



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:53 AM UTC

PDB ID : 4V7P / pdb_00004v7p
Title : Recognition of the amber stop codon by release factor RF1.
Authors : Korostelev, A.; Zhu, J.; Asahara, H.; Noller, H.F.
Deposited on : 2010-04-29
Resolution : 3.62 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

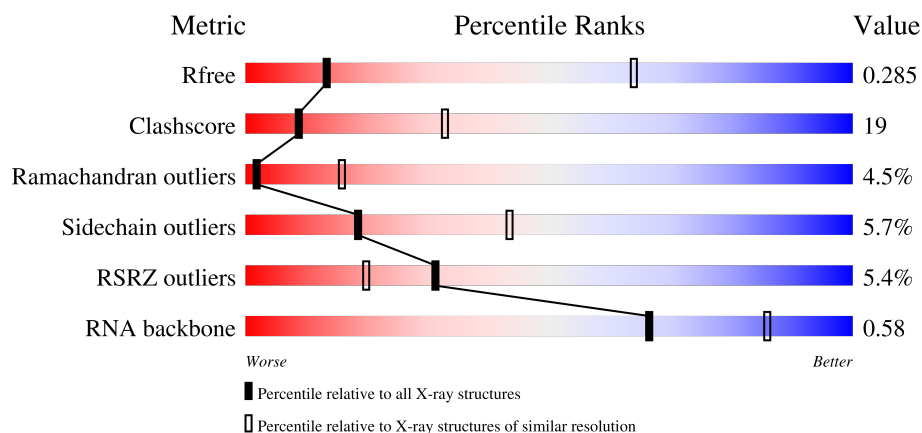
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)
RNA backbone	3983	1018 (4.18-3.06)

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

Mol	Chain	Length	Quality of chain
1	AA	1504	3% 48% 45% 7%
1	DA	1504	3% 47% 45% 7%
2	AB	234	3% 48% 47% 5%
2	DB	234	5% 48% 47% 5%

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	DC	206	
4	AD	208	
4	DD	208	
5	AE	151	
5	DE	151	
6	AF	101	
6	DF	101	
7	AG	155	
7	DG	155	
8	AH	138	
8	DH	138	
9	AI	127	
9	DI	127	
10	AJ	98	
10	DJ	98	
11	AK	119	
11	DK	119	
12	AL	124	
12	DL	124	
13	AM	117	
13	DM	117	
14	AN	60	
14	DN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	DO	88	
16	AP	83	
16	DP	83	
17	AQ	99	
17	DQ	99	
18	AR	70	
18	DR	70	
19	AS	78	
19	DS	78	
20	AT	99	
20	DT	99	
21	AU	24	
21	DU	24	
22	AV	354	
22	DV	354	
23	AW	77	
23	DW	77	
24	AX	7	
25	BA	2879	
25	CA	2879	
26	BB	119	
26	CB	119	
27	BC	275	
27	CC	275	
28	BD	206	

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Mol	Chain	Length	Quality of chain
28	CD	206	
29	BE	205	
29	CE	205	
30	BF	181	
30	CF	181	
31	BG	180	
31	CG	180	
32	BH	148	
32	CH	148	
33	BI	173	
33	CI	173	
34	BJ	139	
34	CJ	139	
35	BK	122	
35	CK	122	
36	BL	150	
36	CL	150	
37	BM	141	
37	CM	141	
38	BN	117	
38	CN	117	
39	BO	111	
39	CO	111	
40	BP	146	
40	CP	146	

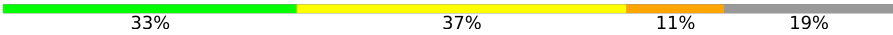
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Mol	Chain	Length	Quality of chain
41	BQ	116	
41	CQ	116	
42	BR	101	
42	CR	101	
43	BS	112	
43	CS	112	
44	BT	96	
44	CT	96	
45	BU	109	
45	CU	109	
46	BV	206	
46	CV	206	
47	BW	84	
47	CW	84	
48	BX	98	
48	CX	98	
49	BY	72	
49	CY	72	
50	BZ	59	
50	CZ	59	
51	B1	71	
51	C1	71	
52	B2	59	
52	C2	59	
53	B3	54	

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Mol	Chain	Length	Quality of chain
53	C3	54	
54	B4	48	
54	C4	48	
55	B5	64	
55	C5	64	
56	DX	9	

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	1612	-	-	-	X
57	MG	BA	2987	-	-	-	X
57	MG	BA	3054	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	DA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	DB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	DC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	DD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
5	DE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	DF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	DG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	DH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	DI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	DK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	DL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
13	DM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	DN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	DO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	DP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	DQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	DR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	DS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	DT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	DU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			
22	DV	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

- Molecule 23 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	DW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	7	Total	C	N	O	P	0	0	0
			149	68	29	46	6			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
25	CA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	conflict	GB AE017221.1
BA	2825	U	G	conflict	GB AE017221.1
CA	1142	U	C	conflict	GB AE017221.1
CA	2825	U	G	conflict	GB AE017221.1

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
26	CB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	CC	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	CD	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
29	CE	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	CF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
31	CG	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			
32	CH	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BI	32	Total	C	N	O	0	0	0
			253	157	49	47			
33	CI	32	Total	C	N	O	0	0	0
			253	157	49	47			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BJ	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
34	CJ	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
35	CK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
37	CM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	CN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BO	98	Total	C	N	O	0	0	0
			770	486	154	130			
39	CO	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BP	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
40	CP	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
41	CQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	deletion	UNP Q72L76
CQ	?	-	PHE	deletion	UNP Q72L76

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	CR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
43	CS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
44	CT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BU	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	CU	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CV	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	CW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BX	88	Total	C	N	O	0	0	0
			694	435	141	118			
48	CX	88	Total	C	N	O	0	0	0
			694	435	141	118			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			
49	CY	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
50	CZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B1	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			
51	C1	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			
52	C2	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			
53	C3	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
54	C4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B5	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	C5	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DX	9	Total	C	N	O	P	0	0	0
			193	88	39	58	8			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	64	Total	Mg	0	0
			64	64		

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AT	1	Total 1	Mg 1	0	0
57	AV	1	Total 1	Mg 1	0	0
57	AW	3	Total 3	Mg 3	0	0
57	BA	176	Total 176	Mg 176	0	0
57	BB	2	Total 2	Mg 2	0	0
57	BK	1	Total 1	Mg 1	0	0
57	BM	1	Total 1	Mg 1	0	0
57	B2	1	Total 1	Mg 1	0	0
57	CA	125	Total 125	Mg 125	0	0
57	CB	2	Total 2	Mg 2	0	0
57	CM	1	Total 1	Mg 1	0	0
57	CY	1	Total 1	Mg 1	0	0
57	DA	30	Total 30	Mg 30	0	0
57	DW	1	Total 1	Mg 1	0	0

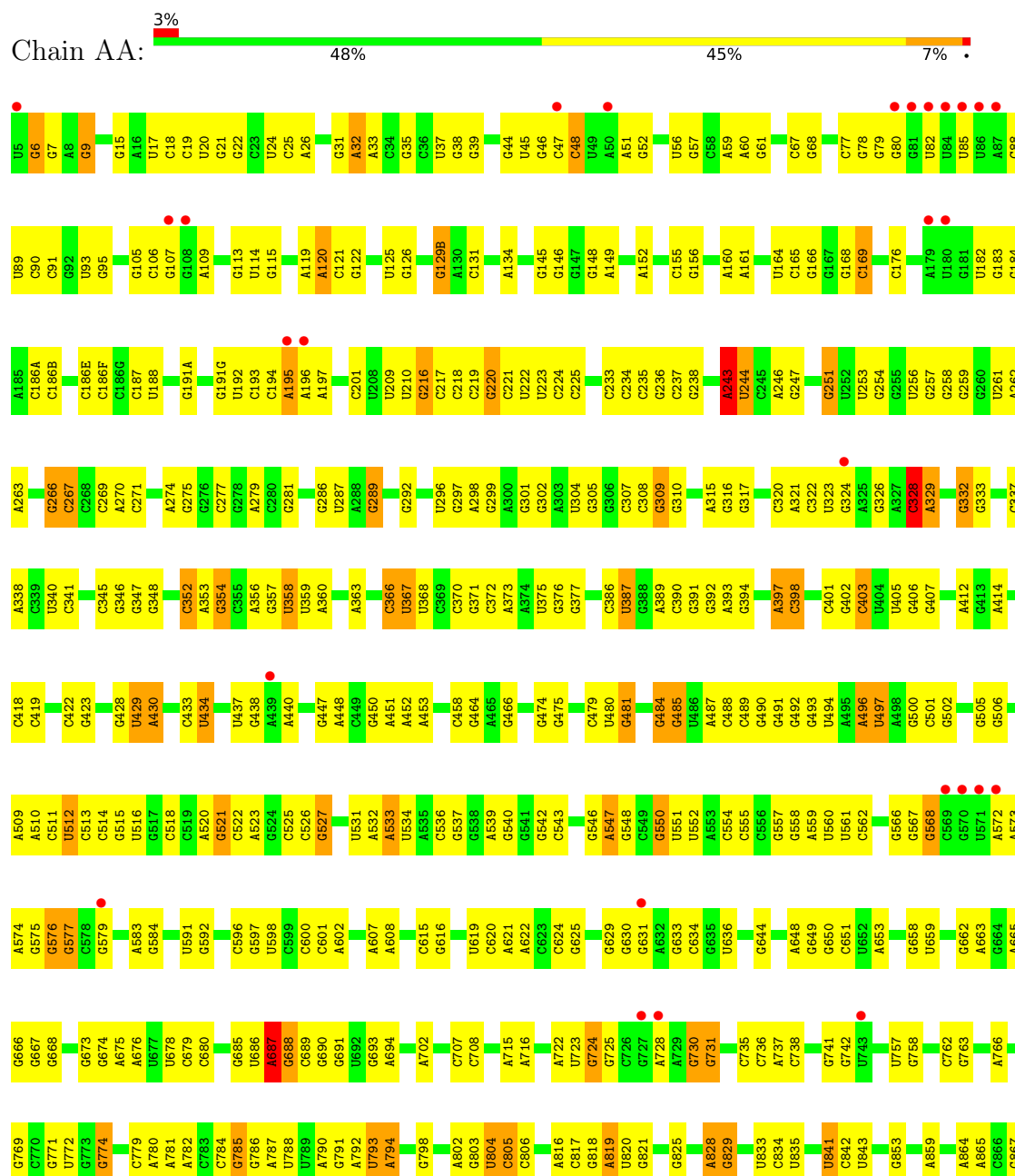
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

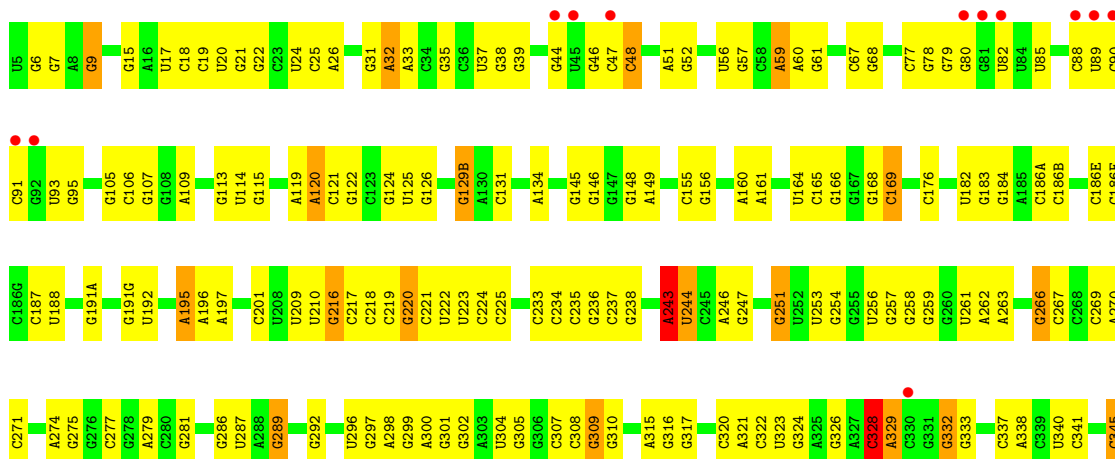
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total 1	Zn 1	0	0
58	AN	1	Total 1	Zn 1	0	0
58	DD	1	Total 1	Zn 1	0	0
58	DN	1	Total 1	Zn 1	0	0

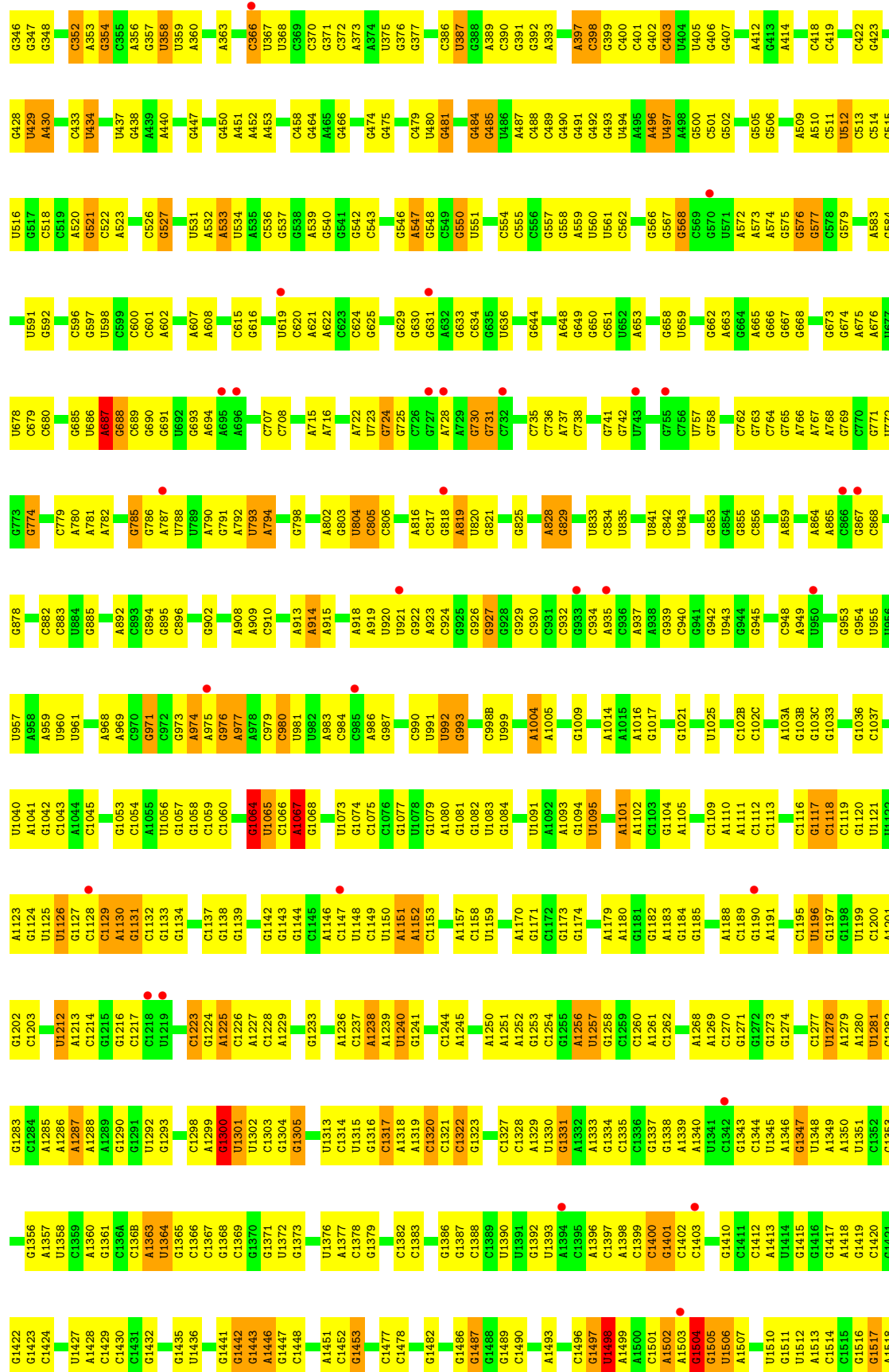
3 Residue-property plots

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

• Molecule 1: 16S rRNA (1504-MER)

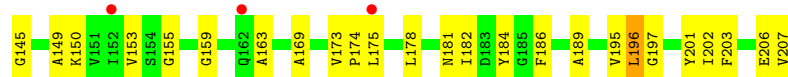




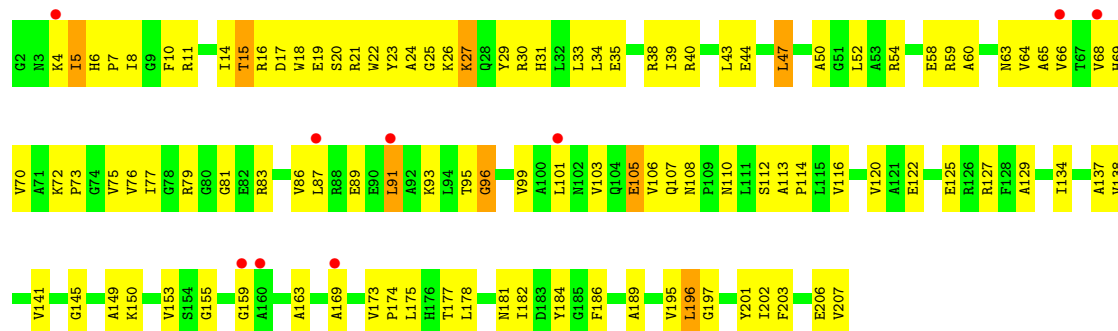


S233	S234	S235	V239	Q240	L158	I162	F163	V164	D166	P167	T168	K169	E170	A171	E176	A177	K179	I182	P183	V184	I185	A186	L187	T190	D191	S192	D193	P194	I196	V197	D198	I199	I200	I201	N204	D205	I208	I211	Q212	L213	S216	R217	A218	V219	D220	L221	I222	I223	G228	S233	P234	S235	V239	Q240	L158	I162	F163	V164	D166	P167	T168	K169	E170	A171	E176	A177	K179	I182	P183	V184	I185	A186	L187	T190	D191	S192	D193	P194	I196	V197	D198	I199	I200	I201	N204	D205	I208	I211	Q212	L213	S216	R217	A218	V219	D220	L221	I222	I223	G228	R82	M83	E84	R87	A88	G89	M90	F91	Y92	V93	N94	Q95	R96	W97	L98	M101	L102	T103	N104	I108	R111	V112	H113	R114	L115	E116	L117	E118	F122	A123	S124	P125	E126	R130	P131	V136	R137	L138	K139	H140	E141	L142	G146	L145	R147	S150	R153	L154	T155	R82	M83	E84	R87	A88	G89	M90	F91	Y92	V93	N94	Q95	R96	W97	L98	M101	L102	T103	N104	I108	R111	V112	H113	R114	L115	E116	L117	E118	F122	A123	S124	P125	E126	R130	P131	V136	R137	L138	K139	H140	E141	L142	G146	L145	R147	S150	R153	L154	T155	V7	K8	L11	E12	V15	F17	G18	H19	E20	R21	K22	N25	P26	K27	F28	A29	R30	Y31	I32	R36	H40	I41	I42	T47	L51	E52	R53	T54	F55	R56	F57	I58	F59	D60	R64	T67	I68	L69	V71	G72	T73	K74	K75	Q76	A77	Q78	D79	I80	R81
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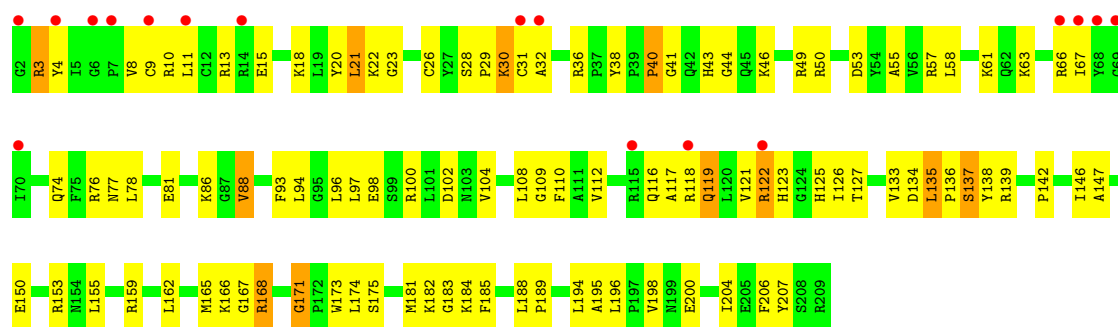
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G228	L154	D79	K8
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S233	L158	M83	L11
F234		E84	E12
S235			A13
	T162		G14
V239	F163	R87	V15
Q240	V164	A88	H16
	V165	G89	F17
	D166	M90	G18
	P167	P91	H19
	T168	Y92	E20
	K169	V93	R21
	E170	N94	K22
	A171	Q95	
		R96	N25
	E176	W97	F26
	A177	L98	K27
	R178		F28
	K179	M101	A29
		L102	R30
	T182	T103	Y31
	F183	M104	I32
	V184		
	I185	T108	R36
	A186		
	L187	R111	H40
		V112	I41
	T190	H113	I42
	D191	R114	D43
	S192	L115	L44
	D193	E116	Q45
	P194	E117	K46
	D195	L118	T47
	L196		
	V197	F122	L51
	D198	A123	E52
	Y199	S124	R53
	T200	P125	T54
	T201	E126	F55
	F202	R130	R56
	G203	P131	F57
	D205		I58
		Q135	E59
	I208	V136	D60
		R137	
	T211	L138	R64
	Q212	K139	T67
	L213	H140	I68
	T214	E141	L69
	L215	L142	F70
	S216		V71
	R217	L145	G72
	A218	Q146	T73
	V219	K147	K74
	D220		K75
	L221	S150	A76
	F222		Q77



