



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:45 am BST

PDB ID : 4U1U
Title : Crystal structure of the E. coli ribosome bound to quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

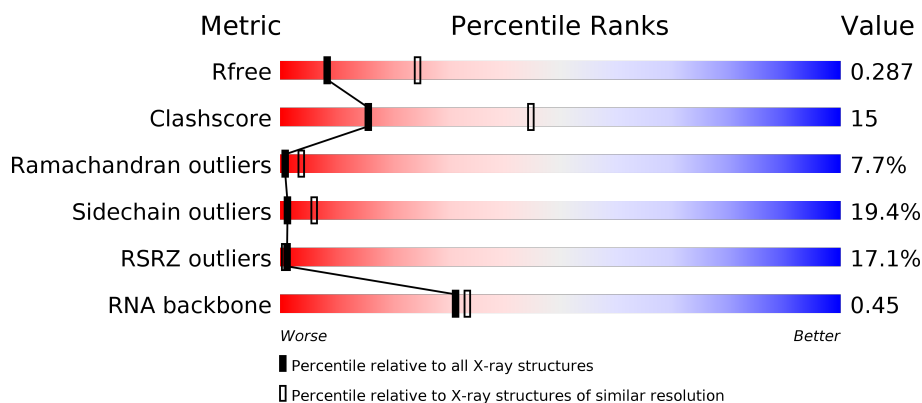
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	1539	
1	CA	1539	
2	AB	218	
2	CB	218	

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
27	DF	177	

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	8	
54	D6	8	

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	004	D6	7	-	-	X	-
55	MG	AA	1614	-	-	-	X
55	MG	AA	1657	-	-	-	X
55	MG	AA	1659	-	-	-	X
55	MG	BA	3015	-	-	-	X
55	MG	BA	3061	-	-	-	X
55	MG	BA	3179	-	-	-	X
55	MG	CA	1633	-	-	-	X
55	MG	DA	3015	-	-	-	X
55	MG	DA	3016	-	-	-	X
55	MG	DA	3025	-	-	-	X
55	MG	DA	3055	-	-	-	X
55	MG	DA	3057	-	-	-	X
55	MG	DA	3060	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3091	-	-	-	X
55	MG	DA	3092	-	-	-	X
55	MG	DA	3119	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3155	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288328 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
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

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

- 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
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	4	Total	Mg	0	0
			4	4		
55	BA	195	Total	Mg	0	0
			195	195		
55	CA	55	Total	Mg	0	0
			55	55		
55	DQ	1	Total	Mg	0	0
			1	1		
55	CM	1	Total	Mg	0	0
			1	1		
55	AA	71	Total	Mg	0	0
			71	71		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	AM	1	Total	Mg	0	0
			1	1		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	619	Total O 619 619	0	0
57	BB	13	Total O 13 13	0	0
57	BC	8	Total O 8 8	0	0
57	BD	3	Total O 3 3	0	0
57	BE	3	Total O 3 3	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BL	5	Total O 5 5	0	0
57	BN	5	Total O 5 5	0	0
57	BS	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0

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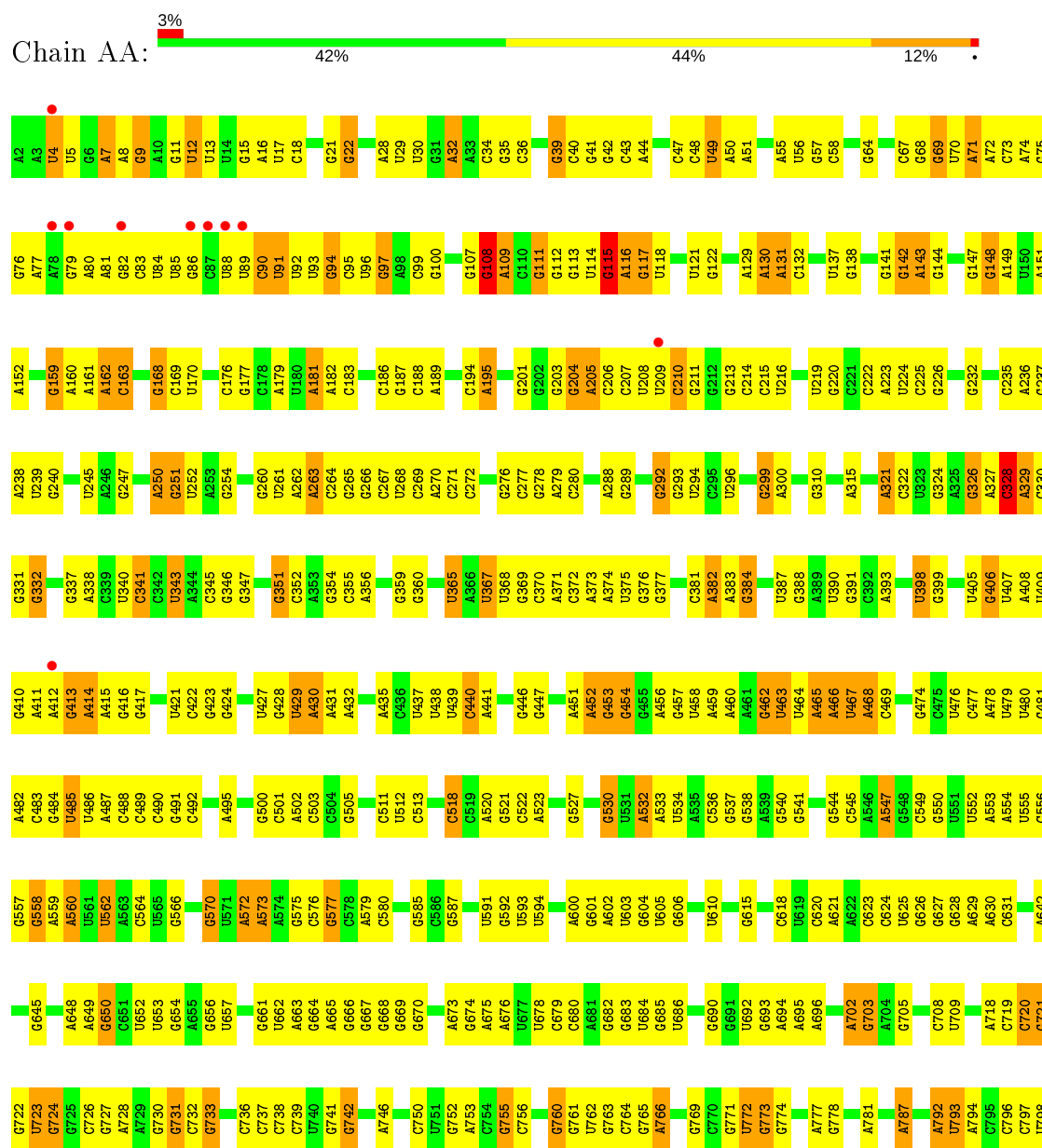
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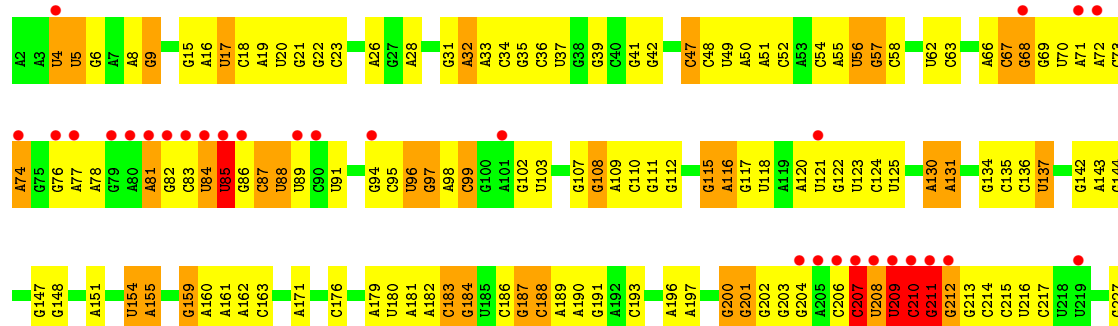
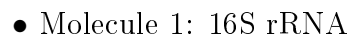
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57	CU	1	Total 1	O 1	0	0
57	DA	612	Total 612	O 612	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	4	Total 4	O 4	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	1	Total 1	O 1	0	0
57	DQ	2	Total 2	O 2	0	0
57	DT	3	Total 3	O 3	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

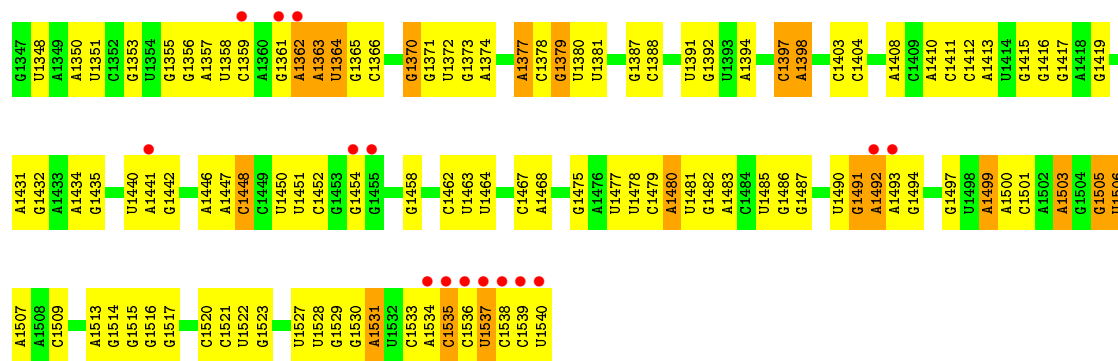
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

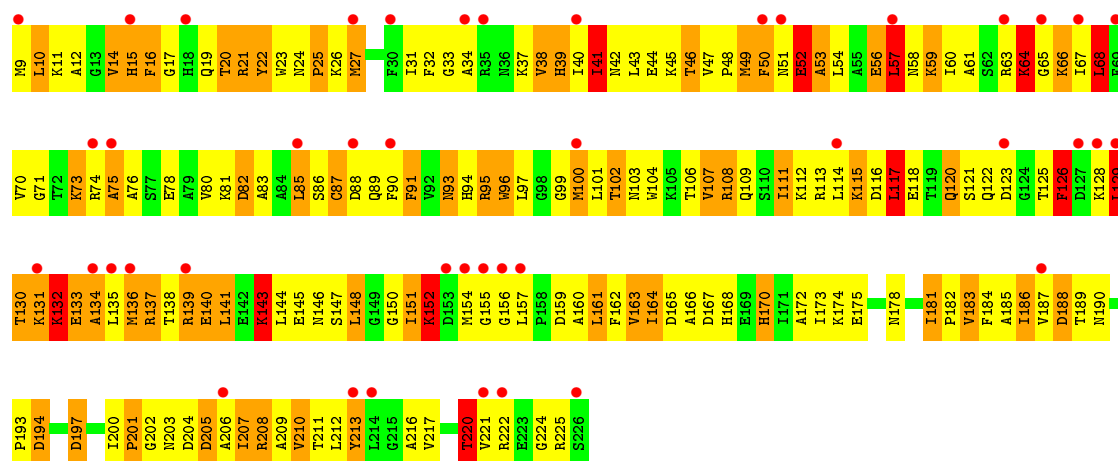
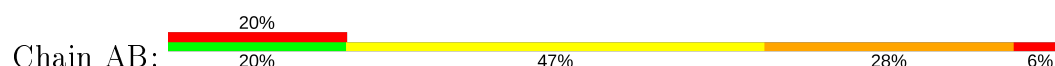




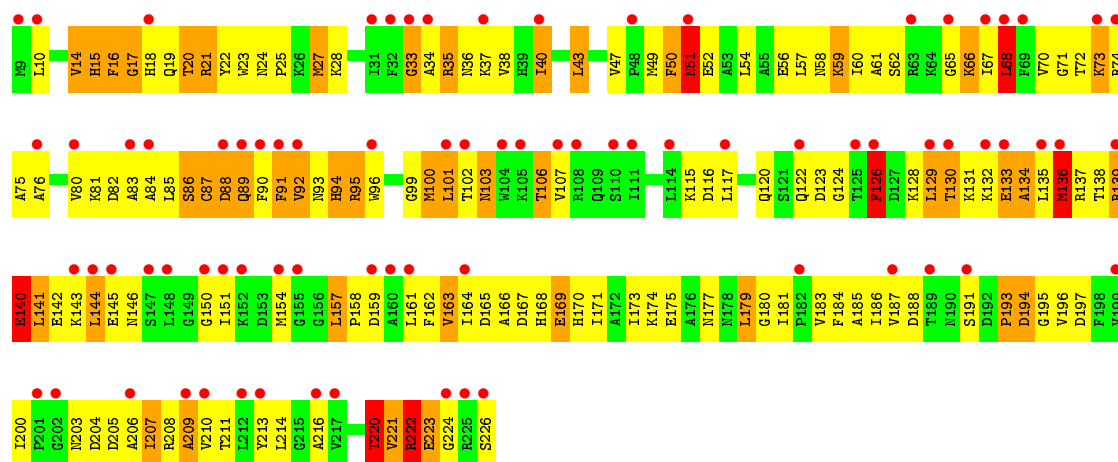
G1282	G1283	G1284	A1285	A1286	A1287	A1288	U1291	G1292	G1293	G1294	U1295	G1296	U1297	U1298	G1300	U1301	G1302	G1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	G1313	G1314	U1315	G1316	G1317	G1318	A1319	G1320	U1321	G1322	G1323	A1324	G1325	U1326	C1327	C1328	U1330	G1331	A1332	A1333	G1334	G1337	G1338	G1342	G1343	G1344	U1345	A1346																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1217	C1218	A1219	G1220	G1221	G1222	G1223	U1224	A1225	C1226	A1227	G1228	A1229	C1230	G1231	U1232	G1233	A1238	A1239	U1240	G1241	G1242	G1243	C1244	C1245	U1246	U1247	A1248	G1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1260	A1261	C1262	C1263	U1264	C1265	G1266	A1269	A1271	G1272	A1273	A1274	U1275	G1276	C1277	G1278	C1279	G1281	A1282	U1283	C1284	C1285	C1286	G1289	G1297	A1298	G1299	A1300	G1301	G1302	A1303	G1305	A1306	C1307	C1308	A1309	G1402	C1403																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C1141	G1142	G1143	G1144	A1145	C1146	C1147	U1148	C1149	A1150	C1151	A1152	G1153	G1154	A1155	A1156	A1157	C1158	U1159	C1160	C1161	G1166	A1167	U1168	A1169	A1170	G1175	A1176	A1177	A1179	A1180	G1181	G1182	U1183	G1184	A1191	C1192	A1196	A1197	C1198	U1199	C1200	A1201	U1202	G1203	A1204	U1205	G1206	G1209	C1210	U1211	C1212	G1213	C1214	C1215	G1216	C1217	G1218	A1219	C1220	A1221	C1222	A1223	C1224	A1225	C1226	A1227	C1228	A1229	C1230	A1231	C1232	A1233	C1234	A1235	C1236	A1237	C1238	A1239	C1240	A1241	C1242	A1243	C1244	A1245	C1246	A1247	C1248	A1249	C1250	A1251	C1252	A1253	C1254	A1255	C1256	A1257	C1258	A1259	C1260	A1261	C1262	A1263	C1264	A1265	C1266	A1267	C1268	A1269	C1270	A1271	C1272	A1273	C1274	A1275	C1276	A1277	C1278	A1279	C1280	A1281	C1282	A1283	C1284	A1285	C1286	A1287	C1288	A1289	C1290	A1291	C1292	A1293	C1294	A1295	C1296	A1297	C1298	A1299	C1300	A1301	C1302	A1303	C1304	A1305	C1306	A1307	C1308	A1309	C1310	A1311	C1312	A1313	C1314	A1315	C1316	A1317	C1318	A1319	C1320	A1321	C1322	A1323	C1324	A1325	C1326	A1327	C1328	A1329	C1330	A1331	C1332	A1333	C1334	A1335	C1336	A1337	C1338	A1339	C1340	A1341	C1342	A1343	C1344	A1345	C1346	A1347	C1348	A1349	C1350	A1351	C1352	A1353	C1354	A1355	C1356	A1357	C1358	A1359	C1360	A1361	C1362	A1363	C1364	A1365	C1366	A1367	C1368	A1369	C1370	A1371	C1372	A1373	C1374	A1375	C1376	A1377	C1378	A1379	C1380	A1381	C1382	A1383	C1384	A1385	C1386	A1387	C1388	A1389	C1390	A1391	C1392	A1393	C1394	A1395	C1396	A1397	C1398	A1399	C1400	A1401	C1402	A1403	C1404	A1405	C1406	A1407	C1408	A1409	C1410	A1411	C1412	A1413	C1414	A1415	C1416	A1417	C1418	A1419	C1420	A1421	C1422	A1423	C1424	A1425	C1426	A1427	C1428	A1429	C1430	A1431	C1432	A1433	C1434	A1435	C1436	A1437	C1438	A1439	C1440	A1441	C1442	A1443	C1444	A1445	C1446	A1447	C1448	A1449	C1450	A1451	C1452	A1453	C1454	A1455	C1456	A1457	C1458	A1459	C1460	A1461	C1462	A1463	C1464	A1465	C1466	A1467	C1468	A1469	C1470	A1471	C1472	A1473	C1474	A1475	C1476	A1477	C1478	A1479	C1480	A1481	C1482	A1483	C1484	A1485	C1486	A1487	C1488	A1489	C1490	A1491	C1492	A1493	C1494	A1495	C1496	A1497	C1498	A1499	C1500	A1501	C1502	A1503	C1504	A1505	C1506	A1507	C1508	A1509	C1510	A1511	C1512	A1513	C1514	A1515	C1516	A1517	C1518	A1519	C1520	A1521	C1522	A1523	C1524	A1525	C1526	A1527	C1528	A1529	C1530	A1531	C1532	A1533	C1534	A1535	C1536	A1537	C1538	A1539	C1540	A1541	C1542	A1543	C1544	A1545	C1546	A1547	C1548	A1549	C1550	A1551	C1552	A1553	C1554	A1555	C1556	A1557	C1558	A1559	C1560	A1561	C1562	A1563	C1564	A1565	C1566	A1567	C1568	A1569	C1570	A1571	C1572	A1573	C1574	A1575	C1576	A1577	C1578	A1579	C1580	A1581	C1582	A1583	C1584	A1585	C1586	A1587	C1588	A1589	C1590	A1591	C1592	A1593	C1594	A1595	C1596	A1597	C1598	A1599	C1600	A1601	C1602	A1603	C1604	A1605	C1606	A1607	C1608	A1609	C1610	A1611	C1612	A1613	C1614	A1615	C1616	A1617	C1618	A1619	C1620	A1621	C1622	A1623	C1624	A1625	C1626	A1627	C1628	A1629	C1630	A1631	C1632	A1633	C1634	A1635	C1636	A1637	C1638	A1639	C1640	A1641	C1642	A1643	C1644	A1645	C1646	A1647	C1648	A1649	C1650	A1651	C1652	A1653	C1654	A1655	C1656	A1657	C1658	A1659	C1660	A1661	C1662	A1663	C1664	A1665	C1666	A1667	C1668	A1669	C1670	A1671	C1672	A1673	C1674	A1675	C1676	A1677	C1678	A1679	C1680	A1681	C1682	A1683	C1684	A1685	C1686	A1687	C1688	A1689	C1690	A1691	C1692	A1693	C1694	A1695	C1696	A1697	C1698	A1699	C1700	A1701	C1702	A1703	C1704	A1705	C1706	A1707	C1708	A1709	C1710	A1711	C1712	A1713	C1714	A1715	C1716	A1717	C1718	A1719	C1720	A1721	C1722	A1723	C1724	A1725	C1726	A1727	C1728	A1729	C1730	A1731	C1732	A1733	C1734	A1735	C1736	A1737	C1738	A1739	C1740	A1741	C1742	A1743	C1744	A1745	C1746	A1747	C1748	A1749	C1750	A1751	C1752	A1753	C1754	A1755	C1756	A1757	C1758	A1759	C1760	A1761	C1762	A1763	C1764	A1765	C1766	A1767	C1768	A1769	C1770	A1771	C1772	A1773	C1774	A1775	C1776	A1777	C1778	A1779	C1780	A1781	C1782	A1783	C1784	A1785	C1786	A1787	C1788	A1789	C1790	A1791	C1792	A1793	C1794	A1795	C1796	A1797	C1798	A1799	C1800	A1801	C1802	A1803	C1804	A1805	C1806	A1807	C1808	A1809	C1810	A1811	C1812	A1813	C1814	A1815	C1816	A1817	C1818	A1819	C1820	A1821	C1822	A1823	C1824	A1825	C1826	A1827	C1828	A1829	C1830	A1831	C1832	A1833	C1834	A1835	C1836	A1837	C1838	A1839	C1840	A1841	C1842	A1843	C1844	A1845	C1846	A1847	C1848	A1849	C1850	A1851	C1852	A1853	C1854	A1855	C1856	A1857	C1858	A1859	C1860	A1861	C1862	A1863	C1864	A1865	C1866	A1867	C1868	A1869	C1870	A1871	C1872	A1873	C1874	A1875	C1876	A1877	C1878	A1879	C1880	A1881	C1882	A1883	C1884	A1885	C1886	A1887	C1888	A1889	C1890	A1891	C1892	A1893	C1894	A1895	C1896	A1897	C1898	A1899	C1900	A1901	C1902	A1903	C1904	A1905	C1906	A1907	C1908	A1909	C1910	A1911	C1912	A1913	C1914	A1915	C1916	A1917	C1918	A1919	C1920	A1921	C1922	A1923	C1924	A1925	C1926	A1927	C1928	A1929	C1930	A1931	C1932	A1933	C1934	A1935	C1936	A1937	C1938	A1939	C1940	A1941	C1942	A1943	C1944	A1945	C1946	A1947	C1948	A1949	C1950	A1951	C1952	A1953	C1954	A1955	C1956	A1957	C1958	A1959	C1960	A1961	C1962	A1963	C1964	A1965	C1966	A1967	C1968	A1969	C1970	A1971	C1972	A1973	C1974	A1975	C1976	A1977	C1978	A1979	C1980	A1981	C1982	A1983	C1984	A1985	C1986	A1987	C1988	A1989	C1990	A1991	C1992	A1993	C1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• Molecule 2: 30S ribosomal protein S2

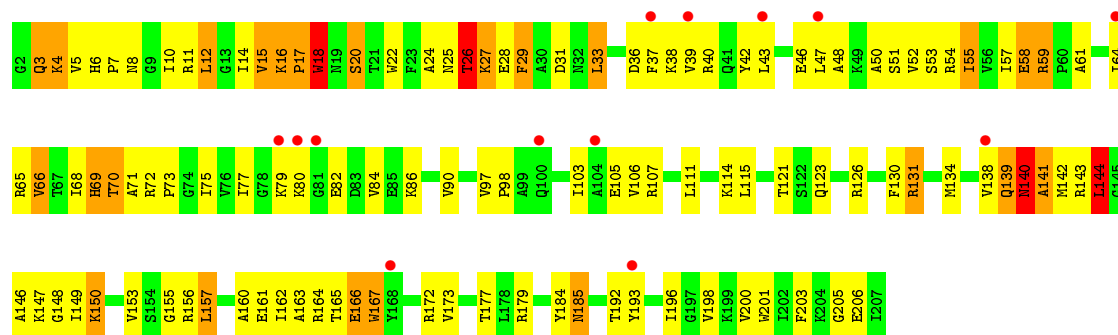


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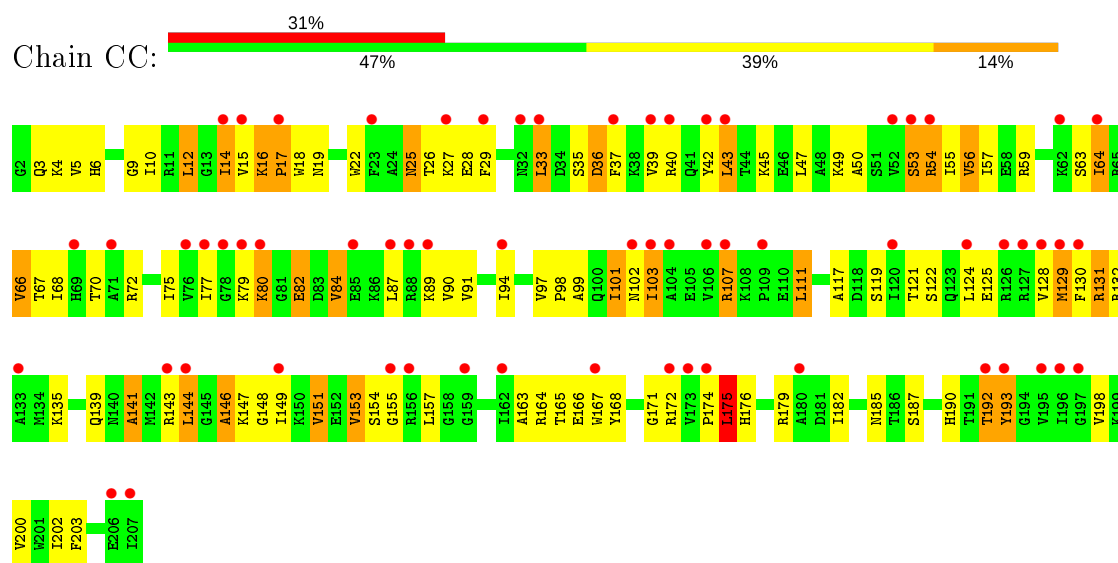


