



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 04:50 AM EDT

PDB ID : 4V54
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-16
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

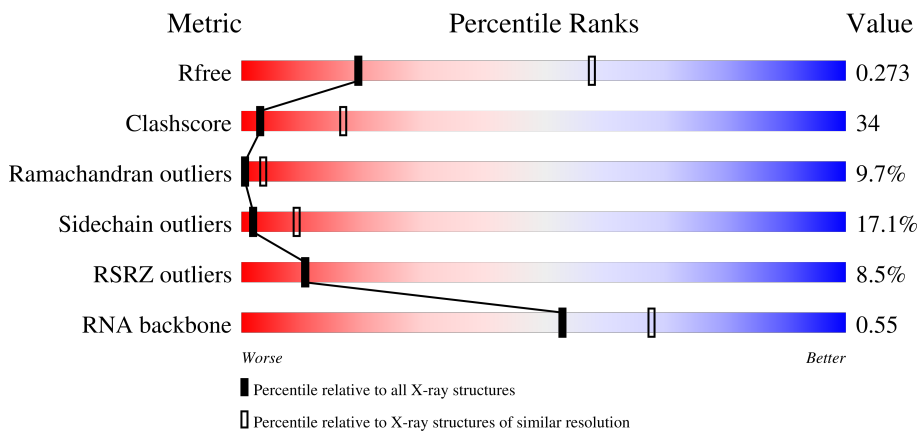
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1542	 27% 60% 13%
1	CA	1542	 26% 61% 12%
2	AC	232	 30% 47% 11% 3% 11%
2	CC	232	 31% 45% 12% 2% 11%

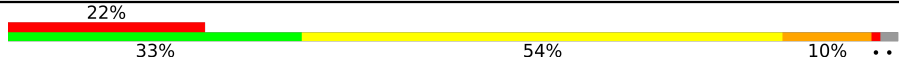
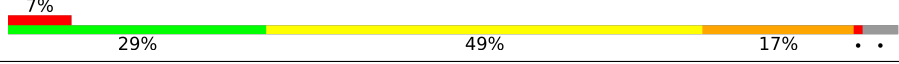
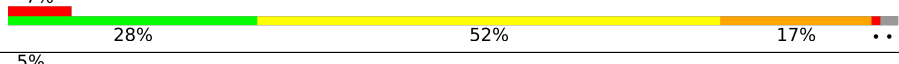
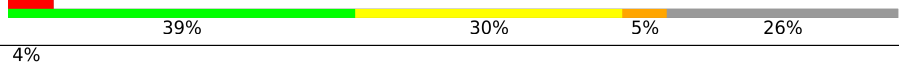
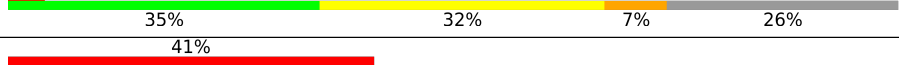
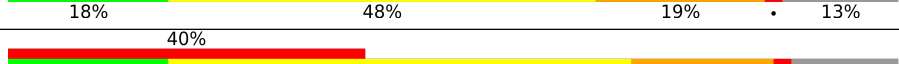
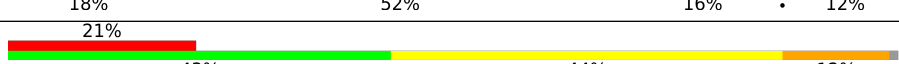
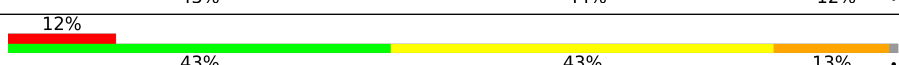
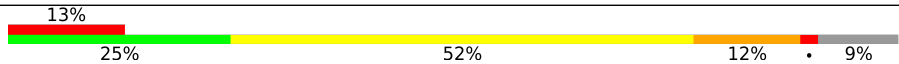
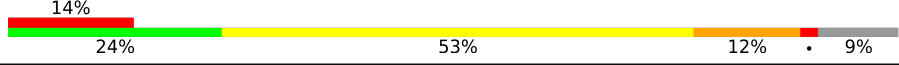
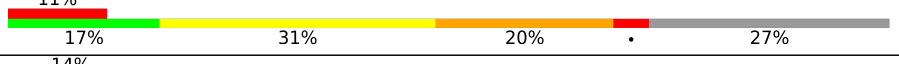

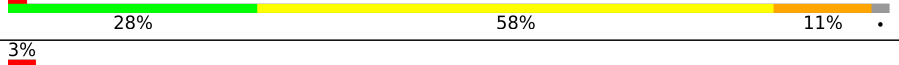

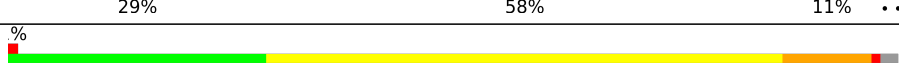


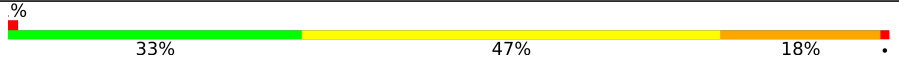
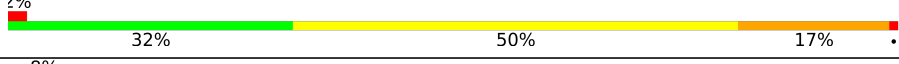
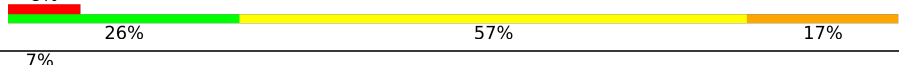
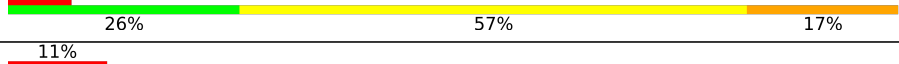
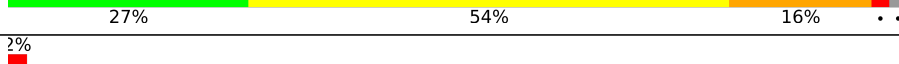
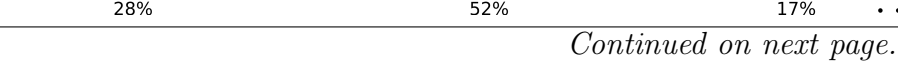


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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

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Mol	Chain	Length	Quality of chain
40	DH	149	28% 18% 56% 22% .
41	BJ	142	9% 22% 60% 16% .
41	DJ	142	9% 23% 59% 15% .
42	BN	127	6% 21% 60% 11% . 6%
42	DN	127	3% 23% 59% 10% . 6%
43	BO	117	30% 32% 58% 9% ..
43	DO	117	12% 32% 56% 10% ..
44	BQ	117	6% 34% 52% 12% .
44	DQ	117	7% 33% 52% 13% .
45	BS	110	8% 28% 53% 19%
45	DS	110	3% 29% 51% 20%
46	BU	103	19% 24% 54% 17% . .
46	DU	103	16% 25% 52% 17% . .
47	BF	178	25% 15% 58% 24% .
47	DF	178	19% 15% 58% 23% .
48	BG	176	24% 27% 49% 20% .
48	DG	176	16% 26% 49% 22% .
49	BR	103	26% 24% 60% 14% .
49	DR	103	9% 25% 56% 17% .
50	BT	100	24% 21% 41% 29% . 7%
50	DT	100	21% 22% 42% 27% . 7%
51	BZ	78	3% 24% 51% 19% . .
51	DZ	78	6% 22% 55% 18% . .
52	BW	84	15% 18% 33% 37% 6% 6%
52	DW	84	15% 17% 36% 36% 6% 6%

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Mol	Chain	Length	Quality of chain
53	B6	185	
53	D6	185	

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
54	MG	AA	2025	-	-	-	X
54	MG	AA	2037	-	-	-	X
54	MG	AA	2059	-	-	-	X
54	MG	BB	3093	-	-	-	X
54	MG	BB	3100	-	-	-	X
54	MG	DB	3058	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286960 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.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

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

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	BZ	77	Total 625	C 388	N 129	O 106	S 2	0	0	0
51	DZ	77	Total 625	C 388	N 129	O 106	S 2	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	60	Total	Mg	0	0
			60	60		
54	BB	110	Total	Mg	0	0
			110	110		
54	CE	1	Total	Mg	0	0
			1	1		
54	CA	61	Total	Mg	0	0
			61	61		
54	DB	111	Total	Mg	0	0
			111	111		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	289	Total	O	0	0
			289	289		
56	AE	4	Total	O	0	0
			4	4		
56	AK	1	Total	O	0	0
			1	1		
56	AL	1	Total	O	0	0
			1	1		
56	AN	3	Total	O	0	0
			3	3		
56	AP	1	Total	O	0	0
			1	1		

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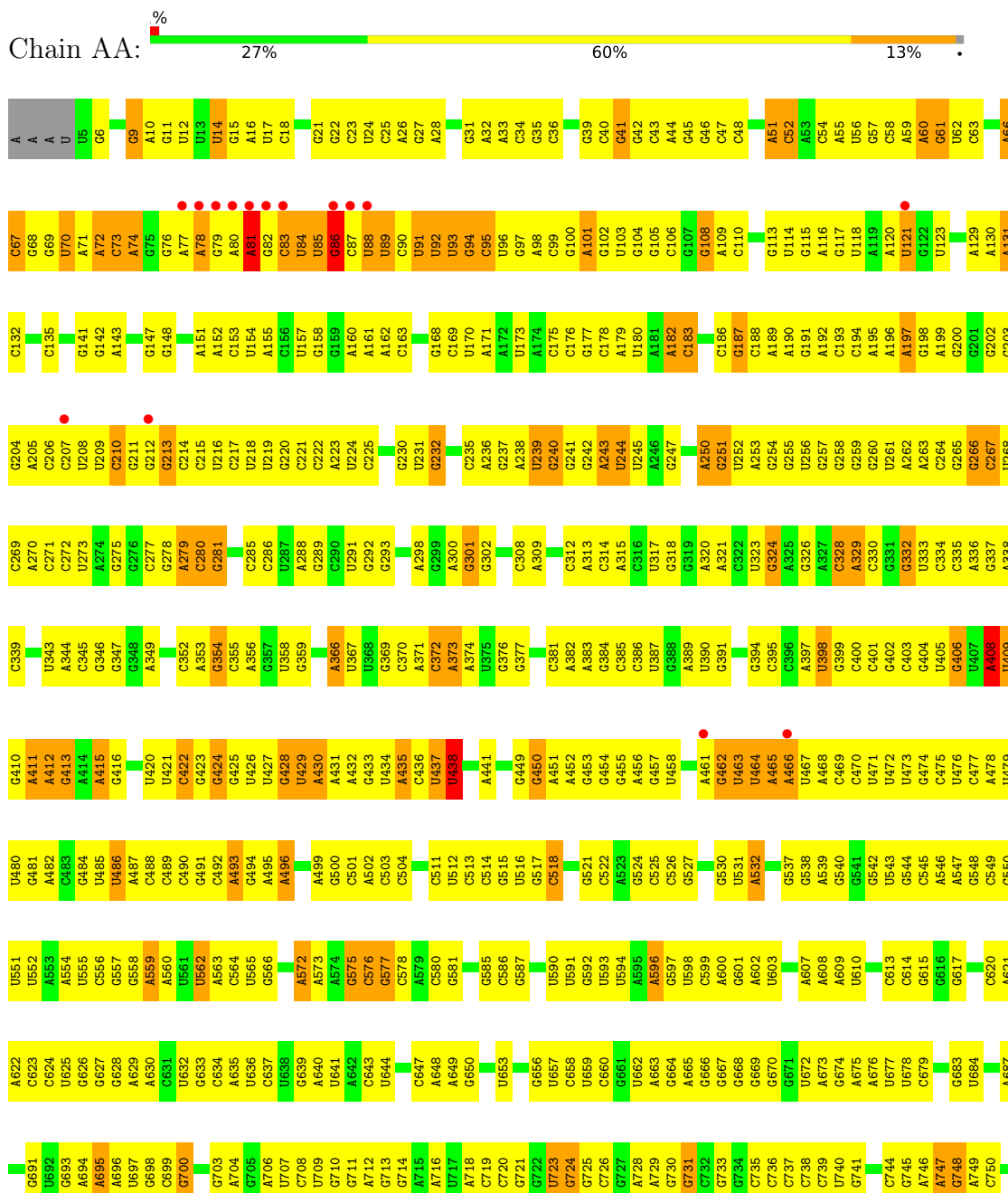
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AT	1	Total O 1 1	0	0
56	BB	495	Total O 495 495	0	0
56	BC	4	Total O 4 4	0	0
56	BD	1	Total O 1 1	0	0
56	BE	3	Total O 3 3	0	0
56	B2	1	Total O 1 1	0	0
56	BL	1	Total O 1 1	0	0
56	BT	1	Total O 1 1	0	0
56	CE	2	Total O 2 2	0	0
56	CK	1	Total O 1 1	0	0
56	CL	1	Total O 1 1	0	0
56	CN	4	Total O 4 4	0	0
56	CT	1	Total O 1 1	0	0
56	CA	300	Total O 300 300	0	0
56	DB	505	Total O 505 505	0	0
56	DC	4	Total O 4 4	0	0
56	DD	1	Total O 1 1	0	0
56	DE	2	Total O 2 2	0	0

3 Residue-property plots [i](#)

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



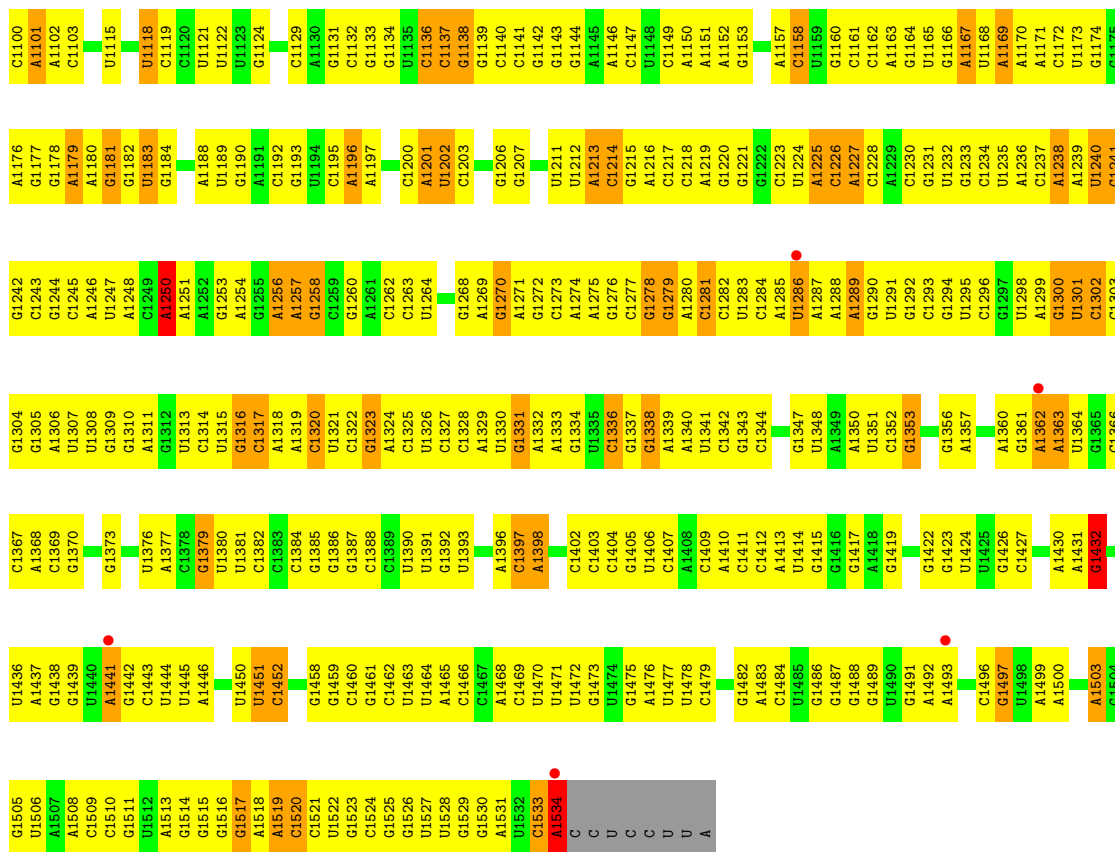
C764	C756	A831	G832	U834	U837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1084	C1085	C1086	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1107	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1157	C1158	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1206	C1207	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1263	C1264	C1268	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1356	C1357	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1380	C1381	C1382	C1383	C1384	C1385	C1389	C1390	C1391	C1392	C1393	C1396	C1397	C1398	C1399	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1416	C1417	C1422	C1423	C1424	C1425	C1426	C1427	C1430	C1431	C1432	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1450	C1451	C1452	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1477	C1478	C1479	C1480	C1481	C1482	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1503	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1533	C1534	C	C	U	C	C	C	U	U	A	A	A	A	U5	G6	G9	A10	G11	G12	U13	U14	G15	A16	U17	C18	G21	G22	C23	U24	U25	A26	G27	A28	G31	A32	A33	C34	G35	C36	G39	C40	G41	C42	C43	A44	C45	U46	U47	C48	A51	C52	A53	C54	A55	U56	C57	C58	U59	U60	A61	U62	C63	G64	A65	A1519	C1520	C1521	U1522	C1523	C1524	C1525	C1526	U1527	C1528	C1529	C1530	C1533	C1534	C	C	U	C	C	U	U	A	U1450	U1451	C1452	U1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	U1477	U1478	C1479	C1480	U1481	C1482	U1485	C1486	C1487	C1488	C1489	U1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	A1503	U1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	A1519
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● Molecule 1: 16S rRNA

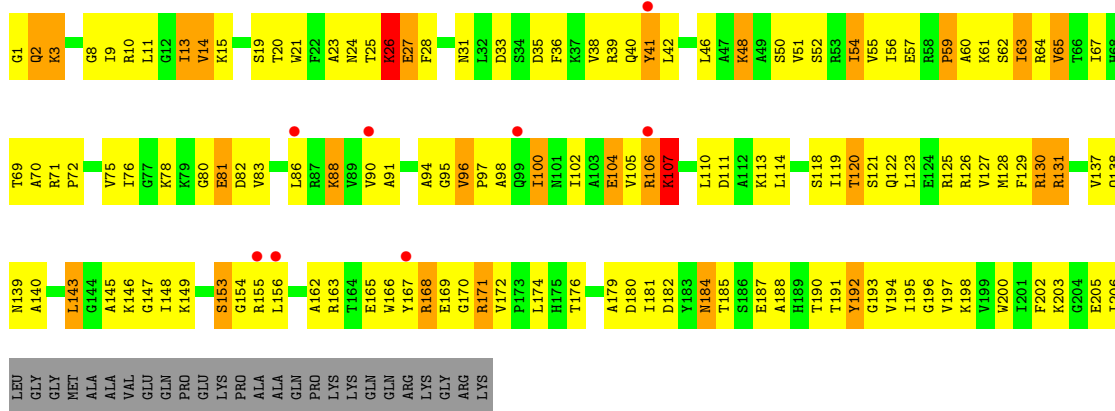


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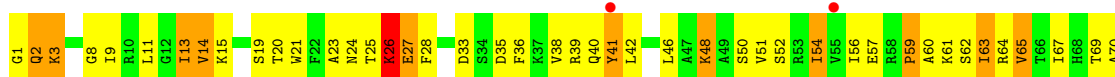
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C1037	A977	A831	U884	C620	C549	C477	U407	G337	C267	G203	A131	U70
G1038	A978	G832	A687	A621	G550	A478	A408	A338	U268	G204	C132	A71
G1039	C979	G833	G691	A622	U551	U479	U409	C339	C269	G205	C135	A205
U1040	C980	U834	G692	G623	U552	U480	C410	U343	A270	C206	G141	C73
G1041	C981	U835	G693	C624	A553	G481	A411	A344	C271	U208	G142	A74
A1042	U982	G836	A694	U625	U554	A482	A412	C345	C272	U209	A143	G75
G1043	A915	U837	A695	U626	C555	C483	G413	G346	U273	C210	G76	G76
A1044	U916	G838	A696	G627	U556	U484	A414	A349	A274	G211	A77	A77
C1045	G917	C839	A697	G628	G557	U485	A415	C352	G275	G212	G147	A78
A1046	U918	C840	U697	A629	U558	U486	C416	A353	G276	G213	G148	G79
G1047	A919	C841	G698	A630	G559	A487	U420	C354	G277	C214	A151	A80
U1048	U920	U842	C699	A631	U560	A488	U421	A355	G278	C215	A152	A81
G1050	U921	U843	G700	C632	U561	C489	U422	C356	A279	C216	A153	A82
A1051	G922	G844	G703	U633	U562	C490	C422	C357	C280	U216	A154	C83
C1052	A923	A845	U704	A633	A563	C491	C423	C358	C281	G217	C153	C83
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G1054	C925	G847	G705	A635	U565	A493	G425	G357	C285	U219	U155	U85
A1055	G926	C848	A706	U636	G566	C494	U426	U358	C286	G220	C156	G86
C1056	G927	G849	U707	C637	G566	C494	U426	G359	U287	G221	U157	C87
G1057	A928	G850	C708	U638	A572	C428	G428	C359	A288	C222	G158	U88
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C1059	C930	G852	G710	A640	A574	A430	U430	A364	C290	U224	A160	C90
G1060	C931	C853	G711	U641	C575	A431	A431	A365	U291	C225	A161	U91
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C1063	C934	C856	G713	U644	C578	C504	U434	U368	A298	G232	G168	G94
G1064	A935	G857	G714	U645	A579	A435	U435	C370	A299	U233	G169	C95
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G1067	G937	G861	U717	A648	G581	U512	U437	A373	G302	C235	A171	A98
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C1072	C942	G866	U722	U653	U593	G517	C449	C381	A312	G240	C176	U103
G1073	A943	A867	G723	G656	U594	C518	C450	A382	C312	G241	C177	G104
U1074	C944	G868	A724	U657	G592	G521	A451	A383	A313	G242	C178	G105
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U1076	C946	U870	C726	U659	U594	A823	G453	C385	A315	U244	U180	G107
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A1092	U962	C884	A742	A675	C611	G542	U470	C400	C330	U261	A196	U123
C1093	G963	G885	C743	A676	C612	U543	C401	C401	G331	G262	A197	C124
G1094	A964	U886	U744	G745	C613	G544	U472	G402	G332	A262	G198	U125
U1095	U965	C887	C745	U677	C614	C545	U473	C403	U333	A263	A199	G126
C1096	G966	A892	G746	U678	C615	C546	U474	G404	G334	G264	G200	G126
U1097	C967	U888	A747	C679	G616	A546	C474	C405	C335	A265	G201	A129
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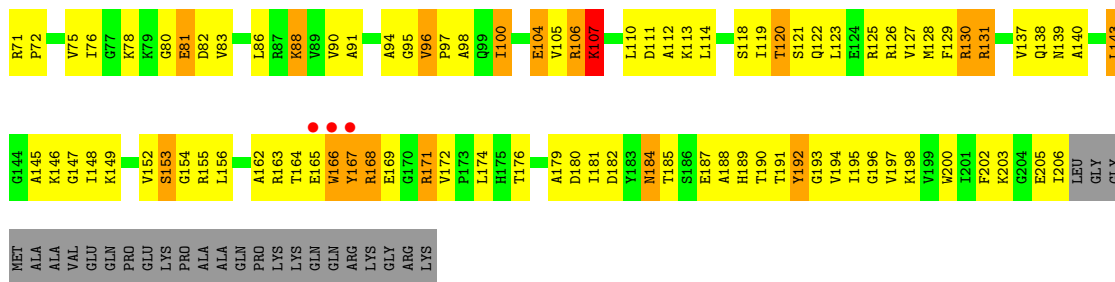