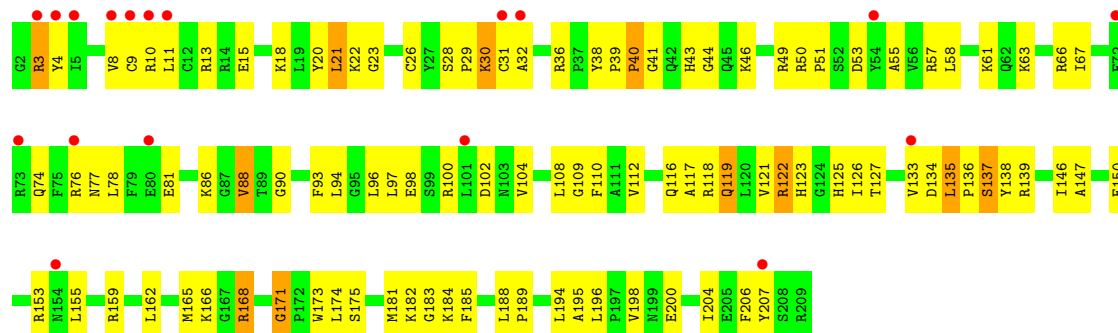
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

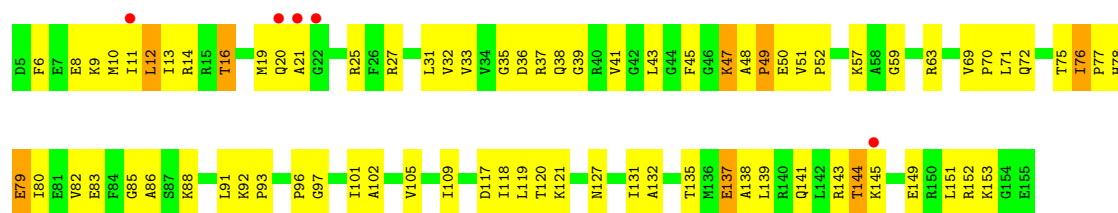


• Molecule 4: 30S ribosomal protein S4

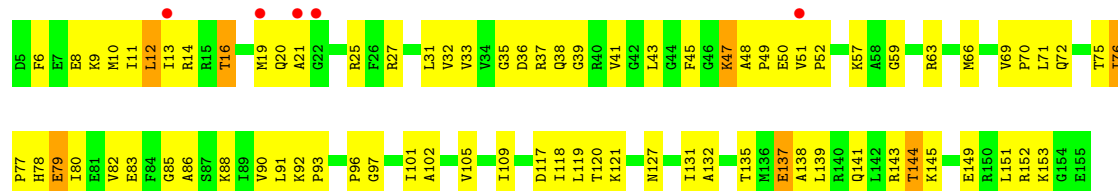


• Molecule 5: 30S ribosomal protein S5

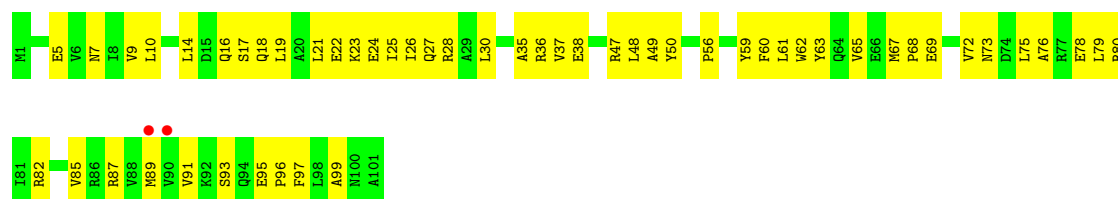




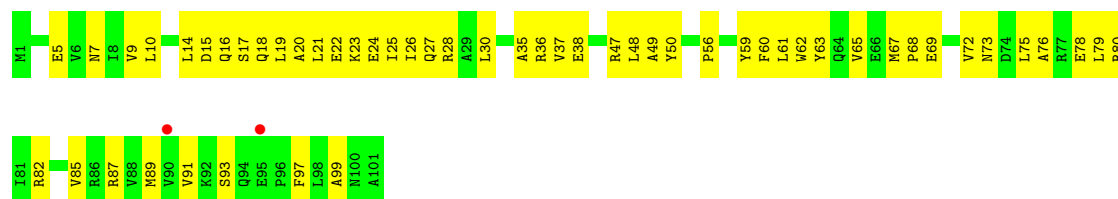
• Molecule 5: 30S ribosomal protein S5



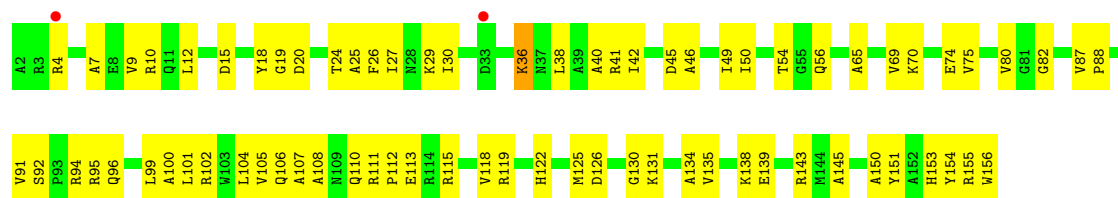
• Molecule 6: 30S ribosomal protein S6



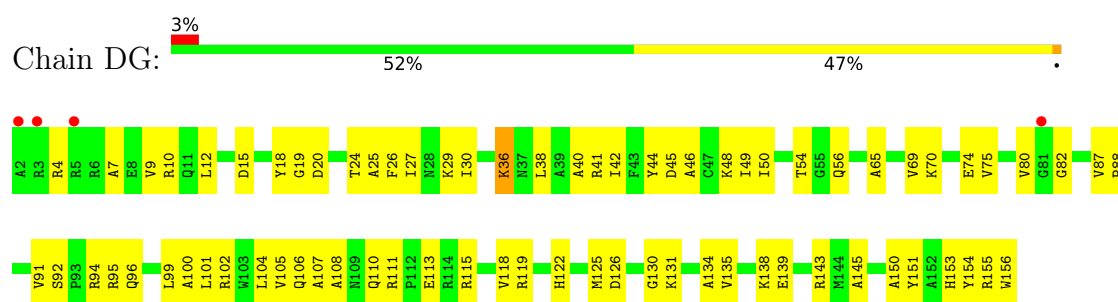
• Molecule 6: 30S ribosomal protein S6



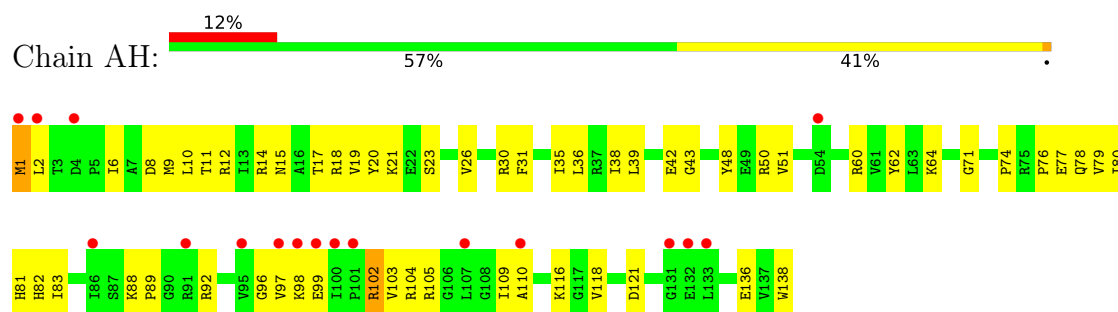
• Molecule 7: 30S ribosomal protein S7



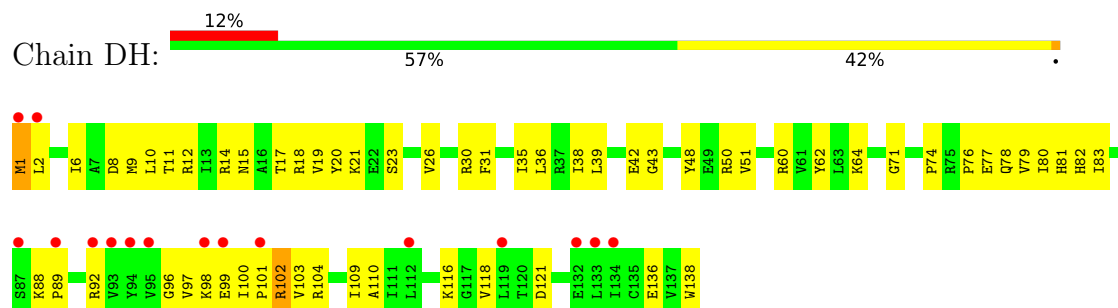
• Molecule 7: 30S ribosomal protein S7



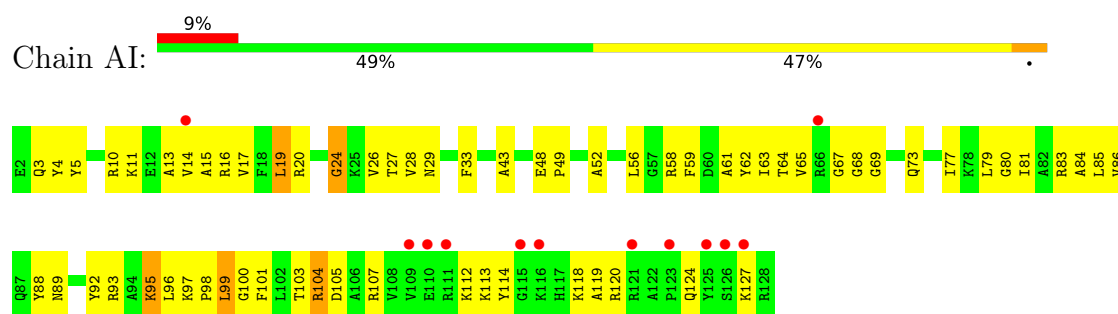
• Molecule 8: 30S ribosomal protein S8



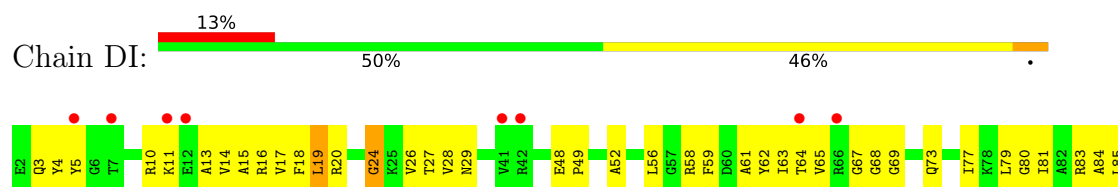
• Molecule 8: 30S ribosomal protein S8

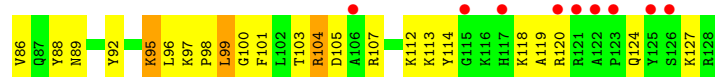


• Molecule 9: 30S ribosomal protein S9

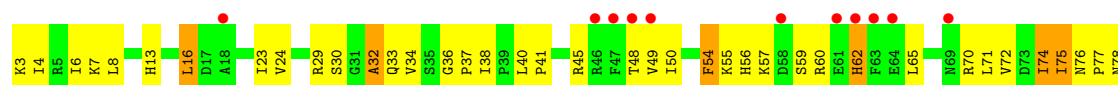


• Molecule 9: 30S ribosomal protein S9

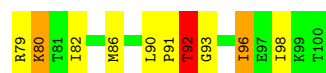
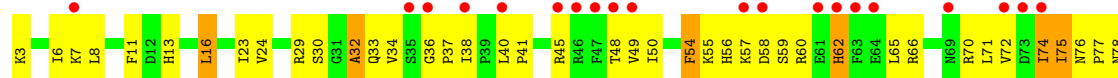




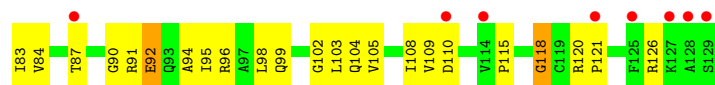
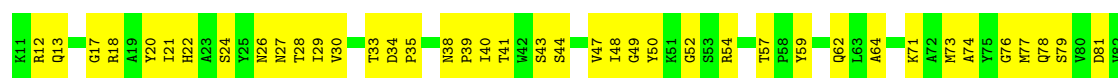
• Molecule 10: 30S ribosomal protein S10



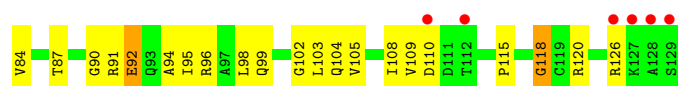
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

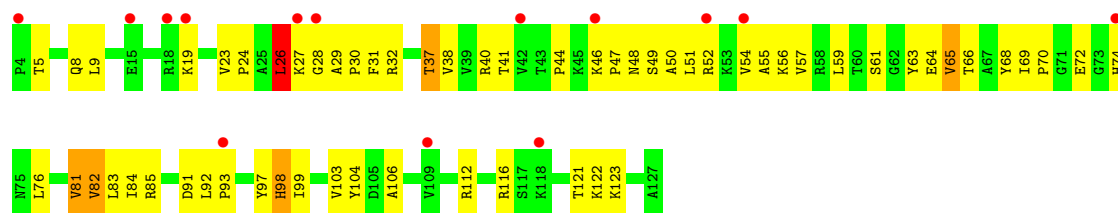


• Molecule 11: 30S ribosomal protein S11

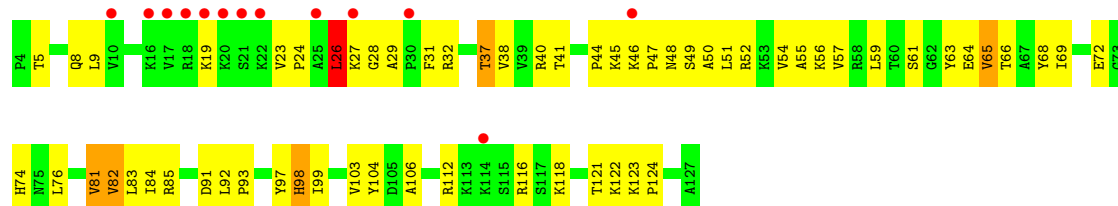


• Molecule 12: 30S ribosomal protein S12

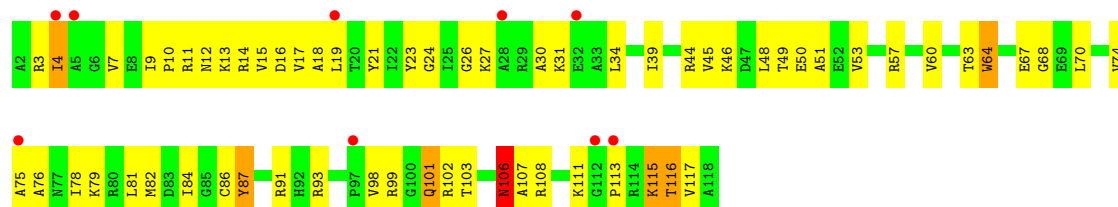




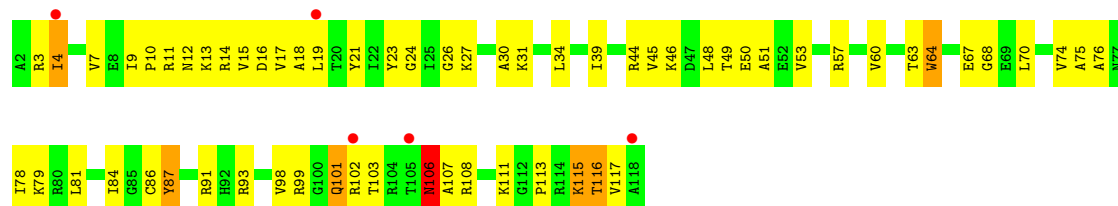
• Molecule 12: 30S ribosomal protein S12



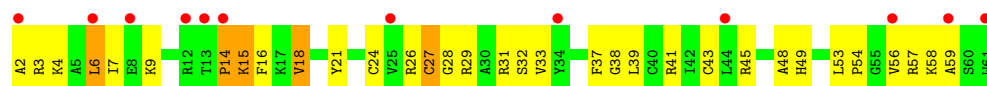
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

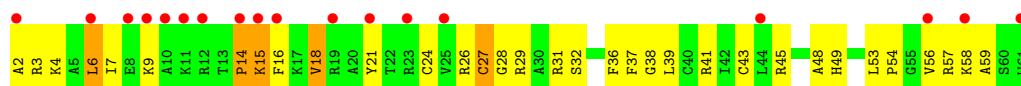


• Molecule 14: 30S ribosomal protein S14

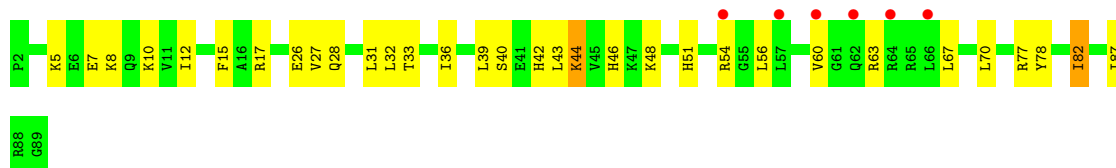


• Molecule 14: 30S ribosomal protein S14

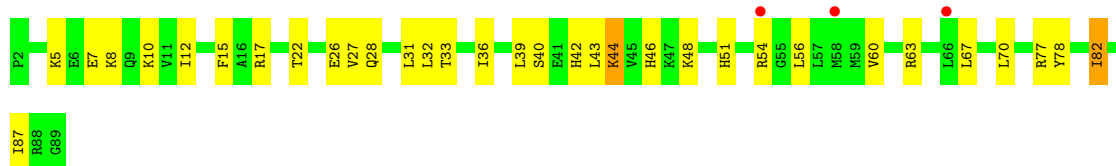




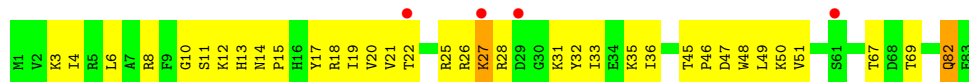
- Molecule 15: 30S ribosomal protein S15



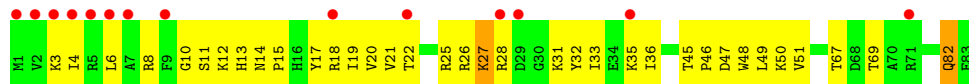
- Molecule 15: 30S ribosomal protein S15



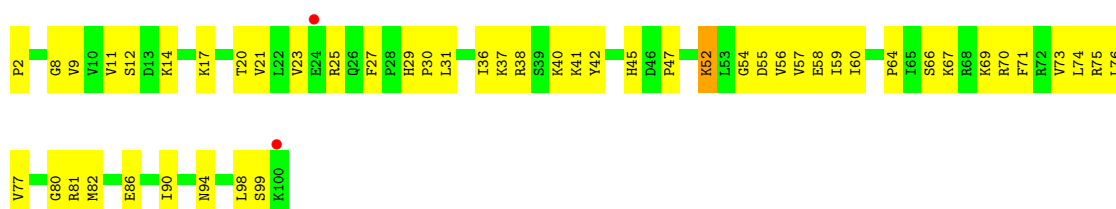
- Molecule 16: 30S ribosomal protein S16



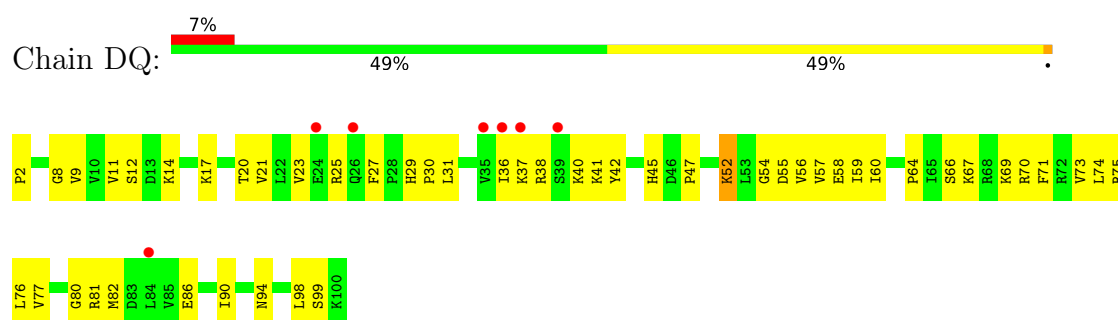
- Molecule 16: 30S ribosomal protein S16



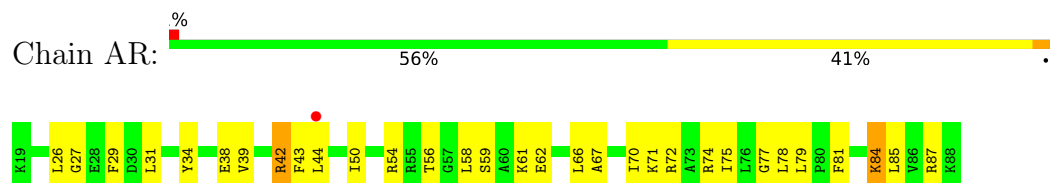
- Molecule 17: 30S ribosomal protein S17



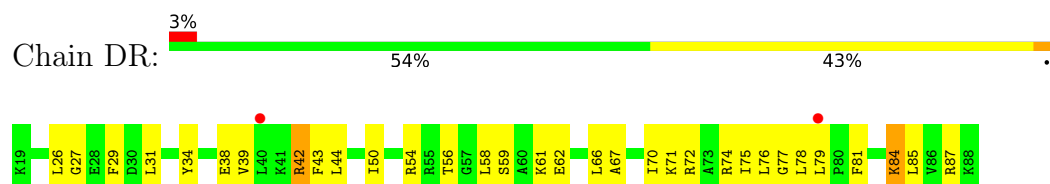
- Molecule 17: 30S ribosomal protein S17