• Molecule 3: 30S ribosomal protein S3

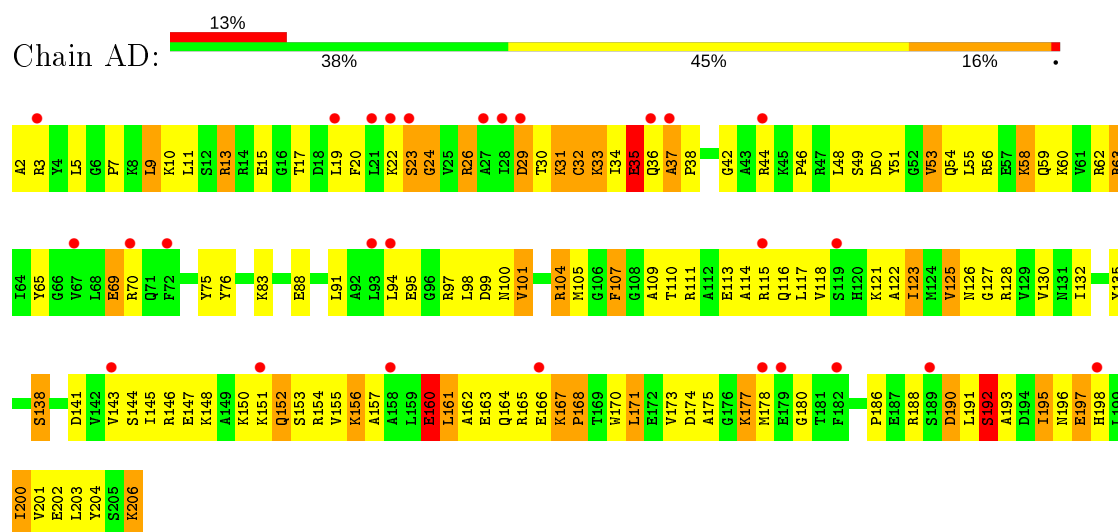




• Molecule 3: 30S ribosomal protein S3

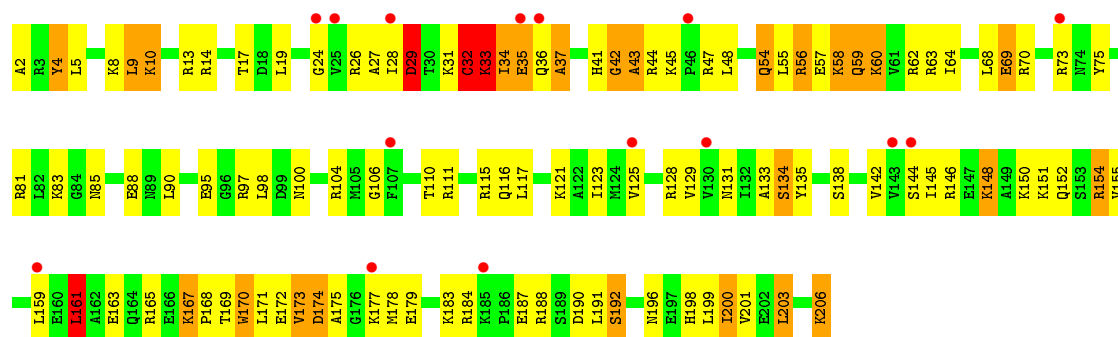


• Molecule 4: 30S ribosomal protein S4

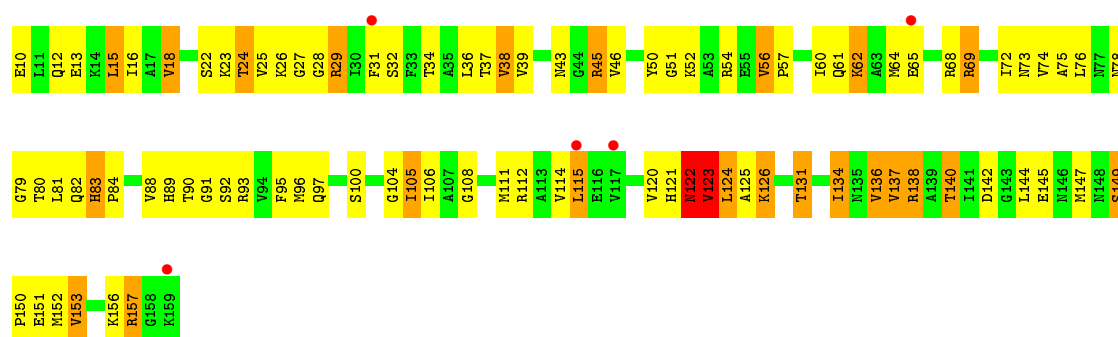


• Molecule 4: 30S ribosomal protein S4

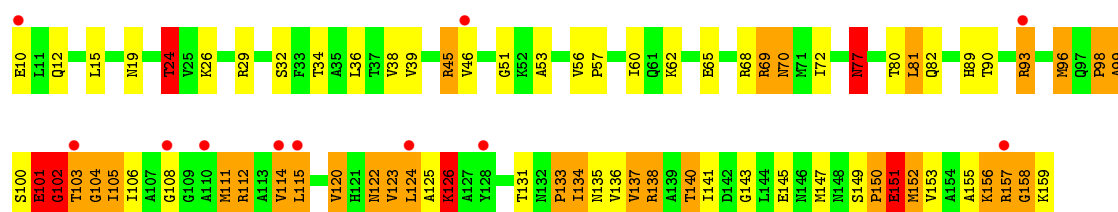




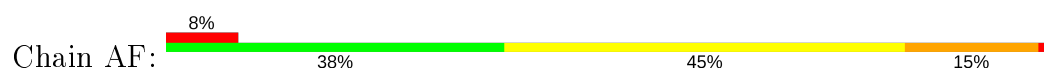
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

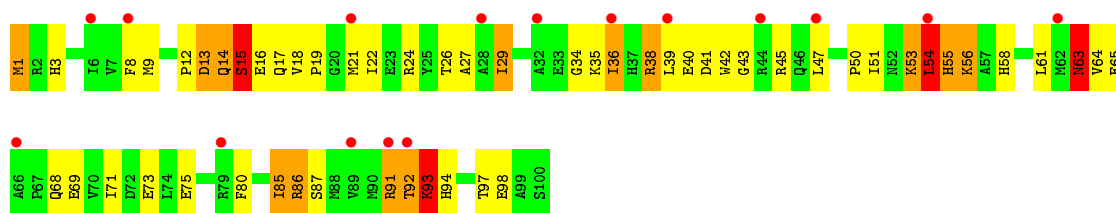


• Molecule 6: 30S ribosomal protein S6

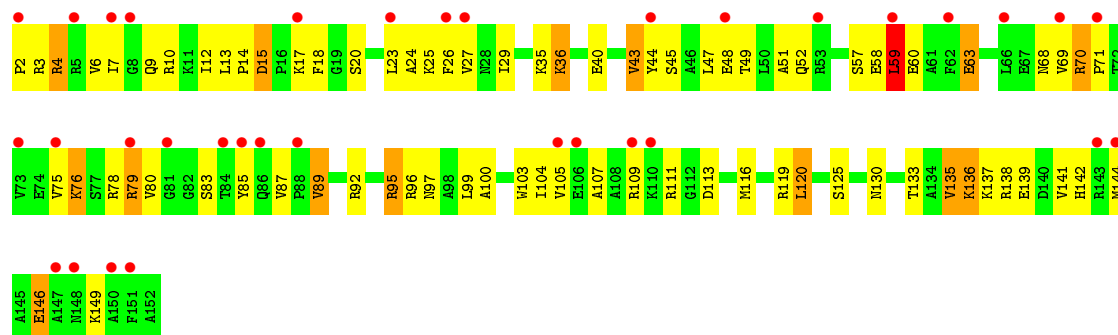


• Molecule 6: 30S ribosomal protein S6

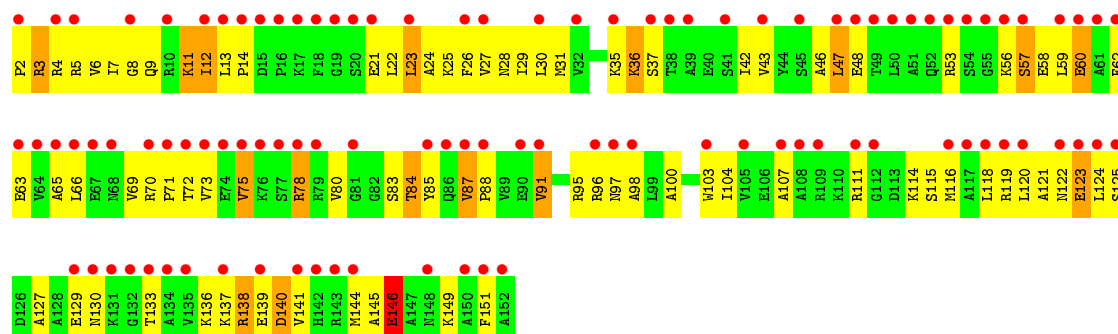




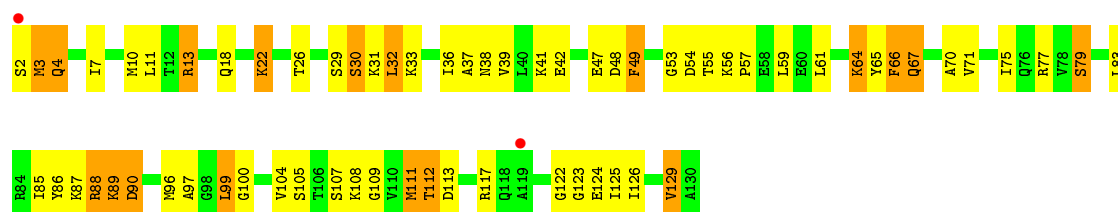
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

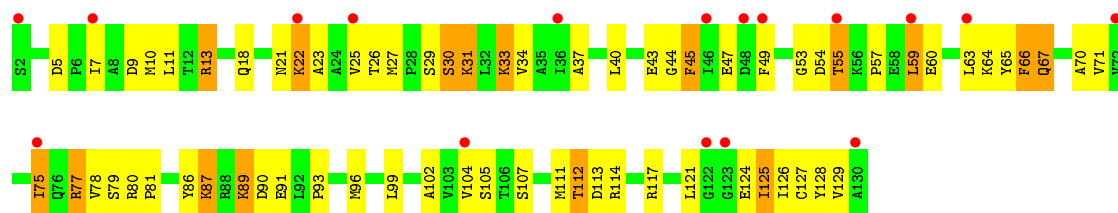


• Molecule 8: 30S ribosomal protein S8

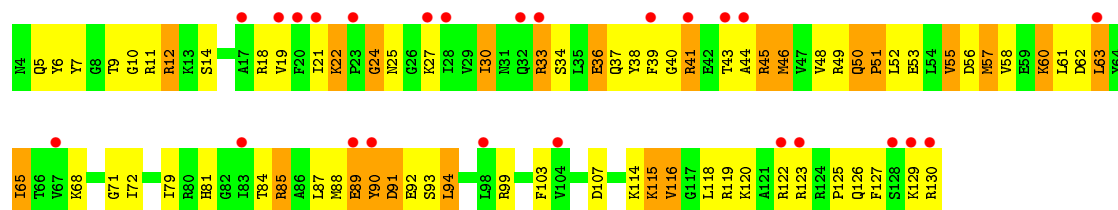


• Molecule 8: 30S ribosomal protein S8

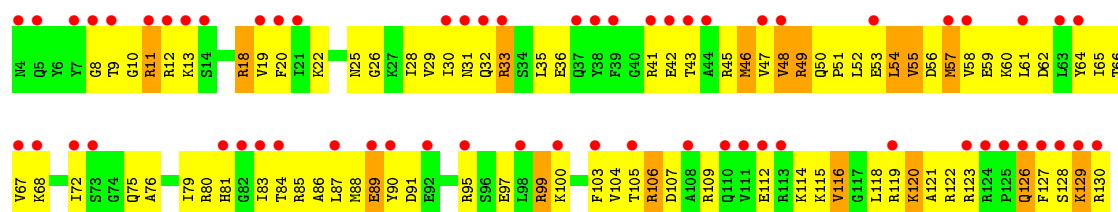




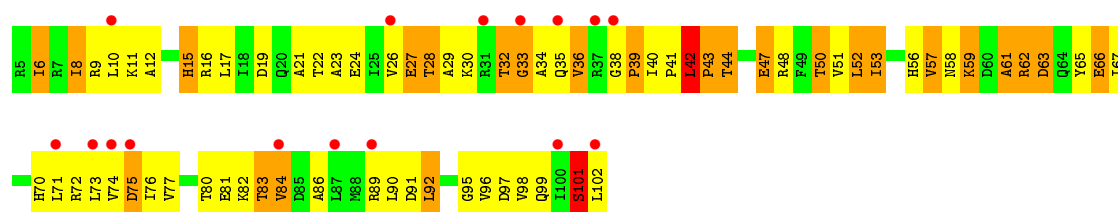
• Molecule 9: 30S ribosomal protein S9



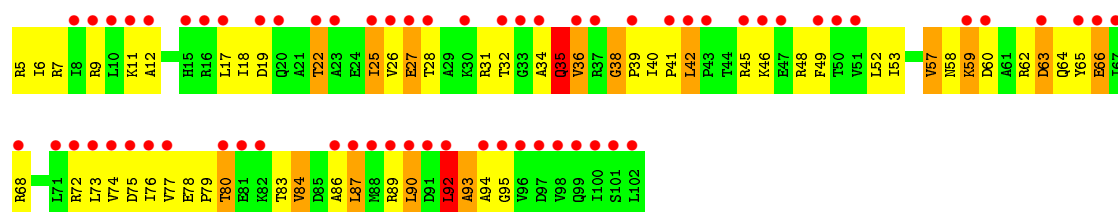
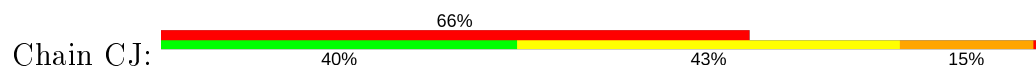
• Molecule 9: 30S ribosomal protein S9



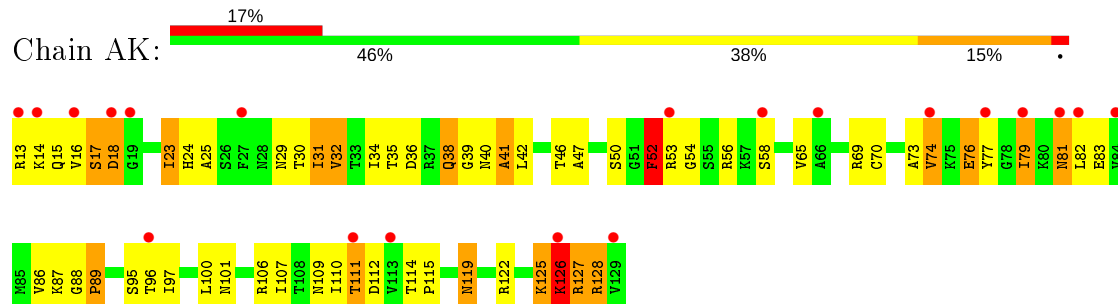
• Molecule 10: 30S ribosomal protein S10



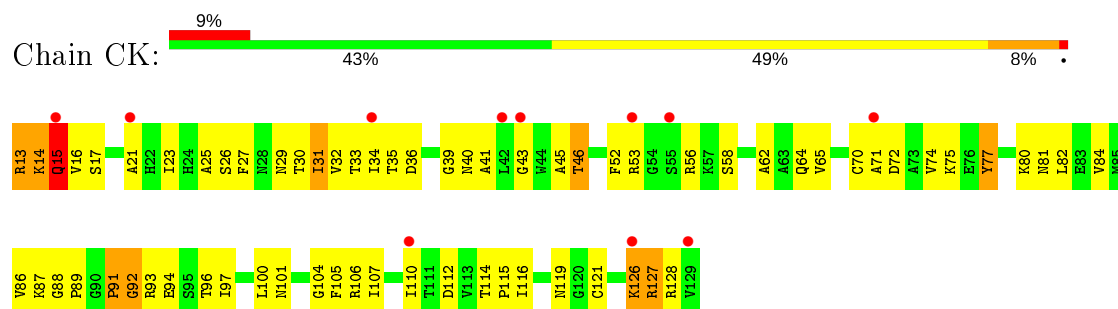
• Molecule 10: 30S ribosomal protein S10



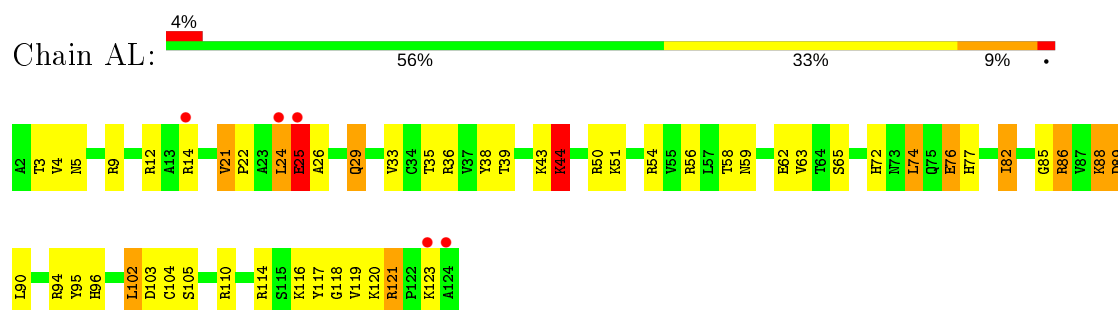
- Molecule 11: 30S ribosomal protein S11



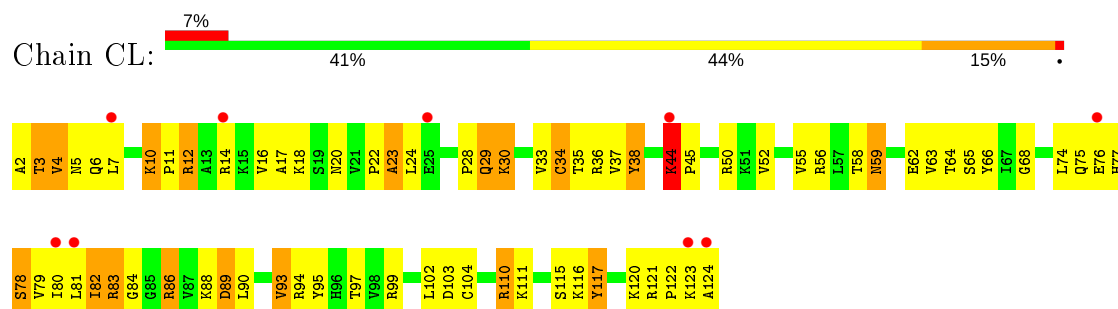
- Molecule 11: 30S ribosomal protein S11



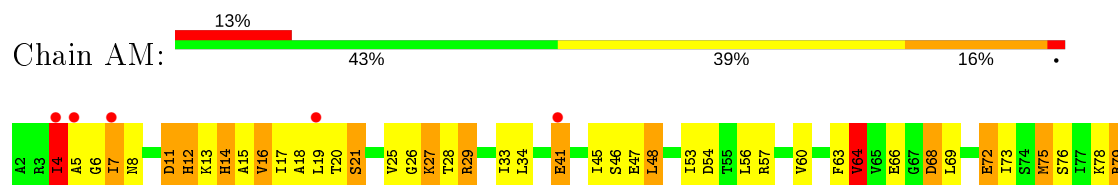
- Molecule 12: 30S ribosomal protein S12

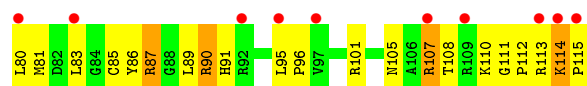


- Molecule 12: 30S ribosomal protein S12

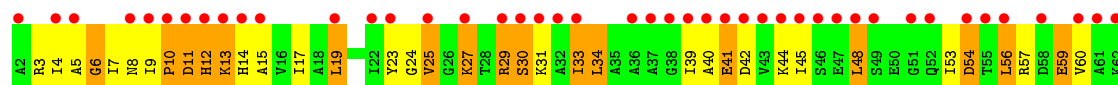
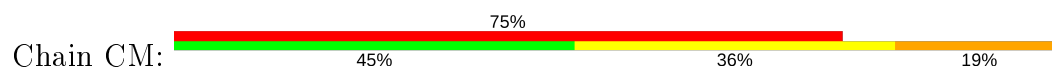


- Molecule 13: 30S ribosomal protein S13

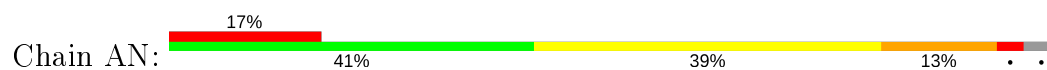




- Molecule 13: 30S ribosomal protein S13



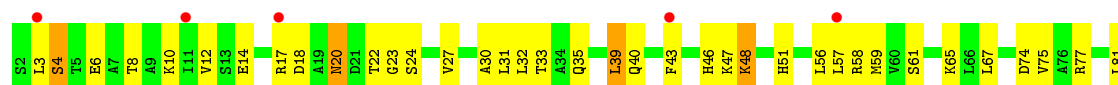
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

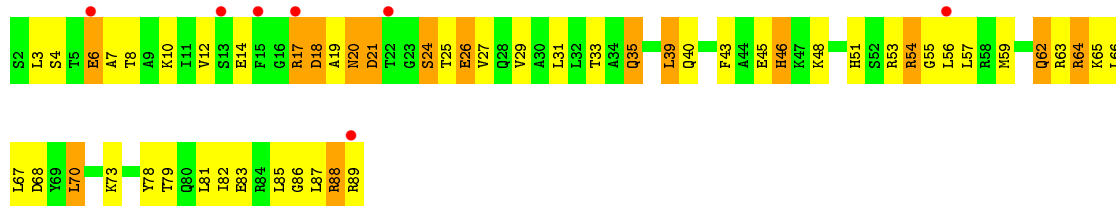


- Molecule 15: 30S ribosomal protein S15

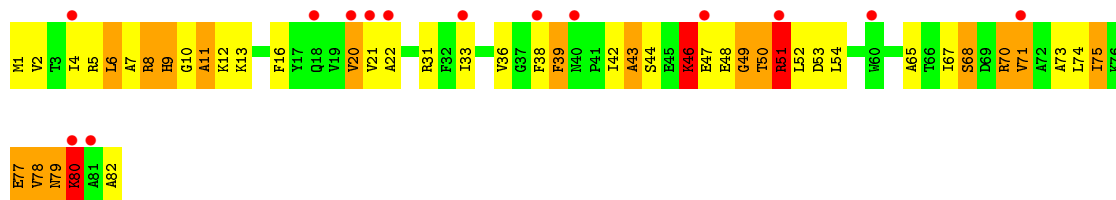
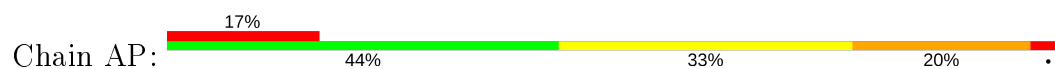


- Molecule 15: 30S ribosomal protein S15

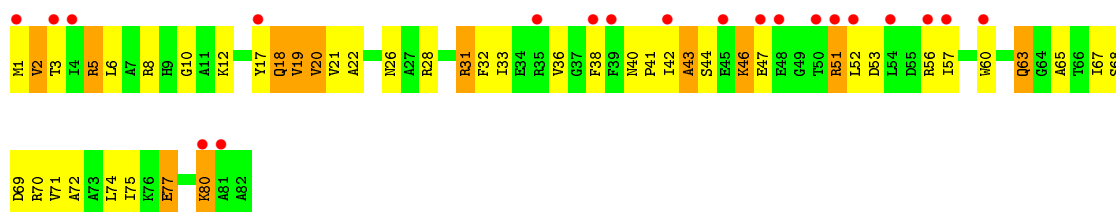




● Molecule 16: 30S ribosomal protein S16



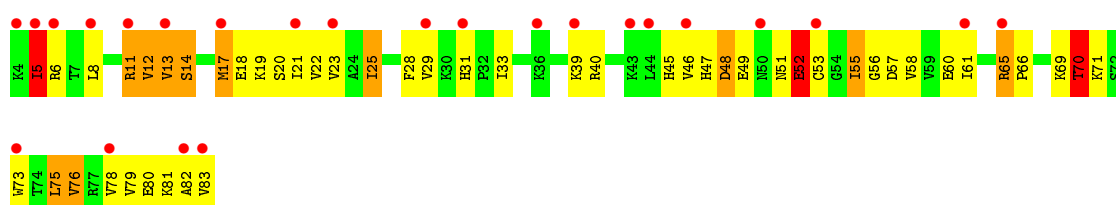
● Molecule 16: 30S ribosomal protein S16



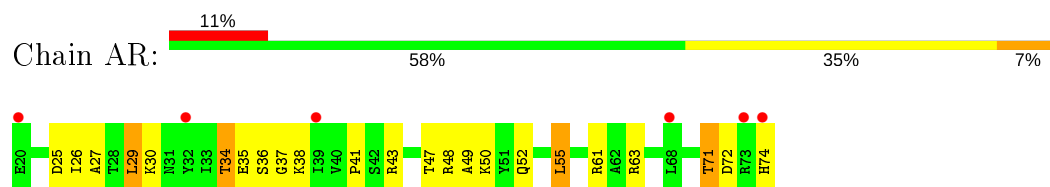
● Molecule 17: 30S ribosomal protein S17



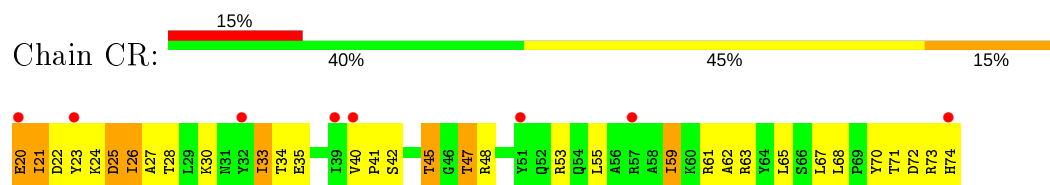
● Molecule 17: 30S ribosomal protein S17



