



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:06 PM GMT

PDB ID : 4U25
Title : Crystal structure of the E. coli ribosome bound to virginiamycin M1.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-06-07
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

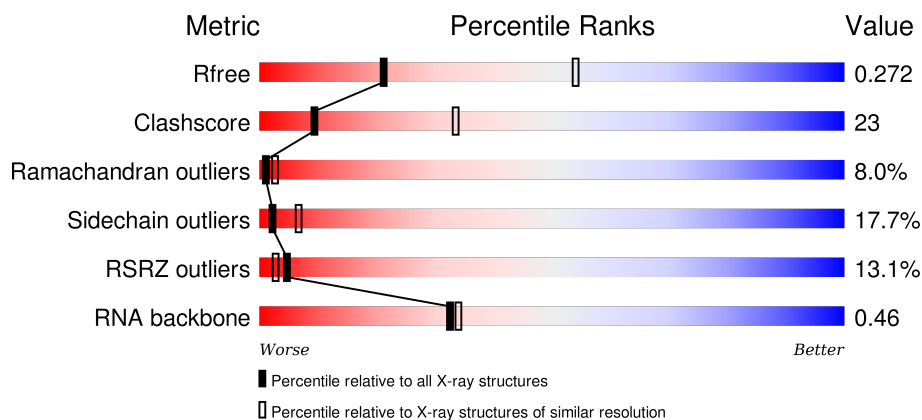
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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. 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	<div> <div>2%</div> <div>32%</div> <div>52%</div> <div>15%</div> </div>
1	CA	1539	<div> <div>4%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
2	AB	218	<div> <div>15%</div> <div>20%</div> <div>50%</div> <div>23%</div> <div>6%</div> </div>
2	CB	218	<div> <div>28%</div> <div>30%</div> <div>51%</div> <div>17%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

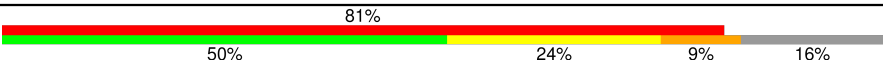
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B5	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1610	-	-	-	X
54	MG	AA	1621	-	-	-	X
54	MG	AA	1634	-	-	-	X
54	MG	AA	1643	-	-	-	X
54	MG	AA	1654	-	-	-	X
54	MG	AA	1662	-	-	-	X
54	MG	AA	1670	-	-	-	X
54	MG	BA	3016	-	-	-	X
54	MG	BA	3035	-	-	-	X
54	MG	BA	3041	-	-	-	X
54	MG	BA	3056	-	-	-	X
54	MG	BA	3058	-	-	-	X
54	MG	BA	3084	-	-	-	X
54	MG	BA	3105	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3110	-	-	-	X
54	MG	BA	3132	-	-	-	X
54	MG	BA	3134	-	-	-	X
54	MG	BA	3137	-	-	-	X
54	MG	BA	3139	-	-	-	X
54	MG	BA	3145	-	-	-	X
54	MG	BA	3147	-	-	-	X
54	MG	BA	3151	-	-	-	X
54	MG	BA	3153	-	-	-	X
54	MG	BA	3155	-	-	-	X
54	MG	BA	3168	-	-	-	X
54	MG	BA	3183	-	-	-	X
54	MG	BA	3185	-	-	-	X
54	MG	CA	1630	-	-	-	X
54	MG	CA	1632	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3009	-	-	-	X
54	MG	DA	3029	-	-	-	X
54	MG	DA	3042	-	-	-	X
54	MG	DA	3050	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3072	-	-	-	X
54	MG	DA	3110	-	-	-	X
54	MG	DA	3114	-	-	-	X
54	MG	DA	3117	-	-	-	X
54	MG	DA	3125	-	-	-	X
55	VIR	BA	3001	-	-	-	X
55	VIR	DA	3001	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288258 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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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				

Continued on next page...

Continued from previous page...

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			

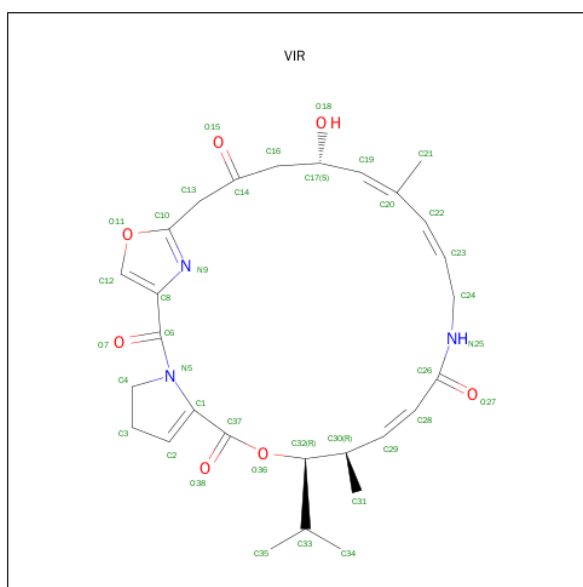
- Molecule 53 is a protein called 50S ribosomal protein L1.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	4	Total	Mg	0	0
			4	4		
54	BA	193	Total	Mg	0	0
			193	193		
54	CA	56	Total	Mg	0	0
			56	56		
54	DQ	1	Total	Mg	0	0
			1	1		
54	BD	1	Total	Mg	0	0
			1	1		
54	DA	166	Total	Mg	0	0
			166	166		
54	AA	71	Total	Mg	0	0
			71	71		
54	BQ	1	Total	Mg	0	0
			1	1		
54	AN	1	Total	Mg	0	0
			1	1		
54	D2	1	Total	Mg	0	0
			1	1		
54	DB	3	Total	Mg	0	0
			3	3		

- Molecule 55 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: C₂₈H₃₅N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total 38	C 28	N 3	O 7	0	0
55	DA	1	Total 38	C 28	N 3	O 7	0	0

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	192	Total O 192 192	0	0
57	AL	2	Total O 2 2	0	0
57	AN	6	Total O 6 6	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	620	Total 620	O 620	0	0
57	BB	13	Total 13	O 13	0	0
57	BC	7	Total 7	O 7	0	0
57	BD	3	Total 3	O 3	0	0
57	BE	4	Total 4	O 4	0	0
57	BF	1	Total 1	O 1	0	0
57	BJ	1	Total 1	O 1	0	0
57	BL	5	Total 5	O 5	0	0
57	BN	3	Total 3	O 3	0	0
57	BQ	1	Total 1	O 1	0	0
57	BS	1	Total 1	O 1	0	0
57	BT	1	Total 1	O 1	0	0
57	BV	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	2	Total 2	O 2	0	0
57	B4	2	Total 2	O 2	0	0
57	CA	191	Total 191	O 191	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	2	Total 2	O 2	0	0
57	CT	2	Total 2	O 2	0	0
57	CU	2	Total 2	O 2	0	0

Continued on next page...