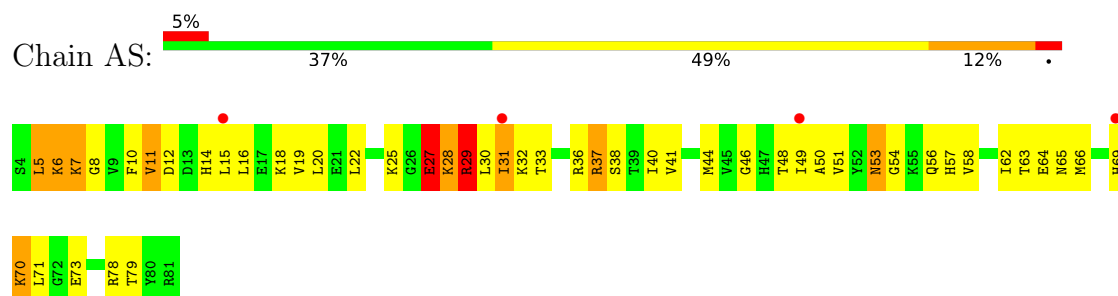
- Molecule 18: 30S ribosomal protein S18



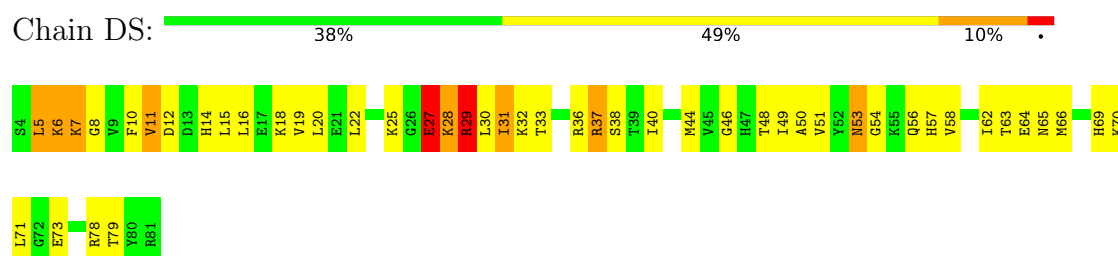
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

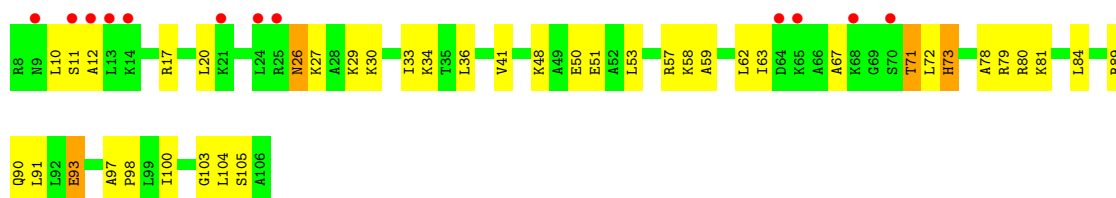


- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

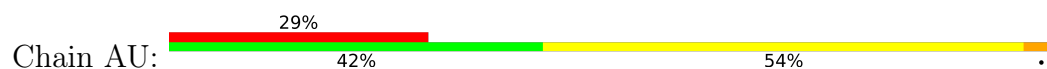




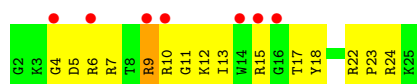
- Molecule 20: 30S ribosomal protein S20



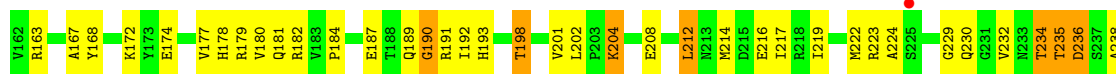
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

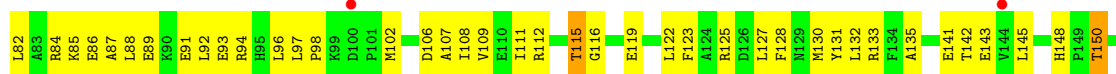


- Molecule 22: Peptide chain release factor 1

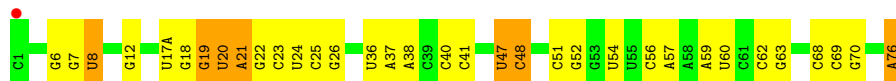




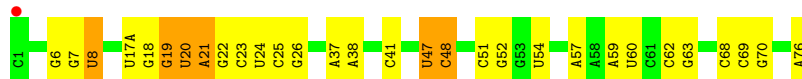
- Molecule 22: Peptide chain release factor 1



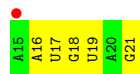
- Molecule 23: P-site tRNA-fMet



- Molecule 23: P-site tRNA-fMet



- Molecule 24: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')

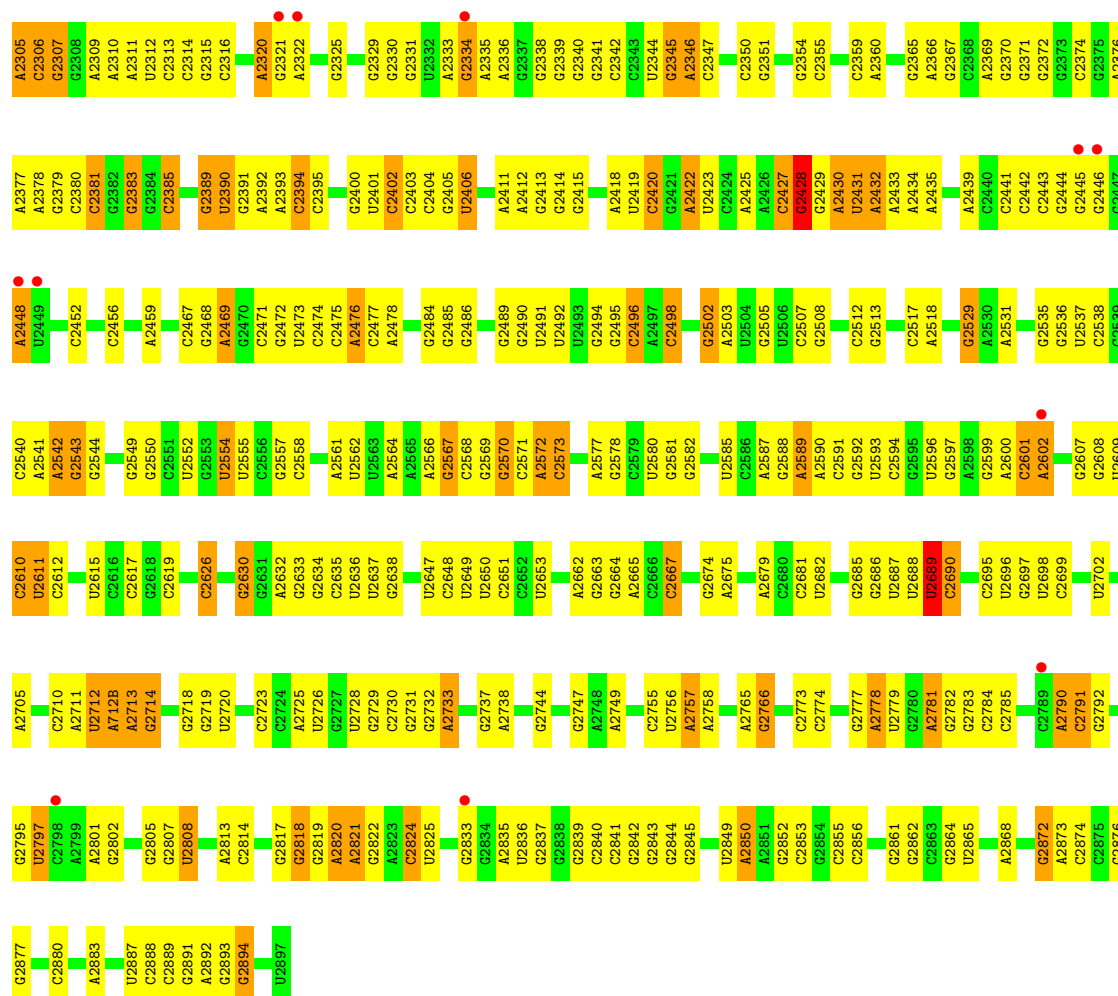


- Molecule 25: 23S ribosomal RNA

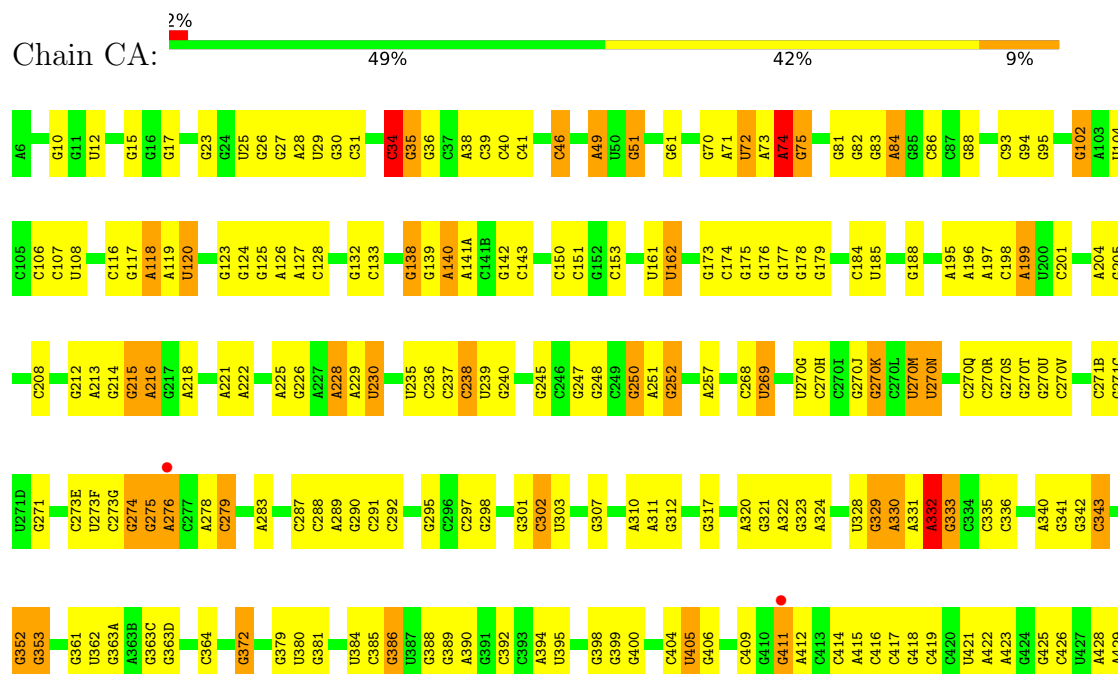






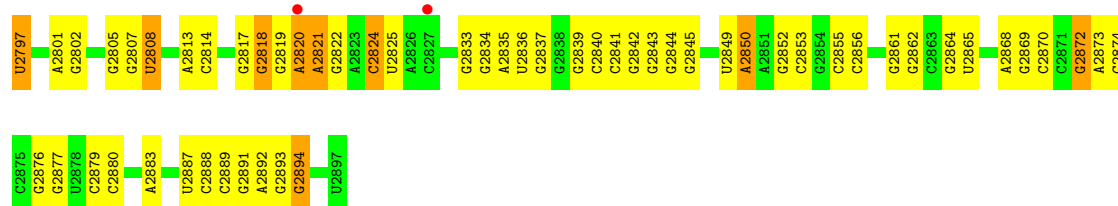


• Molecule 25: 23S ribosomal RNA

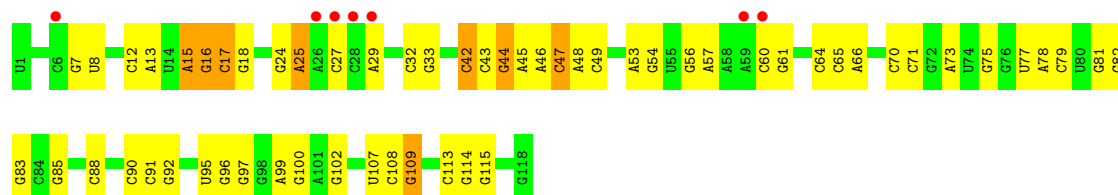




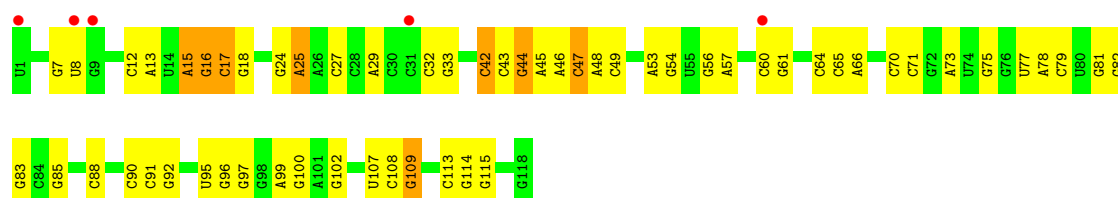
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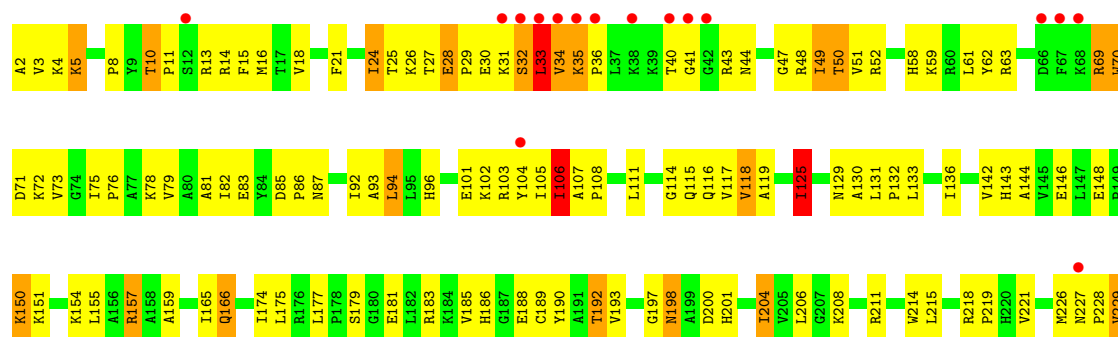
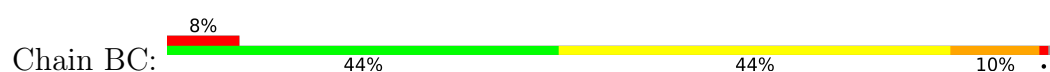
• Molecule 26: 5S ribosomal RNA

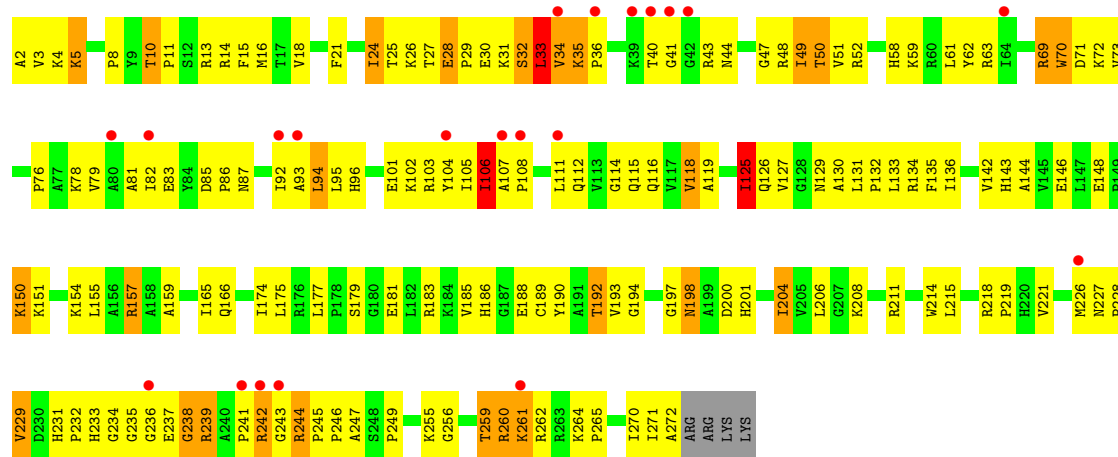


• Molecule 26: 5S ribosomal RNA

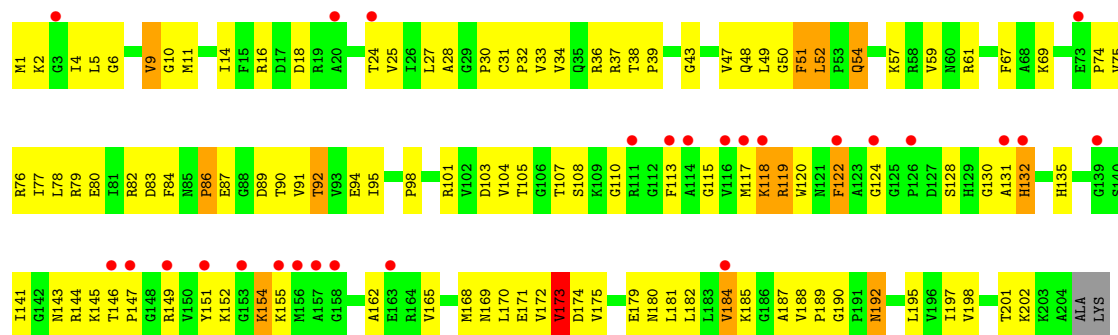


• Molecule 27: 50S ribosomal protein L2

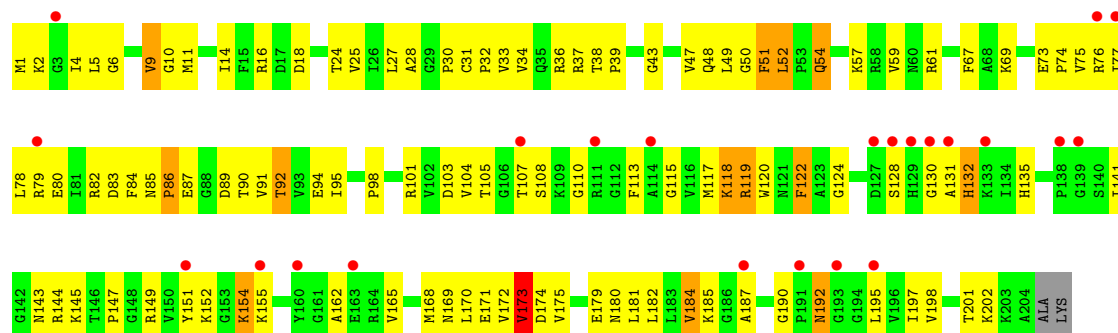




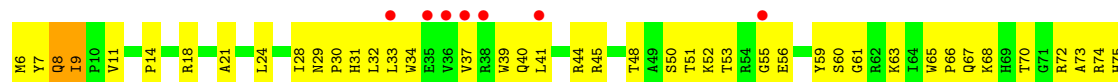
• Molecule 28: 50S ribosomal protein L3

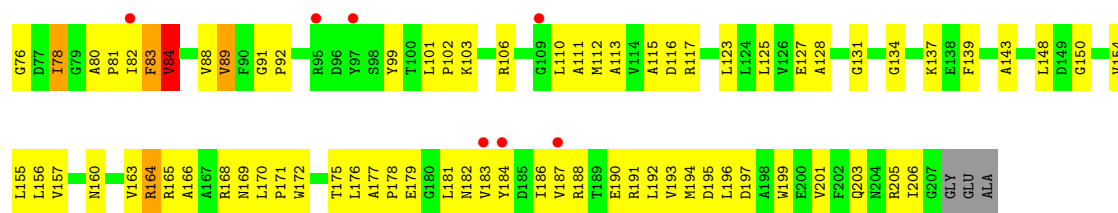


• Molecule 28: 50S ribosomal protein L3

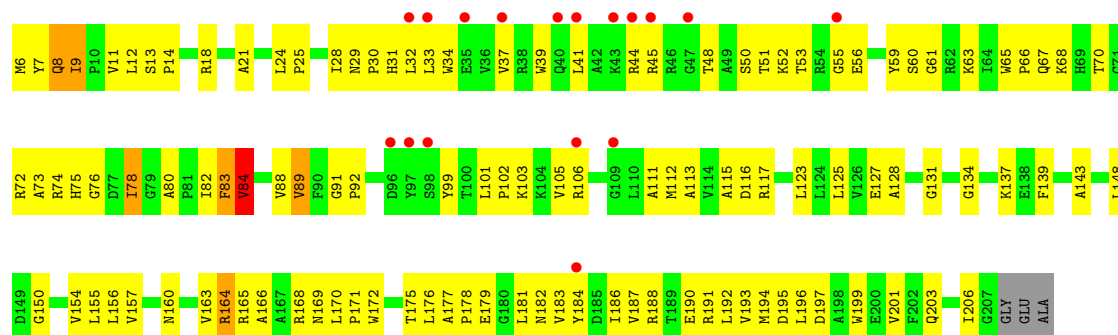
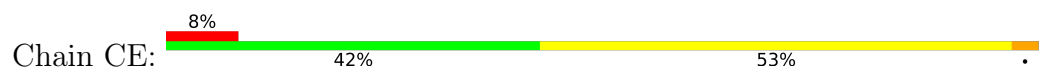


