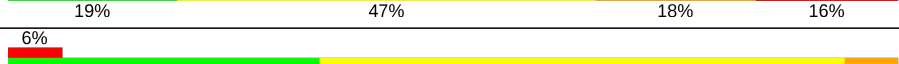
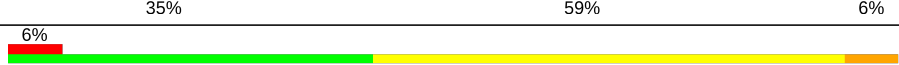
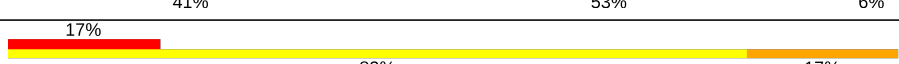
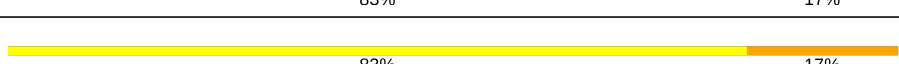
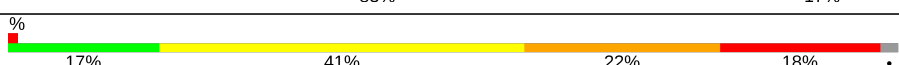
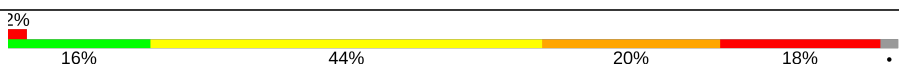
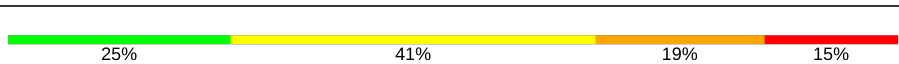
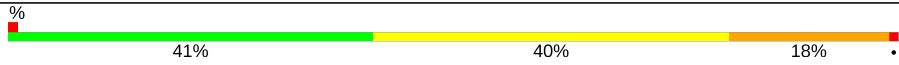


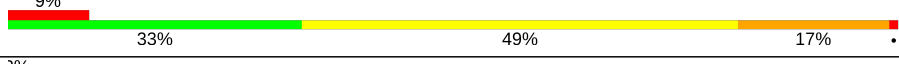

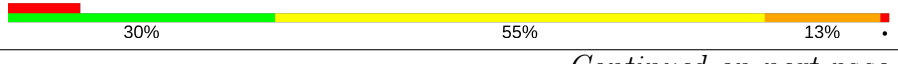

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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	CV	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	
28	BE	201	
28	DE	201	

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Mol	Chain	Length	Quality of chain
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	
40	DQ	118	
41	BR	103	



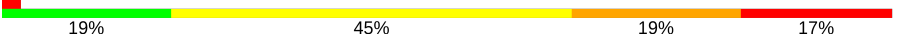
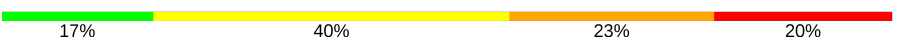
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Mol	Chain	Length	Quality of chain
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	
53	B3	65	
53	D3	65	

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Mol	Chain	Length	Quality of chain
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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
57	MG	AA	1607	-	-	-	X
57	MG	AA	1629	-	-	-	X
57	MG	AA	1631	-	-	-	X
57	MG	AA	1641	-	-	-	X
57	MG	AA	1642	-	-	-	X
57	MG	BA	3002	-	-	-	X
57	MG	BA	3005	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3037	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3071	-	-	-	X
57	MG	BA	3072	-	-	-	X
57	MG	BA	3104	-	-	-	X
57	MG	BA	3105	-	-	-	X
57	MG	BA	3109	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3124	-	-	-	X
57	MG	BA	3132	-	-	-	X
57	MG	BA	3136	-	-	-	X
57	MG	CA	1617	-	-	-	X
57	MG	CA	1625	-	-	-	X
57	MG	CA	1628	-	-	-	X
57	MG	CA	1629	-	-	-	X
57	MG	CA	1637	-	-	-	X
57	MG	CA	1639	-	-	-	X
57	MG	DA	3002	-	-	-	X
57	MG	DA	3041	-	-	-	X
57	MG	DA	3054	-	-	-	X
57	MG	DA	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3071	-	-	-	X
57	MG	DA	3077	-	-	-	X
57	MG	DA	3101	-	-	-	X
57	MG	DA	3109	-	-	-	X
57	MG	DA	3134	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 285420 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
1	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
3	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
7	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
8	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
11	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
13	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
19	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
20	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
22	CV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
23	CW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
26	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
27	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
28	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
30	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
31	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
33	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
35	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
37	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
38	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
39	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
40	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
41	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
42	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
43	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
44	DU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
45	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
46	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
47	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
49	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
50	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 55 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BA	136	Total	Mg	0	0
			136	136		
57	CA	42	Total	Mg	0	0
			42	42		
57	DJ	1	Total	Mg	0	0
			1	1		
57	BD	1	Total	Mg	0	0
			1	1		
57	AA	43	Total	Mg	0	0
			43	43		
57	DA	134	Total	Mg	0	0
			134	134		
57	DC	1	Total	Mg	0	0
			1	1		
57	DB	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	B4	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	5	Total O 5 5	0	0
59	AT	3	Total O 3 3	0	0
59	AU	1	Total O 1 1	0	0
59	AA	195	Total O 195 195	0	0
59	BA	615	Total O 615 615	0	0
59	BB	19	Total O 19 19	0	0
59	BC	7	Total O 7 7	0	0
59	BD	2	Total O 2 2	0	0
59	BE	1	Total O 1 1	0	0
59	BL	4	Total O 4 4	0	0
59	BN	2	Total O 2 2	0	0
59	BQ	1	Total O 1 1	0	0
59	BT	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	B2	2	Total O 2 2	0	0
59	B3	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	2	Total 2	O 2	0	0
59	CE	3	Total 3	O 3	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	196	Total 196	O 196	0	0
59	DC	14	Total 14	O 14	0	0
59	DD	4	Total 4	O 4	0	0
59	DE	2	Total 2	O 2	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	5	Total 5	O 5	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0
59	DA	598	Total 598	O 598	0	0

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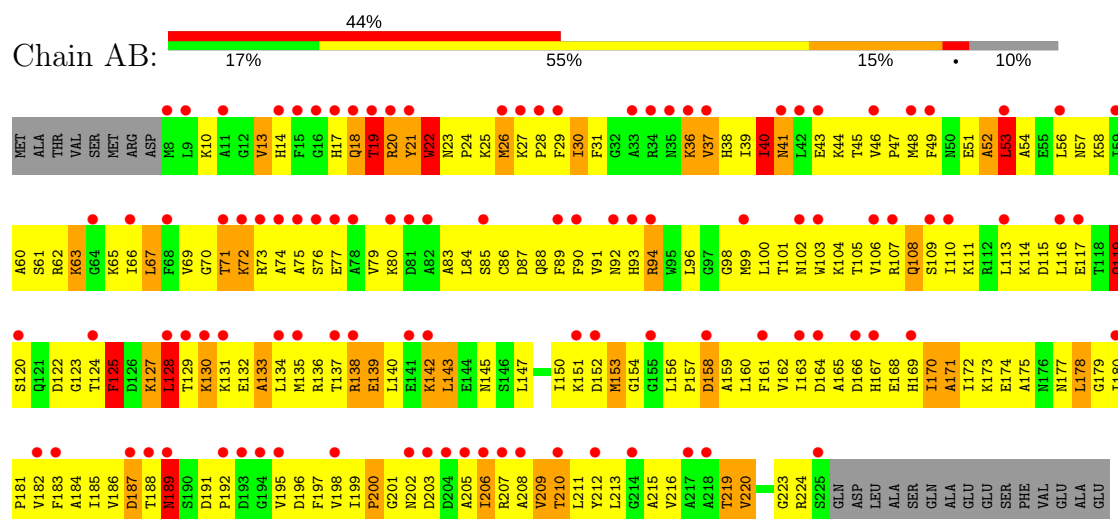
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	4	Total	O	0	0
			4	4		