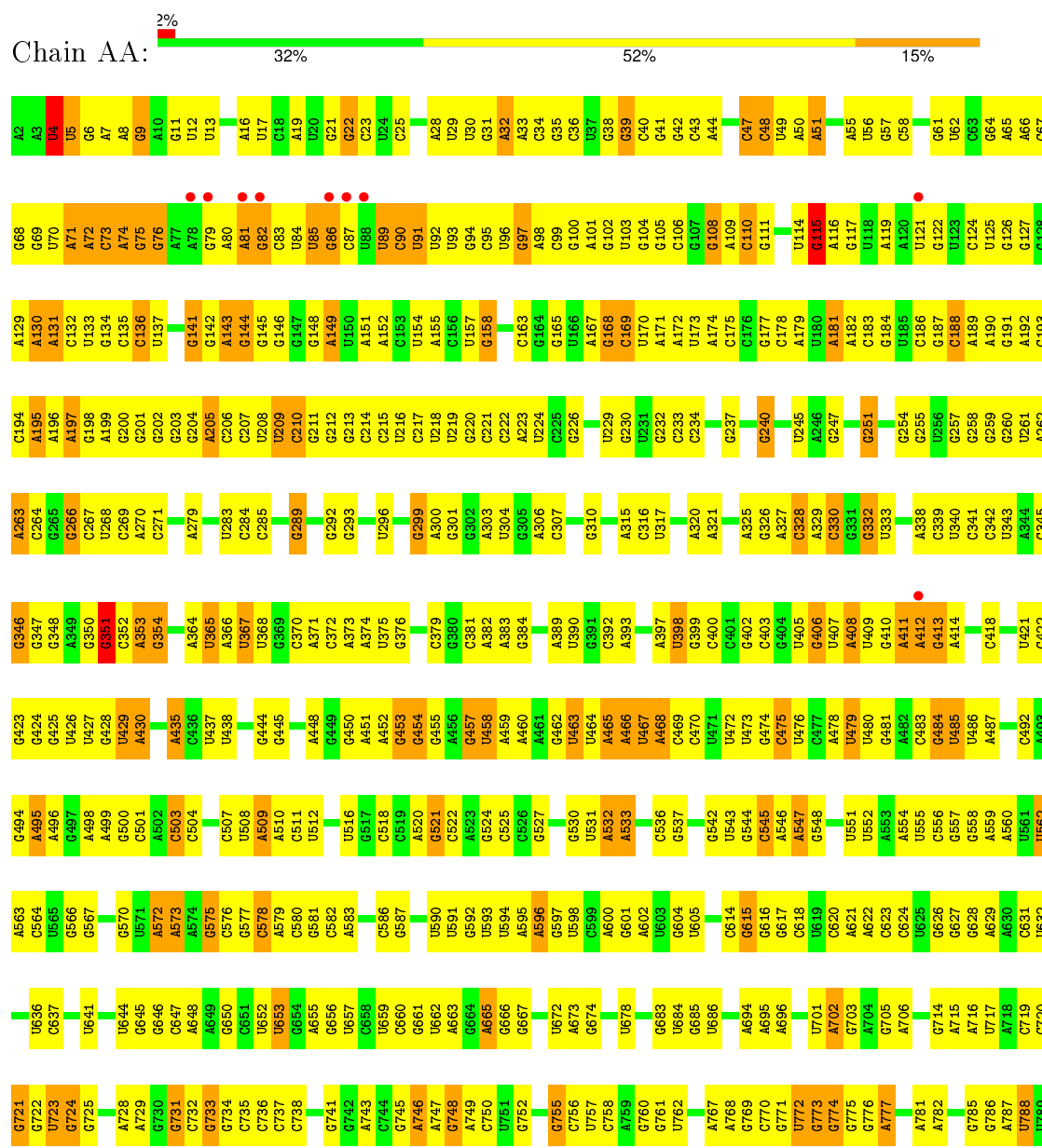
Continued from previous page...

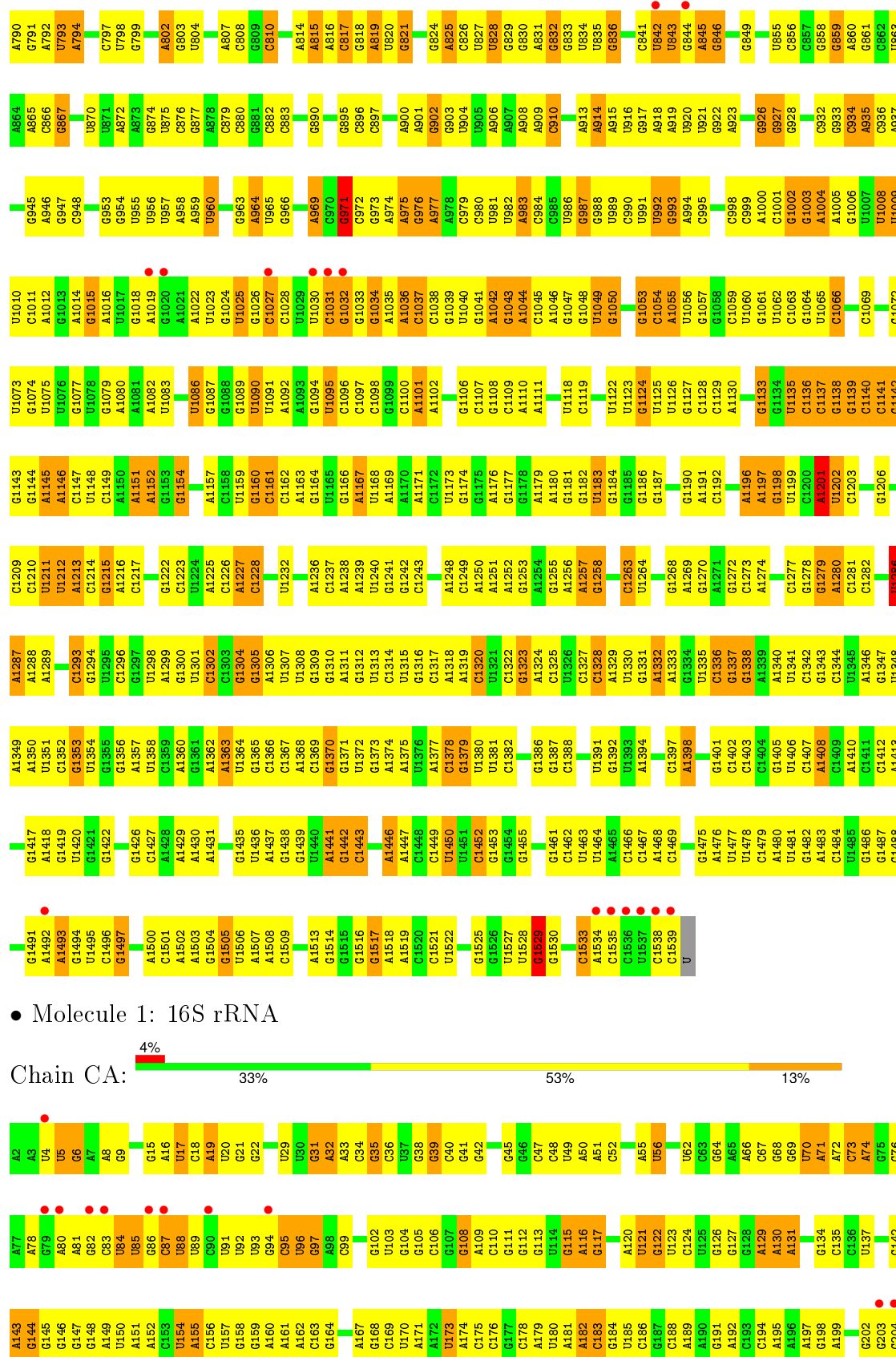
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	12	Total 12	O 12	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DJ	1	Total 1	O 1	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	1	Total 1	O 1	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

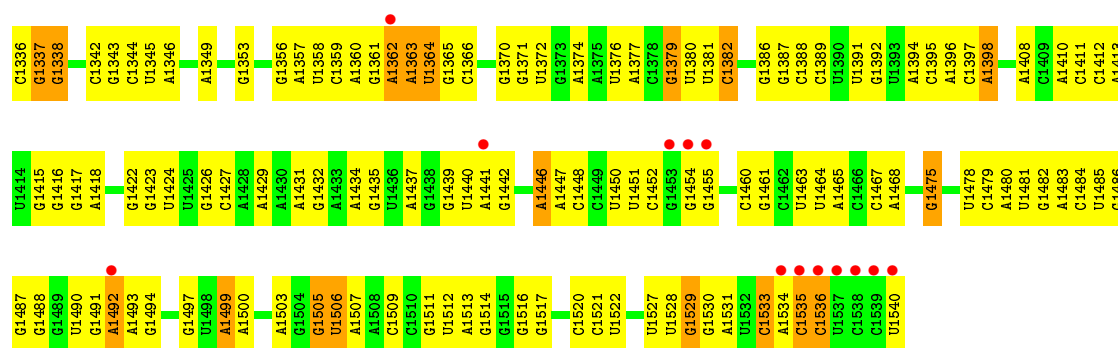
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