• Molecule 29: 50S ribosomal protein L4

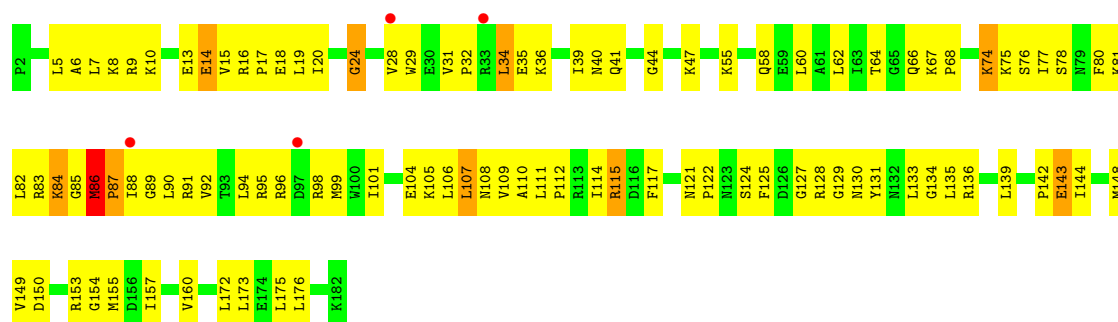




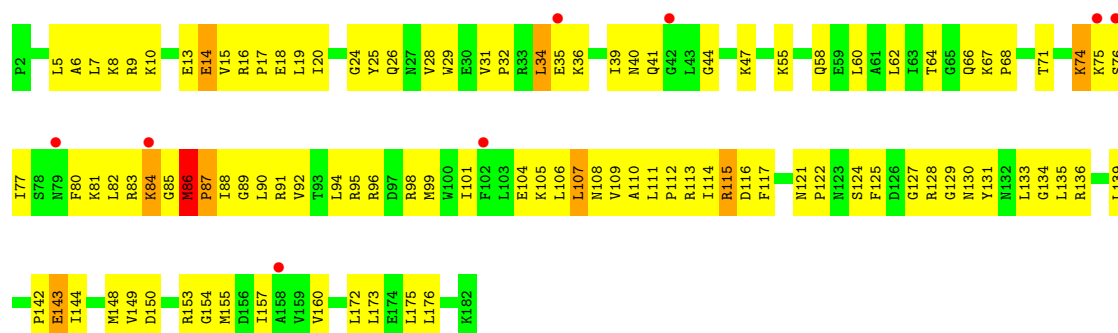
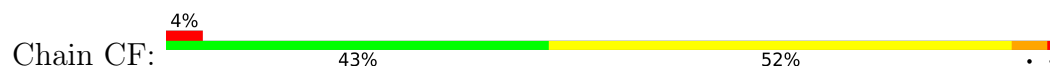
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L5

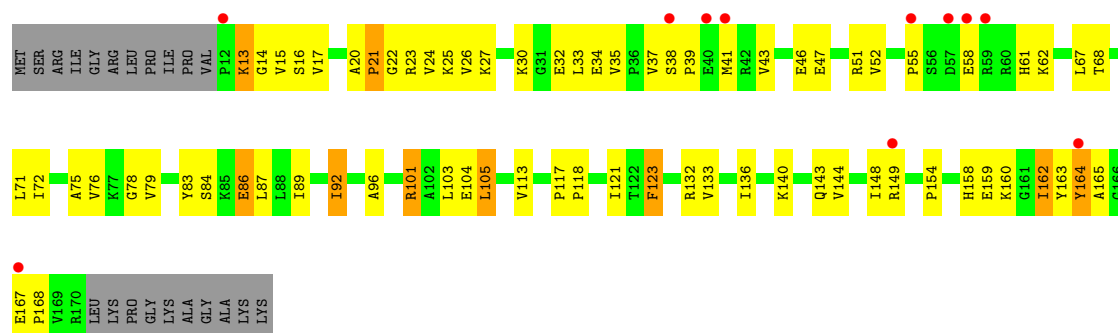


• Molecule 30: 50S ribosomal protein L5

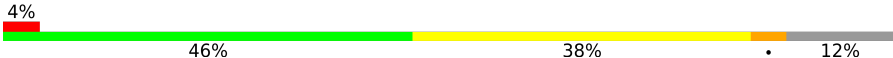


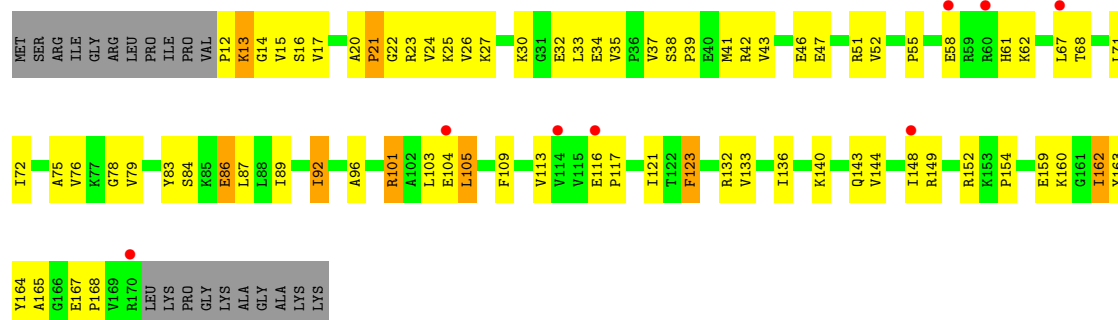
- Molecule 31: 50S ribosomal protein L6

Chain BG: 



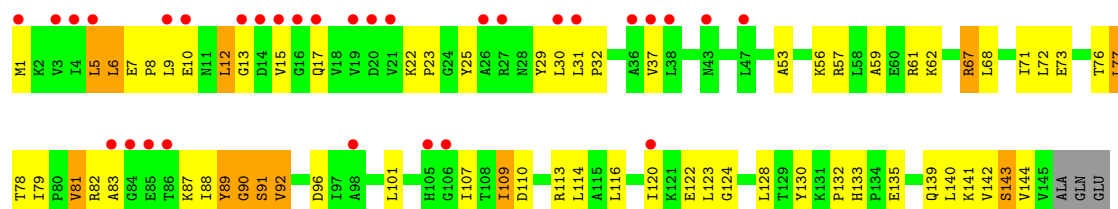
- Molecule 31: 50S ribosomal protein L6

Chain CG: 



- Molecule 32: 50S ribosomal protein L9

Chain BH: 



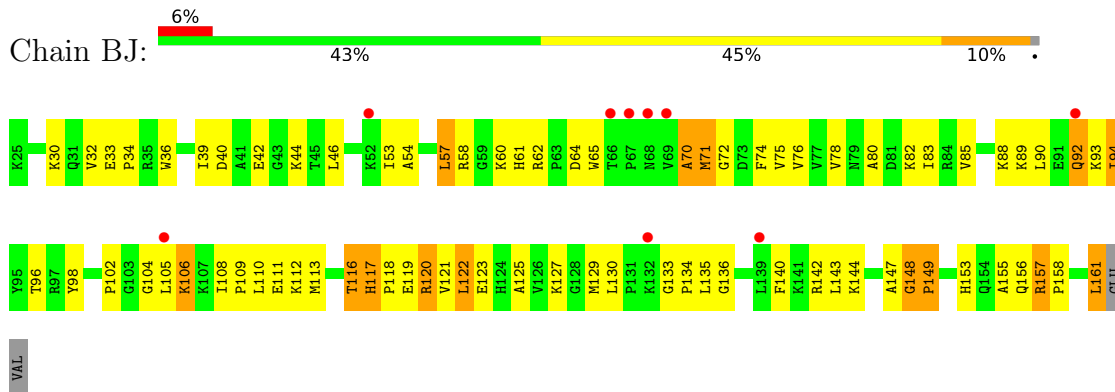
- Molecule 33: 50S ribosomal protein L10



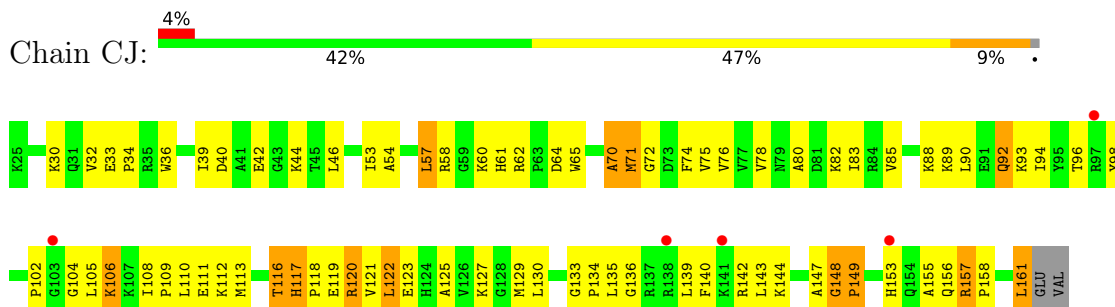
- Molecule 33: 50S ribosomal protein L10



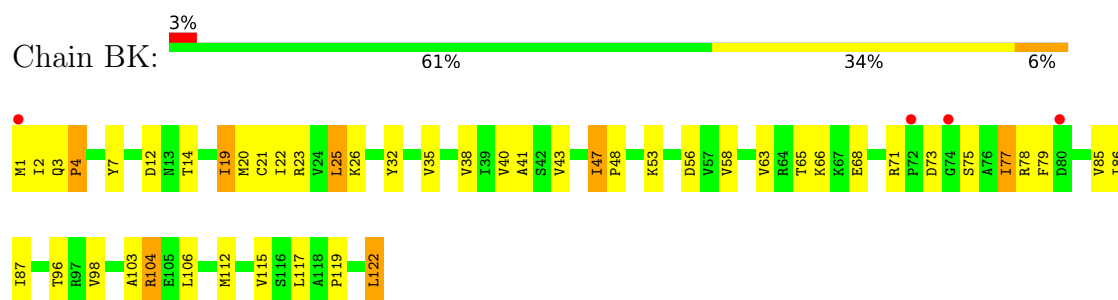
- Molecule 34: 50S ribosomal protein L13



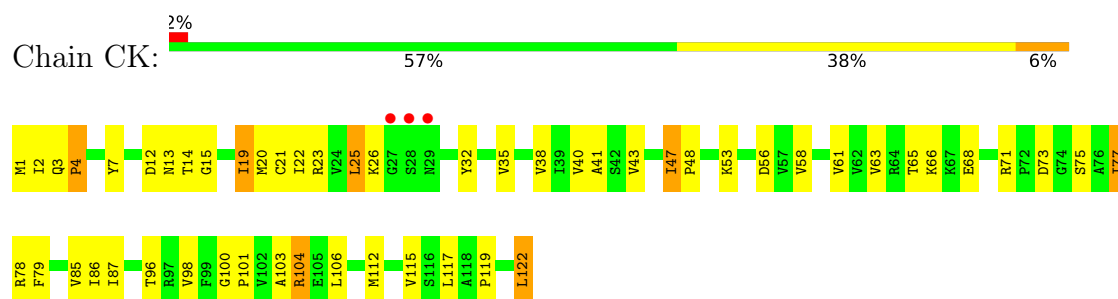
- Molecule 34: 50S ribosomal protein L13



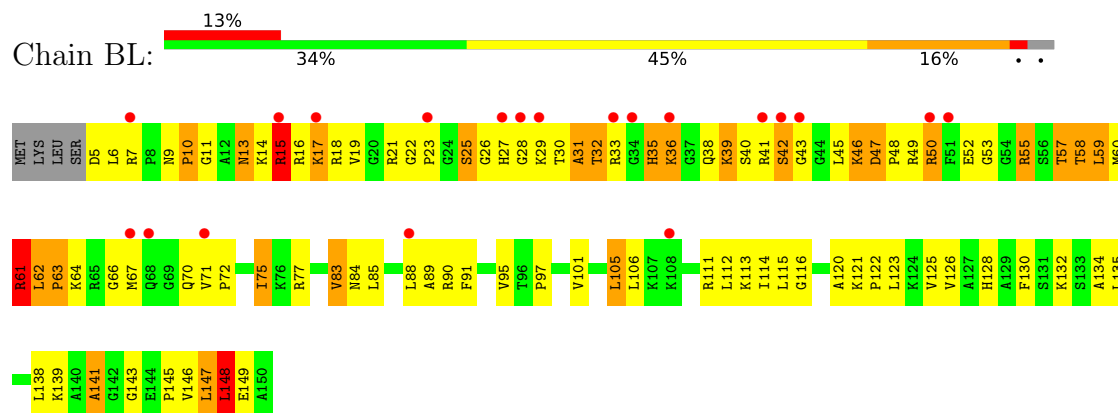
- Molecule 35: 50S ribosomal protein L14



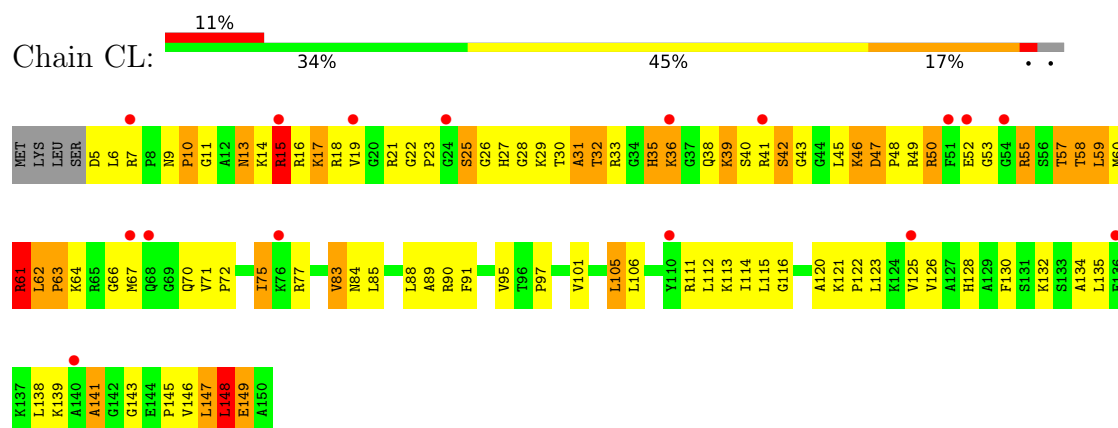
- Molecule 35: 50S ribosomal protein L14



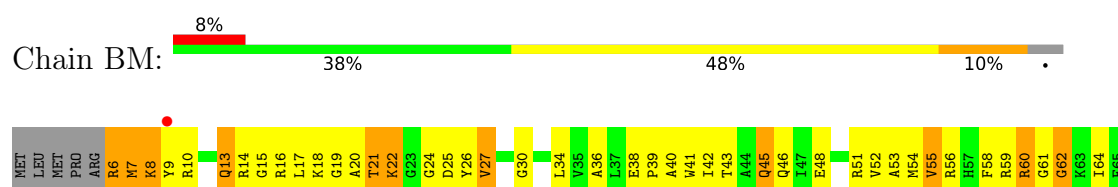
- Molecule 36: 50S ribosomal protein L15



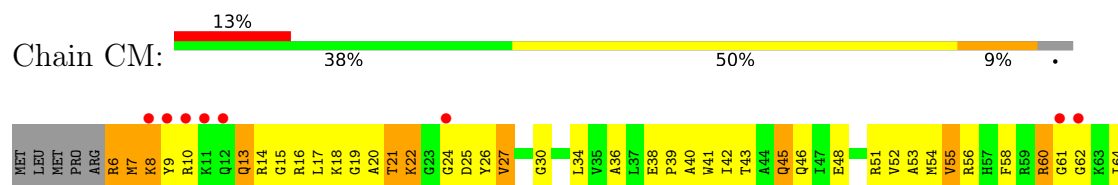
- Molecule 36: 50S ribosomal protein L15



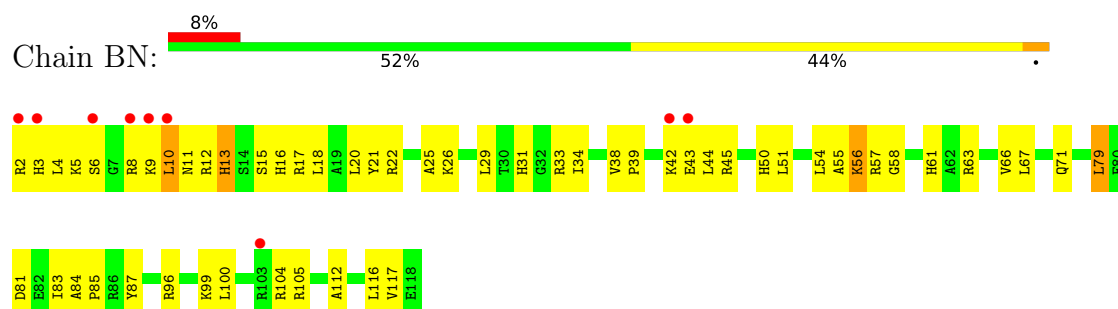
- Molecule 37: 50S ribosomal protein L16



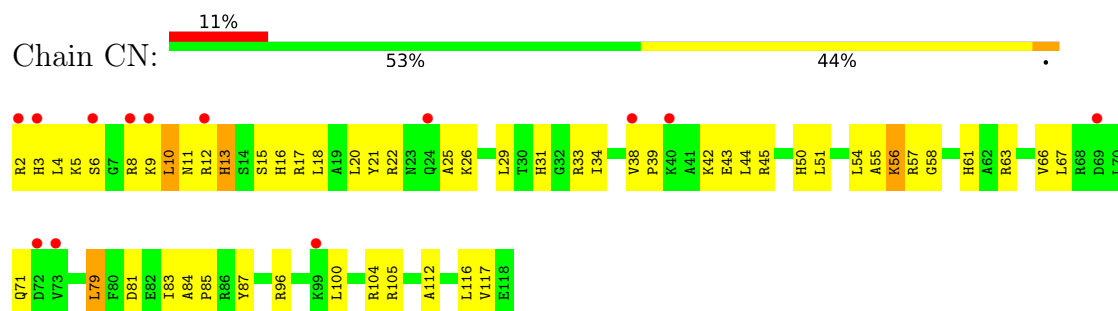
• Molecule 37: 50S ribosomal protein L16



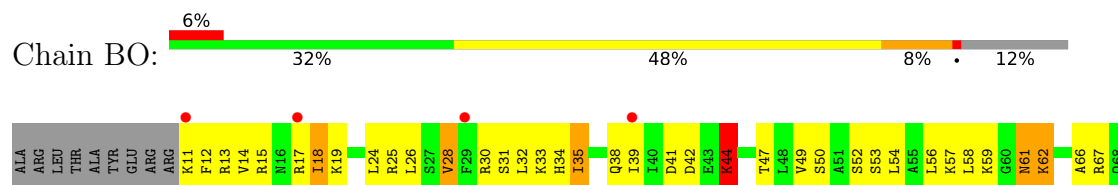
• Molecule 38: 50S ribosomal protein L17

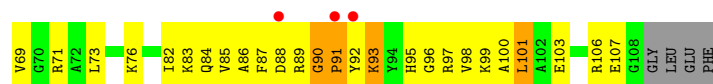


• Molecule 38: 50S ribosomal protein L17

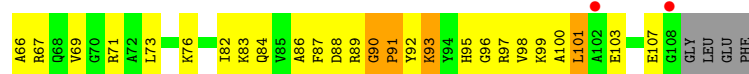
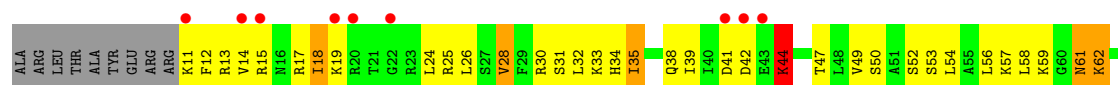


• Molecule 39: 50S ribosomal protein L18

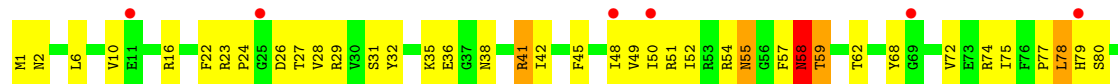




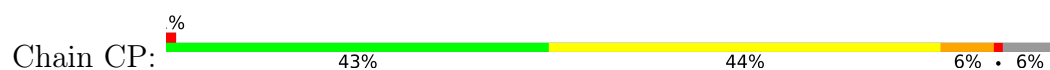
• Molecule 39: 50S ribosomal protein L18



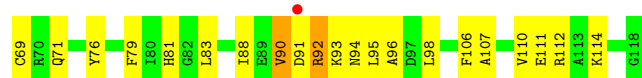
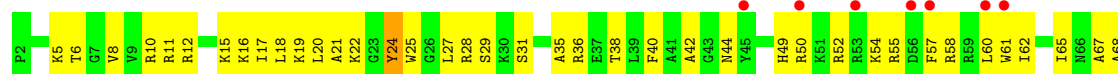
• Molecule 40: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L19

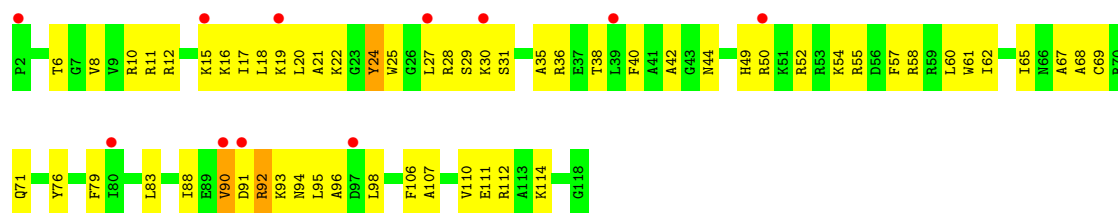


• Molecule 41: 50S ribosomal protein L20

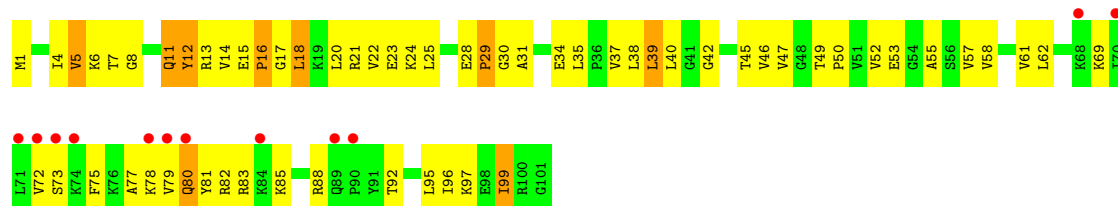
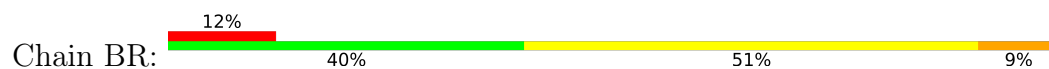


• Molecule 41: 50S ribosomal protein L20

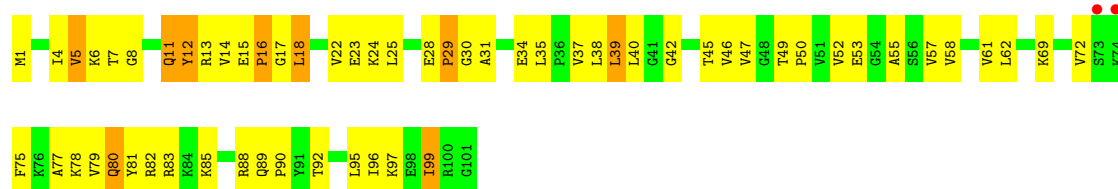
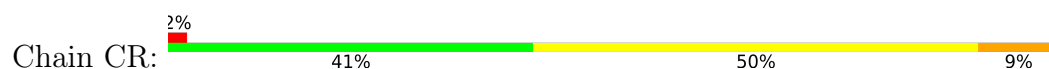