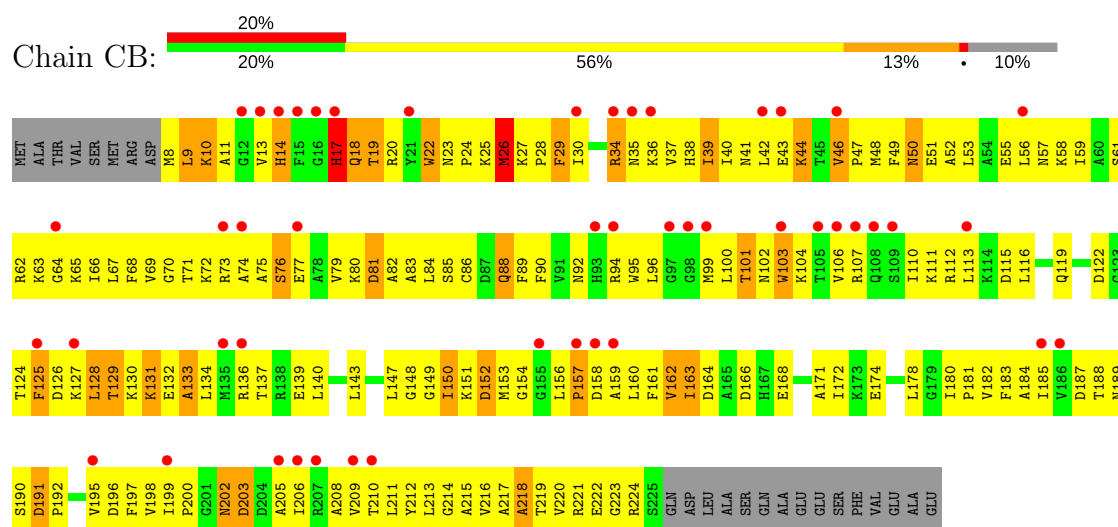
### 3 Residue-property plots

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

#### • Molecule 1: 30S ribosomal protein S2

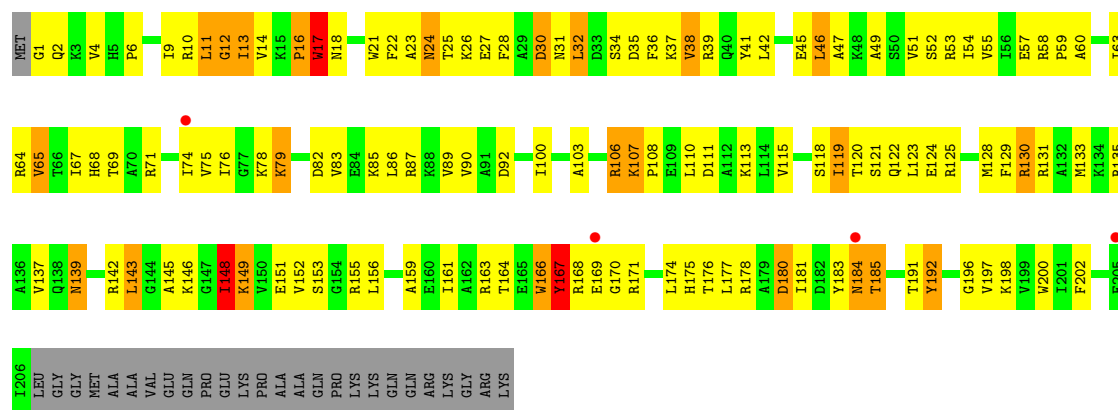


#### • Molecule 1: 30S ribosomal protein S2

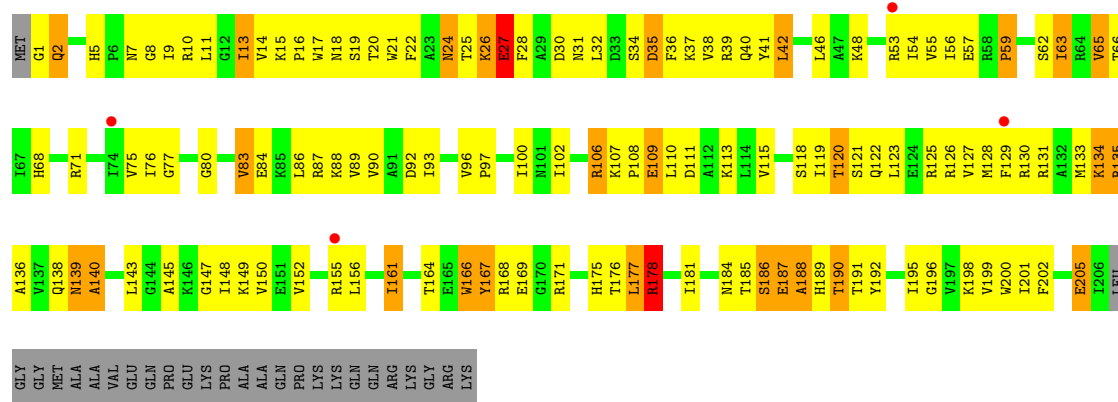


#### • Molecule 2: 30S ribosomal protein S3

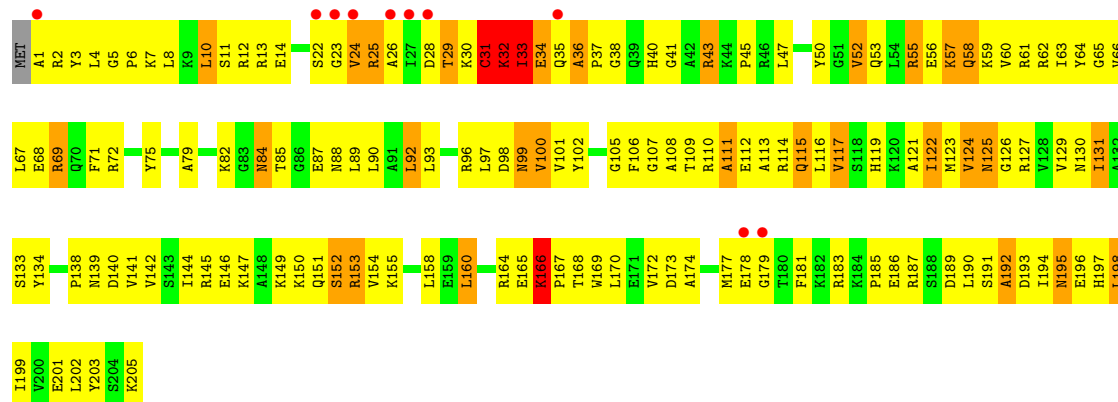




• Molecule 2: 30S ribosomal protein S3

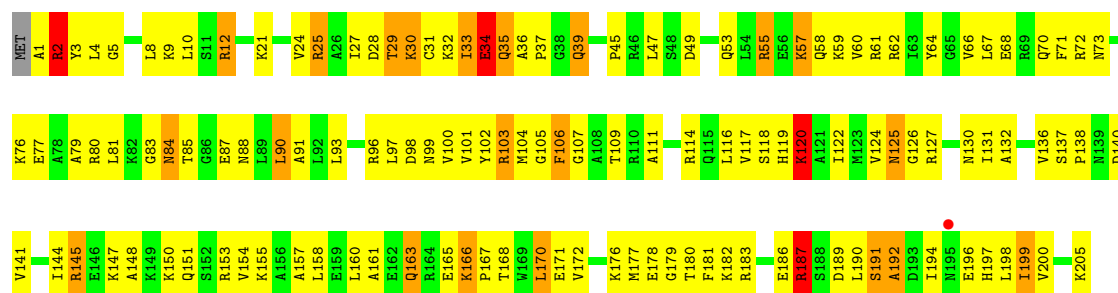


• Molecule 3: 30S ribosomal protein S4

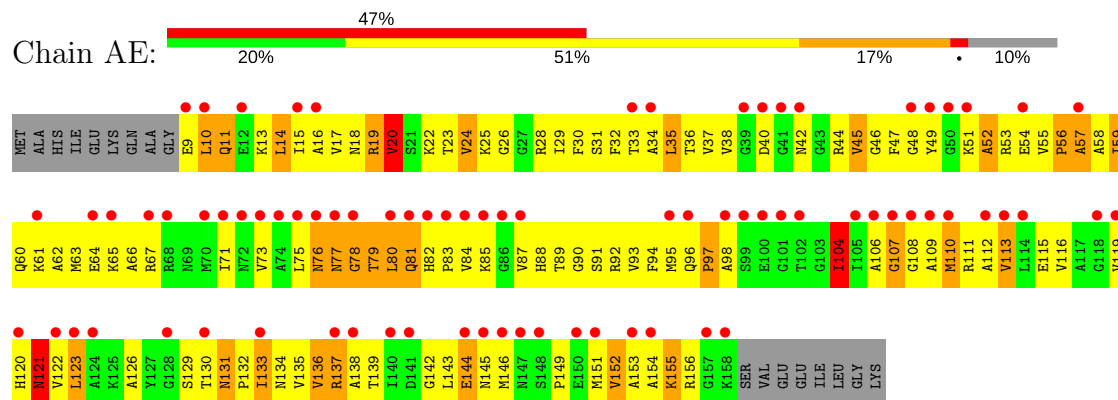


• Molecule 3: 30S ribosomal protein S4

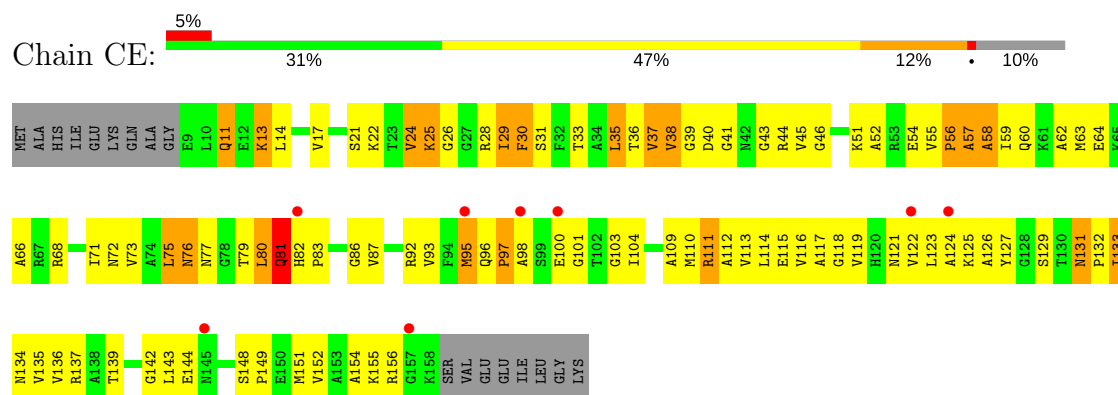




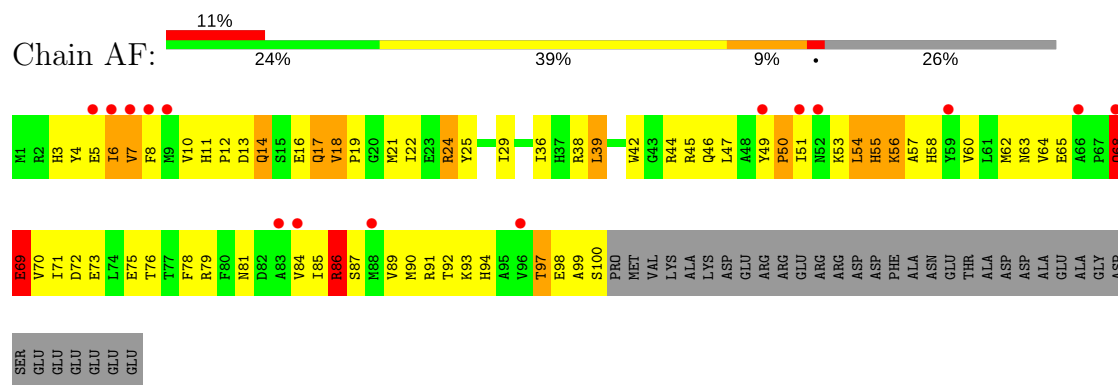
• Molecule 4: 30S ribosomal protein S5



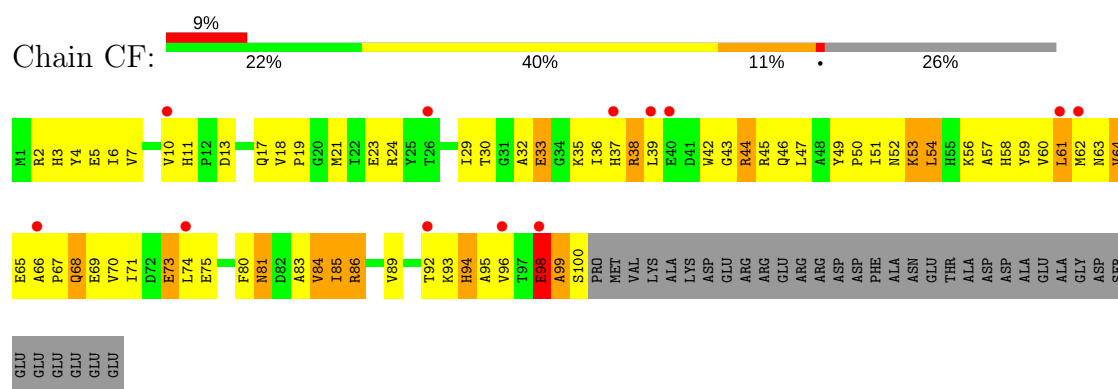
• Molecule 4: 30S ribosomal protein S5



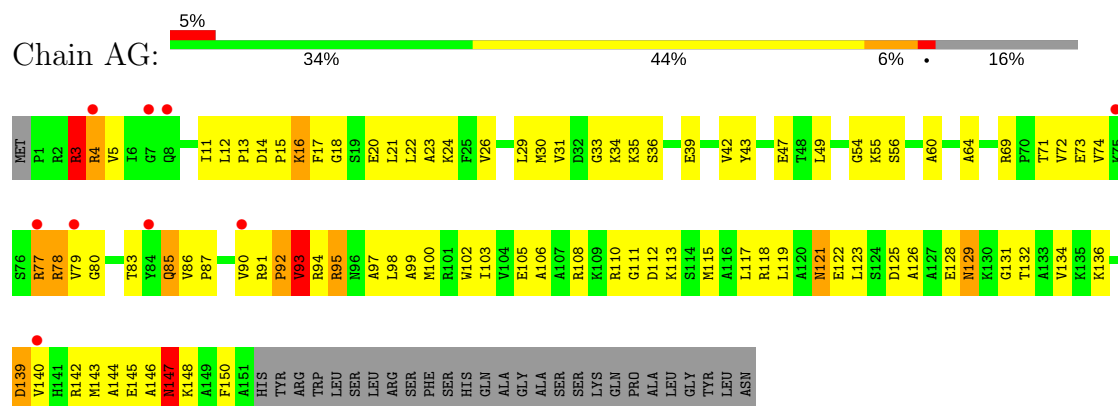
• Molecule 5: 30S ribosomal protein S6



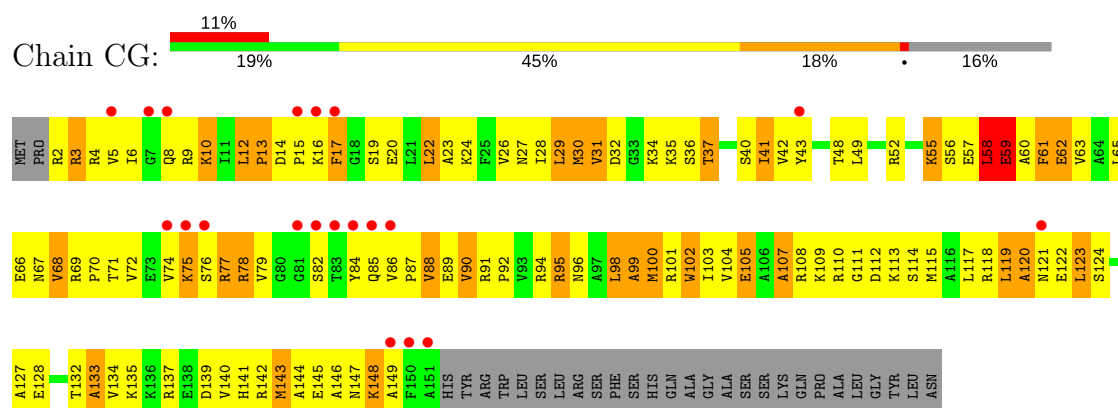
• Molecule 5: 30S ribosomal protein S6



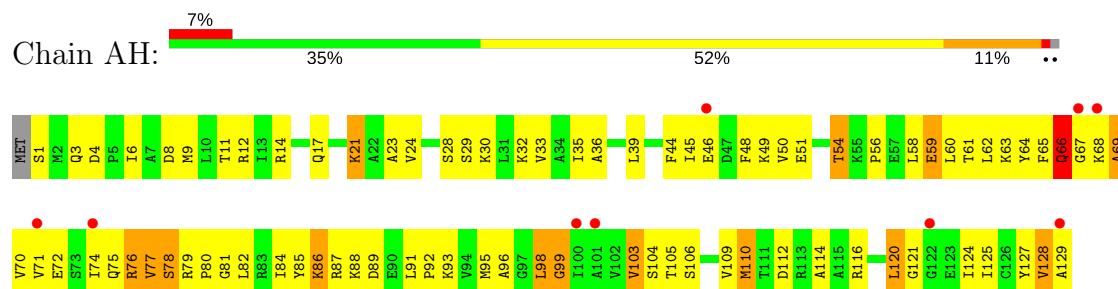
• Molecule 6: 30S ribosomal protein S7



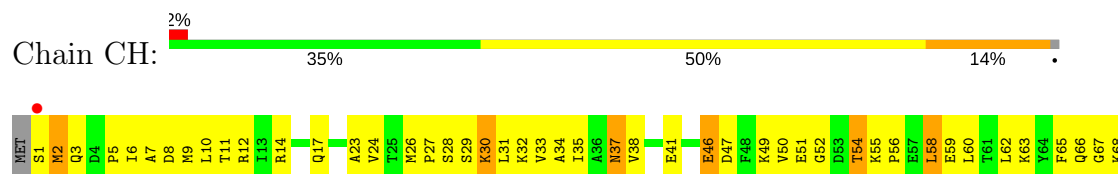
• Molecule 6: 30S ribosomal protein S7



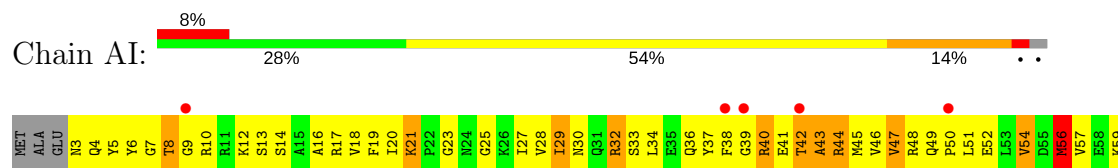
• Molecule 7: 30S ribosomal protein S8



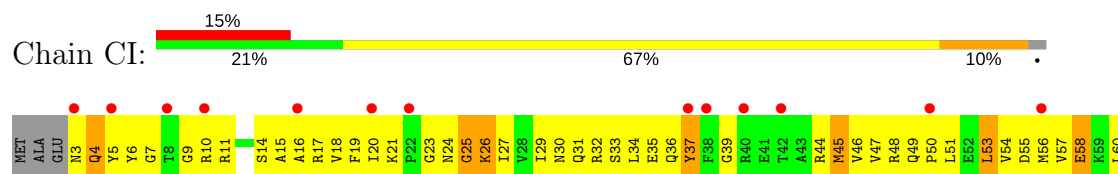
• Molecule 7: 30S ribosomal protein S8



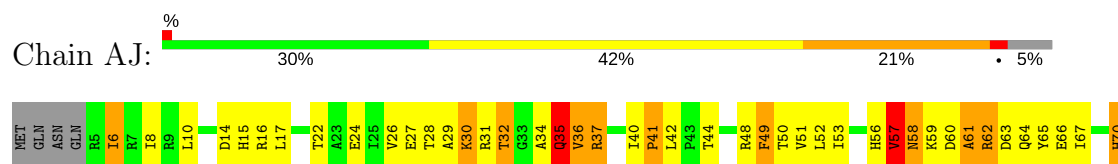
• Molecule 8: 30S ribosomal protein S9



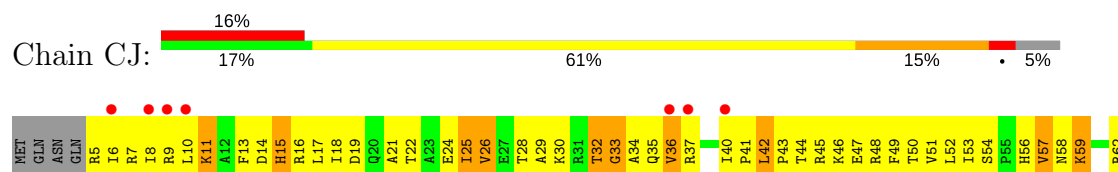
• Molecule 8: 30S ribosomal protein S9

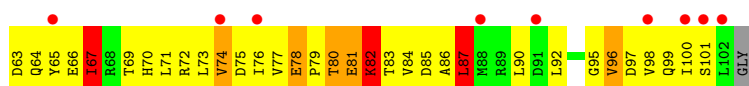


• Molecule 9: 30S ribosomal protein S10

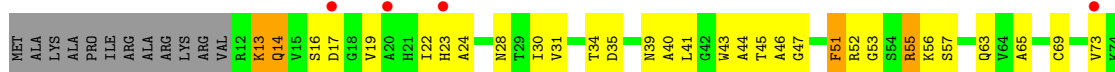


• Molecule 9: 30S ribosomal protein S10





- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

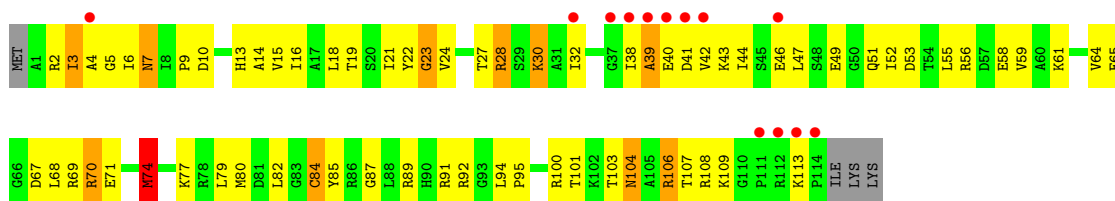


- Molecule 11: 30S ribosomal protein S12

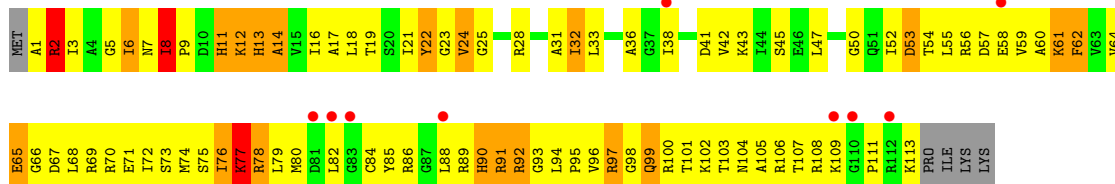


- Molecule 12: 30S ribosomal protein S13

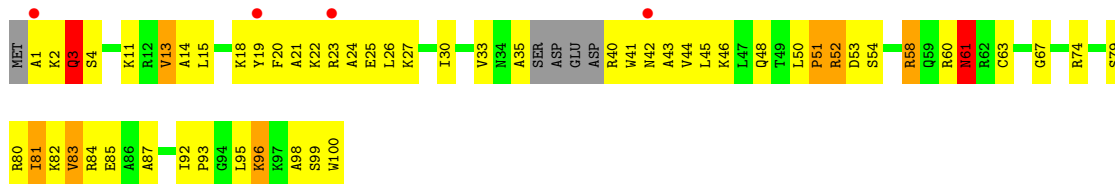
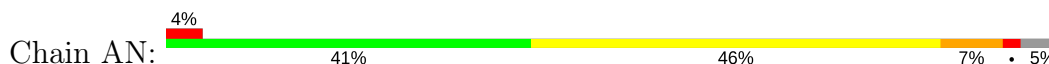




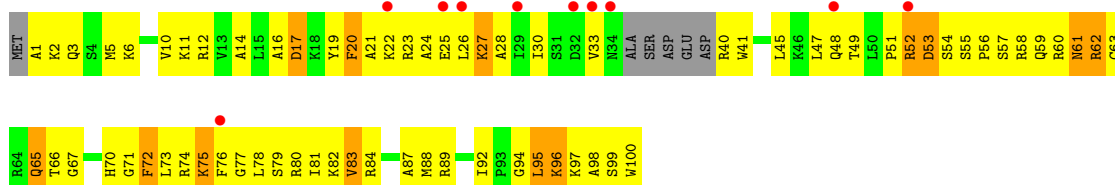
• Molecule 12: 30S ribosomal protein S13



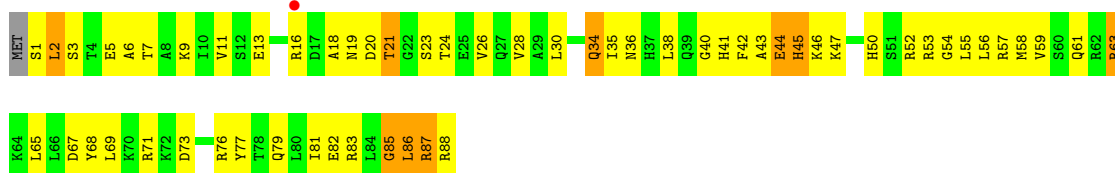
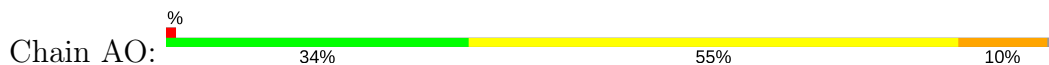
• Molecule 13: 30S ribosomal protein S14



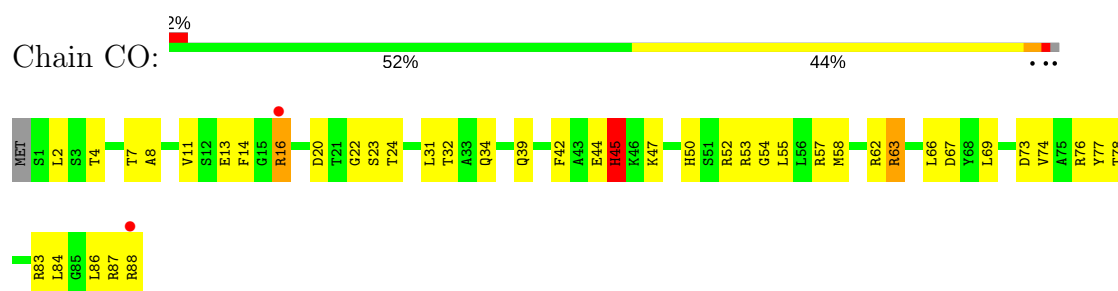
• Molecule 13: 30S ribosomal protein S14



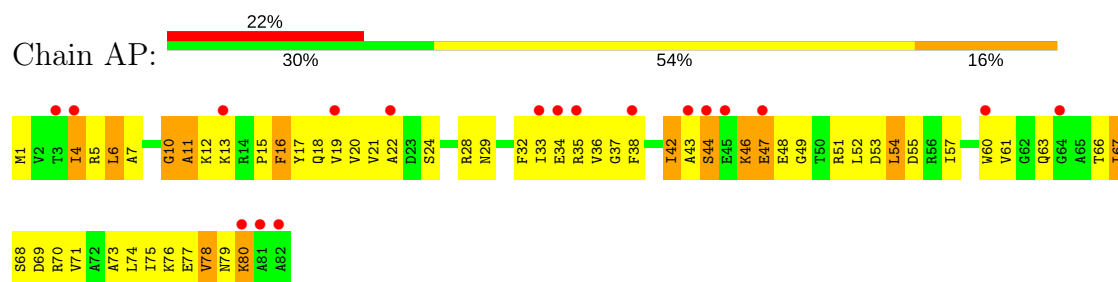
• Molecule 14: 30S ribosomal protein S15



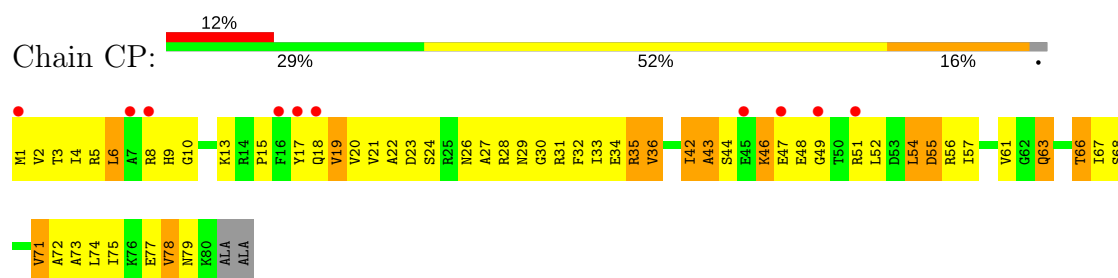
• Molecule 14: 30S ribosomal protein S15



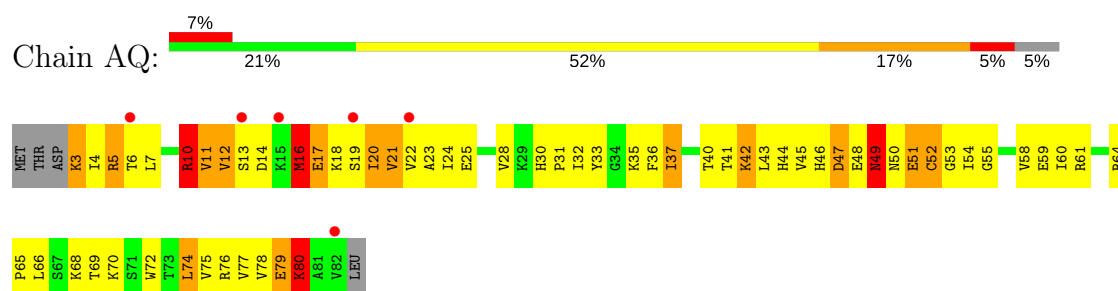
- Molecule 15: 30S ribosomal protein S16



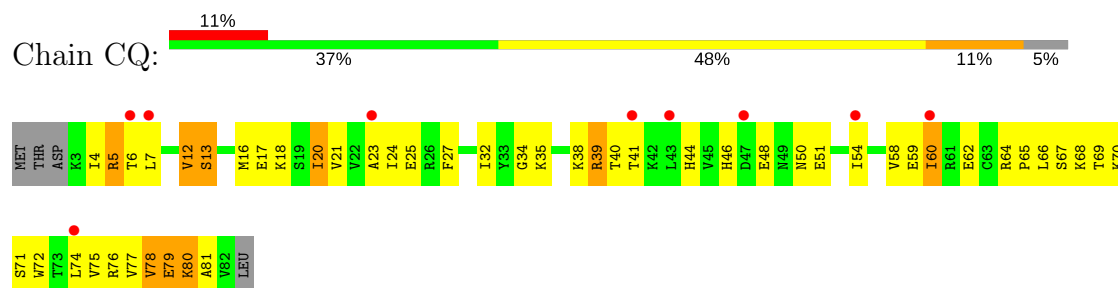
- Molecule 15: 30S ribosomal protein S16



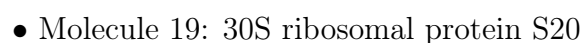
- Molecule 16: 30S ribosomal protein S17

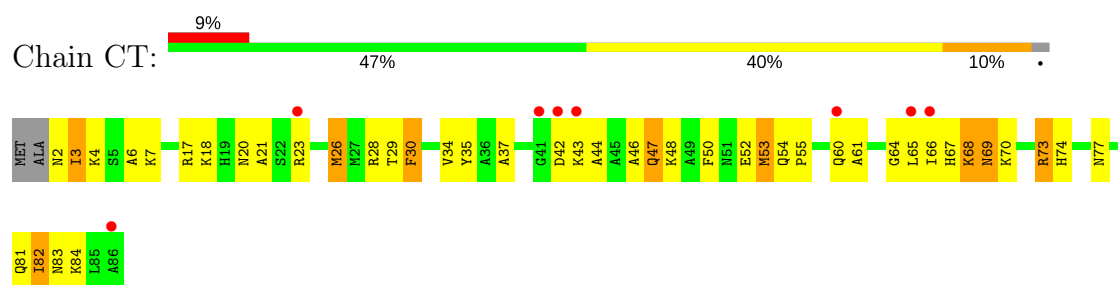


- Molecule 16: 30S ribosomal protein S17

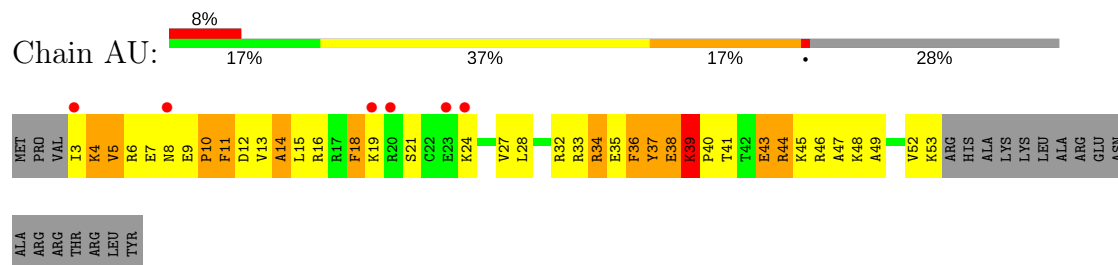


- Molecule 17: 30S ribosomal protein S18

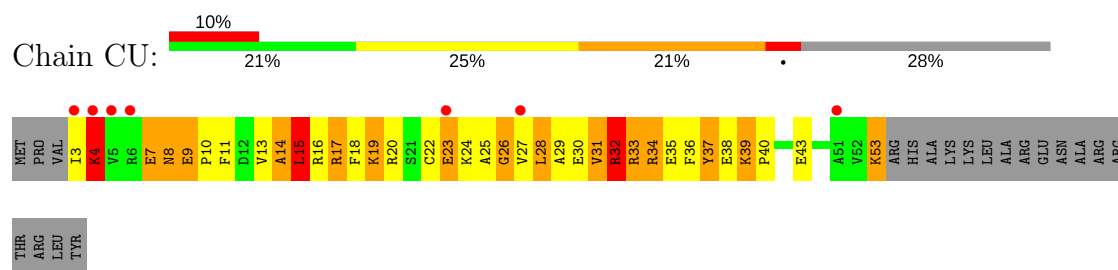




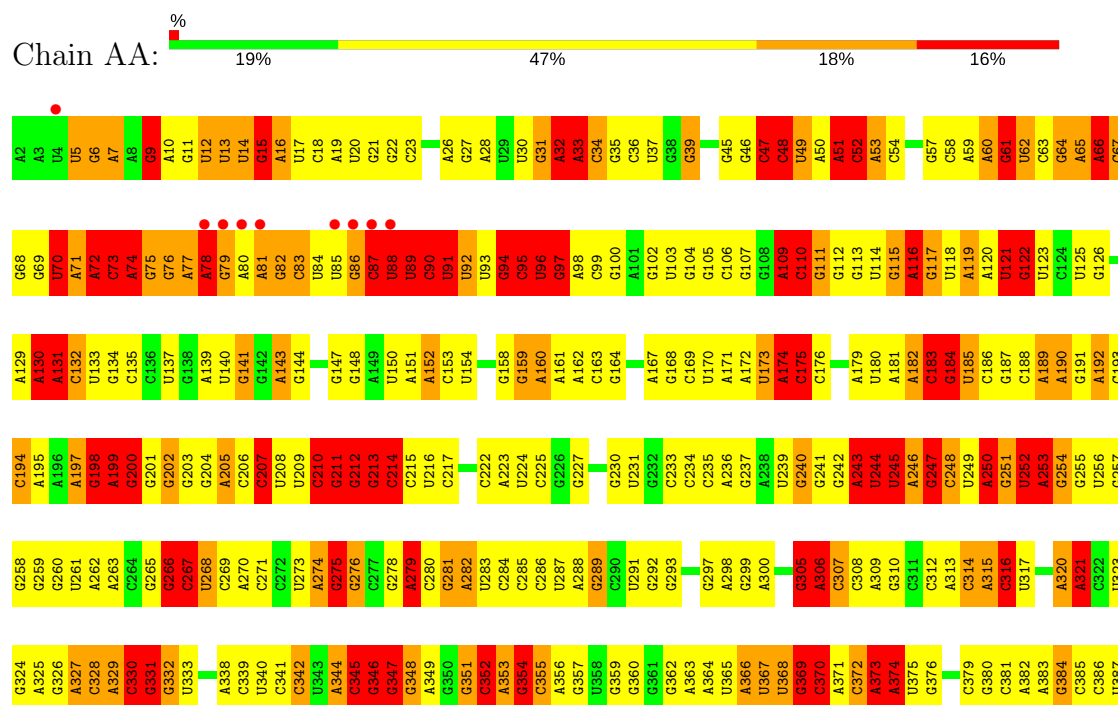
• Molecule 20: 30S ribosomal protein S21



• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S rRNA



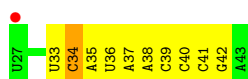
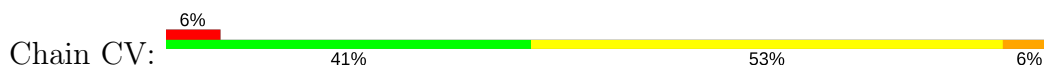
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G1379	U1380	C1316	C1317	A1251	G1187	G1127	G1057	C995	G928	A864	U768	A718	C854	C587	C525	U463	A389
U1381	U1382	C1318	U1189	A1252	A1188	C1128	U1060	A996	G929	A865	U789	C719	A655	G588	C526	U464	U390
C1382	A1319	A1254	G1190	C1253	U1191	C1129	G1061	U997	C930	C866	A790	C720	A656	U589	C527	A465	G391
C1383	C1390	G1255	A1191	A1255	G1192	G1131	U1062	C998	C931	C867	A792	G722	U657	U590	C392	U466	C392
G1384	U1321	A1256	C1063	A1256	C1132	G1132	C1063	A1000	C834	C868	U793	U723	C658	U591	G530	U467	A393
G1385	C1322	A1257	G1064	C1001	G1133	G1133	U1064	C1001	A835	C869	A794	G724	U662	G592	U531	A468	G394
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G1387	A1324	A1197	C1066	G1003	U1135	U1135	C1066	G1003	A937	U871	C796	G726	G664	A594	A533	C470	G399
C1388	C1325	A1198	C1067	A1004	U1136	U1136	C1067	A1004	A938	A872	C797	G727	A665	A595	U534	U471	C400
C1389	C1326	U1198	G1068	A1005	G1137	G1137	C1068	A1005	G939	A873	U798	A728	G666	C596	A535	U472	
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U1391	C1263	C1200	U1070	U1007	G1139	G1139	U1070	U1007	G941	U875	G803	G781	G668	C598	G537	G474	G404
G1392	U1264	A1201	C1071	U1008	G1200	G1200	C1071	U1008	G942	C976	U804	C732	G669	A600	G538	G475	U405
U1393	C1265	U1202	G1072	U1009	A1202	C1141	G1072	U1009	A946	A876	G733	G734	G670	A601	A539	C477	G406
A1394	C1266	C1203	U1073	U1010	A1203	G1142	U1073	U1010	A947	C879	G734	G735	G671	A602	G540	U478	A408
C1395	G1267	A1204	G1074	G1013	U1013	G1143	U1074	G1013	A948	C880	C810	C736	A673	U603	G544	U479	A411
A1396	G1268	U1205	U1075	A1014	A1014	A1145	U1075	A1014	A949	C881	C811	C737	G674	G604	C545	U480	A412
C1397	A1269	G1206	G1077	A1015	A1015	A1146	U1077	A1015	U950	C882	C812	C738	G675	U605	C456	U481	A413
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C1400	G1338	C1209	U1080	U1018	U1018	C1149	U1080	U1018	G954	U884	A815	U740	U678	A608	C548	U484	A415
G1401	A1274	C1210	A1081	G1019	G1019	U1150	A1081	G1019	U955	C885	A816	G741	U679	A609	C549	U485	G416
A1402	A1275	U1211	A1082	A1020	A1020	A1151	U1082	A1020	U956	C886	C817	A747	C679	C613	G550	U486	G417
C1403	G1276	U1212	U1083	A1021	A1021	A1152	U1083	A1021	U957	A889	G818	G748	C680	C614	U551	U487	
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C1405	G1278	C1214	U1085	A1023	A1023	G1154	U1085	A1023	A959	C891	A820	U751	G683	C616	A553	C489	C422
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C1409	U1282	C1218	G1089	U1027	U1027	A1158	G1089	C995	U965	C995	A825	G755	U687	C620	G558	A496	U426
A1410	U1283	A1219	U1090	U1030	U1030	C1159	U1090	C996	U966	C996	C826	G756	U688	A621	C559	C497	G428
C1411	G1284	G1220	U1091	U1031	U1031	C1160	U1091	U967	C967	A900	U827	U757	G690	C622	U560	A498	U429
U1412	A1285	G1221	U1092	G1032	G1032	C1161	U1092	C968	C968	A901	U828	C758	G691	C623	U561	A499	A430
A1413	C1352	G1222	U1093	G1033	G1033	C1162	U1093	C969	A969	C902	G829	A759	U692	C624	U562	G500	A431
U1414	U1286	C1223	U1094	U1034	U1034	A1163	U1094	C970	C970	C903	G830	G760	G693	C625	A563	C501	
C1353	A1287	U1224	U1095	G1035	G1035	G1164	U1095	C971	C971	C904	G831	G761	G694	C626	C364	A502	A435
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G1355	A1289	G1164	U1097	A1037	A1037	G1166	C1097	C973	C973	U905	G833	G763	A695	C628	C365	C504	U437
G1356	U1290	G1165	C1098	C1037	C1037	A1167	C1098	G973	C974	A908	G834	C764	A696	G628	C366	C505	U438
G1417	U1357	U1166	U1099	U1038	U1038	U1167	U1099	G974	A974	A909	G835	G765	A697	U632	C367	G506	U439
A1418	U1358	A1167	C1100	C1039	C1039	U1168	C1100	A975	A975	C910	G836	A766	C569	U633	C368	C507	G440
G1419	U1359	U1168	A1101	U1040	U1040	U1169	A1101	A976	A976	U911	G837	A767	C570	G633	G570	U608	A441
U1420	G1359	C1230	A1102	U1041	U1041	A1170	A1102	G976	G976	C912	U837	A768	C571	U636	G571	U609	G442
G1421	U1297	G1231	C1103	A1042	A1042	C1171	C1103	A977	A977	C913	G838	A769	C572	C637	A572	A510	C511
G1422	A1299	U1232	G1104	A1043	A1043	U1172	G1104	A978	A978	C914	G839	G769	C573	C637	A573	C512	A448
U1423	G1300	C1233	A1105	A1044	A1044	U1173	A1105	C979	C979	A915	G840	C770	G704	C637	A574	U512	G449
U1424	U1301	C1234	G1106	C1045	C1045	U1174	G1106	U982	U982	U916	G841	C771	G705	A640	G574	C513	G450
U1425	C1302	U1235	C1107	C1046	C1046	G1175	C1107	U983	U983	U917	U842	G771	G706	A641	G575	C514	A451
G1426	G1303	A1236	G1108	A1047	A1047	U1176	G1108	A983	A983	C917	U843	G775	G707	A642	C576	C515	A452
G1427	C1304	C1237	U1177	U1048	U1048	G1177	U1177	C984	C984	A918	U844	G776	C708	A643	C577	C516	G453
A1428	G1305	A1238	C1114	G1049	G1049	U1178	C1114	U986	U986	A919	A845	A777	G710	U644	C578	U516	G454
A1429	A1306	A1239	U1115	U1049	U1049	A1179	U1115	U987	U987	U920	G846	A777	G711	U645	A579	C517	G455
A1430	U1307	U1240	U1116	U1050	U1050	A1180	U1116	G987	G987	U921	G847	A781	G712	U646	C580	C518	A456
A1431	C1343	G1241	U1118	G1051	G1051	G1181	U1118	G988	G988	A923	U847	A782	G713	C647	C581	C519	A457
G1432	U1308	U1242	C1119	U1052	U1052	G1182	C1119	U991	U991	C924	C857	C783	G714	A648	C582	A520	A458
A1433	G1309	U1243	U1119	G1053	G1053	U1183	C1119	U992	U992	C925	G858	A784	G715	A649	C583	C522	A459
A1434	U1312	U1244	G1124	G1054	G1054	U1184	G1124	U993	U993	G926	G859	A785	G716	U652	C584	C523	A460
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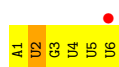
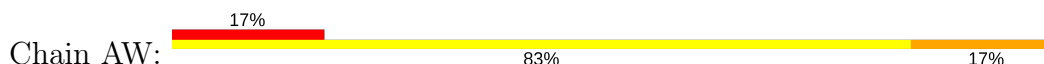
• Molecule 22: P-site tRNA ASL fragment