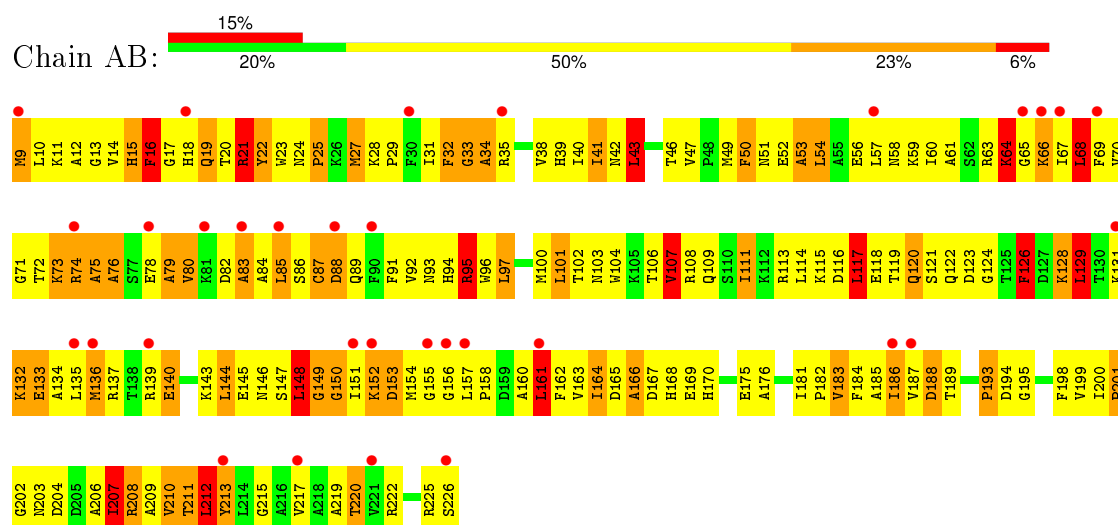




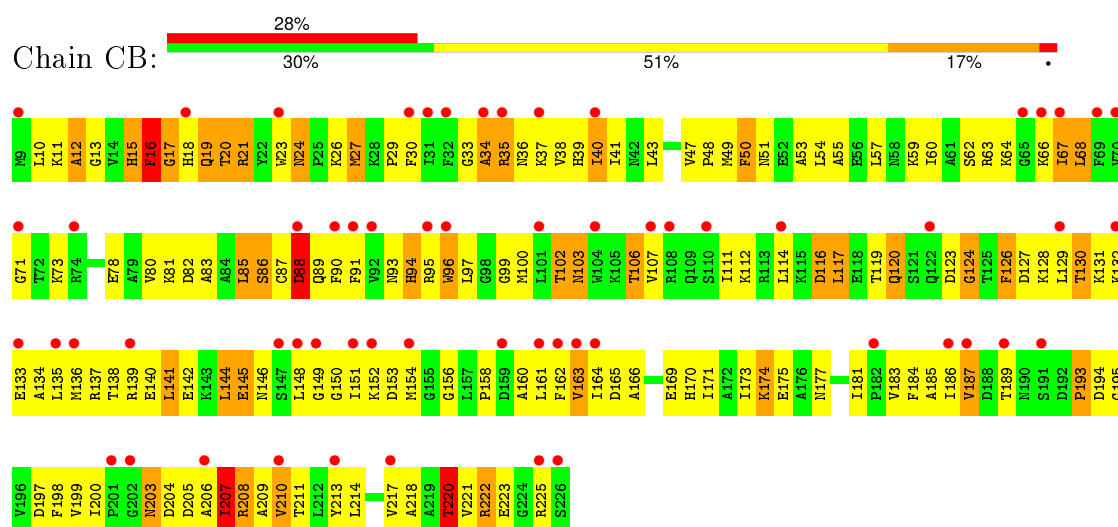




• Molecule 2: 30S ribosomal protein S2

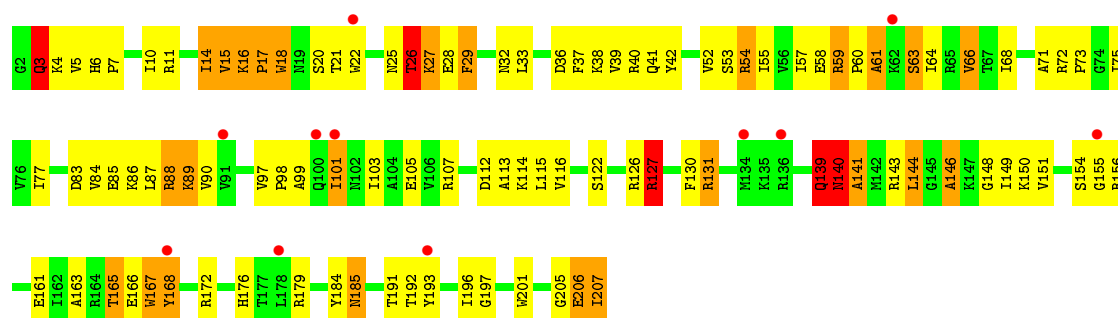


• Molecule 2: 30S ribosomal protein S2

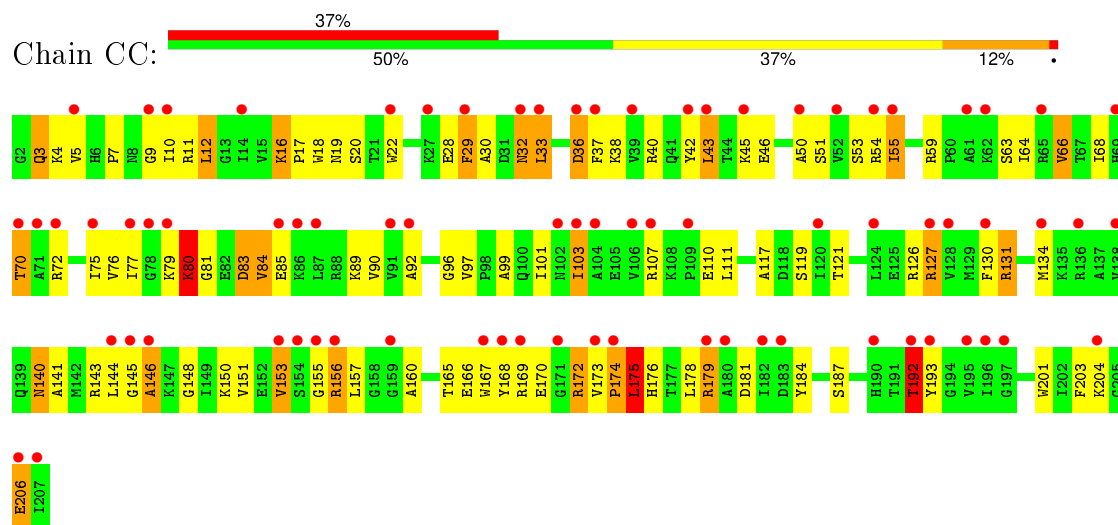


• Molecule 3: 30S ribosomal protein S3

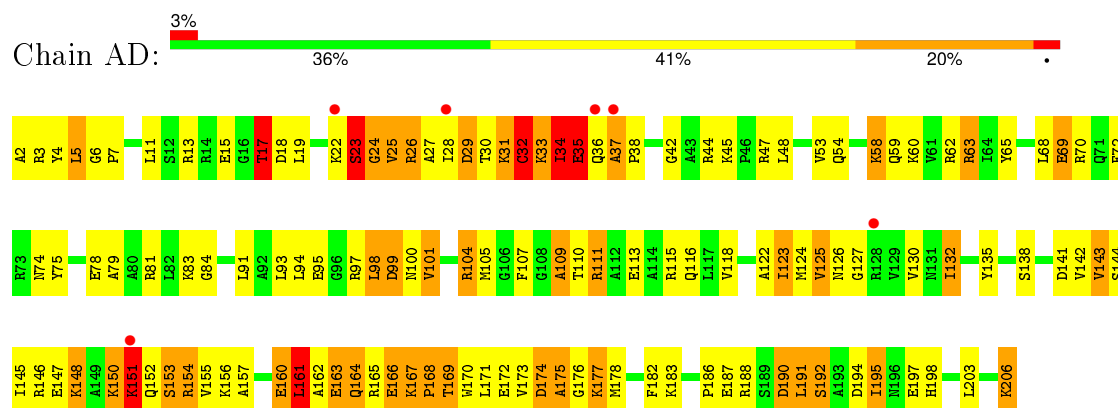




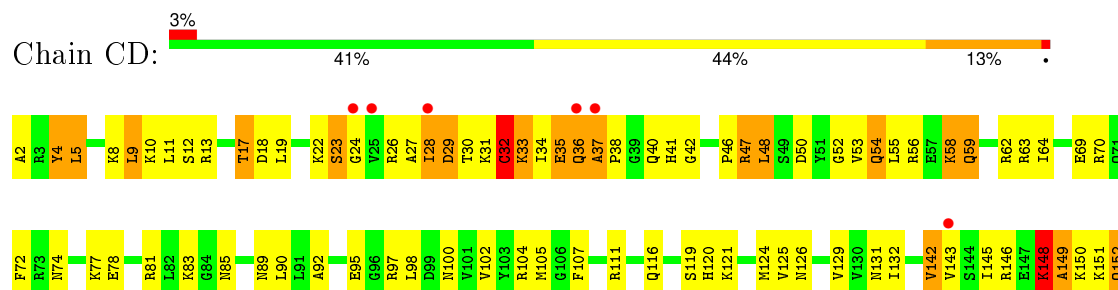
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

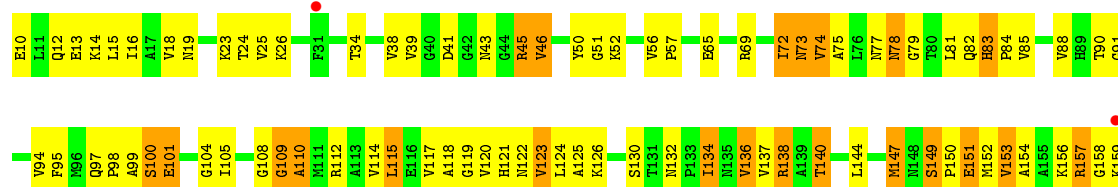