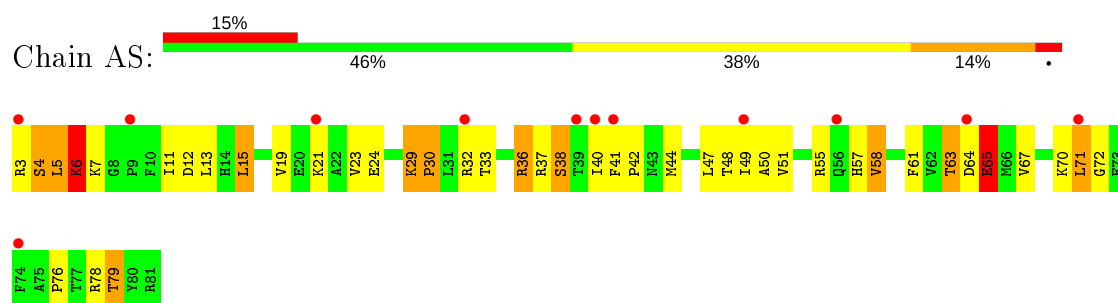
- Molecule 18: 30S ribosomal protein S18



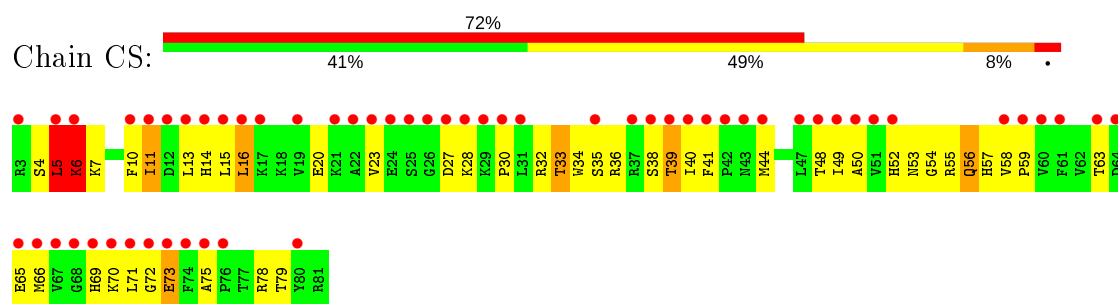
- Molecule 18: 30S ribosomal protein S18



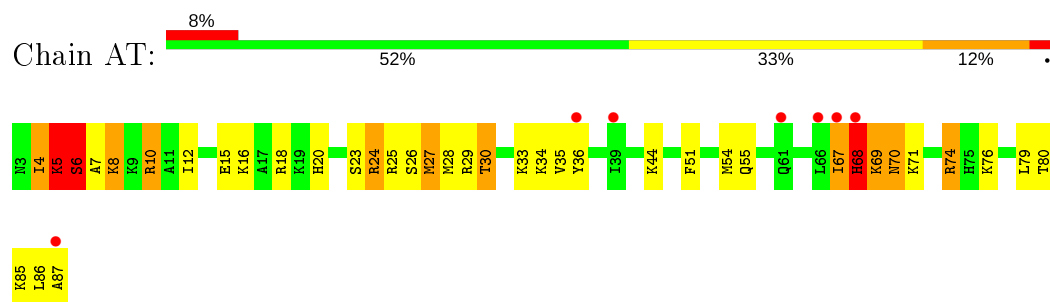
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

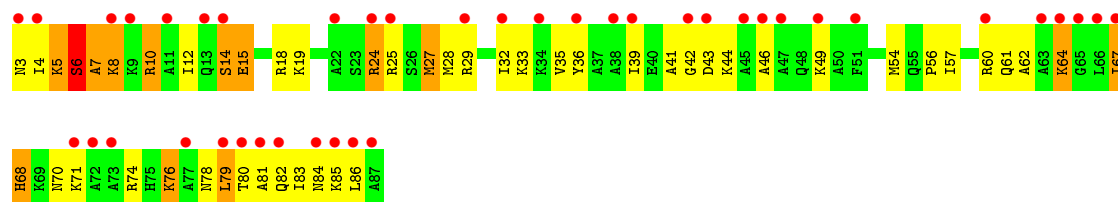


- Molecule 20: 30S ribosomal protein S20

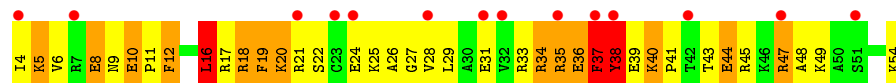


- Molecule 20: 30S ribosomal protein S20

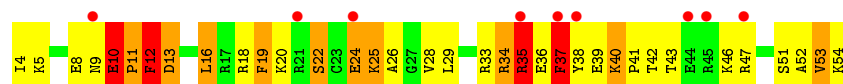




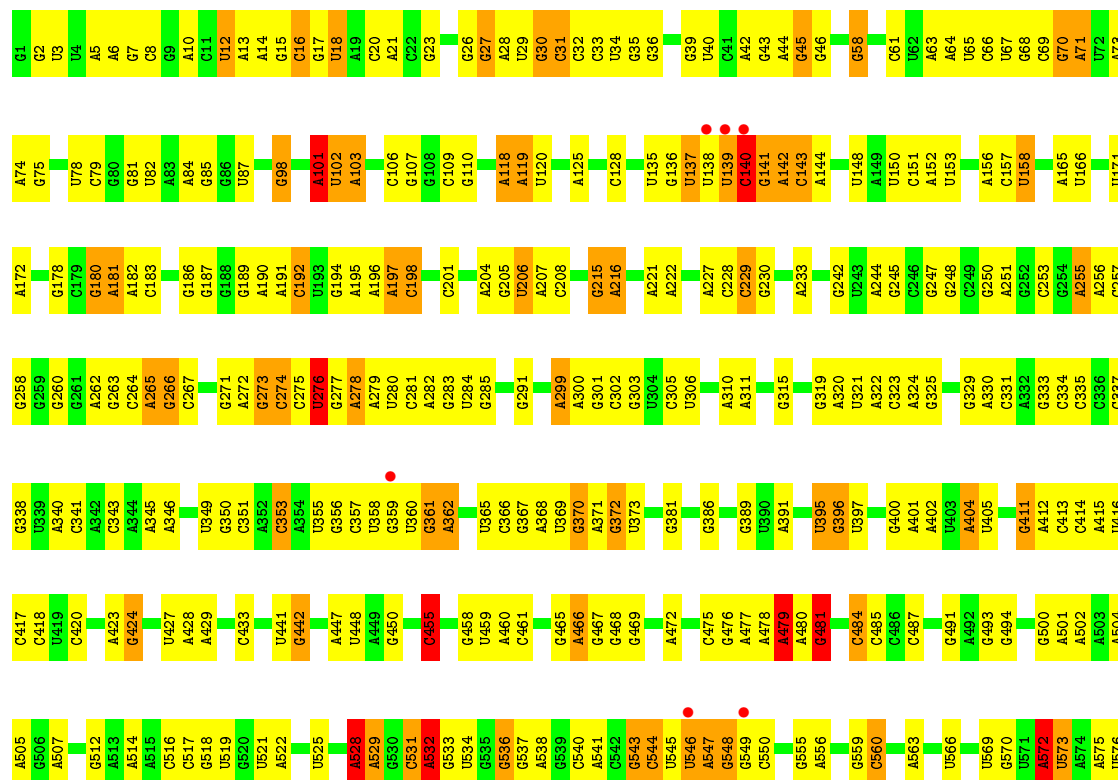
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

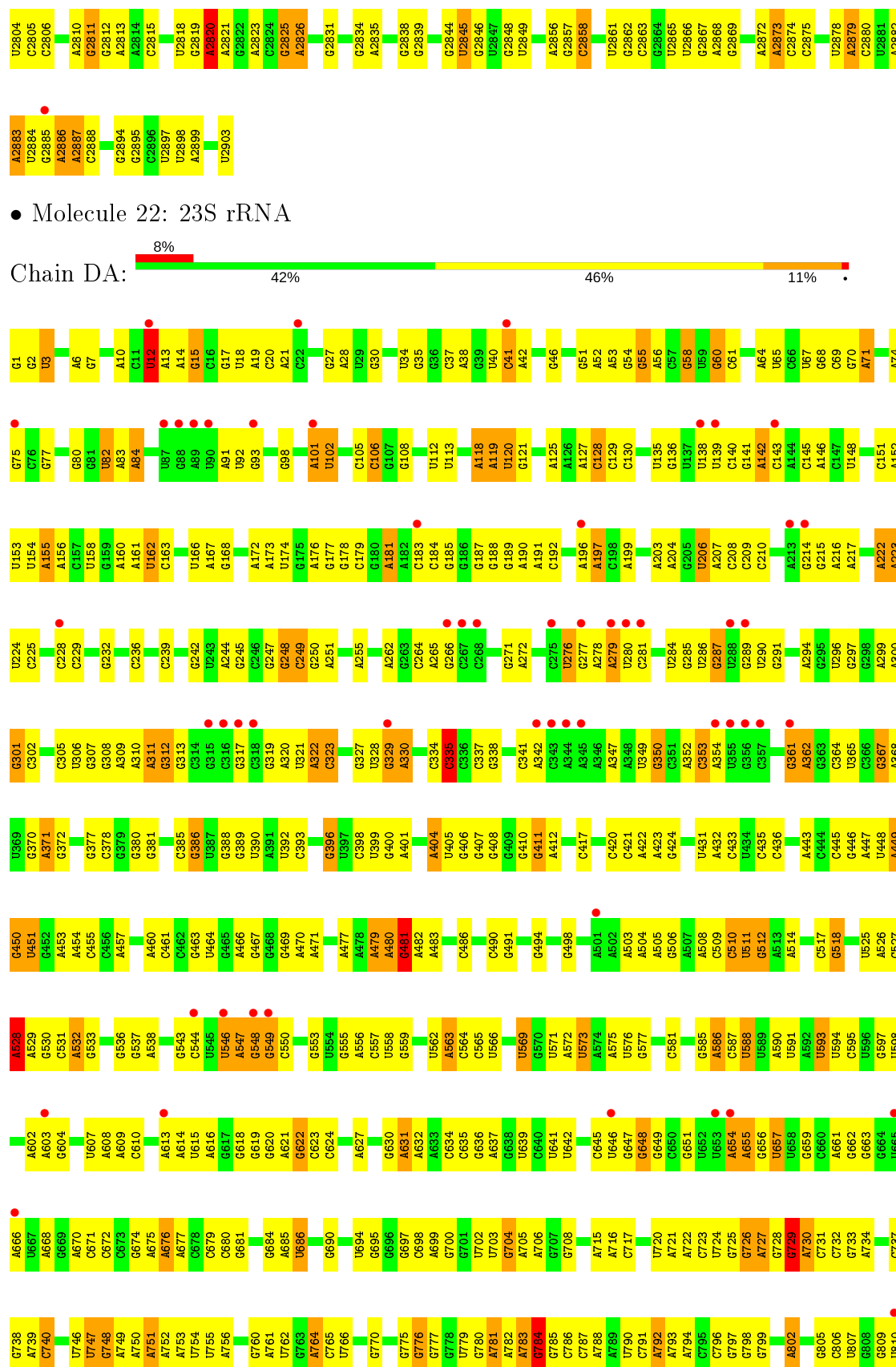


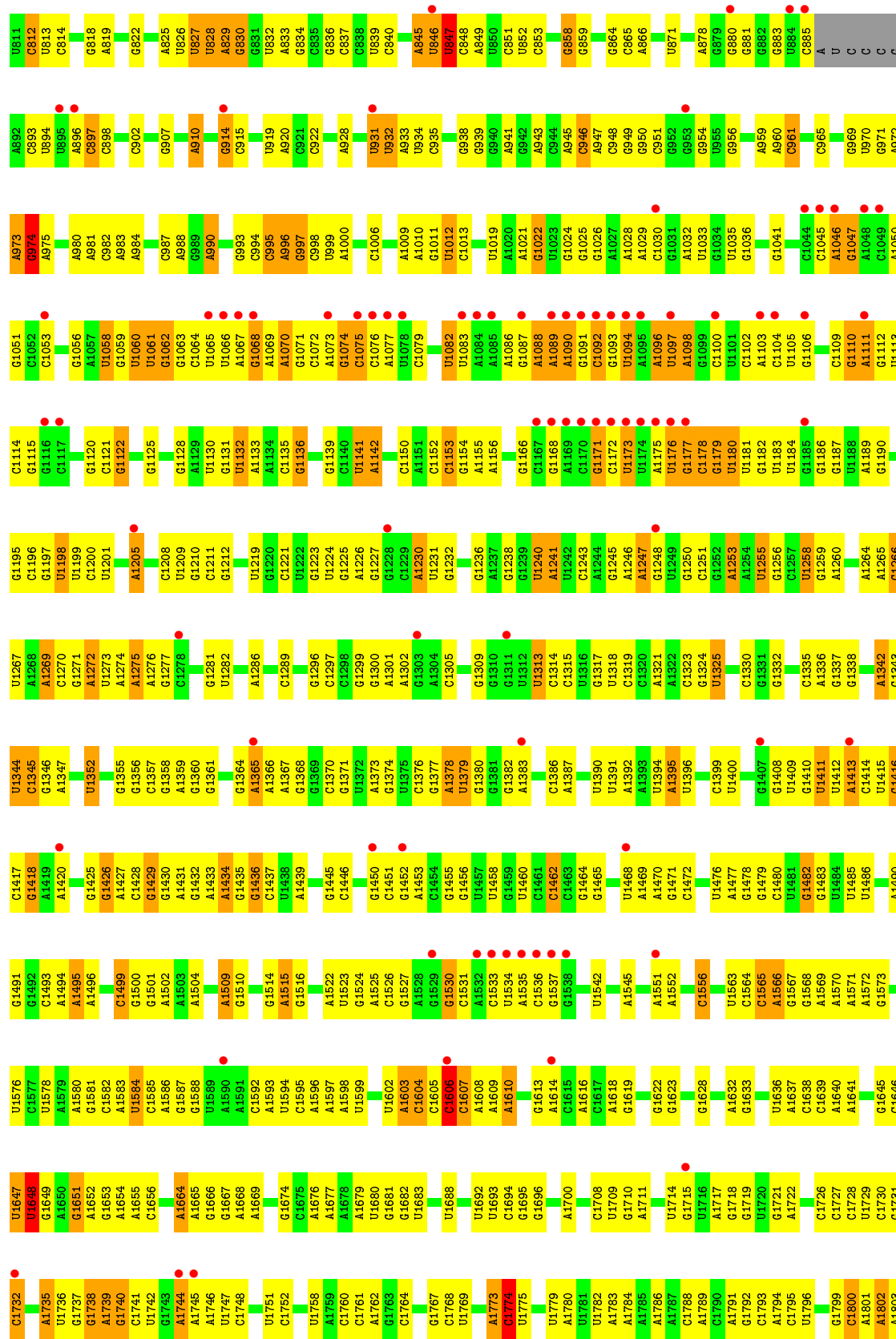
• Molecule 22: 23S rRNA

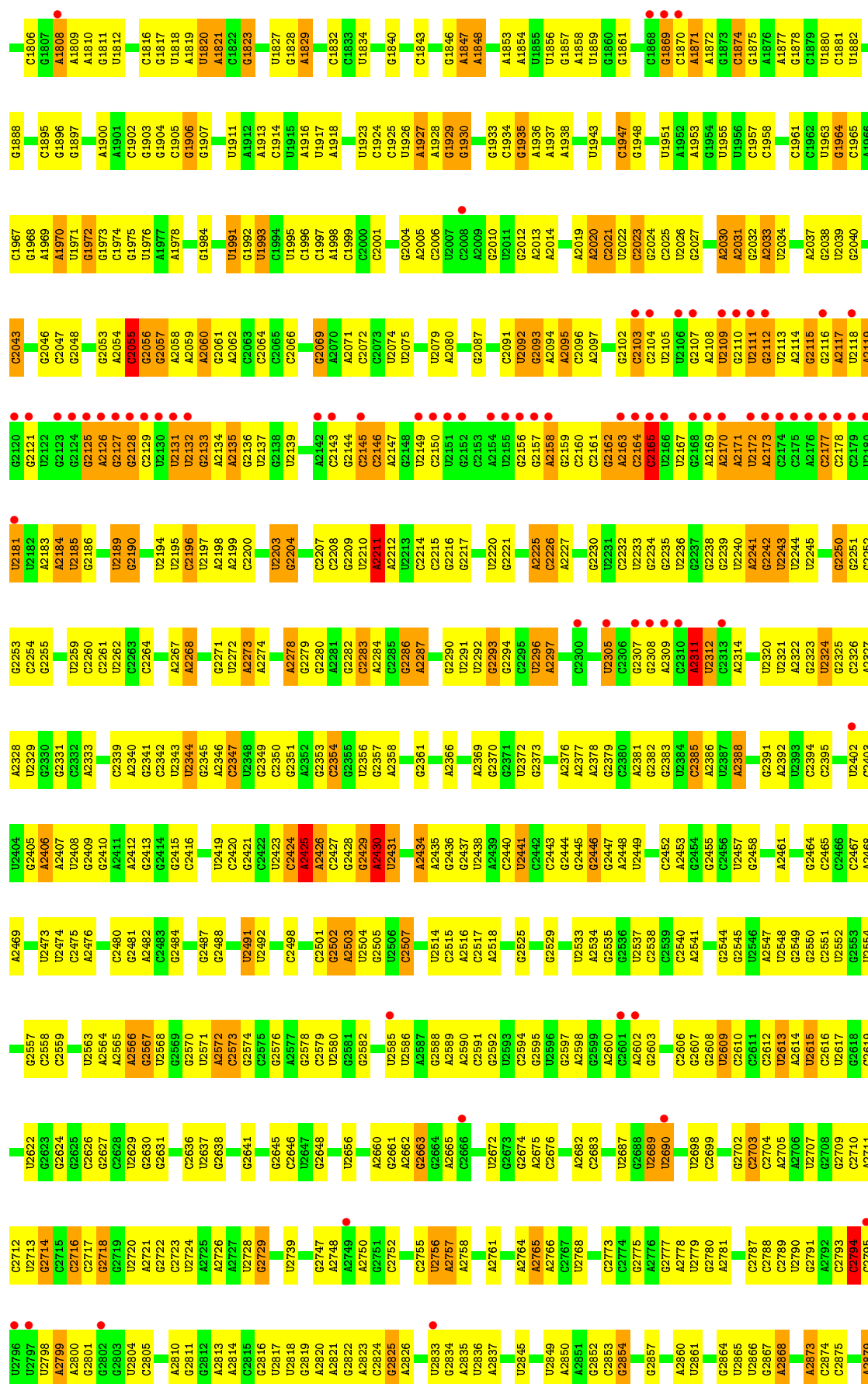


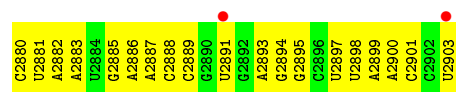
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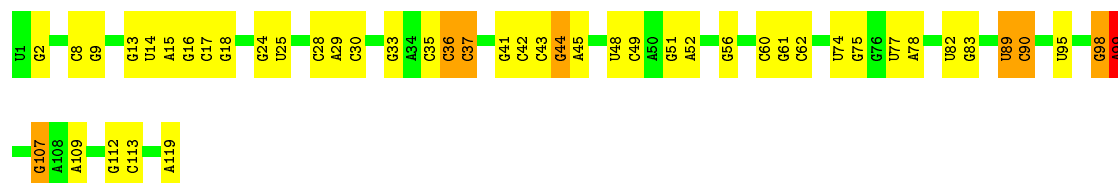