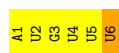
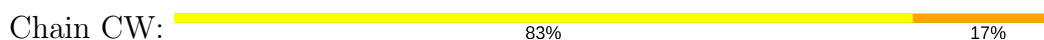
• Molecule 22: P-site tRNA ASL fragment



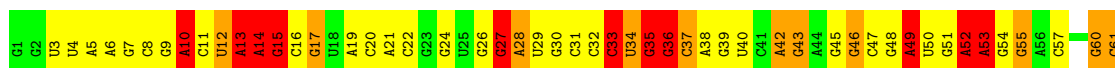
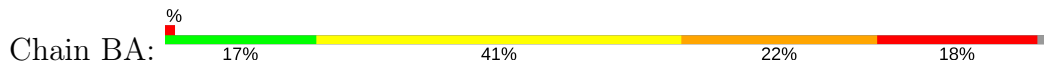
• Molecule 23: messenger RNA



• Molecule 23: messenger RNA

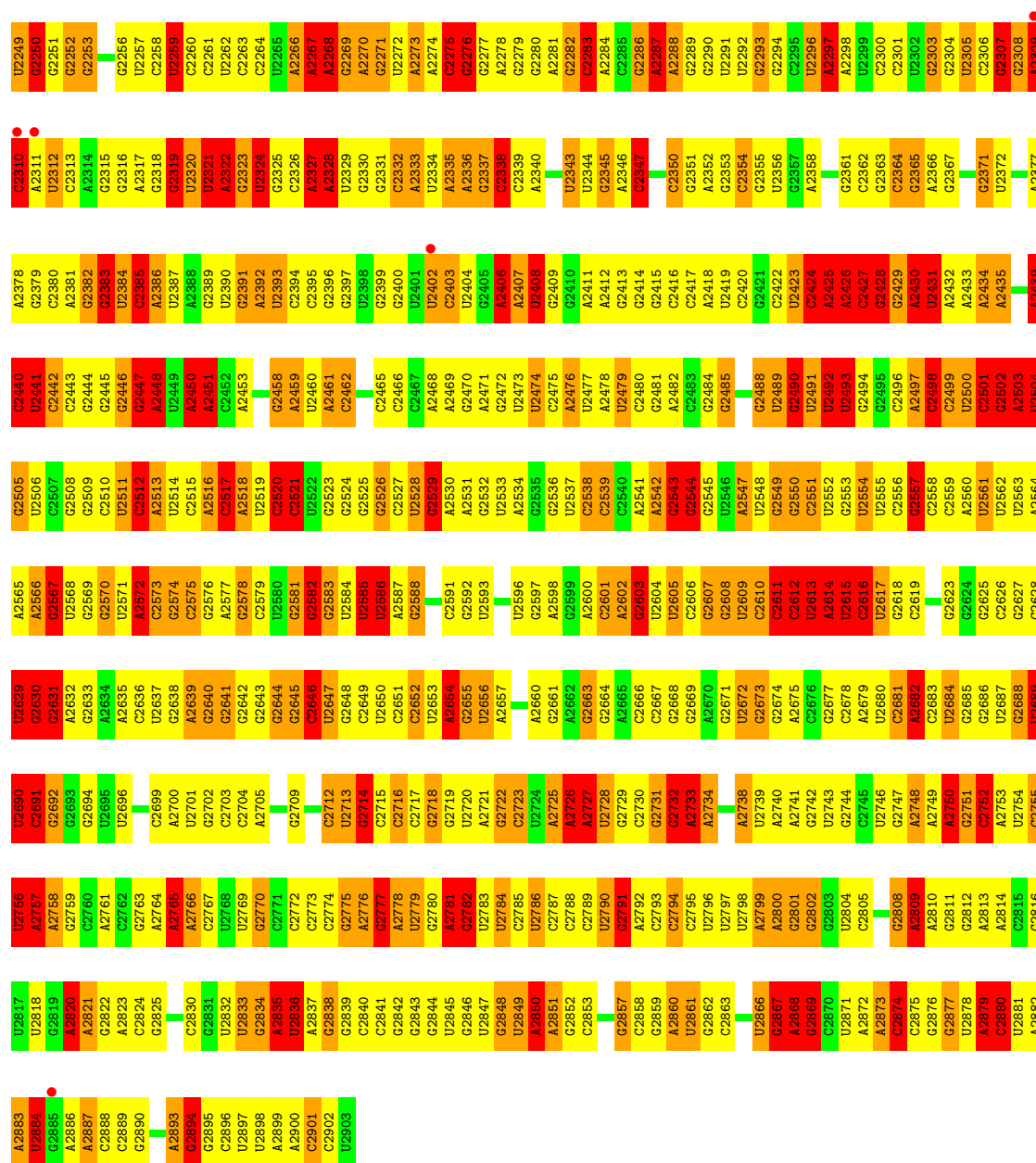


• Molecule 24: 23S rRNA

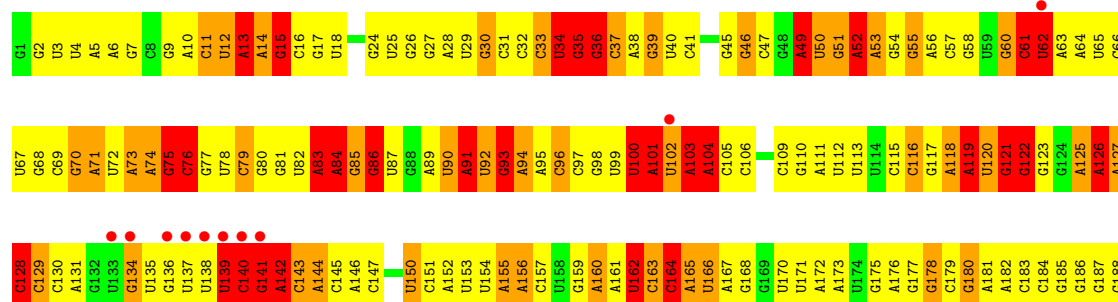
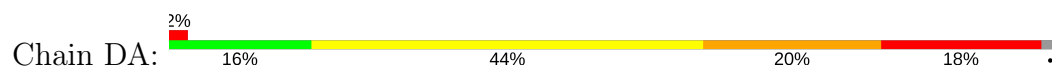






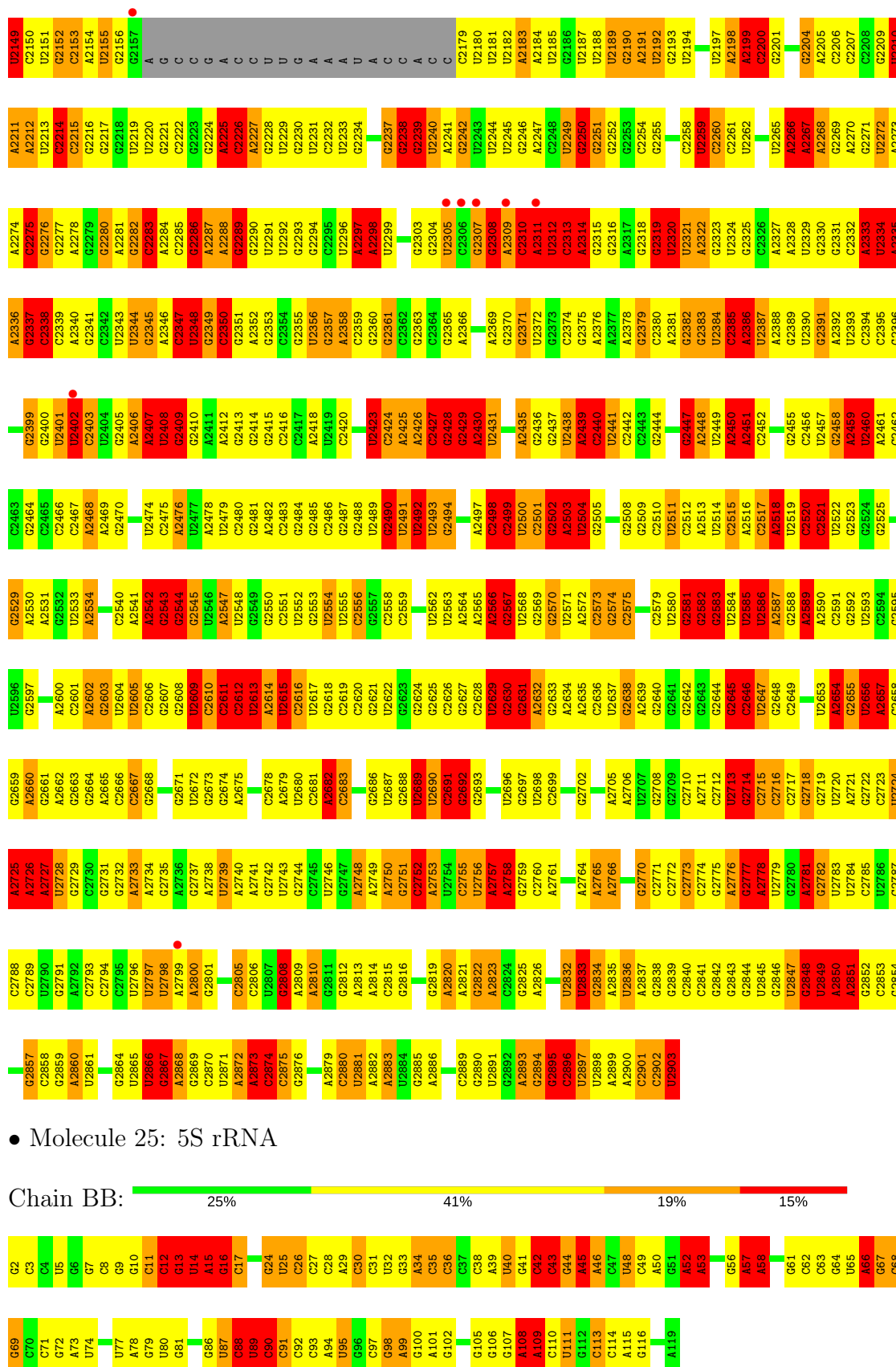


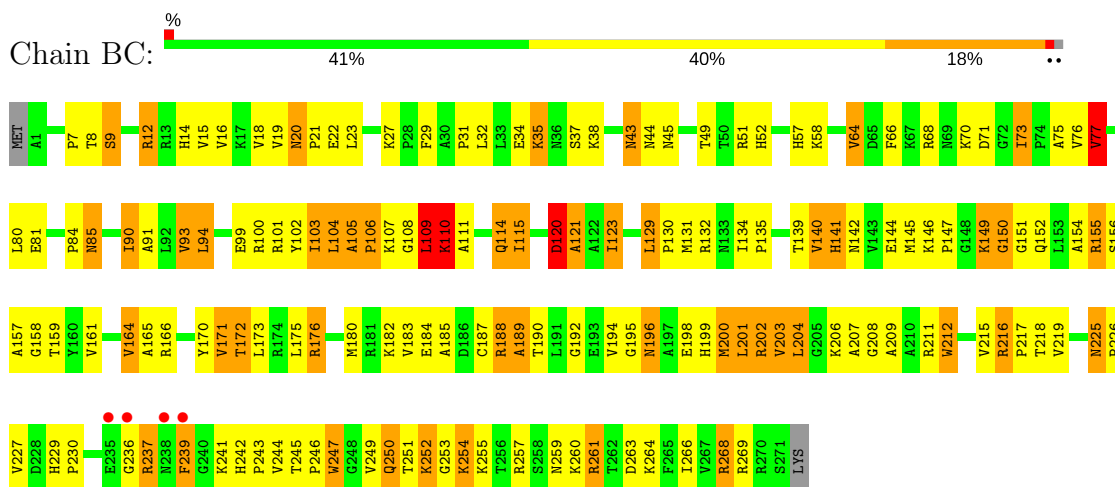
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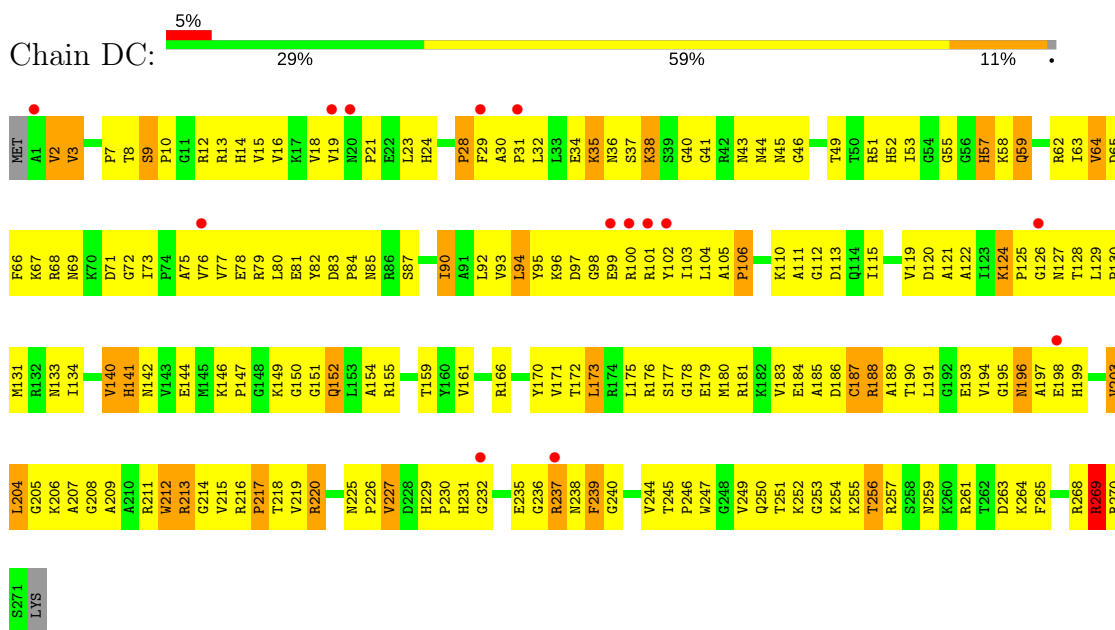
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A1014	U1015	G1016	G1017	U1018	U1019	A1020	A1021	A1022	C1023	U1024	G1025	G1026	A1027	A1028	U1029	C1030	G1031	A1032	U1033	A1034	U1035	G1036	A1039	A1040	G1041	G1042	A1043	C1044	U1045	A1046	G1047	C1048	A1049	C1050	A1051	C1052	C1053	G1054	G1055	C1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	U1064	U1065	U1066	G1067	U1068	U1069	A1070	C1071	C1072	A1073	G1074																																																																																																																																																																																																																																																																																																																																																																													
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G822	G823	U824	A825	U826	U827	U828	A829	G830	A831	U832	A833	G834	C835	U839	C840	G841	U842	G843	A844	A845	U846	U847	G848	A849	U850	C851	G852	A853	A854	A855	G856	U857	A858	C859	A860	A861	G862	U863	A864	C865	A866	C867	U868	G869	U870	U871	U872	C873	G874	U875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248
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C2089	C1958	C1895	A1829	A1701	C1638	C1574	U1513	G1451	G1388	A1327	U1263	U1199
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C2091	A1960	G1897	G1831	G1770	A1640	U1576	A1515	A1453	G1390	C1329	A1265	G1201
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G2093	U1962	A1899	G1833	G1772	G1707	U1578	G1517	G1455	A1392	G1331	U1267	A1203
A2094	U1963	A1900	U1834	A1773	G1643	A1579	C1518	G1456	A1393	G1332	A1268	A1204
A2095	G1964	A1901	G1835	C1774	G1644	A1580	G1519	U1457	G1394	G1333	A1269	A1205
C2096	C1965	G1902	C1836	G1775	G1645	G1581	U1520	U1458	A1395	G1334	G1270	G1206
A2097	A1966	G1903	G1837	G1776	C1646	G1582	U1521	G1459	G1396	C1335	G1271	C1207
U2098	C1967	G1904	G1838	U1777	U1647	A1583	U1522	U1460	A1397	A1336	A1272	C1208
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G2110	U1979	A1918	A1853	G1724	G1661	C1595	C1533	U1473	G1408	A1347	G1283	G1221
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G	U1982	G1922	G1857	C1728	A1665	C1600	U1539	A1477	U1352	U1352	A1287	G1225
A	A2051	G1923	A1858	U1729	G1666	G1601	U1540	G1478	A1353	A1353	G1288	A1226
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C	C2001	U1939	G1875	A1744	U1681	A1616	G1555	G1492	G1430	A1307	A1242	
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U	A2003	C1941	A1877	A1746	U1683	A1618	C1557	A1494	G1432	G1370	G1309	A1246
G	G2004	C1942	U1878	U1747	G1684	G1619	C1558	A1495	G1433	G1371	G1310	A1247
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A	A2013	G1945	U1881	U1751	G1687	U1625	C1561	C1498	G1436	A1374	C1314	G1250
A2014	U1946	U1946	C1816	G1752	U1688	A1626	U1562	G1500	G1437	U1375	C1251	C1251
A2015	C1947	C1947	U1818	G1753	A1689	A1627	C1563	G1501	U1438	G1376	G1315	G1252
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U2017	U2017	U1949	U1886	U1820	G1628	U1628	C1565	A1504	U1440	U1378	G1317	A1254
G2018	C2018	G1950	C1887	A1757	U1693	G1631	A1566	A1505	G1441	U1379	U1319	A1254
A2019	A2019	U1951	G1888	U1758	C1694	G1631	G1567	U1506	G1442	G1380	G1320	U1255
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C2021	C2021	G1953	A1890	C1760	G1696	G1633	A1569	A1508	G1444	A1382	C1257	U1257
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A2082	U2022	U1956	G1892	U1825	G1697	A1634	A1571	A1509	C1446	A1384	C1323	G1259
C2023	C2023	G1955	C1893	A1762	A1698	A1635	A1572	G1510	G1447	A1385	G1324	A1260
G2087	G2087	U1956	C1892	G1763	G1699	U1636	A1571	G1511	G1448	C1386	C1261	U1261
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• Molecule 26: 50S ribosomal protein L2