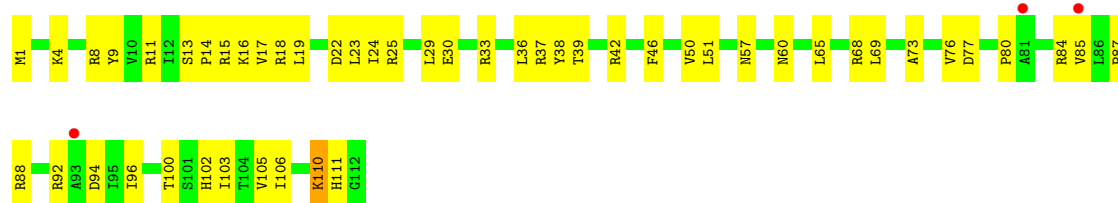
• Molecule 42: 50S ribosomal protein L21



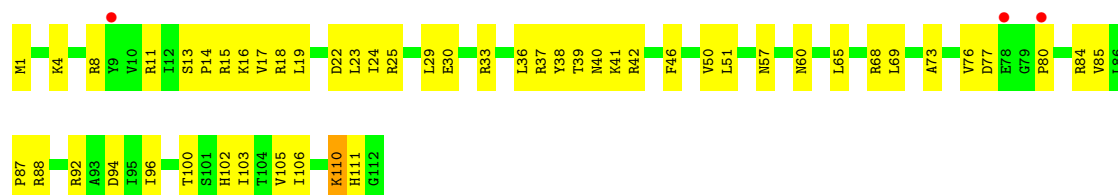
• Molecule 42: 50S ribosomal protein L21



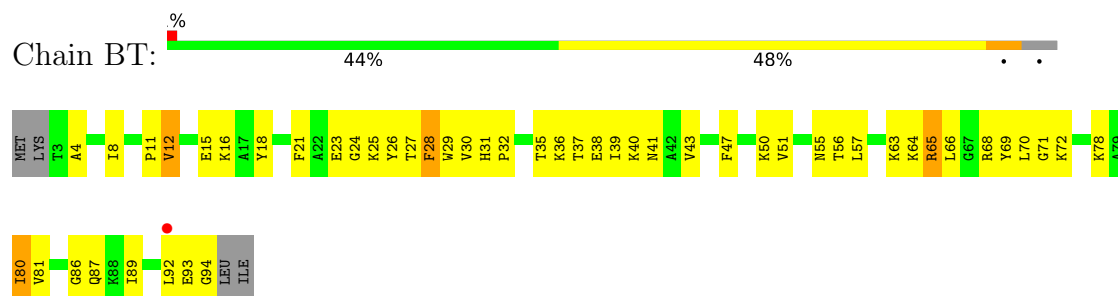
• Molecule 43: 50S ribosomal protein L22



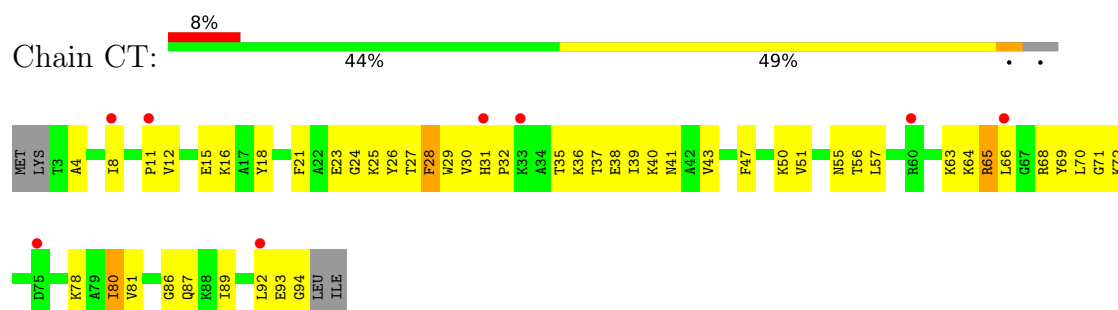
• Molecule 43: 50S ribosomal protein L22



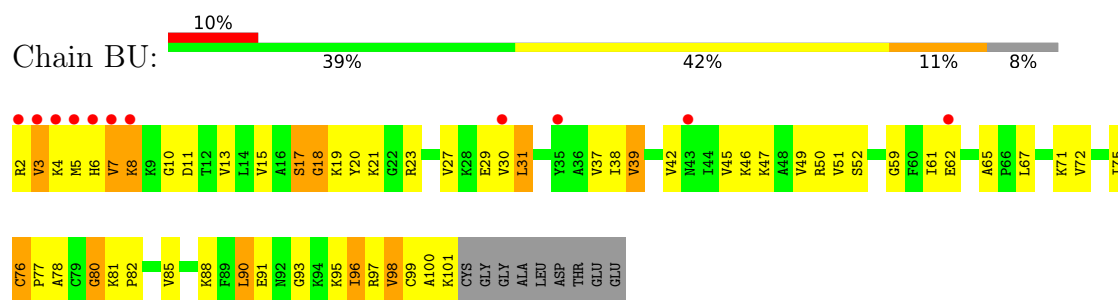
- Molecule 44: 50S ribosomal protein L23



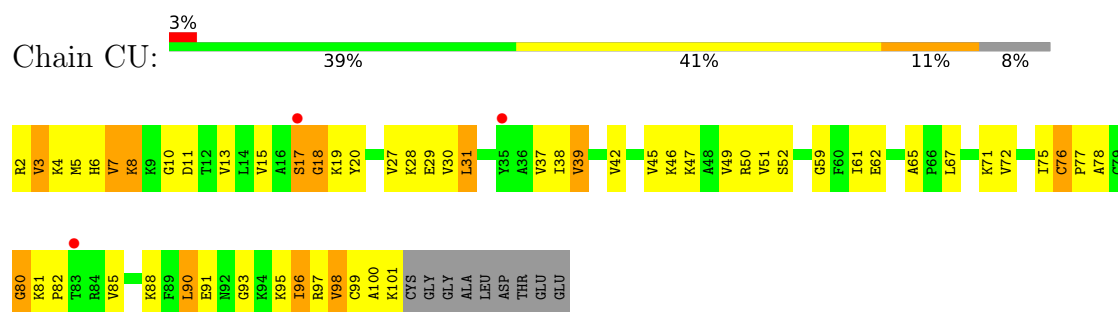
- Molecule 44: 50S ribosomal protein L23



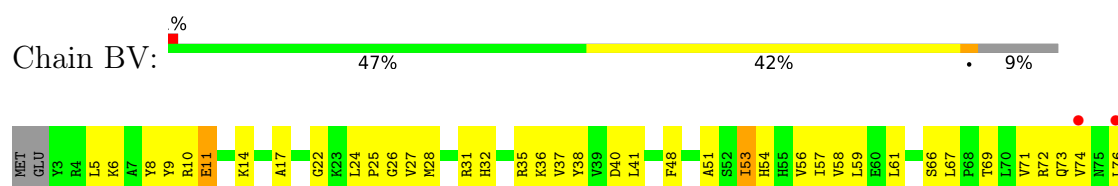
- Molecule 45: 50S ribosomal protein L24

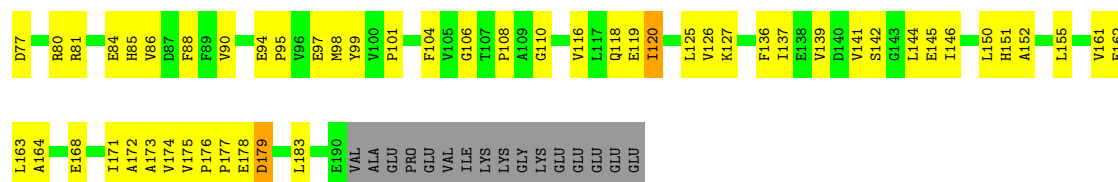


- Molecule 45: 50S ribosomal protein L24

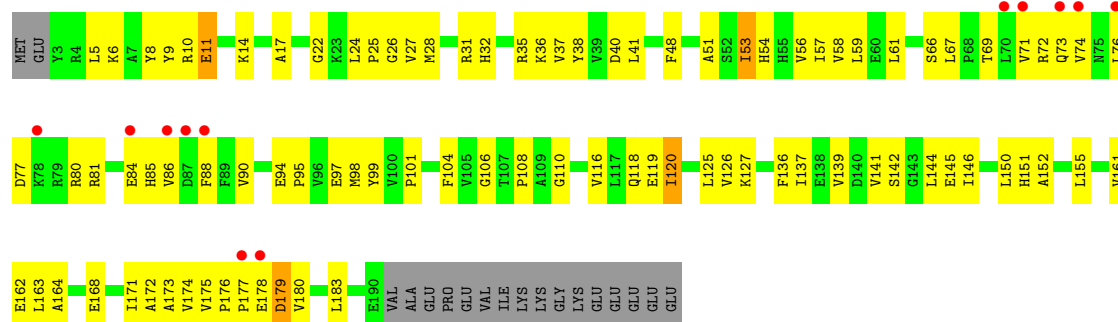


- Molecule 46: 50S ribosomal protein L25

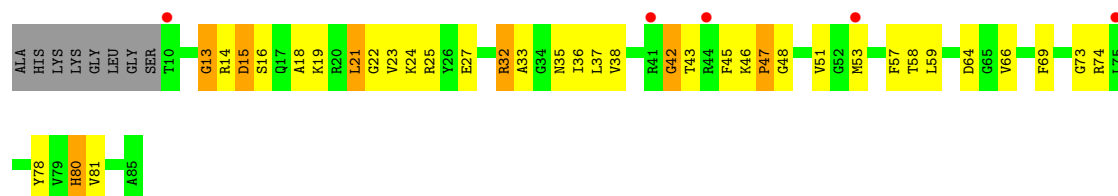




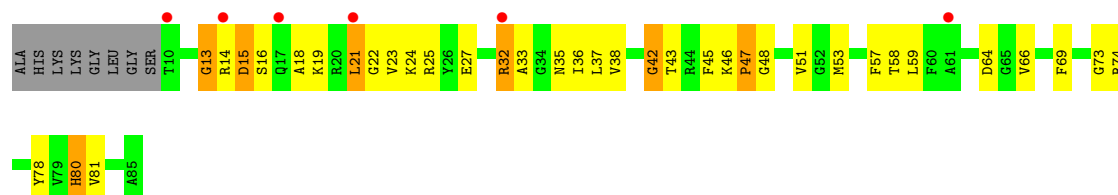
• Molecule 46: 50S ribosomal protein L25



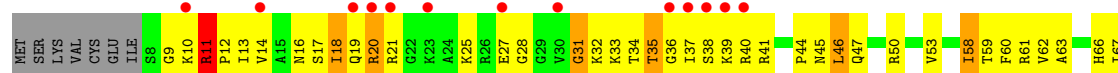
• Molecule 47: 50S ribosomal protein L27

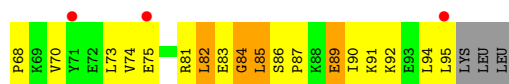


• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28

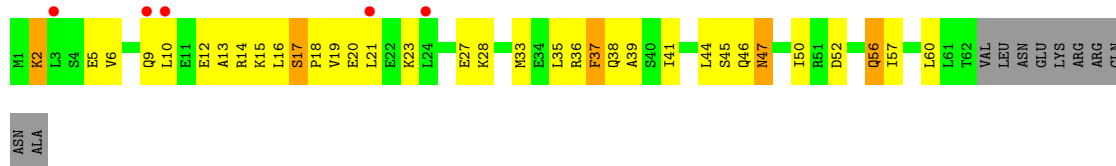




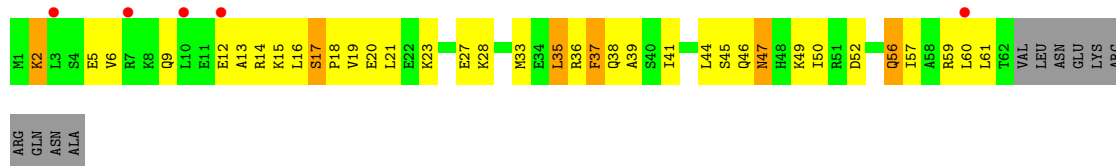
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

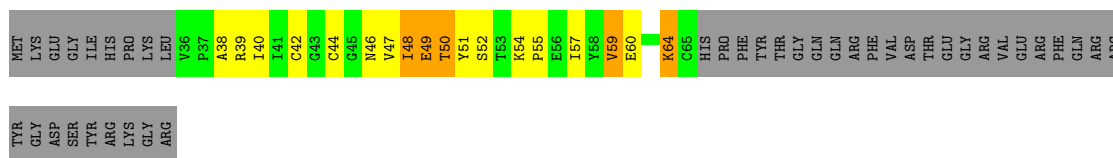


- Molecule 50: 50S ribosomal protein L30



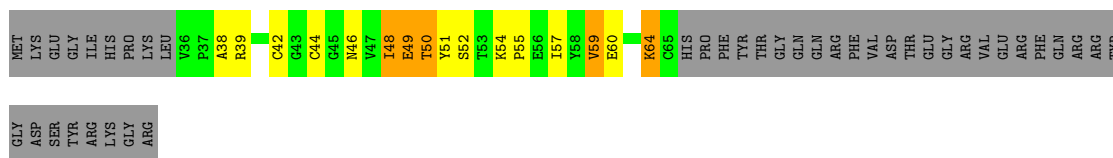
- Molecule 51: 50S ribosomal protein L31

Chain B1: 



- Molecule 51: 50S ribosomal protein L31

Chain C1: 



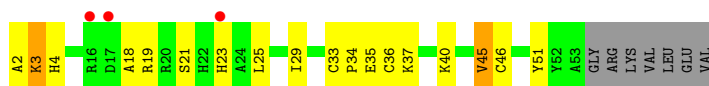
- Molecule 52: 50S ribosomal protein L32

Chain B2: 

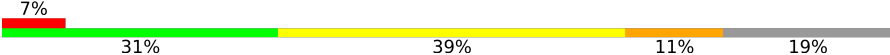


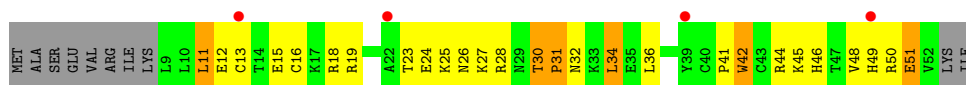
- Molecule 52: 50S ribosomal protein L32

Chain C2: 

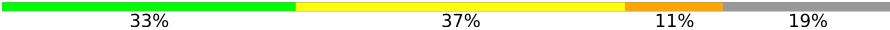


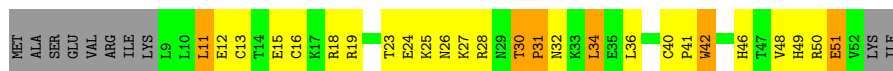
- Molecule 53: 50S ribosomal protein L33

Chain B3: 



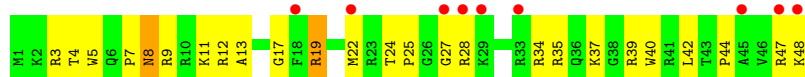
- Molecule 53: 50S ribosomal protein L33

Chain C3: 



- Molecule 54: 50S ribosomal protein L34

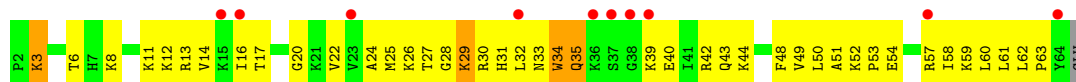
Chain B4: 



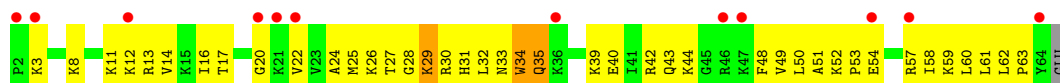
- Molecule 54: 50S ribosomal protein L34



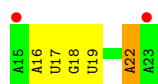
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.38Å 452.70Å 617.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.62 49.95 – 3.62	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.95-3.62) 99.9 (49.95-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.6_289, CNS	Depositor
R, R_{free}	0.260 , 0.291 0.252 , 0.285	Depositor DCC
R_{free} test set	14480 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	130.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	294174	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	AA	0.08	0/36194	0.42	9/56493 (0.0%)
1	DA	0.09	0/36194	0.42	9/56493 (0.0%)
2	AB	0.25	0/1936	0.69	0/2609
2	DB	0.25	0/1936	0.68	0/2609
3	AC	0.26	0/1637	0.65	0/2205
3	DC	0.26	0/1637	0.65	0/2205
4	AD	0.26	0/1733	0.68	0/2318
4	DD	0.25	0/1733	0.68	0/2318
5	AE	0.26	0/1172	0.70	0/1576
5	DE	0.26	0/1172	0.70	0/1576
6	AF	0.24	0/856	0.71	0/1154
6	DF	0.25	0/856	0.71	0/1154
7	AG	0.26	0/1276	0.66	0/1709
7	DG	0.26	0/1276	0.66	0/1709
8	AH	0.26	0/1136	0.73	0/1527
8	DH	0.26	0/1136	0.73	0/1527
9	AI	0.25	0/1029	0.66	0/1378
9	DI	0.25	0/1029	0.67	0/1378
10	AJ	0.26	0/808	0.70	0/1085
10	DJ	0.26	0/808	0.70	0/1085
11	AK	0.26	0/900	0.71	0/1213
11	DK	0.26	0/900	0.71	0/1213
12	AL	0.26	0/987	0.75	0/1320
12	DL	0.26	0/987	0.74	0/1320
13	AM	0.26	0/944	0.70	0/1265
13	DM	0.27	0/944	0.70	0/1265
14	AN	0.28	0/501	0.65	0/664
14	DN	0.28	0/501	0.65	0/664
15	AO	0.27	0/745	0.66	0/992
15	DO	0.28	0/745	0.66	0/992
16	AP	0.27	0/717	0.67	0/963
16	DP	0.26	0/717	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.23	0/837	0.69	0/1117
17	DQ	0.23	0/837	0.69	0/1117
18	AR	0.25	0/579	0.65	0/768
18	DR	0.25	0/579	0.65	0/768
19	AS	0.26	0/643	0.66	0/865
19	DS	0.26	0/643	0.65	0/865
20	AT	0.27	0/764	0.64	0/1006
20	DT	0.27	0/764	0.65	0/1006
21	AU	0.22	0/213	0.65	0/277
21	DU	0.22	0/213	0.65	0/277
22	AV	0.28	0/2850	0.70	0/3829
22	DV	0.28	0/2850	0.70	0/3829
23	AW	0.08	0/1832	0.40	0/2855
23	DW	0.09	0/1832	0.40	0/2855
24	AX	0.09	0/167	0.52	0/259
25	BA	0.10	0/69437	0.46	18/108401 (0.0%)
25	CA	0.10	0/69437	0.46	16/108401 (0.0%)
26	BB	0.08	0/2853	0.43	0/4451
26	CB	0.08	0/2853	0.43	0/4451
27	BC	0.29	0/2154	0.74	0/2905
27	CC	0.29	0/2154	0.74	0/2905
28	BD	0.26	0/1596	0.74	0/2153
28	CD	0.26	0/1596	0.74	0/2153
29	BE	0.28	0/1621	0.71	0/2194
29	CE	0.27	0/1621	0.71	0/2194
30	BF	0.26	0/1500	0.69	1/2017 (0.0%)
30	CF	0.27	0/1500	0.69	1/2017 (0.0%)
31	BG	0.27	0/1245	0.73	1/1682 (0.1%)
31	CG	0.27	0/1245	0.73	1/1682 (0.1%)
32	BH	0.25	0/1147	0.70	0/1552
32	CH	0.25	0/1147	0.69	0/1552
33	BI	0.25	0/251	0.61	0/333
33	CI	0.25	0/251	0.60	0/333
34	BJ	0.25	0/1123	0.73	2/1515 (0.1%)
34	CJ	0.25	0/1123	0.73	2/1515 (0.1%)
35	BK	0.27	0/942	0.73	0/1268
35	CK	0.27	0/942	0.73	0/1268
36	BL	0.29	0/1131	0.75	3/1504 (0.2%)
36	CL	0.29	0/1131	0.75	3/1504 (0.2%)
37	BM	0.27	0/1099	0.72	1/1468 (0.1%)
37	CM	0.27	0/1099	0.73	1/1468 (0.1%)
38	BN	0.28	0/974	0.67	0/1302
38	CN	0.28	0/974	0.67	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BO	0.28	0/778	0.71	1/1036 (0.1%)
39	CO	0.28	0/778	0.72	1/1036 (0.1%)
40	BP	0.26	0/1157	0.69	0/1544
40	CP	0.26	0/1157	0.69	0/1544
41	BQ	0.28	0/970	0.69	0/1290
41	CQ	0.27	0/970	0.69	0/1290
42	BR	0.25	0/790	0.63	0/1057
42	CR	0.25	0/790	0.63	0/1057
43	BS	0.27	0/902	0.67	0/1209
43	CS	0.27	0/902	0.67	0/1209
44	BT	0.26	0/739	0.73	0/993
44	CT	0.26	0/739	0.72	0/993
45	BU	0.26	0/788	0.73	0/1051
45	CU	0.29	0/788	0.73	0/1051
46	BV	0.25	0/1523	0.69	0/2068
46	CV	0.26	0/1523	0.69	0/2068
47	BW	0.23	0/613	0.65	0/816
47	CW	0.23	0/613	0.65	0/816
48	BX	0.27	0/701	0.76	1/932 (0.1%)
48	CX	0.27	0/701	0.78	1/932 (0.1%)
49	BY	0.27	0/522	0.68	0/690
49	CY	0.28	0/522	0.68	0/690
50	BZ	0.25	0/473	0.77	0/634
50	CZ	0.26	0/473	0.77	0/634
51	B1	0.27	0/228	0.66	0/309
51	C1	0.26	0/228	0.66	0/309
52	B2	0.29	0/418	0.74	0/567
52	C2	0.31	0/418	0.75	0/567
53	B3	0.27	0/387	0.67	0/518
53	C3	0.26	0/387	0.67	0/518
54	B4	0.30	0/427	0.80	0/561
54	C4	0.30	0/427	0.80	0/561
55	B5	0.26	0/515	0.62	0/679
55	C5	0.26	0/515	0.62	0/679
56	DX	0.09	0/217	0.48	0/337
All	All	0.17	0/318970	0.53	72/476370 (0.0%)