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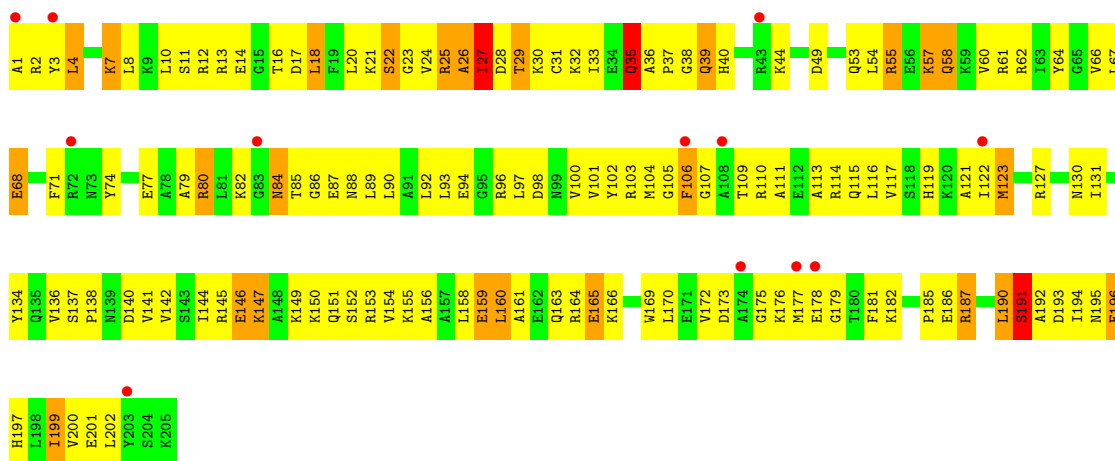


• Molecule 2: 30S ribosomal protein S3

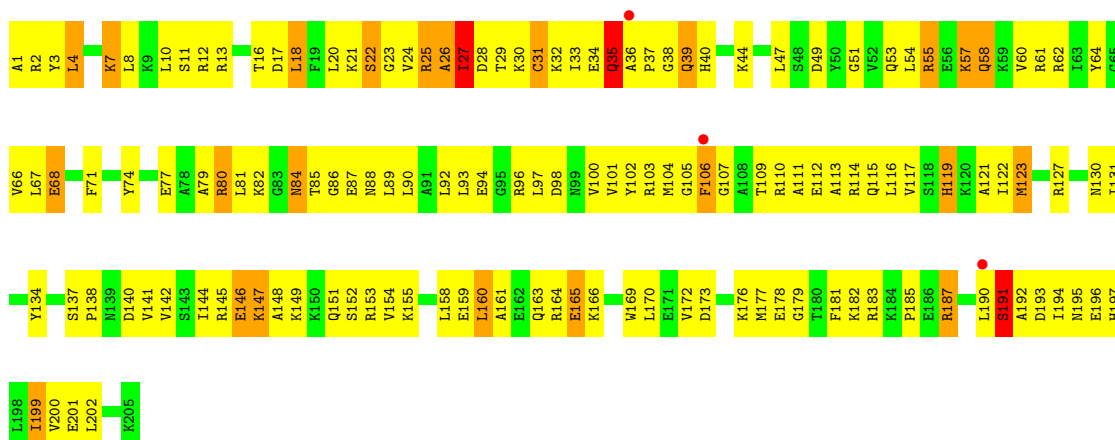




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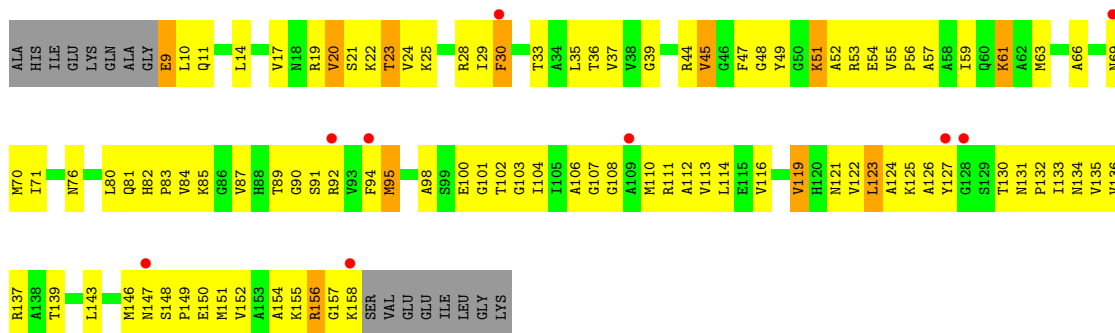


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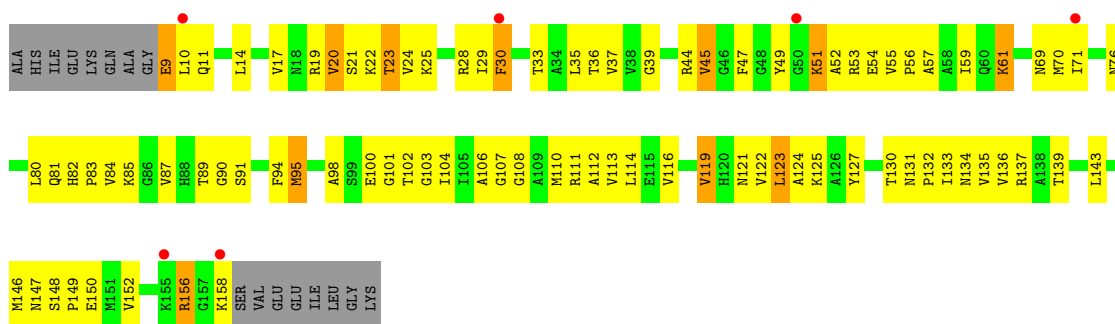


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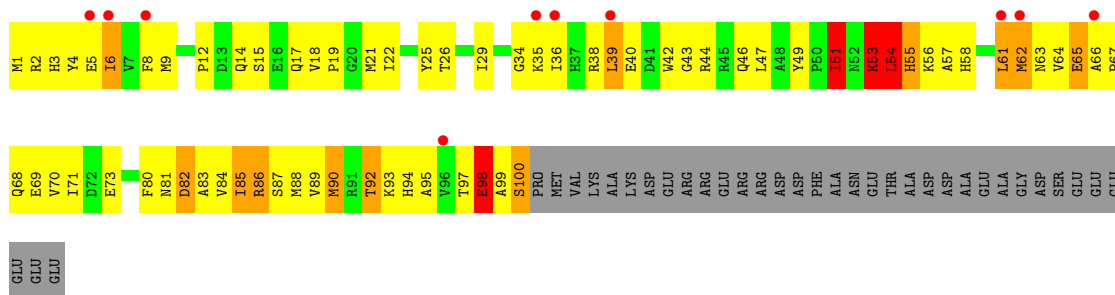
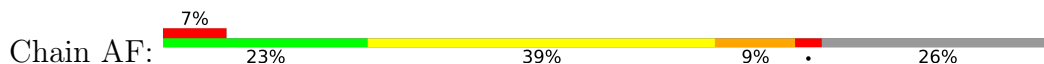




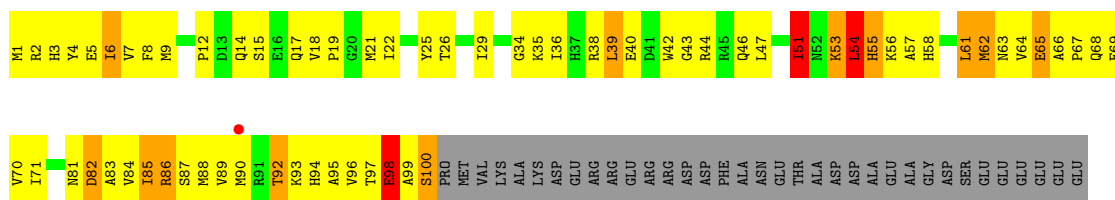
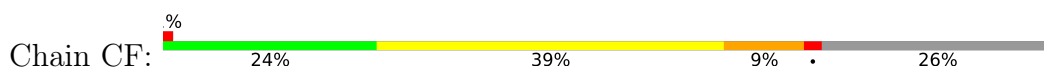
• Molecule 4: 30S ribosomal protein S5



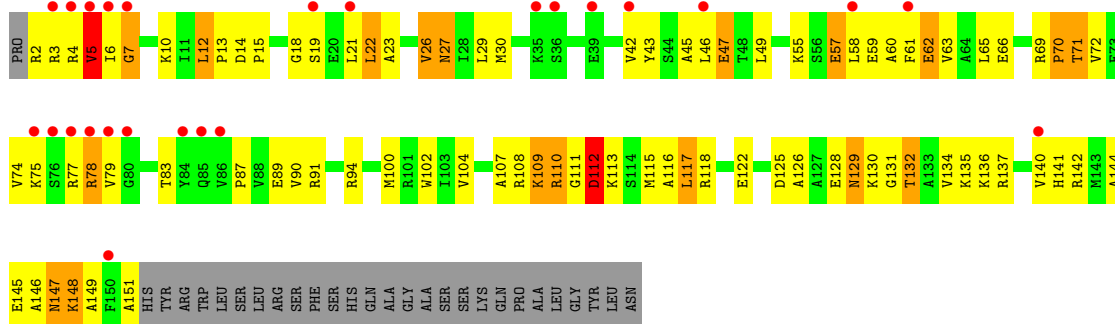
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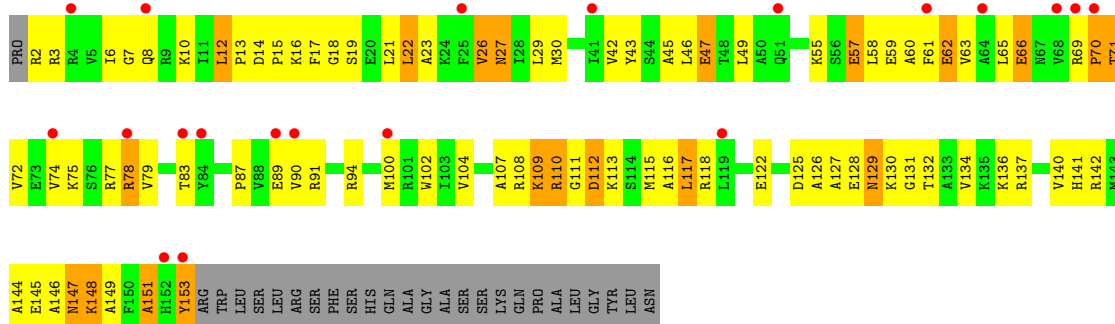
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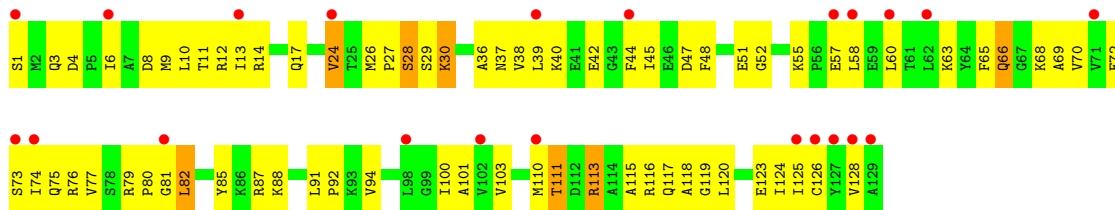
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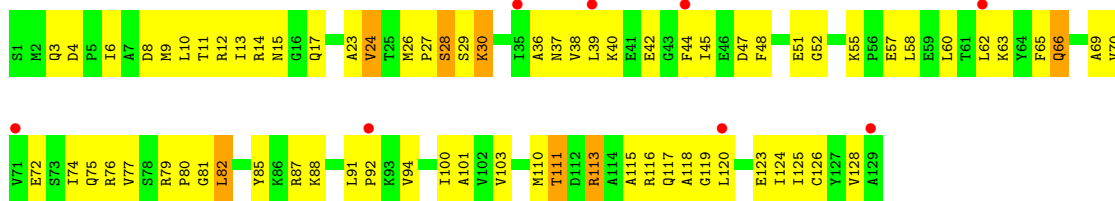
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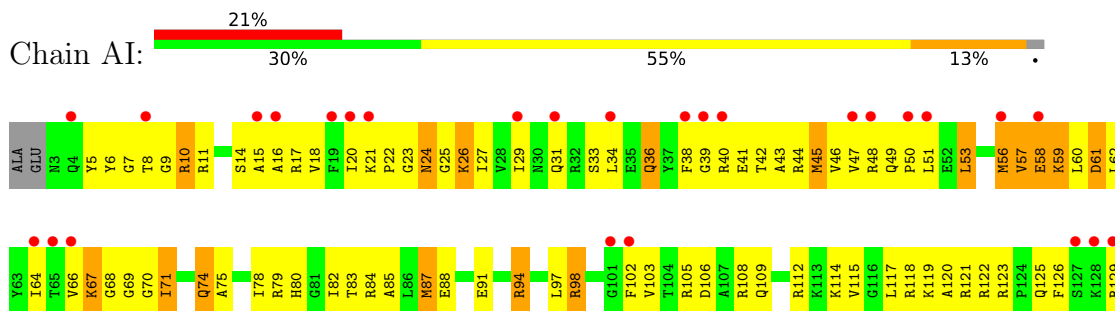
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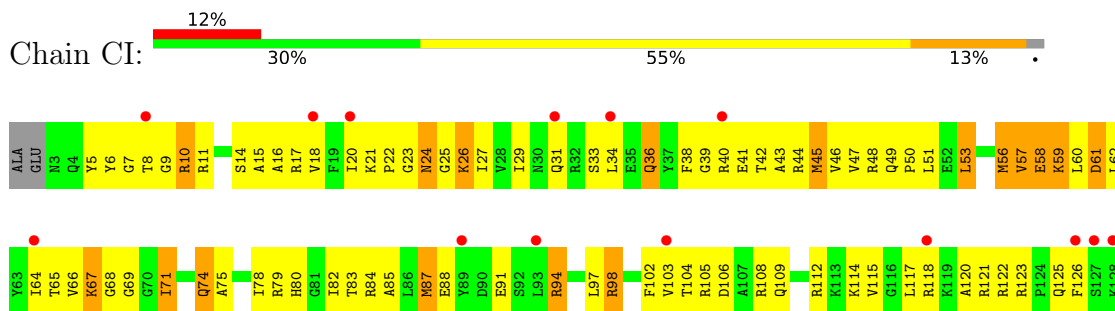
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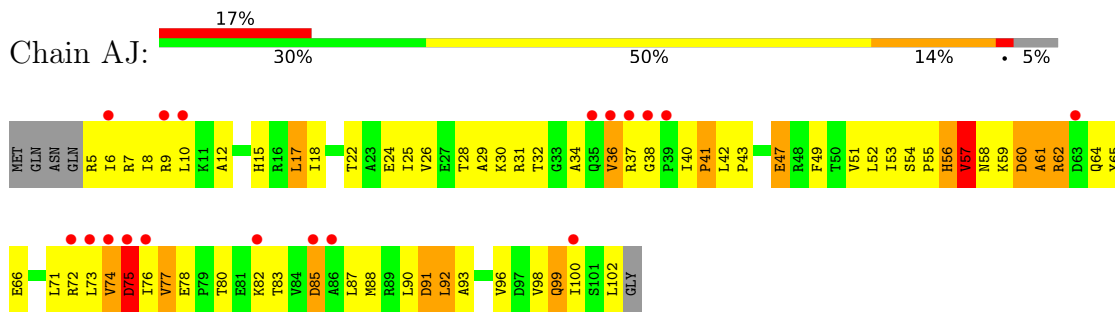
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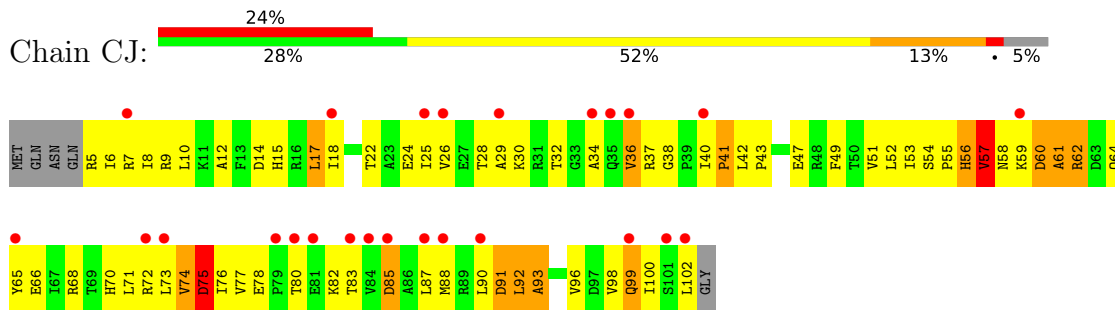
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

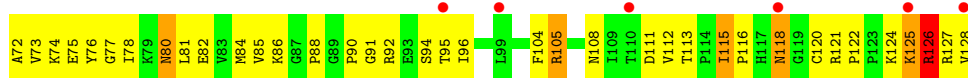
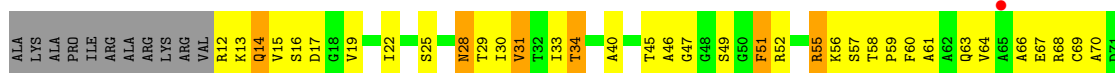


• Molecule 9: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S11

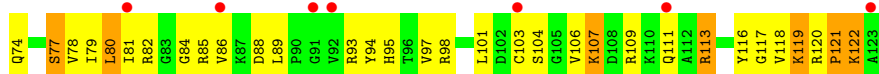
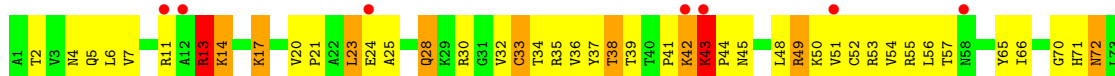
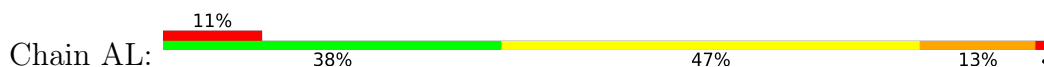




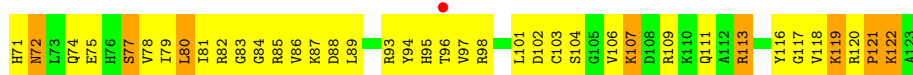
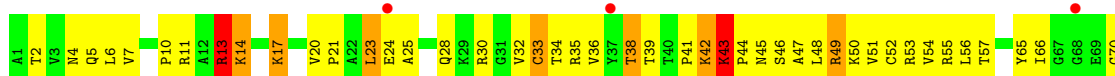
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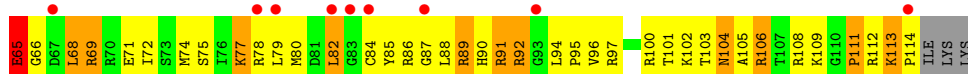
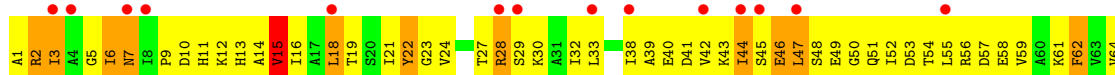
• Molecule 11: 30S ribosomal protein S12



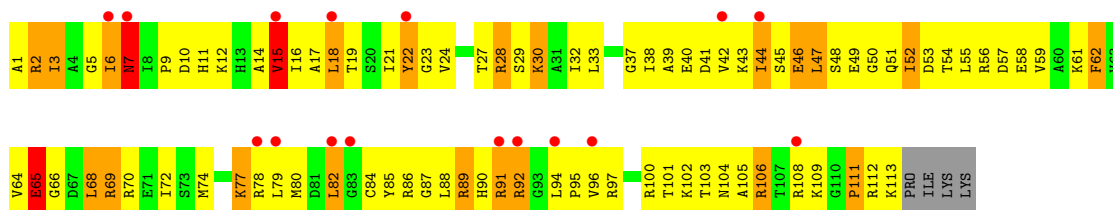
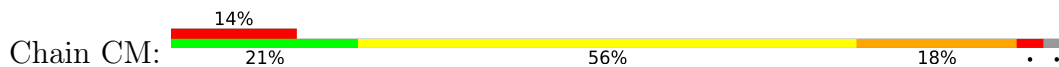
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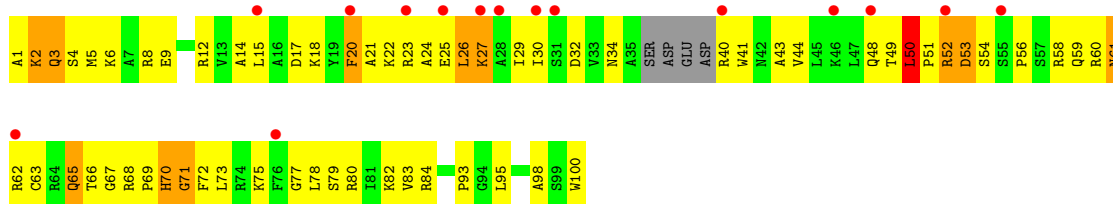
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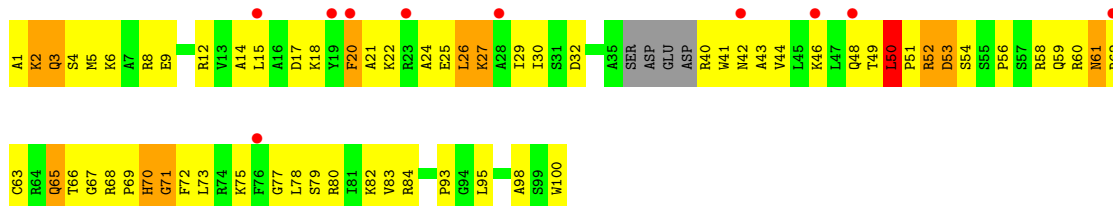
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14