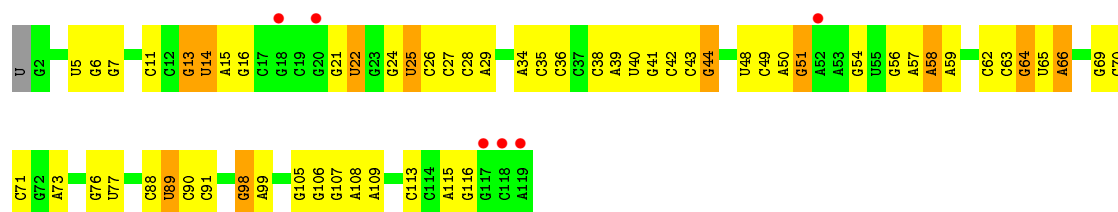




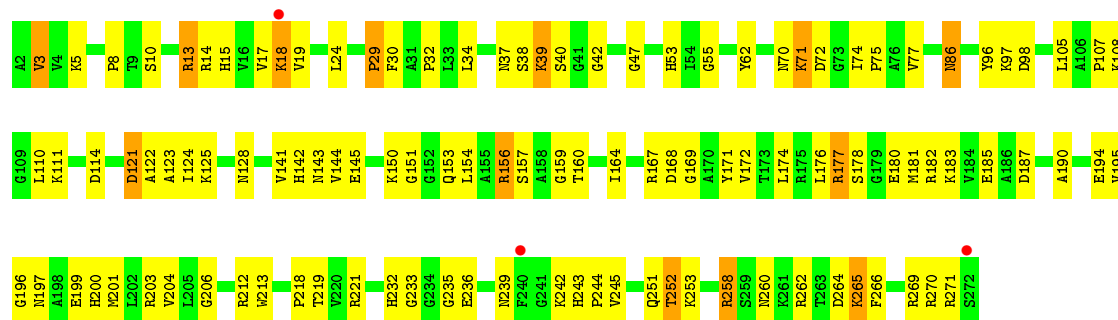
• Molecule 23: 5S rRNA



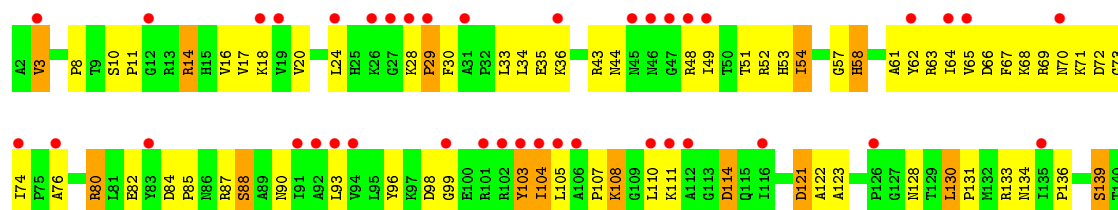
• Molecule 23: 5S rRNA

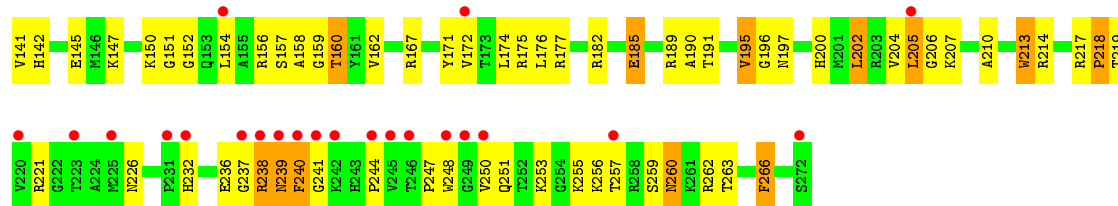


• Molecule 24: 50S ribosomal protein L2



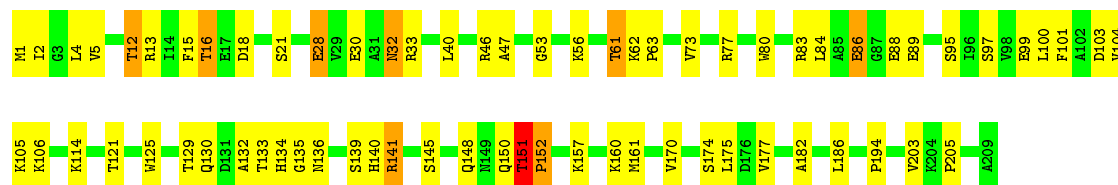
• Molecule 24: 50S ribosomal protein L2





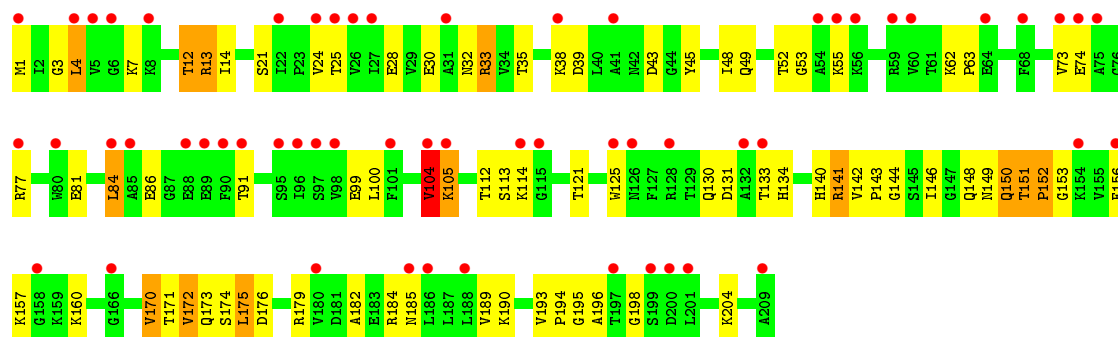
• Molecule 25: 50S ribosomal protein L3

Chain BD: 67% 29%



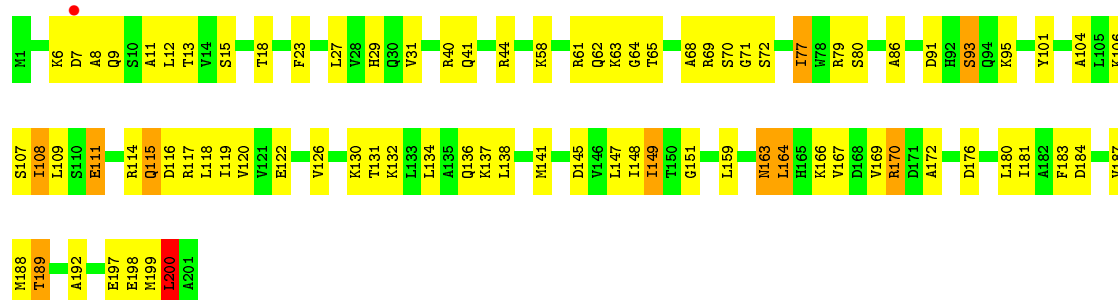
• Molecule 25: 50S ribosomal protein L3

Chain DD: 28% 62% 32% 6%



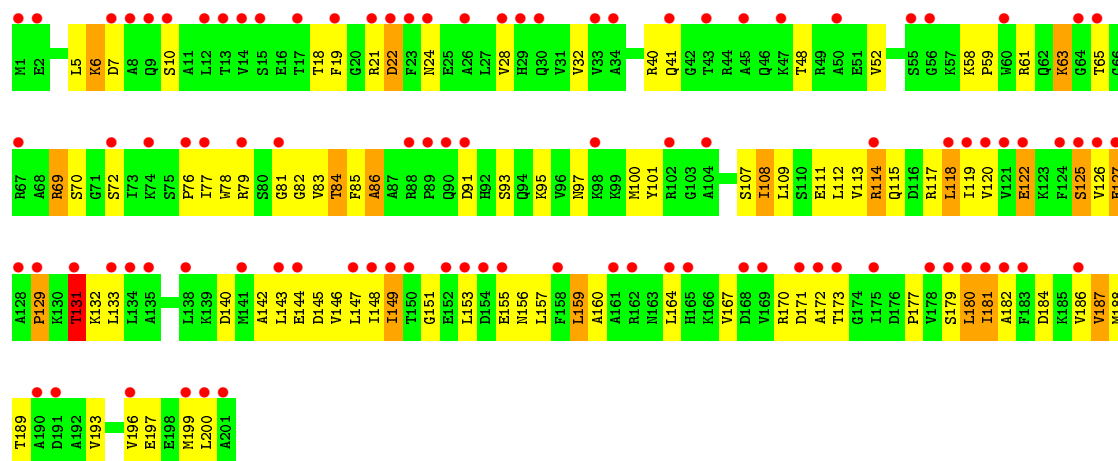
• Molecule 26: 50S ribosomal protein L4

Chain BE: 58% 36% 5%

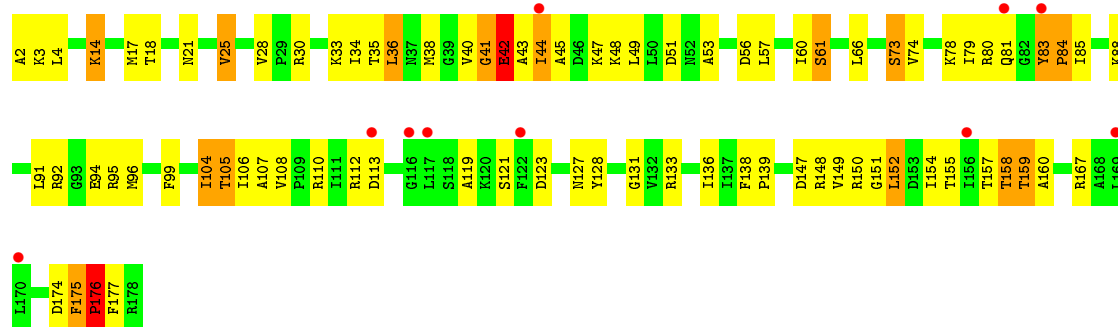


• Molecule 26: 50S ribosomal protein L4

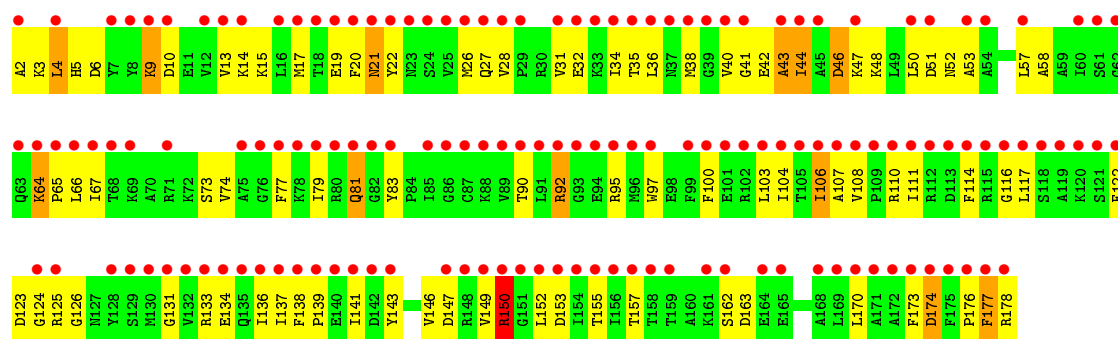
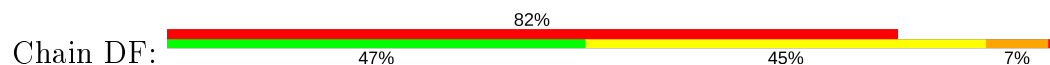
Chain DE: 49% 52% 38% 9%



• Molecule 27: 50S ribosomal protein L5

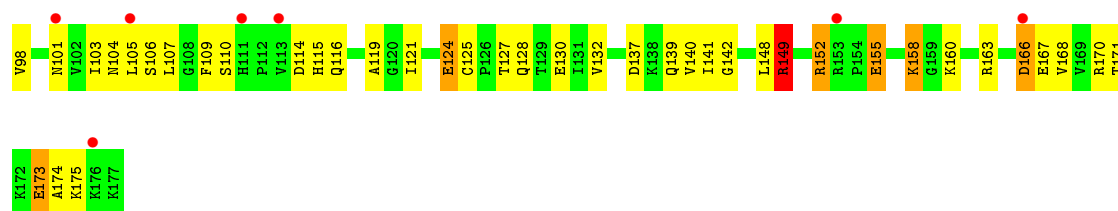


• Molecule 27: 50S ribosomal protein L5

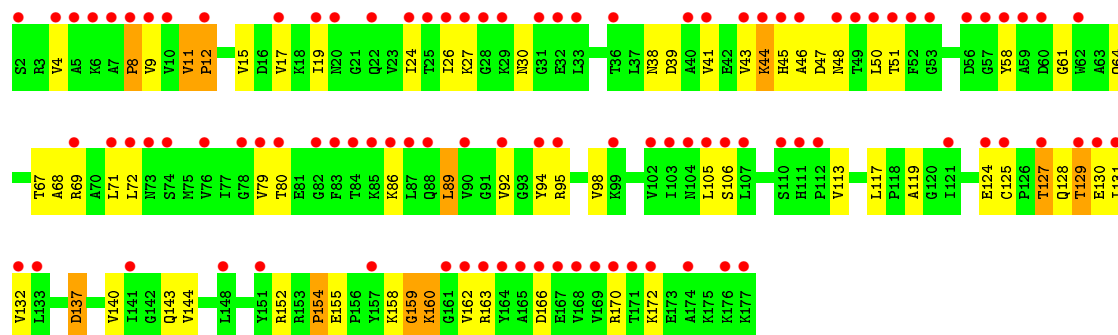


• Molecule 28: 50S ribosomal protein L6

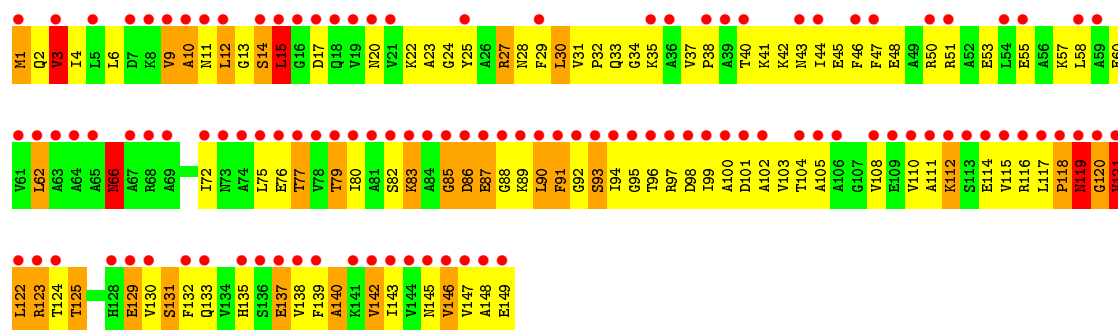
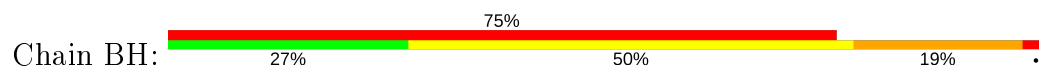




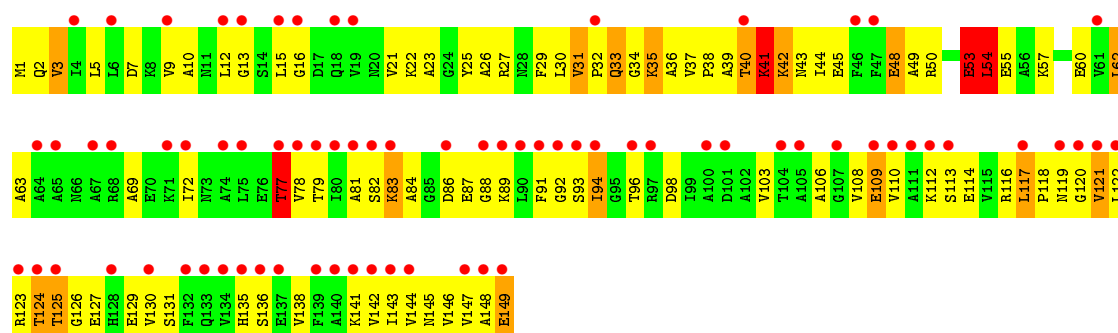
• Molecule 28: 50S ribosomal protein L6



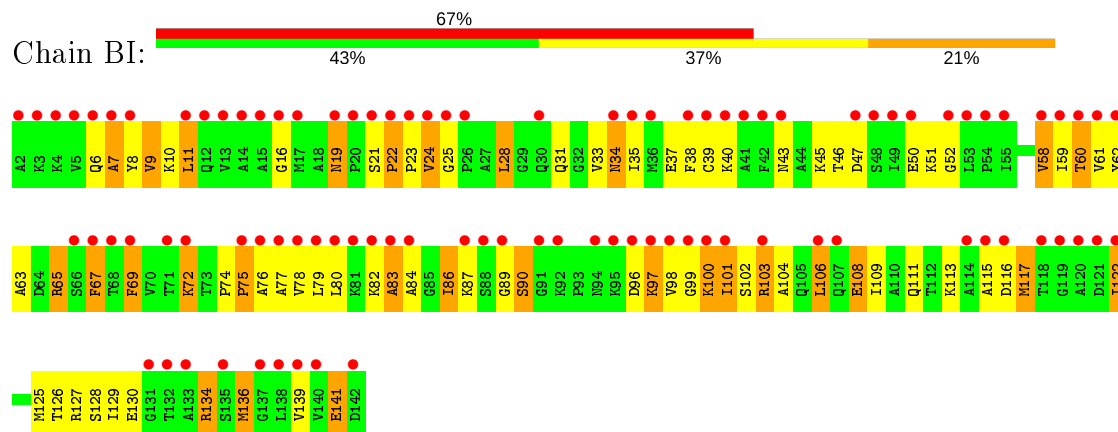
• Molecule 29: 50S ribosomal protein L9



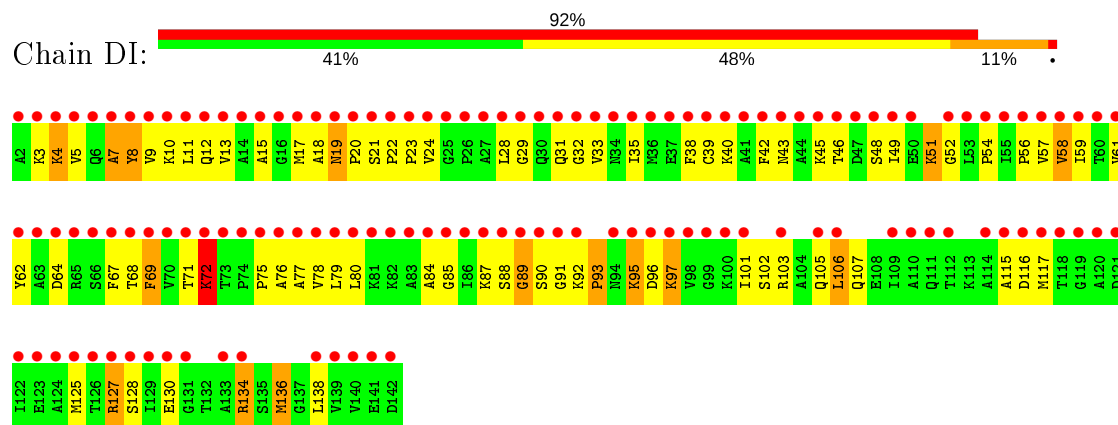
• Molecule 29: 50S ribosomal protein L9



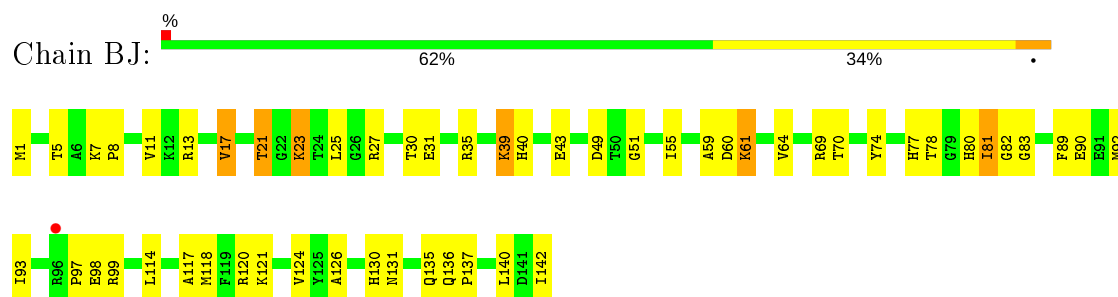
- Molecule 30: 50S ribosomal protein L11



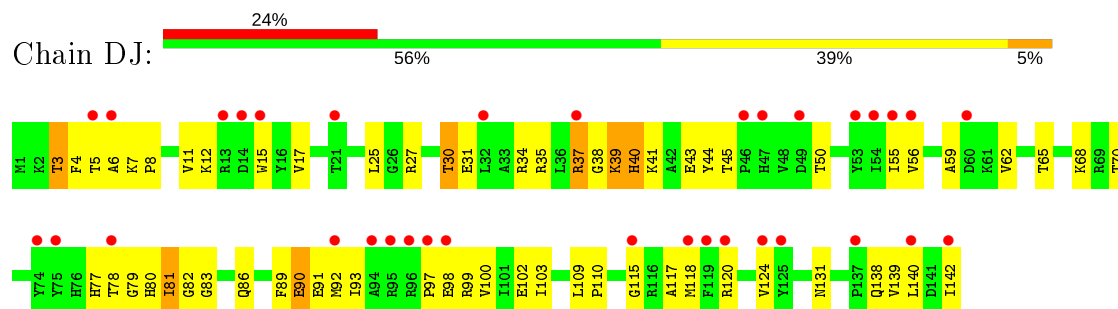
- Molecule 30: 50S ribosomal protein L11



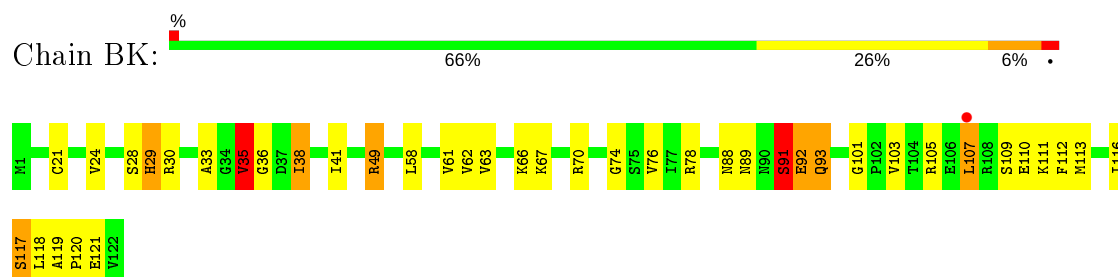
- Molecule 31: 50S ribosomal protein L13



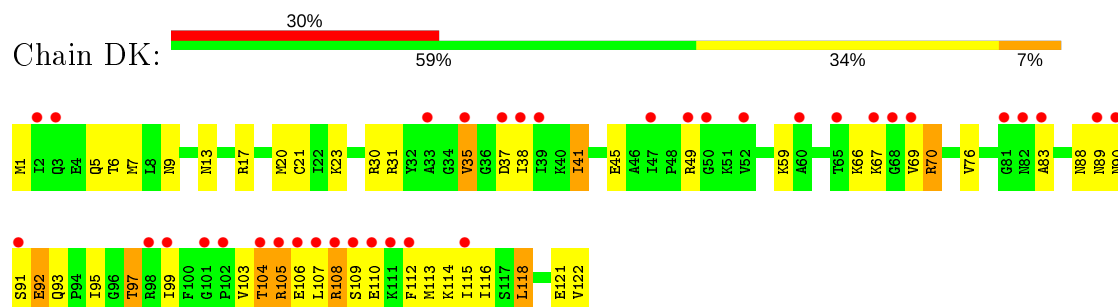
- Molecule 31: 50S ribosomal protein L13



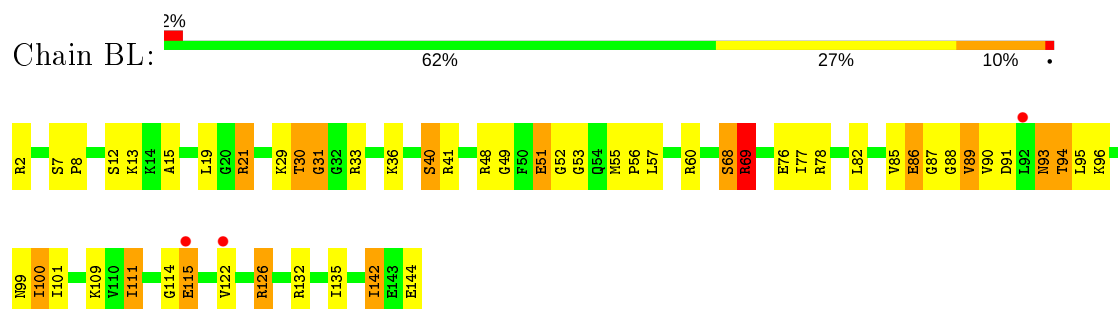
- Molecule 32: 50S ribosomal protein L14



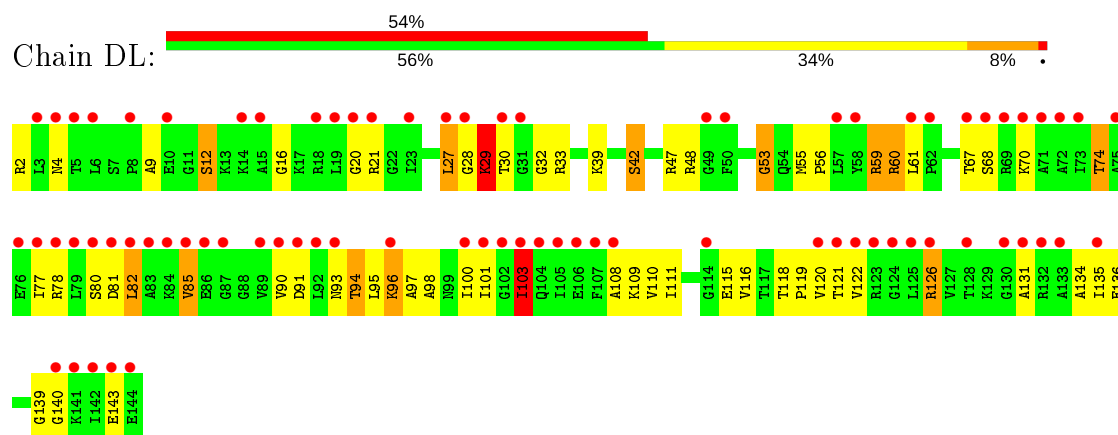
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15

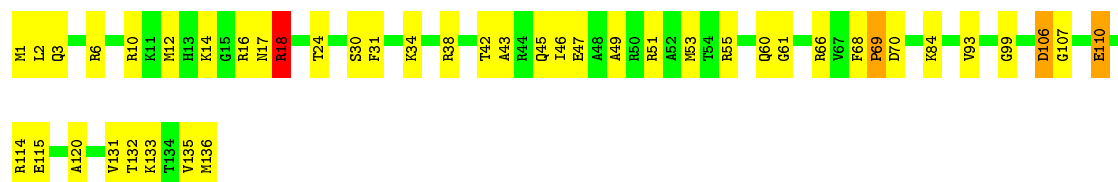


- Molecule 33: 50S ribosomal protein L15

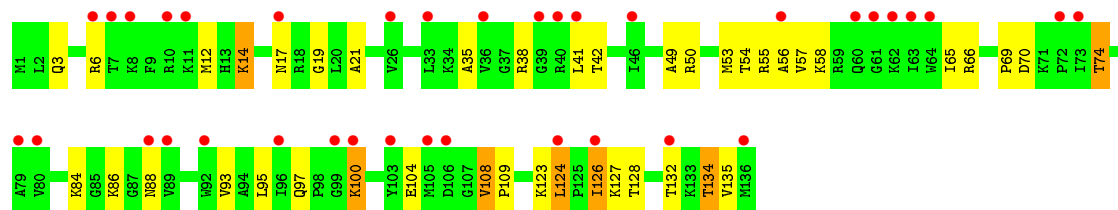


- Molecule 34: 50S ribosomal protein L16

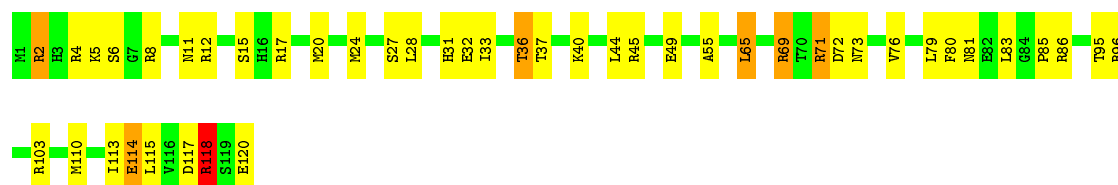




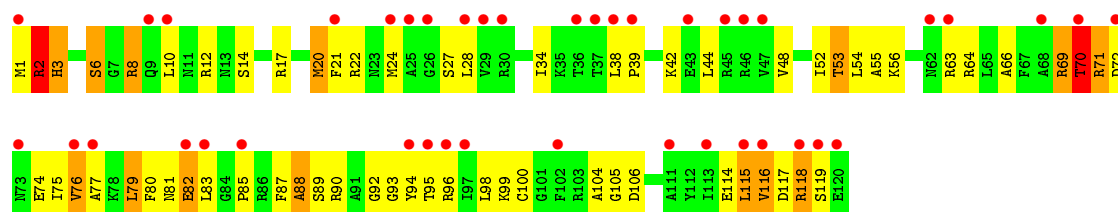
• Molecule 34: 50S ribosomal protein L16



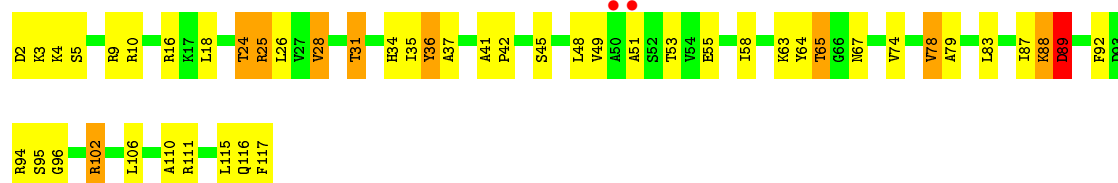
• Molecule 35: 50S ribosomal protein L17



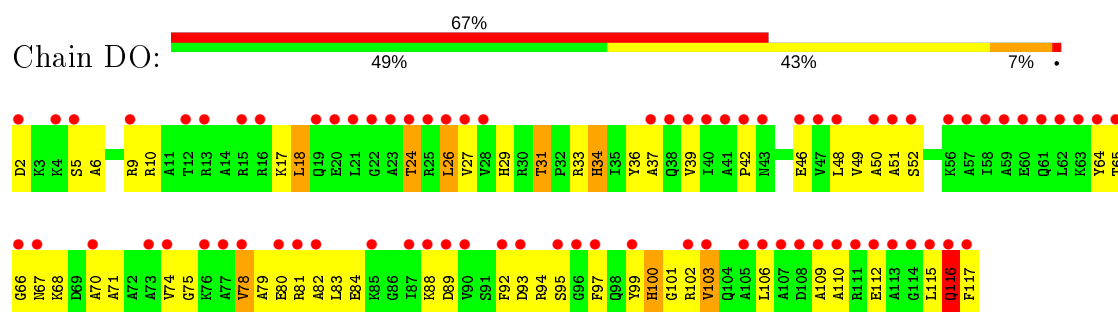
• Molecule 35: 50S ribosomal protein L17



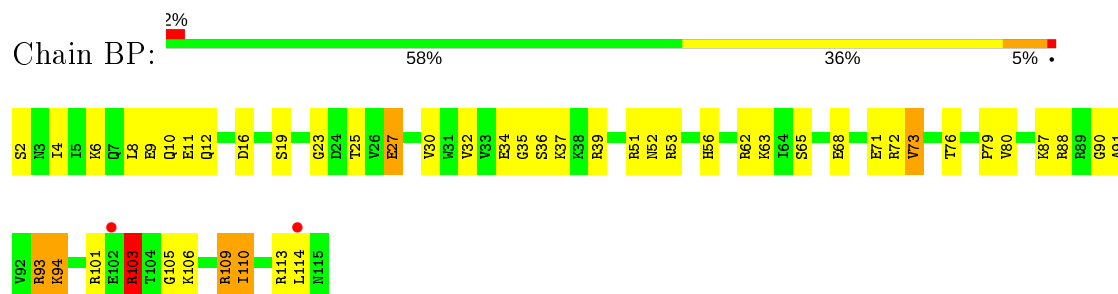
• Molecule 36: 50S ribosomal protein L18