• Molecule 4: 30S ribosomal protein S4

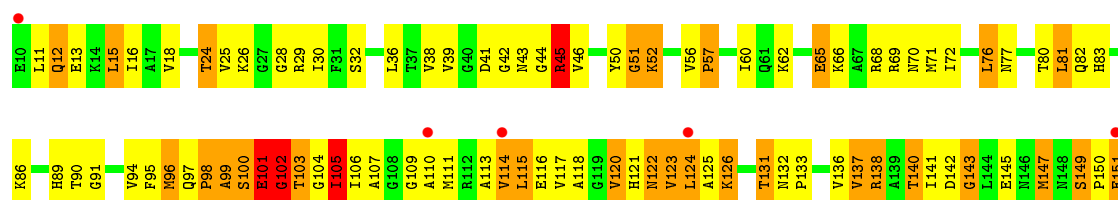




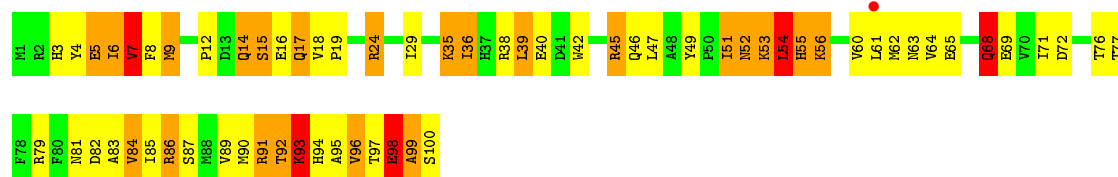
• Molecule 5: 30S ribosomal protein S5



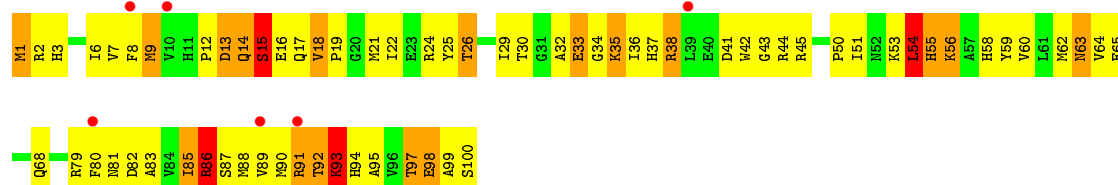
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

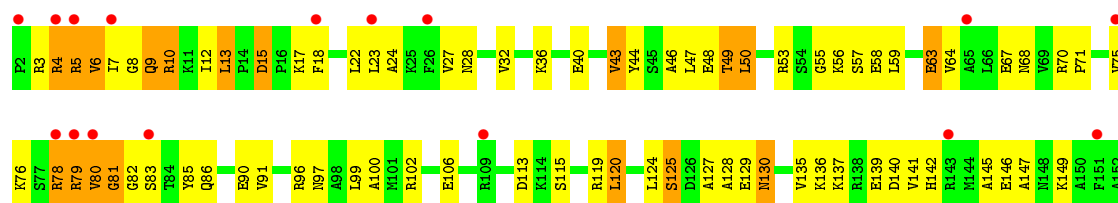


• Molecule 6: 30S ribosomal protein S6

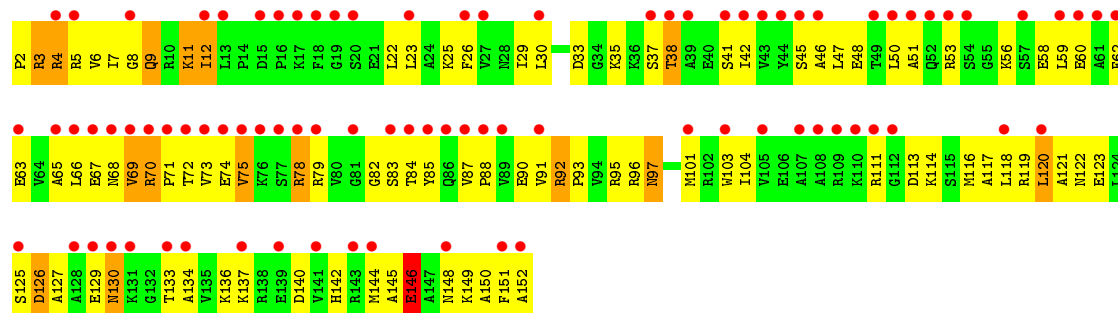


• Molecule 7: 30S ribosomal protein S7

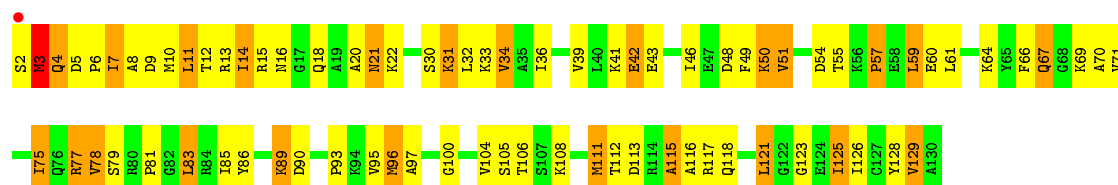
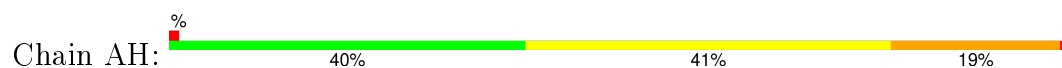