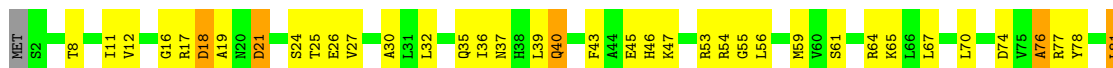
- Molecule 13: 30S ribosomal protein S14

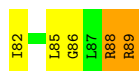


- Molecule 14: 30S ribosomal protein S15

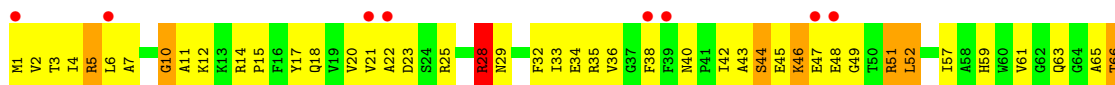


- Molecule 14: 30S ribosomal protein S15

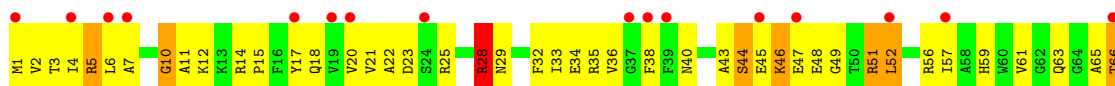




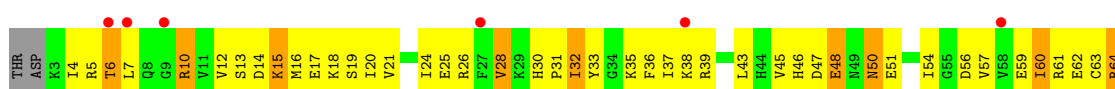
- Molecule 15: 30S ribosomal protein S16



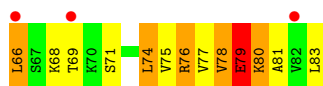
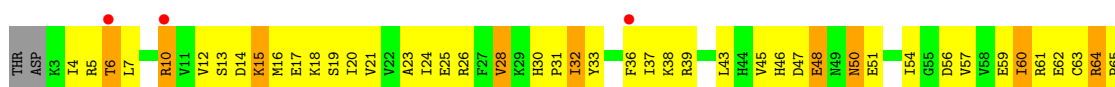
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

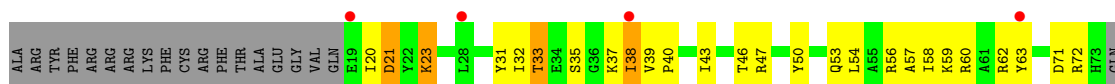


- Molecule 16: 30S ribosomal protein S17

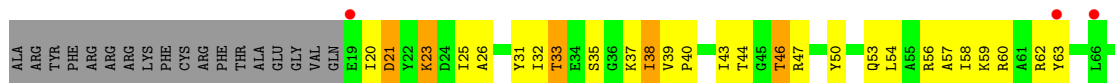


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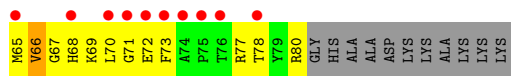
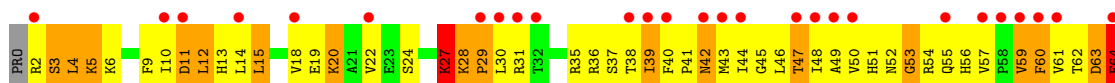
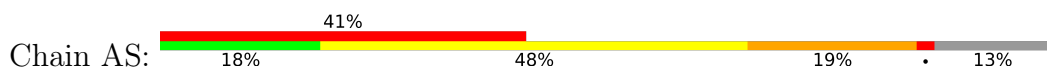




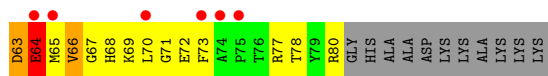
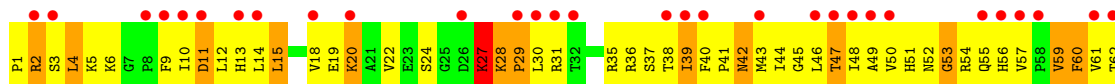
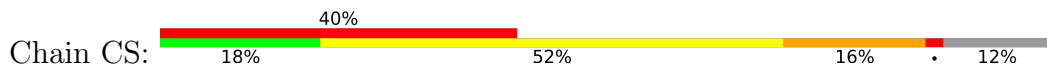
- Molecule 17: 30S ribosomal protein S18



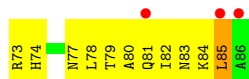
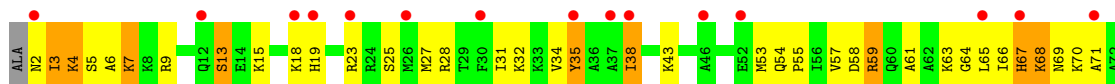
- Molecule 18: 30S ribosomal protein S19



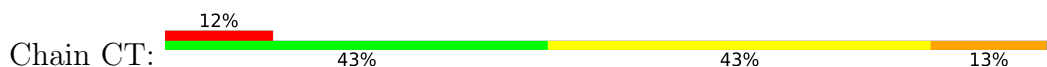
- Molecule 18: 30S ribosomal protein S19

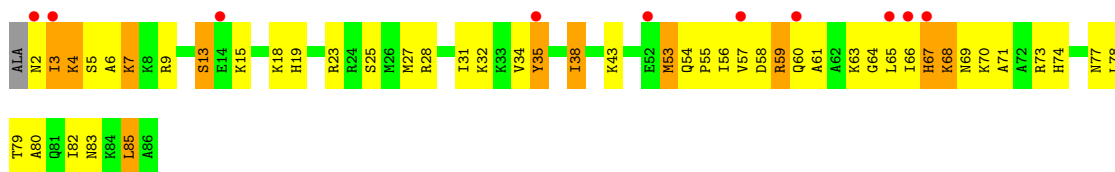


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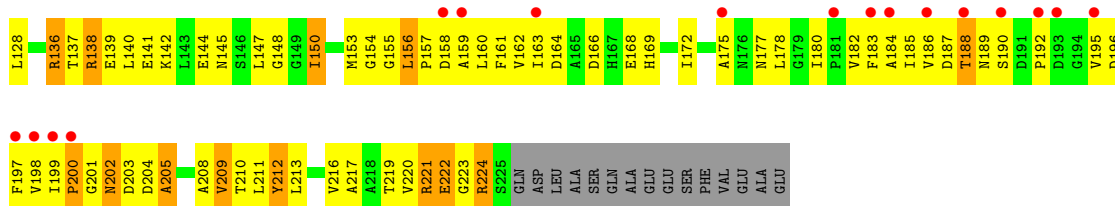
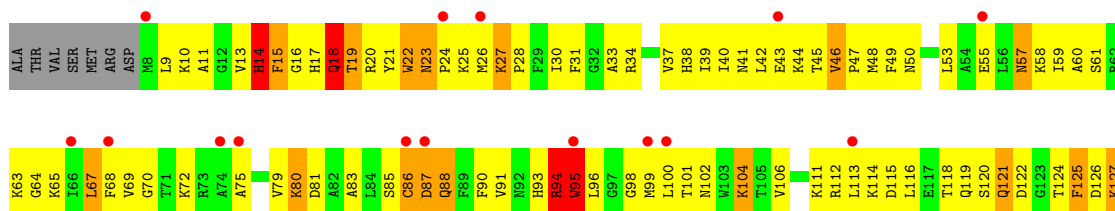


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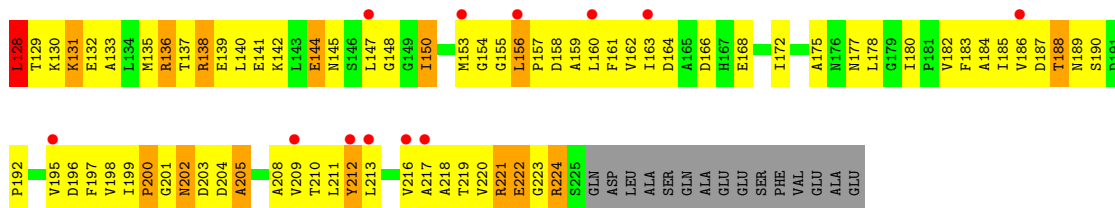
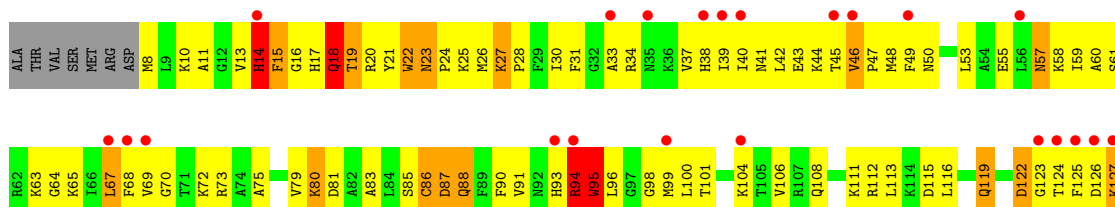




• Molecule 20: 30S ribosomal protein S2



• Molecule 20: 30S ribosomal protein S2



• Molecule 21: 30S ribosomal protein S21



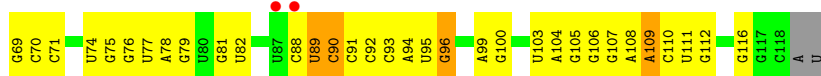
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ARG
ARG
THR
THR
ARG
ARG
LEU
LEU
TYR

• Molecule 21: 30S ribosomal protein S21



ARG
ARG
THR
ARG
ARG
TYR

• Molecule 22: 5S rRNA

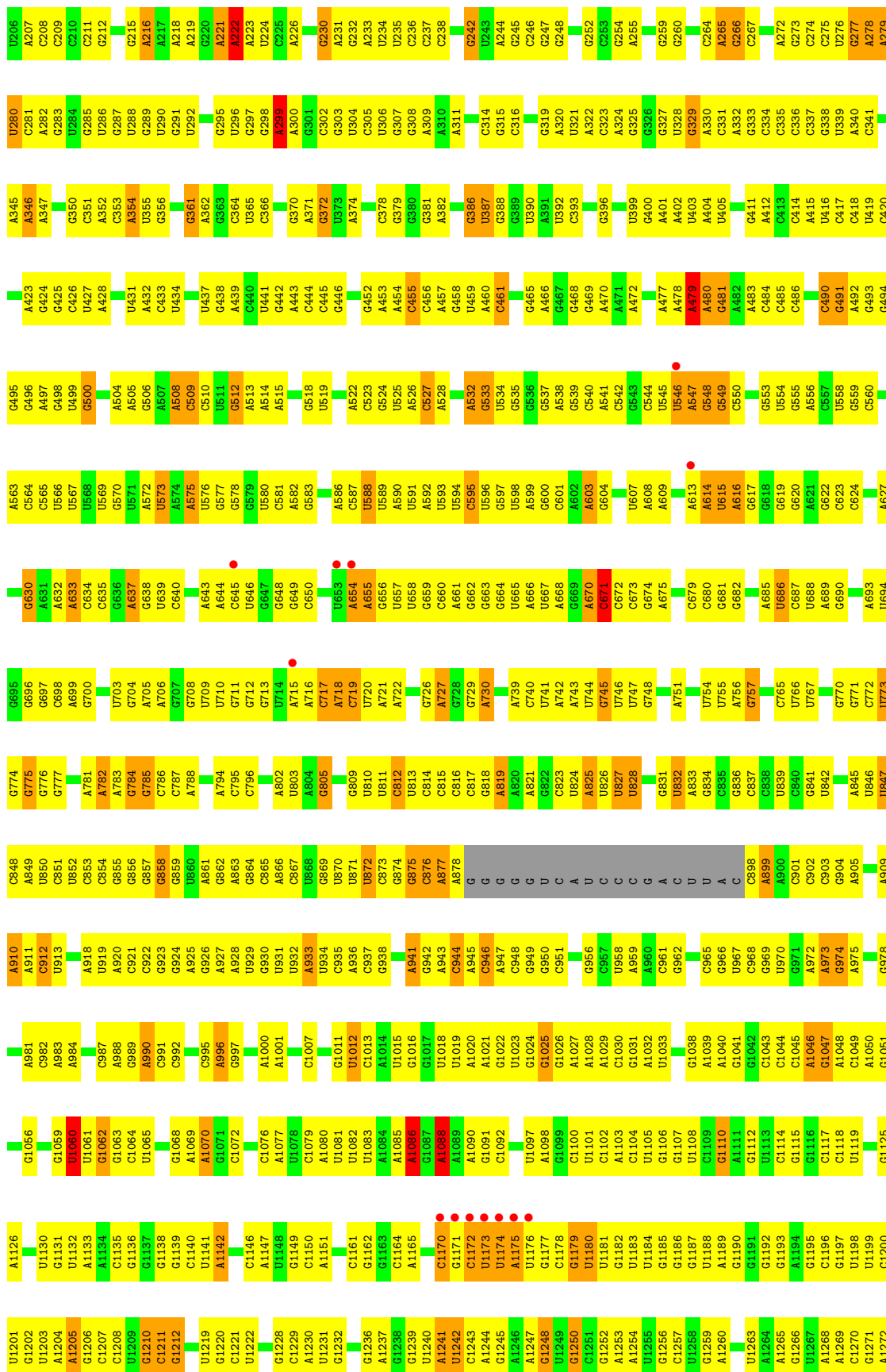


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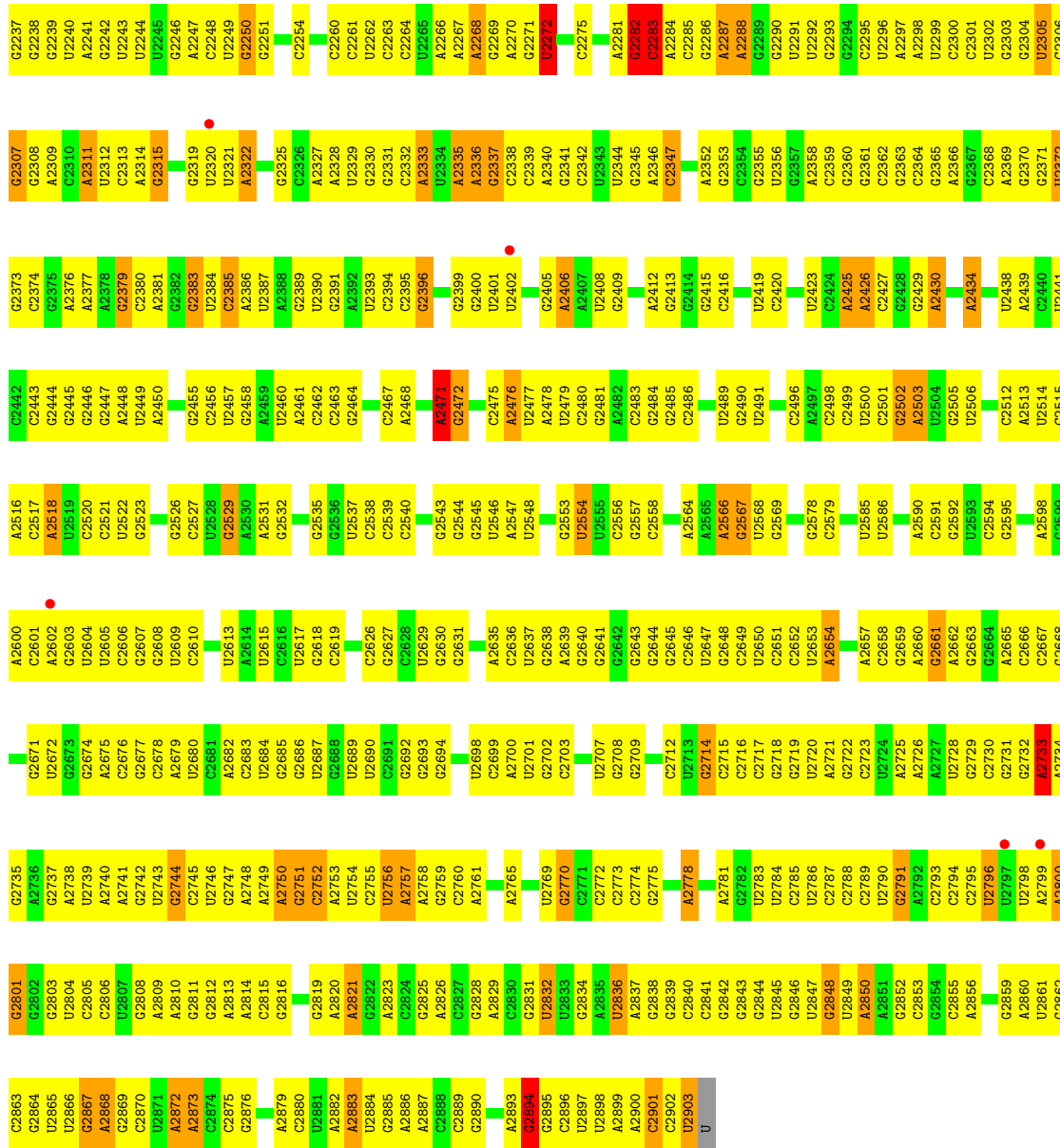