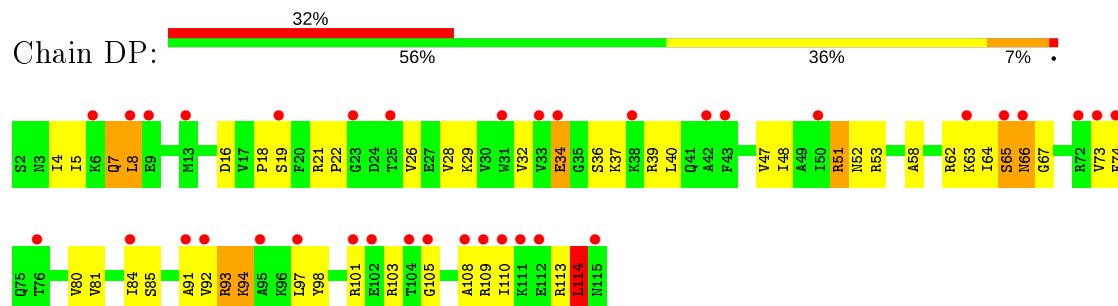
• Molecule 36: 50S ribosomal protein L18



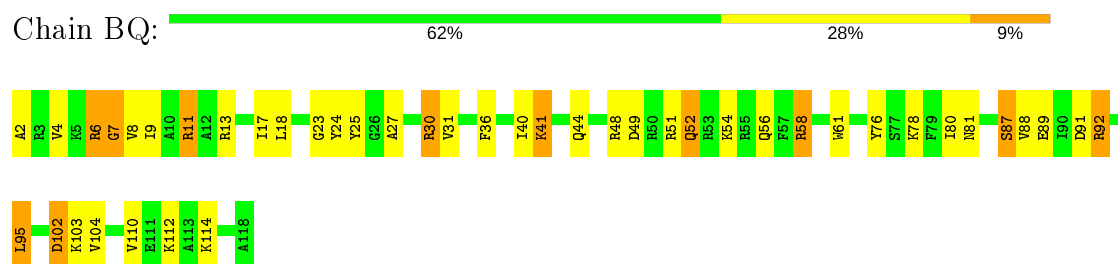
- Molecule 37: 50S ribosomal protein L19



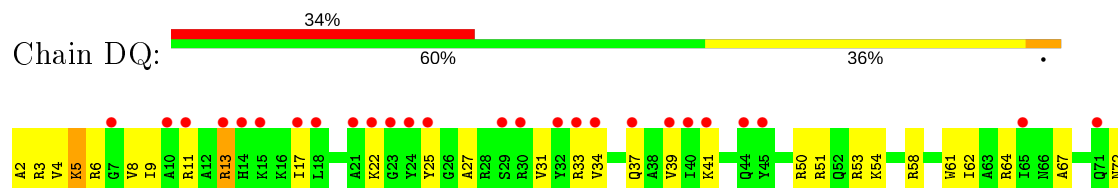
- Molecule 37: 50S ribosomal protein L19

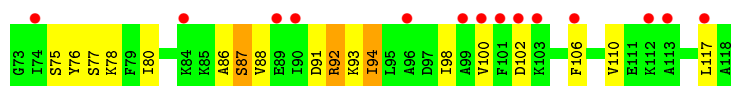


- Molecule 38: 50S ribosomal protein L20

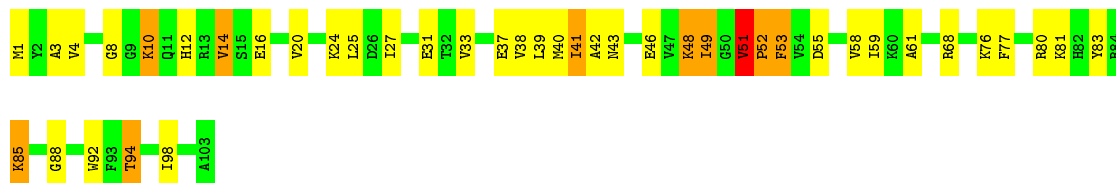


- Molecule 38: 50S ribosomal protein L20

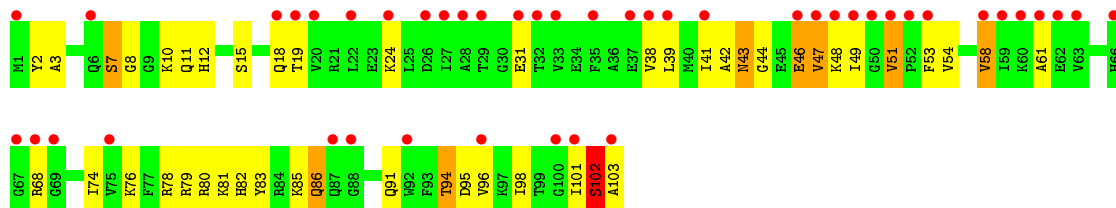




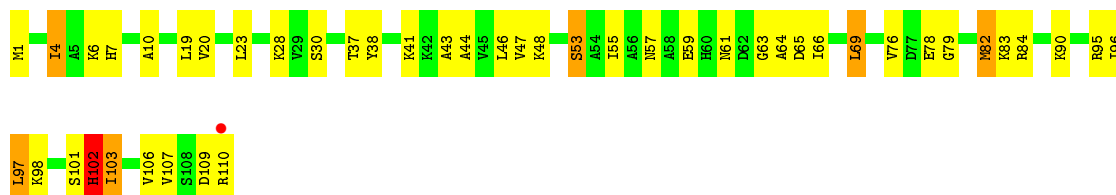
- Molecule 39: 50S ribosomal protein L21



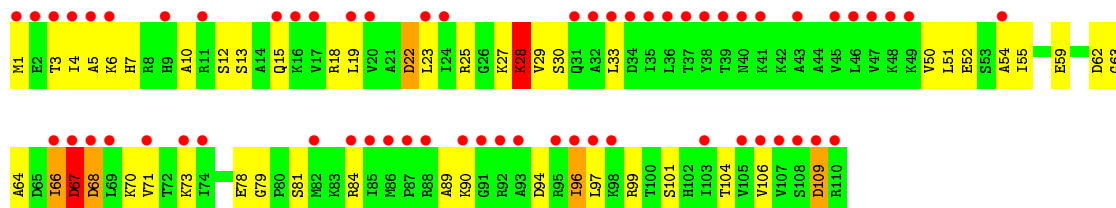
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L22

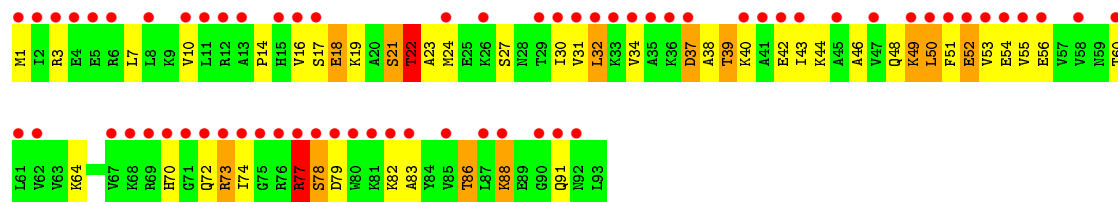
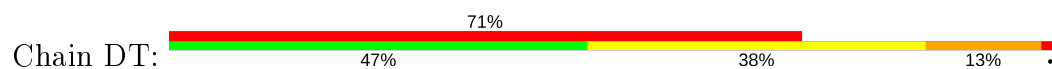


- Molecule 41: 50S ribosomal protein L23

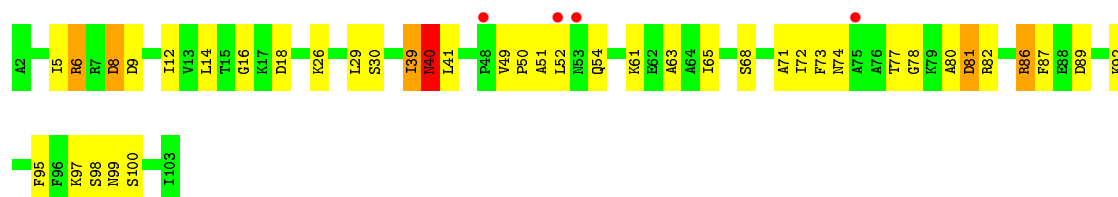




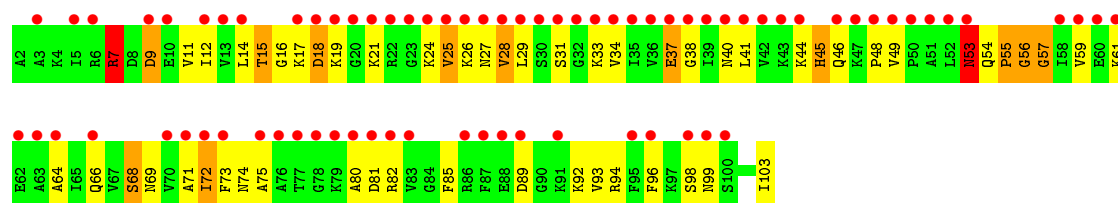
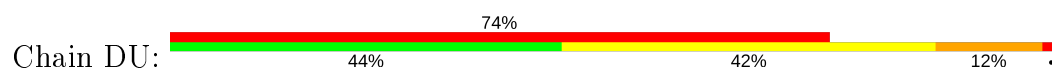
• Molecule 41: 50S ribosomal protein L23



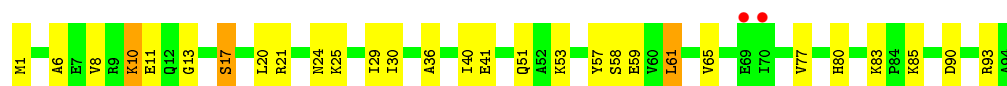
• Molecule 42: 50S ribosomal protein L24



• Molecule 42: 50S ribosomal protein L24

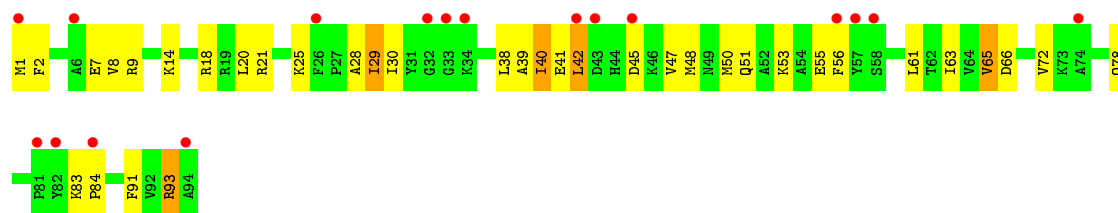


• Molecule 43: 50S ribosomal protein L25

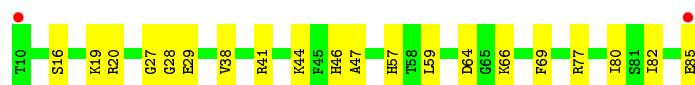
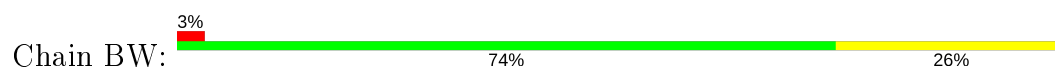


• Molecule 43: 50S ribosomal protein L25

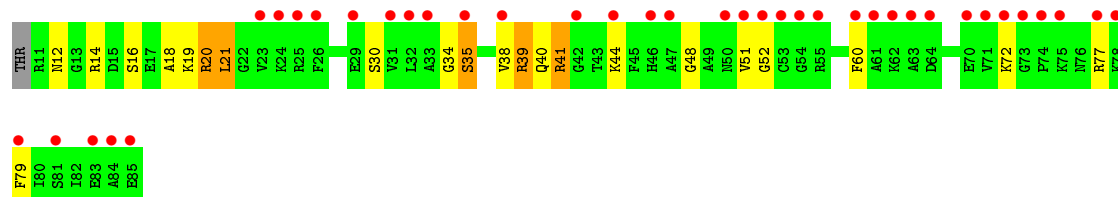
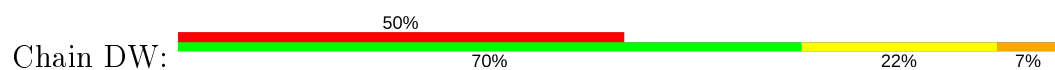




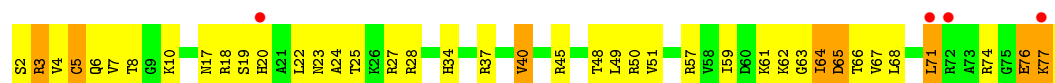
- Molecule 44: 50S ribosomal protein L27



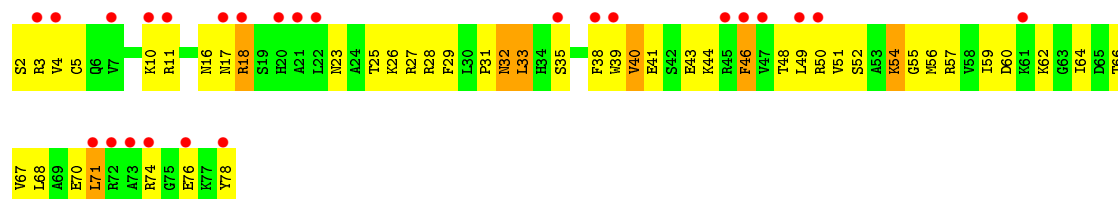
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28



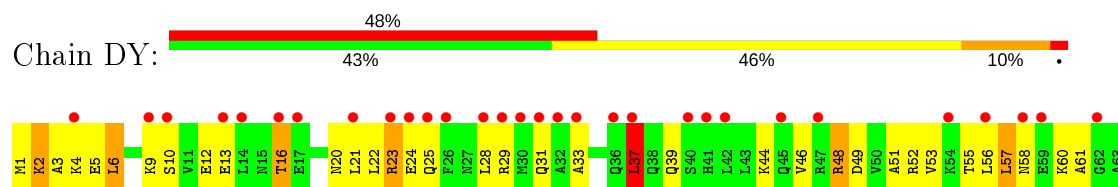
- Molecule 45: 50S ribosomal protein L28



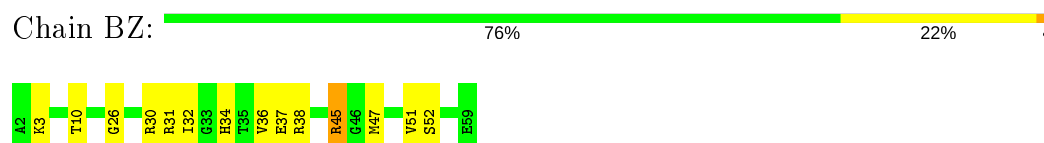
- Molecule 46: 50S ribosomal protein L29



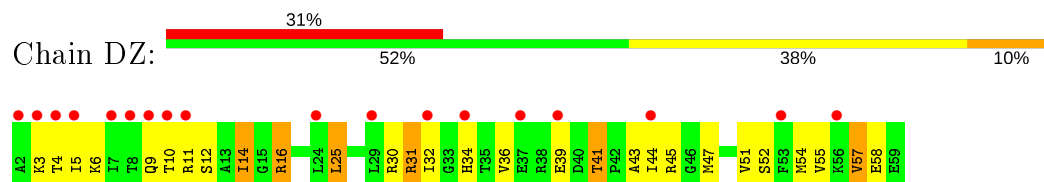
- Molecule 46: 50S ribosomal protein L29



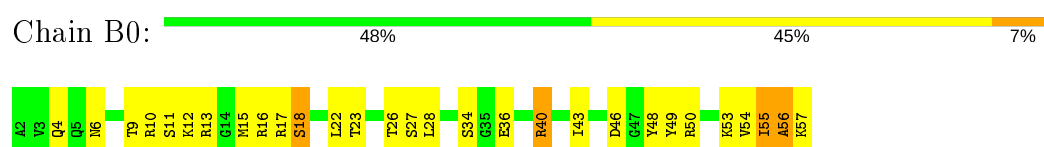
- Molecule 47: 50S ribosomal protein L30



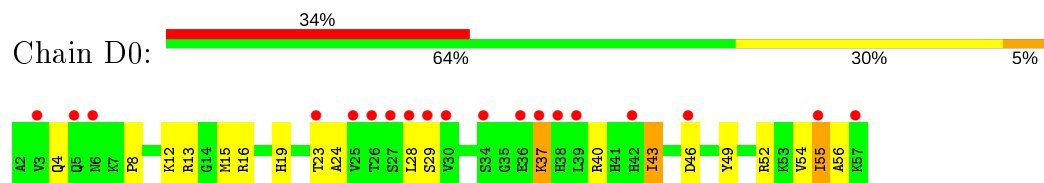
- Molecule 47: 50S ribosomal protein L30



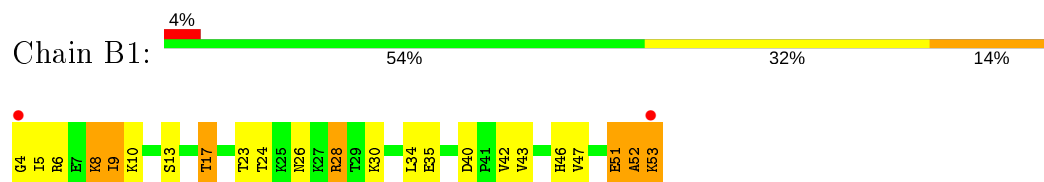
- Molecule 48: 50S ribosomal protein L32



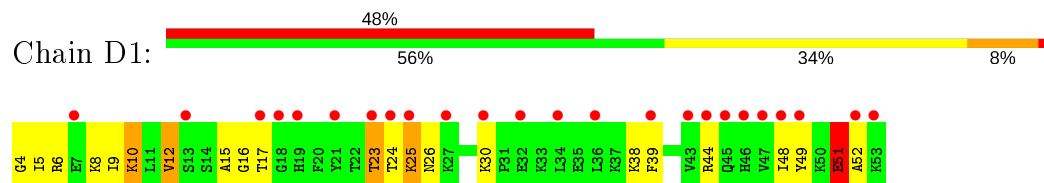
- Molecule 48: 50S ribosomal protein L32



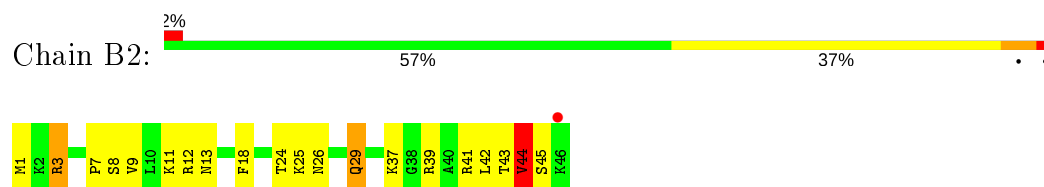
- Molecule 49: 50S ribosomal protein L33



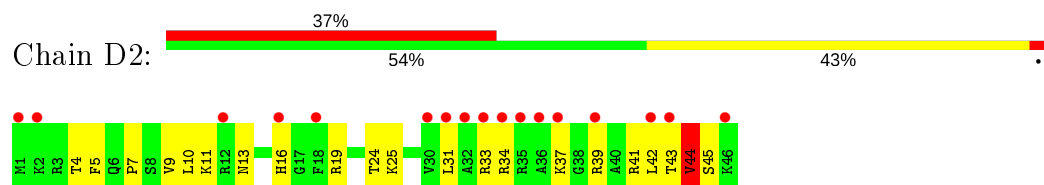
- Molecule 49: 50S ribosomal protein L33



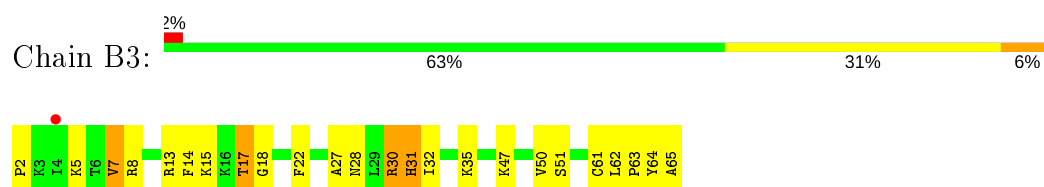
- Molecule 50: 50S ribosomal protein L34



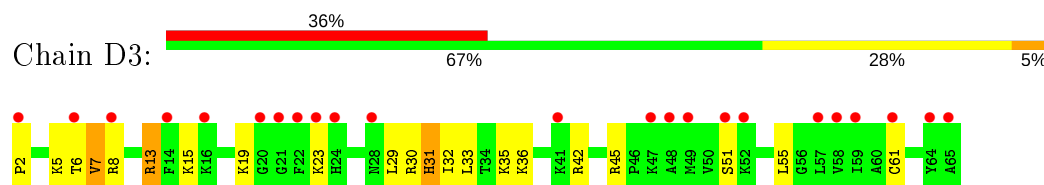
- Molecule 50: 50S ribosomal protein L34



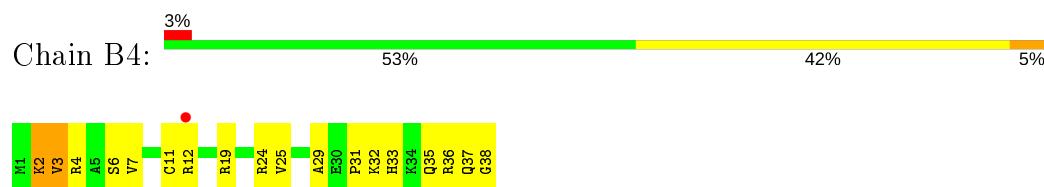
- Molecule 51: 50S ribosomal protein L35



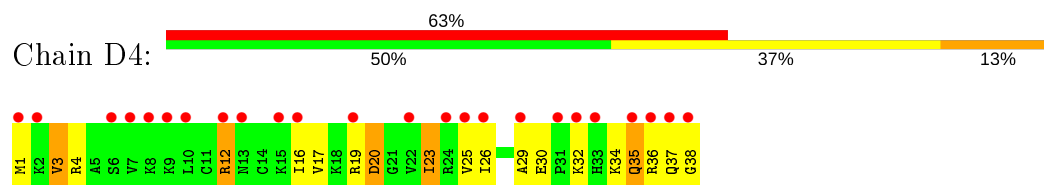
- Molecule 51: 50S ribosomal protein L35



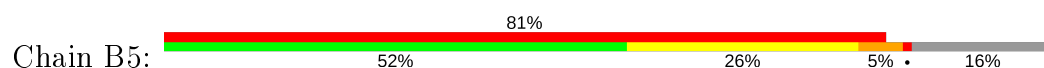
- Molecule 52: 50S ribosomal protein L36

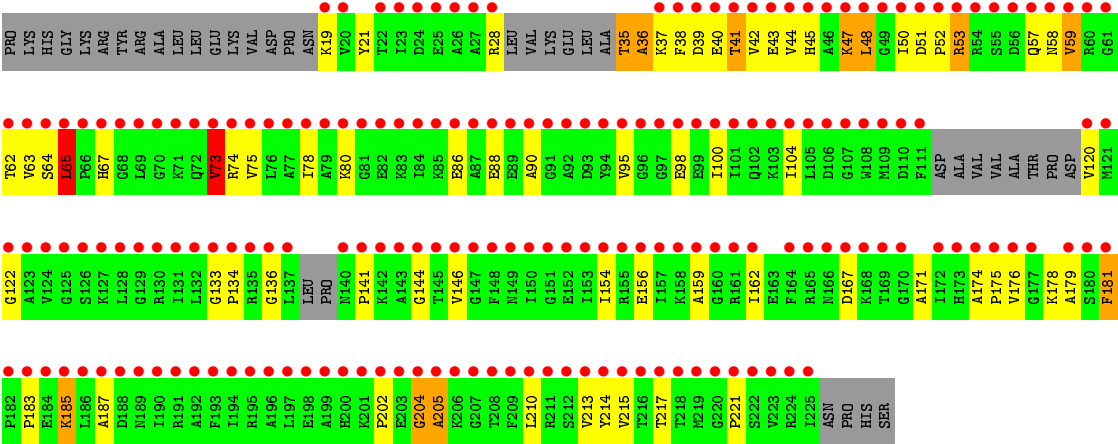


- Molecule 52: 50S ribosomal protein L36

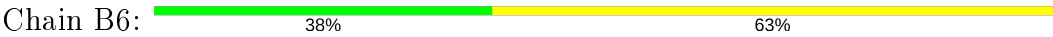


- Molecule 53: 50S ribosomal protein L1

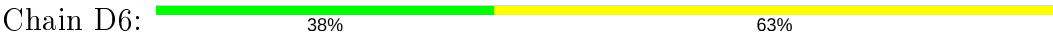




● Molecule 54: Quinupristin



● Molecule 54: Quinupristin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 432.73Å 631.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.68 – 2.95 68.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (68.68-2.95) 93.2 (68.68-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.248 , 0.282 0.252 , 0.287	Depositor DCC
R_{free} test set	4515 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	288328	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DBB, MG, 004, MHV, MHW, MHT, MHU