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1558	A	P-O3'-C3'	8.13	132.39	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1558	A	P-O3'-C3'	7.98	132.17	120.20
48	CX	35	THR	N-CA-C	7.75	118.22	108.45
48	BX	35	THR	N-CA-C	7.67	118.11	108.45
25	CA	1379	A	P-O3'-C3'	7.24	131.06	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32332	0	16318	651	0
1	DA	32332	0	16318	663	0
2	AB	1901	0	1951	96	0
2	DB	1901	0	1951	96	0
3	AC	1613	0	1677	87	0
3	DC	1613	0	1677	88	0
4	AD	1703	0	1765	94	0
4	DD	1703	0	1765	90	0
5	AE	1156	0	1213	60	0
5	DE	1156	0	1213	62	0
6	AF	843	0	857	44	0
6	DF	843	0	857	46	0
7	AG	1257	0	1296	62	0
7	DG	1257	0	1296	63	0
8	AH	1116	0	1177	53	0
8	DH	1116	0	1177	54	0
9	AI	1011	0	1043	62	0
9	DI	1011	0	1043	65	0
10	AJ	795	0	840	59	0
10	DJ	795	0	840	62	0
11	AK	885	0	904	51	0
11	DK	885	0	904	49	0
12	AL	971	0	1057	63	0
12	DL	971	0	1057	65	0
13	AM	934	0	992	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	DM	934	0	992	51	0
14	AN	492	0	532	32	0
14	DN	492	0	531	33	0
15	AO	734	0	771	37	0
15	DO	734	0	771	39	0
16	AP	701	0	720	34	0
16	DP	701	0	720	35	0
17	AQ	824	0	893	41	0
17	DQ	824	0	893	42	0
18	AR	574	0	644	31	0
18	DR	574	0	644	30	0
19	AS	630	0	652	61	0
19	DS	630	0	652	60	0
20	AT	762	0	859	31	0
20	DT	762	0	859	31	0
21	AU	209	0	221	10	0
21	DU	209	0	221	11	0
22	AV	2813	0	2823	184	0
22	DV	2813	0	2823	184	0
23	AW	1640	0	837	25	0
23	DW	1640	0	837	20	0
24	AX	149	0	77	6	0
25	BA	61997	0	31250	1322	0
25	CA	61997	0	31250	1304	0
26	BB	2551	0	1295	64	0
26	CB	2551	0	1295	63	0
27	BC	2104	0	2182	164	0
27	CC	2104	0	2182	170	0
28	BD	1563	0	1629	113	0
28	CD	1563	0	1629	111	0
29	BE	1586	0	1632	105	0
29	CE	1586	0	1632	106	0
30	BF	1475	0	1537	104	0
30	CF	1475	0	1537	106	0
31	BG	1222	0	1282	58	0
31	CG	1222	0	1282	61	0
32	BH	1132	0	1220	56	0
32	CH	1132	0	1220	58	0
33	BI	253	0	275	7	0
33	CI	253	0	275	7	0
34	BJ	1096	0	1168	70	0
34	CJ	1096	0	1168	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BK	932	0	994	49	0
35	CK	932	0	994	52	0
36	BL	1114	0	1187	145	0
36	CL	1114	0	1187	148	0
37	BM	1079	0	1127	84	0
37	CM	1079	0	1127	82	0
38	BN	960	0	1021	63	0
38	CN	960	0	1021	59	0
39	BO	770	0	832	69	0
39	CO	770	0	832	71	0
40	BP	1143	0	1211	68	0
40	CP	1143	0	1211	73	0
41	BQ	953	0	1013	76	0
41	CQ	953	0	1013	76	0
42	BR	779	0	852	70	0
42	CR	779	0	852	72	0
43	BS	891	0	951	43	0
43	CS	891	0	951	41	0
44	BT	725	0	778	45	0
44	CT	725	0	778	46	0
45	BU	775	0	870	75	0
45	CU	775	0	870	75	0
46	BV	1491	0	1513	79	0
46	CV	1491	0	1513	78	0
47	BW	605	0	628	36	0
47	CW	605	0	628	36	0
48	BX	694	0	764	63	0
48	CX	694	0	764	67	0
49	BY	520	0	575	38	0
49	CY	520	0	575	39	0
50	BZ	468	0	523	22	0
50	CZ	468	0	523	21	0
51	B1	225	0	225	17	0
51	C1	225	0	225	20	0
52	B2	404	0	420	19	0
52	C2	404	0	420	20	0
53	B3	380	0	391	23	0
53	C3	380	0	391	24	0
54	B4	419	0	467	26	0
54	C4	419	0	467	24	0
55	B5	507	0	576	55	0
55	C5	507	0	576	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DX	193	0	99	4	0
57	AA	64	0	0	0	0
57	AT	1	0	0	0	0
57	AV	1	0	0	0	0
57	AW	3	0	0	0	0
57	B2	1	0	0	0	0
57	BA	176	0	0	0	0
57	BB	2	0	0	0	0
57	BK	1	0	0	0	0
57	BM	1	0	0	0	0
57	CA	125	0	0	0	0
57	CB	2	0	0	0	0
57	CM	1	0	0	0	0
57	CY	1	0	0	0	0
57	DA	30	0	0	0	0
57	DW	1	0	0	0	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	DD	1	0	0	0	0
58	DN	1	0	0	0	0
All	All	294174	0	201035	9236	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 19.

The worst 5 of 9236 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)
4:AD:166:LYS:HE2	27:CC:134:ARG:HH21	1.20	1.07
36:CL:128:HIS:HA	36:CL:147:LEU:HB3	1.36	1.07
36:BL:128:HIS:HA	36:BL:147:LEU:HB3	1.36	1.07
35:BK:3:GLN:HB2	35:BK:4:PRO:HD2	1.40	1.03
22:DV:302:ILE:HG22	22:DV:303:ARG:H	1.21	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	197 (85%)	28 (12%)	7 (3%)	3	22
2	DB	232/234 (99%)	197 (85%)	28 (12%)	7 (3%)	3	22
3	AC	204/206 (99%)	158 (78%)	36 (18%)	10 (5%)	1	15
3	DC	204/206 (99%)	158 (78%)	36 (18%)	10 (5%)	1	15
4	AD	206/208 (99%)	168 (82%)	29 (14%)	9 (4%)	2	16
4	DD	206/208 (99%)	168 (82%)	29 (14%)	9 (4%)	2	16
5	AE	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	9	37
5	DE	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	9	37
6	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	42
6	DF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	42
7	AG	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	9	37
7	DG	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	9	37
8	AH	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	18	49
8	DH	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	18	49
9	AI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	4	26
9	DI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	4	26
10	AJ	96/98 (98%)	78 (81%)	13 (14%)	5 (5%)	1	14
10	DJ	96/98 (98%)	79 (82%)	12 (12%)	5 (5%)	1	14
11	AK	117/119 (98%)	94 (80%)	20 (17%)	3 (3%)	4	24
11	DK	117/119 (98%)	95 (81%)	19 (16%)	3 (3%)	4	24
12	AL	122/124 (98%)	92 (75%)	25 (20%)	5 (4%)	2	18
12	DL	122/124 (98%)	92 (75%)	25 (20%)	5 (4%)	2	18
13	AM	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	1	14
13	DM	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	1	14
14	AN	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	DN	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	10
15	AO	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
15	DO	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
16	AP	81/83 (98%)	66 (82%)	14 (17%)	1 (1%)	10	39
16	DP	81/83 (98%)	66 (82%)	14 (17%)	1 (1%)	10	39
17	AQ	97/99 (98%)	83 (86%)	12 (12%)	2 (2%)	5	28
17	DQ	97/99 (98%)	83 (86%)	12 (12%)	2 (2%)	5	28
18	AR	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	8	34
18	DR	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	8	34
19	AS	76/78 (97%)	58 (76%)	13 (17%)	5 (7%)	1	11
19	DS	76/78 (97%)	58 (76%)	13 (17%)	5 (7%)	1	11
20	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	18
20	DT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	18
21	AU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	16
21	DU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	16
22	AV	352/354 (99%)	290 (82%)	50 (14%)	12 (3%)	3	21
22	DV	352/354 (99%)	289 (82%)	52 (15%)	11 (3%)	3	22
27	BC	269/275 (98%)	216 (80%)	37 (14%)	16 (6%)	1	12
27	CC	269/275 (98%)	216 (80%)	37 (14%)	16 (6%)	1	12
28	BD	202/206 (98%)	168 (83%)	26 (13%)	8 (4%)	2	18
28	CD	202/206 (98%)	168 (83%)	26 (13%)	8 (4%)	2	18
29	BE	200/205 (98%)	163 (82%)	29 (14%)	8 (4%)	2	18
29	CE	200/205 (98%)	163 (82%)	29 (14%)	8 (4%)	2	18
30	BF	179/181 (99%)	133 (74%)	38 (21%)	8 (4%)	2	16
30	CF	179/181 (99%)	133 (74%)	38 (21%)	8 (4%)	2	16
31	BG	157/180 (87%)	129 (82%)	23 (15%)	5 (3%)	3	21
31	CG	157/180 (87%)	129 (82%)	23 (15%)	5 (3%)	3	21
32	BH	143/148 (97%)	115 (80%)	21 (15%)	7 (5%)	1	15
32	CH	143/148 (97%)	115 (80%)	21 (15%)	7 (5%)	1	15
33	BI	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
33	CI	28/173 (16%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BJ	135/139 (97%)	110 (82%)	16 (12%)	9 (7%)	1	10
34	CJ	135/139 (97%)	109 (81%)	17 (13%)	9 (7%)	1	10
35	BK	120/122 (98%)	105 (88%)	13 (11%)	2 (2%)	7	32
35	CK	120/122 (98%)	105 (88%)	13 (11%)	2 (2%)	7	32
36	BL	144/150 (96%)	97 (67%)	25 (17%)	22 (15%)	0	2
36	CL	144/150 (96%)	97 (67%)	25 (17%)	22 (15%)	0	2
37	BM	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	0	3
37	CM	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	0	3
38	BN	115/117 (98%)	100 (87%)	11 (10%)	4 (4%)	3	21
38	CN	115/117 (98%)	101 (88%)	10 (9%)	4 (4%)	3	21
39	BO	96/111 (86%)	65 (68%)	20 (21%)	11 (12%)	0	3
39	CO	96/111 (86%)	64 (67%)	21 (22%)	11 (12%)	0	3
40	BP	135/146 (92%)	106 (78%)	21 (16%)	8 (6%)	1	12
40	CP	135/146 (92%)	107 (79%)	20 (15%)	8 (6%)	1	12
41	BQ	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	14	44
41	CQ	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	14	44
42	BR	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	12
42	CR	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	12
43	BS	110/112 (98%)	92 (84%)	17 (16%)	1 (1%)	14	44
43	CS	110/112 (98%)	92 (84%)	17 (16%)	1 (1%)	14	44
44	BT	90/96 (94%)	81 (90%)	7 (8%)	2 (2%)	5	28
44	CT	90/96 (94%)	81 (90%)	7 (8%)	2 (2%)	5	28
45	BU	98/109 (90%)	62 (63%)	26 (26%)	10 (10%)	0	4
45	CU	98/109 (90%)	63 (64%)	25 (26%)	10 (10%)	0	4
46	BV	186/206 (90%)	143 (77%)	34 (18%)	9 (5%)	2	15
46	CV	186/206 (90%)	143 (77%)	34 (18%)	9 (5%)	2	15
47	BW	74/84 (88%)	56 (76%)	12 (16%)	6 (8%)	1	7
47	CW	74/84 (88%)	57 (77%)	11 (15%)	6 (8%)	1	7
48	BX	86/98 (88%)	59 (69%)	19 (22%)	8 (9%)	0	5
48	CX	86/98 (88%)	59 (69%)	19 (22%)	8 (9%)	0	5
49	BY	60/72 (83%)	47 (78%)	11 (18%)	2 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	CY	60/72 (83%)	47 (78%)	11 (18%)	2 (3%)	3	21
50	BZ	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
50	CZ	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
51	B1	28/71 (39%)	17 (61%)	8 (29%)	3 (11%)	0	4
51	C1	28/71 (39%)	17 (61%)	8 (29%)	3 (11%)	0	4
52	B2	50/59 (85%)	40 (80%)	8 (16%)	2 (4%)	2	18
52	C2	50/59 (85%)	40 (80%)	8 (16%)	2 (4%)	2	18
53	B3	42/54 (78%)	33 (79%)	4 (10%)	5 (12%)	0	3
53	C3	42/54 (78%)	33 (79%)	4 (10%)	5 (12%)	0	3
54	B4	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
54	C4	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
55	B5	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	5
55	C5	61/64 (95%)	44 (72%)	11 (18%)	6 (10%)	0	5
All	All	11898/12752 (93%)	9614 (81%)	1747 (15%)	537 (4%)	2	16

5 of 537 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	15	THR
4	AD	137	SER
13	AM	106	ASN
14	AN	26	ARG
19	AS	28	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	
2	AB	202/202 (100%)	189 (94%)	13 (6%)	16	41
2	DB	202/202 (100%)	189 (94%)	13 (6%)	16	41
3	AC	160/160 (100%)	156 (98%)	4 (2%)	42	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DC	160/160 (100%)	156 (98%)	4 (2%)	42	59
4	AD	180/180 (100%)	172 (96%)	8 (4%)	25	49
4	DD	180/180 (100%)	172 (96%)	8 (4%)	25	49
5	AE	116/116 (100%)	108 (93%)	8 (7%)	14	39
5	DE	116/116 (100%)	108 (93%)	8 (7%)	14	39
6	AF	90/90 (100%)	88 (98%)	2 (2%)	45	62
6	DF	90/90 (100%)	88 (98%)	2 (2%)	45	62
7	AG	126/126 (100%)	125 (99%)	1 (1%)	73	74
7	DG	126/126 (100%)	125 (99%)	1 (1%)	73	74
8	AH	119/119 (100%)	114 (96%)	5 (4%)	26	49
8	DH	119/119 (100%)	114 (96%)	5 (4%)	26	49
9	AI	98/98 (100%)	93 (95%)	5 (5%)	21	46
9	DI	98/98 (100%)	93 (95%)	5 (5%)	21	46
10	AJ	88/88 (100%)	82 (93%)	6 (7%)	14	39
10	DJ	88/88 (100%)	82 (93%)	6 (7%)	14	39
11	AK	90/90 (100%)	89 (99%)	1 (1%)	65	71
11	DK	90/90 (100%)	89 (99%)	1 (1%)	65	71
12	AL	104/104 (100%)	97 (93%)	7 (7%)	15	40
12	DL	104/104 (100%)	97 (93%)	7 (7%)	15	40
13	AM	94/94 (100%)	89 (95%)	5 (5%)	20	45
13	DM	94/94 (100%)	89 (95%)	5 (5%)	20	45
14	AN	49/49 (100%)	46 (94%)	3 (6%)	17	42
14	DN	49/49 (100%)	46 (94%)	3 (6%)	17	42
15	AO	79/79 (100%)	76 (96%)	3 (4%)	29	51
15	DO	79/79 (100%)	76 (96%)	3 (4%)	29	51
16	AP	72/72 (100%)	70 (97%)	2 (3%)	38	57
16	DP	72/72 (100%)	70 (97%)	2 (3%)	38	57
17	AQ	94/94 (100%)	92 (98%)	2 (2%)	47	62
17	DQ	94/94 (100%)	92 (98%)	2 (2%)	47	62
18	AR	61/61 (100%)	59 (97%)	2 (3%)	33	54
18	DR	61/61 (100%)	59 (97%)	2 (3%)	33	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	69/69 (100%)	61 (88%)	8 (12%)	5	23
19	DS	69/69 (100%)	61 (88%)	8 (12%)	5	23
20	AT	76/76 (100%)	72 (95%)	4 (5%)	20	45
20	DT	76/76 (100%)	72 (95%)	4 (5%)	20	45
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	DU	19/19 (100%)	19 (100%)	0	100	100
22	AV	299/299 (100%)	274 (92%)	25 (8%)	10	33
22	DV	299/299 (100%)	273 (91%)	26 (9%)	9	32
27	BC	213/217 (98%)	191 (90%)	22 (10%)	7	28
27	CC	213/217 (98%)	191 (90%)	22 (10%)	7	28
28	BD	165/166 (99%)	153 (93%)	12 (7%)	13	37
28	CD	165/166 (99%)	153 (93%)	12 (7%)	13	37
29	BE	161/162 (99%)	155 (96%)	6 (4%)	30	52
29	CE	161/162 (99%)	155 (96%)	6 (4%)	30	52
30	BF	155/155 (100%)	147 (95%)	8 (5%)	21	45
30	CF	155/155 (100%)	147 (95%)	8 (5%)	21	45
31	BG	132/148 (89%)	126 (96%)	6 (4%)	24	48
31	CG	132/148 (89%)	126 (96%)	6 (4%)	24	48
32	BH	122/124 (98%)	113 (93%)	9 (7%)	13	37
32	CH	122/124 (98%)	113 (93%)	9 (7%)	13	37
33	BI	27/135 (20%)	26 (96%)	1 (4%)	30	52
33	CI	27/135 (20%)	26 (96%)	1 (4%)	30	52
34	BJ	116/118 (98%)	108 (93%)	8 (7%)	14	39
34	CJ	116/118 (98%)	108 (93%)	8 (7%)	14	39
35	BK	100/100 (100%)	93 (93%)	7 (7%)	14	39
35	CK	100/100 (100%)	93 (93%)	7 (7%)	14	39
36	BL	112/116 (97%)	96 (86%)	16 (14%)	3	16
36	CL	112/116 (97%)	96 (86%)	16 (14%)	3	16
37	BM	106/111 (96%)	98 (92%)	8 (8%)	12	37
37	CM	106/111 (96%)	98 (92%)	8 (8%)	12	37
38	BN	100/100 (100%)	96 (96%)	4 (4%)	28	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	CN	100/100 (100%)	96 (96%)	4 (4%)	28	50
39	BO	77/87 (88%)	74 (96%)	3 (4%)	28	51
39	CO	77/87 (88%)	74 (96%)	3 (4%)	28	51
40	BP	121/128 (94%)	112 (93%)	9 (7%)	13	37
40	CP	121/128 (94%)	112 (93%)	9 (7%)	13	37
41	BQ	92/92 (100%)	89 (97%)	3 (3%)	33	54
41	CQ	92/92 (100%)	89 (97%)	3 (3%)	33	54
42	BR	82/82 (100%)	74 (90%)	8 (10%)	7	29
42	CR	82/82 (100%)	74 (90%)	8 (10%)	7	29
43	BS	91/91 (100%)	87 (96%)	4 (4%)	25	49
43	CS	91/91 (100%)	87 (96%)	4 (4%)	25	49
44	BT	74/78 (95%)	69 (93%)	5 (7%)	14	39
44	CT	74/78 (95%)	70 (95%)	4 (5%)	20	44
45	BU	84/90 (93%)	81 (96%)	3 (4%)	31	53
45	CU	84/90 (93%)	81 (96%)	3 (4%)	31	53
46	BV	163/179 (91%)	162 (99%)	1 (1%)	78	77
46	CV	163/179 (91%)	162 (99%)	1 (1%)	78	77
47	BW	61/66 (92%)	59 (97%)	2 (3%)	33	54
47	CW	61/66 (92%)	59 (97%)	2 (3%)	33	54
48	BX	73/83 (88%)	65 (89%)	8 (11%)	6	25
48	CX	73/83 (88%)	64 (88%)	9 (12%)	4	21
49	BY	58/67 (87%)	54 (93%)	4 (7%)	14	39
49	CY	58/67 (87%)	54 (93%)	4 (7%)	14	39
50	BZ	51/51 (100%)	48 (94%)	3 (6%)	18	43
50	CZ	51/51 (100%)	48 (94%)	3 (6%)	18	43
51	B1	27/63 (43%)	23 (85%)	4 (15%)	3	15
51	C1	27/63 (43%)	23 (85%)	4 (15%)	3	15
52	B2	45/51 (88%)	43 (96%)	2 (4%)	25	49
52	C2	45/51 (88%)	44 (98%)	1 (2%)	45	62
53	B3	43/52 (83%)	39 (91%)	4 (9%)	8	30
53	C3	43/52 (83%)	39 (91%)	4 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B4	41/41 (100%)	38 (93%)	3 (7%)	13	37
54	C4	41/41 (100%)	38 (93%)	3 (7%)	13	37
55	B5	53/54 (98%)	52 (98%)	1 (2%)	50	64
55	C5	53/54 (98%)	52 (98%)	1 (2%)	50	64
All	All	10060/10584 (95%)	9484 (94%)	576 (6%)	18	43

5 of 576 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	DB	71	VAL
22	DV	332	LEU
3	DC	91	LEU
2	DB	27	LYS
12	DL	98	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
6	DF	32	ASN
9	DI	23	ASN
19	DS	53	ASN
38	BN	71	GLN
38	BN	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	198 (13%)	14 (0%)
1	DA	1503/1504 (99%)	198 (13%)	14 (0%)
23	AW	76/77 (98%)	9 (11%)	0
23	DW	76/77 (98%)	9 (11%)	0
24	AX	6/7 (85%)	1 (16%)	0
25	BA	2878/2879 (99%)	429 (14%)	18 (0%)
25	CA	2878/2879 (99%)	430 (14%)	19 (0%)
26	BB	118/119 (99%)	12 (10%)	0
26	CB	118/119 (99%)	12 (10%)	0
56	DX	8/9 (88%)	2 (25%)	0
All	All	9164/9174 (99%)	1300 (14%)	65 (0%)