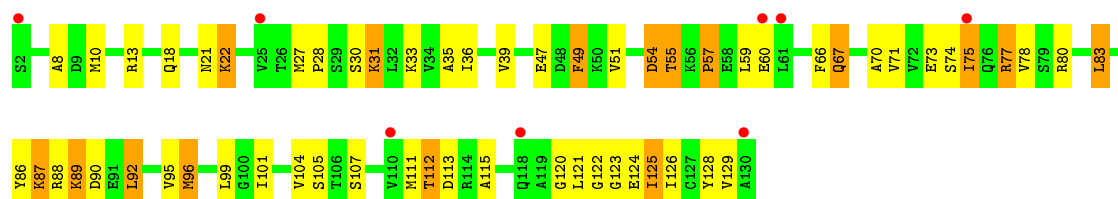
• Molecule 7: 30S ribosomal protein S7



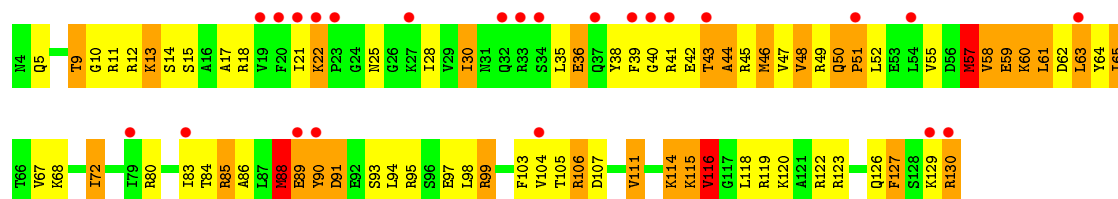
• Molecule 8: 30S ribosomal protein S8



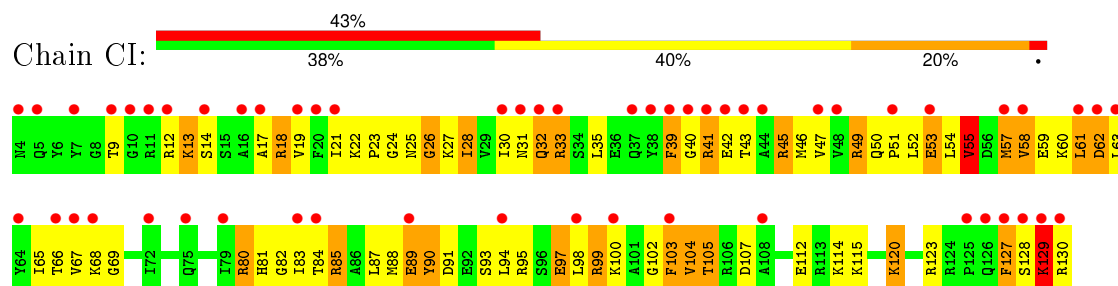
• Molecule 8: 30S ribosomal protein S8



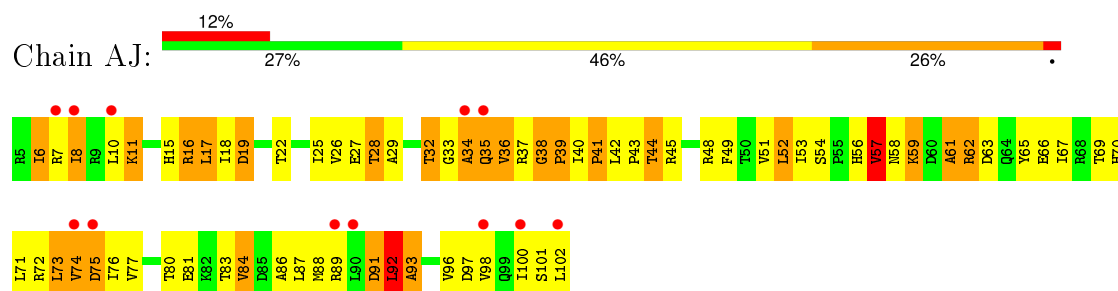
• Molecule 9: 30S ribosomal protein S9



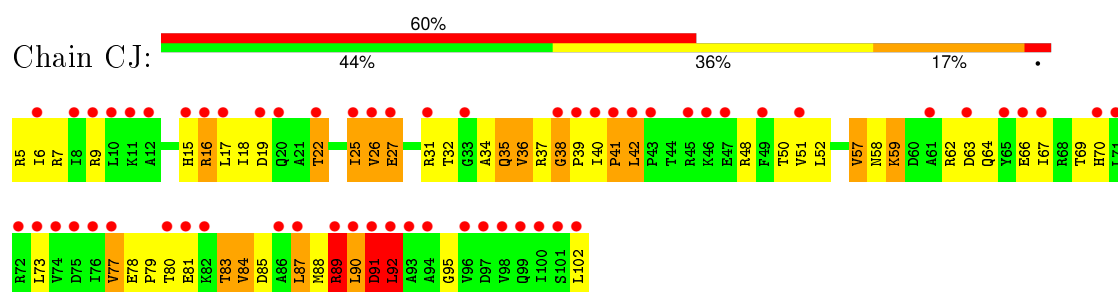
- Molecule 9: 30S ribosomal protein S9



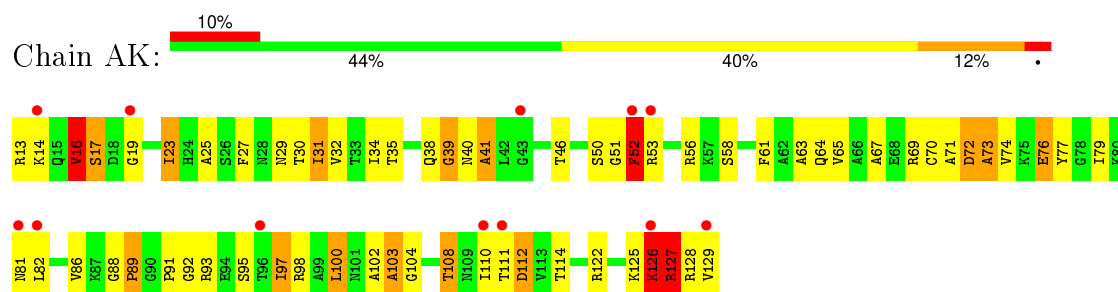
- Molecule 10: 30S ribosomal protein S10



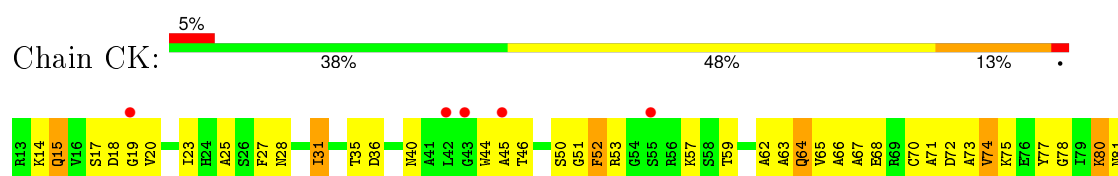
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