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	0.44	0/36944	1.04	74/57632 (0.1%)
1	CA	0.39	0/36966	0.99	74/57666 (0.1%)
2	AB	0.36	0/1736	0.72	1/2338 (0.0%)
2	CB	0.33	0/1736	0.70	0/2338
3	AC	0.35	0/1652	0.65	2/2225 (0.1%)
3	CC	0.32	0/1652	0.58	1/2225 (0.0%)
4	AD	0.35	0/1665	0.68	0/2227
4	CD	0.38	0/1665	0.71	1/2227 (0.0%)
5	AE	0.38	0/1119	0.74	0/1504
5	CE	0.37	0/1119	0.73	0/1504
6	AF	0.39	0/836	0.71	2/1128 (0.2%)
6	CF	0.34	0/836	0.68	0/1128
7	AG	0.32	0/1196	0.59	0/1602
7	CG	0.31	0/1196	0.56	0/1602
8	AH	0.36	0/989	0.67	0/1326
8	CH	0.30	0/989	0.59	0/1326
9	AI	0.32	0/1034	0.65	1/1375 (0.1%)
9	CI	0.32	0/1034	0.64	0/1375
10	AJ	0.35	0/797	0.65	0/1077
10	CJ	0.30	0/797	0.66	2/1077 (0.2%)
11	AK	0.35	0/893	0.63	0/1205
11	CK	0.32	0/893	0.63	0/1205
12	AL	0.39	0/969	0.69	0/1300
12	CL	0.35	0/969	0.72	0/1300
13	AM	0.33	0/893	0.69	0/1193
13	CM	0.33	0/893	0.65	0/1193
14	AN	0.31	0/785	0.66	0/1043
14	CN	0.29	0/785	0.57	0/1043
15	AO	0.31	0/718	0.61	0/959
15	CO	0.30	0/718	0.61	0/959
16	AP	0.39	0/659	0.72	1/884 (0.1%)
16	CP	0.33	0/659	0.59	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.72	1/881 (0.1%)
17	CQ	0.38	0/658	0.63	0/881
18	AR	0.31	0/463	0.60	0/621
18	CR	0.30	0/463	0.57	0/621
19	AS	0.32	0/653	0.63	0/877
19	CS	0.33	0/653	0.59	0/877
20	AT	0.36	0/671	0.64	0/888
20	CT	0.32	0/671	0.62	0/888
21	AU	0.43	0/431	0.75	0/570
21	CU	0.45	0/431	0.78	0/570
22	BA	0.68	6/69659 (0.0%)	1.32	534/108672 (0.5%)
22	DA	0.38	0/69659	0.99	76/108672 (0.1%)
23	BB	0.62	1/2850 (0.0%)	1.22	7/4444 (0.2%)
23	DB	0.32	0/2828	0.92	2/4410 (0.0%)
24	BC	0.45	0/2122	0.71	0/2852
24	DC	0.34	0/2122	0.62	0/2852
25	BD	0.50	0/1586	0.74	1/2134 (0.0%)
25	DD	0.32	0/1586	0.59	0/2134
26	BE	0.42	0/1571	0.70	0/2113
26	DE	0.34	0/1571	0.62	1/2113 (0.0%)
27	BF	0.37	0/1435	0.63	0/1926
27	DF	0.30	0/1435	0.56	0/1926
28	BG	0.39	0/1343	0.69	1/1816 (0.1%)
28	DG	0.31	0/1343	0.55	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.38	0/1046	0.69	0/1410
30	DI	0.35	0/1046	0.67	0/1410
31	BJ	0.49	0/1152	0.70	0/1551
31	DJ	0.31	0/1152	0.59	0/1551
32	BK	0.51	0/948	0.73	0/1268
32	DK	0.34	0/948	0.58	0/1268
33	BL	0.45	0/1054	0.80	2/1403 (0.1%)
33	DL	0.32	0/1054	0.62	0/1403
34	BM	0.48	0/1093	0.73	1/1460 (0.1%)
34	DM	0.30	0/1093	0.57	0/1460
35	BN	0.47	0/974	0.77	0/1301
35	DN	0.33	0/974	0.59	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.29	0/902	0.53	0/1209
37	BP	0.47	0/929	0.72	1/1242 (0.1%)
37	DP	0.32	0/929	0.59	1/1242 (0.1%)
38	BQ	0.56	0/960	0.73	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.32	0/960	0.53	0/1278
39	BR	0.53	0/829	0.82	1/1107 (0.1%)
39	DR	0.34	0/829	0.66	0/1107
40	BS	0.71	2/864 (0.2%)	0.89	2/1156 (0.2%)
40	DS	0.33	0/864	0.63	0/1156
41	BT	0.45	0/745	0.70	0/994
41	DT	0.33	0/745	0.61	0/994
42	BU	0.43	0/788	0.72	0/1051
42	DU	0.37	0/788	0.61	0/1051
43	BV	0.40	0/766	0.67	1/1025 (0.1%)
43	DV	0.28	0/766	0.54	0/1025
44	BW	0.52	0/587	0.69	0/776
44	DW	0.29	0/576	0.54	0/762
45	BX	0.39	0/635	0.67	0/848
45	DX	0.32	0/635	0.61	0/848
46	BY	0.39	0/510	0.76	0/677
46	DY	0.32	0/510	0.64	0/677
47	BZ	0.52	0/453	0.74	0/605
47	DZ	0.30	0/453	0.56	0/605
48	B0	0.52	0/450	0.75	0/599
48	D0	0.31	0/450	0.61	0/599
49	B1	0.44	0/417	0.69	0/554
49	D1	0.32	0/417	0.56	0/554
50	B2	0.48	0/380	0.80	0/498
50	D2	0.30	0/380	0.58	0/498
51	B3	0.43	0/513	0.71	0/676
51	D3	0.29	0/513	0.49	0/676
52	B4	0.52	0/303	0.66	0/397
52	D4	0.37	0/303	0.58	0/397
53	B5	0.32	0/1145	0.69	1/1556 (0.1%)
54	B6	1.71	0/13	2.43	1/15 (6.7%)
54	D6	1.45	0/13	2.67	2/15 (13.3%)
All	All	0.47	9/310652 (0.0%)	1.01	796/464396 (0.2%)

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
2	CB	0	1
5	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	2
6	CF	0	1
11	AK	0	1
11	CK	0	1
12	CL	0	2
21	AU	0	2
21	CU	0	1
25	BD	0	1
25	DD	0	1
26	BE	0	1
40	BS	0	1
All	All	0	16

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-9.06	1.32	1.37
22	BA	1142	A	N9-C4	-8.98	1.32	1.37
40	BS	102	HIS	CB-CG	-6.45	1.38	1.50
22	BA	1936	A	N9-C4	-5.92	1.34	1.37
23	BB	99	A	N9-C4	-5.46	1.34	1.37

The worst 5 of 796 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	984	A	C2-N3-C4	-12.57	104.31	110.60
1	AA	1054	C	O5'-P-OP2	-12.23	94.69	105.70
22	BA	1936	A	C2-N3-C4	-10.65	105.28	110.60
25	BD	151	THR	C-N-CD	-10.63	97.20	120.60
22	BA	1142	A	C2-N3-C4	-10.48	105.36	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	123	VAL	Peptide
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	608	14
1	CA	33015	0	16616	645	0
2	AB	1705	0	1732	135	0
2	CB	1705	0	1732	109	0
3	AC	1625	0	1696	75	0
3	CC	1625	0	1696	67	0
4	AD	1643	0	1707	93	0
4	CD	1643	0	1707	74	0
5	AE	1106	0	1148	60	0
5	CE	1106	0	1148	72	0
6	AF	818	0	808	37	0
6	CF	818	0	808	35	0
7	AG	1182	0	1238	47	0
7	CG	1182	0	1238	49	0
8	AH	979	0	1031	38	0
8	CH	979	0	1031	43	0
9	AI	1022	0	1070	51	0
9	CI	1022	0	1070	64	0
10	AJ	787	0	828	60	0
10	CJ	787	0	828	44	0
11	AK	877	0	887	54	0
11	CK	877	0	887	39	0
12	AL	955	0	1016	38	0
12	CL	955	0	1016	48	0
13	AM	884	0	941	49	0
13	CM	884	0	941	40	0
14	AN	774	0	824	44	0
14	CN	774	0	824	44	0
15	AO	710	0	728	20	0
15	CO	710	0	728	38	0
16	AP	649	0	666	34	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	30	0
17	CQ	649	0	691	33	0
18	AR	456	0	478	12	0
18	CR	456	0	478	25	0
19	AS	638	0	665	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	31	0
20	AT	665	0	714	31	0
20	CT	665	0	714	34	0
21	AU	426	0	449	39	0
21	CU	426	0	449	29	0
22	BA	62195	0	31280	1058	0
22	DA	62195	0	31280	1193	1
23	BB	2549	0	1291	19	0
23	DB	2529	0	1281	44	0
24	BC	2083	0	2154	76	0
24	DC	2083	0	2154	94	0
25	BD	1565	0	1616	48	0
25	DD	1565	0	1616	55	0
26	BE	1552	0	1619	47	0
26	DE	1552	0	1619	63	0
27	BF	1411	0	1444	51	0
27	DF	1411	0	1444	50	0
28	BG	1323	0	1371	44	0
28	DG	1323	0	1371	39	0
29	BH	1110	0	1145	196	0
29	DH	1110	0	1148	91	13
30	BI	1032	0	1085	52	0
30	DI	1032	0	1085	54	0
31	BJ	1129	0	1162	28	0
31	DJ	1129	0	1162	48	0
32	BK	939	0	1012	30	0
32	DK	939	0	1012	29	0
33	BL	1045	0	1117	38	0
33	DL	1045	0	1117	46	0
34	BM	1074	0	1157	30	0
34	DM	1074	0	1157	20	0
35	BN	961	0	1000	35	0
35	DN	961	0	1000	47	0
36	BO	892	0	923	25	0
36	DO	892	0	923	42	0
37	BP	917	0	962	39	0
37	DP	917	0	962	34	0
38	BQ	947	0	1019	35	0
38	DQ	947	0	1019	44	0
39	BR	816	0	839	37	0
39	DR	816	0	839	34	0
40	BS	857	0	922	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	25	0
41	BT	739	0	807	27	0
41	DT	739	0	807	27	0
42	BU	780	0	831	18	0
42	DU	780	0	831	44	0
43	BV	753	0	780	14	0
43	DV	753	0	780	27	0
44	BW	580	0	594	14	0
44	DW	569	0	581	18	0
45	BX	625	0	652	29	0
45	DX	625	0	652	46	0
46	BY	509	0	543	25	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	7	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	20	0
48	D0	444	0	458	16	0
49	B1	410	0	440	15	0
49	D1	410	0	440	14	0
50	B2	377	0	418	13	0
50	D2	377	0	418	14	0
51	B3	504	0	572	18	0
51	D3	504	0	572	17	0
52	B4	302	0	341	15	0
52	D4	302	0	340	12	0
53	B5	1142	0	865	27	0
54	B6	73	0	64	5	0
54	D6	73	0	64	7	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	6	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AT	2	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	619	0	0	59	0
57	BB	13	0	0	1	0
57	BC	8	0	0	1	0
57	BD	3	0	0	2	0
57	BE	3	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	5	0	0	1	0
57	BN	5	0	0	1	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	10	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	1	0
57	D0	1	0	0	0	0
57	D2	2	0	0	1	0
57	D3	1	0	0	0	0
57	D4	1	0	0	0	0
57	DA	612	0	0	63	0
57	DB	13	0	0	0	0
57	DC	7	0	0	1	0
57	DD	4	0	0	1	0
57	DE	4	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DQ	2	0	0	0	0
57	DT	3	0	0	0	0
57	DV	1	0	0	0	0
All	All	288328	0	192913	6784	14

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 15.

The worst 5 of 6784 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)
29:BH:83:LYS:HD2	1:CA:55:A:O2'	1.21	1.29
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
29:BH:123:ARG:O	29:BH:124:THR:CG2	2.01	1.09
29:BH:97:ARG:HD2	1:CA:369:G:O2'	1.51	1.09

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.50	0.70
1:AA:55:A:N1	29:DH:91:PHE:CE1[4_455]	1.60	0.60
1:AA:55:A:N3	29:DH:91:PHE:CZ[4_455]	1.66	0.54
1:AA:55:A:C2	29:DH:91:PHE:CE1[4_455]	1.70	0.50
1:AA:55:A:C2	29:DH:91:PHE:CZ[4_455]	1.71	0.49

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	130 (60%)	40 (18%)	46 (21%)	0	0
2	CB	216/218 (99%)	134 (62%)	47 (22%)	35 (16%)	0	0
3	AC	204/206 (99%)	158 (78%)	30 (15%)	16 (8%)	1	3
3	CC	204/206 (99%)	156 (76%)	33 (16%)	15 (7%)	1	4
4	AD	203/205 (99%)	150 (74%)	29 (14%)	24 (12%)	0	1
4	CD	203/205 (99%)	152 (75%)	29 (14%)	22 (11%)	0	1
5	AE	148/150 (99%)	112 (76%)	20 (14%)	16 (11%)	0	1
5	CE	148/150 (99%)	103 (70%)	20 (14%)	25 (17%)	0	0
6	AF	98/100 (98%)	72 (74%)	15 (15%)	11 (11%)	0	1
6	CF	98/100 (98%)	69 (70%)	14 (14%)	15 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	30 (20%)	9 (6%)	1	7
7	CG	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	1	7
8	AH	127/129 (98%)	94 (74%)	26 (20%)	7 (6%)	2	8
8	CH	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	2	8
9	AI	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	1	4
9	CI	125/127 (98%)	97 (78%)	20 (16%)	8 (6%)	1	5
10	AJ	96/98 (98%)	67 (70%)	12 (12%)	17 (18%)	0	0
10	CJ	96/98 (98%)	70 (73%)	14 (15%)	12 (12%)	0	1
11	AK	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	3
11	CK	115/117 (98%)	85 (74%)	21 (18%)	9 (8%)	1	3
12	AL	121/123 (98%)	96 (79%)	19 (16%)	6 (5%)	2	10
12	CL	121/123 (98%)	97 (80%)	13 (11%)	11 (9%)	1	2
13	AM	112/114 (98%)	85 (76%)	16 (14%)	11 (10%)	0	2
13	CM	112/114 (98%)	82 (73%)	19 (17%)	11 (10%)	0	2
14	AN	92/100 (92%)	61 (66%)	20 (22%)	11 (12%)	0	1
14	CN	92/100 (92%)	61 (66%)	15 (16%)	16 (17%)	0	0
15	AO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	17
15	CO	86/88 (98%)	68 (79%)	14 (16%)	4 (5%)	2	11
16	AP	80/82 (98%)	49 (61%)	15 (19%)	16 (20%)	0	0
16	CP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	2	10
17	AQ	78/80 (98%)	57 (73%)	11 (14%)	10 (13%)	0	1
17	CQ	78/80 (98%)	53 (68%)	17 (22%)	8 (10%)	0	2
18	AR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	4
18	CR	53/55 (96%)	40 (76%)	8 (15%)	5 (9%)	0	2
19	AS	77/79 (98%)	55 (71%)	14 (18%)	8 (10%)	0	2
19	CS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	3	14
20	AT	83/85 (98%)	66 (80%)	12 (14%)	5 (6%)	1	7
20	CT	83/85 (98%)	68 (82%)	9 (11%)	6 (7%)	1	4
21	AU	49/51 (96%)	29 (59%)	9 (18%)	11 (22%)	0	0
21	CU	49/51 (96%)	29 (59%)	6 (12%)	14 (29%)	0	0
24	BC	269/271 (99%)	217 (81%)	41 (15%)	11 (4%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	209 (78%)	42 (16%)	18 (7%)	1	5
25	BD	207/209 (99%)	183 (88%)	19 (9%)	5 (2%)	6	26
25	DD	207/209 (99%)	173 (84%)	29 (14%)	5 (2%)	6	26
26	BE	199/201 (99%)	171 (86%)	22 (11%)	6 (3%)	4	20
26	DE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	5
27	BF	175/177 (99%)	144 (82%)	23 (13%)	8 (5%)	2	11
27	DF	175/177 (99%)	146 (83%)	17 (10%)	12 (7%)	1	4
28	BG	174/176 (99%)	147 (84%)	15 (9%)	12 (7%)	1	4
28	DG	174/176 (99%)	138 (79%)	25 (14%)	11 (6%)	1	6
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	2
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	80 (58%)	44 (32%)	15 (11%)	0	1
31	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	3	16
31	DJ	140/142 (99%)	123 (88%)	15 (11%)	2 (1%)	11	39
32	BK	120/122 (98%)	98 (82%)	13 (11%)	9 (8%)	1	4
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	2	10
33	BL	141/143 (99%)	109 (77%)	20 (14%)	12 (8%)	1	3
33	DL	141/143 (99%)	105 (74%)	29 (21%)	7 (5%)	2	10
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	10	38
34	DM	134/136 (98%)	112 (84%)	19 (14%)	3 (2%)	6	28
35	BN	118/120 (98%)	96 (81%)	21 (18%)	1 (1%)	19	53
35	DN	118/120 (98%)	97 (82%)	11 (9%)	10 (8%)	1	3
36	BO	114/116 (98%)	95 (83%)	15 (13%)	4 (4%)	3	17
36	DO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	3	17
37	BP	112/114 (98%)	98 (88%)	9 (8%)	5 (4%)	2	12
37	DP	112/114 (98%)	91 (81%)	16 (14%)	5 (4%)	2	12
38	BQ	115/117 (98%)	107 (93%)	3 (3%)	5 (4%)	2	12
38	DQ	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	17	51
39	BR	101/103 (98%)	86 (85%)	8 (8%)	7 (7%)	1	4
39	DR	101/103 (98%)	77 (76%)	20 (20%)	4 (4%)	3	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	5	22
40	DS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	11
41	BT	91/93 (98%)	70 (77%)	13 (14%)	8 (9%)	1	3
41	DT	91/93 (98%)	70 (77%)	9 (10%)	12 (13%)	0	1
42	BU	100/102 (98%)	80 (80%)	12 (12%)	8 (8%)	1	3
42	DU	100/102 (98%)	73 (73%)	17 (17%)	10 (10%)	0	2
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14	46
43	DV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	6	28
44	BW	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
44	DW	73/76 (96%)	65 (89%)	6 (8%)	2 (3%)	5	23
45	BX	75/77 (97%)	72 (96%)	1 (1%)	2 (3%)	5	23
45	DX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	23
46	BY	61/63 (97%)	40 (66%)	12 (20%)	9 (15%)	0	1
46	DY	61/63 (97%)	49 (80%)	8 (13%)	4 (7%)	1	5
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3	16
48	B0	54/56 (96%)	46 (85%)	5 (9%)	3 (6%)	2	8
48	D0	54/56 (96%)	41 (76%)	11 (20%)	2 (4%)	3	15
49	B1	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	3
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	1	6
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	12
50	D2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	12
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	36
51	D3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	36
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	1 (3%)	2 (6%)	2	8
53	B5	183/228 (80%)	94 (51%)	54 (30%)	35 (19%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	2 (100%)	0	0	100	100
All	All	11422/11688 (98%)	8887 (78%)	1654 (14%)	881 (8%)	1	4

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS
2	AB	73	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	113 (63%)	67 (37%)	0	0
2	CB	180/180 (100%)	129 (72%)	51 (28%)	0	1
3	AC	170/170 (100%)	132 (78%)	38 (22%)	1	3
3	CC	170/170 (100%)	131 (77%)	39 (23%)	1	3
4	AD	172/172 (100%)	129 (75%)	43 (25%)	0	2
4	CD	172/172 (100%)	138 (80%)	34 (20%)	1	6
5	AE	113/113 (100%)	85 (75%)	28 (25%)	0	2
5	CE	113/113 (100%)	85 (75%)	28 (25%)	0	2
6	AF	87/87 (100%)	64 (74%)	23 (26%)	0	2
6	CF	87/87 (100%)	63 (72%)	24 (28%)	0	1
7	AG	124/124 (100%)	94 (76%)	30 (24%)	0	2
7	CG	124/124 (100%)	91 (73%)	33 (27%)	0	2
8	AH	104/104 (100%)	79 (76%)	25 (24%)	0	2
8	CH	104/104 (100%)	83 (80%)	21 (20%)	1	5
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	1
9	CI	105/105 (100%)	77 (73%)	28 (27%)	0	2
10	AJ	86/86 (100%)	64 (74%)	22 (26%)	0	2
10	CJ	86/86 (100%)	67 (78%)	19 (22%)	1	3
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	2
11	CK	90/90 (100%)	69 (77%)	21 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	84 (82%)	19 (18%)	1	7
12	CL	103/103 (100%)	78 (76%)	25 (24%)	0	2
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	6
13	CM	92/92 (100%)	70 (76%)	22 (24%)	0	2
14	AN	79/83 (95%)	61 (77%)	18 (23%)	1	3
14	CN	79/83 (95%)	68 (86%)	11 (14%)	3	14
15	AO	75/76 (99%)	59 (79%)	16 (21%)	1	4
15	CO	75/76 (99%)	57 (76%)	18 (24%)	0	2
16	AP	65/65 (100%)	52 (80%)	13 (20%)	1	5
16	CP	65/65 (100%)	49 (75%)	16 (25%)	0	2
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	1
17	CQ	74/74 (100%)	53 (72%)	21 (28%)	0	1
18	AR	48/48 (100%)	41 (85%)	7 (15%)	3	13
18	CR	48/48 (100%)	39 (81%)	9 (19%)	1	7
19	AS	70/70 (100%)	57 (81%)	13 (19%)	1	7
19	CS	70/70 (100%)	55 (79%)	15 (21%)	1	4
20	AT	65/65 (100%)	46 (71%)	19 (29%)	0	1
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	2
21	AU	44/44 (100%)	27 (61%)	17 (39%)	0	0
21	CU	44/44 (100%)	32 (73%)	12 (27%)	0	1
24	BC	216/216 (100%)	190 (88%)	26 (12%)	5	19
24	DC	216/216 (100%)	180 (83%)	36 (17%)	2	9
25	BD	164/164 (100%)	147 (90%)	17 (10%)	7	24
25	DD	164/164 (100%)	144 (88%)	20 (12%)	5	19
26	BE	165/165 (100%)	138 (84%)	27 (16%)	2	9
26	DE	165/165 (100%)	133 (81%)	32 (19%)	1	6
27	BF	148/148 (100%)	121 (82%)	27 (18%)	1	7
27	DF	148/148 (100%)	118 (80%)	30 (20%)	1	5
28	BG	137/137 (100%)	117 (85%)	20 (15%)	3	13
28	DG	137/137 (100%)	123 (90%)	14 (10%)	7	25
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	3
30	BI	109/109 (100%)	86 (79%)	23 (21%)	1	4
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	3
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	6	22
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	5	19
32	BK	103/103 (100%)	93 (90%)	10 (10%)	8	28
32	DK	103/103 (100%)	90 (87%)	13 (13%)	4	17
33	BL	102/102 (100%)	85 (83%)	17 (17%)	2	9
33	DL	102/102 (100%)	81 (79%)	21 (21%)	1	4
34	BM	109/109 (100%)	97 (89%)	12 (11%)	6	22
34	DM	109/109 (100%)	97 (89%)	12 (11%)	6	22
35	BN	100/100 (100%)	87 (87%)	13 (13%)	4	16
35	DN	100/100 (100%)	83 (83%)	17 (17%)	2	9
36	BO	86/86 (100%)	64 (74%)	22 (26%)	0	2
36	DO	86/86 (100%)	72 (84%)	14 (16%)	2	9
37	BP	99/99 (100%)	88 (89%)	11 (11%)	6	22
37	DP	99/99 (100%)	80 (81%)	19 (19%)	1	6
38	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	9
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	13
39	BR	84/84 (100%)	73 (87%)	11 (13%)	4	16
39	DR	84/84 (100%)	70 (83%)	14 (17%)	2	9
40	BS	93/93 (100%)	78 (84%)	15 (16%)	2	10
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	8
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	12
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	8
42	BU	83/83 (100%)	68 (82%)	15 (18%)	1	7
42	DU	83/83 (100%)	64 (77%)	19 (23%)	1	3
43	BV	78/78 (100%)	66 (85%)	12 (15%)	2	11
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	14
44	BW	57/58 (98%)	53 (93%)	4 (7%)	15	43
44	DW	56/58 (97%)	49 (88%)	7 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	7
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	7
46	BY	55/55 (100%)	48 (87%)	7 (13%)	4	17
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	4
47	BZ	48/48 (100%)	43 (90%)	5 (10%)	7	24
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	4
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	12
48	D0	47/47 (100%)	42 (89%)	5 (11%)	6	24
49	B1	45/45 (100%)	38 (84%)	7 (16%)	2	11
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	15
50	B2	38/38 (100%)	32 (84%)	6 (16%)	2	10
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	10
51	B3	51/51 (100%)	46 (90%)	5 (10%)	8	27
51	D3	51/51 (100%)	46 (90%)	5 (10%)	8	27
52	B4	34/34 (100%)	30 (88%)	4 (12%)	5	20
52	D4	34/34 (100%)	28 (82%)	6 (18%)	2	8
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	4
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7570 (81%)	1820 (19%)	1	6

5 of 1820 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	81	ASP
4	CD	138	SER
39	DR	43	ASN
45	BX	48	THR
2	CB	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
45	BX	34	HIS

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Mol	Chain	Res	Type
3	CC	176	HIS
41	DT	59	ASN
2	CB	18	HIS
2	CB	51	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	357 (23%)	16 (1%)
1	CA	1538/1539 (99%)	337 (21%)	9 (0%)
22	BA	2895/2903 (99%)	563 (19%)	28 (0%)
22	DA	2895/2903 (99%)	643 (22%)	34 (1%)
23	BB	118/119 (99%)	23 (19%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	1948 (21%)	87 (0%)

5 of 1948 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	13	U

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2286	G
1	CA	559	A
22	DA	2296	U
22	BA	2326	C
1	CA	96	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	004	D6	7	54	9,10,11	0.55	0	9,12,14	0.56	0
54	MHU	B6	5	54	14,15,16	1.71	3 (21%)	18,19,21	1.55	4 (22%)
54	MHV	B6	6	54	7,9,10	1.41	1 (14%)	7,11,13	3.59	3 (42%)
54	MHW	D6	1	54	9,9,10	1.76	1 (11%)	10,11,13	3.43	4 (40%)
54	MHW	B6	1	54	9,9,10	1.63	1 (11%)	10,11,13	2.52	4 (40%)
54	004	B6	7	54	9,10,11	1.50	1 (11%)	9,12,14	2.51	4 (44%)
54	DBB	D6	3	54	4,5,6	1.15	0	1,5,7	2.63	1 (100%)
54	MHU	D6	5	54	14,15,16	1.93	3 (21%)	18,19,21	2.11	2 (11%)
54	MHV	D6	6	54	7,9,10	0.93	0	7,11,13	3.83	4 (57%)
54	DBB	B6	3	54	4,5,6	1.48	1 (25%)	1,5,7	2.96	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	004	D6	7	54	-	2/4/6/8	0/1/1/1
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	004	B6	7	54	-	1/4/6/8	0/1/1/1
54	DBB	D6	3	54	-	0/3/4/6	-
54	MHU	D6	5	54	-	0/9/12/14	0/1/1/1
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	DBB	B6	3	54	-	0/3/4/6	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	5	MHU	CZ-NZ	5.60	1.50	1.37
54	B6	5	MHU	CZ-NZ	5.08	1.49	1.37
54	D6	1	MHW	CA-C	4.31	1.53	1.48
54	B6	7	004	CB-CA	-4.21	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	1	MHW	CA-C	3.78	1.52	1.48