5 of 1300 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	DA	484	G
1	DA	687	A
25	BA	1830	C
25	BA	1678	G
1	DA	1064	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 414 ligands modelled in this entry, 414 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1504/1504 (100%)	-0.21	43 (2%)	53	32	99, 172, 294, 492	0
1	DA	1504/1504 (100%)	-0.23	42 (2%)	55	33	92, 174, 297, 495	0
2	AB	234/234 (100%)	-0.24	6 (2%)	57	35	141, 239, 344, 376	0
2	DB	234/234 (100%)	-0.03	12 (5%)	33	21	122, 210, 294, 383	0
3	AC	206/206 (100%)	0.03	12 (5%)	29	18	116, 224, 305, 369	0
3	DC	206/206 (100%)	-0.17	9 (4%)	39	23	104, 199, 279, 314	0
4	AD	208/208 (100%)	0.27	17 (8%)	17	13	103, 180, 260, 329	0
4	DD	208/208 (100%)	0.47	18 (8%)	16	12	100, 192, 286, 330	0
5	AE	151/151 (100%)	-0.02	5 (3%)	49	29	115, 194, 274, 320	0
5	DE	151/151 (100%)	-0.20	5 (3%)	49	29	112, 173, 263, 312	0
6	AF	101/101 (100%)	-0.47	2 (1%)	65	40	121, 210, 285, 343	0
6	DF	101/101 (100%)	-0.31	2 (1%)	65	40	99, 169, 251, 279	0
7	AG	155/155 (100%)	-0.33	2 (1%)	75	49	115, 218, 295, 339	0
7	DG	155/155 (100%)	-0.28	4 (2%)	57	35	123, 203, 287, 375	0
8	AH	138/138 (100%)	0.59	17 (12%)	8	9	97, 193, 268, 342	0
8	DH	138/138 (100%)	0.51	16 (11%)	9	9	110, 185, 269, 354	0
9	AI	127/127 (100%)	0.26	12 (9%)	14	12	114, 236, 311, 356	0
9	DI	127/127 (100%)	0.63	17 (13%)	7	7	112, 221, 309, 373	0
10	AJ	98/98 (100%)	0.75	14 (14%)	6	7	149, 231, 311, 408	0
10	DJ	98/98 (100%)	0.84	20 (20%)	3	3	135, 215, 306, 339	0
11	AK	119/119 (100%)	0.05	8 (6%)	24	16	92, 173, 278, 341	0
11	DK	119/119 (100%)	0.15	7 (5%)	28	18	107, 164, 241, 317	0
12	AL	124/124 (100%)	0.55	14 (11%)	10	9	94, 147, 231, 327	0
12	DL	124/124 (100%)	0.40	13 (10%)	11	11	77, 151, 233, 395	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	117/117 (100%)	0.13	9 (7%) 19 14	142, 235, 332, 396	0
13	DM	117/117 (100%)	0.11	5 (4%) 40 24	121, 218, 300, 332	0
14	AN	60/60 (100%)	0.99	12 (20%) 3 3	135, 207, 347, 354	0
14	DN	60/60 (100%)	1.75	18 (30%) 1 1	112, 186, 256, 288	0
15	AO	88/88 (100%)	0.10	6 (6%) 23 16	113, 177, 253, 318	0
15	DO	88/88 (100%)	-0.11	3 (3%) 48 29	76, 170, 222, 312	0
16	AP	83/83 (100%)	0.31	4 (4%) 35 22	96, 168, 232, 363	0
16	DP	83/83 (100%)	0.71	14 (16%) 4 5	119, 196, 272, 331	0
17	AQ	99/99 (100%)	-0.12	2 (2%) 65 40	114, 162, 240, 267	0
17	DQ	99/99 (100%)	0.27	7 (7%) 22 15	111, 176, 266, 362	0
18	AR	70/70 (100%)	-0.31	1 (1%) 73 47	122, 206, 275, 318	0
18	DR	70/70 (100%)	-0.32	2 (2%) 53 32	96, 176, 241, 287	0
19	AS	78/78 (100%)	0.10	4 (5%) 33 21	132, 234, 327, 378	0
19	DS	78/78 (100%)	0.13	0 100 100	143, 217, 319, 367	0
20	AT	99/99 (100%)	0.50	12 (12%) 8 9	103, 160, 245, 342	0
20	DT	99/99 (100%)	0.67	15 (15%) 5 6	125, 200, 284, 326	0
21	AU	24/24 (100%)	1.18	7 (29%) 1 1	148, 244, 303, 312	0
21	DU	24/24 (100%)	1.46	7 (29%) 1 1	131, 228, 310, 325	0
22	AV	354/354 (100%)	-0.11	16 (4%) 38 23	75, 180, 316, 397	0
22	DV	354/354 (100%)	-0.04	14 (3%) 42 25	60, 172, 340, 419	0
23	AW	77/77 (100%)	-0.47	1 (1%) 75 49	117, 172, 228, 282	0
23	DW	77/77 (100%)	-0.48	1 (1%) 75 49	114, 152, 205, 327	0
24	AX	7/7 (100%)	0.17	1 (14%) 6 7	131, 140, 172, 230	0
25	BA	2879/2879 (100%)	-0.26	91 (3%) 50 30	66, 133, 337, 509	0
25	CA	2879/2879 (100%)	-0.31	65 (2%) 61 37	63, 130, 320, 567	0
26	BB	119/119 (100%)	0.02	7 (5%) 28 18	132, 211, 322, 386	0
26	CB	119/119 (100%)	0.02	5 (4%) 40 24	139, 208, 302, 358	0
27	BC	271/275 (98%)	0.17	21 (7%) 19 14	52, 127, 184, 306	0
27	CC	271/275 (98%)	0.11	21 (7%) 19 14	44, 112, 187, 280	0
28	BD	204/206 (99%)	0.53	27 (13%) 7 8	75, 135, 219, 307	0
28	CD	204/206 (99%)	0.48	23 (11%) 10 9	77, 158, 268, 353	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BE	202/205 (98%)	0.02	14 (6%) 23 16	73, 148, 237, 316	0
29	CE	202/205 (98%)	0.16	17 (8%) 17 13	54, 127, 207, 321	0
30	BF	181/181 (100%)	-0.04	4 (2%) 62 38	116, 229, 328, 395	0
30	CF	181/181 (100%)	-0.09	8 (4%) 39 23	132, 225, 320, 387	0
31	BG	159/180 (88%)	0.03	11 (6%) 23 16	110, 232, 345, 379	0
31	CG	159/180 (88%)	0.10	8 (5%) 34 21	103, 186, 271, 358	0
32	BH	145/148 (97%)	0.90	31 (21%) 2 3	105, 224, 381, 471	0
32	CH	145/148 (97%)	0.21	10 (6%) 23 16	119, 232, 379, 479	0
33	BI	32/173 (18%)	0.09	0 100 100	161, 262, 354, 447	0
33	CI	32/173 (18%)	0.11	3 (9%) 14 12	151, 286, 381, 418	0
34	BJ	137/139 (98%)	0.28	9 (6%) 24 16	100, 160, 238, 322	0
34	CJ	137/139 (98%)	0.23	5 (3%) 46 27	76, 163, 235, 340	0
35	BK	122/122 (100%)	-0.04	4 (3%) 49 29	64, 129, 174, 262	0
35	CK	122/122 (100%)	0.01	3 (2%) 58 35	75, 147, 215, 267	0
36	BL	146/150 (97%)	0.48	20 (13%) 6 7	68, 167, 254, 359	0
36	CL	146/150 (97%)	0.43	16 (10%) 10 10	43, 165, 270, 378	0
37	BM	136/141 (96%)	0.48	11 (8%) 18 13	80, 165, 256, 385	0
37	CM	136/141 (96%)	0.60	19 (13%) 6 7	60, 157, 256, 354	0
38	BN	117/117 (100%)	0.48	9 (7%) 19 14	79, 132, 239, 320	0
38	CN	117/117 (100%)	0.59	13 (11%) 10 10	82, 150, 252, 325	0
39	BO	98/111 (88%)	0.31	7 (7%) 22 15	106, 207, 288, 378	0
39	CO	98/111 (88%)	0.33	11 (11%) 10 10	115, 197, 296, 380	0
40	BP	137/146 (93%)	0.24	10 (7%) 21 15	67, 151, 253, 327	0
40	CP	137/146 (93%)	-0.08	2 (1%) 72 46	93, 164, 281, 335	0
41	BQ	116/116 (100%)	0.32	8 (6%) 23 16	77, 154, 235, 363	0
41	CQ	116/116 (100%)	0.34	11 (9%) 14 12	66, 147, 252, 322	0
42	BR	101/101 (100%)	0.28	12 (11%) 9 9	94, 183, 280, 337	0
42	CR	101/101 (100%)	-0.20	2 (1%) 65 40	51, 163, 271, 316	0
43	BS	112/112 (100%)	0.07	3 (2%) 56 34	71, 120, 201, 275	0
43	CS	112/112 (100%)	0.06	3 (2%) 56 34	63, 131, 191, 266	0
44	BT	92/96 (95%)	0.07	1 (1%) 78 53	68, 140, 191, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CT	92/96 (95%)	0.12	8 (8%) 16 12	64, 132, 204, 258	0
45	BU	100/109 (91%)	0.63	11 (11%) 10 10	91, 177, 297, 414	0
45	CU	100/109 (91%)	0.23	3 (3%) 52 31	76, 157, 321, 358	0
46	BV	188/206 (91%)	-0.33	2 (1%) 78 53	118, 210, 291, 347	0
46	CV	188/206 (91%)	-0.01	12 (6%) 25 17	89, 206, 296, 359	0
47	BW	76/84 (90%)	0.11	5 (6%) 24 16	94, 154, 226, 291	0
47	CW	76/84 (90%)	0.23	6 (7%) 18 13	86, 147, 208, 248	0
48	BX	88/98 (89%)	0.73	16 (18%) 3 4	64, 141, 224, 317	0
48	CX	88/98 (89%)	0.23	7 (7%) 18 13	64, 139, 229, 290	0
49	BY	62/72 (86%)	0.33	5 (8%) 18 13	97, 176, 273, 392	0
49	CY	62/72 (86%)	0.19	5 (8%) 18 13	81, 148, 293, 400	0
50	BZ	59/59 (100%)	0.61	7 (11%) 9 9	102, 179, 276, 480	0
50	CZ	59/59 (100%)	0.07	1 (1%) 69 43	82, 158, 257, 334	0
51	B1	30/71 (42%)	-0.49	0 100 100	182, 257, 349, 389	0
51	C1	30/71 (42%)	-0.43	0 100 100	183, 270, 342, 359	0
52	B2	52/59 (88%)	0.28	4 (7%) 19 14	78, 155, 263, 316	0
52	C2	52/59 (88%)	-0.14	3 (5%) 29 18	80, 150, 280, 315	0
53	B3	44/54 (81%)	0.71	4 (9%) 15 12	180, 285, 354, 375	0
53	C3	44/54 (81%)	0.24	0 100 100	158, 285, 358, 393	0
54	B4	48/48 (100%)	0.64	9 (18%) 3 4	62, 103, 179, 239	0
54	C4	48/48 (100%)	0.39	3 (6%) 26 17	65, 95, 156, 236	0
55	B5	63/64 (98%)	0.73	10 (15%) 5 6	72, 135, 204, 249	0
55	C5	63/64 (98%)	0.73	12 (19%) 3 3	81, 138, 215, 262	0
56	DX	9/9 (100%)	1.17	2 (22%) 2 2	125, 132, 226, 255	0
All	All	21276/21926 (97%)	-0.00	1158 (5%) 31 20	43, 165, 303, 567	0