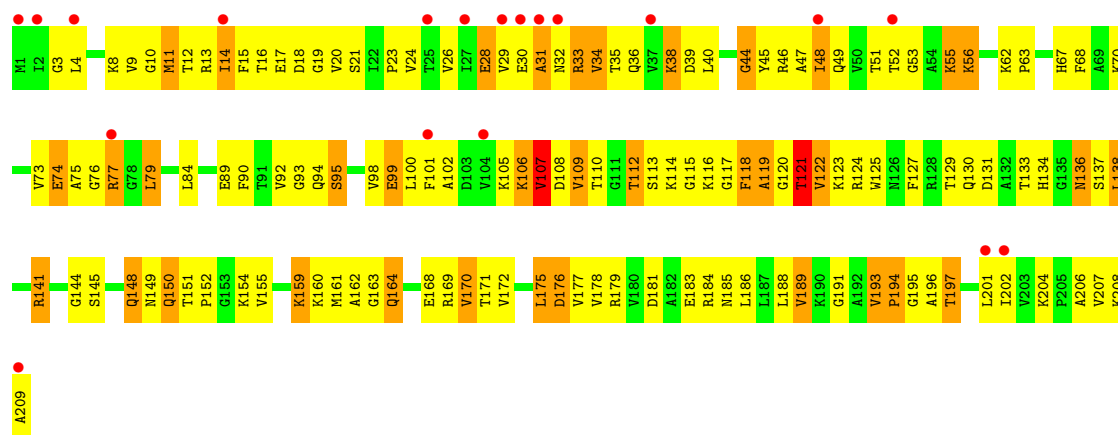


• Molecule 27: 50S ribosomal protein L3

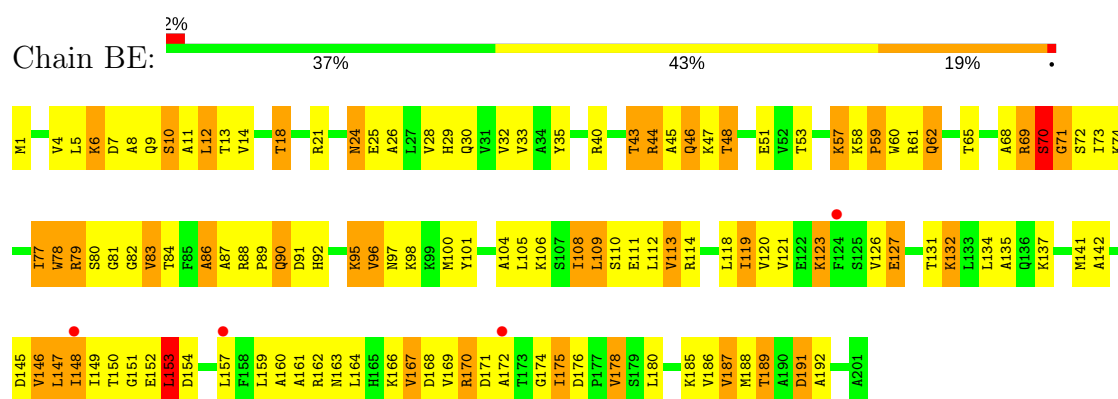


• Molecule 27: 50S ribosomal protein L3

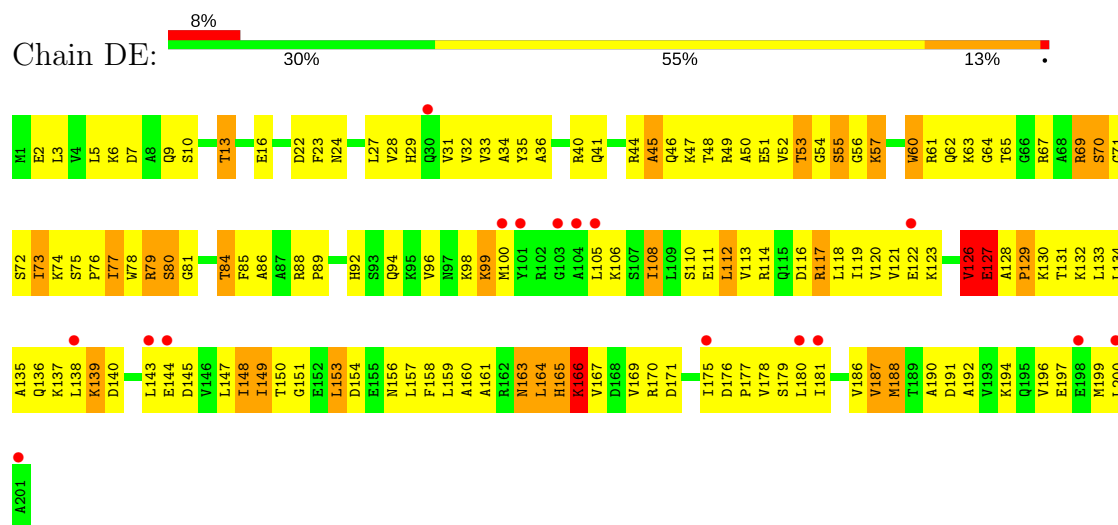




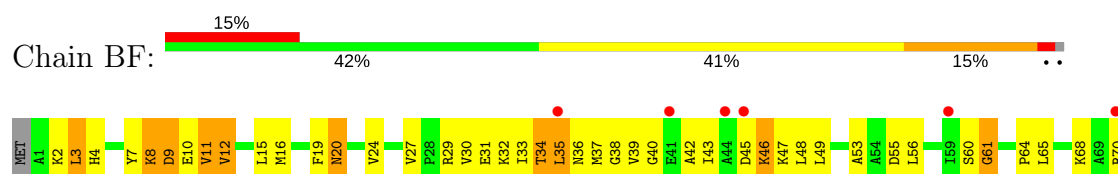
• Molecule 28: 50S ribosomal protein L4

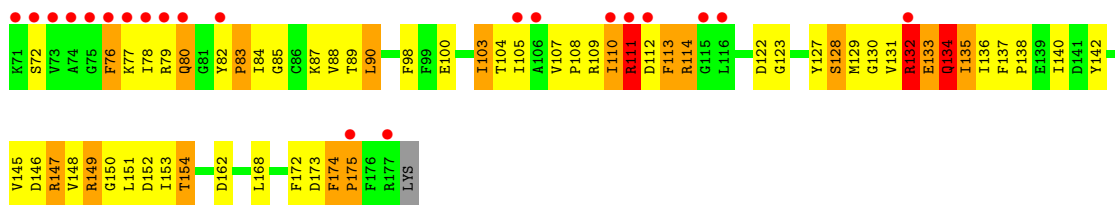


• Molecule 28: 50S ribosomal protein L4

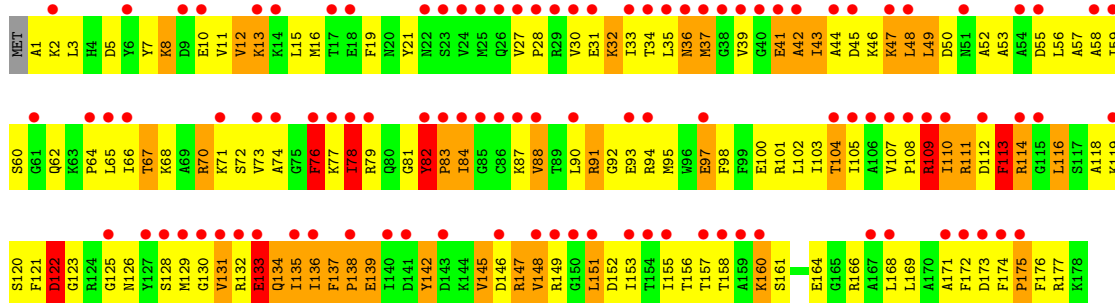


• Molecule 29: 50S ribosomal protein L5

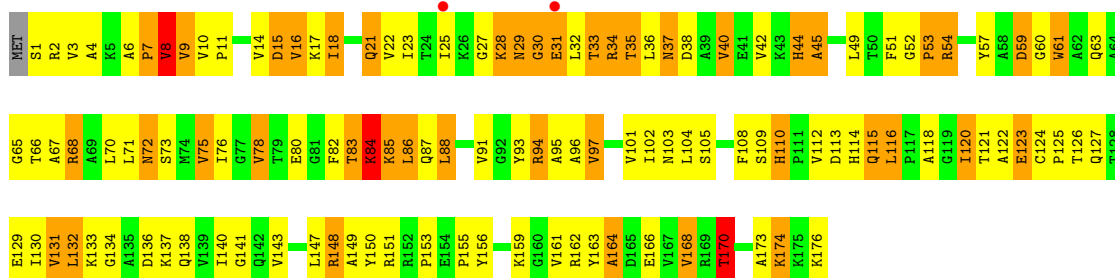




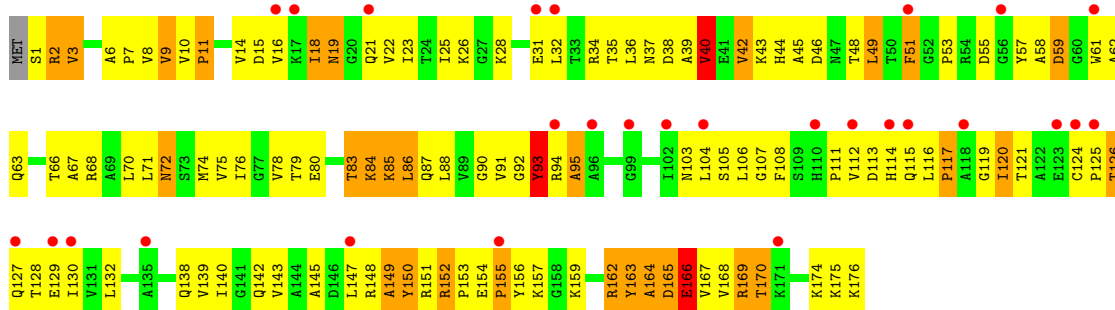
• Molecule 29: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L6

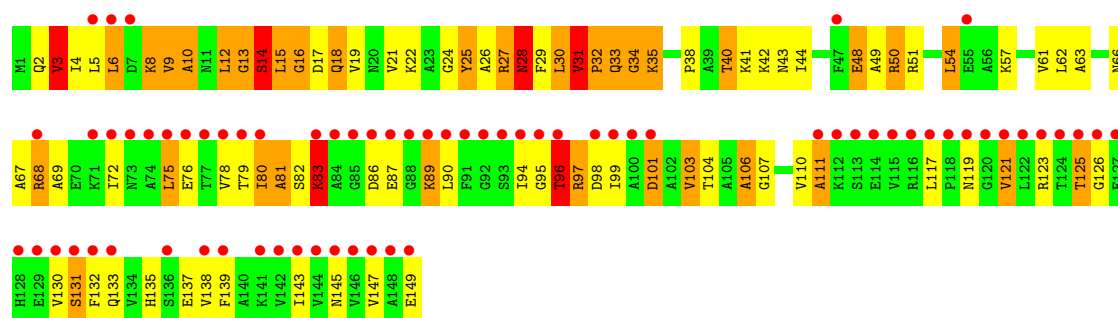


• Molecule 30: 50S ribosomal protein L6

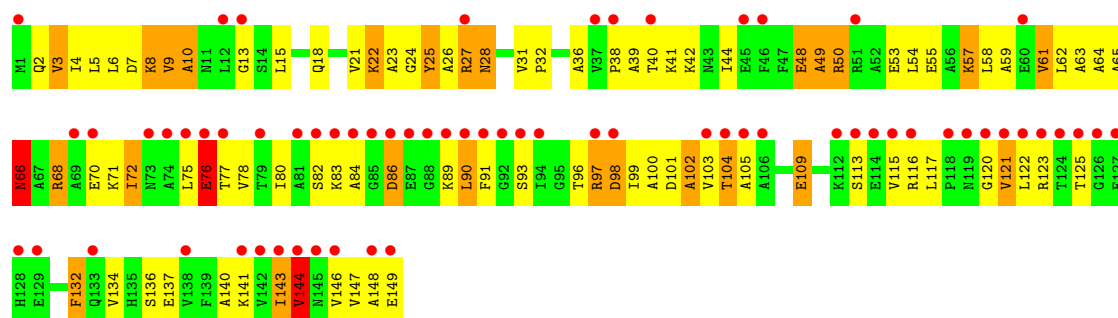


• Molecule 31: 50S ribosomal protein L9

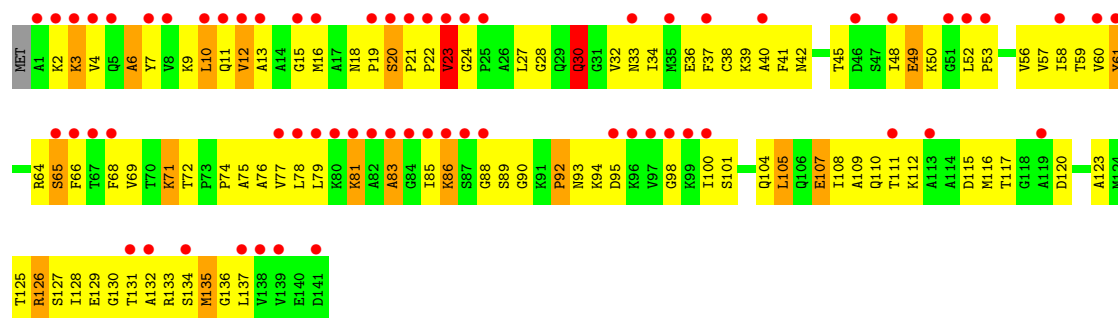




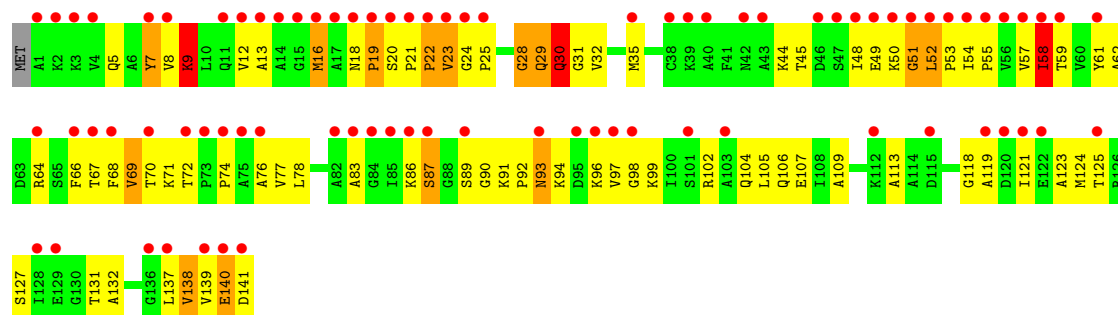
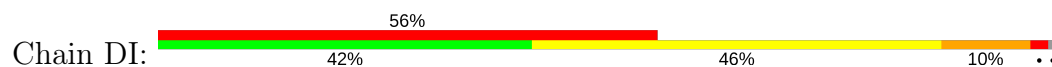
• Molecule 31: 50S ribosomal protein L9



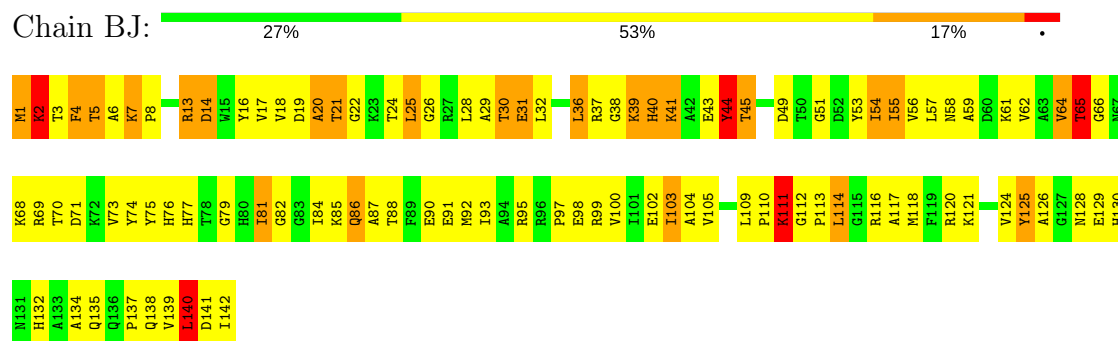
• Molecule 32: 50S ribosomal protein L11



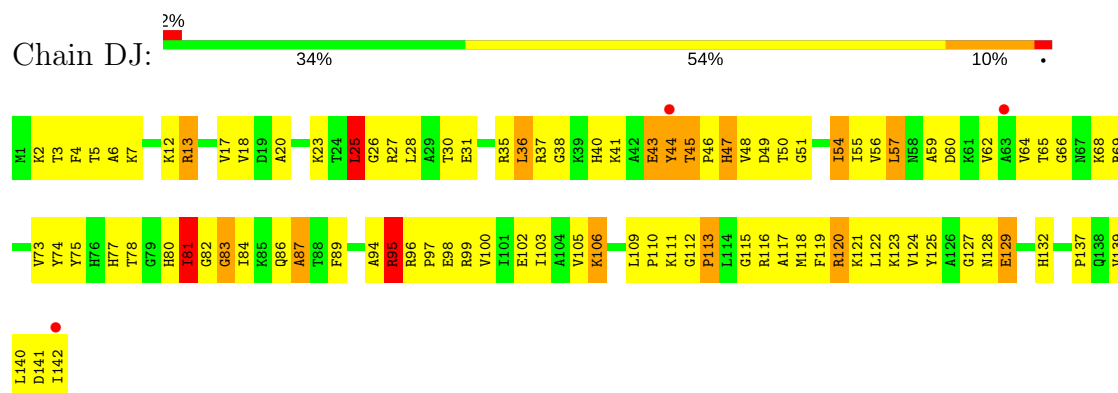
• Molecule 32: 50S ribosomal protein L11



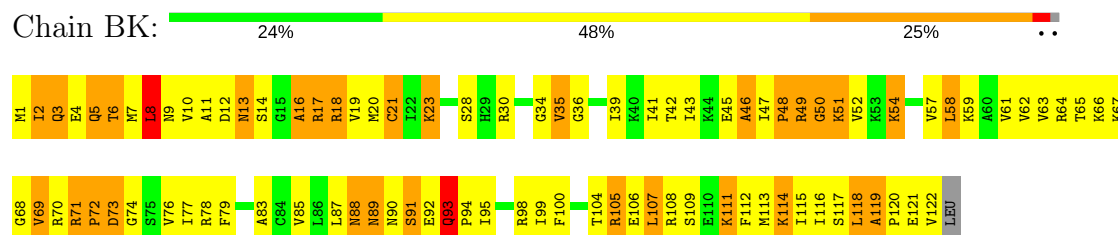
- Molecule 33: 50S ribosomal protein L13



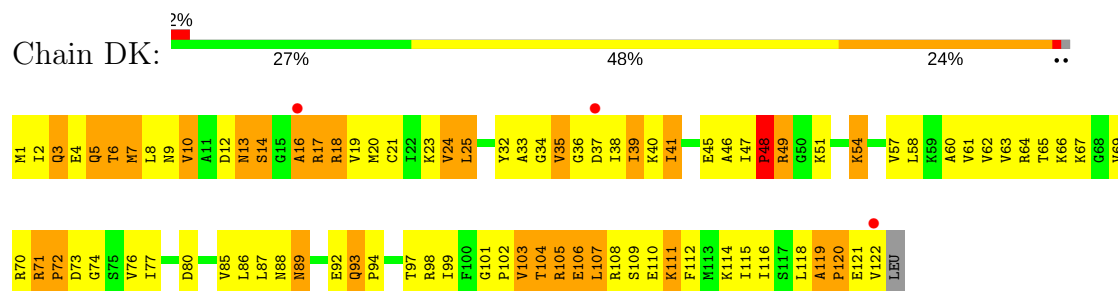
- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14

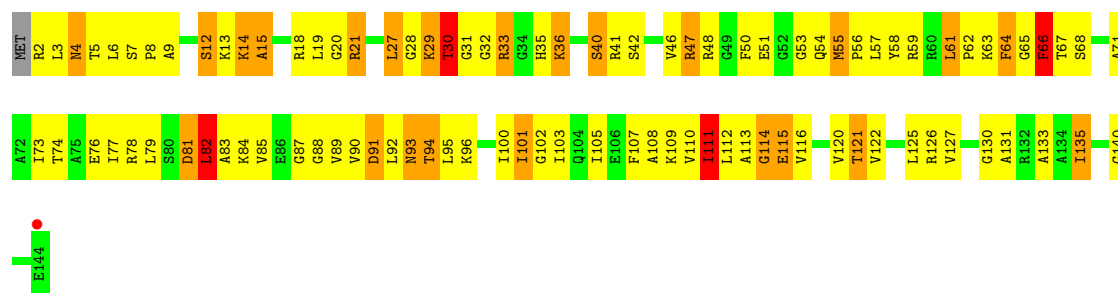


- Molecule 34: 50S ribosomal protein L14

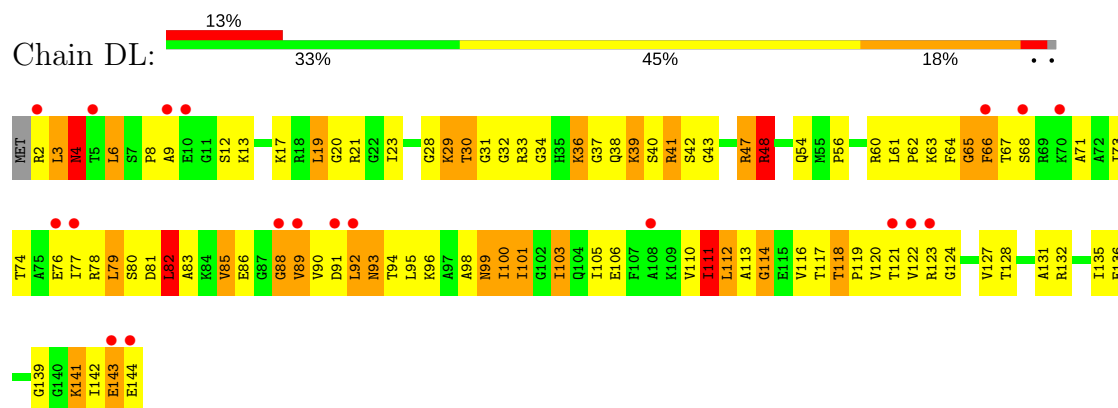


- Molecule 35: 50S ribosomal protein L15

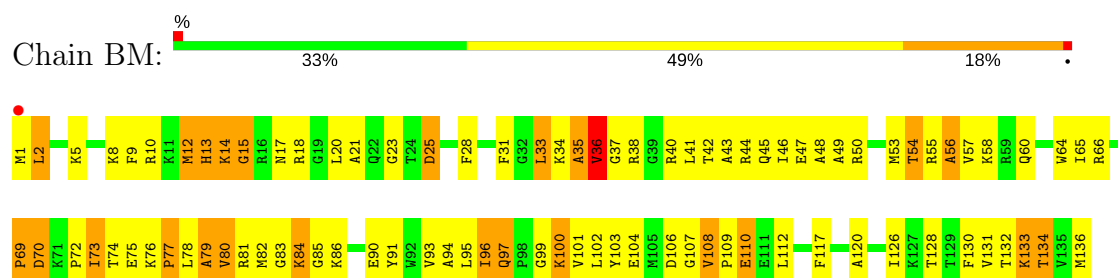




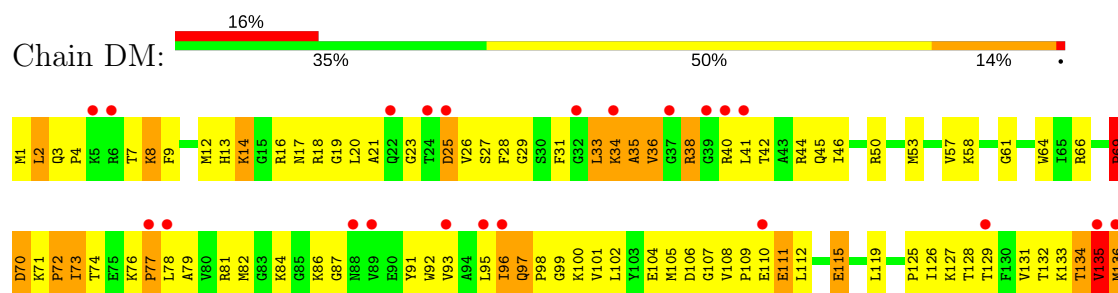
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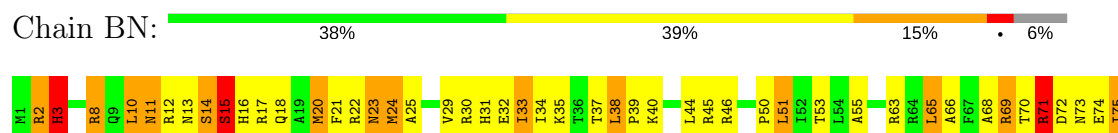
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

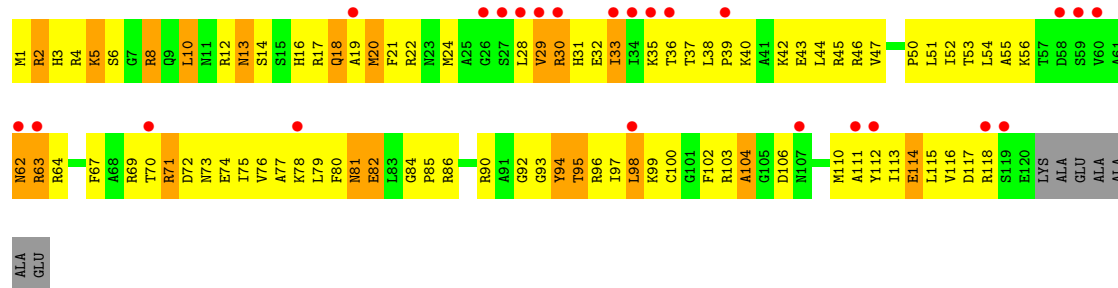


- Molecule 37: 50S ribosomal protein L17

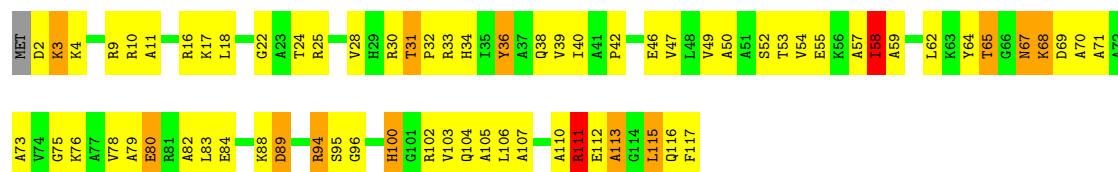




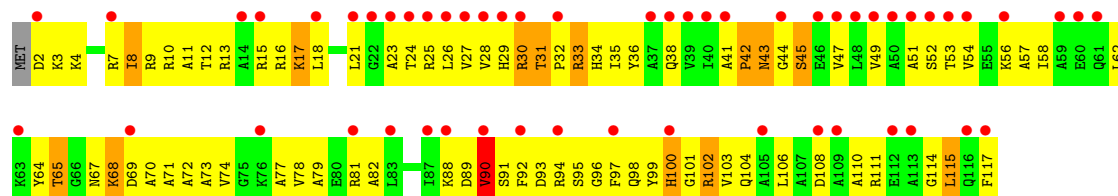
• Molecule 37: 50S ribosomal protein L17



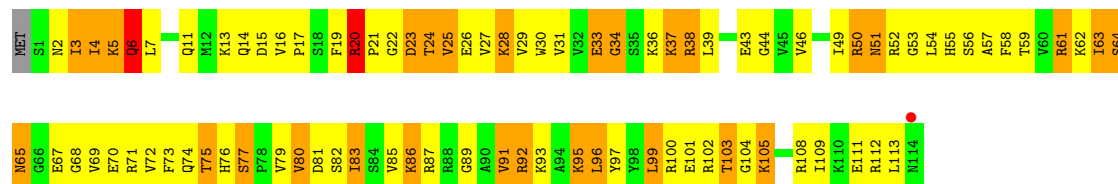
• Molecule 38: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L18

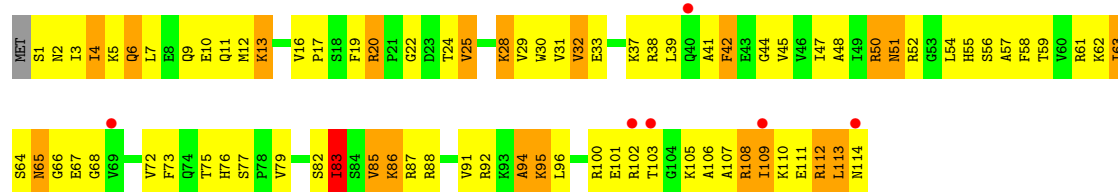


• Molecule 39: 50S ribosomal protein L19



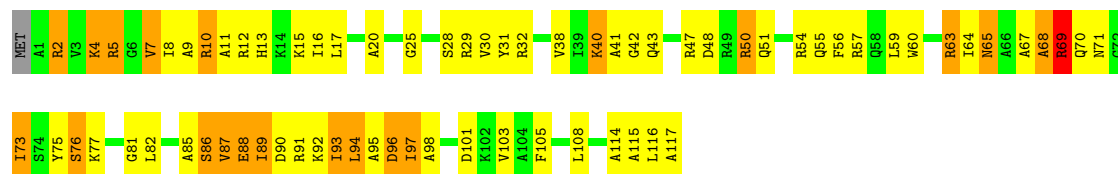
• Molecule 39: 50S ribosomal protein L19





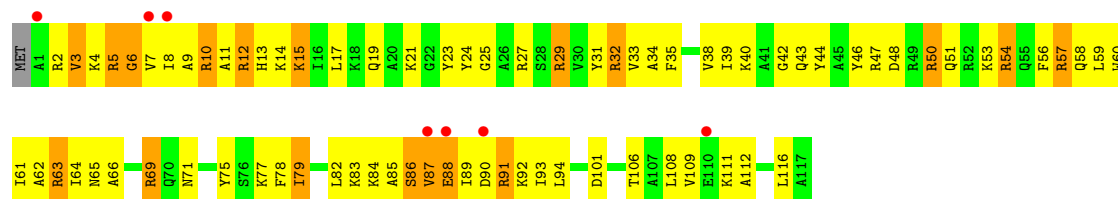
• Molecule 40: 50S ribosomal protein L20

Chain BQ: 39% 42% 17% ..