• Molecule 23: 23S rRNA



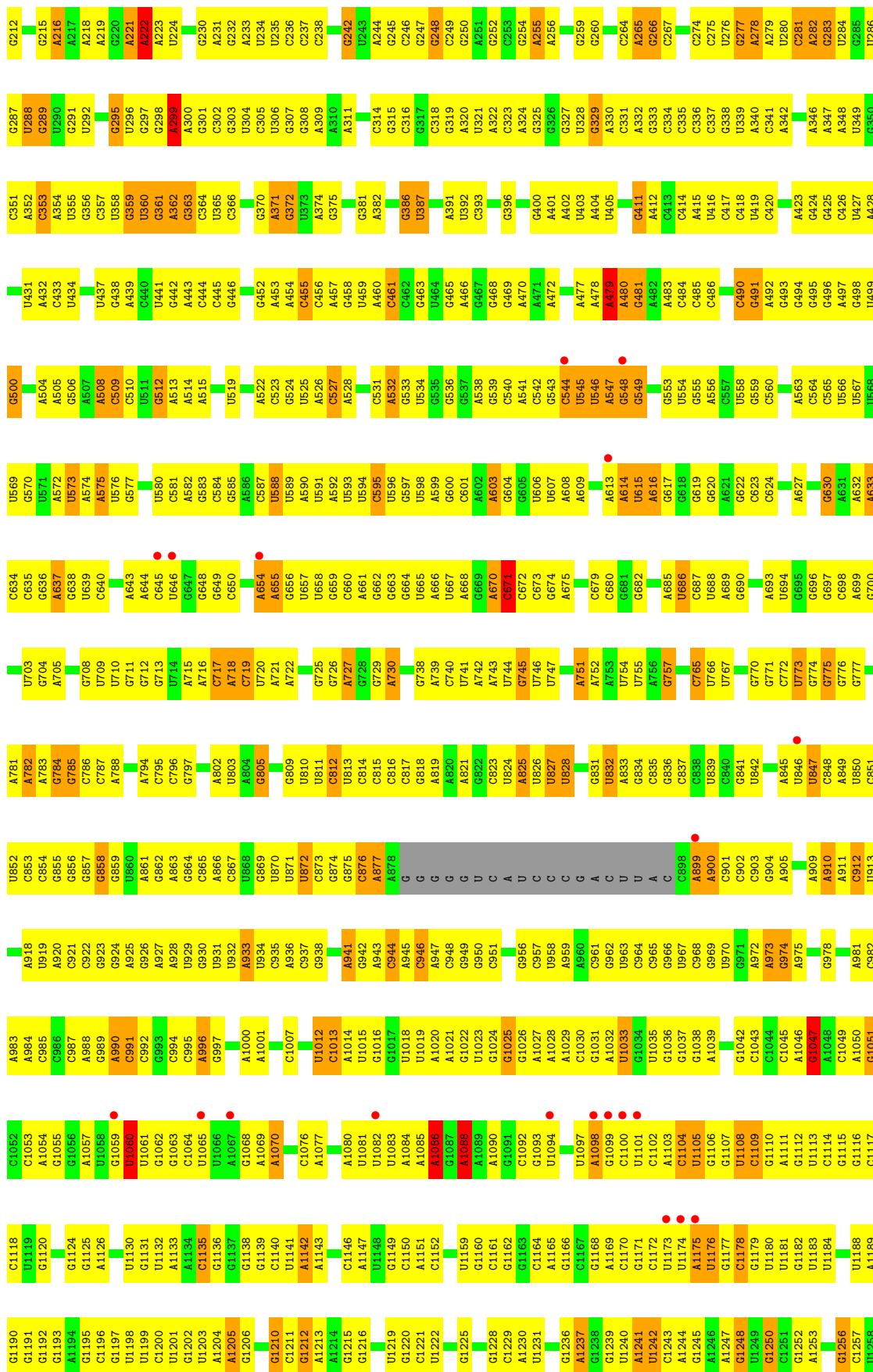


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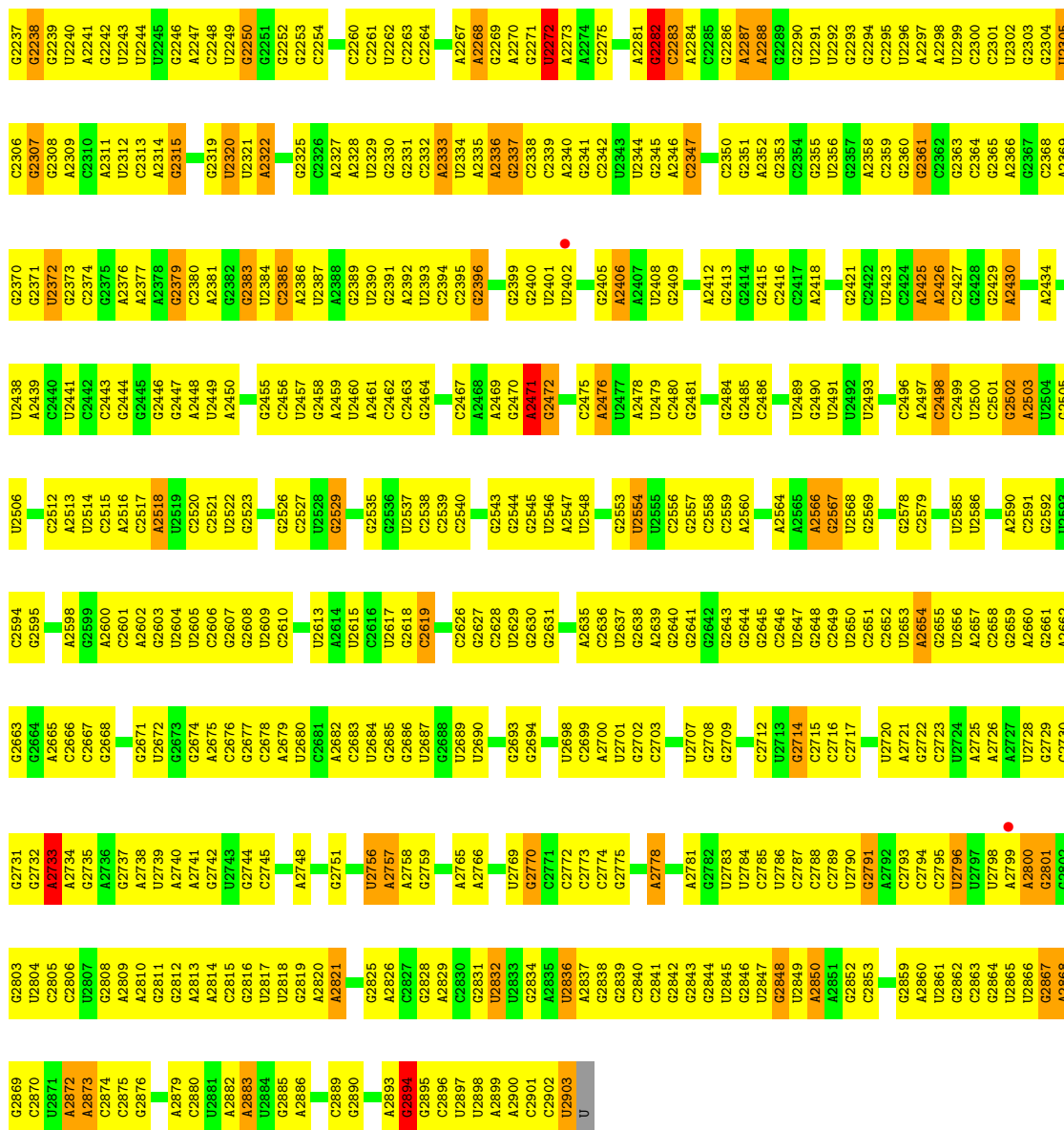


• Molecule 23: 23S rRNA

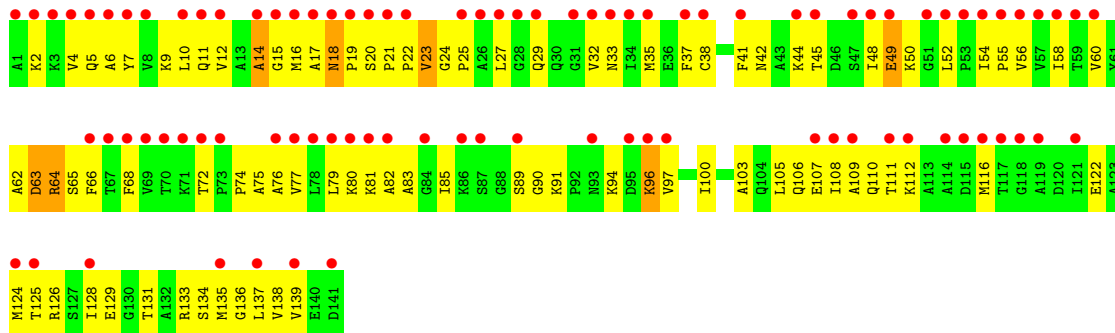




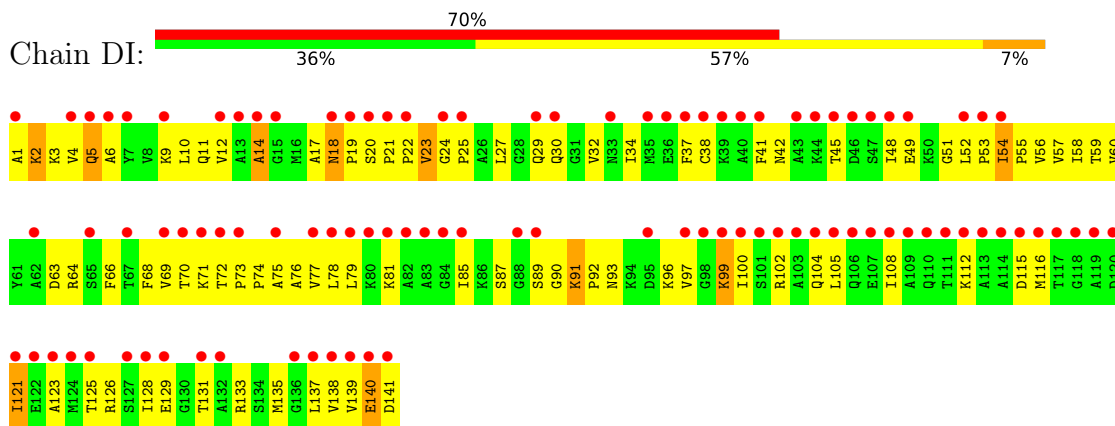
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A	U2274	C2042	C1891	U1963	U1742	U1742	A1678	A1591	G1524	C1386	C1386	C1320
C	U2275	A2042	C1892	G1964	G1743	G1743	A1678	C1592	A1525	A1387	A1387	A1321
U	U2276	C2043	U1898	C1967	A1744	A1744	A1679	A1593	C1526	U1388	U1388	A1322
C	U2277	A	U1899	U1968	A1745	A1745	U1680	A1594	G1527	G1389	G1389	C1323
A	U2278	U	U1820	U1968	A1746	A1746	G1681	U1595	A1528	U1390	U1390	G1324



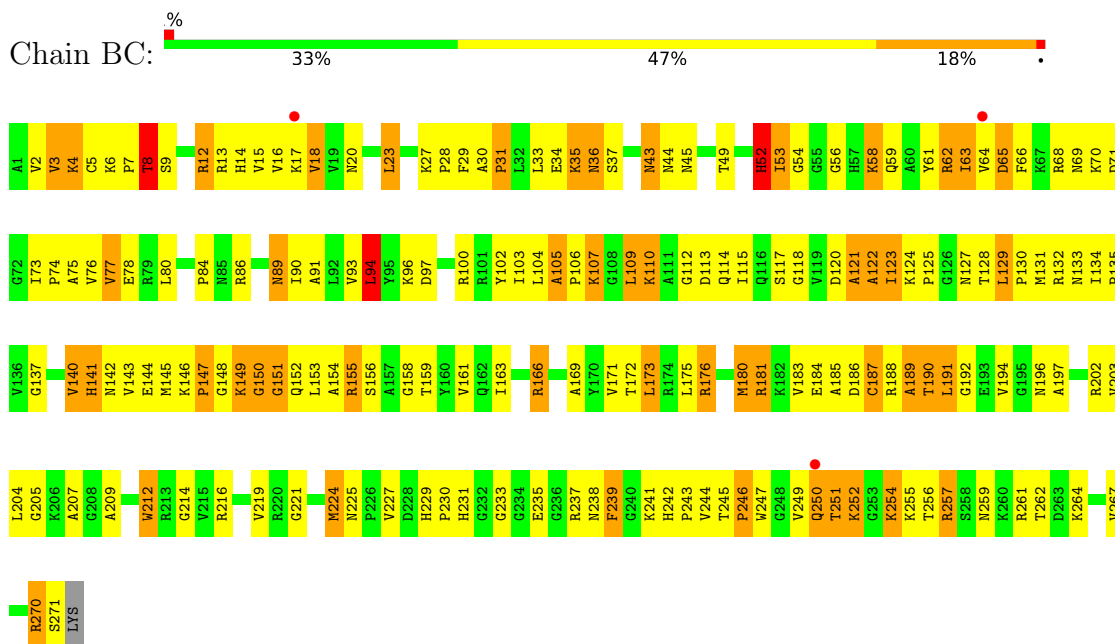
• Molecule 24: 50S ribosomal protein L11



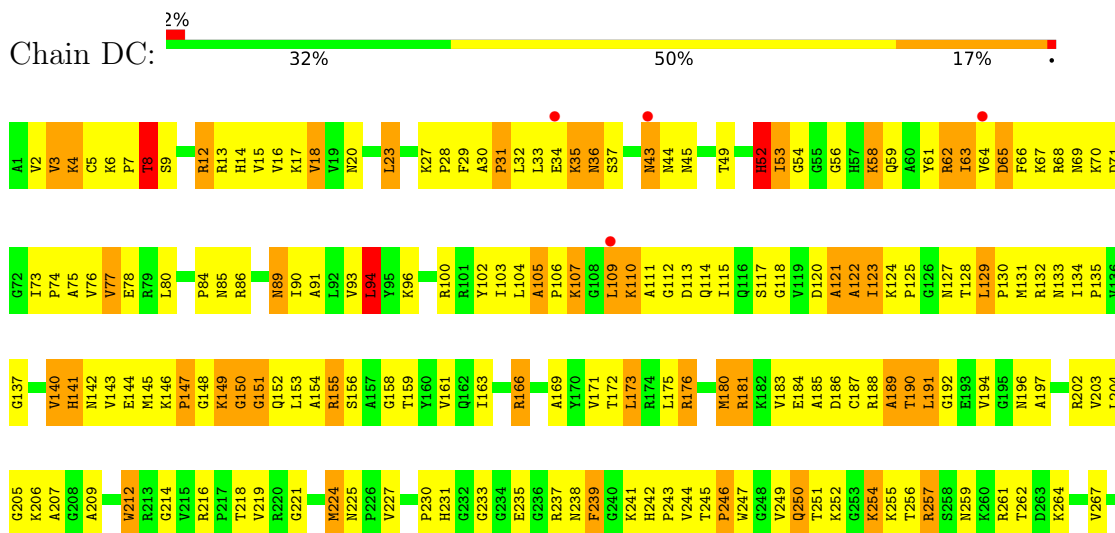
• Molecule 24: 50S ribosomal protein L11



• Molecule 25: 50S ribosomal protein L2

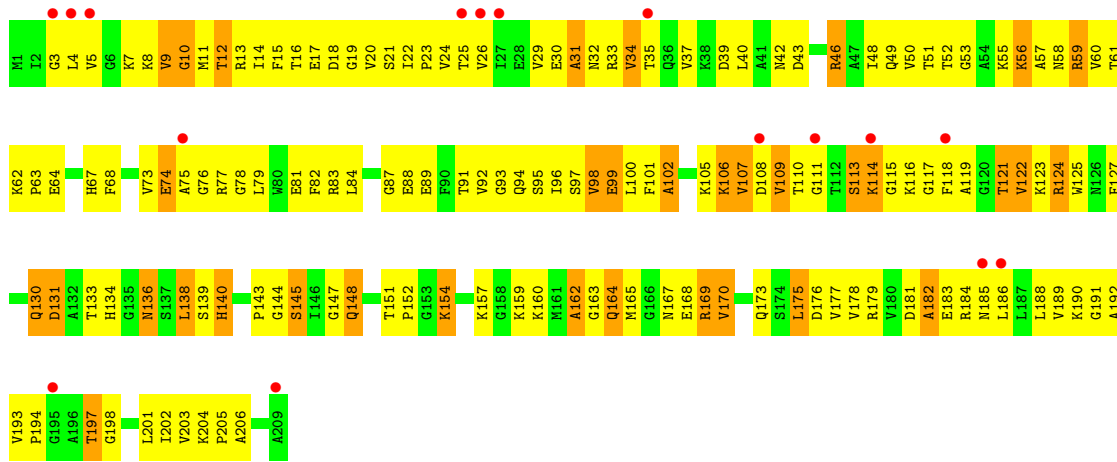


• Molecule 25: 50S ribosomal protein L2

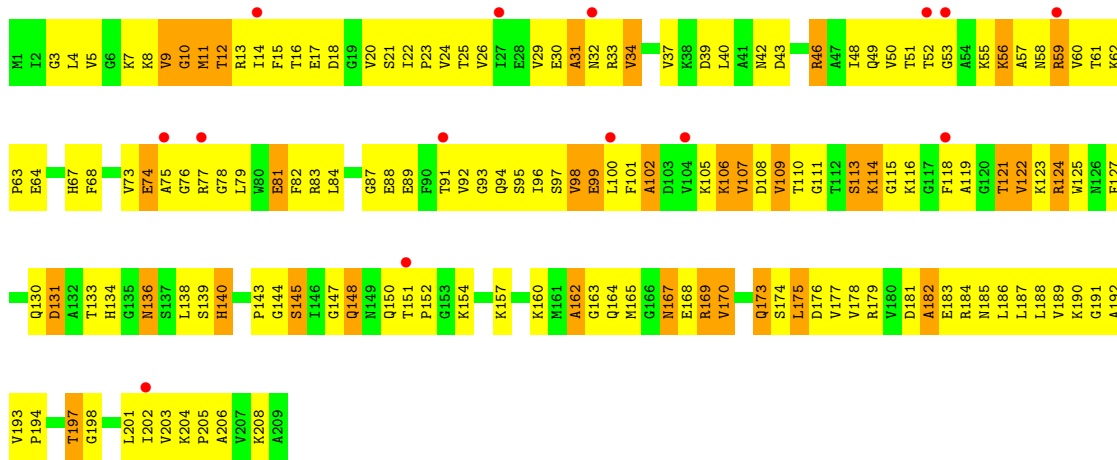




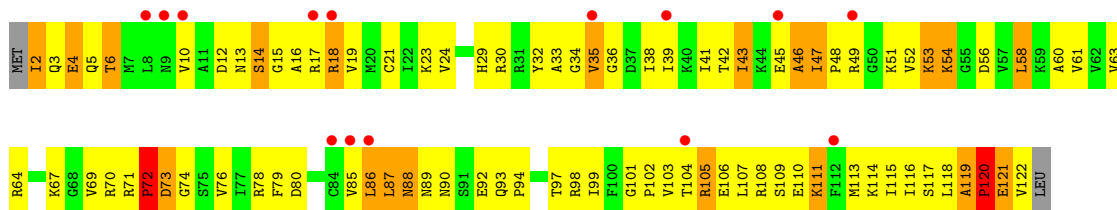
• Molecule 26: 50S ribosomal protein L3



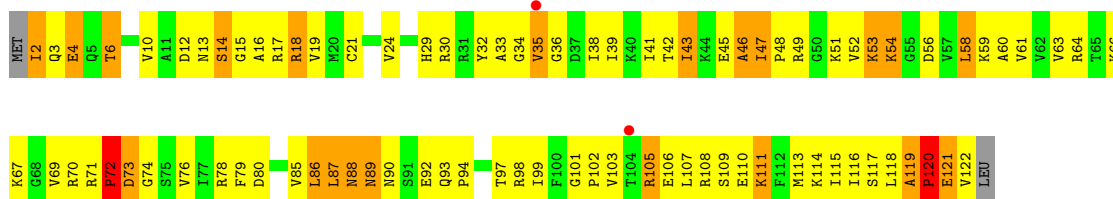
• Molecule 26: 50S ribosomal protein L3



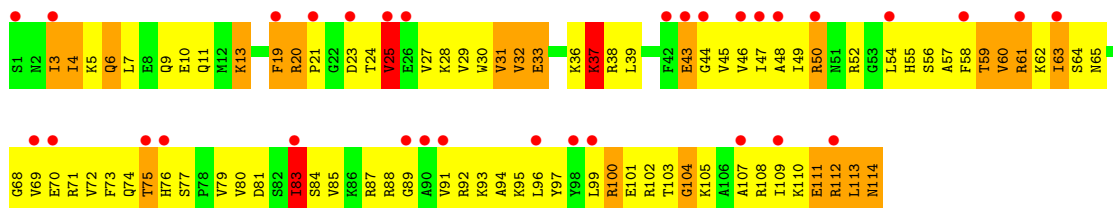
• Molecule 27: 50S ribosomal protein L14



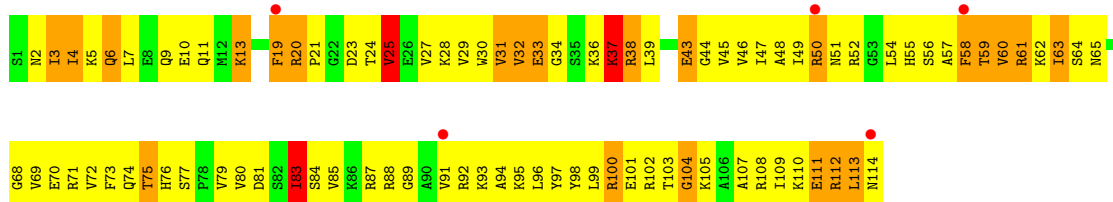
- Molecule 27: 50S ribosomal protein L14



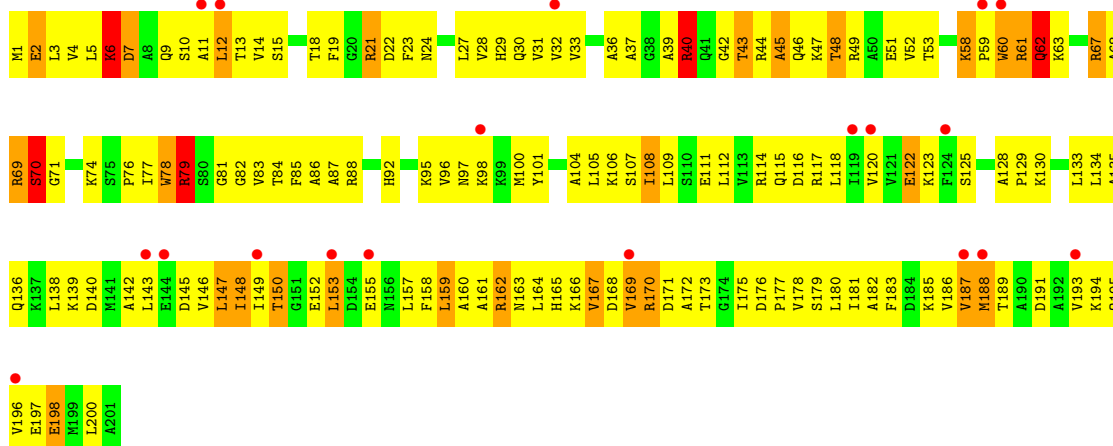
- Molecule 28: 50S ribosomal protein L19



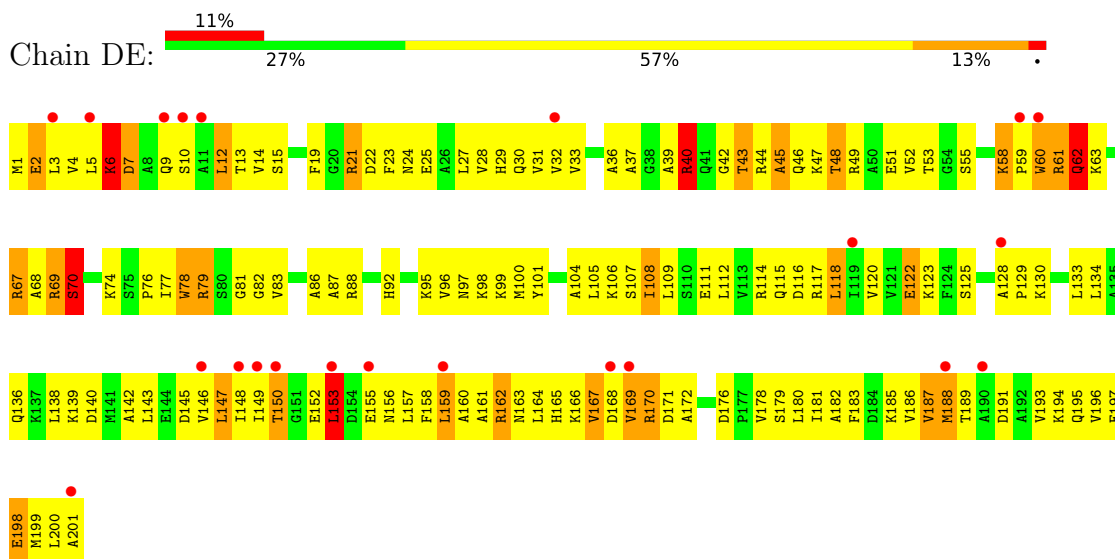
- Molecule 28: 50S ribosomal protein L19