The worst 5 of 1158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	DH	132	GLU	11.5
42	BR	70	ILE	11.1
14	DN	14	PRO	10.4
37	CM	10	ARG	10.1
38	BN	3	HIS	9.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	2963	1/1	0.26	0.18	132,132,132,132	0
57	MG	DA	1623	1/1	0.42	0.19	151,151,151,151	0
57	MG	BA	2913	1/1	0.45	0.36	88,88,88,88	0
57	MG	BA	3015	1/1	0.46	0.29	107,107,107,107	0
57	MG	CA	2937	1/1	0.49	0.23	124,124,124,124	0
57	MG	CA	2953	1/1	0.53	0.27	135,135,135,135	0
57	MG	BA	2990	1/1	0.54	0.26	120,120,120,120	0
57	MG	AA	1606	1/1	0.57	0.36	112,112,112,112	0
57	MG	AA	1619	1/1	0.58	0.28	160,160,160,160	0
57	MG	BA	3003	1/1	0.59	0.30	63,63,63,63	0
57	MG	DA	1625	1/1	0.60	0.25	104,104,104,104	0
57	MG	CA	2935	1/1	0.61	0.12	90,90,90,90	0
57	MG	BA	2968	1/1	0.62	0.22	106,106,106,106	0
57	MG	AA	1612	1/1	0.63	0.40	126,126,126,126	0
57	MG	DA	1615	1/1	0.65	0.15	84,84,84,84	0
57	MG	AA	1655	1/1	0.65	0.09	102,102,102,102	0
57	MG	BA	3067	1/1	0.65	0.30	126,126,126,126	0
57	MG	CA	2997	1/1	0.66	0.13	78,78,78,78	0
57	MG	CA	2951	1/1	0.66	0.21	81,81,81,81	0
57	MG	AW	103	1/1	0.67	0.23	93,93,93,93	0
57	MG	AA	1607	1/1	0.67	0.19	128,128,128,128	0
57	MG	CB	201	1/1	0.68	0.21	82,82,82,82	0
57	MG	AA	1654	1/1	0.68	0.28	130,130,130,130	0
57	MG	DA	1626	1/1	0.68	0.27	119,119,119,119	0
57	MG	CA	2992	1/1	0.69	0.18	106,106,106,106	0
57	MG	CA	2926	1/1	0.70	0.20	70,70,70,70	0
57	MG	BA	3017	1/1	0.70	0.11	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1639	1/1	0.70	0.26	104,104,104,104	0
57	MG	CY	101	1/1	0.70	0.35	61,61,61,61	0
57	MG	BA	2961	1/1	0.71	0.26	83,83,83,83	0
57	MG	CA	3023	1/1	0.71	0.11	142,142,142,142	0
57	MG	BA	2937	1/1	0.72	0.27	83,83,83,83	0
57	MG	BA	3054	1/1	0.73	0.45	106,106,106,106	0
57	MG	BA	3014	1/1	0.74	0.18	110,110,110,110	0
57	MG	BA	2986	1/1	0.74	0.11	114,114,114,114	0
57	MG	AA	1631	1/1	0.74	0.34	128,128,128,128	0
57	MG	BA	2971	1/1	0.74	0.21	123,123,123,123	0
57	MG	CM	201	1/1	0.75	0.21	96,96,96,96	0
57	MG	BA	2947	1/1	0.75	0.19	77,77,77,77	0
57	MG	CA	2907	1/1	0.75	0.33	65,65,65,65	0
57	MG	BA	2943	1/1	0.76	0.32	85,85,85,85	0
57	MG	BA	3036	1/1	0.76	0.20	114,114,114,114	0
57	MG	CA	2929	1/1	0.76	0.23	102,102,102,102	0
57	MG	BA	3051	1/1	0.76	0.33	120,120,120,120	0
57	MG	BA	2987	1/1	0.76	0.51	125,125,125,125	0
57	MG	BA	2963	1/1	0.76	0.25	75,75,75,75	0
57	MG	BA	3016	1/1	0.77	0.29	89,89,89,89	0
57	MG	AV	401	1/1	0.77	0.35	91,91,91,91	0
57	MG	CA	2988	1/1	0.77	0.23	72,72,72,72	0
57	MG	AA	1660	1/1	0.77	0.13	143,143,143,143	0
57	MG	CA	2996	1/1	0.77	0.15	84,84,84,84	0
57	MG	BA	3044	1/1	0.77	0.23	87,87,87,87	0
57	MG	CA	2919	1/1	0.77	0.26	72,72,72,72	0
57	MG	CA	3014	1/1	0.78	0.24	104,104,104,104	0
57	MG	BA	2979	1/1	0.78	0.24	71,71,71,71	0
57	MG	DA	1617	1/1	0.78	0.07	139,139,139,139	0
57	MG	CA	3024	1/1	0.78	0.10	120,120,120,120	0
57	MG	CA	2970	1/1	0.78	0.08	103,103,103,103	0
57	MG	CA	2932	1/1	0.78	0.19	81,81,81,81	0
57	MG	BA	2918	1/1	0.79	0.18	111,111,111,111	0
57	MG	BA	2949	1/1	0.79	0.24	89,89,89,89	0
57	MG	BA	2992	1/1	0.79	0.18	80,80,80,80	0
57	MG	BB	201	1/1	0.79	0.16	102,102,102,102	0
57	MG	BA	2939	1/1	0.79	0.23	86,86,86,86	0
57	MG	BA	2936	1/1	0.79	0.21	106,106,106,106	0
57	MG	AA	1649	1/1	0.80	0.17	106,106,106,106	0
57	MG	AA	1618	1/1	0.80	0.23	87,87,87,87	0
57	MG	BA	3050	1/1	0.80	0.05	114,114,114,114	0
57	MG	CA	2974	1/1	0.81	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	2978	1/1	0.81	0.28	90,90,90,90	0
57	MG	BA	2945	1/1	0.81	0.29	100,100,100,100	0
57	MG	CA	2989	1/1	0.81	0.16	81,81,81,81	0
57	MG	BA	2994	1/1	0.81	0.28	82,82,82,82	0
57	MG	BA	2930	1/1	0.81	0.17	94,94,94,94	0
57	MG	BA	3026	1/1	0.81	0.13	84,84,84,84	0
57	MG	BA	2984	1/1	0.81	0.13	45,45,45,45	0
57	MG	BA	3068	1/1	0.81	0.06	88,88,88,88	0
57	MG	DA	1614	1/1	0.82	0.16	74,74,74,74	0
57	MG	BA	2933	1/1	0.82	0.18	83,83,83,83	0
57	MG	DA	1628	1/1	0.82	0.10	103,103,103,103	0
57	MG	AA	1646	1/1	0.83	0.17	82,82,82,82	0
57	MG	BA	2998	1/1	0.83	0.27	90,90,90,90	0
57	MG	BA	3020	1/1	0.83	0.14	85,85,85,85	0
57	MG	BA	3022	1/1	0.83	0.07	95,95,95,95	0
57	MG	BA	3024	1/1	0.83	0.23	88,88,88,88	0
57	MG	CA	2948	1/1	0.83	0.16	107,107,107,107	0
57	MG	DA	1621	1/1	0.83	0.16	96,96,96,96	0
57	MG	BA	3075	1/1	0.83	0.07	72,72,72,72	0
57	MG	BA	2989	1/1	0.83	0.14	84,84,84,84	0
57	MG	AA	1602	1/1	0.83	0.13	91,91,91,91	0
57	MG	BA	2931	1/1	0.83	0.13	99,99,99,99	0
57	MG	CA	2921	1/1	0.84	0.18	62,62,62,62	0
57	MG	BA	2965	1/1	0.84	0.38	97,97,97,97	0
57	MG	BA	2950	1/1	0.84	0.14	89,89,89,89	0
57	MG	CA	2955	1/1	0.84	0.15	88,88,88,88	0
57	MG	AA	1616	1/1	0.84	0.19	84,84,84,84	0
57	MG	CA	3003	1/1	0.84	0.16	111,111,111,111	0
57	MG	CA	2914	1/1	0.84	0.12	48,48,48,48	0
57	MG	CA	2973	1/1	0.84	0.14	95,95,95,95	0
57	MG	AA	1637	1/1	0.84	0.23	65,65,65,65	0
57	MG	CA	2943	1/1	0.84	0.36	55,55,55,55	0
57	MG	DA	1612	1/1	0.85	0.05	107,107,107,107	0
57	MG	BA	3040	1/1	0.85	0.12	118,118,118,118	0
57	MG	BA	2911	1/1	0.85	0.27	62,62,62,62	0
57	MG	CA	2945	1/1	0.85	0.10	84,84,84,84	0
57	MG	CA	2911	1/1	0.85	0.14	77,77,77,77	0
57	MG	CB	202	1/1	0.85	0.13	79,79,79,79	0
57	MG	BA	3034	1/1	0.85	0.07	72,72,72,72	0
57	MG	BA	2914	1/1	0.85	0.25	57,57,57,57	0
57	MG	DA	1608	1/1	0.85	0.06	90,90,90,90	0
57	MG	BA	2934	1/1	0.86	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	2906	1/1	0.86	0.25	72,72,72,72	0
57	MG	AA	1641	1/1	0.86	0.18	82,82,82,82	0
57	MG	BA	2902	1/1	0.86	0.25	71,71,71,71	0
57	MG	BA	2922	1/1	0.86	0.25	76,76,76,76	0
57	MG	CA	2918	1/1	0.86	0.19	51,51,51,51	0
57	MG	CA	2949	1/1	0.86	0.33	57,57,57,57	0
57	MG	CA	2993	1/1	0.86	0.14	92,92,92,92	0
57	MG	BA	2970	1/1	0.86	0.23	101,101,101,101	0
57	MG	CA	2952	1/1	0.86	0.10	88,88,88,88	0
57	MG	CA	3000	1/1	0.86	0.20	82,82,82,82	0
57	MG	BA	2940	1/1	0.86	0.26	104,104,104,104	0
57	MG	CA	3007	1/1	0.86	0.15	84,84,84,84	0
57	MG	BA	3070	1/1	0.86	0.09	108,108,108,108	0
57	MG	BA	2977	1/1	0.86	0.14	79,79,79,79	0
57	MG	BA	3018	1/1	0.87	0.13	103,103,103,103	0
57	MG	BK	201	1/1	0.87	0.22	102,102,102,102	0
57	MG	CA	2936	1/1	0.87	0.11	64,64,64,64	0
57	MG	CA	2902	1/1	0.87	0.20	61,61,61,61	0
57	MG	AA	1642	1/1	0.87	0.08	67,67,67,67	0
57	MG	DA	1607	1/1	0.87	0.08	110,110,110,110	0
57	MG	BA	2999	1/1	0.87	0.22	84,84,84,84	0
57	MG	BA	2955	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	1613	1/1	0.87	0.14	72,72,72,72	0
57	MG	BA	2906	1/1	0.87	0.21	54,54,54,54	0
57	MG	AA	1647	1/1	0.87	0.09	92,92,92,92	0
57	MG	BA	2941	1/1	0.87	0.16	63,63,63,63	0
57	MG	BA	3071	1/1	0.87	0.07	107,107,107,107	0
57	MG	BA	2967	1/1	0.87	0.56	111,111,111,111	0
57	MG	CA	2956	1/1	0.87	0.15	107,107,107,107	0
57	MG	BA	3076	1/1	0.87	0.07	100,100,100,100	0
57	MG	CA	2967	1/1	0.87	0.11	94,94,94,94	0
57	MG	AA	1620	1/1	0.88	0.08	60,60,60,60	0
57	MG	BA	3058	1/1	0.88	0.14	60,60,60,60	0
57	MG	BA	2956	1/1	0.88	0.13	77,77,77,77	0
57	MG	CA	2903	1/1	0.88	0.26	69,69,69,69	0
57	MG	CA	2954	1/1	0.88	0.22	72,72,72,72	0
57	MG	DA	1610	1/1	0.88	0.08	77,77,77,77	0
57	MG	BA	2912	1/1	0.88	0.17	57,57,57,57	0
57	MG	AA	1623	1/1	0.88	0.09	88,88,88,88	0
57	MG	CA	2960	1/1	0.88	0.06	63,63,63,63	0
57	MG	CA	2908	1/1	0.88	0.27	81,81,81,81	0
57	MG	CA	2965	1/1	0.88	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	1620	1/1	0.88	0.10	68,68,68,68	0
57	MG	AW	101	1/1	0.88	0.27	77,77,77,77	0
57	MG	CA	3021	1/1	0.88	0.23	85,85,85,85	0
57	MG	BA	3009	1/1	0.88	0.12	103,103,103,103	0
57	MG	CA	2915	1/1	0.88	0.27	73,73,73,73	0
57	MG	BA	2978	1/1	0.88	0.13	87,87,87,87	0
57	MG	BA	3006	1/1	0.89	0.13	70,70,70,70	0
57	MG	CA	2959	1/1	0.89	0.07	51,51,51,51	0
57	MG	BA	2919	1/1	0.89	0.18	61,61,61,61	0
57	MG	BA	2953	1/1	0.89	0.15	66,66,66,66	0
57	MG	BA	3057	1/1	0.89	0.24	88,88,88,88	0
57	MG	CA	3001	1/1	0.89	0.08	40,40,40,40	0
57	MG	AA	1640	1/1	0.89	0.35	142,142,142,142	0
57	MG	AA	1662	1/1	0.89	0.04	110,110,110,110	0
57	MG	CA	2924	1/1	0.89	0.22	57,57,57,57	0
57	MG	BA	2916	1/1	0.89	0.05	88,88,88,88	0
57	MG	AA	1621	1/1	0.89	0.15	67,67,67,67	0
57	MG	CA	2980	1/1	0.89	0.07	57,57,57,57	0
57	MG	CA	2983	1/1	0.89	0.13	55,55,55,55	0
57	MG	BA	3019	1/1	0.89	0.16	94,94,94,94	0
57	MG	CA	2910	1/1	0.89	0.28	65,65,65,65	0
57	MG	DW	101	1/1	0.89	0.26	83,83,83,83	0
57	MG	CA	2913	1/1	0.90	0.24	78,78,78,78	0
57	MG	CA	3005	1/1	0.90	0.14	67,67,67,67	0
57	MG	BA	2985	1/1	0.90	0.18	82,82,82,82	0
57	MG	CA	3009	1/1	0.90	0.09	60,60,60,60	0
57	MG	BA	3061	1/1	0.90	0.07	77,77,77,77	0
57	MG	CA	3015	1/1	0.90	0.09	98,98,98,98	0
57	MG	BA	2957	1/1	0.90	0.23	81,81,81,81	0
57	MG	AA	1661	1/1	0.90	0.18	105,105,105,105	0
57	MG	CA	2920	1/1	0.90	0.45	69,69,69,69	0
57	MG	CA	3025	1/1	0.90	0.14	97,97,97,97	0
57	MG	AA	1652	1/1	0.90	0.13	79,79,79,79	0
57	MG	CA	2923	1/1	0.90	0.20	56,56,56,56	0
57	MG	AA	1663	1/1	0.90	0.10	86,86,86,86	0
57	MG	BA	2928	1/1	0.90	0.19	67,67,67,67	0
57	MG	AA	1636	1/1	0.90	0.08	76,76,76,76	0
57	MG	BA	2996	1/1	0.90	0.15	58,58,58,58	0
57	MG	DA	1609	1/1	0.90	0.12	95,95,95,95	0
57	MG	CA	2934	1/1	0.90	0.11	57,57,57,57	0
57	MG	CA	2979	1/1	0.90	0.08	79,79,79,79	0
57	MG	AA	1615	1/1	0.90	0.07	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1608	1/1	0.90	0.14	126,126,126,126	0
57	MG	BA	3002	1/1	0.90	0.20	78,78,78,78	0
57	MG	BA	2976	1/1	0.90	0.27	84,84,84,84	0
57	MG	CA	2944	1/1	0.90	0.21	55,55,55,55	0
57	MG	BA	2915	1/1	0.90	0.23	62,62,62,62	0
57	MG	CA	2994	1/1	0.90	0.08	60,60,60,60	0
57	MG	DA	1624	1/1	0.90	0.06	97,97,97,97	0
57	MG	BA	2901	1/1	0.90	0.31	57,57,57,57	0
57	MG	CA	2909	1/1	0.90	0.24	81,81,81,81	0
57	MG	BA	2917	1/1	0.90	0.24	54,54,54,54	0
57	MG	DA	1630	1/1	0.90	0.05	87,87,87,87	0
57	MG	BA	2938	1/1	0.90	0.16	78,78,78,78	0
57	MG	BA	3060	1/1	0.91	0.06	57,57,57,57	0
57	MG	BA	3008	1/1	0.91	0.06	79,79,79,79	0
57	MG	BA	3025	1/1	0.91	0.47	115,115,115,115	0
57	MG	AA	1627	1/1	0.91	0.04	109,109,109,109	0
57	MG	BA	3029	1/1	0.91	0.12	83,83,83,83	0
57	MG	DA	1603	1/1	0.91	0.29	85,85,85,85	0
57	MG	DA	1606	1/1	0.91	0.17	62,62,62,62	0
57	MG	CA	2916	1/1	0.91	0.13	92,92,92,92	0
57	MG	BA	3011	1/1	0.91	0.12	97,97,97,97	0
57	MG	BA	3074	1/1	0.91	0.10	64,64,64,64	0
57	MG	AA	1617	1/1	0.91	0.11	61,61,61,61	0
57	MG	BA	3037	1/1	0.91	0.17	67,67,67,67	0
57	MG	AA	1644	1/1	0.91	0.05	73,73,73,73	0
57	MG	BA	2981	1/1	0.91	0.06	72,72,72,72	0
57	MG	B2	101	1/1	0.91	0.05	96,96,96,96	0
57	MG	DA	1616	1/1	0.91	0.20	93,93,93,93	0
57	MG	BA	3046	1/1	0.91	0.10	71,71,71,71	0
57	MG	BA	2951	1/1	0.91	0.27	71,71,71,71	0
57	MG	CA	2933	1/1	0.91	0.25	64,64,64,64	0
57	MG	CA	3013	1/1	0.91	0.07	88,88,88,88	0
57	MG	BA	2908	1/1	0.91	0.14	48,48,48,48	0
57	MG	BA	2942	1/1	0.91	0.15	50,50,50,50	0
57	MG	CA	3016	1/1	0.91	0.08	99,99,99,99	0
57	MG	DA	1627	1/1	0.91	0.10	77,77,77,77	0
57	MG	BA	2925	1/1	0.91	0.13	39,39,39,39	0
57	MG	CA	2975	1/1	0.91	0.18	81,81,81,81	0
57	MG	AA	1626	1/1	0.91	0.06	108,108,108,108	0
57	MG	BA	2932	1/1	0.92	0.15	68,68,68,68	0
57	MG	CA	2999	1/1	0.92	0.10	58,58,58,58	0
57	MG	BA	3038	1/1	0.92	0.12	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	2966	1/1	0.92	0.11	79,79,79,79	0
57	MG	BA	3065	1/1	0.92	0.13	114,114,114,114	0
57	MG	CA	2946	1/1	0.92	0.08	80,80,80,80	0
57	MG	CA	2971	1/1	0.92	0.22	48,48,48,48	0
57	MG	CA	2947	1/1	0.92	0.08	81,81,81,81	0
57	MG	BA	3039	1/1	0.92	0.15	90,90,90,90	0
57	MG	BA	2991	1/1	0.92	0.07	48,48,48,48	0
57	MG	AA	1634	1/1	0.92	0.09	75,75,75,75	0
57	MG	BA	2907	1/1	0.92	0.11	50,50,50,50	0
57	MG	BA	3047	1/1	0.92	0.08	41,41,41,41	0
57	MG	CA	2982	1/1	0.92	0.07	77,77,77,77	0
57	MG	AA	1635	1/1	0.92	0.03	85,85,85,85	0
57	MG	BA	2909	1/1	0.92	0.21	82,82,82,82	0
57	MG	AA	1630	1/1	0.92	0.06	96,96,96,96	0
57	MG	CA	2957	1/1	0.92	0.17	63,63,63,63	0
57	MG	AA	1609	1/1	0.92	0.10	86,86,86,86	0
57	MG	BA	2962	1/1	0.92	0.15	50,50,50,50	0
57	MG	CA	2962	1/1	0.92	0.12	68,68,68,68	0
57	MG	BA	3048	1/1	0.93	0.11	98,98,98,98	0
57	MG	BM	201	1/1	0.93	0.12	105,105,105,105	0
57	MG	AA	1629	1/1	0.93	0.10	71,71,71,71	0
57	MG	BA	2903	1/1	0.93	0.18	44,44,44,44	0
57	MG	CA	2958	1/1	0.93	0.17	56,56,56,56	0
57	MG	BA	2944	1/1	0.93	0.14	78,78,78,78	0
57	MG	BA	2904	1/1	0.93	0.21	35,35,35,35	0
57	MG	CA	2998	1/1	0.93	0.14	73,73,73,73	0
57	MG	AA	1603	1/1	0.93	0.17	85,85,85,85	0
57	MG	BA	3028	1/1	0.93	0.16	95,95,95,95	0
57	MG	AA	1664	1/1	0.93	0.05	87,87,87,87	0
57	MG	CA	3002	1/1	0.93	0.10	71,71,71,71	0
57	MG	BA	3062	1/1	0.93	0.09	89,89,89,89	0
57	MG	CA	2940	1/1	0.93	0.07	44,44,44,44	0
57	MG	AA	1613	1/1	0.93	0.16	105,105,105,105	0
57	MG	CA	2912	1/1	0.93	0.11	38,38,38,38	0
57	MG	AA	1658	1/1	0.93	0.07	58,58,58,58	0
57	MG	BA	3012	1/1	0.93	0.04	54,54,54,54	0
57	MG	AW	102	1/1	0.93	0.12	77,77,77,77	0
57	MG	BA	2954	1/1	0.93	0.14	77,77,77,77	0
57	MG	CA	3020	1/1	0.93	0.18	89,89,89,89	0
57	MG	BA	2993	1/1	0.93	0.13	57,57,57,57	0
57	MG	CA	3022	1/1	0.93	0.14	59,59,59,59	0
57	MG	AA	1610	1/1	0.93	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1611	1/1	0.93	0.06	62,62,62,62	0
57	MG	BA	2997	1/1	0.93	0.05	87,87,87,87	0
57	MG	AA	1633	1/1	0.94	0.07	76,76,76,76	0
57	MG	AT	201	1/1	0.94	0.11	98,98,98,98	0
57	MG	CA	2927	1/1	0.94	0.18	60,60,60,60	0
57	MG	BA	3041	1/1	0.94	0.05	65,65,65,65	0
57	MG	CA	2930	1/1	0.94	0.10	53,53,53,53	0
57	MG	BB	202	1/1	0.94	0.03	81,81,81,81	0
57	MG	BA	2958	1/1	0.94	0.04	77,77,77,77	0
57	MG	BA	2960	1/1	0.94	0.11	56,56,56,56	0
57	MG	BA	2924	1/1	0.94	0.17	60,60,60,60	0
57	MG	CA	2976	1/1	0.94	0.10	119,119,119,119	0
57	MG	CA	2977	1/1	0.94	0.10	82,82,82,82	0
57	MG	CA	2901	1/1	0.94	0.24	39,39,39,39	0
57	MG	BA	2980	1/1	0.94	0.10	70,70,70,70	0
57	MG	BA	3049	1/1	0.94	0.15	100,100,100,100	0
57	MG	DA	1601	1/1	0.94	0.19	62,62,62,62	0
57	MG	CA	2981	1/1	0.94	0.07	74,74,74,74	0
57	MG	CA	2905	1/1	0.94	0.20	50,50,50,50	0
57	MG	AA	1659	1/1	0.94	0.05	81,81,81,81	0
57	MG	CA	2984	1/1	0.94	0.08	78,78,78,78	0
57	MG	CA	2987	1/1	0.94	0.23	64,64,64,64	0
57	MG	BA	3021	1/1	0.94	0.16	88,88,88,88	0
57	MG	BA	2982	1/1	0.94	0.16	43,43,43,43	0
57	MG	BA	2983	1/1	0.94	0.15	77,77,77,77	0
57	MG	AA	1645	1/1	0.94	0.07	98,98,98,98	0
57	MG	BA	3004	1/1	0.94	0.08	92,92,92,92	0
57	MG	BA	3027	1/1	0.94	0.13	69,69,69,69	0
57	MG	AA	1624	1/1	0.94	0.14	74,74,74,74	0
57	MG	DA	1618	1/1	0.94	0.15	112,112,112,112	0
57	MG	DA	1619	1/1	0.94	0.07	89,89,89,89	0
57	MG	BA	3007	1/1	0.94	0.04	55,55,55,55	0
57	MG	BA	3066	1/1	0.94	0.12	98,98,98,98	0
57	MG	AA	1614	1/1	0.94	0.04	68,68,68,68	0
57	MG	CA	2917	1/1	0.94	0.16	74,74,74,74	0
57	MG	BA	3035	1/1	0.94	0.06	77,77,77,77	0
57	MG	AA	1656	1/1	0.94	0.14	88,88,88,88	0
57	MG	BA	2969	1/1	0.94	0.11	41,41,41,41	0
57	MG	CA	3006	1/1	0.94	0.09	74,74,74,74	0
57	MG	BA	3072	1/1	0.94	0.07	83,83,83,83	0
57	MG	BA	2910	1/1	0.94	0.28	56,56,56,56	0
57	MG	AA	1657	1/1	0.95	0.11	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	2921	1/1	0.95	0.15	65,65,65,65	0
57	MG	CA	2950	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3059	1/1	0.95	0.11	82,82,82,82	0
57	MG	AA	1653	1/1	0.95	0.04	89,89,89,89	0
57	MG	BA	2905	1/1	0.95	0.29	43,43,43,43	0
57	MG	CA	2985	1/1	0.95	0.04	49,49,49,49	0
57	MG	AA	1651	1/1	0.95	0.04	68,68,68,68	0
57	MG	CA	2904	1/1	0.95	0.12	27,27,27,27	0
57	MG	CA	2928	1/1	0.95	0.12	66,66,66,66	0
57	MG	DA	1602	1/1	0.95	0.20	84,84,84,84	0
57	MG	CA	2991	1/1	0.95	0.11	72,72,72,72	0
57	MG	DA	1604	1/1	0.95	0.10	96,96,96,96	0
57	MG	DA	1605	1/1	0.95	0.09	75,75,75,75	0
57	MG	BA	3043	1/1	0.95	0.06	60,60,60,60	0
57	MG	BA	3005	1/1	0.95	0.11	54,54,54,54	0
57	MG	CA	2931	1/1	0.95	0.18	71,71,71,71	0
57	MG	CA	2995	1/1	0.95	0.10	69,69,69,69	0
57	MG	BA	2927	1/1	0.95	0.26	53,53,53,53	0
57	MG	BA	3030	1/1	0.95	0.08	80,80,80,80	0
57	MG	BA	3069	1/1	0.95	0.09	60,60,60,60	0
57	MG	BA	3032	1/1	0.95	0.04	62,62,62,62	0
57	MG	BA	3033	1/1	0.95	0.16	92,92,92,92	0
57	MG	BA	2995	1/1	0.95	0.07	87,87,87,87	0
57	MG	CA	2968	1/1	0.95	0.16	77,77,77,77	0
57	MG	CA	2969	1/1	0.95	0.07	48,48,48,48	0
57	MG	CA	2938	1/1	0.95	0.07	60,60,60,60	0
57	MG	CA	2939	1/1	0.95	0.09	40,40,40,40	0
57	MG	CA	2972	1/1	0.95	0.06	75,75,75,75	0
57	MG	CA	3008	1/1	0.95	0.04	74,74,74,74	0
57	MG	BA	3073	1/1	0.95	0.06	71,71,71,71	0
57	MG	BA	2935	1/1	0.95	0.19	80,80,80,80	0
57	MG	BA	3052	1/1	0.95	0.09	74,74,74,74	0
57	MG	BA	2988	1/1	0.95	0.09	54,54,54,54	0
57	MG	BA	3055	1/1	0.95	0.11	80,80,80,80	0
57	MG	CA	3019	1/1	0.95	0.03	71,71,71,71	0
57	MG	BA	3056	1/1	0.95	0.25	81,81,81,81	0
57	MG	AA	1632	1/1	0.96	0.06	55,55,55,55	0
57	MG	BA	2966	1/1	0.96	0.09	51,51,51,51	0
57	MG	CA	3012	1/1	0.96	0.07	57,57,57,57	0
57	MG	AA	1605	1/1	0.96	0.11	61,61,61,61	0
57	MG	CA	2990	1/1	0.96	0.16	68,68,68,68	0
57	MG	BA	3023	1/1	0.96	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	2948	1/1	0.96	0.10	44,44,44,44	0
57	MG	CA	3017	1/1	0.96	0.05	76,76,76,76	0
57	MG	CA	3018	1/1	0.96	0.03	65,65,65,65	0
57	MG	AA	1650	1/1	0.96	0.11	124,124,124,124	0
57	MG	BA	3010	1/1	0.96	0.15	80,80,80,80	0
57	MG	BA	2959	1/1	0.96	0.10	43,43,43,43	0
57	MG	BA	3063	1/1	0.96	0.06	69,69,69,69	0
57	MG	BA	2926	1/1	0.96	0.05	56,56,56,56	0
57	MG	BA	2973	1/1	0.96	0.08	63,63,63,63	0
57	MG	BA	2975	1/1	0.96	0.17	48,48,48,48	0
57	MG	DA	1622	1/1	0.96	0.09	67,67,67,67	0
57	MG	BA	3031	1/1	0.96	0.08	101,101,101,101	0
57	MG	BA	3000	1/1	0.96	0.08	54,54,54,54	0
57	MG	AA	1638	1/1	0.96	0.03	68,68,68,68	0
57	MG	CA	2925	1/1	0.96	0.10	100,100,100,100	0
57	MG	CA	3004	1/1	0.96	0.13	57,57,57,57	0
57	MG	AA	1625	1/1	0.96	0.07	77,77,77,77	0
57	MG	DA	1629	1/1	0.96	0.10	85,85,85,85	0
57	MG	AA	1628	1/1	0.96	0.12	65,65,65,65	0
57	MG	CA	2986	1/1	0.96	0.08	96,96,96,96	0
57	MG	AA	1601	1/1	0.97	0.17	57,57,57,57	0
57	MG	AA	1643	1/1	0.97	0.02	85,85,85,85	0
57	MG	BA	2929	1/1	0.97	0.06	34,34,34,34	0
57	MG	BA	2952	1/1	0.97	0.12	51,51,51,51	0
57	MG	CA	2942	1/1	0.97	0.11	66,66,66,66	0
57	MG	BA	2972	1/1	0.97	0.06	87,87,87,87	0
57	MG	BA	3042	1/1	0.97	0.03	80,80,80,80	0
57	MG	BA	2923	1/1	0.97	0.13	42,42,42,42	0
57	MG	AA	1604	1/1	0.97	0.13	78,78,78,78	0
57	MG	BA	3045	1/1	0.97	0.06	76,76,76,76	0
57	MG	BA	2964	1/1	0.97	0.03	69,69,69,69	0
57	MG	CA	2964	1/1	0.97	0.07	65,65,65,65	0
57	MG	BA	2946	1/1	0.97	0.22	45,45,45,45	0
57	MG	AA	1648	1/1	0.97	0.04	62,62,62,62	0
57	MG	BA	2920	1/1	0.97	0.07	23,23,23,23	0
57	MG	DA	1611	1/1	0.98	0.08	89,89,89,89	0
57	MG	BA	3064	1/1	0.98	0.03	56,56,56,56	0
57	MG	CA	2961	1/1	0.98	0.07	47,47,47,47	0
57	MG	BA	2974	1/1	0.98	0.04	27,27,27,27	0
57	MG	BA	3053	1/1	0.98	0.06	73,73,73,73	0
57	MG	CA	2922	1/1	0.98	0.12	43,43,43,43	0
57	MG	AA	1622	1/1	0.98	0.08	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	AN	101	1/1	0.98	0.03	163,163,163,163	0
57	MG	CA	2941	1/1	0.99	0.08	36,36,36,36	0
57	MG	BA	3001	1/1	0.99	0.09	54,54,54,54	0
57	MG	BA	3013	1/1	0.99	0.08	78,78,78,78	0
57	MG	CA	3010	1/1	0.99	0.07	70,70,70,70	0
58	ZN	AD	301	1/1	0.99	0.18	92,92,92,92	0
57	MG	CA	3011	1/1	0.99	0.02	40,40,40,40	0
58	ZN	DD	301	1/1	0.99	0.18	99,99,99,99	0
58	ZN	DN	101	1/1	0.99	0.03	162,162,162,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.