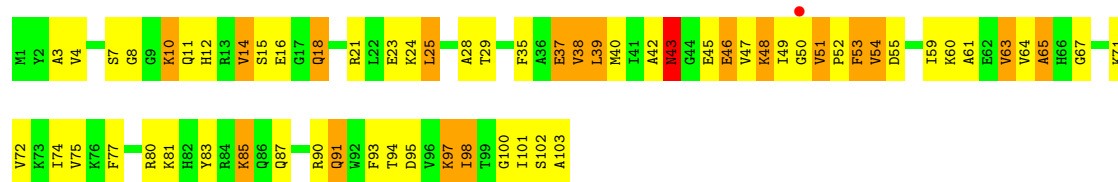
• Molecule 40: 50S ribosomal protein L20

Chain DQ: 6% 34% 50% 15% .



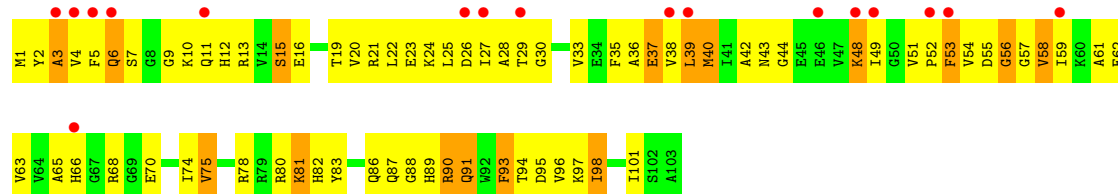
• Molecule 41: 50S ribosomal protein L21

Chain BR: % 39% 43% 17% .

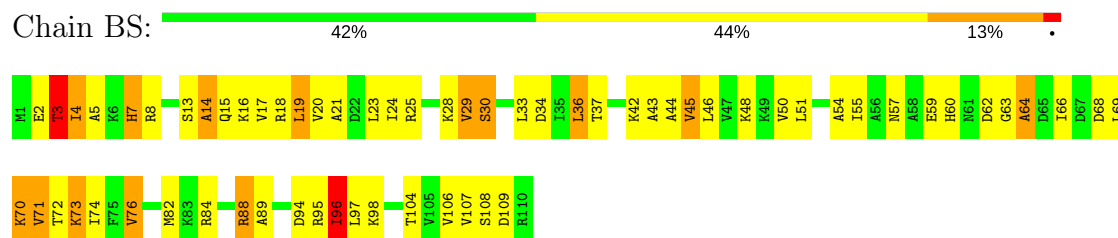


• Molecule 41: 50S ribosomal protein L21

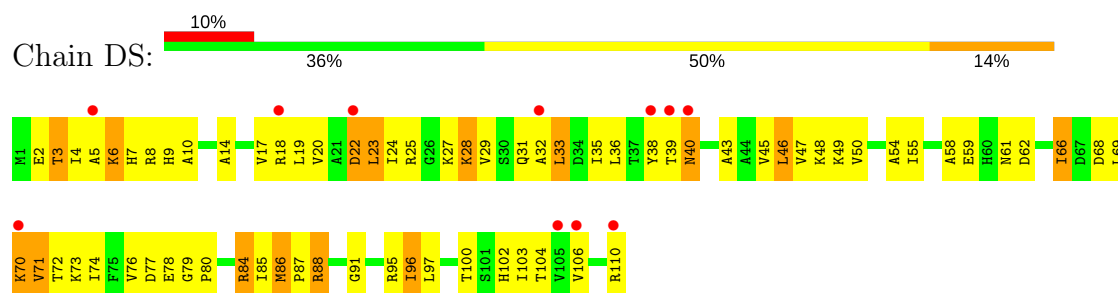
Chain DR: 17% 28% 56% 16%



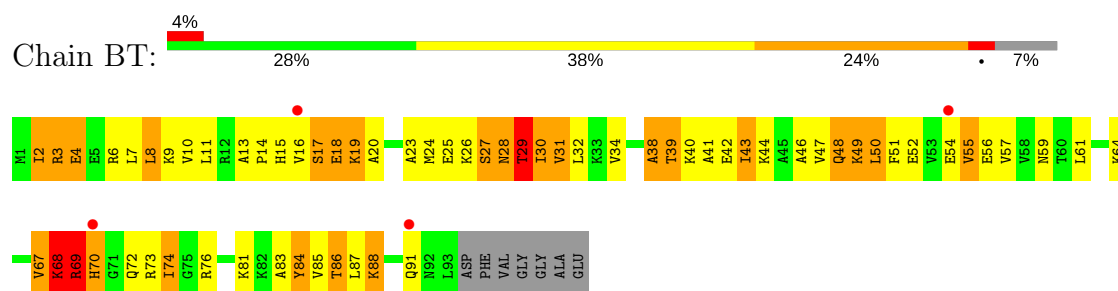
• Molecule 42: 50S ribosomal protein L22



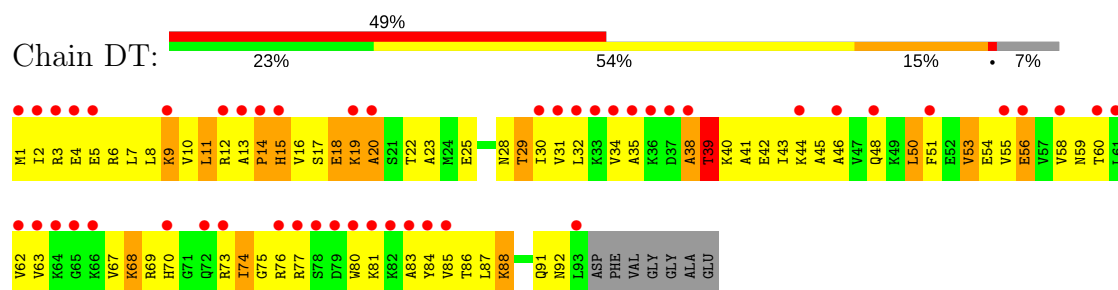
• Molecule 42: 50S ribosomal protein L22



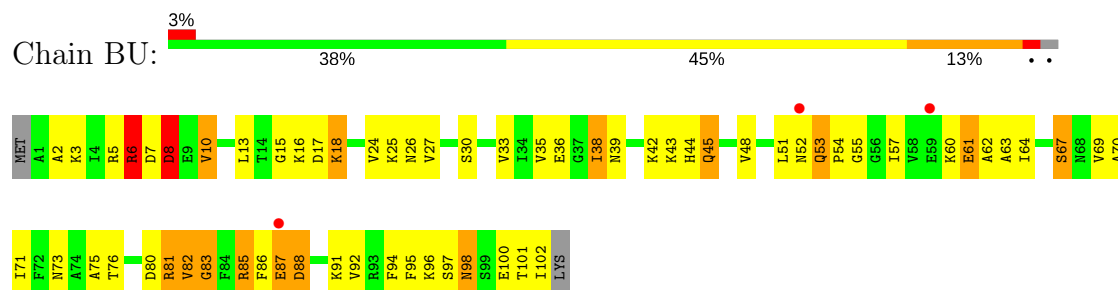
• Molecule 43: 50S ribosomal protein L23



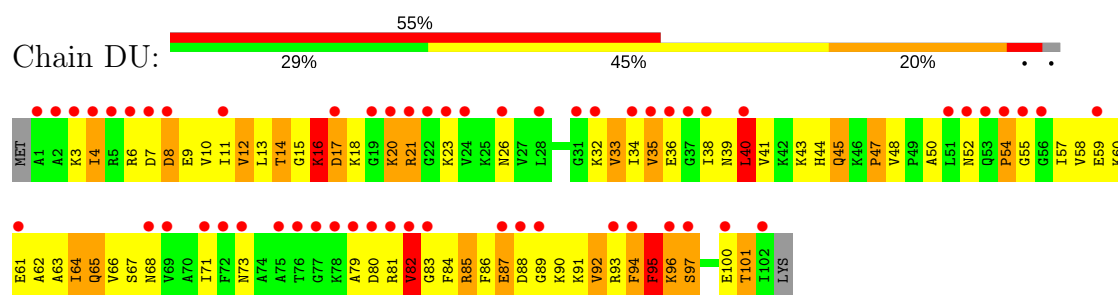
• Molecule 43: 50S ribosomal protein L23



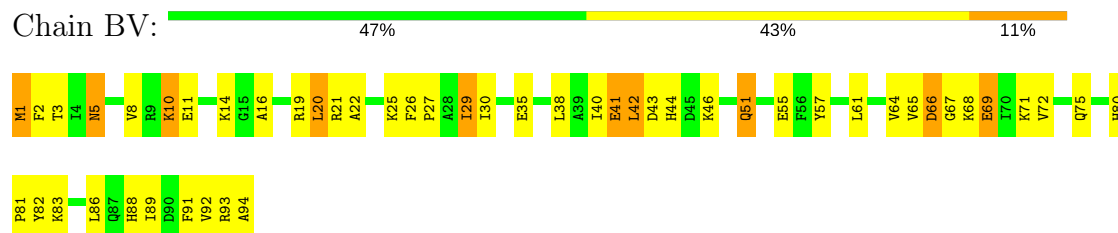
• Molecule 44: 50S ribosomal protein L24



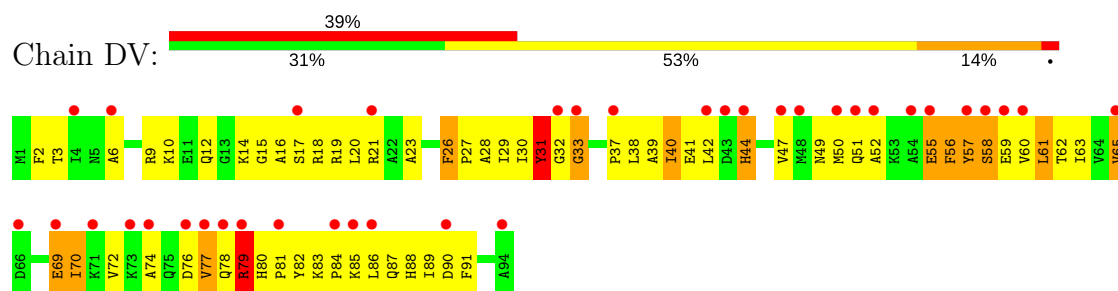
• Molecule 44: 50S ribosomal protein L24



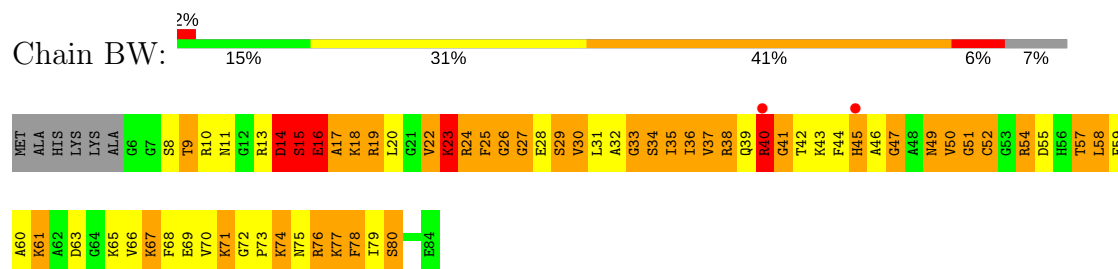
- Molecule 45: 50S ribosomal protein L25



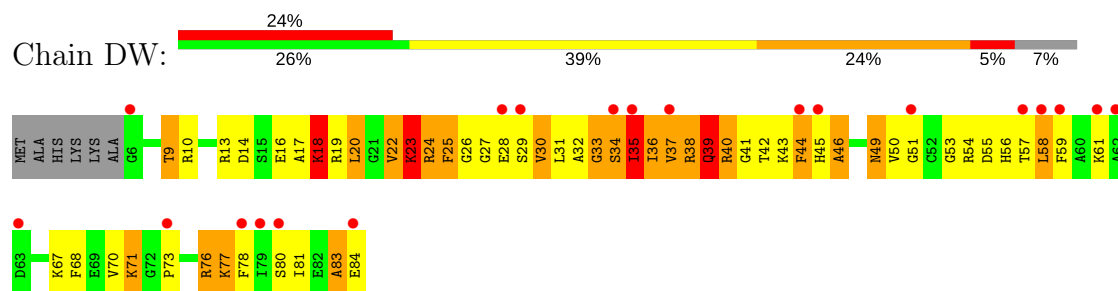
- Molecule 45: 50S ribosomal protein L25



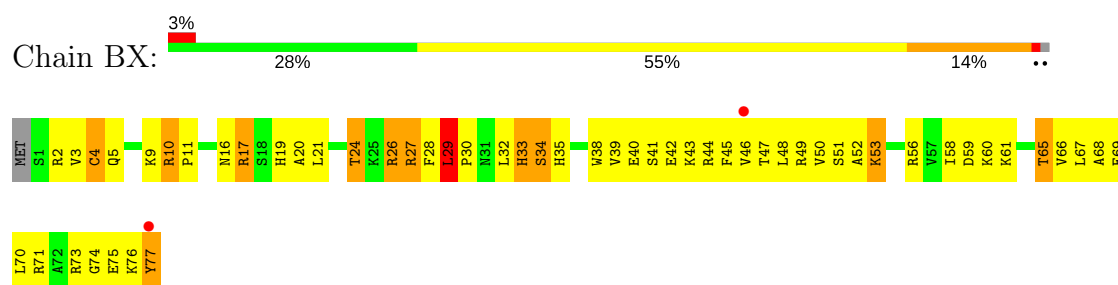
- Molecule 46: 50S ribosomal protein L27



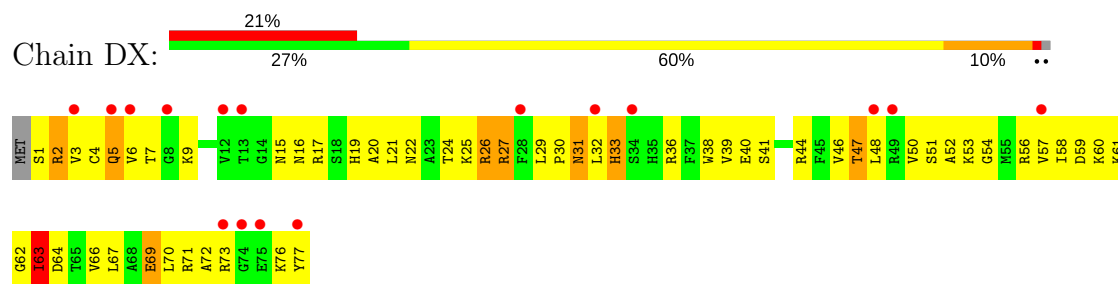
- Molecule 46: 50S ribosomal protein L27



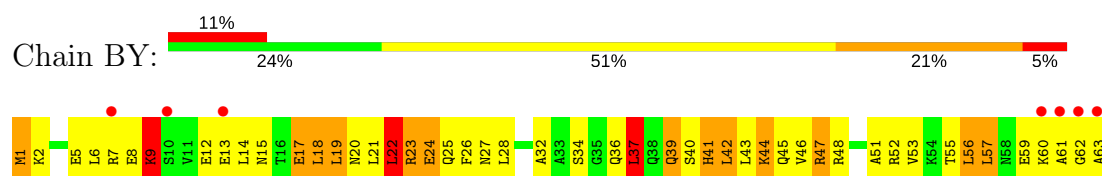
- Molecule 47: 50S ribosomal protein L28



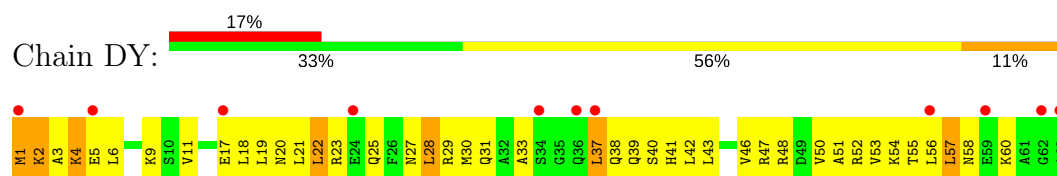
• Molecule 47: 50S ribosomal protein L28



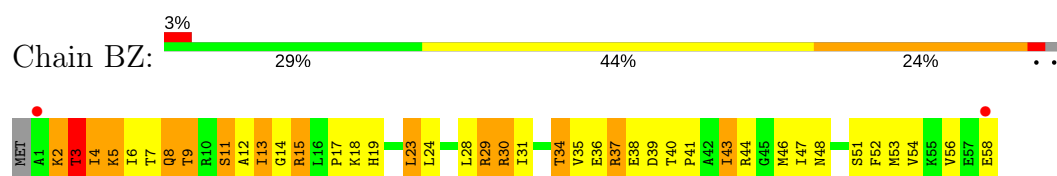
• Molecule 48: 50S ribosomal protein L29



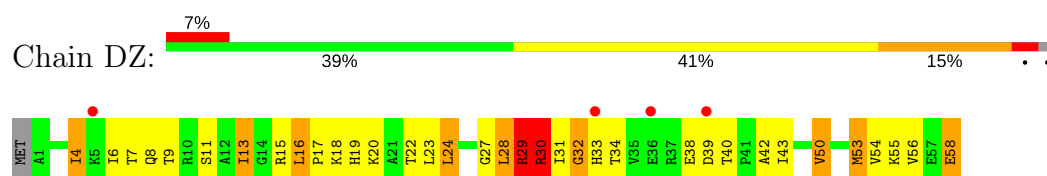
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30



• Molecule 49: 50S ribosomal protein L30

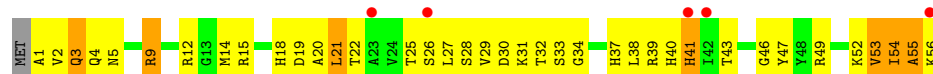


• Molecule 50: 50S ribosomal protein L32





- Molecule 50: 50S ribosomal protein L32



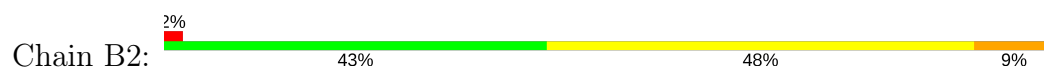
- Molecule 51: 50S ribosomal protein L33



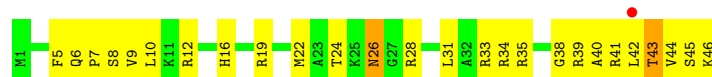
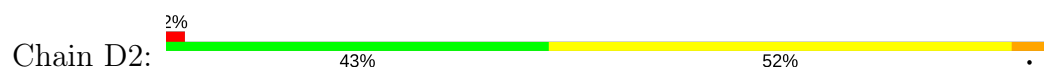
- Molecule 51: 50S ribosomal protein L33



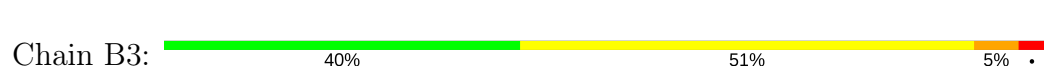
- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34

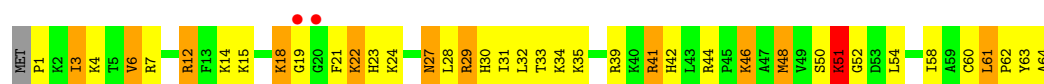


- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35





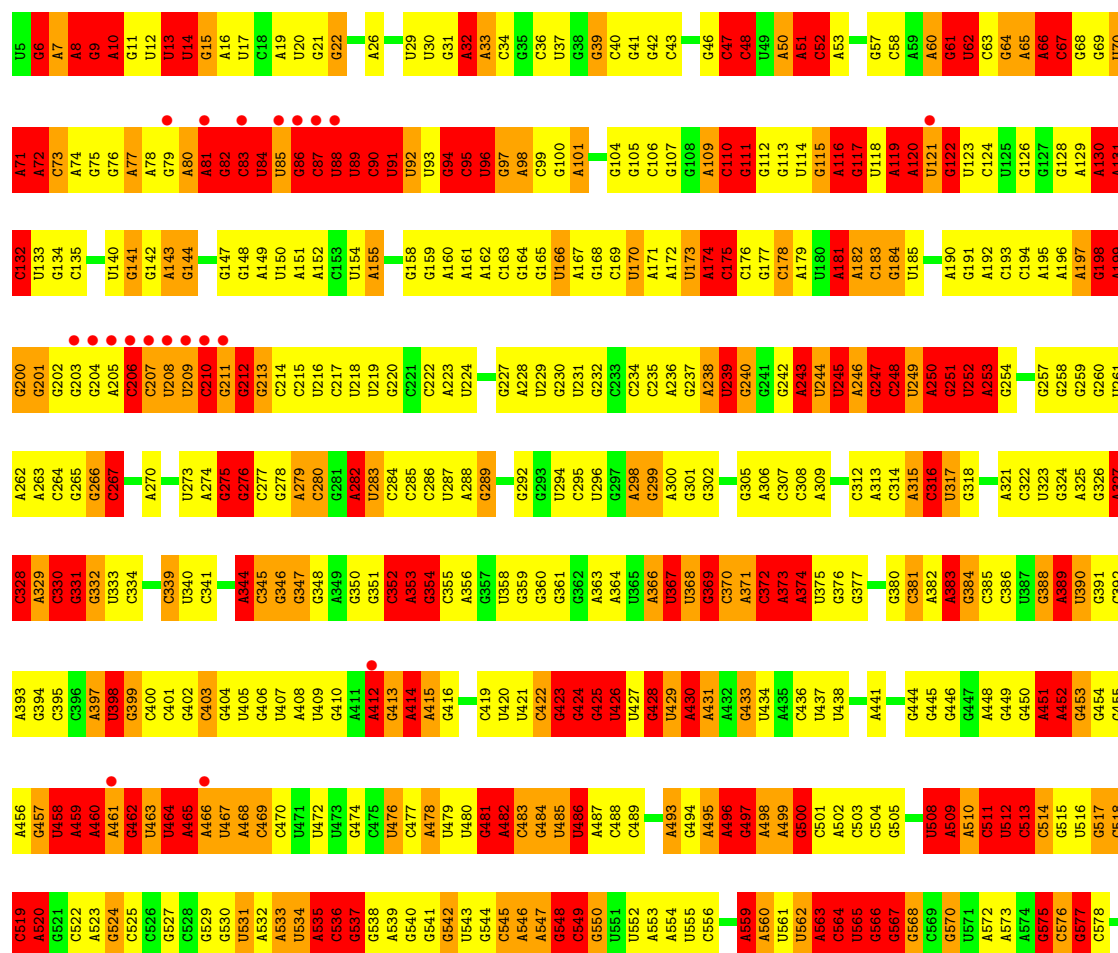
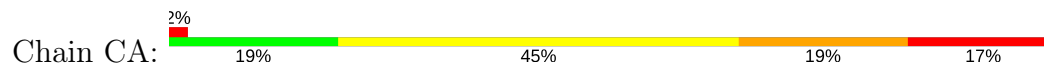
- Molecule 54: 50S ribosomal protein L36