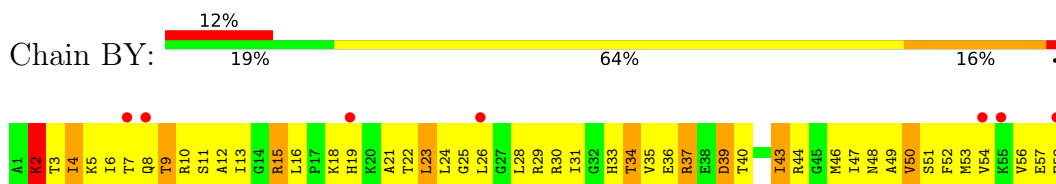
- Molecule 29: 50S ribosomal protein L4



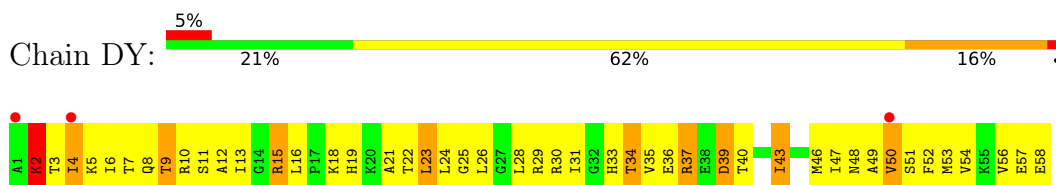
- Molecule 29: 50S ribosomal protein L4



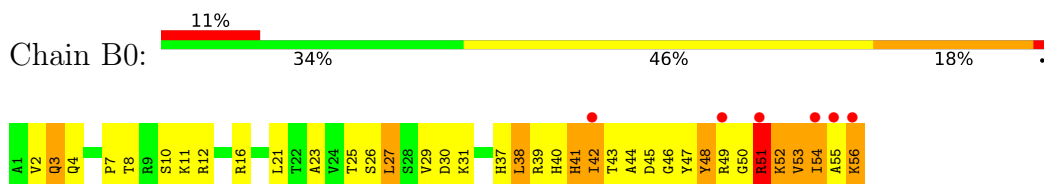
- Molecule 30: 50S ribosomal protein L30



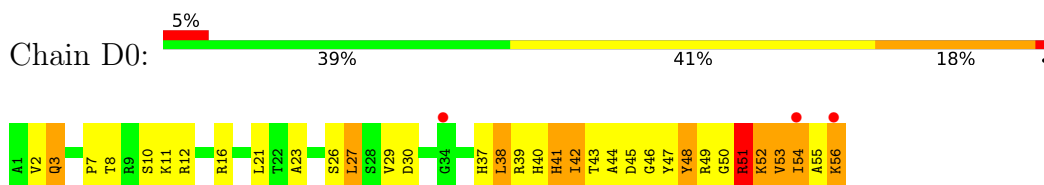
- Molecule 30: 50S ribosomal protein L30



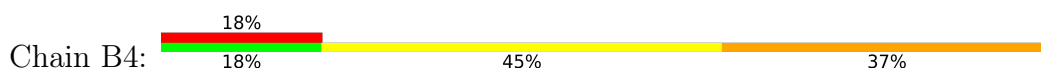
- Molecule 31: 50S ribosomal protein L32



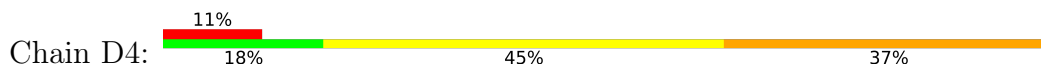
- Molecule 31: 50S ribosomal protein L32



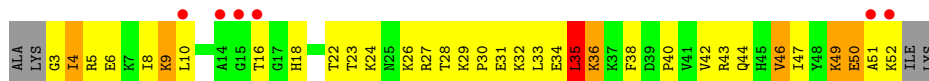
- Molecule 32: 50S ribosomal protein L36



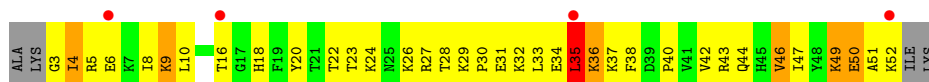
- Molecule 32: 50S ribosomal protein L36



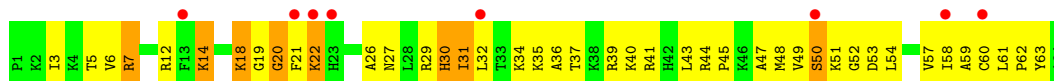
- Molecule 33: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L33



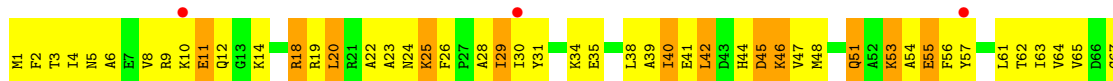
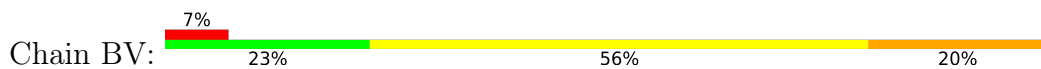
- Molecule 34: 50S ribosomal protein L35

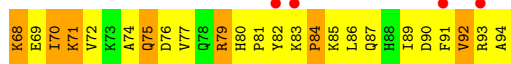


- Molecule 34: 50S ribosomal protein L35

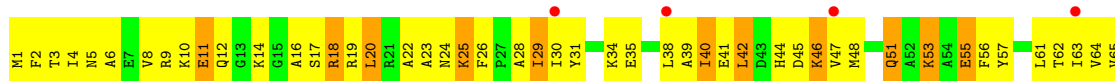


- Molecule 35: 50S ribosomal protein L25

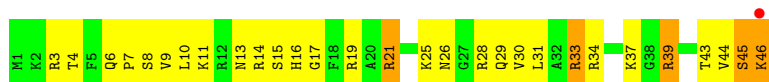




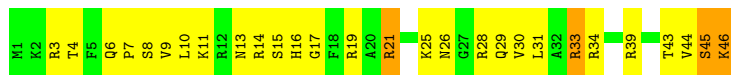
• Molecule 35: 50S ribosomal protein L25



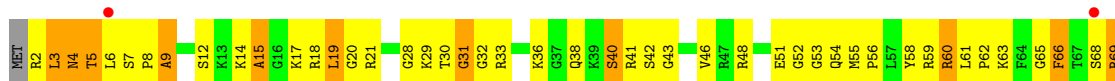
• Molecule 36: 50S ribosomal protein L34



• Molecule 36: 50S ribosomal protein L34

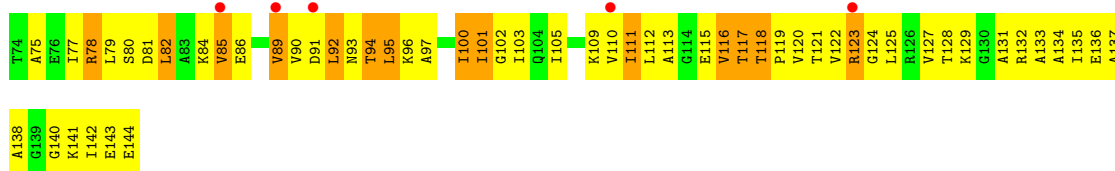


• Molecule 37: 50S ribosomal protein L15

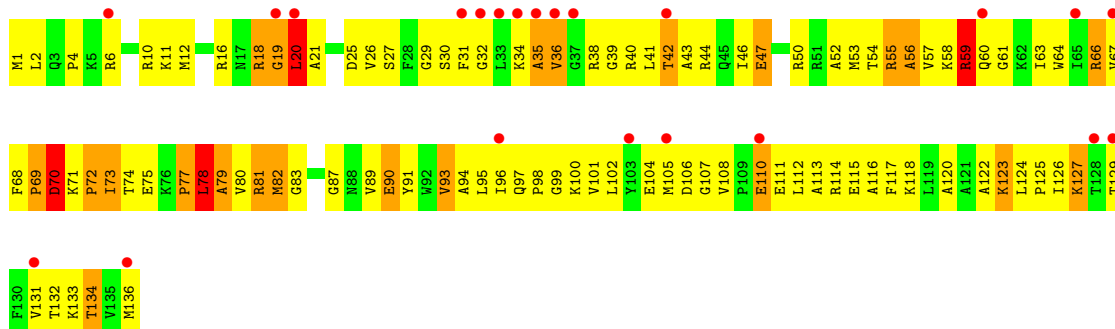


• Molecule 37: 50S ribosomal protein L15

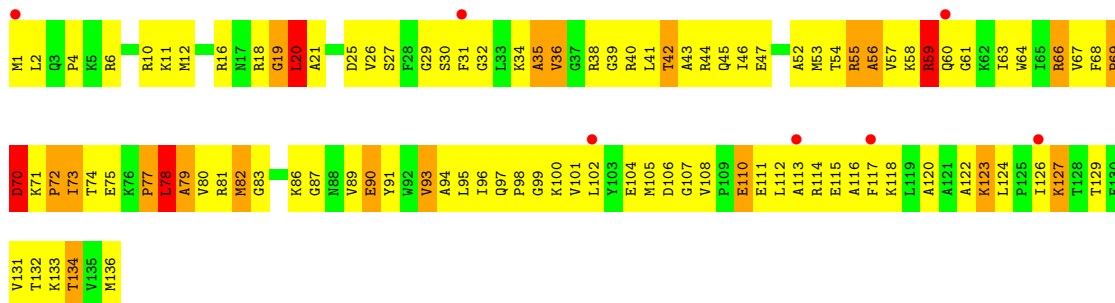




• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L29

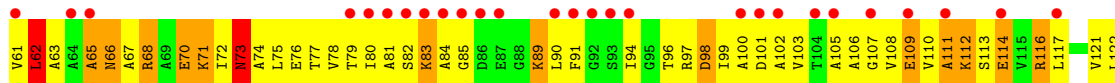
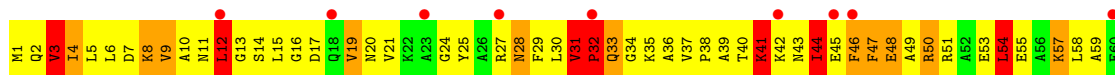
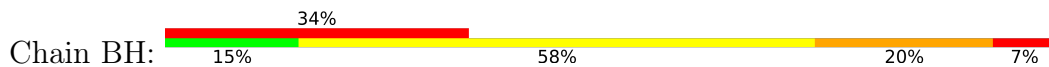


• Molecule 39: 50S ribosomal protein L29





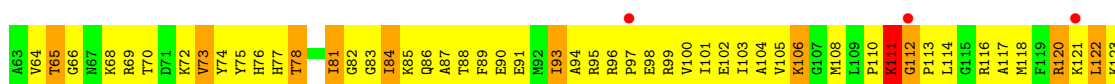
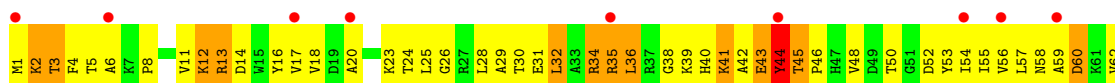
• Molecule 40: 50S ribosomal protein L9



• Molecule 40: 50S ribosomal protein L9



• Molecule 41: 50S ribosomal protein L13

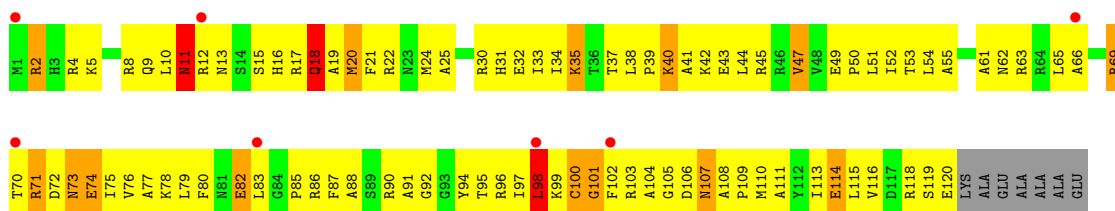


• Molecule 41: 50S ribosomal protein L13

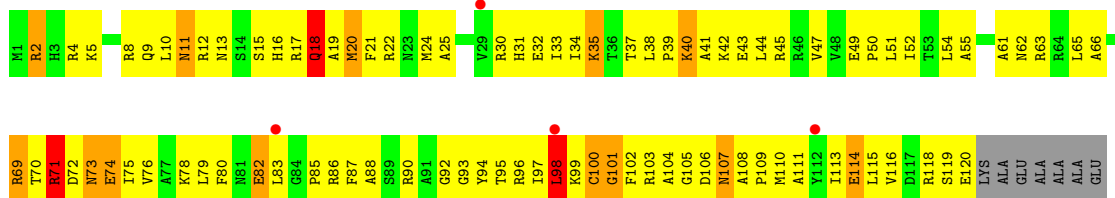
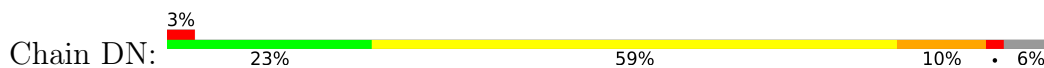




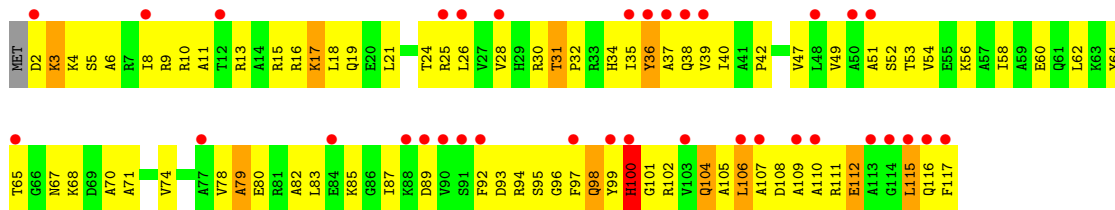
• Molecule 42: 50S ribosomal protein L17



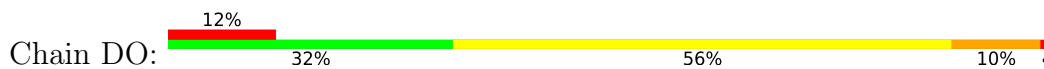
• Molecule 42: 50S ribosomal protein L17

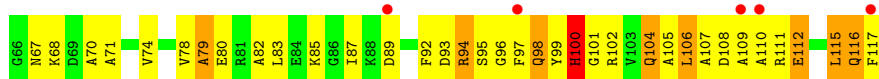


• Molecule 43: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L18

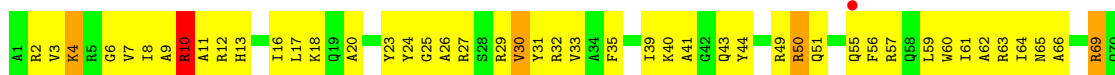




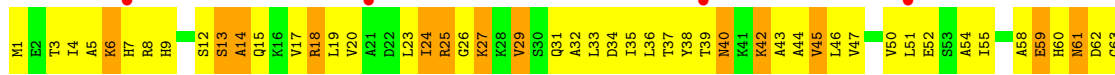
• Molecule 44: 50S ribosomal protein L20



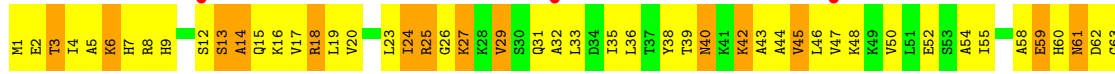
• Molecule 44: 50S ribosomal protein L20



• Molecule 45: 50S ribosomal protein L22

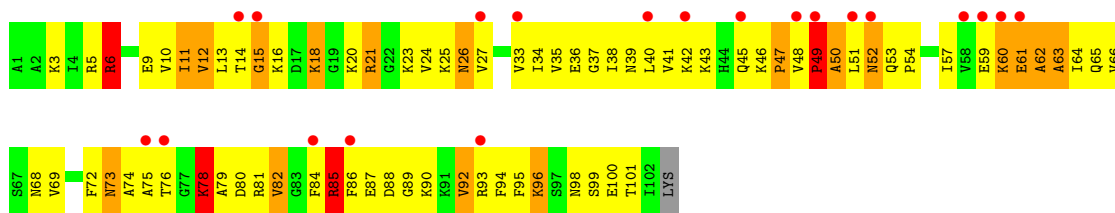


• Molecule 45: 50S ribosomal protein L22

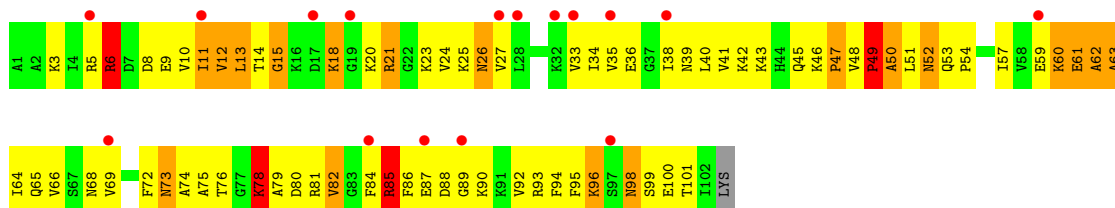


• Molecule 46: 50S ribosomal protein L24

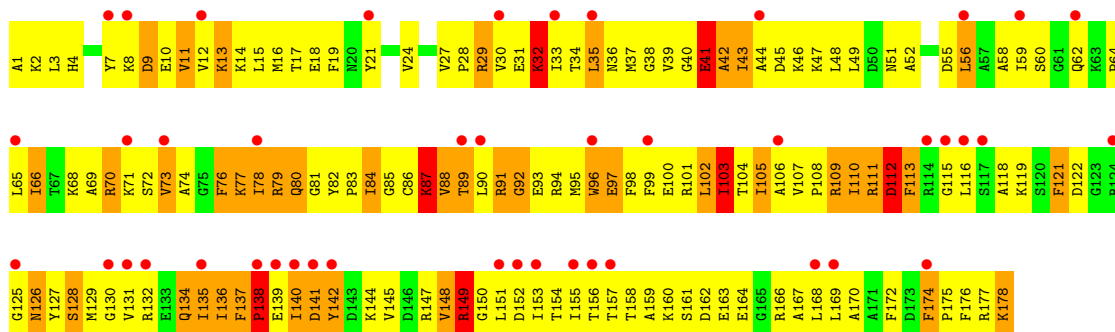
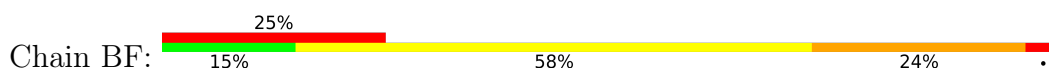




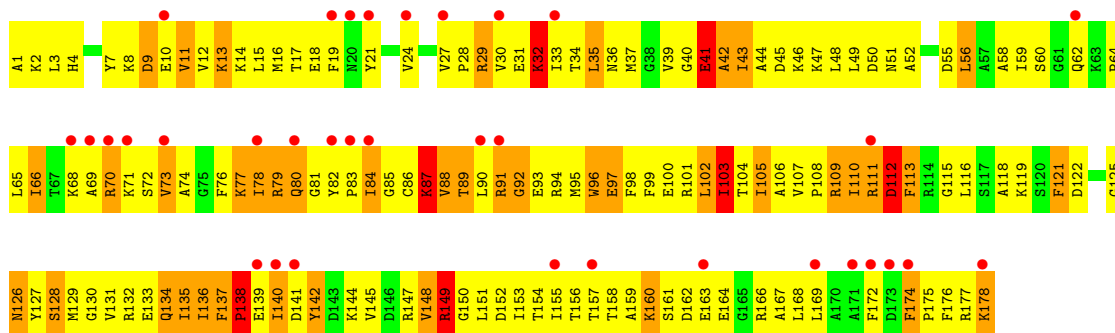
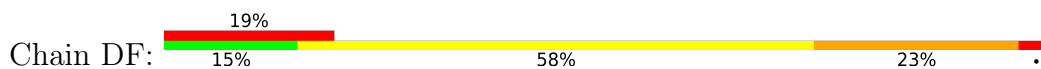
- Molecule 46: 50S ribosomal protein L24



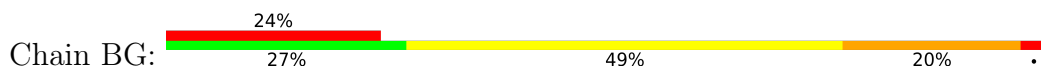
- Molecule 47: 50S ribosomal protein L5

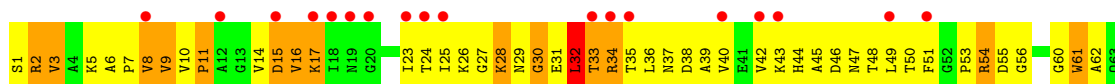


- Molecule 47: 50S ribosomal protein L5

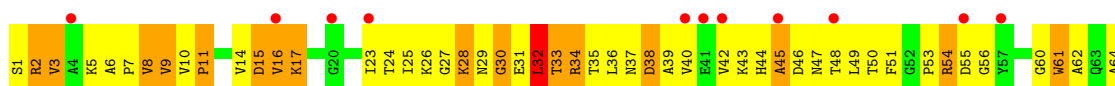


- Molecule 48: 50S ribosomal protein L6

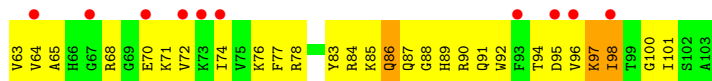
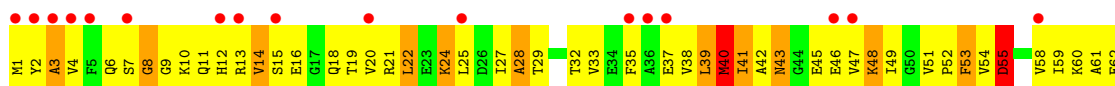




- Molecule 48: 50S ribosomal protein L6



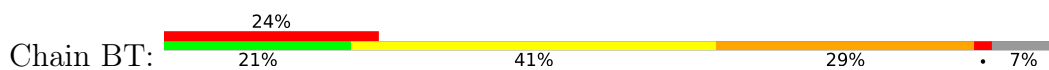
- Molecule 49: 50S ribosomal protein L21