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-8.94	90.50	110.03
54	B6	6	MHV	CD2-CE-N	-8.15	92.22	110.03
54	D6	5	MHU	CG-CB-CA	7.90	124.94	113.63
54	D6	1	MHW	CD-CE-N	7.04	134.92	123.43
54	D6	1	MHW	O-C-CA	-5.68	118.84	124.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	7	004	C-CA-CB-CG1
54	D6	7	004	C-CA-CB-CG2
54	B6	7	004	C-CA-CB-CG1

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	D6	7	004	6	0
54	B6	5	MHU	1	0
54	D6	6	MHV	3	0
54	B6	3	DBB	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	0.07	46 (2%) 50 34	15, 50, 134, 177	0
1	CA	1539/1539 (100%)	0.42	117 (7%) 13 7	29, 71, 143, 177	0
2	AB	218/218 (100%)	1.00	43 (19%) 1 0	39, 71, 98, 131	0
2	CB	218/218 (100%)	1.53	79 (36%) 0 0	55, 80, 108, 126	0
3	AC	206/206 (100%)	0.36	13 (6%) 20 11	36, 56, 81, 95	0
3	CC	206/206 (100%)	1.57	63 (30%) 0 0	52, 73, 93, 114	0
4	AD	205/205 (100%)	0.80	27 (13%) 3 2	33, 55, 80, 109	0
4	CD	205/205 (100%)	0.38	15 (7%) 15 8	23, 40, 75, 93	0
5	AE	150/150 (100%)	0.43	5 (3%) 46 30	32, 49, 82, 111	0
5	CE	150/150 (100%)	0.65	11 (7%) 15 8	35, 56, 83, 105	0
6	AF	100/100 (100%)	0.34	8 (8%) 12 7	34, 55, 75, 85	0
6	CF	100/100 (100%)	0.88	16 (16%) 1 1	44, 72, 97, 105	0
7	AG	151/151 (100%)	1.14	34 (22%) 0 0	48, 73, 96, 107	0
7	CG	151/151 (100%)	3.14	101 (66%) 0 0	75, 92, 105, 113	0
8	AH	129/129 (100%)	0.31	2 (1%) 72 55	28, 47, 71, 80	0
8	CH	129/129 (100%)	0.91	17 (13%) 3 2	46, 63, 83, 90	0
9	AI	127/127 (100%)	1.07	25 (19%) 1 0	42, 68, 96, 115	0
9	CI	127/127 (100%)	2.14	62 (48%) 0 0	64, 87, 106, 131	0
10	AJ	98/98 (100%)	1.07	16 (16%) 1 1	42, 62, 93, 120	0
10	CJ	98/98 (100%)	3.36	65 (66%) 0 0	66, 89, 108, 122	0
11	AK	117/117 (100%)	0.90	20 (17%) 1 1	29, 61, 88, 106	0
11	CK	117/117 (100%)	0.62	11 (9%) 8 5	35, 63, 82, 91	0
12	AL	123/123 (100%)	0.41	5 (4%) 37 24	23, 36, 72, 102	0
12	CL	123/123 (100%)	0.80	9 (7%) 15 8	38, 50, 80, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	AM	114/114 (100%)	0.66	15 (13%)	3	2	43, 66, 91, 105	0
13	CM	114/114 (100%)	3.44	85 (74%)	0	0	80, 98, 113, 118	0
14	AN	96/100 (96%)	0.81	17 (17%)	1	1	39, 56, 93, 108	0
14	CN	96/100 (96%)	2.80	57 (59%)	0	0	60, 88, 106, 119	0
15	AO	88/88 (100%)	0.46	6 (6%)	17	10	31, 49, 66, 99	0
15	CO	88/88 (100%)	0.74	7 (7%)	12	7	42, 62, 84, 108	0
16	AP	82/82 (100%)	0.95	14 (17%)	1	1	35, 46, 80, 103	0
16	CP	82/82 (100%)	1.57	20 (24%)	0	0	43, 61, 87, 105	0
17	AQ	80/80 (100%)	0.66	6 (7%)	14	8	30, 55, 85, 123	0
17	CQ	80/80 (100%)	1.59	24 (30%)	0	0	42, 69, 97, 108	0
18	AR	55/55 (100%)	0.68	6 (10%)	5	3	38, 51, 76, 113	0
18	CR	55/55 (100%)	0.92	8 (14%)	2	1	40, 54, 83, 113	0
19	AS	79/79 (100%)	0.88	12 (15%)	2	1	45, 66, 92, 97	0
19	CS	79/79 (100%)	4.00	57 (72%)	0	0	79, 98, 113, 126	0
20	AT	85/85 (100%)	0.72	7 (8%)	11	6	35, 48, 74, 115	0
20	CT	85/85 (100%)	2.31	41 (48%)	0	0	52, 69, 91, 98	0
21	AU	51/51 (100%)	1.51	14 (27%)	0	0	49, 70, 92, 105	0
21	CU	51/51 (100%)	1.06	9 (17%)	1	1	43, 67, 92, 107	0
22	BA	2897/2903 (99%)	0.32	125 (4%)	35	22	3, 18, 128, 196	0
22	DA	2897/2903 (99%)	0.60	218 (7%)	14	8	42, 82, 142, 182	0
23	BB	119/119 (100%)	-0.24	0	100	100	6, 26, 52, 94	0
23	DB	118/119 (99%)	0.37	6 (5%)	28	17	68, 109, 131, 143	0
24	BC	271/271 (100%)	0.06	3 (1%)	80	65	8, 24, 44, 65	0
24	DC	271/271 (100%)	1.27	62 (22%)	0	0	40, 60, 76, 84	0
25	BD	209/209 (100%)	0.08	0	100	100	4, 15, 42, 69	0
25	DD	209/209 (100%)	1.40	58 (27%)	0	0	47, 64, 83, 99	0
26	BE	201/201 (100%)	0.05	1 (0%)	91	81	4, 27, 54, 95	0
26	DE	201/201 (100%)	2.16	98 (48%)	0	0	38, 76, 96, 108	0
27	BF	177/177 (100%)	0.40	10 (5%)	24	15	23, 44, 86, 104	0
27	DF	177/177 (100%)	3.92	146 (82%)	0	0	79, 97, 113, 125	0
28	BG	176/176 (100%)	0.48	12 (6%)	17	10	21, 39, 66, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.44	99 (56%) 0 0	66, 85, 103, 117	0
29	BH	149/149 (100%)	4.62	112 (75%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.43	74 (49%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.81	94 (66%) 0 0	80, 104, 120, 136	0
30	DI	141/141 (100%)	5.67	130 (92%) 0 0	91, 110, 121, 124	0
31	BJ	142/142 (100%)	-0.06	1 (0%) 87 76	5, 12, 32, 54	0
31	DJ	142/142 (100%)	1.30	34 (23%) 0 0	49, 64, 80, 96	0
32	BK	122/122 (100%)	-0.07	1 (0%) 86 73	7, 16, 40, 68	0
32	DK	122/122 (100%)	1.40	36 (29%) 0 0	47, 60, 81, 95	0
33	BL	143/143 (100%)	0.13	3 (2%) 63 46	4, 26, 49, 80	0
33	DL	143/143 (100%)	2.46	77 (53%) 0 0	45, 72, 90, 111	0
34	BM	136/136 (100%)	-0.07	0 100 100	6, 16, 34, 93	0
34	DM	136/136 (100%)	1.28	36 (26%) 0 0	40, 64, 82, 110	0
35	BN	120/120 (100%)	-0.05	0 100 100	7, 13, 25, 70	0
35	DN	120/120 (100%)	1.87	41 (34%) 0 0	50, 71, 88, 109	0
36	BO	116/116 (100%)	0.12	2 (1%) 70 53	18, 29, 52, 59	0
36	DO	116/116 (100%)	3.13	78 (67%) 0 0	64, 86, 100, 113	0
37	BP	114/114 (100%)	0.08	2 (1%) 68 51	10, 22, 49, 73	0
37	DP	114/114 (100%)	1.42	36 (31%) 0 0	51, 66, 84, 91	0
38	BQ	117/117 (100%)	-0.03	0 100 100	3, 8, 21, 57	0
38	DQ	117/117 (100%)	1.49	40 (34%) 0 0	46, 65, 79, 83	0
39	BR	103/103 (100%)	-0.09	0 100 100	4, 15, 37, 64	0
39	DR	103/103 (100%)	2.01	45 (43%) 0 0	49, 72, 86, 96	0
40	BS	110/110 (100%)	0.02	1 (0%) 84 71	4, 9, 27, 89	0
40	DS	110/110 (100%)	2.49	61 (55%) 0 0	53, 69, 89, 97	0
41	BT	93/93 (100%)	0.57	7 (7%) 14 8	15, 28, 83, 100	0
41	DT	93/93 (100%)	3.17	66 (70%) 0 0	60, 79, 102, 111	0
42	BU	102/102 (100%)	0.16	4 (3%) 39 25	15, 32, 62, 95	0
42	DU	102/102 (100%)	4.12	75 (73%) 0 0	61, 82, 103, 109	0
43	BV	94/94 (100%)	0.01	2 (2%) 63 46	11, 24, 48, 59	0
43	DV	94/94 (100%)	1.11	17 (18%) 1 1	60, 78, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	0.13	2 (2%) 56 39	10, 17, 37, 56	0
44	DW	75/76 (98%)	2.25	38 (50%) 0 0	49, 75, 86, 107	0
45	BX	77/77 (100%)	0.15	4 (5%) 27 17	11, 28, 53, 81	0
45	DX	77/77 (100%)	1.54	25 (32%) 0 0	49, 66, 84, 89	0
46	BY	63/63 (100%)	0.59	5 (7%) 12 7	21, 42, 71, 93	0
46	DY	63/63 (100%)	2.32	30 (47%) 0 0	63, 86, 95, 104	0
47	BZ	58/58 (100%)	-0.02	0 100 100	7, 11, 34, 40	0
47	DZ	58/58 (100%)	1.32	18 (31%) 0 0	50, 69, 82, 89	0
48	B0	56/56 (100%)	-0.09	0 100 100	4, 14, 38, 77	0
48	D0	56/56 (100%)	2.01	19 (33%) 0 0	49, 69, 90, 106	0
49	B1	50/50 (100%)	0.24	2 (4%) 38 25	19, 33, 61, 95	0
49	D1	50/50 (100%)	2.12	24 (48%) 0 0	63, 79, 91, 103	0
50	B2	46/46 (100%)	0.09	1 (2%) 62 45	8, 14, 22, 97	0
50	D2	46/46 (100%)	1.96	17 (36%) 0 0	47, 64, 78, 100	0
51	B3	64/64 (100%)	0.17	1 (1%) 72 55	10, 16, 26, 37	0
51	D3	64/64 (100%)	1.76	23 (35%) 0 0	53, 67, 79, 83	0
52	B4	38/38 (100%)	0.40	1 (2%) 56 39	13, 23, 38, 60	0
52	D4	38/38 (100%)	2.95	24 (63%) 0 0	56, 71, 84, 96	0
53	B5	191/228 (83%)	7.09	185 (96%) 0 0	71, 107, 119, 133	0
54	B6	2/8 (25%)	0.31	0 100 100	6, 6, 6, 8	0
54	D6	2/8 (25%)	1.02	0 100 100	41, 41, 41, 44	0
All	All	20738/20810 (99%)	0.94	3547 (17%) 1 1	3, 61, 117, 196	0

The worst 5 of 3547 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BH	96	THR	24.1
53	B5	111	PHE	22.9
30	DI	2	ALA	21.9
22	BA	2184	A	20.6
29	BH	113	SER	20.3