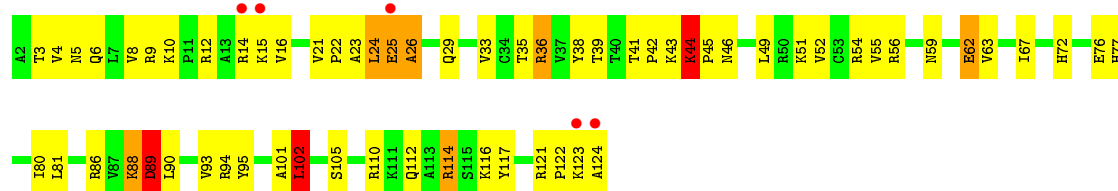


- Molecule 11: 30S ribosomal protein S11

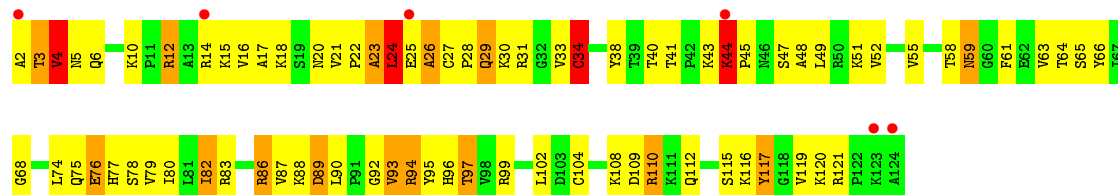




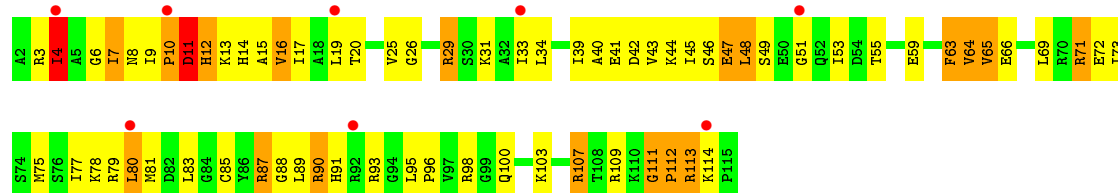
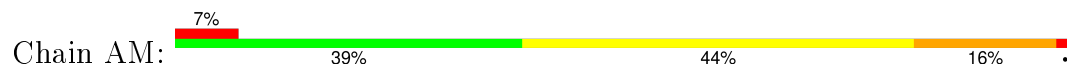
• Molecule 12: 30S ribosomal protein S12



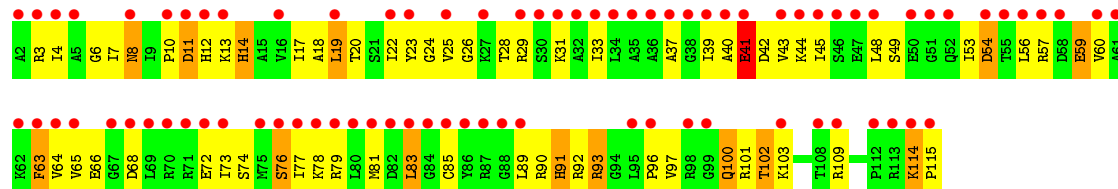
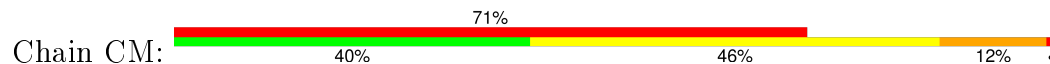
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

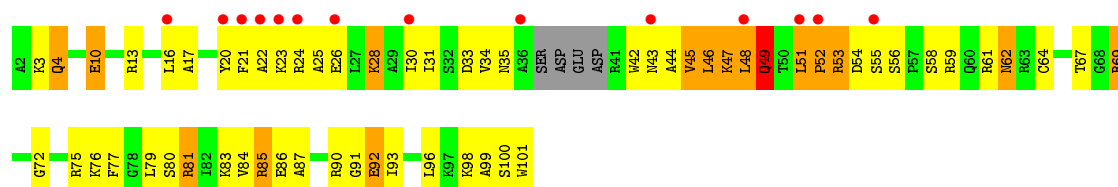


• Molecule 13: 30S ribosomal protein S13

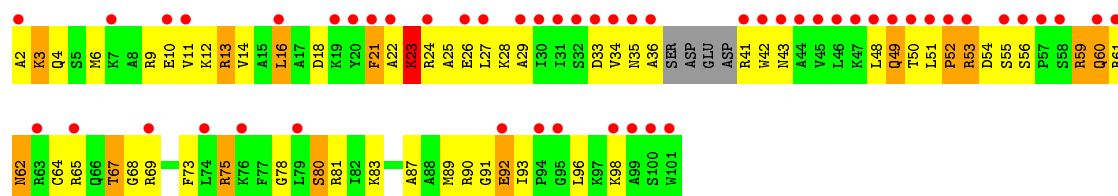


• Molecule 14: 30S ribosomal protein S14

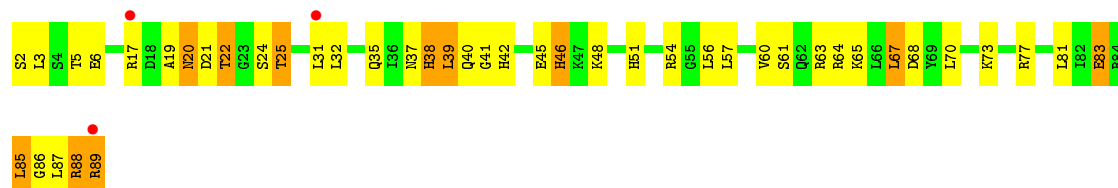




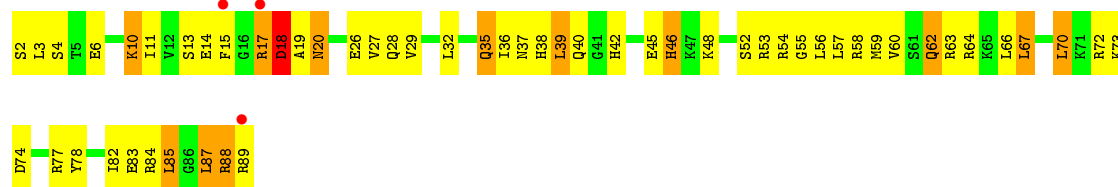
• Molecule 14: 30S ribosomal protein S14



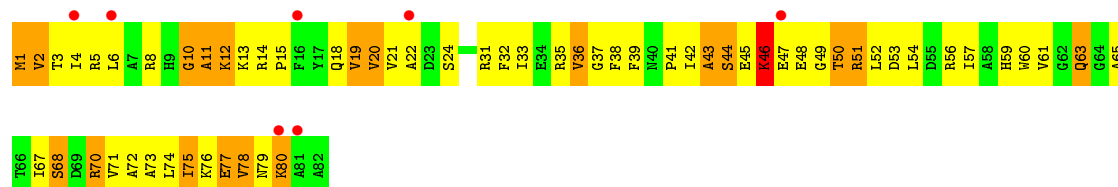
• Molecule 15: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S15