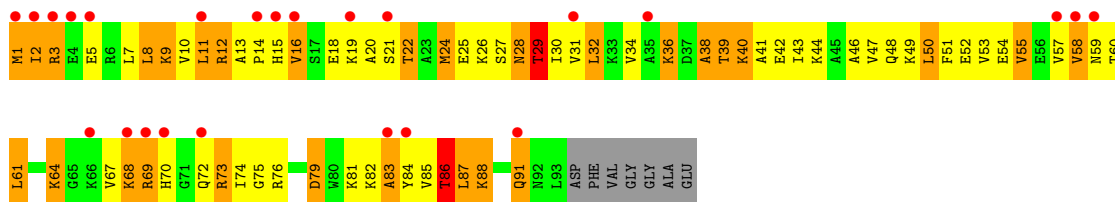


- Molecule 49: 50S ribosomal protein L21

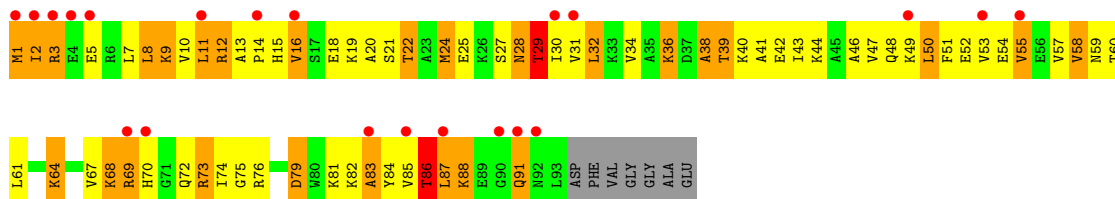
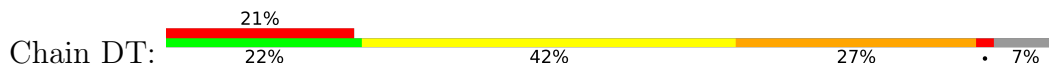


- Molecule 50: 50S ribosomal protein L23

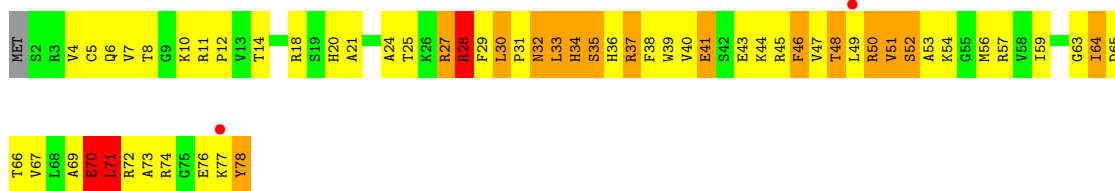




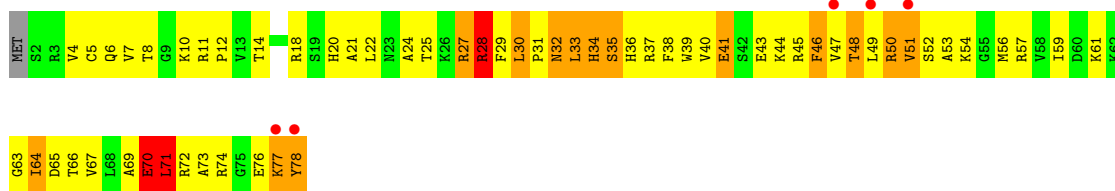
• Molecule 50: 50S ribosomal protein L23



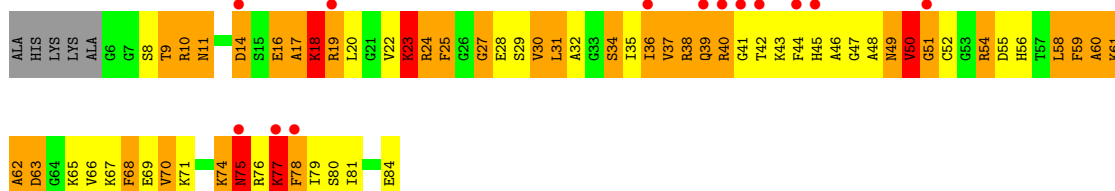
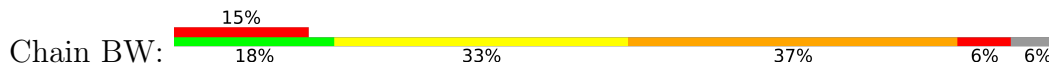
• Molecule 51: 50S ribosomal protein L28



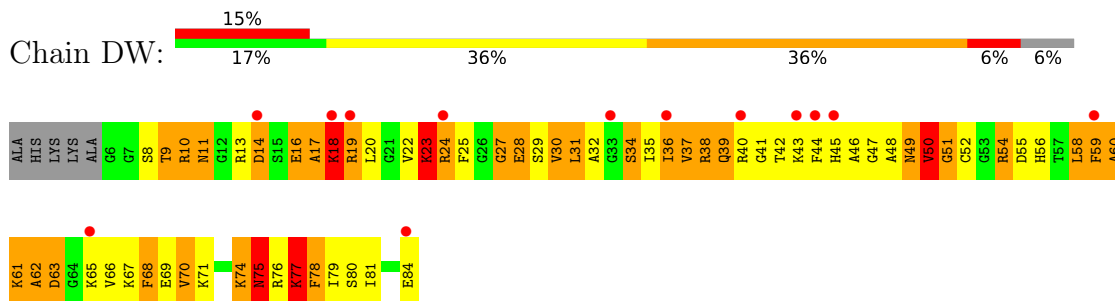
• Molecule 51: 50S ribosomal protein L28



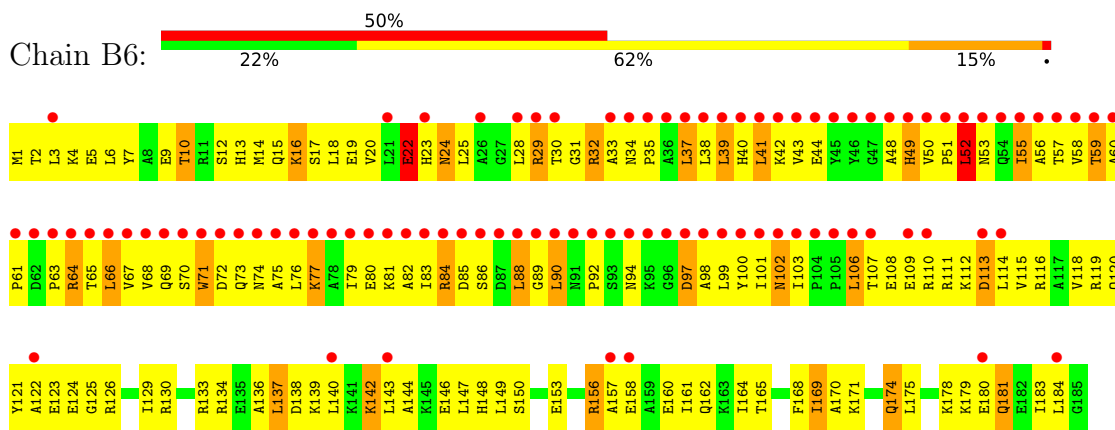
• Molecule 52: 50S ribosomal protein L27



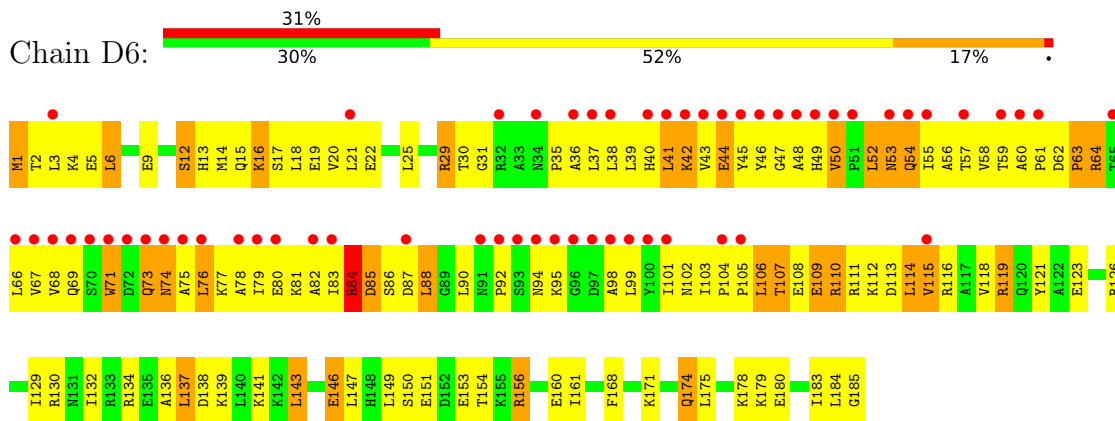
● Molecule 52: 50S ribosomal protein L27



● Molecule 53: ribosome recycling factor



● Molecule 53: ribosome recycling factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.90Å 378.20Å 736.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 82.86 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.00-3.30) 87.2 (82.86-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.304 0.248 , 0.273	Depositor DCC
R_{free} test set	35399 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtrriage
Anisotropy	0.393	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	286960	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% 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 i

5.1 Standard geometry i

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

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	0.26	0/36762	0.75	11/57350 (0.0%)
1	CA	0.26	0/36762	0.75	18/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.45	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.44	0/1043
13	CN	0.24	0/785	0.44	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.45	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.24	0/666	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.23	0/671	0.40	0/888
19	CT	0.23	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.25	0/2803	0.74	1/4371 (0.0%)
22	DA	0.25	0/2803	0.74	1/4371 (0.0%)
23	BB	0.28	6/68314 (0.0%)	0.77	55/106569 (0.1%)
23	DB	0.28	8/68314 (0.0%)	0.78	51/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.25	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.50	0/605
30	DY	0.23	0/453	0.50	0/605
31	B0	0.22	0/450	0.56	0/599
31	D0	0.22	0/450	0.56	0/599
32	B4	0.23	0/303	0.47	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.48	0/498
36	D2	0.26	0/380	0.48	0/498
37	BL	0.23	0/1054	0.49	0/1403
37	DL	0.23	0/1054	0.49	0/1403
38	BM	0.25	0/1093	0.49	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.49	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.25	0/960	0.49	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.47	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.48	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.49	0/1107
49	DR	0.25	0/829	0.49	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.23	0/744	0.55	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.52	0/797
52	DW	0.28	0/603	0.52	0/797
53	B6	0.24	0/1497	0.48	0/2017
53	D6	0.23	0/1497	0.48	0/2017
All	All	0.26	14/309354 (0.0%)	0.70	137/462003 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	14
1	CA	0	13
23	BB	0	29

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	29
All	All	0	85

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.41	1.26	1.41
23	DB	1086	A	C5-C6	-16.29	1.26	1.41
23	DB	1088	A	C6-N1	-10.64	1.28	1.35
23	BB	1088	A	C6-N1	-10.54	1.28	1.35
23	DB	1060	U	C2-N3	7.91	1.43	1.37

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.30	75.55	110.70
23	BB	2204	G	O5'-P-OP2	-27.99	77.11	110.70
23	BB	2791	G	O5'-P-OP1	-27.68	77.49	110.70
23	DB	2791	G	O5'-P-OP2	-27.63	77.54	110.70
23	DB	2791	G	O5'-P-OP1	18.08	132.40	110.70

There are no chirality outliers.

5 of 85 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	81	A	Sidechain

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	32831	0	16521	1174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32831	0	16521	1151	0
2	AC	1624	0	1699	141	0
2	CC	1624	0	1699	138	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	155	0
4	AE	1105	0	1148	107	0
4	CE	1105	0	1148	102	0
5	AF	817	0	808	85	0
5	CF	817	0	808	82	0
6	AG	1174	0	1230	102	0
6	CG	1196	0	1246	91	0
7	AH	979	0	1034	62	0
7	CH	979	0	1034	62	0
8	AI	1022	0	1070	123	0
8	CI	1022	0	1070	126	0
9	AJ	786	0	828	76	0
9	CJ	786	0	828	76	0
10	AK	877	0	887	84	0
10	CK	877	0	887	73	0
11	AL	955	0	1019	85	0
11	CL	955	0	1019	92	0
12	AM	883	0	944	104	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	95	0
14	AO	714	0	734	46	0
14	CO	714	0	734	51	0
15	AP	649	0	666	60	0
15	CP	638	0	656	60	0
16	AQ	648	0	691	64	0
16	CQ	657	0	702	65	0
17	AR	455	0	478	36	0
17	CR	455	0	478	37	0
18	AS	637	0	665	89	0
18	CS	644	0	675	91	0
19	AT	665	0	714	45	0
19	CT	665	0	714	44	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	198	0
21	AU	425	0	449	69	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	83	0
23	BB	60995	0	30679	2163	0
23	DB	60995	0	30677	2184	0
24	BI	1032	0	1088	112	0
24	DI	1032	0	1088	183	0
25	BC	2082	0	2157	232	0
25	DC	2082	0	2157	232	0
26	BD	1565	0	1616	186	0
26	DD	1565	0	1616	184	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	113	0
28	BP	917	0	965	136	0
28	DP	917	0	965	145	0
29	BE	1552	0	1619	188	0
29	DE	1552	0	1619	191	0
30	BY	449	0	491	52	0
30	DY	449	0	491	52	0
31	B0	444	0	461	39	0
31	D0	444	0	461	31	0
32	B4	302	0	340	50	0
32	D4	302	0	340	53	0
33	B1	409	0	440	51	0
33	D1	409	0	440	43	0
34	B3	504	0	574	54	0
34	D3	504	0	574	57	0
35	BV	753	0	780	86	0
35	DV	753	0	780	84	0
36	B2	377	0	418	34	0
36	D2	377	0	418	32	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	120	0
38	DM	1074	0	1157	118	0
39	BX	509	0	543	56	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	220	0
40	DH	1111	0	1148	161	0
41	BJ	1129	0	1162	156	0
41	DJ	1129	0	1162	161	0
42	BN	960	0	1000	111	0
42	DN	960	0	1000	108	0
43	BO	892	0	923	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	81	0
44	BQ	947	0	1022	125	0
44	DQ	947	0	1022	136	0
45	BS	857	0	922	94	0
45	DS	857	0	922	93	0
46	BU	779	0	834	111	0
46	DU	779	0	834	111	0
47	BF	1420	0	1460	242	0
47	DF	1420	0	1460	233	0
48	BG	1323	0	1374	158	0
48	DG	1323	0	1374	159	0
49	BR	816	0	839	85	0
49	DR	816	0	839	96	0
50	BT	738	0	807	120	0
50	DT	738	0	807	115	0
51	BZ	625	0	652	63	0
51	DZ	625	0	652	61	0
52	BW	596	0	610	138	0
52	DW	596	0	610	152	0
53	B6	1478	0	1526	204	0
53	D6	1478	0	1526	177	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	289	0	0	1	0
56	AE	4	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	3	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	B2	1	0	0	0	0
56	BB	495	0	0	5	0
56	BC	4	0	0	0	0
56	BD	1	0	0	0	0
56	BE	3	0	0	0	0
56	BL	1	0	0	0	0
56	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CA	300	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	1	0	0	0	0
56	CN	4	0	0	0	0
56	CT	1	0	0	0	0
56	DB	505	0	0	7	0
56	DC	4	0	0	1	0
56	DD	1	0	0	0	0
56	DE	2	0	0	0	0
All	All	286960	0	193714	16198	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 34.

The worst 5 of 16198 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)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.39	1.17
13:CN:63:CYS:HB3	13:CN:67:GLY:H	1.09	1.16
13:AN:63:CYS:HB3	13:AN:67:GLY:H	1.05	1.15
10:AK:124:LYS:HA	21:AU:34:ARG:HB3	1.27	1.14
29:DE:21:ARG:HD2	29:DE:107:SER:HB3	1.30	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	152 (74%)	36 (18%)	16 (8%)	1 6
2	CC	204/232 (88%)	151 (74%)	37 (18%)	16 (8%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	1	9
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	1	10
4	AE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	7	32
4	CE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	7	32
5	AF	98/135 (73%)	71 (72%)	18 (18%)	9 (9%)	1	4
5	CF	98/135 (73%)	69 (70%)	21 (21%)	8 (8%)	1	5
6	AG	148/178 (83%)	114 (77%)	28 (19%)	6 (4%)	3	17
6	CG	150/178 (84%)	118 (79%)	25 (17%)	7 (5%)	2	14
7	AH	127/129 (98%)	106 (84%)	17 (13%)	4 (3%)	4	23
7	CH	127/129 (98%)	105 (83%)	18 (14%)	4 (3%)	4	23
8	AI	125/129 (97%)	92 (74%)	28 (22%)	5 (4%)	3	18
8	CI	125/129 (97%)	93 (74%)	28 (22%)	4 (3%)	4	22
9	AJ	96/103 (93%)	73 (76%)	13 (14%)	10 (10%)	0	3
9	CJ	96/103 (93%)	74 (77%)	12 (12%)	10 (10%)	0	3
10	AK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	2	16
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	13
11	AL	121/123 (98%)	84 (69%)	28 (23%)	9 (7%)	1	7
11	CL	121/123 (98%)	86 (71%)	25 (21%)	10 (8%)	1	5
12	AM	112/117 (96%)	85 (76%)	16 (14%)	11 (10%)	0	3
12	CM	111/117 (95%)	83 (75%)	17 (15%)	11 (10%)	0	3
13	AN	92/100 (92%)	65 (71%)	19 (21%)	8 (9%)	1	5
13	CN	92/100 (92%)	66 (72%)	18 (20%)	8 (9%)	1	5
14	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	3	21
14	CO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	6	29
15	AP	80/82 (98%)	62 (78%)	10 (12%)	8 (10%)	0	3
15	CP	78/82 (95%)	61 (78%)	11 (14%)	6 (8%)	1	6
16	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	2	13
16	CQ	79/83 (95%)	60 (76%)	15 (19%)	4 (5%)	2	13
17	AR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
17	CR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
18	AS	77/91 (85%)	59 (77%)	12 (16%)	6 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	6
19	AT	83/86 (96%)	64 (77%)	15 (18%)	4 (5%)	2	14
19	CT	83/86 (96%)	65 (78%)	14 (17%)	4 (5%)	2	14
20	AB	216/240 (90%)	153 (71%)	48 (22%)	15 (7%)	1	8
20	CB	216/240 (90%)	150 (69%)	49 (23%)	17 (8%)	1	6
21	AU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
21	CU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	20
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	4	24
25	BC	269/272 (99%)	176 (65%)	61 (23%)	32 (12%)	0	2
25	DC	269/272 (99%)	177 (66%)	59 (22%)	33 (12%)	0	1
26	BD	207/209 (99%)	123 (59%)	56 (27%)	28 (14%)	0	1
26	DD	207/209 (99%)	122 (59%)	55 (27%)	30 (14%)	0	1
27	BK	119/123 (97%)	80 (67%)	25 (21%)	14 (12%)	0	2
27	DK	119/123 (97%)	81 (68%)	24 (20%)	14 (12%)	0	2
28	BP	112/114 (98%)	68 (61%)	29 (26%)	15 (13%)	0	1
28	DP	112/114 (98%)	69 (62%)	28 (25%)	15 (13%)	0	1
29	BE	199/201 (99%)	126 (63%)	54 (27%)	19 (10%)	0	4
29	DE	199/201 (99%)	127 (64%)	52 (26%)	20 (10%)	0	3
30	BY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	3
30	DY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	3
31	B0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
31	D0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
32	B4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
32	D4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	6 (12%)	5 (10%)	0	3
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	3
34	B3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	3
34	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	3
35	BV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	4	22
35	DV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	6	29
36	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	2	15
37	BL	141/144 (98%)	92 (65%)	31 (22%)	18 (13%)	0	1
37	DL	141/144 (98%)	94 (67%)	28 (20%)	19 (14%)	0	1
38	BM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
38	DM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
39	BX	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	8
39	DX	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	8
40	BH	147/149 (99%)	74 (50%)	50 (34%)	23 (16%)	0	1
40	DH	147/149 (99%)	92 (63%)	38 (26%)	17 (12%)	0	2
41	BJ	140/142 (99%)	96 (69%)	31 (22%)	13 (9%)	0	4
41	DJ	140/142 (99%)	95 (68%)	32 (23%)	13 (9%)	0	4
42	BN	118/127 (93%)	84 (71%)	25 (21%)	9 (8%)	1	6
42	DN	118/127 (93%)	82 (70%)	25 (21%)	11 (9%)	0	4
43	BO	114/117 (97%)	87 (76%)	21 (18%)	6 (5%)	2	12
43	DO	114/117 (97%)	86 (75%)	21 (18%)	7 (6%)	1	10
44	BQ	115/117 (98%)	81 (70%)	21 (18%)	13 (11%)	0	2
44	DQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	3
45	BS	108/110 (98%)	72 (67%)	21 (19%)	15 (14%)	0	1
45	DS	108/110 (98%)	73 (68%)	20 (18%)	15 (14%)	0	1
46	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
46	DU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
47	BF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
47	DF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
48	BG	174/176 (99%)	108 (62%)	41 (24%)	25 (14%)	0	1
48	DG	174/176 (99%)	109 (63%)	39 (22%)	26 (15%)	0	1
49	BR	101/103 (98%)	74 (73%)	16 (16%)	11 (11%)	0	2
49	DR	101/103 (98%)	73 (72%)	17 (17%)	11 (11%)	0	2
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	1
50	DT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
51	BZ	75/78 (96%)	50 (67%)	16 (21%)	9 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	3
52	BW	77/84 (92%)	32 (42%)	20 (26%)	25 (32%)	0	0
52	DW	77/84 (92%)	33 (43%)	18 (23%)	26 (34%)	0	0
53	B6	183/185 (99%)	140 (76%)	36 (20%)	7 (4%)	3	19
53	D6	183/185 (99%)	146 (80%)	28 (15%)	9 (5%)	2	14
All	All	11607/12284 (94%)	8146 (70%)	2335 (20%)	1126 (10%)	0	3

5 of 1126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	100	ILE
2	AC	104	GLU