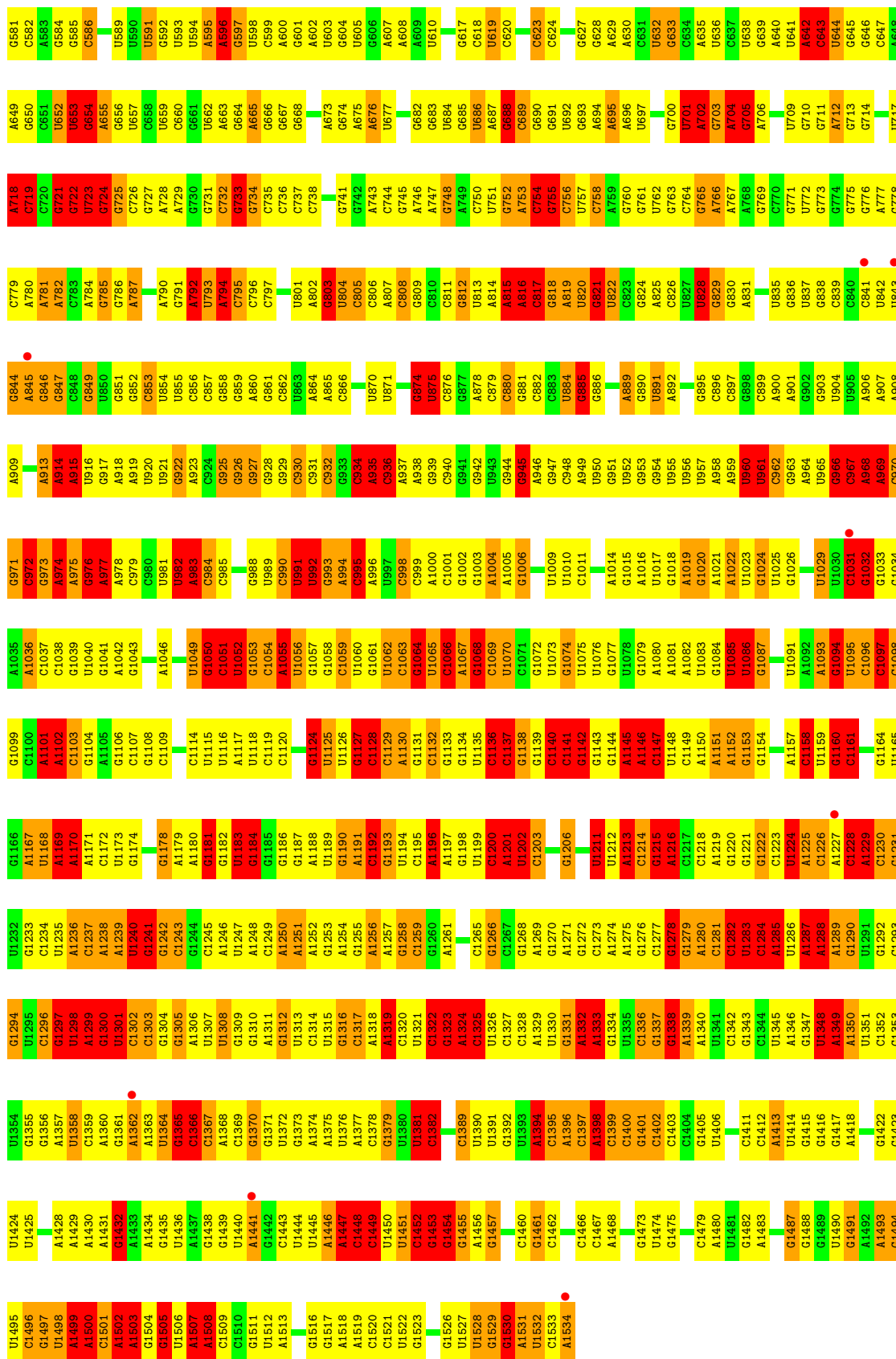


- Molecule 54: 50S ribosomal protein L36



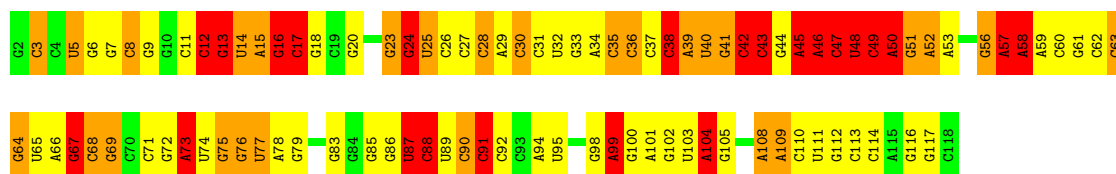
- Molecule 55: 16S rRNA





- Molecule 56: 5S rRNA

Frequency	Percentage
Daily	17%
Often	40%
Sometimes	23%
Never	20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.72Å 435.07Å 628.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.71 – 3.81 75.71 – 3.81	Depositor EDS
% Data completeness (in resolution range)	78.6 (75.71-3.81) 78.7 (75.71-3.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.207 , 0.253 0.217 , 0.261	Depositor DCC
$R_{free}$ test set	8852 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	285420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	AB	0.27	0/1735	0.48	0/2338
1	CB	0.28	0/1735	0.52	0/2338
2	AC	0.28	0/1651	0.50	0/2225
2	CC	0.29	0/1651	0.48	0/2225
3	AD	0.29	0/1665	0.48	0/2227
3	CD	0.36	0/1665	0.53	0/2227
4	AE	0.35	0/1118	0.64	1/1504 (0.1%)
4	CE	0.34	0/1118	0.55	0/1504
5	AF	0.27	0/835	0.49	0/1128
5	CF	0.26	0/835	0.48	0/1128
6	AG	0.26	0/1195	0.45	0/1602
6	CG	0.30	0/1187	0.51	0/1591
7	AH	0.31	0/989	0.49	0/1326
7	CH	0.30	0/989	0.50	0/1326
8	AI	0.26	0/1034	0.46	0/1375
8	CI	0.26	0/1034	0.46	0/1375
9	AJ	0.26	0/796	0.49	0/1077
9	CJ	0.26	0/796	0.50	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.30	0/893	0.52	0/1205
11	AL	0.34	0/969	0.60	0/1300
11	CL	0.30	0/969	0.56	0/1300
12	AM	0.27	0/892	0.54	1/1193 (0.1%)
12	CM	0.36	0/884	1.04	4/1181 (0.3%)
13	AN	0.25	0/785	0.45	0/1043
13	CN	0.26	0/780	0.45	0/1036
14	AO	0.25	0/722	0.45	0/964
14	CO	0.26	0/722	0.47	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.49	0/870
16	AQ	0.32	0/657	0.57	0/881
16	CQ	0.31	0/657	0.49	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.25	0/462	0.46	0/621
17	CR	0.31	0/462	0.49	0/621
18	AS	0.25	0/652	0.44	0/877
18	CS	0.25	0/652	0.46	0/877
19	AT	0.30	0/671	0.51	0/888
19	CT	0.27	0/671	0.46	0/888
20	AU	0.28	0/430	0.53	0/570
20	CU	0.33	0/430	0.57	0/570
21	AA	0.57	0/36834	1.45	646/57462 (1.1%)
22	AV	0.56	0/401	1.20	2/622 (0.3%)
22	CV	0.55	0/401	1.18	1/622 (0.2%)
23	AW	0.76	0/138	1.54	3/212 (1.4%)
23	CW	0.79	0/138	1.93	4/212 (1.9%)
24	BA	0.77	12/68626 (0.0%)	1.70	1788/107056 (1.7%)
24	DA	0.57	3/68314 (0.0%)	1.49	1376/106569 (1.3%)
25	BB	0.71	0/2828	1.59	62/4410 (1.4%)
26	BC	0.47	0/2121	0.73	1/2852 (0.0%)
26	DC	0.35	0/2121	0.58	0/2852
27	BD	0.52	0/1586	0.81	1/2134 (0.0%)
27	DD	0.32	0/1586	0.60	0/2134
28	BE	0.45	0/1571	0.67	0/2113
28	DE	0.33	0/1571	0.53	0/2113
29	BF	0.44	1/1434 (0.1%)	0.62	1/1926 (0.1%)
29	DF	0.45	3/1444 (0.2%)	0.79	5/1937 (0.3%)
30	BG	0.38	0/1343	0.64	0/1816
30	DG	0.28	0/1343	0.50	0/1816
31	BH	0.48	1/1122 (0.1%)	0.62	1/1515 (0.1%)
31	DH	0.39	0/1122	0.54	0/1515
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.24	0/1046	0.44	0/1410
33	BJ	0.56	0/1152	0.77	1/1551 (0.1%)
33	DJ	0.37	0/1152	0.62	0/1551
34	BK	0.53	0/947	0.82	1/1268 (0.1%)
34	DK	0.35	0/947	0.61	0/1268
35	BL	0.47	0/1054	0.76	1/1403 (0.1%)
35	DL	0.34	0/1054	0.58	0/1403
36	BM	0.50	0/1093	0.70	0/1460
36	DM	0.45	0/1093	0.63	0/1460
37	BN	0.48	0/973	0.73	1/1301 (0.1%)
37	DN	0.32	0/973	0.56	0/1301
38	BO	0.41	0/902	0.61	0/1209
38	DO	0.44	0/902	0.71	2/1209 (0.2%)
39	BP	0.48	0/929	0.74	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DP	0.33	0/929	0.52	0/1242
40	BQ	0.58	0/960	0.74	0/1278
40	DQ	0.36	0/960	0.54	0/1278
41	BR	0.57	0/829	0.77	0/1107
41	DR	0.38	0/829	0.58	0/1107
42	BS	0.54	0/864	0.78	0/1156
42	DS	0.30	0/864	0.56	0/1156
43	BT	0.44	0/744	0.67	0/994
43	DT	0.27	0/744	0.51	0/994
44	BU	0.42	0/787	0.71	1/1051 (0.1%)
44	DU	0.35	0/787	0.56	1/1051 (0.1%)
45	BV	0.47	0/766	0.68	0/1025
45	DV	0.68	3/766 (0.4%)	0.81	3/1025 (0.3%)
46	BW	0.54	0/603	0.84	0/797
46	DW	0.34	0/603	0.55	0/797
47	BX	0.41	0/635	0.68	1/848 (0.1%)
47	DX	0.32	0/635	0.55	0/848
48	BY	0.42	0/510	0.67	0/677
48	DY	0.28	0/510	0.49	0/677
49	BZ	0.47	0/453	0.73	0/605
49	DZ	0.32	0/453	0.58	0/605
50	B0	0.40	0/450	0.70	0/599
50	D0	0.31	0/450	0.55	0/599
51	B1	0.40	0/416	0.59	0/554
51	D1	0.31	0/416	0.49	0/554
52	B2	0.48	0/380	0.80	0/498
52	D2	0.31	0/380	0.53	0/498
53	B3	0.46	0/513	0.67	0/676
53	D3	0.36	0/513	0.57	0/676
54	B4	0.50	0/303	0.80	0/397
54	D4	0.41	0/303	0.60	0/397
55	CA	0.55	1/36762 (0.0%)	1.45	694/57350 (1.2%)
56	DB	0.68	4/2803 (0.1%)	1.79	112/4371 (2.6%)
All	All	0.57	28/307815 (0.0%)	1.37	4715/460233 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	BD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
36	DM	0	1
All	All	0	4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-11.34	1.31	1.37
45	DV	31	TYR	CE1-CZ	10.97	1.52	1.38
24	DA	1060	U	C2-N3	7.54	1.43	1.37
24	BA	1142	A	C8-N7	7.36	1.36	1.31
24	BA	2857	G	N3-C4	7.16	1.40	1.35

The worst 5 of 4715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	CM	2	ARG	NE-CZ-NH1	-22.49	109.06	120.30
24	BA	2447	G	C6-N1-C2	-18.42	114.05	125.10
12	CM	2	ARG	NE-CZ-NH2	17.95	129.28	120.30
24	BA	1330	C	N1-C1'-C2'	-17.28	91.53	114.00
56	DB	104	A	C8-N9-C4	-16.28	99.29	105.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	10	GLY	Peptide
27	BD	9	VAL	Peptide
29	DF	78	ILE	Peptide
36	DM	135	VAL	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	AB	1704	0	1732	269	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	1704	0	1732	208	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	159	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	143	0
4	AE	1105	0	1148	242	0
4	CE	1105	0	1148	122	0
5	AF	817	0	808	78	0
5	CF	817	0	808	79	0
6	AG	1181	0	1240	98	0
6	CG	1174	0	1230	151	0
7	AH	979	0	1034	118	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	116	0
8	CI	1022	0	1070	141	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	124	0
10	AK	877	0	887	85	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	102	0
12	AM	883	0	944	71	0
12	CM	876	0	937	137	0
13	AN	774	0	827	80	0
13	CN	769	0	822	89	0
14	AO	714	0	737	54	0
14	CO	714	0	737	40	0
15	AP	649	0	666	55	0
15	CP	638	0	656	65	0
16	AQ	648	0	691	82	0
16	CQ	648	0	691	47	0
17	AR	455	0	478	42	0
17	CR	455	0	478	40	0
18	AS	637	0	665	51	0
18	CS	637	0	665	78	0
19	AT	665	0	714	59	0
19	CT	665	0	714	47	0
20	AU	425	0	449	68	0
20	CU	425	0	449	76	0
21	AA	32895	0	16553	1701	0
22	AV	360	0	185	10	0
22	CV	360	0	185	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	125	0	63	4	0
23	CW	125	0	63	6	0
24	BA	61274	0	30819	3143	0
24	DA	60995	0	30677	3530	0
25	BB	2529	0	1281	108	0
26	BC	2082	0	2157	200	0
26	DC	2082	0	2157	211	0
27	BD	1565	0	1616	189	0
27	DD	1565	0	1616	165	0
28	BE	1552	0	1619	150	0
28	DE	1552	0	1619	167	0
29	BF	1410	0	1447	123	0
29	DF	1420	0	1460	197	0
30	BG	1323	0	1374	163	0
30	DG	1323	0	1374	147	0
31	BH	1111	0	1148	109	0
31	DH	1111	0	1148	106	0
32	BI	1032	0	1088	110	0
32	DI	1032	0	1088	67	0
33	BJ	1129	0	1162	158	0
33	DJ	1129	0	1162	118	0
34	BK	938	0	1012	113	0
34	DK	938	0	1012	112	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	142	0
36	BM	1074	0	1157	111	0
36	DM	1074	0	1157	109	0
37	BN	960	0	1000	99	0
37	DN	960	0	1000	115	0
38	BO	892	0	923	67	0
38	DO	892	0	923	155	0
39	BP	917	0	965	134	0
39	DP	917	0	965	106	0
40	BQ	947	0	1022	130	0
40	DQ	947	0	1022	129	0
41	BR	816	0	839	88	0
41	DR	816	0	839	97	0
42	BS	857	0	922	69	0
42	DS	857	0	922	69	0
43	BT	738	0	807	108	0
43	DT	738	0	807	93	0
44	BU	779	0	834	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DU	779	0	834	107	0
45	BV	753	0	780	53	0
45	DV	753	0	780	118	0
46	BW	596	0	610	179	0
46	DW	596	0	610	120	0
47	BX	625	0	655	69	0
47	DX	625	0	655	73	0
48	BY	509	0	543	67	0
48	DY	509	0	543	62	0
49	BZ	449	0	491	46	0
49	DZ	449	0	491	38	0
50	B0	444	0	461	32	0
50	D0	444	0	461	52	0
51	B1	409	0	440	37	0
51	D1	409	0	440	33	0
52	B2	377	0	418	32	0
52	D2	377	0	418	33	0
53	B3	504	0	574	46	0
53	D3	504	0	574	50	0
54	B4	302	0	340	32	0
54	D4	302	0	340	24	0
55	CA	32831	0	16521	1808	0
56	DB	2507	0	1270	203	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	DA	134	0	0	0	0
57	DB	1	0	0	0	0
57	DC	1	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	195	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	1	0
59	AN	5	0	0	0	0
59	AT	3	0	0	0	0
59	AU	1	0	0	0	0
59	B2	2	0	0	0	0
59	B3	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B4	2	0	0	0	0
59	BA	615	0	0	31	0
59	BB	19	0	0	0	0
59	BC	7	0	0	1	0
59	BD	2	0	0	3	0
59	BE	1	0	0	1	0
59	BL	4	0	0	1	0
59	BN	2	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	1	0
59	BV	1	0	0	1	0
59	CA	196	0	0	4	0
59	CE	3	0	0	1	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	598	0	0	14	0
59	DB	4	0	0	0	0
59	DC	14	0	0	2	0
59	DD	4	0	0	0	0
59	DE	2	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	5	0	0	0	0
59	DN	2	0	0	0	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	285420	0	191332	18973	0

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 40.

The worst 5 of 18973 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)
24:DA:1439:A:C2	24:DA:1552:A:C6	2.21	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DA:1439:A:N1	24:DA:1552:A:C5	2.03	1.26
24:DA:1439:A:C2	24:DA:1552:A:C5	2.25	1.25
38:DO:100:HIS:CE1	56:DB:48:U:O2'	1.89	1.25
38:DO:30:ARG:HB2	38:DO:30:ARG:NH1	1.53	1.21

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	
1	AB	216/241 (90%)	128 (59%)	60 (28%)	28 (13%)	0	6
1	CB	216/241 (90%)	145 (67%)	49 (23%)	22 (10%)	1	11
2	AC	204/233 (88%)	139 (68%)	51 (25%)	14 (7%)	1	22
2	CC	204/233 (88%)	146 (72%)	41 (20%)	17 (8%)	1	16
3	AD	203/206 (98%)	126 (62%)	52 (26%)	25 (12%)	0	7
3	CD	203/206 (98%)	141 (70%)	40 (20%)	22 (11%)	0	10
4	AE	148/167 (89%)	100 (68%)	31 (21%)	17 (12%)	0	8
4	CE	148/167 (89%)	98 (66%)	37 (25%)	13 (9%)	1	15
5	AF	98/135 (73%)	62 (63%)	25 (26%)	11 (11%)	0	9
5	CF	98/135 (73%)	65 (66%)	21 (21%)	12 (12%)	0	7
6	AG	149/179 (83%)	109 (73%)	29 (20%)	11 (7%)	1	20
6	CG	148/179 (83%)	80 (54%)	44 (30%)	24 (16%)	0	4
7	AH	127/130 (98%)	97 (76%)	22 (17%)	8 (6%)	1	25
7	CH	127/130 (98%)	96 (76%)	24 (19%)	7 (6%)	2	28
8	AI	125/130 (96%)	80 (64%)	34 (27%)	11 (9%)	1	15
8	CI	125/130 (96%)	86 (69%)	33 (26%)	6 (5%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	12 (12%)	15 (16%)	0	4
9	CJ	96/103 (93%)	61 (64%)	20 (21%)	15 (16%)	0	4
10	AK	115/129 (89%)	86 (75%)	22 (19%)	7 (6%)	2	25
10	CK	115/129 (89%)	74 (64%)	31 (27%)	10 (9%)	1	15
11	AL	121/124 (98%)	80 (66%)	24 (20%)	17 (14%)	0	5
11	CL	121/124 (98%)	86 (71%)	25 (21%)	10 (8%)	1	16
12	AM	112/118 (95%)	87 (78%)	16 (14%)	9 (8%)	1	17
12	CM	111/118 (94%)	65 (59%)	30 (27%)	16 (14%)	0	5
13	AN	92/101 (91%)	58 (63%)	25 (27%)	9 (10%)	1	13
13	CN	91/101 (90%)	59 (65%)	24 (26%)	8 (9%)	1	15
14	AO	86/89 (97%)	64 (74%)	17 (20%)	5 (6%)	2	26
14	CO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	15	58
15	AP	80/82 (98%)	54 (68%)	15 (19%)	11 (14%)	0	5
15	CP	78/82 (95%)	56 (72%)	14 (18%)	8 (10%)	0	11
16	AQ	78/84 (93%)	48 (62%)	21 (27%)	9 (12%)	0	8
16	CQ	78/84 (93%)	59 (76%)	13 (17%)	6 (8%)	1	19
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	4	35
17	CR	53/75 (71%)	44 (83%)	6 (11%)	3 (6%)	2	26
18	AS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	2	29
18	CS	77/92 (84%)	54 (70%)	19 (25%)	4 (5%)	2	29
19	AT	83/87 (95%)	55 (66%)	21 (25%)	7 (8%)	1	16
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	4	37
20	AU	49/71 (69%)	22 (45%)	18 (37%)	9 (18%)	0	3
20	CU	49/71 (69%)	20 (41%)	17 (35%)	12 (24%)	0	1
26	BC	269/273 (98%)	184 (68%)	59 (22%)	26 (10%)	1	13
26	DC	269/273 (98%)	181 (67%)	60 (22%)	28 (10%)	0	11
27	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	4
27	DD	207/209 (99%)	132 (64%)	45 (22%)	30 (14%)	0	5
28	BE	199/201 (99%)	151 (76%)	24 (12%)	24 (12%)	0	7
28	DE	199/201 (99%)	130 (65%)	43 (22%)	26 (13%)	0	6
29	BF	175/179 (98%)	133 (76%)	25 (14%)	17 (10%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	97 (55%)	45 (26%)	34 (19%)	0	2
30	BG	174/177 (98%)	112 (64%)	35 (20%)	27 (16%)	0	4
30	DG	174/177 (98%)	105 (60%)	41 (24%)	28 (16%)	0	4
31	BH	147/149 (99%)	62 (42%)	54 (37%)	31 (21%)	0	2
31	DH	147/149 (99%)	76 (52%)	50 (34%)	21 (14%)	0	5
32	BI	139/142 (98%)	84 (60%)	44 (32%)	11 (8%)	1	18
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	5
33	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	1	12
33	DJ	140/142 (99%)	95 (68%)	33 (24%)	12 (9%)	1	16
34	BK	120/123 (98%)	84 (70%)	18 (15%)	18 (15%)	0	4
34	DK	120/123 (98%)	80 (67%)	21 (18%)	19 (16%)	0	4
35	BL	141/144 (98%)	101 (72%)	28 (20%)	12 (8%)	1	16
35	DL	141/144 (98%)	83 (59%)	37 (26%)	21 (15%)	0	5
36	BM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	9
36	DM	134/136 (98%)	92 (69%)	25 (19%)	17 (13%)	0	7
37	BN	118/127 (93%)	87 (74%)	21 (18%)	10 (8%)	1	16
37	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	11
38	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	18
38	DO	114/117 (97%)	76 (67%)	29 (25%)	9 (8%)	1	18
39	BP	112/115 (97%)	71 (63%)	22 (20%)	19 (17%)	0	4
39	DP	112/115 (97%)	67 (60%)	28 (25%)	17 (15%)	0	4
40	BQ	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	18
40	DQ	115/118 (98%)	79 (69%)	26 (23%)	10 (9%)	1	15
41	BR	101/103 (98%)	79 (78%)	14 (14%)	8 (8%)	1	18
41	DR	101/103 (98%)	72 (71%)	19 (19%)	10 (10%)	1	12
42	BS	108/110 (98%)	76 (70%)	27 (25%)	5 (5%)	3	31
42	DS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	16
43	BT	91/100 (91%)	53 (58%)	23 (25%)	15 (16%)	0	4
43	DT	91/100 (91%)	48 (53%)	28 (31%)	15 (16%)	0	4
44	BU	100/104 (96%)	71 (71%)	13 (13%)	16 (16%)	0	4
44	DU	100/104 (96%)	51 (51%)	28 (28%)	21 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	8	47
45	DV	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1	19
46	BW	77/85 (91%)	29 (38%)	22 (29%)	26 (34%)	0	0
46	DW	77/85 (91%)	32 (42%)	27 (35%)	18 (23%)	0	1
47	BX	75/78 (96%)	59 (79%)	13 (17%)	3 (4%)	3	34
47	DX	75/78 (96%)	48 (64%)	21 (28%)	6 (8%)	1	17
48	BY	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	6
48	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	16
49	BZ	56/59 (95%)	39 (70%)	13 (23%)	4 (7%)	1	21
49	DZ	56/59 (95%)	31 (55%)	18 (32%)	7 (12%)	0	7
50	B0	54/57 (95%)	39 (72%)	9 (17%)	6 (11%)	0	9
50	D0	54/57 (95%)	40 (74%)	8 (15%)	6 (11%)	0	9
51	B1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	16
51	D1	48/55 (87%)	35 (73%)	9 (19%)	4 (8%)	1	16
52	B2	44/46 (96%)	35 (80%)	8 (18%)	1 (2%)	7	46
52	D2	44/46 (96%)	32 (73%)	7 (16%)	5 (11%)	0	8
53	B3	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	5	39
53	D3	62/65 (95%)	39 (63%)	17 (27%)	6 (10%)	1	13
54	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	16
54	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	5
All	All	11238/11970 (94%)	7499 (67%)	2485 (22%)	1254 (11%)	0	9

5 of 1254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	40	ILE
1	AB	71	THR
1	AB	72	LYS