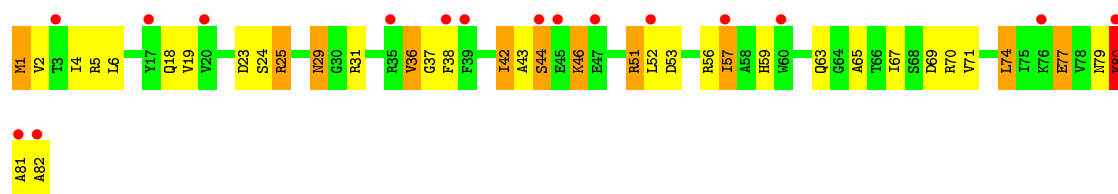


• Molecule 16: 30S ribosomal protein S16

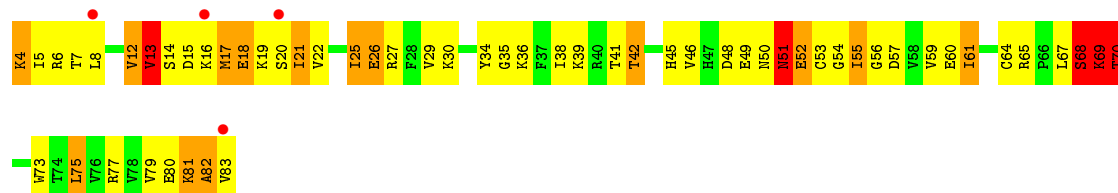


• Molecule 16: 30S ribosomal protein S16

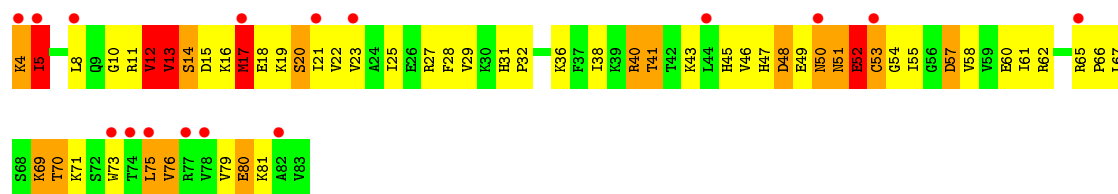




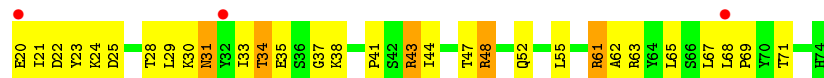
- Molecule 17: 30S ribosomal protein S17



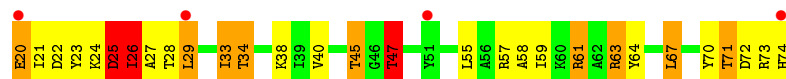
- Molecule 17: 30S ribosomal protein S17



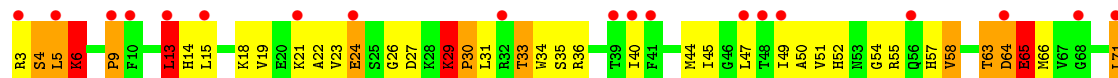
- Molecule 18: 30S ribosomal protein S18

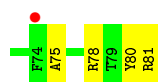


- Molecule 18: 30S ribosomal protein S18

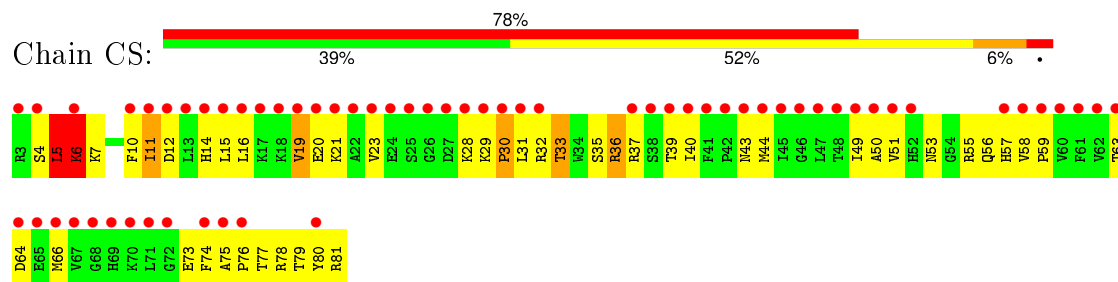


- Molecule 19: 30S ribosomal protein S19

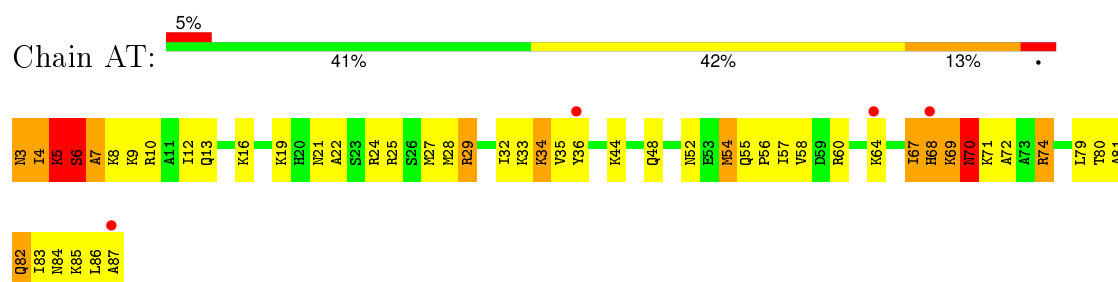




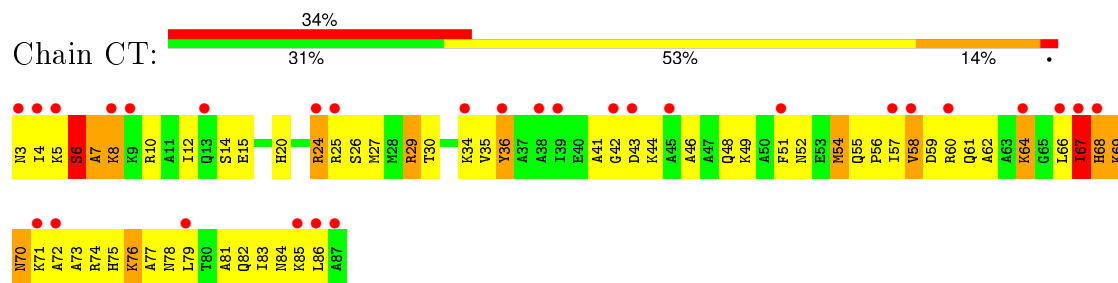
- Molecule 19: 30S ribosomal protein S19



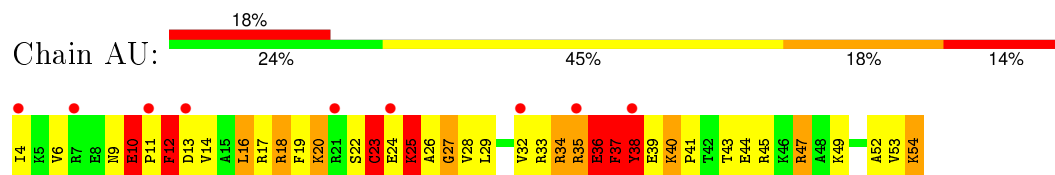
- Molecule 20: 30S ribosomal protein S20



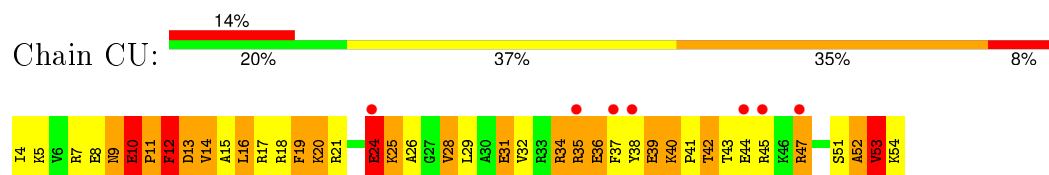
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