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

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	MHW	D6	1	9/10	0.77	0.33	49,54,56,59	0
54	MHU	D6	5	15/16	0.89	0.36	37,42,54,56	0
54	004	D6	7	10/11	0.90	0.20	38,42,48,48	0
54	DBB	D6	3	6/7	0.91	0.28	37,40,41,43	0
54	MHV	D6	6	9/10	0.92	0.16	39,40,42,43	0
54	MHW	B6	1	9/10	0.95	0.21	12,14,18,21	0
54	004	B6	7	10/11	0.97	0.29	3,6,7,10	0
54	MHU	B6	5	15/16	0.97	0.23	0,5,18,21	0
54	DBB	B6	3	6/7	0.97	0.22	6,8,10,15	0
54	MHV	B6	6	9/10	0.98	0.16	2,6,13,14	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	1636	1/1	0.30	0.26	79,79,79,79	0
55	MG	CA	1609	1/1	0.31	0.21	58,58,58,58	0
55	MG	DA	3005	1/1	0.35	0.23	66,66,66,66	0
55	MG	DA	3048	1/1	0.36	0.20	51,51,51,51	0
55	MG	DA	3070	1/1	0.38	0.34	58,58,58,58	0
55	MG	DA	3046	1/1	0.47	0.25	53,53,53,53	0
55	MG	DA	3004	1/1	0.47	0.33	64,64,64,64	0
55	MG	DA	3060	1/1	0.47	1.17	61,61,61,61	0
55	MG	DA	3099	1/1	0.49	0.18	53,53,53,53	0
55	MG	CA	1604	1/1	0.51	0.17	70,70,70,70	0
55	MG	CA	1602	1/1	0.52	0.10	61,61,61,61	0
55	MG	DA	3102	1/1	0.53	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3131	1/1	0.53	0.90	71,71,71,71	0
55	MG	DA	3001	1/1	0.53	0.19	43,43,43,43	0
55	MG	DA	3155	1/1	0.57	0.74	44,44,44,44	0
55	MG	BA	3044	1/1	0.57	0.15	20,20,20,20	0
55	MG	DA	3163	1/1	0.57	0.31	51,51,51,51	0
55	MG	DA	3127	1/1	0.58	0.13	47,47,47,47	0
55	MG	CA	1611	1/1	0.59	0.19	55,55,55,55	0
55	MG	BA	3015	1/1	0.59	0.41	52,52,52,52	0
55	MG	DA	3136	1/1	0.60	0.10	57,57,57,57	0
55	MG	CA	1635	1/1	0.60	0.18	76,76,76,76	0
55	MG	DA	3077	1/1	0.61	0.08	59,59,59,59	0
55	MG	BA	3004	1/1	0.62	0.15	33,33,33,33	0
55	MG	CA	1638	1/1	0.62	0.21	55,55,55,55	0
55	MG	AA	1638	1/1	0.62	0.12	51,51,51,51	0
55	MG	DA	3106	1/1	0.62	0.13	56,56,56,56	0
55	MG	DA	3049	1/1	0.63	0.10	49,49,49,49	0
55	MG	DA	3040	1/1	0.64	0.26	57,57,57,57	0
55	MG	DA	3056	1/1	0.64	0.24	51,51,51,51	0
55	MG	AA	1614	1/1	0.64	0.44	53,53,53,53	0
55	MG	DA	3023	1/1	0.64	0.18	35,35,35,35	0
55	MG	DA	3086	1/1	0.65	0.13	53,53,53,53	0
55	MG	AA	1624	1/1	0.65	0.17	39,39,39,39	0
55	MG	AA	1657	1/1	0.65	0.61	40,40,40,40	0
55	MG	DA	3009	1/1	0.65	0.12	57,57,57,57	0
55	MG	AA	1630	1/1	0.65	0.20	49,49,49,49	0
55	MG	DA	3111	1/1	0.66	0.12	42,42,42,42	0
55	MG	DA	3015	1/1	0.66	0.64	56,56,56,56	0
55	MG	DA	3041	1/1	0.66	0.36	53,53,53,53	0
55	MG	DA	3113	1/1	0.66	0.16	42,42,42,42	0
55	MG	DA	3043	1/1	0.66	0.21	54,54,54,54	0
55	MG	DA	3091	1/1	0.67	0.65	71,71,71,71	0
55	MG	DA	3016	1/1	0.67	0.41	53,53,53,53	0
55	MG	DA	3135	1/1	0.67	0.25	47,47,47,47	0
55	MG	CA	1633	1/1	0.67	0.45	54,54,54,54	0
55	MG	DA	3119	1/1	0.68	0.63	68,68,68,68	0
55	MG	AA	1608	1/1	0.68	0.21	24,24,24,24	0
55	MG	DA	3093	1/1	0.68	0.14	65,65,65,65	0
55	MG	BA	3045	1/1	0.68	0.20	13,13,13,13	0
55	MG	DA	3087	1/1	0.69	0.14	51,51,51,51	0
55	MG	DA	3010	1/1	0.69	0.11	48,48,48,48	0
55	MG	DA	3026	1/1	0.69	0.10	53,53,53,53	0
55	MG	BA	3052	1/1	0.70	0.15	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1621	1/1	0.70	0.11	53,53,53,53	0
55	MG	DA	3115	1/1	0.70	0.18	58,58,58,58	0
55	MG	DA	3047	1/1	0.70	0.31	66,66,66,66	0
55	MG	DA	3121	1/1	0.70	0.16	41,41,41,41	0
55	MG	AA	1615	1/1	0.70	0.12	46,46,46,46	0
55	MG	DA	3090	1/1	0.71	0.20	58,58,58,58	0
55	MG	BA	3029	1/1	0.71	0.11	15,15,15,15	0
55	MG	DA	3018	1/1	0.71	0.18	57,57,57,57	0
55	MG	CA	1652	1/1	0.71	0.17	39,39,39,39	0
55	MG	DA	3078	1/1	0.71	0.10	64,64,64,64	0
55	MG	DA	3143	1/1	0.71	0.30	46,46,46,46	0
55	MG	BA	3168	1/1	0.71	0.32	18,18,18,18	0
55	MG	AA	1610	1/1	0.72	0.16	49,49,49,49	0
55	MG	BA	3048	1/1	0.72	0.09	16,16,16,16	0
55	MG	CA	1617	1/1	0.72	0.15	35,35,35,35	0
55	MG	DA	3025	1/1	0.73	0.45	49,49,49,49	0
55	MG	CA	1637	1/1	0.73	0.38	51,51,51,51	0
55	MG	AA	1634	1/1	0.73	0.17	36,36,36,36	0
55	MG	CA	1601	1/1	0.73	0.11	33,33,33,33	0
55	MG	BA	3188	1/1	0.74	0.18	27,27,27,27	0
55	MG	DA	3103	1/1	0.74	0.13	48,48,48,48	0
55	MG	BA	3057	1/1	0.75	0.20	20,20,20,20	0
55	MG	DA	3124	1/1	0.75	0.38	59,59,59,59	0
55	MG	DA	3045	1/1	0.75	0.21	53,53,53,53	0
55	MG	DA	3034	1/1	0.76	0.30	56,56,56,56	0
55	MG	DA	3055	1/1	0.76	0.50	53,53,53,53	0
55	MG	DA	3033	1/1	0.76	0.23	45,45,45,45	0
55	MG	BA	3023	1/1	0.76	0.15	15,15,15,15	0
55	MG	CA	1605	1/1	0.76	0.37	57,57,57,57	0
55	MG	BB	201	1/1	0.76	0.10	28,28,28,28	0
55	MG	DA	3062	1/1	0.77	0.14	44,44,44,44	0
55	MG	AA	1659	1/1	0.77	0.52	34,34,34,34	0
55	MG	DA	3037	1/1	0.77	0.10	45,45,45,45	0
55	MG	BA	3085	1/1	0.77	0.15	7,7,7,7	0
55	MG	DA	3117	1/1	0.77	0.06	49,49,49,49	0
55	MG	AA	1617	1/1	0.77	0.18	44,44,44,44	0
55	MG	BA	3079	1/1	0.77	0.11	28,28,28,28	0
55	MG	DA	3104	1/1	0.77	0.14	54,54,54,54	0
55	MG	BA	3098	1/1	0.77	0.34	58,58,58,58	0
55	MG	BA	3179	1/1	0.77	0.47	39,39,39,39	0
55	MG	AA	1631	1/1	0.77	0.13	42,42,42,42	0
55	MG	DA	3092	1/1	0.77	0.44	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3057	1/1	0.78	0.62	54,54,54,54	0
55	MG	BA	3009	1/1	0.78	0.13	6,6,6,6	0
55	MG	DA	3011	1/1	0.78	0.17	46,46,46,46	0
55	MG	DA	3013	1/1	0.78	0.37	45,45,45,45	0
55	MG	AA	1637	1/1	0.78	0.18	18,18,18,18	0
55	MG	DA	3054	1/1	0.78	0.28	44,44,44,44	0
55	MG	CA	1606	1/1	0.78	0.29	52,52,52,52	0
55	MG	DA	3084	1/1	0.78	0.30	56,56,56,56	0
55	MG	AA	1623	1/1	0.78	0.13	42,42,42,42	0
55	MG	CA	1628	1/1	0.78	0.39	64,64,64,64	0
55	MG	BA	3108	1/1	0.78	0.28	1,1,1,1	0
55	MG	AA	1648	1/1	0.78	0.29	38,38,38,38	0
55	MG	BA	3047	1/1	0.78	0.14	34,34,34,34	0
55	MG	AA	1632	1/1	0.78	0.14	40,40,40,40	0
55	MG	BA	3025	1/1	0.78	0.25	40,40,40,40	0
55	MG	BA	3061	1/1	0.79	0.47	55,55,55,55	0
55	MG	CM	201	1/1	0.79	0.32	46,46,46,46	0
55	MG	DA	3160	1/1	0.79	0.30	35,35,35,35	0
55	MG	DA	3021	1/1	0.79	0.12	38,38,38,38	0
55	MG	BA	3154	1/1	0.79	0.20	29,29,29,29	0
55	MG	BA	3030	1/1	0.79	0.28	10,10,10,10	0
55	MG	DA	3061	1/1	0.79	0.98	53,53,53,53	0
55	MG	DA	3159	1/1	0.80	0.17	39,39,39,39	0
55	MG	DA	3076	1/1	0.80	0.33	48,48,48,48	0
55	MG	BA	3150	1/1	0.80	0.24	42,42,42,42	0
55	MG	AA	1605	1/1	0.80	0.16	32,32,32,32	0
55	MG	DA	3024	1/1	0.80	0.17	45,45,45,45	0
55	MG	DA	3007	1/1	0.80	0.26	54,54,54,54	0
55	MG	DA	3031	1/1	0.80	0.23	50,50,50,50	0
55	MG	BA	3090	1/1	0.80	0.08	17,17,17,17	0
55	MG	DA	3095	1/1	0.80	0.10	49,49,49,49	0
55	MG	DA	3028	1/1	0.80	0.09	50,50,50,50	0
55	MG	DA	3012	1/1	0.80	0.16	40,40,40,40	0
55	MG	AA	1620	1/1	0.80	0.11	44,44,44,44	0
55	MG	DA	3133	1/1	0.81	0.58	57,57,57,57	0
55	MG	DA	3038	1/1	0.81	0.09	42,42,42,42	0
55	MG	CA	1626	1/1	0.81	0.08	42,42,42,42	0
55	MG	DA	3017	1/1	0.81	0.13	40,40,40,40	0
55	MG	DA	3006	1/1	0.81	0.37	64,64,64,64	0
55	MG	AA	1635	1/1	0.81	0.18	37,37,37,37	0
55	MG	DA	3029	1/1	0.81	0.27	41,41,41,41	0
55	MG	BA	3087	1/1	0.81	0.10	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3080	1/1	0.81	0.11	39,39,39,39	0
55	MG	AA	1618	1/1	0.81	0.11	35,35,35,35	0
55	MG	DA	3118	1/1	0.81	0.12	45,45,45,45	0
55	MG	BA	3019	1/1	0.82	0.24	3,3,3,3	0
55	MG	BB	203	1/1	0.82	0.09	10,10,10,10	0
55	MG	CA	1655	1/1	0.82	0.60	44,44,44,44	0
55	MG	DA	3079	1/1	0.82	0.11	62,62,62,62	0
55	MG	BA	3060	1/1	0.82	0.37	33,33,33,33	0
55	MG	AA	1639	1/1	0.82	0.06	51,51,51,51	0
55	MG	DA	3137	1/1	0.82	0.46	42,42,42,42	0
55	MG	AA	1644	1/1	0.82	0.26	32,32,32,32	0
55	MG	DA	3044	1/1	0.82	0.10	61,61,61,61	0
55	MG	BA	3008	1/1	0.82	0.12	9,9,9,9	0
55	MG	DA	3110	1/1	0.82	0.37	57,57,57,57	0
55	MG	CA	1631	1/1	0.82	0.25	62,62,62,62	0
55	MG	AA	1627	1/1	0.83	0.34	43,43,43,43	0
55	MG	DA	3158	1/1	0.83	0.16	55,55,55,55	0
55	MG	BA	3003	1/1	0.83	0.11	20,20,20,20	0
55	MG	BA	3077	1/1	0.83	0.08	26,26,26,26	0
55	MG	CA	1603	1/1	0.83	0.14	44,44,44,44	0
55	MG	BA	3175	1/1	0.83	0.18	27,27,27,27	0
55	MG	CA	1627	1/1	0.83	0.12	59,59,59,59	0
55	MG	BA	3120	1/1	0.83	0.16	7,7,7,7	0
55	MG	DA	3112	1/1	0.83	0.28	52,52,52,52	0
55	MG	DA	3167	1/1	0.83	0.12	59,59,59,59	0
55	MG	DA	3116	1/1	0.83	0.20	51,51,51,51	0
55	MG	DA	3027	1/1	0.84	0.44	51,51,51,51	0
55	MG	BA	3076	1/1	0.84	0.19	17,17,17,17	0
55	MG	AA	1612	1/1	0.84	0.14	24,24,24,24	0
55	MG	BA	3103	1/1	0.84	0.12	9,9,9,9	0
55	MG	AA	1669	1/1	0.84	0.54	43,43,43,43	0
55	MG	BA	3031	1/1	0.84	0.14	8,8,8,8	0
55	MG	BA	3010	1/1	0.84	0.15	3,3,3,3	0
55	MG	DA	3036	1/1	0.84	0.16	61,61,61,61	0
55	MG	DA	3073	1/1	0.84	0.10	37,37,37,37	0
55	MG	DA	3162	1/1	0.84	0.44	46,46,46,46	0
55	MG	BA	3161	1/1	0.84	0.22	24,24,24,24	0
55	MG	CA	1629	1/1	0.85	0.08	63,63,63,63	0
55	MG	DA	3074	1/1	0.85	0.10	41,41,41,41	0
55	MG	CA	1654	1/1	0.85	0.14	26,26,26,26	0
55	MG	DA	3069	1/1	0.85	0.08	63,63,63,63	0
55	MG	DA	3014	1/1	0.85	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1624	1/1	0.85	0.13	33,33,33,33	0
55	MG	DB	203	1/1	0.85	0.06	56,56,56,56	0
55	MG	DA	3032	1/1	0.85	0.06	49,49,49,49	0
55	MG	DA	3122	1/1	0.85	0.18	42,42,42,42	0
55	MG	DA	3094	1/1	0.85	0.30	59,59,59,59	0
55	MG	DA	3125	1/1	0.85	0.17	51,51,51,51	0
55	MG	DA	3151	1/1	0.85	0.40	45,45,45,45	0
55	MG	AA	1667	1/1	0.85	0.20	37,37,37,37	0
55	MG	AA	1604	1/1	0.86	0.10	45,45,45,45	0
55	MG	BA	3051	1/1	0.86	0.12	6,6,6,6	0
55	MG	BA	3123	1/1	0.86	0.13	18,18,18,18	0
55	MG	BA	3195	1/1	0.86	0.12	20,20,20,20	0
55	MG	DA	3066	1/1	0.86	0.11	39,39,39,39	0
55	MG	DA	3142	1/1	0.86	0.34	38,38,38,38	0
55	MG	BA	3133	1/1	0.86	0.39	40,40,40,40	0
55	MG	DA	3068	1/1	0.86	0.19	52,52,52,52	0
55	MG	BA	3075	1/1	0.86	0.15	15,15,15,15	0
55	MG	DA	3138	1/1	0.86	0.72	41,41,41,41	0
55	MG	DA	3008	1/1	0.86	0.42	51,51,51,51	0
55	MG	BA	3073	1/1	0.86	0.12	13,13,13,13	0
55	MG	CA	1650	1/1	0.86	0.48	40,40,40,40	0
55	MG	DA	3134	1/1	0.86	0.10	34,34,34,34	0
55	MG	BA	3119	1/1	0.86	0.34	21,21,21,21	0
55	MG	DQ	201	1/1	0.86	0.26	32,32,32,32	0
55	MG	DA	3123	1/1	0.87	0.17	47,47,47,47	0
55	MG	DA	3098	1/1	0.87	0.57	63,63,63,63	0
55	MG	DA	3130	1/1	0.87	0.09	51,51,51,51	0
55	MG	BA	3116	1/1	0.87	0.31	11,11,11,11	0
55	MG	DA	3154	1/1	0.87	0.13	45,45,45,45	0
55	MG	BA	3134	1/1	0.87	0.17	8,8,8,8	0
55	MG	AA	1616	1/1	0.87	0.10	42,42,42,42	0
55	MG	BA	3093	1/1	0.87	0.16	16,16,16,16	0
55	MG	BA	3007	1/1	0.87	0.08	25,25,25,25	0
55	MG	DA	3166	1/1	0.87	0.15	34,34,34,34	0
55	MG	CA	1614	1/1	0.87	0.09	44,44,44,44	0
55	MG	DA	3083	1/1	0.88	0.27	61,61,61,61	0
55	MG	AA	1619	1/1	0.88	0.26	43,43,43,43	0
55	MG	BA	3091	1/1	0.88	0.07	28,28,28,28	0
55	MG	BA	3105	1/1	0.88	0.19	4,4,4,4	0
55	MG	BA	3040	1/1	0.88	0.45	7,7,7,7	0
55	MG	BA	3128	1/1	0.88	0.22	9,9,9,9	0
55	MG	DA	3097	1/1	0.88	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3126	1/1	0.88	0.28	7,7,7,7	0
55	MG	DA	3100	1/1	0.88	0.07	43,43,43,43	0
55	MG	AA	1668	1/1	0.88	0.18	18,18,18,18	0
55	MG	CA	1630	1/1	0.88	0.26	66,66,66,66	0
55	MG	DA	3059	1/1	0.88	0.35	53,53,53,53	0
55	MG	DA	3132	1/1	0.88	0.10	45,45,45,45	0
55	MG	AA	1652	1/1	0.88	0.20	43,43,43,43	0
55	MG	BA	3125	1/1	0.88	0.20	8,8,8,8	0
55	MG	CA	1615	1/1	0.88	0.16	35,35,35,35	0
55	MG	BA	3038	1/1	0.88	0.14	8,8,8,8	0
55	MG	BA	3071	1/1	0.89	0.16	11,11,11,11	0
55	MG	BA	3082	1/1	0.89	0.19	15,15,15,15	0
55	MG	BA	3002	1/1	0.89	0.08	15,15,15,15	0
55	MG	BA	3151	1/1	0.89	0.20	31,31,31,31	0
55	MG	BA	3055	1/1	0.89	0.22	23,23,23,23	0
55	MG	BA	3110	1/1	0.89	0.08	23,23,23,23	0
55	MG	CA	1634	1/1	0.89	0.07	49,49,49,49	0
55	MG	BA	3109	1/1	0.89	0.20	9,9,9,9	0
55	MG	AA	1646	1/1	0.89	0.19	44,44,44,44	0
55	MG	CA	1608	1/1	0.89	0.30	50,50,50,50	0
55	MG	DA	3126	1/1	0.89	0.14	57,57,57,57	0
55	MG	DA	3002	1/1	0.89	0.42	52,52,52,52	0
55	MG	BA	3066	1/1	0.89	0.13	6,6,6,6	0
55	MG	BA	3099	1/1	0.89	0.14	3,3,3,3	0
55	MG	BA	3034	1/1	0.89	0.20	18,18,18,18	0
55	MG	CA	1607	1/1	0.89	0.10	42,42,42,42	0
55	MG	DA	3146	1/1	0.89	0.21	35,35,35,35	0
55	MG	BA	3115	1/1	0.89	0.20	35,35,35,35	0
55	MG	BA	3027	1/1	0.89	0.09	22,22,22,22	0
55	MG	BA	3140	1/1	0.89	0.20	14,14,14,14	0
55	MG	CA	1613	1/1	0.90	0.15	19,19,19,19	0
55	MG	DA	3071	1/1	0.90	0.27	59,59,59,59	0
55	MG	BA	3064	1/1	0.90	0.17	2,2,2,2	0
55	MG	BA	3187	1/1	0.90	0.17	28,28,28,28	0
55	MG	BA	3054	1/1	0.90	0.12	5,5,5,5	0
55	MG	DA	3148	1/1	0.90	0.26	45,45,45,45	0
55	MG	BA	3190	1/1	0.90	0.25	33,33,33,33	0
55	MG	AA	1613	1/1	0.90	0.11	20,20,20,20	0
55	MG	DA	3120	1/1	0.90	0.09	49,49,49,49	0
55	MG	BA	3185	1/1	0.90	0.18	11,11,11,11	0
55	MG	BA	3036	1/1	0.90	0.19	19,19,19,19	0
55	MG	BA	3111	1/1	0.90	0.11	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3051	1/1	0.90	0.07	35,35,35,35	0
55	MG	AA	1665	1/1	0.90	0.17	34,34,34,34	0
55	MG	DB	202	1/1	0.90	0.05	42,42,42,42	0
55	MG	BA	3160	1/1	0.90	0.26	7,7,7,7	0
55	MG	DA	3107	1/1	0.90	0.14	49,49,49,49	0
55	MG	DA	3149	1/1	0.90	0.32	36,36,36,36	0
55	MG	CA	1651	1/1	0.90	0.15	48,48,48,48	0
55	MG	BA	3068	1/1	0.90	0.17	6,6,6,6	0
55	MG	AA	1602	1/1	0.90	0.07	33,33,33,33	0
55	MG	BA	3145	1/1	0.90	0.21	15,15,15,15	0
55	MG	BA	3114	1/1	0.90	0.20	19,19,19,19	0
55	MG	AA	1607	1/1	0.91	0.15	33,33,33,33	0
55	MG	BA	3049	1/1	0.91	0.14	9,9,9,9	0
55	MG	AA	1643	1/1	0.91	0.16	19,19,19,19	0
55	MG	CA	1625	1/1	0.91	0.21	25,25,25,25	0
55	MG	BA	3139	1/1	0.91	0.40	1,1,1,1	0
55	MG	CA	1646	1/1	0.91	0.14	40,40,40,40	0
55	MG	BA	3042	1/1	0.91	0.17	6,6,6,6	0
55	MG	DA	3128	1/1	0.91	0.10	57,57,57,57	0
55	MG	AA	1622	1/1	0.91	0.27	21,21,21,21	0
55	MG	BA	3102	1/1	0.91	0.33	23,23,23,23	0
55	MG	BA	3138	1/1	0.91	0.41	4,4,4,4	0
55	MG	BA	3012	1/1	0.91	0.21	4,4,4,4	0
55	MG	DA	3052	1/1	0.91	0.08	35,35,35,35	0
55	MG	CA	1649	1/1	0.91	0.16	35,35,35,35	0
55	MG	BA	3033	1/1	0.91	0.25	4,4,4,4	0
55	MG	BA	3132	1/1	0.91	0.18	27,27,27,27	0
55	MG	BA	3181	1/1	0.91	0.22	14,14,14,14	0
55	MG	BA	3178	1/1	0.91	0.46	20,20,20,20	0
55	MG	BA	3094	1/1	0.91	0.05	17,17,17,17	0
55	MG	BA	3170	1/1	0.91	0.29	35,35,35,35	0
55	MG	DA	3042	1/1	0.91	0.11	49,49,49,49	0
55	MG	AA	1666	1/1	0.91	0.22	30,30,30,30	0
55	MG	BA	3014	1/1	0.91	0.11	6,6,6,6	0
55	MG	BA	3080	1/1	0.91	0.10	18,18,18,18	0
55	MG	AA	1640	1/1	0.91	0.06	39,39,39,39	0
55	MG	BA	3086	1/1	0.91	0.22	9,9,9,9	0
55	MG	AA	1664	1/1	0.91	0.19	36,36,36,36	0
55	MG	BA	3028	1/1	0.92	0.11	4,4,4,4	0
55	MG	BA	3101	1/1	0.92	0.14	2,2,2,2	0
55	MG	BA	3159	1/1	0.92	0.19	19,19,19,19	0
55	MG	BA	3083	1/1	0.92	0.21	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3021	1/1	0.92	0.16	1,1,1,1	0
55	MG	DB	201	1/1	0.92	0.06	69,69,69,69	0
55	MG	DA	3152	1/1	0.92	0.16	41,41,41,41	0
55	MG	CA	1620	1/1	0.92	0.10	46,46,46,46	0
55	MG	BA	3016	1/1	0.92	0.07	17,17,17,17	0
55	MG	AA	1626	1/1	0.92	0.19	26,26,26,26	0
55	MG	BA	3050	1/1	0.92	0.11	11,11,11,11	0
55	MG	BA	3113	1/1	0.92	0.32	10,10,10,10	0
55	MG	BA	3155	1/1	0.92	0.27	15,15,15,15	0
55	MG	DA	3161	1/1	0.92	0.10	42,42,42,42	0
55	MG	AA	1601	1/1	0.92	0.14	49,49,49,49	0
55	MG	DA	3003	1/1	0.92	0.09	52,52,52,52	0
55	MG	BA	3180	1/1	0.92	0.26	25,25,25,25	0
55	MG	DA	3105	1/1	0.92	0.17	37,37,37,37	0
55	MG	BA	3078	1/1	0.92	0.10	33,33,33,33	0
55	MG	BA	3020	1/1	0.92	0.11	7,7,7,7	0
55	MG	CA	1632	1/1	0.92	0.13	54,54,54,54	0
55	MG	AA	1655	1/1	0.92	0.12	34,34,34,34	0
55	MG	DA	3088	1/1	0.92	0.29	51,51,51,51	0
55	MG	BA	3166	1/1	0.92	0.21	25,25,25,25	0
55	MG	CA	1618	1/1	0.92	0.16	28,28,28,28	0
55	MG	DA	3053	1/1	0.92	0.12	43,43,43,43	0
55	MG	CA	1623	1/1	0.93	0.29	40,40,40,40	0
55	MG	DA	3096	1/1	0.93	0.17	52,52,52,52	0
55	MG	BA	3176	1/1	0.93	0.14	24,24,24,24	0
55	MG	AM	201	1/1	0.93	0.28	29,29,29,29	0
55	MG	BA	3067	1/1	0.93	0.20	5,5,5,5	0
55	MG	DA	3022	1/1	0.93	0.16	54,54,54,54	0
55	MG	BA	3092	1/1	0.93	0.09	20,20,20,20	0
55	MG	BA	3035	1/1	0.93	0.15	2,2,2,2	0
55	MG	DA	3085	1/1	0.93	0.10	42,42,42,42	0
55	MG	DA	3150	1/1	0.93	0.21	42,42,42,42	0
55	MG	BA	3191	1/1	0.93	0.24	35,35,35,35	0
55	MG	CA	1641	1/1	0.93	0.83	46,46,46,46	0
55	MG	DA	3081	1/1	0.93	0.15	43,43,43,43	0
55	MG	BA	3121	1/1	0.93	0.08	22,22,22,22	0
55	MG	BA	3163	1/1	0.93	0.23	27,27,27,27	0
55	MG	DA	3063	1/1	0.93	0.19	41,41,41,41	0
55	MG	AA	1628	1/1	0.93	0.04	37,37,37,37	0
55	MG	CA	1619	1/1	0.93	0.11	26,26,26,26	0
55	MG	CA	1648	1/1	0.93	0.19	42,42,42,42	0
55	MG	DA	3039	1/1	0.93	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3100	1/1	0.93	0.14	6,6,6,6	0
55	MG	AA	1663	1/1	0.93	0.16	35,35,35,35	0
55	MG	DA	3165	1/1	0.93	0.38	34,34,34,34	0
55	MG	BA	3182	1/1	0.93	0.21	22,22,22,22	0
55	MG	AA	1671	1/1	0.93	0.20	35,35,35,35	0
55	MG	CA	1616	1/1	0.93	0.11	29,29,29,29	0
55	MG	AA	1621	1/1	0.93	0.06	33,33,33,33	0
55	MG	AA	1662	1/1	0.93	0.19	41,41,41,41	0
55	MG	BA	3162	1/1	0.93	0.19	21,21,21,21	0
55	MG	BA	3013	1/1	0.93	0.19	0,0,0,0	0
55	MG	DA	3109	1/1	0.93	0.24	37,37,37,37	0
55	MG	BA	3131	1/1	0.93	0.11	35,35,35,35	0
55	MG	DA	3141	1/1	0.93	0.20	28,28,28,28	0
55	MG	BA	3177	1/1	0.94	0.09	24,24,24,24	0
55	MG	BA	3158	1/1	0.94	0.18	20,20,20,20	0
55	MG	CA	1647	1/1	0.94	0.19	24,24,24,24	0
55	MG	BA	3046	1/1	0.94	0.22	8,8,8,8	0
55	MG	DA	3153	1/1	0.94	0.49	52,52,52,52	0
55	MG	AA	1661	1/1	0.94	0.20	22,22,22,22	0
55	MG	CA	1639	1/1	0.94	0.12	34,34,34,34	0
55	MG	BA	3058	1/1	0.94	0.08	13,13,13,13	0
55	MG	BA	3088	1/1	0.94	0.16	32,32,32,32	0
55	MG	DA	3065	1/1	0.94	0.06	33,33,33,33	0
55	MG	AA	1633	1/1	0.94	0.09	31,31,31,31	0
55	MG	AA	1650	1/1	0.94	0.17	35,35,35,35	0
55	MG	BA	3122	1/1	0.94	0.24	2,2,2,2	0
55	MG	BA	3112	1/1	0.94	0.16	11,11,11,11	0
55	MG	BA	3024	1/1	0.94	0.14	7,7,7,7	0
55	MG	DA	3129	1/1	0.94	0.11	38,38,38,38	0
55	MG	DA	3114	1/1	0.94	0.32	64,64,64,64	0
55	MG	DA	3147	1/1	0.94	0.19	49,49,49,49	0
55	MG	DA	3089	1/1	0.94	0.22	58,58,58,58	0
55	MG	DA	3050	1/1	0.94	0.07	29,29,29,29	0
55	MG	BA	3192	1/1	0.94	0.16	15,15,15,15	0
55	MG	AA	1660	1/1	0.94	0.22	40,40,40,40	0
55	MG	CA	1642	1/1	0.94	0.27	27,27,27,27	0
55	MG	BA	3006	1/1	0.94	0.10	20,20,20,20	0
55	MG	BB	202	1/1	0.94	0.08	11,11,11,11	0
55	MG	BA	3011	1/1	0.94	0.07	13,13,13,13	0
55	MG	BA	3084	1/1	0.94	0.12	12,12,12,12	0
55	MG	BA	3173	1/1	0.94	0.19	20,20,20,20	0
55	MG	BA	3142	1/1	0.94	0.41	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1656	1/1	0.94	0.12	37,37,37,37	0
55	MG	BA	3059	1/1	0.94	0.14	16,16,16,16	0
55	MG	BA	3089	1/1	0.94	0.10	12,12,12,12	0
55	MG	BA	3167	1/1	0.94	0.15	28,28,28,28	0
55	MG	BA	3070	1/1	0.94	0.25	9,9,9,9	0
55	MG	DA	3020	1/1	0.95	0.37	42,42,42,42	0
55	MG	CA	1640	1/1	0.95	0.21	23,23,23,23	0
55	MG	DA	3145	1/1	0.95	0.10	37,37,37,37	0
55	MG	BA	3174	1/1	0.95	0.12	20,20,20,20	0
55	MG	BA	3129	1/1	0.95	0.16	5,5,5,5	0
55	MG	DA	3101	1/1	0.95	0.10	40,40,40,40	0
55	MG	AA	1641	1/1	0.95	0.17	20,20,20,20	0
55	MG	BA	3169	1/1	0.95	0.12	24,24,24,24	0
55	MG	BA	3001	1/1	0.95	0.08	10,10,10,10	0
55	MG	DA	3067	1/1	0.95	0.10	49,49,49,49	0
55	MG	CA	1622	1/1	0.95	0.05	40,40,40,40	0
55	MG	DA	3019	1/1	0.95	0.16	47,47,47,47	0
55	MG	AA	1603	1/1	0.95	0.15	34,34,34,34	0
55	MG	BA	3146	1/1	0.95	0.25	23,23,23,23	0
55	MG	DA	3157	1/1	0.95	0.39	47,47,47,47	0
55	MG	BA	3074	1/1	0.95	0.07	20,20,20,20	0
55	MG	AA	1653	1/1	0.95	0.30	24,24,24,24	0
55	MG	AA	1629	1/1	0.95	0.12	43,43,43,43	0
55	MG	BA	3172	1/1	0.95	0.20	23,23,23,23	0
55	MG	DA	3030	1/1	0.95	0.15	44,44,44,44	0
55	MG	BA	3148	1/1	0.95	0.24	16,16,16,16	0
55	MG	BA	3130	1/1	0.95	0.24	4,4,4,4	0
55	MG	AA	1606	1/1	0.95	0.09	31,31,31,31	0
55	MG	AA	1654	1/1	0.95	0.32	40,40,40,40	0
55	MG	BA	3153	1/1	0.95	0.30	2,2,2,2	0
55	MG	BA	3039	1/1	0.95	0.18	1,1,1,1	0
55	MG	DA	3072	1/1	0.95	0.12	42,42,42,42	0
55	MG	DA	3108	1/1	0.95	0.18	35,35,35,35	0
55	MG	BA	3032	1/1	0.95	0.17	8,8,8,8	0
55	MG	BA	3018	1/1	0.96	0.09	27,27,27,27	0
55	MG	BA	3124	1/1	0.96	0.24	21,21,21,21	0
55	MG	AA	1609	1/1	0.96	0.08	20,20,20,20	0
55	MG	AA	1642	1/1	0.96	0.13	24,24,24,24	0
55	MG	AA	1651	1/1	0.96	0.27	32,32,32,32	0
55	MG	BA	3136	1/1	0.96	0.13	24,24,24,24	0
55	MG	CA	1610	1/1	0.96	0.09	47,47,47,47	0
55	MG	BA	3022	1/1	0.96	0.16	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3157	1/1	0.96	0.27	26,26,26,26	0
55	MG	DA	3035	1/1	0.96	0.15	38,38,38,38	0
55	MG	BA	3118	1/1	0.96	0.07	11,11,11,11	0
55	MG	DA	3140	1/1	0.96	0.43	37,37,37,37	0
55	MG	DA	3156	1/1	0.96	0.13	30,30,30,30	0
55	MG	CA	1643	1/1	0.96	0.28	44,44,44,44	0
55	MG	BA	3106	1/1	0.96	0.33	0,0,0,0	0
55	MG	CA	1653	1/1	0.96	0.31	47,47,47,47	0
55	MG	DA	3058	1/1	0.96	0.04	37,37,37,37	0
55	MG	DA	3064	1/1	0.96	0.08	38,38,38,38	0
55	MG	AA	1649	1/1	0.96	0.22	27,27,27,27	0
56	ZN	B4	101	1/1	0.96	0.20	131,131,131,131	0
55	MG	BA	3135	1/1	0.96	0.09	17,17,17,17	0
55	MG	BA	3062	1/1	0.96	0.21	3,3,3,3	0
55	MG	CA	1644	1/1	0.96	0.25	32,32,32,32	0
55	MG	BA	3164	1/1	0.96	0.45	21,21,21,21	0
55	MG	BA	3143	1/1	0.96	0.29	7,7,7,7	0
55	MG	BA	3184	1/1	0.96	0.18	23,23,23,23	0
55	MG	AA	1658	1/1	0.96	0.08	33,33,33,33	0
55	MG	BA	3053	1/1	0.96	0.20	4,4,4,4	0
55	MG	BA	3127	1/1	0.96	0.09	1,1,1,1	0
55	MG	DA	3075	1/1	0.96	0.11	48,48,48,48	0
55	MG	BA	3041	1/1	0.96	0.12	11,11,11,11	0
55	MG	DA	3164	1/1	0.96	0.13	47,47,47,47	0
55	MG	BA	3183	1/1	0.96	0.17	24,24,24,24	0
55	MG	BA	3171	1/1	0.96	0.14	29,29,29,29	0
56	ZN	D4	101	1/1	0.97	0.05	79,79,79,79	0
55	MG	BA	3096	1/1	0.97	0.11	5,5,5,5	0
55	MG	BA	3069	1/1	0.97	0.07	39,39,39,39	0
55	MG	BA	3065	1/1	0.97	0.12	7,7,7,7	0
55	MG	BA	3095	1/1	0.97	0.09	8,8,8,8	0
55	MG	BA	3152	1/1	0.97	0.22	11,11,11,11	0
55	MG	AA	1625	1/1	0.97	0.07	31,31,31,31	0
55	MG	AA	1636	1/1	0.97	0.20	26,26,26,26	0
55	MG	BA	3107	1/1	0.97	0.20	6,6,6,6	0
55	MG	BA	3056	1/1	0.97	0.11	10,10,10,10	0
55	MG	BA	3144	1/1	0.97	0.19	25,25,25,25	0
55	MG	BA	3005	1/1	0.97	0.05	31,31,31,31	0
55	MG	DA	3082	1/1	0.97	0.06	50,50,50,50	0
55	MG	BA	3189	1/1	0.97	0.20	3,3,3,3	0
55	MG	BA	3017	1/1	0.97	0.13	6,6,6,6	0
55	MG	BA	3097	1/1	0.97	0.19	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1670	1/1	0.97	0.38	26,26,26,26	0
55	MG	BA	3104	1/1	0.97	0.20	1,1,1,1	0
55	MG	BA	3193	1/1	0.97	0.12	12,12,12,12	0
55	MG	DA	3144	1/1	0.97	0.04	52,52,52,52	0
55	MG	CA	1645	1/1	0.97	0.19	41,41,41,41	0
55	MG	BA	3165	1/1	0.97	0.16	2,2,2,2	0
55	MG	BA	3026	1/1	0.97	0.07	7,7,7,7	0
55	MG	BA	3149	1/1	0.97	0.15	1,1,1,1	0
55	MG	BA	3156	1/1	0.98	0.24	12,12,12,12	0
55	MG	DA	3139	1/1	0.98	0.35	31,31,31,31	0
55	MG	AA	1611	1/1	0.98	0.07	18,18,18,18	0
55	MG	BA	3063	1/1	0.98	0.19	0,0,0,0	0
55	MG	CA	1612	1/1	0.98	0.05	30,30,30,30	0
55	MG	BB	204	1/1	0.98	0.29	4,4,4,4	0
55	MG	BA	3141	1/1	0.98	0.41	4,4,4,4	0
55	MG	AA	1645	1/1	0.98	0.13	39,39,39,39	0
55	MG	BA	3147	1/1	0.98	0.46	13,13,13,13	0
55	MG	BA	3186	1/1	0.98	0.35	18,18,18,18	0
55	MG	BA	3081	1/1	0.98	0.18	1,1,1,1	0
55	MG	AA	1647	1/1	0.98	0.18	39,39,39,39	0
55	MG	BA	3117	1/1	0.98	0.15	4,4,4,4	0
55	MG	BA	3072	1/1	0.98	0.20	4,4,4,4	0
55	MG	BA	3037	1/1	0.98	0.23	2,2,2,2	0
55	MG	BA	3137	1/1	0.99	0.45	4,4,4,4	0
55	MG	BA	3194	1/1	0.99	0.17	28,28,28,28	0
55	MG	BA	3043	1/1	0.99	0.08	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.