### 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	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	2	14
1	CB	180/199 (90%)	157 (87%)	23 (13%)	5	29
2	AC	170/190 (90%)	148 (87%)	22 (13%)	5	29
2	CC	170/190 (90%)	153 (90%)	17 (10%)	9	39
3	AD	172/173 (99%)	144 (84%)	28 (16%)	3	20
3	CD	172/173 (99%)	146 (85%)	26 (15%)	3	23
4	AE	113/126 (90%)	90 (80%)	23 (20%)	1	11
4	CE	113/126 (90%)	97 (86%)	16 (14%)	4	26
5	AF	87/116 (75%)	77 (88%)	10 (12%)	6	34
5	CF	87/116 (75%)	78 (90%)	9 (10%)	8	38
6	AG	124/147 (84%)	116 (94%)	8 (6%)	20	57
6	CG	123/147 (84%)	97 (79%)	26 (21%)	1	10
7	AH	104/105 (99%)	92 (88%)	12 (12%)	6	34
7	CH	104/105 (99%)	87 (84%)	17 (16%)	3	20
8	AI	105/107 (98%)	88 (84%)	17 (16%)	3	20
8	CI	105/107 (98%)	91 (87%)	14 (13%)	4	28
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	3	20
9	CJ	86/90 (96%)	74 (86%)	12 (14%)	4	26
10	AK	90/99 (91%)	81 (90%)	9 (10%)	9	39
10	CK	90/99 (91%)	73 (81%)	17 (19%)	2	13
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	16
11	CL	103/104 (99%)	85 (82%)	18 (18%)	2	16
12	AM	92/96 (96%)	87 (95%)	5 (5%)	26	63
12	CM	91/96 (95%)	75 (82%)	16 (18%)	2	16
13	AN	79/84 (94%)	74 (94%)	5 (6%)	21	58
13	CN	79/84 (94%)	67 (85%)	12 (15%)	3	22
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	43
14	CO	76/77 (99%)	71 (93%)	5 (7%)	19	57
15	AP	65/65 (100%)	59 (91%)	6 (9%)	11	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	11	43
16	AQ	74/78 (95%)	57 (77%)	17 (23%)	1	7
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	4	27
17	AR	48/65 (74%)	47 (98%)	1 (2%)	59	82
17	CR	48/65 (74%)	45 (94%)	3 (6%)	21	58
18	AS	70/79 (89%)	62 (89%)	8 (11%)	7	34
18	CS	70/79 (89%)	59 (84%)	11 (16%)	3	22
19	AT	65/66 (98%)	56 (86%)	9 (14%)	4	27
19	CT	65/66 (98%)	58 (89%)	7 (11%)	7	37
20	AU	44/61 (72%)	36 (82%)	8 (18%)	2	14
20	CU	44/61 (72%)	33 (75%)	11 (25%)	1	6
26	BC	216/218 (99%)	177 (82%)	39 (18%)	2	15
26	DC	216/218 (99%)	191 (88%)	25 (12%)	6	33
27	BD	164/164 (100%)	133 (81%)	31 (19%)	2	13
27	DD	164/164 (100%)	144 (88%)	20 (12%)	6	31
28	BE	165/165 (100%)	128 (78%)	37 (22%)	1	8
28	DE	165/165 (100%)	150 (91%)	15 (9%)	11	44
29	BF	148/150 (99%)	129 (87%)	19 (13%)	5	29
29	DF	149/150 (99%)	121 (81%)	28 (19%)	2	13
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	9
30	DG	137/138 (99%)	120 (88%)	17 (12%)	5	30
31	BH	114/114 (100%)	98 (86%)	16 (14%)	4	26
31	DH	114/114 (100%)	97 (85%)	17 (15%)	3	23
32	BI	109/110 (99%)	92 (84%)	17 (16%)	3	22
32	DI	109/110 (99%)	102 (94%)	7 (6%)	20	57
33	BJ	116/116 (100%)	91 (78%)	25 (22%)	1	9
33	DJ	116/116 (100%)	105 (90%)	11 (10%)	10	42
34	BK	103/104 (99%)	82 (80%)	21 (20%)	1	11
34	DK	103/104 (99%)	85 (82%)	18 (18%)	2	16
35	BL	102/103 (99%)	77 (76%)	25 (24%)	1	6
35	DL	102/103 (99%)	87 (85%)	15 (15%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	89 (82%)	20 (18%)	2	14
36	DM	109/109 (100%)	96 (88%)	13 (12%)	6	32
37	BN	100/103 (97%)	78 (78%)	22 (22%)	1	9
37	DN	100/103 (97%)	87 (87%)	13 (13%)	5	29
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	12
38	DO	86/87 (99%)	76 (88%)	10 (12%)	6	33
39	BP	99/100 (99%)	77 (78%)	22 (22%)	1	8
39	DP	99/100 (99%)	91 (92%)	8 (8%)	14	49
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	2	15
40	DQ	89/90 (99%)	78 (88%)	11 (12%)	5	30
41	BR	84/84 (100%)	68 (81%)	16 (19%)	2	13
41	DR	84/84 (100%)	72 (86%)	12 (14%)	4	25
42	BS	93/93 (100%)	76 (82%)	17 (18%)	2	14
42	DS	93/93 (100%)	80 (86%)	13 (14%)	4	26
43	BT	80/84 (95%)	63 (79%)	17 (21%)	1	9
43	DT	80/84 (95%)	75 (94%)	5 (6%)	21	58
44	BU	83/85 (98%)	73 (88%)	10 (12%)	6	31
44	DU	83/85 (98%)	72 (87%)	11 (13%)	4	28
45	BV	78/78 (100%)	64 (82%)	14 (18%)	2	15
45	DV	78/78 (100%)	65 (83%)	13 (17%)	2	19
46	BW	59/63 (94%)	39 (66%)	20 (34%)	0	1
46	DW	59/63 (94%)	43 (73%)	16 (27%)	0	4
47	BX	67/68 (98%)	56 (84%)	11 (16%)	2	19
47	DX	67/68 (98%)	58 (87%)	9 (13%)	4	28
48	BY	55/55 (100%)	41 (74%)	14 (26%)	0	6
48	DY	55/55 (100%)	51 (93%)	4 (7%)	16	53
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	3
49	DZ	48/49 (98%)	39 (81%)	9 (19%)	2	13
50	B0	47/48 (98%)	43 (92%)	4 (8%)	12	48
50	D0	47/48 (98%)	41 (87%)	6 (13%)	5	29
51	B1	45/49 (92%)	35 (78%)	10 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	11	45
52	B2	38/38 (100%)	32 (84%)	6 (16%)	3	21
52	D2	38/38 (100%)	34 (90%)	4 (10%)	8	37
53	B3	51/52 (98%)	45 (88%)	6 (12%)	6	32
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2	16
54	B4	34/34 (100%)	29 (85%)	5 (15%)	3	24
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	24
All	All	9331/9756 (96%)	7927 (85%)	1404 (15%)	3	23

5 of 1404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BS	29	VAL
1	CB	19	THR
42	DS	22	ASP
43	BT	17	SER
47	BX	24	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	51	GLN
3	CD	125	ASN
44	DU	53	GLN
46	BW	49	ASN
1	CB	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	474 (30%)	0
22	AV	16/17 (94%)	0	0
22	CV	16/17 (94%)	1 (6%)	0
23	AW	5/6 (83%)	3 (60%)	0
23	CW	5/6 (83%)	2 (40%)	0
24	BA	2850/2903 (98%)	958 (33%)	0
24	DA	2837/2903 (97%)	1000 (35%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	BB	117/118 (99%)	33 (28%)	0
55	CA	1529/1530 (99%)	519 (33%)	0
56	DB	116/117 (99%)	42 (36%)	0
All	All	9023/9150 (98%)	3032 (33%)	0

5 of 3032 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

There are no RNA pucker outliers to report.

## 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 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AB	218/241 (90%)	2.67	105 (48%) 0 1	206, 268, 283, 298	0
1	CB	218/241 (90%)	0.97	48 (22%) 1 1	146, 174, 199, 216	0
2	AC	206/233 (88%)	0.31	4 (1%) 67 58	106, 135, 169, 198	0
2	CC	206/233 (88%)	0.21	4 (1%) 67 58	111, 140, 177, 195	0
3	AD	205/206 (99%)	0.20	10 (4%) 30 24	102, 139, 185, 204	0
3	CD	205/206 (99%)	-0.26	1 (0%) 90 86	86, 109, 140, 157	0
4	AE	150/167 (89%)	2.98	79 (52%) 0 1	102, 214, 237, 255	0
4	CE	150/167 (89%)	0.44	8 (5%) 27 22	86, 134, 166, 209	0
5	AF	100/135 (74%)	0.64	15 (15%) 3 3	140, 166, 186, 192	0
5	CF	100/135 (74%)	0.72	12 (12%) 5 6	140, 170, 200, 208	0
6	AG	151/179 (84%)	0.48	9 (5%) 23 17	128, 157, 186, 202	0
6	CG	150/179 (83%)	0.49	20 (13%) 4 4	115, 165, 204, 219	0
7	AH	129/130 (99%)	0.47	9 (6%) 17 13	102, 134, 158, 182	0
7	CH	129/130 (99%)	0.23	3 (2%) 61 51	106, 135, 159, 174	0
8	AI	127/130 (97%)	0.47	10 (7%) 13 11	108, 158, 190, 210	0
8	CI	127/130 (97%)	0.74	19 (14%) 3 3	114, 174, 206, 221	0
9	AJ	98/103 (95%)	0.15	1 (1%) 82 74	105, 150, 194, 211	0
9	CJ	98/103 (95%)	0.82	16 (16%) 2 3	113, 165, 210, 220	0
10	AK	117/129 (90%)	0.85	16 (13%) 3 4	100, 149, 183, 200	0
10	CK	117/129 (90%)	0.60	11 (9%) 9 8	89, 133, 167, 192	0
11	AL	123/124 (99%)	0.16	4 (3%) 47 37	75, 95, 132, 157	0
11	CL	123/124 (99%)	0.09	2 (1%) 72 63	83, 101, 132, 151	0
12	AM	114/118 (96%)	0.54	13 (11%) 6 6	122, 182, 213, 232	0
12	CM	113/118 (95%)	0.62	9 (7%) 13 11	133, 193, 225, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/101 (95%)	0.25	4 (4%) 37 29	111, 142, 184, 210	0
13	CN	95/101 (94%)	0.56	10 (10%) 7 6	117, 149, 199, 207	0
14	AO	88/89 (98%)	0.15	1 (1%) 80 72	105, 133, 163, 199	0
14	CO	88/89 (98%)	0.13	2 (2%) 61 51	113, 141, 174, 197	0
15	AP	82/82 (100%)	0.93	18 (21%) 1 1	95, 127, 165, 208	0
15	CP	80/82 (97%)	0.87	10 (12%) 4 5	98, 122, 156, 189	0
16	AQ	80/84 (95%)	0.74	6 (7%) 15 12	69, 100, 142, 159	0
16	CQ	80/84 (95%)	0.93	9 (11%) 6 6	72, 111, 142, 159	0
17	AR	55/75 (73%)	0.61	7 (12%) 4 5	129, 148, 180, 190	0
17	CR	55/75 (73%)	0.87	8 (14%) 3 3	131, 150, 170, 182	0
18	AS	79/92 (85%)	0.82	13 (16%) 2 3	140, 176, 210, 235	0
18	CS	79/92 (85%)	1.24	16 (20%) 1 2	151, 182, 215, 230	0
19	AT	85/87 (97%)	0.15	0 100 100	89, 121, 149, 180	0
19	CT	85/87 (97%)	0.66	8 (9%) 9 8	115, 153, 185, 206	0
20	AU	51/71 (71%)	0.61	6 (11%) 5 6	98, 145, 201, 208	0
20	CU	51/71 (71%)	0.65	7 (13%) 3 4	104, 139, 173, 193	0
21	AA	1533/1533 (100%)	-0.49	15 (0%) 82 74	65, 123, 208, 301	0
22	AV	17/17 (100%)	-0.16	1 (5%) 23 17	102, 112, 149, 197	0
22	CV	17/17 (100%)	-0.22	1 (5%) 23 17	99, 104, 145, 179	0
23	AW	6/6 (100%)	0.56	1 (16%) 2 3	100, 109, 120, 155	0
23	CW	6/6 (100%)	0.21	0 100 100	98, 105, 123, 130	0
24	BA	2854/2903 (98%)	-0.43	40 (1%) 75 66	36, 66, 188, 342	0
24	DA	2841/2903 (97%)	-0.08	57 (2%) 65 56	79, 132, 236, 340	0
25	BB	118/118 (100%)	-0.65	0 100 100	52, 81, 113, 162	0
26	BC	271/273 (99%)	-0.12	4 (1%) 74 64	44, 80, 122, 159	0
26	DC	271/273 (99%)	0.44	14 (5%) 28 22	89, 133, 164, 189	0
27	BD	209/209 (100%)	-0.14	0 100 100	37, 59, 105, 146	0
27	DD	209/209 (100%)	0.50	19 (9%) 10 8	83, 131, 164, 186	0
28	BE	201/201 (100%)	-0.04	4 (1%) 65 56	38, 84, 131, 164	0
28	DE	201/201 (100%)	0.51	16 (7%) 13 11	95, 171, 212, 250	0
29	BF	177/179 (98%)	0.99	27 (15%) 2 3	90, 148, 201, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DF	178/179 (99%)	2.88	103 (57%) 0 1	250, 278, 301, 305	0
30	BG	176/177 (99%)	0.02	2 (1%) 80 72	66, 91, 135, 160	0
30	DG	176/177 (99%)	0.99	28 (15%) 2 3	120, 148, 177, 204	0
31	BH	149/149 (100%)	3.03	69 (46%) 0 1	89, 262, 290, 299	0
31	DH	149/149 (100%)	2.49	66 (44%) 0 1	156, 244, 279, 286	0
32	BI	141/142 (99%)	2.25	64 (45%) 0 1	237, 306, 364, 376	0
32	DI	141/142 (99%)	2.79	80 (56%) 0 1	277, 331, 367, 378	0
33	BJ	142/142 (100%)	-0.30	0 100 100	41, 57, 102, 157	0
33	DJ	142/142 (100%)	0.20	3 (2%) 64 54	92, 115, 142, 181	0
34	BK	122/123 (99%)	-0.23	0 100 100	41, 56, 110, 177	0
34	DK	122/123 (99%)	0.51	3 (2%) 58 47	93, 115, 144, 173	0
35	BL	143/144 (99%)	-0.22	1 (0%) 87 82	38, 77, 119, 160	0
35	DL	143/144 (99%)	0.70	19 (13%) 4 4	93, 155, 197, 209	0
36	BM	136/136 (100%)	-0.13	1 (0%) 87 82	41, 67, 114, 152	0
36	DM	136/136 (100%)	0.90	22 (16%) 2 3	80, 107, 142, 164	0
37	BN	120/127 (94%)	-0.12	0 100 100	46, 63, 84, 138	0
37	DN	120/127 (94%)	1.09	24 (20%) 1 2	122, 154, 180, 217	0
38	BO	116/117 (99%)	-0.28	0 100 100	73, 84, 124, 149	0
38	DO	116/117 (99%)	2.06	54 (46%) 0 1	165, 197, 217, 225	0
39	BP	114/115 (99%)	-0.21	1 (0%) 84 77	49, 67, 123, 152	0
39	DP	114/115 (99%)	0.46	6 (5%) 27 22	117, 137, 163, 182	0
40	BQ	117/118 (99%)	-0.49	0 100 100	40, 58, 100, 127	0
40	DQ	117/118 (99%)	0.47	7 (5%) 23 17	97, 119, 143, 172	0
41	BR	103/103 (100%)	-0.11	1 (0%) 82 74	39, 70, 116, 158	0
41	DR	103/103 (100%)	0.86	17 (16%) 2 3	96, 133, 157, 164	0
42	BS	110/110 (100%)	-0.37	0 100 100	41, 58, 95, 161	0
42	DS	110/110 (100%)	0.68	11 (10%) 8 7	98, 141, 173, 188	0
43	BT	93/100 (93%)	0.38	4 (4%) 36 28	56, 95, 135, 165	0
43	DT	93/100 (93%)	2.17	49 (52%) 0 1	144, 196, 226, 237	0
44	BU	102/104 (98%)	0.27	3 (2%) 52 41	77, 105, 139, 194	0
44	DU	102/104 (98%)	2.36	57 (55%) 0 1	174, 208, 248, 279	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	BV	94/94 (100%)	0.02	0 100 100	60, 81, 115, 143	0
45	DV	94/94 (100%)	1.79	37 (39%) 0 1	125, 188, 226, 239	0
46	BW	79/85 (92%)	0.09	2 (2%) 58 47	50, 75, 131, 168	0
46	DW	79/85 (92%)	1.22	20 (25%) 1 1	88, 134, 164, 184	0
47	BX	77/78 (98%)	-0.26	2 (2%) 56 45	50, 84, 126, 147	0
47	DX	77/78 (98%)	0.92	16 (20%) 1 2	110, 157, 187, 203	0
48	BY	63/63 (100%)	0.22	7 (11%) 6 6	87, 109, 154, 163	0
48	DY	63/63 (100%)	0.91	11 (17%) 2 2	196, 218, 251, 257	0
49	BZ	58/59 (98%)	-0.07	2 (3%) 46 36	49, 63, 106, 145	0
49	DZ	58/59 (98%)	0.50	4 (6%) 18 13	97, 116, 142, 155	0
50	B0	56/57 (98%)	-0.48	0 100 100	40, 63, 119, 143	0
50	D0	56/57 (98%)	0.53	5 (8%) 10 8	93, 152, 190, 202	0
51	B1	50/55 (90%)	0.38	1 (2%) 65 56	63, 91, 117, 156	0
51	D1	50/55 (90%)	1.18	11 (22%) 1 1	113, 142, 173, 179	0
52	B2	46/46 (100%)	-0.30	1 (2%) 62 53	50, 61, 80, 165	0
52	D2	46/46 (100%)	0.20	1 (2%) 62 53	118, 137, 161, 174	0
53	B3	64/65 (98%)	-0.28	0 100 100	45, 63, 98, 133	0
53	D3	64/65 (98%)	0.45	2 (3%) 49 39	105, 123, 146, 174	0
54	B4	38/38 (100%)	-0.16	0 100 100	54, 68, 100, 118	0
54	D4	38/38 (100%)	0.82	1 (2%) 56 45	95, 117, 138, 142	0
55	CA	1530/1530 (100%)	-0.27	28 (1%) 69 60	77, 126, 214, 305	0
56	DB	117/117 (100%)	-0.41	0 100 100	87, 166, 194, 210	0
All	All	20477/21120 (96%)	0.23	1598 (7%) 14 11	36, 125, 246, 378	0

The worst 5 of 1598 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	BH	92	GLY	21.9
31	DH	92	GLY	21.4
31	DH	93	SER	20.7
29	DF	129	MET	20.6
31	BH	119	ASN	18.2