5.3.2 Protein sidechains [i](#)

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	AC	170/189 (90%)	145 (85%)	25 (15%)	3	14
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	14
3	AD	172/172 (100%)	138 (80%)	34 (20%)	1	5
3	CD	172/172 (100%)	138 (80%)	34 (20%)	1	5
4	AE	113/125 (90%)	99 (88%)	14 (12%)	4	19
4	CE	113/125 (90%)	99 (88%)	14 (12%)	4	19
5	AF	87/116 (75%)	70 (80%)	17 (20%)	1	5
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1	5
6	AG	123/146 (84%)	101 (82%)	22 (18%)	2	8
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2	8
7	AH	104/104 (100%)	95 (91%)	9 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CH	104/104 (100%)	96 (92%)	8 (8%)	13	38
8	AI	105/106 (99%)	86 (82%)	19 (18%)	1	7
8	CI	105/106 (99%)	86 (82%)	19 (18%)	1	7
9	AJ	86/90 (96%)	75 (87%)	11 (13%)	4	18
9	CJ	86/90 (96%)	76 (88%)	10 (12%)	5	22
10	AK	90/98 (92%)	74 (82%)	16 (18%)	2	8
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	8
11	AL	103/103 (100%)	87 (84%)	16 (16%)	2	12
11	CL	103/103 (100%)	87 (84%)	16 (16%)	2	12
12	AM	92/95 (97%)	71 (77%)	21 (23%)	1	3
12	CM	91/95 (96%)	69 (76%)	22 (24%)	0	2
13	AN	79/83 (95%)	71 (90%)	8 (10%)	7	27
13	CN	79/83 (95%)	71 (90%)	8 (10%)	7	27
14	AO	76/77 (99%)	70 (92%)	6 (8%)	12	37
14	CO	76/77 (99%)	70 (92%)	6 (8%)	12	37
15	AP	65/65 (100%)	57 (88%)	8 (12%)	4	20
15	CP	65/65 (100%)	56 (86%)	9 (14%)	3	16
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	1	5
16	CQ	75/77 (97%)	60 (80%)	15 (20%)	1	5
17	AR	48/64 (75%)	43 (90%)	5 (10%)	7	25
17	CR	48/64 (75%)	43 (90%)	5 (10%)	7	25
18	AS	70/78 (90%)	53 (76%)	17 (24%)	0	2
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	3
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	9
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2	9
20	AB	180/198 (91%)	145 (81%)	35 (19%)	1	5
20	CB	180/198 (91%)	144 (80%)	36 (20%)	1	5
21	AU	44/60 (73%)	28 (64%)	16 (36%)	0	0
21	CU	44/60 (73%)	27 (61%)	17 (39%)	0	0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59	78
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BC	216/217 (100%)	186 (86%)	30 (14%)	3	16
25	DC	216/217 (100%)	187 (87%)	29 (13%)	4	16
26	BD	164/164 (100%)	146 (89%)	18 (11%)	6	24
26	DD	164/164 (100%)	148 (90%)	16 (10%)	8	29
27	BK	102/104 (98%)	84 (82%)	18 (18%)	2	8
27	DK	102/104 (98%)	84 (82%)	18 (18%)	2	8
28	BP	99/99 (100%)	78 (79%)	21 (21%)	1	4
28	DP	99/99 (100%)	78 (79%)	21 (21%)	1	4
29	BE	165/165 (100%)	136 (82%)	29 (18%)	2	8
29	DE	165/165 (100%)	137 (83%)	28 (17%)	2	9
30	BY	48/48 (100%)	41 (85%)	7 (15%)	3	14
30	DY	48/48 (100%)	41 (85%)	7 (15%)	3	14
31	B0	47/47 (100%)	37 (79%)	10 (21%)	1	4
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	4
32	B4	34/34 (100%)	26 (76%)	8 (24%)	1	3
32	D4	34/34 (100%)	26 (76%)	8 (24%)	1	3
33	B1	45/48 (94%)	39 (87%)	6 (13%)	4	17
33	D1	45/48 (94%)	39 (87%)	6 (13%)	4	17
34	B3	51/51 (100%)	47 (92%)	4 (8%)	12	38
34	D3	51/51 (100%)	47 (92%)	4 (8%)	12	38
35	BV	78/78 (100%)	59 (76%)	19 (24%)	0	2
35	DV	78/78 (100%)	59 (76%)	19 (24%)	0	2
36	B2	38/38 (100%)	32 (84%)	6 (16%)	2	11
36	D2	38/38 (100%)	32 (84%)	6 (16%)	2	11
37	BL	102/103 (99%)	92 (90%)	10 (10%)	8	29
37	DL	102/103 (99%)	92 (90%)	10 (10%)	8	29
38	BM	109/109 (100%)	90 (83%)	19 (17%)	2	8
38	DM	109/109 (100%)	90 (83%)	19 (17%)	2	8
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	4
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	4
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DH	114/114 (100%)	82 (72%)	32 (28%)	0	1
41	BJ	116/116 (100%)	96 (83%)	20 (17%)	2	9
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	12
42	BN	100/103 (97%)	84 (84%)	16 (16%)	2	11
42	DN	100/103 (97%)	84 (84%)	16 (16%)	2	11
43	BO	86/87 (99%)	74 (86%)	12 (14%)	3	16
43	DO	86/87 (99%)	72 (84%)	14 (16%)	2	10
44	BQ	89/89 (100%)	78 (88%)	11 (12%)	4	19
44	DQ	89/89 (100%)	78 (88%)	11 (12%)	4	19
45	BS	93/93 (100%)	82 (88%)	11 (12%)	5	21
45	DS	93/93 (100%)	82 (88%)	11 (12%)	5	21
46	BU	83/84 (99%)	71 (86%)	12 (14%)	3	14
46	DU	83/84 (99%)	70 (84%)	13 (16%)	2	12
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	3
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	3
48	BG	137/137 (100%)	106 (77%)	31 (23%)	1	3
48	DG	137/137 (100%)	105 (77%)	32 (23%)	1	3
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	12
49	DR	84/84 (100%)	71 (84%)	13 (16%)	2	12
50	BT	80/84 (95%)	59 (74%)	21 (26%)	0	2
50	DT	80/84 (95%)	59 (74%)	21 (26%)	0	2
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	3
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	3
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	1
52	DW	59/62 (95%)	43 (73%)	16 (27%)	0	1
53	B6	157/157 (100%)	126 (80%)	31 (20%)	1	5
53	D6	157/157 (100%)	121 (77%)	36 (23%)	1	3
All	All	9647/10014 (96%)	7996 (83%)	1651 (17%)	2	9

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	83	THR

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Mol	Chain	Res	Type
21	CU	38	GLU
52	DW	10	ARG
8	CI	61	ASP
6	CG	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 342 such sidechains are listed below:

Mol	Chain	Res	Type
20	CB	88	GLN
38	DM	60	GLN
24	DI	33	ASN
28	DP	114	ASN
42	DN	73	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	248 (16%)	28 (1%)
1	CA	1529/1542 (99%)	239 (15%)	25 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	19 (16%)	0
23	BB	2837/2904 (97%)	448 (15%)	20 (0%)
23	DB	2837/2904 (97%)	432 (15%)	19 (0%)
All	All	8964/9132 (98%)	1404 (15%)	92 (1%)

5 of 1404 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	429	U
1	CA	1397	C
1	CA	484	G

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Mol	Chain	Res	Type
1	CA	1065	U
23	DB	162	U

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 345 ligands modelled in this entry, 345 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	1530/1542 (99%)	-0.10	22 (1%) 75 75	20, 68, 149, 180	0
1	CA	1530/1542 (99%)	-0.20	9 (0%) 89 90	10, 51, 126, 180	0
2	AC	206/232 (88%)	0.45	8 (3%) 39 37	24, 58, 114, 180	0
2	CC	206/232 (88%)	0.36	5 (2%) 59 56	28, 67, 117, 175	0
3	AD	205/205 (100%)	0.51	12 (5%) 22 22	22, 77, 137, 154	0
3	CD	205/205 (100%)	0.19	3 (1%) 73 72	15, 53, 129, 160	0
4	AE	150/166 (90%)	0.41	9 (6%) 21 21	16, 62, 116, 154	0
4	CE	150/166 (90%)	0.40	6 (4%) 38 36	20, 50, 105, 159	0
5	AF	100/135 (74%)	0.58	10 (10%) 7 7	33, 73, 126, 163	0
5	CF	100/135 (74%)	0.24	1 (1%) 82 82	20, 63, 115, 146	0
6	AG	150/178 (84%)	0.76	25 (16%) 1 1	40, 87, 140, 168	0
6	CG	152/178 (85%)	0.74	20 (13%) 3 3	21, 80, 132, 169	0
7	AH	129/129 (100%)	0.90	22 (17%) 1 1	34, 71, 116, 137	0
7	CH	129/129 (100%)	0.46	8 (6%) 20 20	18, 50, 96, 131	0
8	AI	127/129 (98%)	1.01	27 (21%) 0 1	23, 81, 151, 180	0
8	CI	127/129 (98%)	0.73	15 (11%) 4 4	26, 82, 135, 180	0
9	AJ	98/103 (95%)	1.13	18 (18%) 1 1	21, 74, 134, 180	0
9	CJ	98/103 (95%)	1.30	25 (25%) 0 0	34, 83, 136, 163	0
10	AK	117/128 (91%)	0.39	7 (5%) 21 21	19, 57, 100, 155	0
10	CK	117/128 (91%)	0.20	2 (1%) 70 68	18, 48, 100, 142	0
11	AL	123/123 (100%)	0.92	14 (11%) 5 4	29, 68, 124, 169	0
11	CL	123/123 (100%)	0.46	4 (3%) 46 44	10, 44, 107, 159	0
12	AM	114/117 (97%)	1.10	23 (20%) 1 1	48, 105, 157, 171	0
12	CM	113/117 (96%)	0.86	16 (14%) 2 2	44, 98, 149, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.93	15 (15%) 2 2	31, 77, 136, 171	0
13	CN	96/100 (96%)	0.82	10 (10%) 6 6	31, 78, 137, 161	0
14	AO	88/89 (98%)	0.35	2 (2%) 60 59	33, 67, 119, 173	0
14	CO	88/89 (98%)	0.05	0 100 100	18, 53, 105, 133	0
15	AP	82/82 (100%)	1.16	13 (15%) 1 2	38, 78, 140, 157	0
15	CP	80/82 (97%)	1.29	18 (22%) 0 1	16, 44, 124, 180	0
16	AQ	80/83 (96%)	0.78	6 (7%) 14 13	47, 86, 139, 155	0
16	CQ	81/83 (97%)	0.63	6 (7%) 14 14	25, 56, 117, 151	0
17	AR	55/74 (74%)	0.78	4 (7%) 15 15	27, 66, 125, 149	0
17	CR	55/74 (74%)	0.57	3 (5%) 25 23	24, 51, 105, 154	0
18	AS	79/91 (86%)	1.98	37 (46%) 0 0	61, 116, 158, 179	0
18	CS	80/91 (87%)	1.96	36 (45%) 0 0	54, 107, 165, 177	0
19	AT	85/86 (98%)	1.22	18 (21%) 0 1	52, 92, 133, 180	0
19	CT	85/86 (98%)	0.77	10 (11%) 4 4	24, 52, 103, 156	0
20	AB	218/240 (90%)	0.83	32 (14%) 2 2	29, 88, 139, 180	0
20	CB	218/240 (90%)	0.75	34 (15%) 2 2	40, 92, 143, 161	0
21	AU	51/70 (72%)	0.98	8 (15%) 2 2	36, 90, 150, 153	0
21	CU	51/70 (72%)	0.97	10 (19%) 1 1	26, 74, 136, 174	0
22	BA	117/120 (97%)	-0.26	3 (2%) 56 53	46, 80, 115, 168	0
22	DA	117/120 (97%)	-0.10	4 (3%) 45 43	35, 69, 110, 178	0
23	BB	2841/2904 (97%)	-0.04	51 (1%) 68 67	16, 56, 145, 180	0
23	DB	2841/2904 (97%)	-0.07	35 (1%) 79 78	7, 44, 142, 180	0
24	BI	141/141 (100%)	2.92	90 (63%) 0 0	62, 152, 180, 180	0
24	DI	141/141 (100%)	3.47	98 (69%) 0 0	85, 155, 180, 180	0
25	BC	271/272 (99%)	0.43	3 (1%) 80 81	9, 45, 87, 170	0
25	DC	271/272 (99%)	0.37	5 (1%) 68 67	5, 37, 75, 125	0
26	BD	209/209 (100%)	0.62	16 (7%) 13 12	22, 66, 124, 167	0
26	DD	209/209 (100%)	0.49	14 (6%) 17 17	10, 44, 112, 139	0
27	BK	121/123 (98%)	0.84	14 (11%) 4 4	16, 67, 120, 154	0
27	DK	121/123 (98%)	0.35	2 (1%) 70 68	8, 39, 93, 152	0
28	BP	114/114 (100%)	1.17	32 (28%) 0 0	27, 77, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.43	5 (4%) 34 33	5, 42, 104, 160	0
29	BE	201/201 (100%)	0.64	19 (9%) 8 8	16, 67, 132, 148	0
29	DE	201/201 (100%)	0.56	22 (10%) 5 5	5, 65, 124, 156	0
30	BY	58/58 (100%)	0.78	7 (12%) 4 3	42, 73, 129, 143	0
30	DY	58/58 (100%)	0.58	3 (5%) 27 25	9, 58, 127, 150	0
31	B0	56/56 (100%)	0.61	6 (10%) 6 5	33, 71, 126, 141	0
31	D0	56/56 (100%)	0.53	3 (5%) 25 24	11, 45, 122, 170	0
32	B4	38/38 (100%)	1.04	7 (18%) 1 1	23, 75, 134, 149	0
32	D4	38/38 (100%)	0.82	4 (10%) 6 6	29, 54, 106, 125	0
33	B1	50/54 (92%)	0.97	6 (12%) 4 3	43, 79, 117, 132	0
33	D1	50/54 (92%)	0.82	4 (8%) 12 11	34, 66, 111, 135	0
34	B3	64/64 (100%)	0.73	8 (12%) 3 3	31, 51, 91, 115	0
34	D3	64/64 (100%)	0.47	1 (1%) 72 70	20, 40, 75, 110	0
35	BV	94/94 (100%)	0.72	7 (7%) 14 14	32, 90, 135, 169	0
35	DV	94/94 (100%)	0.52	7 (7%) 14 14	28, 74, 131, 167	0
36	B2	46/46 (100%)	0.52	1 (2%) 62 60	13, 40, 87, 121	0
36	D2	46/46 (100%)	0.28	0 100 100	10, 32, 67, 131	0
37	BL	143/144 (99%)	0.58	8 (5%) 24 23	13, 64, 117, 161	0
37	DL	143/144 (99%)	0.41	5 (3%) 44 42	13, 54, 108, 133	0
38	BM	136/136 (100%)	0.88	22 (16%) 1 2	24, 68, 124, 174	0
38	DM	136/136 (100%)	0.57	7 (5%) 28 26	13, 46, 109, 131	0
39	BX	63/63 (100%)	0.74	7 (11%) 5 5	20, 86, 141, 171	0
39	DX	63/63 (100%)	0.48	4 (6%) 20 20	38, 84, 134, 172	0
40	BH	149/149 (100%)	1.73	50 (33%) 0 0	37, 121, 160, 180	0
40	DH	149/149 (100%)	1.42	42 (28%) 0 0	20, 108, 147, 180	0
41	BJ	142/142 (100%)	0.76	13 (9%) 9 9	25, 73, 126, 137	0
41	DJ	142/142 (100%)	0.68	13 (9%) 9 9	19, 55, 104, 167	0
42	BN	120/127 (94%)	0.45	7 (5%) 23 22	20, 65, 117, 173	0
42	DN	120/127 (94%)	0.42	4 (3%) 46 44	8, 40, 80, 125	0
43	BO	116/117 (99%)	1.40	35 (30%) 0 0	27, 82, 128, 179	0
43	DO	116/117 (99%)	0.87	14 (12%) 4 3	19, 68, 119, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.53	7 (5%) 21 21	5, 64, 111, 163	0
44	DQ	117/117 (100%)	0.42	8 (6%) 17 17	14, 48, 96, 180	0
45	BS	110/110 (100%)	0.62	9 (8%) 11 11	15, 58, 112, 161	0
45	DS	110/110 (100%)	0.56	3 (2%) 54 52	8, 42, 101, 132	0
46	BU	102/103 (99%)	1.08	20 (19%) 1 1	26, 75, 130, 171	0
46	DU	102/103 (99%)	0.99	16 (15%) 2 2	26, 83, 143, 180	0
47	BF	178/178 (100%)	1.30	44 (24%) 0 0	42, 113, 160, 180	0
47	DF	178/178 (100%)	1.06	34 (19%) 1 1	38, 97, 155, 180	0
48	BG	176/176 (100%)	1.13	42 (23%) 0 0	51, 103, 141, 162	0
48	DG	176/176 (100%)	0.87	28 (15%) 1 2	34, 91, 142, 169	0
49	BR	103/103 (100%)	1.43	27 (26%) 0 0	27, 86, 128, 157	0
49	DR	103/103 (100%)	0.71	9 (8%) 10 10	18, 76, 122, 148	0
50	BT	93/100 (93%)	1.24	24 (25%) 0 0	31, 70, 134, 164	0
50	DT	93/100 (93%)	1.25	21 (22%) 0 1	21, 66, 136, 173	0
51	BZ	77/78 (98%)	0.68	2 (2%) 56 53	22, 50, 93, 129	0
51	DZ	77/78 (98%)	0.38	5 (6%) 18 18	17, 46, 95, 130	0
52	BW	79/84 (94%)	1.05	13 (16%) 1 2	29, 81, 126, 153	0
52	DW	79/84 (94%)	1.14	13 (16%) 1 2	20, 59, 119, 135	0
53	B6	185/185 (100%)	2.71	93 (50%) 0 0	33, 116, 167, 180	0
53	D6	185/185 (100%)	1.65	58 (31%) 0 0	19, 88, 157, 180	0
All	All	20787/21416 (97%)	0.44	1757 (8%) 10 10	5, 63, 142, 180	0