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3062	1/1	0.69	1.05	27.84	85,85,85,85	0
57	MG	DA	3134	1/1	0.82	1.43	26.25	126,126,126,126	0
57	MG	DA	3077	1/1	0.92	0.67	21.95	86,86,86,86	0
57	MG	DA	3109	1/1	0.65	0.45	21.61	92,92,92,92	0
57	MG	BA	3037	1/1	0.85	0.36	17.52	42,42,42,42	0
57	MG	BA	3058	1/1	0.83	0.49	16.57	44,44,44,44	0
57	MG	BA	3071	1/1	0.83	0.36	15.81	38,38,38,38	0
57	MG	BA	3041	1/1	0.94	0.26	11.89	43,43,43,43	0
57	MG	CA	1625	1/1	0.85	0.33	11.43	86,86,86,86	0
57	MG	DA	3054	1/1	0.86	0.39	10.05	88,88,88,88	0
57	MG	CA	1629	1/1	0.87	0.51	8.99	111,111,111,111	0
57	MG	BA	3005	1/1	0.87	0.21	8.96	73,73,73,73	0
57	MG	AA	1607	1/1	0.19	0.36	7.70	88,88,88,88	0
57	MG	BA	3136	1/1	0.98	0.44	6.94	47,47,47,47	0
57	MG	BA	3124	1/1	0.82	0.55	6.73	41,41,41,41	0
57	MG	CA	1628	1/1	0.90	0.35	6.15	79,79,79,79	0
57	MG	BA	3118	1/1	0.96	0.24	6.10	42,42,42,42	0
57	MG	BA	3002	1/1	0.93	0.32	6.03	47,47,47,47	0
57	MG	AA	1642	1/1	0.87	0.20	5.43	74,74,74,74	0
57	MG	DA	3002	1/1	0.91	0.30	5.38	125,125,125,125	0
57	MG	DA	3071	1/1	0.74	0.60	5.33	94,94,94,94	0
57	MG	BA	3105	1/1	0.95	0.21	5.26	38,38,38,38	0
57	MG	AA	1631	1/1	0.92	0.27	4.39	98,98,98,98	0
57	MG	DA	3041	1/1	0.70	0.26	3.96	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3072	1/1	0.94	0.22	3.51	38,38,38,38	0
57	MG	BA	3109	1/1	0.95	0.21	3.43	42,42,42,42	0
57	MG	AA	1641	1/1	0.83	0.33	3.43	89,89,89,89	0
57	MG	CA	1637	1/1	0.98	0.31	3.11	83,83,83,83	0
57	MG	AA	1629	1/1	0.90	0.23	2.92	129,129,129,129	0
57	MG	DA	3101	1/1	0.93	0.26	2.76	82,82,82,82	0
57	MG	BA	3104	1/1	0.97	0.20	2.62	38,38,38,38	0
57	MG	CA	1639	1/1	0.84	0.24	2.52	165,165,165,165	0
57	MG	CA	1617	1/1	0.67	0.45	2.06	130,130,130,130	0
57	MG	BA	3028	1/1	0.85	0.21	2.05	39,39,39,39	0
57	MG	CA	1604	1/1	0.91	0.13	2.00	106,106,106,106	0
57	MG	DA	3107	1/1	0.68	0.23	1.98	130,130,130,130	0
57	MG	CA	1613	1/1	0.87	0.24	1.88	79,79,79,79	0
57	MG	CA	1630	1/1	0.90	0.28	1.87	79,79,79,79	0
57	MG	CA	1607	1/1	0.83	0.23	1.78	89,89,89,89	0
57	MG	AA	1604	1/1	0.80	0.12	1.42	126,126,126,126	0
57	MG	DA	3053	1/1	0.90	0.24	1.41	101,101,101,101	0
57	MG	BB	202	1/1	0.94	0.17	1.25	114,114,114,114	0
57	MG	CA	1618	1/1	0.92	0.21	1.15	108,108,108,108	0
57	MG	CA	1641	1/1	0.97	0.18	0.88	91,91,91,91	0
57	MG	BA	3132	1/1	0.94	0.45	0.83	42,42,42,42	0
57	MG	BA	3059	1/1	0.96	0.20	0.82	50,50,50,50	0
57	MG	DA	3104	1/1	0.93	0.22	0.78	107,107,107,107	0
57	MG	DA	3003	1/1	0.92	0.23	0.77	94,94,94,94	0
57	MG	BA	3130	1/1	0.97	0.17	0.68	49,49,49,49	0
57	MG	CA	1621	1/1	0.96	0.19	0.67	85,85,85,85	0
57	MG	DA	3094	1/1	0.90	0.18	0.63	126,126,126,126	0
57	MG	DA	3129	1/1	0.87	0.28	0.46	83,83,83,83	0
57	MG	BA	3038	1/1	0.95	0.17	0.44	42,42,42,42	0
57	MG	BA	3008	1/1	0.99	0.17	0.42	43,43,43,43	0
57	MG	DA	3027	1/1	0.84	0.18	0.35	87,87,87,87	0
57	MG	DA	3025	1/1	0.97	0.19	0.25	105,105,105,105	0
57	MG	BA	3048	1/1	0.94	0.16	0.23	74,74,74,74	0
57	MG	DA	3086	1/1	0.70	0.21	0.16	148,148,148,148	0
57	MG	AA	1613	1/1	0.97	0.15	0.15	74,74,74,74	0
57	MG	BA	3128	1/1	0.96	0.15	0.14	52,52,52,52	0
57	MG	BA	3101	1/1	0.97	0.17	0.12	38,38,38,38	0
57	MG	DA	3050	1/1	0.90	0.20	-0.09	148,148,148,148	0
57	MG	BA	3108	1/1	0.98	0.14	-0.35	40,40,40,40	0
57	MG	BA	3107	1/1	0.89	0.18	-0.45	49,49,49,49	0
57	MG	AA	1625	1/1	0.79	0.15	-0.62	90,90,90,90	0
57	MG	DA	3085	1/1	0.60	0.15	-0.71	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1622	1/1	0.97	0.15	-0.72	85,85,85,85	0
57	MG	DA	3105	1/1	0.96	0.17	-0.79	91,91,91,91	0
57	MG	AA	1611	1/1	0.94	0.15	-0.82	91,91,91,91	0
57	MG	DA	3046	1/1	0.92	0.17	-0.86	142,142,142,142	0
57	MG	BA	3051	1/1	0.96	0.12	-0.88	39,39,39,39	0
57	MG	DA	3019	1/1	0.84	0.13	-0.98	150,150,150,150	0
57	MG	AA	1617	1/1	0.85	0.10	-1.00	123,123,123,123	0
57	MG	DA	3039	1/1	0.98	0.15	-1.03	104,104,104,104	0
57	MG	BA	3114	1/1	0.92	0.13	-1.05	73,73,73,73	0
57	MG	DA	3106	1/1	0.92	0.14	-1.07	92,92,92,92	0
58	ZN	B4	101	1/1	0.98	0.11	-1.08	79,79,79,79	0
57	MG	DA	3116	1/1	0.85	0.17	-1.10	98,98,98,98	0
57	MG	BA	3134	1/1	0.92	0.14	-1.21	38,38,38,38	0
57	MG	CA	1642	1/1	0.86	0.12	-1.26	102,102,102,102	0
57	MG	DA	3125	1/1	0.96	0.16	-1.44	90,90,90,90	0
57	MG	DA	3068	1/1	0.80	0.16	-1.46	86,86,86,86	0
57	MG	BA	3024	1/1	0.93	0.13	-1.46	42,42,42,42	0
57	MG	DA	3070	1/1	0.82	0.14	-1.52	94,94,94,94	0
57	MG	BD	301	1/1	0.95	0.13	-1.59	39,39,39,39	0
57	MG	BA	3013	1/1	0.97	0.12	-1.66	38,38,38,38	0
58	ZN	D4	101	1/1	0.99	0.04	-1.68	79,79,79,79	0
57	MG	CA	1631	1/1	0.94	0.14	-1.69	91,91,91,91	0
57	MG	AA	1606	1/1	0.90	0.12	-1.73	96,96,96,96	0
57	MG	CA	1609	1/1	0.85	0.17	-1.78	96,96,96,96	0
57	MG	CA	1634	1/1	0.78	0.11	-1.84	97,97,97,97	0
57	MG	BA	3066	1/1	0.98	0.14	-1.91	43,43,43,43	0
57	MG	BA	3116	1/1	0.96	0.14	-1.91	38,38,38,38	0
57	MG	CA	1616	1/1	0.78	0.13	-2.03	136,136,136,136	0
57	MG	DA	3044	1/1	0.98	0.14	-2.05	116,116,116,116	0
57	MG	BA	3022	1/1	0.94	0.11	-2.11	38,38,38,38	0
57	MG	BA	3018	1/1	0.96	0.06	-2.15	67,67,67,67	0
57	MG	BA	3050	1/1	0.98	0.12	-2.15	40,40,40,40	0
57	MG	BA	3110	1/1	0.96	0.10	-2.16	50,50,50,50	0
57	MG	DA	3098	1/1	0.94	0.15	-2.21	87,87,87,87	0
57	MG	DA	3113	1/1	0.93	0.14	-2.24	86,86,86,86	0
57	MG	DA	3024	1/1	0.95	0.14	-2.27	90,90,90,90	0
57	MG	CA	1606	1/1	0.68	0.14	-2.29	85,85,85,85	0
57	MG	DA	3026	1/1	0.94	0.14	-2.34	88,88,88,88	0
57	MG	BA	3063	1/1	0.92	0.11	-2.34	37,37,37,37	0
57	MG	BA	3012	1/1	0.96	0.14	-2.36	38,38,38,38	0
57	MG	BA	3120	1/1	0.94	0.12	-2.39	41,41,41,41	0
57	MG	DA	3052	1/1	0.88	0.15	-2.40	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3018	1/1	0.92	0.14	-2.55	106,106,106,106	0
57	MG	DA	3013	1/1	0.93	0.14	-2.62	93,93,93,93	0
57	MG	DA	3081	1/1	0.81	0.14	-2.66	87,87,87,87	0
57	MG	BA	3023	1/1	0.97	0.08	-2.69	41,41,41,41	0
57	MG	DA	3132	1/1	0.93	0.09	-2.70	94,94,94,94	0
57	MG	BA	3040	1/1	0.85	0.15	-2.78	41,41,41,41	0
57	MG	AA	1634	1/1	0.98	0.10	-2.78	102,102,102,102	0
57	MG	AA	1643	1/1	0.95	0.10	-2.93	81,81,81,81	0
57	MG	DA	3074	1/1	0.92	0.11	-3.06	98,98,98,98	0
57	MG	BA	3025	1/1	0.86	0.10	-3.14	41,41,41,41	0
57	MG	BA	3080	1/1	0.88	0.13	-3.19	74,74,74,74	0
57	MG	DA	3057	1/1	0.83	0.14	-3.27	92,92,92,92	0
57	MG	BA	3078	1/1	0.95	0.08	-3.29	86,86,86,86	0
57	MG	AA	1616	1/1	0.96	0.10	-3.31	126,126,126,126	0
57	MG	DA	3102	1/1	0.94	0.11	-3.31	84,84,84,84	0
57	MG	BA	3054	1/1	0.97	0.11	-3.47	44,44,44,44	0
57	MG	BA	3069	1/1	0.95	0.11	-3.51	52,52,52,52	0
57	MG	AA	1609	1/1	0.95	0.12	-3.59	91,91,91,91	0
57	MG	BA	3097	1/1	0.97	0.10	-3.67	49,49,49,49	0
57	MG	BA	3017	1/1	0.99	0.09	-4.78	39,39,39,39	0
57	MG	DA	3042	1/1	0.94	0.14	-6.18	101,101,101,101	0
57	MG	BA	3036	1/1	0.95	0.07	-6.28	47,47,47,47	0
57	MG	DA	3063	1/1	0.97	0.13	-6.98	92,92,92,92	0
57	MG	BA	3129	1/1	0.98	0.08	-8.33	39,39,39,39	0
57	MG	DA	3033	1/1	0.94	0.17	-	94,94,94,94	0
57	MG	DA	3131	1/1	0.69	0.88	-	103,103,103,103	0
57	MG	CA	1612	1/1	0.69	0.33	-	86,86,86,86	0
57	MG	CA	1623	1/1	0.93	0.21	-	89,89,89,89	0
57	MG	DA	3092	1/1	0.96	0.20	-	102,102,102,102	0
57	MG	AA	1618	1/1	0.69	0.17	-	104,104,104,104	0
57	MG	BA	3091	1/1	0.93	0.10	-	69,69,69,69	0
57	MG	DA	3031	1/1	0.86	0.39	-	98,98,98,98	0
57	MG	AA	1630	1/1	0.76	0.13	-	79,79,79,79	0
57	MG	BA	3123	1/1	0.89	0.17	-	63,63,63,63	0
57	MG	DA	3088	1/1	0.68	0.21	-	101,101,101,101	0
57	MG	BA	3031	1/1	0.99	0.14	-	42,42,42,42	0
57	MG	DA	3020	1/1	0.91	0.16	-	153,153,153,153	0
57	MG	BA	3113	1/1	0.96	0.16	-	38,38,38,38	0
57	MG	BA	3061	1/1	0.96	0.50	-	39,39,39,39	0
57	MG	DA	3065	1/1	0.52	1.84	-	84,84,84,84	0
57	MG	BA	3099	1/1	0.90	0.21	-	41,41,41,41	0
57	MG	CA	1602	1/1	0.81	0.39	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3072	1/1	0.92	0.13	-	84,84,84,84	0
57	MG	BA	3082	1/1	0.99	0.12	-	38,38,38,38	0
57	MG	CA	1638	1/1	0.79	0.12	-	141,141,141,141	0
57	MG	CA	1608	1/1	0.91	0.22	-	86,86,86,86	0
57	MG	BA	3093	1/1	0.93	0.27	-	84,84,84,84	0
57	MG	BA	3103	1/1	0.98	0.10	-	64,64,64,64	0
57	MG	BA	3126	1/1	0.96	0.25	-	57,57,57,57	0
57	MG	BA	3095	1/1	0.82	0.30	-	75,75,75,75	0
57	MG	DA	3017	1/1	0.82	0.53	-	102,102,102,102	0
57	MG	DA	3112	1/1	0.49	0.70	-	115,115,115,115	0
57	MG	AA	1620	1/1	0.88	0.20	-	144,144,144,144	0
57	MG	DA	3021	1/1	0.82	0.68	-	132,132,132,132	0
57	MG	DA	3061	1/1	0.94	0.43	-	84,84,84,84	0
57	MG	BA	3083	1/1	0.97	0.05	-	43,43,43,43	0
57	MG	BA	3074	1/1	0.98	0.07	-	38,38,38,38	0
57	MG	BA	3046	1/1	0.86	0.17	-	63,63,63,63	0
57	MG	BA	3034	1/1	0.96	0.19	-	40,40,40,40	0
57	MG	DA	3064	1/1	0.79	0.50	-	87,87,87,87	0
57	MG	DA	3082	1/1	0.91	0.29	-	83,83,83,83	0
57	MG	BA	3089	1/1	0.95	0.11	-	50,50,50,50	0
57	MG	DA	3099	1/1	0.71	0.80	-	98,98,98,98	0
57	MG	AA	1603	1/1	0.96	0.12	-	76,76,76,76	0
57	MG	BA	3035	1/1	0.86	0.20	-	55,55,55,55	0
57	MG	DA	3049	1/1	0.88	0.16	-	150,150,150,150	0
57	MG	BA	3042	1/1	0.93	0.14	-	56,56,56,56	0
57	MG	DA	3095	1/1	0.92	0.13	-	159,159,159,159	0
57	MG	CA	1622	1/1	0.77	0.11	-	138,138,138,138	0
57	MG	CA	1610	1/1	0.86	0.10	-	129,129,129,129	0
57	MG	BB	204	1/1	0.93	0.17	-	57,57,57,57	0
57	MG	AA	1628	1/1	0.81	0.33	-	107,107,107,107	0
57	MG	DA	3069	1/1	0.96	0.13	-	86,86,86,86	0
57	MG	BA	3021	1/1	0.97	0.10	-	42,42,42,42	0
57	MG	AA	1612	1/1	0.96	0.12	-	82,82,82,82	0
57	MG	DA	3012	1/1	0.88	0.31	-	96,96,96,96	0
57	MG	DA	3133	1/1	0.63	0.67	-	115,115,115,115	0
57	MG	BA	3122	1/1	0.98	0.18	-	40,40,40,40	0
57	MG	BA	3016	1/1	0.99	0.33	-	39,39,39,39	0
57	MG	BA	3015	1/1	0.82	0.64	-	38,38,38,38	0
57	MG	DA	3010	1/1	0.91	0.13	-	108,108,108,108	0
57	MG	AA	1621	1/1	0.69	0.19	-	67,67,67,67	0
57	MG	BA	3011	1/1	0.94	0.38	-	44,44,44,44	0
57	MG	DA	3090	1/1	0.58	0.34	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3016	1/1	0.66	1.17	-	96,96,96,96	0
57	MG	BA	3086	1/1	0.92	0.14	-	43,43,43,43	0
57	MG	DA	3123	1/1	0.97	0.16	-	93,93,93,93	0
57	MG	DA	3130	1/1	0.96	0.66	-	85,85,85,85	0
57	MG	BA	3049	1/1	0.94	0.12	-	45,45,45,45	0
57	MG	AA	1635	1/1	0.89	0.10	-	114,114,114,114	0
57	MG	DA	3029	1/1	0.87	0.29	-	108,108,108,108	0
57	MG	BA	3006	1/1	0.95	0.11	-	88,88,88,88	0
57	MG	DA	3006	1/1	0.84	0.21	-	149,149,149,149	0
57	MG	DA	3056	1/1	0.97	0.17	-	101,101,101,101	0
57	MG	BA	3102	1/1	0.86	0.31	-	40,40,40,40	0
57	MG	BA	3009	1/1	0.95	0.13	-	46,46,46,46	0
57	MG	AA	1619	1/1	0.20	0.84	-	136,136,136,136	0
57	MG	AA	1602	1/1	0.95	0.23	-	79,79,79,79	0
57	MG	BA	3019	1/1	0.92	0.12	-	70,70,70,70	0
57	MG	CA	1635	1/1	0.91	0.09	-	114,114,114,114	0
57	MG	BA	3014	1/1	0.94	0.30	-	38,38,38,38	0
57	MG	DA	3115	1/1	0.89	0.21	-	84,84,84,84	0
57	MG	AA	1636	1/1	0.70	0.38	-	120,120,120,120	0
57	MG	BA	3062	1/1	0.87	0.52	-	38,38,38,38	0
57	MG	BA	3106	1/1	0.95	0.14	-	40,40,40,40	0
57	MG	BA	3039	1/1	0.94	0.11	-	40,40,40,40	0
57	MG	AA	1601	1/1	0.92	0.08	-	111,111,111,111	0
57	MG	DA	3051	1/1	0.92	0.21	-	177,177,177,177	0
57	MG	DA	3014	1/1	0.90	0.35	-	90,90,90,90	0
57	MG	BA	3117	1/1	0.95	0.14	-	56,56,56,56	0
57	MG	DA	3008	1/1	0.90	0.22	-	177,177,177,177	0
57	MG	CA	1627	1/1	0.80	0.24	-	106,106,106,106	0
57	MG	BA	3119	1/1	0.83	0.35	-	52,52,52,52	0
57	MG	BA	3096	1/1	0.96	0.09	-	45,45,45,45	0
57	MG	BA	3077	1/1	0.91	0.31	-	45,45,45,45	0
57	MG	DA	3078	1/1	0.87	0.31	-	79,79,79,79	0
57	MG	BA	3127	1/1	0.96	0.05	-	40,40,40,40	0
57	MG	DA	3100	1/1	0.84	0.55	-	149,149,149,149	0
57	MG	BA	3081	1/1	0.95	0.17	-	40,40,40,40	0
57	MG	BA	3075	1/1	0.86	0.47	-	40,40,40,40	0
57	MG	BA	3004	1/1	0.95	0.25	-	69,69,69,69	0
57	MG	DA	3007	1/1	0.48	0.35	-	192,192,192,192	0
57	MG	BA	3115	1/1	0.78	0.31	-	49,49,49,49	0
57	MG	DA	3047	1/1	0.55	0.20	-	148,148,148,148	0
57	MG	BA	3032	1/1	0.92	0.13	-	40,40,40,40	0
57	MG	DA	3030	1/1	0.96	0.50	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DB	201	1/1	0.79	0.31	-	108,108,108,108	0
57	MG	DA	3060	1/1	0.23	0.54	-	96,96,96,96	0
57	MG	CA	1615	1/1	0.83	0.38	-	118,118,118,118	0
57	MG	DA	3022	1/1	0.92	0.21	-	105,105,105,105	0
57	MG	BA	3068	1/1	0.97	0.19	-	52,52,52,52	0
57	MG	DA	3005	1/1	0.81	0.12	-	157,157,157,157	0
57	MG	AA	1626	1/1	0.95	0.23	-	107,107,107,107	0
57	MG	BA	3057	1/1	0.98	0.34	-	42,42,42,42	0
57	MG	BA	3090	1/1	0.90	0.13	-	47,47,47,47	0
57	MG	BA	3052	1/1	0.85	0.13	-	38,38,38,38	0
57	MG	BA	3033	1/1	0.96	0.12	-	40,40,40,40	0
57	MG	DA	3110	1/1	0.34	1.51	-	82,82,82,82	0
57	MG	DA	3004	1/1	0.61	1.92	-	150,150,150,150	0
57	MG	DA	3036	1/1	0.96	0.13	-	84,84,84,84	0
57	MG	BA	3065	1/1	0.94	0.25	-	38,38,38,38	0
57	MG	BA	3030	1/1	0.94	0.45	-	41,41,41,41	0
57	MG	CA	1633	1/1	0.97	0.12	-	101,101,101,101	0
57	MG	BA	3047	1/1	0.93	0.15	-	63,63,63,63	0
57	MG	DA	3119	1/1	0.89	0.16	-	138,138,138,138	0
57	MG	BA	3064	1/1	0.96	0.10	-	38,38,38,38	0
57	MG	BA	3044	1/1	0.88	0.10	-	71,71,71,71	0
57	MG	DA	3009	1/1	0.73	0.20	-	121,121,121,121	0
57	MG	DA	3124	1/1	0.89	0.19	-	133,133,133,133	0
57	MG	CA	1636	1/1	0.89	0.75	-	88,88,88,88	0
57	MG	BB	203	1/1	0.98	0.09	-	57,57,57,57	0
57	MG	BA	3112	1/1	0.84	0.22	-	46,46,46,46	0
57	MG	DA	3028	1/1	0.94	0.95	-	103,103,103,103	0
57	MG	DA	3043	1/1	0.87	0.19	-	107,107,107,107	0
57	MG	AA	1605	1/1	0.95	0.09	-	103,103,103,103	0
57	MG	CA	1619	1/1	0.86	0.83	-	119,119,119,119	0
57	MG	CA	1614	1/1	0.84	0.23	-	114,114,114,114	0
57	MG	DA	3103	1/1	0.93	0.20	-	91,91,91,91	0
57	MG	DA	3127	1/1	0.93	0.22	-	104,104,104,104	0
57	MG	BA	3060	1/1	0.89	0.31	-	39,39,39,39	0
57	MG	DA	3023	1/1	0.88	0.65	-	101,101,101,101	0
57	MG	BA	3067	1/1	0.98	0.09	-	40,40,40,40	0
57	MG	DA	3034	1/1	0.94	0.21	-	89,89,89,89	0
57	MG	CA	1605	1/1	0.95	0.21	-	89,89,89,89	0
57	MG	BA	3100	1/1	0.97	0.09	-	59,59,59,59	0
57	MG	DA	3037	1/1	0.92	0.17	-	83,83,83,83	0
57	MG	DA	3059	1/1	0.78	0.46	-	88,88,88,88	0
57	MG	AA	1610	1/1	0.95	0.16	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3053	1/1	0.95	0.12	-	41,41,41,41	0
57	MG	BA	3020	1/1	0.98	0.10	-	46,46,46,46	0
57	MG	DA	3108	1/1	0.90	0.26	-	82,82,82,82	0
57	MG	CA	1620	1/1	0.88	0.26	-	93,93,93,93	0
57	MG	DA	3066	1/1	0.84	0.34	-	92,92,92,92	0
57	MG	DA	3084	1/1	0.68	0.15	-	157,157,157,157	0
57	MG	BA	3084	1/1	0.88	0.55	-	49,49,49,49	0
57	MG	DA	3055	1/1	0.98	0.16	-	85,85,85,85	0
57	MG	DA	3126	1/1	0.77	0.48	-	99,99,99,99	0
57	MG	BA	3001	1/1	0.91	0.15	-	45,45,45,45	0
57	MG	DA	3048	1/1	0.86	0.19	-	131,131,131,131	0
57	MG	DA	3114	1/1	0.97	0.08	-	98,98,98,98	0
57	MG	BA	3121	1/1	0.92	0.10	-	45,45,45,45	0
57	MG	DA	3058	1/1	0.92	0.14	-	96,96,96,96	0
57	MG	DA	3075	1/1	0.80	0.11	-	255,255,255,255	0
57	MG	DA	3089	1/1	0.79	0.30	-	110,110,110,110	0
57	MG	BA	3076	1/1	0.94	0.15	-	47,47,47,47	0
57	MG	BA	3045	1/1	0.90	0.25	-	62,62,62,62	0
57	MG	DA	3096	1/1	0.90	0.63	-	120,120,120,120	0
57	MG	AA	1615	1/1	0.95	0.08	-	117,117,117,117	0
57	MG	BA	3131	1/1	0.76	0.75	-	48,48,48,48	0
57	MG	DA	3083	1/1	0.91	0.22	-	121,121,121,121	0
57	MG	BA	3087	1/1	0.97	0.11	-	45,45,45,45	0
57	MG	BA	3094	1/1	0.88	0.12	-	75,75,75,75	0
57	MG	BA	3125	1/1	0.97	0.17	-	40,40,40,40	0
57	MG	BA	3088	1/1	0.95	0.07	-	58,58,58,58	0
57	MG	AA	1623	1/1	0.92	0.21	-	108,108,108,108	0
57	MG	BA	3135	1/1	0.86	0.48	-	43,43,43,43	0
57	MG	AA	1640	1/1	0.89	0.12	-	132,132,132,132	0
57	MG	AA	1639	1/1	0.96	0.06	-	119,119,119,119	0
57	MG	CA	1626	1/1	0.92	0.14	-	110,110,110,110	0
57	MG	AA	1632	1/1	0.89	0.16	-	95,95,95,95	0
57	MG	DA	3117	1/1	0.91	0.15	-	90,90,90,90	0
57	MG	BA	3092	1/1	0.89	0.19	-	108,108,108,108	0
57	MG	DA	3097	1/1	0.86	0.20	-	119,119,119,119	0
57	MG	DA	3015	1/1	0.82	0.23	-	88,88,88,88	0
57	MG	DA	3091	1/1	0.94	0.13	-	93,93,93,93	0
57	MG	BA	3027	1/1	0.98	0.06	-	41,41,41,41	0
57	MG	BA	3085	1/1	0.95	0.53	-	42,42,42,42	0
57	MG	DA	3040	1/1	0.88	0.49	-	102,102,102,102	0
57	MG	AA	1637	1/1	0.81	0.21	-	87,87,87,87	0
57	MG	BA	3056	1/1	0.92	0.34	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3079	1/1	0.80	0.09	-	89,89,89,89	0
57	MG	DJ	201	1/1	0.87	0.43	-	101,101,101,101	0
57	MG	AA	1633	1/1	0.96	0.13	-	107,107,107,107	0
57	MG	DA	3067	1/1	0.96	0.16	-	86,86,86,86	0
57	MG	BA	3133	1/1	0.86	0.57	-	53,53,53,53	0
57	MG	CA	1611	1/1	0.96	0.09	-	93,93,93,93	0
57	MG	BA	3026	1/1	0.84	0.35	-	41,41,41,41	0
57	MG	DA	3032	1/1	0.86	0.27	-	87,87,87,87	0
57	MG	DC	301	1/1	0.53	0.38	-	103,103,103,103	0
57	MG	AA	1627	1/1	0.91	0.58	-	109,109,109,109	0
57	MG	BB	201	1/1	0.81	0.57	-	105,105,105,105	0
57	MG	DA	3011	1/1	0.88	0.55	-	110,110,110,110	0
57	MG	DA	3087	1/1	0.96	0.09	-	88,88,88,88	0
57	MG	BA	3029	1/1	0.96	0.10	-	38,38,38,38	0
57	MG	BA	3055	1/1	0.97	0.13	-	44,44,44,44	0
57	MG	DA	3080	1/1	0.94	0.53	-	84,84,84,84	0
57	MG	DA	3093	1/1	0.53	0.52	-	93,93,93,93	0
57	MG	DA	3045	1/1	0.80	0.20	-	141,141,141,141	0
57	MG	BA	3073	1/1	0.98	0.08	-	43,43,43,43	0
57	MG	BA	3111	1/1	0.83	0.15	-	38,38,38,38	0
57	MG	CA	1640	1/1	0.94	0.41	-	87,87,87,87	0
57	MG	DA	3001	1/1	0.95	0.22	-	115,115,115,115	0
57	MG	BA	3007	1/1	0.83	0.22	-	90,90,90,90	0
57	MG	DA	3121	1/1	0.93	0.22	-	97,97,97,97	0
57	MG	BA	3043	1/1	0.97	0.15	-	56,56,56,56	0
57	MG	DA	3073	1/1	0.93	0.28	-	98,98,98,98	0
57	MG	DA	3079	1/1	0.95	0.22	-	90,90,90,90	0
57	MG	DA	3120	1/1	0.85	0.66	-	96,96,96,96	0
57	MG	DA	3038	1/1	0.93	0.17	-	108,108,108,108	0
57	MG	DA	3122	1/1	0.96	0.23	-	142,142,142,142	0
57	MG	BA	3010	1/1	0.95	0.09	-	46,46,46,46	0
57	MG	BA	3070	1/1	0.57	0.19	-	140,140,140,140	0
57	MG	DA	3035	1/1	0.87	0.21	-	88,88,88,88	0
57	MG	DA	3076	1/1	-0.05	1.26	-	109,109,109,109	0
57	MG	DA	3128	1/1	0.72	0.56	-	100,100,100,100	0
57	MG	DA	3111	1/1	0.88	0.21	-	164,164,164,164	0
57	MG	CA	1632	1/1	0.69	0.15	-	125,125,125,125	0
57	MG	AA	1608	1/1	0.96	0.24	-	82,82,82,82	0
57	MG	AA	1614	1/1	0.92	0.24	-	113,113,113,113	0
57	MG	CA	1624	1/1	0.71	0.92	-	79,79,79,79	0
57	MG	CA	1603	1/1	0.77	0.39	-	92,92,92,92	0
57	MG	BA	3003	1/1	0.98	0.07	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1624	1/1	0.75	0.21	-	94,94,94,94	0
57	MG	AA	1638	1/1	0.91	0.14	-	81,81,81,81	0
57	MG	DA	3118	1/1	0.96	0.32	-	99,99,99,99	0
57	MG	CA	1601	1/1	0.80	0.07	-	142,142,142,142	0
57	MG	BA	3098	1/1	0.97	0.64	-	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.