The worst 5 of 1757 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	81	ALA	13.1
53	D6	72	ASP	11.6
24	BI	1	ALA	11.3
24	DI	85	ILE	10.8
24	DI	99	LYS	10.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
54	MG	BB	3093	1/1	0.21	0.64	38,38,38,38	1
54	MG	DB	3059	1/1	0.39	0.15	65,65,65,65	1
54	MG	AA	2025	1/1	0.42	0.70	54,54,54,54	1
54	MG	DB	3060	1/1	0.48	0.10	89,89,89,89	0
54	MG	AA	2059	1/1	0.51	2.00	127,127,127,127	0
54	MG	BB	3100	1/1	0.51	0.58	75,75,75,75	1
54	MG	AA	2039	1/1	0.52	0.37	108,108,108,108	0
54	MG	DB	3052	1/1	0.55	0.35	114,114,114,114	0
54	MG	BB	3010	1/1	0.61	0.15	70,70,70,70	0
54	MG	BB	3081	1/1	0.62	0.23	35,35,35,35	0
54	MG	BB	3042	1/1	0.63	0.10	123,123,123,123	0
54	MG	BB	3097	1/1	0.65	0.13	101,101,101,101	0
54	MG	DB	3066	1/1	0.65	0.28	63,63,63,63	1
54	MG	BB	3037	1/1	0.68	0.10	23,23,23,23	0
54	MG	AA	2014	1/1	0.69	0.13	101,101,101,101	0
54	MG	DB	3030	1/1	0.69	0.35	47,47,47,47	0
54	MG	AA	2037	1/1	0.69	1.61	139,139,139,139	0
54	MG	BB	3046	1/1	0.70	0.17	69,69,69,69	0
55	ZN	B4	101	1/1	0.70	0.09	55,55,55,55	0
54	MG	AA	2023	1/1	0.71	0.30	32,32,32,32	1
54	MG	DB	3058	1/1	0.71	2.01	145,145,145,145	0
54	MG	AA	2043	1/1	0.71	0.11	42,42,42,42	0
54	MG	CA	1634	1/1	0.72	0.11	32,32,32,32	0
54	MG	BB	3008	1/1	0.72	0.24	93,93,93,93	0
54	MG	BB	3049	1/1	0.73	0.14	26,26,26,26	0
54	MG	AA	2026	1/1	0.75	0.16	5,5,5,5	1
54	MG	DB	3015	1/1	0.75	0.11	60,60,60,60	0
54	MG	CA	1623	1/1	0.75	0.18	101,101,101,101	0
54	MG	DB	3022	1/1	0.76	0.17	32,32,32,32	0
54	MG	BB	3090	1/1	0.76	0.18	78,78,78,78	0
54	MG	CA	1641	1/1	0.77	0.21	61,61,61,61	0
54	MG	CA	1615	1/1	0.77	0.14	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	2042	1/1	0.78	0.12	32,32,32,32	0
54	MG	DB	3064	1/1	0.78	0.15	37,37,37,37	0
54	MG	CA	1633	1/1	0.78	0.12	42,42,42,42	0
54	MG	CA	1654	1/1	0.78	0.15	52,52,52,52	0
54	MG	AA	2022	1/1	0.79	0.29	77,77,77,77	0
54	MG	AA	2053	1/1	0.79	0.17	46,46,46,46	0
54	MG	BB	3073	1/1	0.80	0.17	70,70,70,70	0
54	MG	CA	1619	1/1	0.80	0.10	51,51,51,51	0
54	MG	CA	1622	1/1	0.80	0.08	46,46,46,46	0
54	MG	DB	3085	1/1	0.81	0.12	5,5,5,5	0
54	MG	CA	1608	1/1	0.82	0.11	106,106,106,106	0
54	MG	BB	3079	1/1	0.82	0.12	63,63,63,63	0
54	MG	CA	1635	1/1	0.83	0.07	55,55,55,55	0
54	MG	BB	3094	1/1	0.83	0.09	21,21,21,21	0
54	MG	DB	3074	1/1	0.83	0.08	30,30,30,30	0
54	MG	AA	2002	1/1	0.83	0.14	85,85,85,85	0
54	MG	DB	3034	1/1	0.83	0.19	82,82,82,82	0
54	MG	BB	3031	1/1	0.84	0.11	46,46,46,46	0
54	MG	AA	2050	1/1	0.84	0.12	101,101,101,101	0
54	MG	AA	2008	1/1	0.84	0.16	94,94,94,94	0
54	MG	AA	2018	1/1	0.84	0.07	78,78,78,78	0
54	MG	BB	3047	1/1	0.84	0.11	70,70,70,70	0
54	MG	AA	2012	1/1	0.84	0.06	63,63,63,63	0
54	MG	CA	1648	1/1	0.84	0.15	47,47,47,47	0
54	MG	BB	3051	1/1	0.84	0.11	35,35,35,35	0
54	MG	DB	3013	1/1	0.84	0.22	47,47,47,47	0
54	MG	AA	2030	1/1	0.84	0.09	102,102,102,102	0
54	MG	DB	3100	1/1	0.84	0.11	17,17,17,17	0
54	MG	DB	3110	1/1	0.84	0.26	40,40,40,40	0
54	MG	BB	3017	1/1	0.84	0.15	59,59,59,59	0
54	MG	AA	2049	1/1	0.85	0.08	90,90,90,90	0
54	MG	AA	2019	1/1	0.85	0.13	120,120,120,120	0
54	MG	BB	3014	1/1	0.85	0.14	58,58,58,58	0
54	MG	AA	2032	1/1	0.85	0.43	64,64,64,64	0
54	MG	DB	3063	1/1	0.85	0.15	28,28,28,28	0
54	MG	AA	2045	1/1	0.85	0.07	63,63,63,63	0
54	MG	BB	3028	1/1	0.86	0.17	46,46,46,46	0
54	MG	AA	2047	1/1	0.86	0.48	126,126,126,126	0
54	MG	BB	3102	1/1	0.86	0.09	38,38,38,38	0
54	MG	BB	3053	1/1	0.86	0.07	61,61,61,61	0
54	MG	CA	1627	1/1	0.86	0.37	5,5,5,5	1
54	MG	CA	1652	1/1	0.86	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BB	3099	1/1	0.87	0.12	51,51,51,51	0
54	MG	DB	3048	1/1	0.87	0.11	41,41,41,41	0
54	MG	DB	3068	1/1	0.87	0.16	8,8,8,8	0
54	MG	BB	3044	1/1	0.87	0.14	70,70,70,70	0
54	MG	DB	3083	1/1	0.87	0.14	72,72,72,72	0
54	MG	BB	3054	1/1	0.87	0.10	57,57,57,57	0
54	MG	BB	3061	1/1	0.87	0.07	38,38,38,38	0
54	MG	DB	3025	1/1	0.87	0.13	28,28,28,28	0
54	MG	BB	3087	1/1	0.87	0.25	100,100,100,100	0
54	MG	CA	1660	1/1	0.88	0.08	96,96,96,96	0
54	MG	BB	3077	1/1	0.88	0.07	36,36,36,36	0
54	MG	DB	3045	1/1	0.88	0.08	61,61,61,61	0
54	MG	DB	3097	1/1	0.88	0.13	32,32,32,32	0
54	MG	BB	3104	1/1	0.88	0.14	20,20,20,20	0
54	MG	AA	2035	1/1	0.88	0.10	102,102,102,102	0
54	MG	CA	1611	1/1	0.88	0.11	81,81,81,81	0
54	MG	CA	1644	1/1	0.89	0.11	52,52,52,52	0
54	MG	CA	1616	1/1	0.89	0.09	42,42,42,42	0
54	MG	DB	3057	1/1	0.89	0.09	40,40,40,40	0
54	MG	AA	2046	1/1	0.89	0.09	46,46,46,46	0
54	MG	BB	3032	1/1	0.89	0.12	34,34,34,34	0
54	MG	BB	3033	1/1	0.89	0.19	94,94,94,94	0
54	MG	DB	3003	1/1	0.89	0.16	29,29,29,29	0
54	MG	BB	3016	1/1	0.89	0.18	34,34,34,34	0
54	MG	BB	3052	1/1	0.89	0.09	25,25,25,25	0
54	MG	BB	3038	1/1	0.89	0.10	98,98,98,98	0
54	MG	BB	3009	1/1	0.89	0.14	87,87,87,87	0
54	MG	DB	3029	1/1	0.89	0.15	67,67,67,67	0
54	MG	CA	1638	1/1	0.89	0.12	90,90,90,90	0
54	MG	DB	3032	1/1	0.89	0.12	33,33,33,33	0
54	MG	DB	3033	1/1	0.89	0.12	20,20,20,20	0
54	MG	AA	2044	1/1	0.89	0.09	47,47,47,47	0
54	MG	CA	1643	1/1	0.89	0.08	20,20,20,20	0
54	MG	AA	2006	1/1	0.90	0.06	71,71,71,71	0
54	MG	BB	3056	1/1	0.90	0.07	31,31,31,31	0
54	MG	DB	3055	1/1	0.90	0.12	17,17,17,17	0
54	MG	AA	2028	1/1	0.90	0.10	66,66,66,66	0
54	MG	BB	3068	1/1	0.90	0.12	43,43,43,43	0
54	MG	CA	1637	1/1	0.90	0.10	53,53,53,53	0
54	MG	BB	3070	1/1	0.90	0.10	35,35,35,35	0
54	MG	AA	2057	1/1	0.90	0.62	93,93,93,93	0
54	MG	BB	3110	1/1	0.90	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1658	1/1	0.91	0.19	33,33,33,33	0
54	MG	CA	1628	1/1	0.91	0.11	38,38,38,38	0
54	MG	AA	2060	1/1	0.91	0.05	75,75,75,75	0
54	MG	BB	3059	1/1	0.91	0.11	32,32,32,32	0
54	MG	CE	201	1/1	0.91	0.20	102,102,102,102	0
54	MG	DB	3017	1/1	0.91	0.13	18,18,18,18	0
54	MG	DB	3018	1/1	0.91	0.12	23,23,23,23	0
54	MG	BB	3007	1/1	0.91	0.11	74,74,74,74	0
54	MG	BB	3062	1/1	0.91	0.18	41,41,41,41	0
54	MG	BB	3063	1/1	0.91	0.14	52,52,52,52	0
54	MG	BB	3039	1/1	0.91	0.15	43,43,43,43	0
54	MG	AA	2027	1/1	0.91	0.21	62,62,62,62	0
54	MG	AA	2056	1/1	0.91	0.32	46,46,46,46	0
54	MG	DB	3090	1/1	0.91	0.07	49,49,49,49	0
54	MG	DB	3095	1/1	0.91	0.38	19,19,19,19	1
54	MG	BB	3076	1/1	0.91	0.07	43,43,43,43	0
54	MG	BB	3034	1/1	0.91	0.13	35,35,35,35	0
54	MG	CA	1657	1/1	0.91	0.12	62,62,62,62	0
54	MG	DB	3050	1/1	0.91	0.05	70,70,70,70	0
54	MG	BB	3003	1/1	0.92	0.11	47,47,47,47	0
54	MG	BB	3005	1/1	0.92	0.10	24,24,24,24	0
54	MG	CA	1624	1/1	0.92	0.10	22,22,22,22	0
54	MG	BB	3015	1/1	0.92	0.10	40,40,40,40	0
54	MG	AA	2058	1/1	0.92	0.06	88,88,88,88	0
54	MG	CA	1629	1/1	0.92	0.07	20,20,20,20	1
54	MG	AA	2051	1/1	0.92	0.11	80,80,80,80	0
54	MG	DB	3073	1/1	0.92	0.10	29,29,29,29	0
54	MG	CA	1659	1/1	0.92	0.11	64,64,64,64	0
54	MG	DB	3079	1/1	0.92	0.08	34,34,34,34	0
54	MG	BB	3025	1/1	0.92	0.13	49,49,49,49	0
54	MG	CA	1661	1/1	0.92	0.06	49,49,49,49	0
54	MG	AA	2031	1/1	0.92	0.09	51,51,51,51	0
54	MG	BB	3085	1/1	0.92	0.16	56,56,56,56	0
54	MG	DB	3054	1/1	0.92	0.08	25,25,25,25	0
54	MG	CA	1620	1/1	0.92	0.06	58,58,58,58	0
54	MG	DB	3108	1/1	0.92	0.11	11,11,11,11	0
54	MG	DB	3056	1/1	0.92	0.10	11,11,11,11	0
54	MG	CA	1621	1/1	0.92	0.41	110,110,110,110	0
54	MG	AA	2020	1/1	0.93	0.09	84,84,84,84	0
54	MG	BB	3078	1/1	0.93	0.10	47,47,47,47	0
54	MG	AA	2038	1/1	0.93	0.11	63,63,63,63	0
54	MG	DB	3062	1/1	0.93	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3024	1/1	0.93	0.13	30,30,30,30	0
54	MG	BB	3029	1/1	0.93	0.11	28,28,28,28	0
54	MG	BB	3084	1/1	0.93	0.14	38,38,38,38	0
54	MG	BB	3108	1/1	0.93	0.11	37,37,37,37	0
54	MG	CA	1626	1/1	0.93	0.30	42,42,42,42	1
54	MG	CA	1656	1/1	0.93	0.10	22,22,22,22	0
54	MG	DB	3077	1/1	0.93	0.17	51,51,51,51	0
54	MG	BB	3030	1/1	0.93	0.07	40,40,40,40	0
54	MG	DB	3080	1/1	0.93	0.15	29,29,29,29	0
54	MG	DB	3082	1/1	0.93	0.10	21,21,21,21	0
54	MG	DB	3037	1/1	0.93	0.16	45,45,45,45	0
54	MG	AA	2021	1/1	0.93	0.08	52,52,52,52	0
54	MG	BB	3089	1/1	0.93	0.08	38,38,38,38	0
54	MG	CA	1610	1/1	0.93	0.07	56,56,56,56	0
54	MG	AA	2011	1/1	0.93	0.08	45,45,45,45	0
54	MG	DB	3099	1/1	0.93	0.18	15,15,15,15	0
54	MG	BB	3024	1/1	0.93	0.10	47,47,47,47	0
54	MG	DB	3102	1/1	0.93	0.13	15,15,15,15	0
54	MG	DB	3006	1/1	0.93	0.15	26,26,26,26	0
54	MG	DB	3109	1/1	0.93	0.09	35,35,35,35	0
54	MG	CA	1636	1/1	0.93	0.12	63,63,63,63	0
54	MG	BB	3057	1/1	0.93	0.27	37,37,37,37	0
54	MG	DB	3051	1/1	0.94	0.17	25,25,25,25	0
54	MG	CA	1606	1/1	0.94	0.09	59,59,59,59	0
54	MG	AA	2034	1/1	0.94	0.11	40,40,40,40	0
54	MG	BB	3080	1/1	0.94	0.09	57,57,57,57	0
54	MG	AA	2024	1/1	0.94	0.08	61,61,61,61	0
54	MG	AA	2013	1/1	0.94	0.10	85,85,85,85	0
54	MG	BB	3002	1/1	0.94	0.11	12,12,12,12	0
54	MG	AA	2052	1/1	0.94	0.07	50,50,50,50	0
54	MG	BB	3018	1/1	0.94	0.14	45,45,45,45	0
54	MG	BB	3019	1/1	0.94	0.07	37,37,37,37	0
54	MG	BB	3092	1/1	0.94	0.05	51,51,51,51	0
54	MG	DB	3011	1/1	0.94	0.17	16,16,16,16	0
54	MG	DB	3012	1/1	0.94	0.18	23,23,23,23	0
54	MG	BB	3040	1/1	0.94	0.19	60,60,60,60	0
54	MG	AA	2015	1/1	0.94	0.13	86,86,86,86	0
54	MG	DB	3016	1/1	0.94	0.09	28,28,28,28	0
54	MG	BB	3095	1/1	0.94	0.07	25,25,25,25	0
54	MG	BB	3096	1/1	0.94	0.07	37,37,37,37	0
54	MG	BB	3006	1/1	0.94	0.08	28,28,28,28	0
54	MG	BB	3069	1/1	0.94	0.08	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BB	3045	1/1	0.94	0.05	41,41,41,41	0
54	MG	DB	3026	1/1	0.94	0.14	41,41,41,41	0
54	MG	DB	3088	1/1	0.94	0.12	28,28,28,28	0
54	MG	BB	3101	1/1	0.94	0.10	22,22,22,22	0
54	MG	DB	3091	1/1	0.94	0.12	29,29,29,29	0
54	MG	DB	3092	1/1	0.94	0.11	65,65,65,65	0
54	MG	BB	3072	1/1	0.94	0.10	44,44,44,44	0
54	MG	BB	3027	1/1	0.94	0.14	34,34,34,34	0
54	MG	BB	3106	1/1	0.94	0.10	36,36,36,36	0
54	MG	AA	2055	1/1	0.94	0.11	54,54,54,54	0
54	MG	AA	2016	1/1	0.94	0.10	50,50,50,50	0
54	MG	DB	3104	1/1	0.94	0.09	28,28,28,28	0
54	MG	DB	3106	1/1	0.94	0.10	9,9,9,9	0
54	MG	DB	3039	1/1	0.94	0.07	34,34,34,34	0
54	MG	AA	2041	1/1	0.94	0.04	40,40,40,40	0
54	MG	CA	1601	1/1	0.94	0.11	9,9,9,9	0
54	MG	CA	1605	1/1	0.94	0.13	38,38,38,38	0
54	MG	DB	3028	1/1	0.95	0.14	29,29,29,29	0
54	MG	BB	3055	1/1	0.95	0.18	41,41,41,41	0
54	MG	DB	3070	1/1	0.95	0.12	26,26,26,26	0
54	MG	CA	1603	1/1	0.95	0.10	29,29,29,29	0
54	MG	BB	3013	1/1	0.95	0.08	36,36,36,36	0
54	MG	AA	2017	1/1	0.95	0.29	75,75,75,75	0
54	MG	BB	3026	1/1	0.95	0.09	28,28,28,28	0
54	MG	CA	1609	1/1	0.95	0.11	56,56,56,56	0
54	MG	BB	3035	1/1	0.95	0.10	41,41,41,41	0
54	MG	DB	3004	1/1	0.95	0.15	17,17,17,17	0
54	MG	BB	3048	1/1	0.95	0.08	30,30,30,30	0
54	MG	DB	3049	1/1	0.95	0.11	26,26,26,26	0
54	MG	CA	1614	1/1	0.95	0.12	58,58,58,58	0
54	MG	AA	2005	1/1	0.95	0.07	36,36,36,36	0
54	MG	BB	3065	1/1	0.95	0.06	40,40,40,40	0
54	MG	DB	3094	1/1	0.95	0.09	39,39,39,39	0
54	MG	CA	1640	1/1	0.95	0.11	43,43,43,43	0
54	MG	DB	3096	1/1	0.95	0.16	30,30,30,30	0
54	MG	CA	1617	1/1	0.95	0.12	21,21,21,21	0
54	MG	BB	3050	1/1	0.95	0.11	28,28,28,28	0
54	MG	BB	3001	1/1	0.95	0.08	35,35,35,35	0
54	MG	DB	3020	1/1	0.95	0.20	14,14,14,14	0
54	MG	CA	1647	1/1	0.95	0.09	102,102,102,102	0
54	MG	DB	3023	1/1	0.95	0.09	33,33,33,33	0
54	MG	DB	3061	1/1	0.95	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	2010	1/1	0.95	0.07	36,36,36,36	0
54	MG	AA	2029	1/1	0.95	0.08	40,40,40,40	0
54	MG	BB	3004	1/1	0.95	0.09	52,52,52,52	0
54	MG	BB	3107	1/1	0.96	0.08	31,31,31,31	0
54	MG	BB	3075	1/1	0.96	0.14	37,37,37,37	0
54	MG	CA	1646	1/1	0.96	0.11	46,46,46,46	0
54	MG	DB	3065	1/1	0.96	0.09	12,12,12,12	0
54	MG	BB	3109	1/1	0.96	0.09	42,42,42,42	0
54	MG	BB	3064	1/1	0.96	0.10	31,31,31,31	0
54	MG	CA	1650	1/1	0.96	0.16	41,41,41,41	0
54	MG	DB	3071	1/1	0.96	0.13	57,57,57,57	0
54	MG	DB	3072	1/1	0.96	0.10	23,23,23,23	0
54	MG	CA	1651	1/1	0.96	0.07	50,50,50,50	0
54	MG	BB	3022	1/1	0.96	0.05	44,44,44,44	0
54	MG	BB	3067	1/1	0.96	0.09	45,45,45,45	0
54	MG	DB	3078	1/1	0.96	0.11	45,45,45,45	0
54	MG	BB	3011	1/1	0.96	0.09	30,30,30,30	0
54	MG	AA	2040	1/1	0.96	0.10	56,56,56,56	0
54	MG	AA	2054	1/1	0.96	0.05	49,49,49,49	0
54	MG	CA	1607	1/1	0.96	0.06	37,37,37,37	0
54	MG	DB	3084	1/1	0.96	0.20	34,34,34,34	0
54	MG	BB	3082	1/1	0.96	0.15	38,38,38,38	0
54	MG	DB	3042	1/1	0.96	0.11	45,45,45,45	0
54	MG	CA	1630	1/1	0.96	0.10	39,39,39,39	0
54	MG	DB	3046	1/1	0.96	0.06	22,22,22,22	0
54	MG	CA	1632	1/1	0.96	0.18	41,41,41,41	0
54	MG	DB	3093	1/1	0.96	0.12	6,6,6,6	0
54	MG	BB	3071	1/1	0.96	0.07	25,25,25,25	0
54	MG	DB	3005	1/1	0.96	0.05	56,56,56,56	0
54	MG	AA	2048	1/1	0.96	0.11	27,27,27,27	0
54	MG	DB	3008	1/1	0.96	0.14	33,33,33,33	0
54	MG	DB	3053	1/1	0.96	0.09	28,28,28,28	0
54	MG	BB	3021	1/1	0.96	0.12	43,43,43,43	0
54	MG	DB	3101	1/1	0.96	0.16	5,5,5,5	0
54	MG	CA	1612	1/1	0.96	0.08	46,46,46,46	0
54	MG	CA	1613	1/1	0.96	0.07	39,39,39,39	0
54	MG	BB	3103	1/1	0.96	0.09	20,20,20,20	0
54	MG	DB	3107	1/1	0.96	0.06	34,34,34,34	0
54	MG	BB	3088	1/1	0.96	0.09	75,75,75,75	0
54	MG	BB	3074	1/1	0.96	0.14	21,21,21,21	0
54	MG	CA	1642	1/1	0.96	0.04	63,63,63,63	0
54	MG	DB	3019	1/1	0.96	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BB	3036	1/1	0.97	0.08	39,39,39,39	0
54	MG	DB	3014	1/1	0.97	0.07	21,21,21,21	0
54	MG	BB	3105	1/1	0.97	0.16	65,65,65,65	0
54	MG	BB	3066	1/1	0.97	0.07	21,21,21,21	0
54	MG	BB	3091	1/1	0.97	0.11	31,31,31,31	0
54	MG	CA	1631	1/1	0.97	0.09	38,38,38,38	0
54	MG	CA	1653	1/1	0.97	0.04	55,55,55,55	0
54	MG	AA	2004	1/1	0.97	0.19	36,36,36,36	0
54	MG	DB	3086	1/1	0.97	0.19	26,26,26,26	0
54	MG	CA	1655	1/1	0.97	0.09	28,28,28,28	0
54	MG	DB	3089	1/1	0.97	0.21	50,50,50,50	0
54	MG	AA	2033	1/1	0.97	0.07	40,40,40,40	0
54	MG	BB	3020	1/1	0.97	0.12	20,20,20,20	0
54	MG	BB	3058	1/1	0.97	0.14	33,33,33,33	0
54	MG	CA	1618	1/1	0.97	0.07	18,18,18,18	0
54	MG	AA	2009	1/1	0.97	0.12	21,21,21,21	0
54	MG	BB	3083	1/1	0.97	0.10	30,30,30,30	0
54	MG	BB	3041	1/1	0.97	0.10	22,22,22,22	0
54	MG	DB	3031	1/1	0.97	0.09	17,17,17,17	0
54	MG	AA	2007	1/1	0.97	0.08	42,42,42,42	0
54	MG	BB	3086	1/1	0.97	0.20	45,45,45,45	0
54	MG	BB	3043	1/1	0.97	0.16	53,53,53,53	0
54	MG	DB	3067	1/1	0.97	0.09	18,18,18,18	0
54	MG	DB	3103	1/1	0.97	0.09	26,26,26,26	0
54	MG	CA	1625	1/1	0.97	0.10	19,19,19,19	0
54	MG	DB	3069	1/1	0.97	0.13	21,21,21,21	0
54	MG	DB	3038	1/1	0.97	0.15	26,26,26,26	0
54	MG	DB	3010	1/1	0.97	0.10	19,19,19,19	0
54	MG	CA	1645	1/1	0.97	0.09	45,45,45,45	0
54	MG	DB	3044	1/1	0.97	0.06	12,12,12,12	0
54	MG	DB	3111	1/1	0.97	0.19	51,51,51,51	0
54	MG	BB	3023	1/1	0.97	0.07	23,23,23,23	0
55	ZN	D4	101	1/1	0.97	0.07	55,55,55,55	0
54	MG	CA	1602	1/1	0.98	0.20	34,34,34,34	0
54	MG	BB	3098	1/1	0.98	0.13	30,30,30,30	0
54	MG	DB	3021	1/1	0.98	0.12	21,21,21,21	0
54	MG	DB	3001	1/1	0.98	0.11	9,9,9,9	0
54	MG	DB	3002	1/1	0.98	0.06	11,11,11,11	0
54	MG	DB	3035	1/1	0.98	0.11	57,57,57,57	0
54	MG	AA	2036	1/1	0.98	0.10	65,65,65,65	0
54	MG	DB	3087	1/1	0.98	0.11	54,54,54,54	0
54	MG	DB	3105	1/1	0.98	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1649	1/1	0.98	0.07	80,80,80,80	0
54	MG	AA	2001	1/1	0.98	0.07	29,29,29,29	0
54	MG	DB	3040	1/1	0.98	0.09	9,9,9,9	0
54	MG	DB	3041	1/1	0.98	0.13	36,36,36,36	0
54	MG	DB	3027	1/1	0.98	0.19	27,27,27,27	0
54	MG	DB	3043	1/1	0.98	0.10	8,8,8,8	0
54	MG	AA	2003	1/1	0.98	0.13	31,31,31,31	0
54	MG	BB	3012	1/1	0.98	0.09	32,32,32,32	0
54	MG	DB	3007	1/1	0.99	0.08	30,30,30,30	0
54	MG	CA	1604	1/1	0.99	0.10	36,36,36,36	0
54	MG	DB	3009	1/1	0.99	0.15	17,17,17,17	0
54	MG	DB	3075	1/1	0.99	0.06	33,33,33,33	0
54	MG	DB	3076	1/1	0.99	0.07	17,17,17,17	0
54	MG	DB	3047	1/1	0.99	0.15	13,13,13,13	0
54	MG	DB	3098	1/1	0.99	0.10	29,29,29,29	0
54	MG	CA	1639	1/1	0.99	0.12	24,24,24,24	0
54	MG	DB	3036	1/1	0.99	0.12	25,25,25,25	0
54	MG	BB	3060	1/1	0.99	0.10	47,47,47,47	0
54	MG	DB	3081	1/1	0.99	0.11	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.