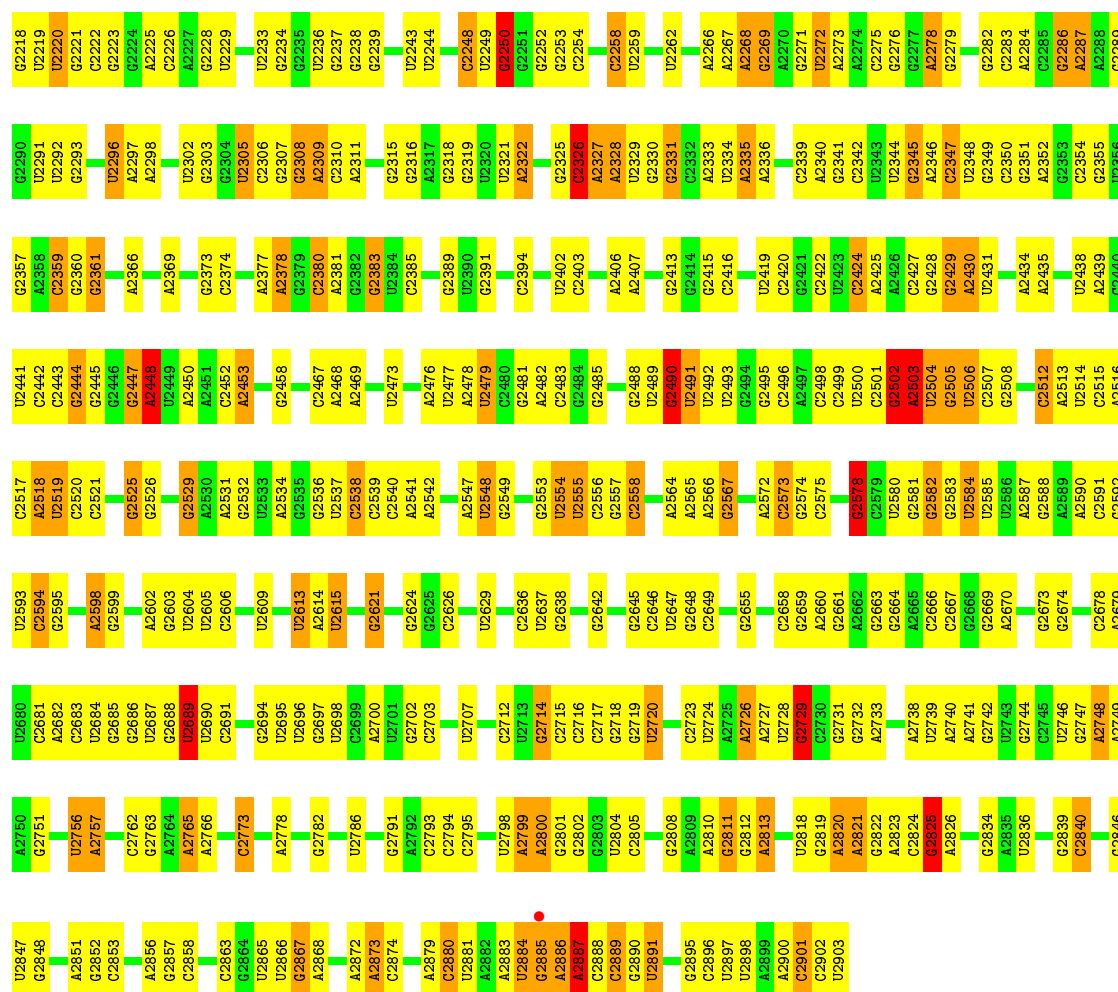
- Molecule 21: 30S ribosomal protein S21



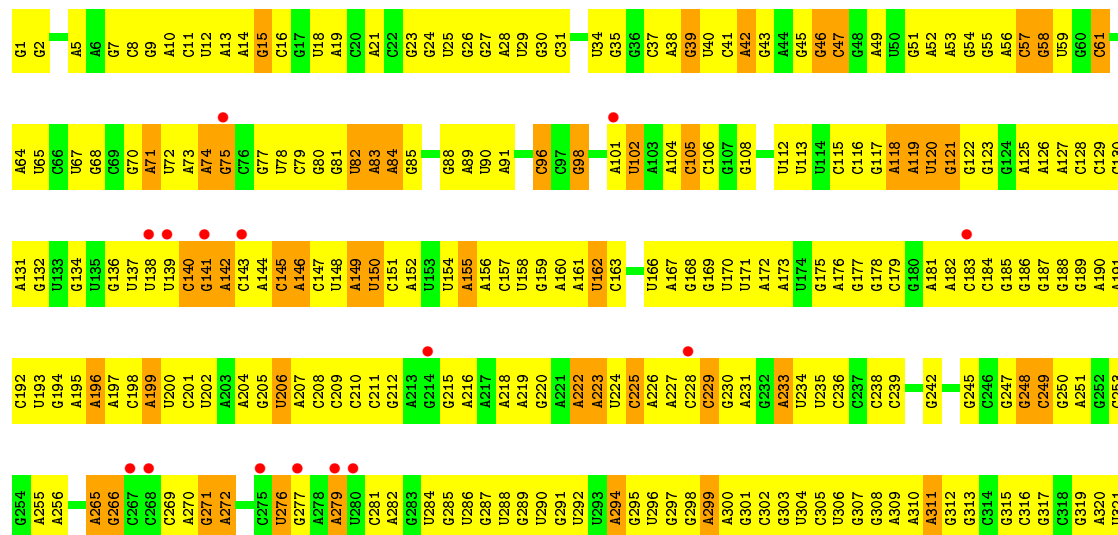
- Molecule 22: 23S rRNA



U2155	A2094	A1876	G1656	A1572	A1494	G1421	G1351	G1278	U1198	G1135
G2156	A2097	A1877	U1657	G1573	A1495	G1422	U1352	G1279	U1199	G1136
A2157	U2097	G1878	G1658	C1574	A1496	G1423	A1353	G1280	U1203	G1137
A2158	U2098	A1879	G1659	C1575	G1499	G1426	A1354	G1283	G1206	G1138
G2159	G2023	U1880	G1660	C1576	G1500	A1427	G1355	G1284	G1207	G1139
G2160	G2024	A1881	G1661	C1577	G1501	A1428	G1356	A1284	U1141	G1140
G2161	G2025	U1882	U1662	U1578	G1502	G1429	G1357	A1285	C1207	U1141
A2162	A2030	U1883	G1663	C1582	A1503	G1430	G1358	A1286	C1208	A1142
A2163	A2031	G1884	A1664	A1583	A1504	A1431	A1359	A1287	U1209	A1143
C2164	G2032	U1885	G1665	A1584	A1505	G1432	G1360	G1288	G1210	A1144
C2165	A2033	G1886	G1666	A1585	A1506	A1433	G1361	G1289	U1210	C1145
U2166	U2034	U1887	A1667	C1586	G1507	A1434	G1362	G1291	G1223	G1146
U2167	G2035	A1889	A1668	A1587	A1508	G1435	G1363	G1292	U1224	G1147
U2168	A2108	A1890	A1669	G1588	A1509	G1436	G1364	G1293	G1225	U1148
G2169	U2109	G1891	G1674	U1589	G1510	G1437	A1365	U1294	G1149	U1149
A2170	U2110	G1892	A1675	A1593	U1513	A1439	A1366	G1295	G1226	C1150
U2171	U2111	A1893	A1676	U1594	G1514	U1440	A1367	G1296	G1227	A1151
U2172	G2112	U1894	A1677	C1595	A1515	U1441	G1368	G1297	C1229	C1152
A2173	U2113	G1900	A1678	G1601	G1516	U1442	G1371	G1298	U1232	C1153
C2174	A2114	U1906	A1679	U1602	U1523	U1443	U1372	G1299	G1233	G1154
G2175	G2115	G1907	A1680	A1603	U1524	U1444	A1373	A1301	A1237	A1156
A2176	G2044	C1908	G1681	A1604	A1525	G1445	G1374	A1302	G1238	G1157
C2177	G2045	G1909	G1682	C1604	G1526	G1446	U1375	G1303	G1239	G1158
A2178	G2048	U1910	U1683	G1605	C1526	G1447	C1376	A1304	U1240	U1159
C2179	U2118	U1911	G1686	C1606	G1527	G1448	G1377	G1305	G1160	G1160
U2180	G2120	U1912	G1687	A1607	A1528	G1449	A1378	U1241	A1241	G1164
U2181	G2121	A1913	A1688	A1608	G1529	G1450	G1379	U1242	U1242	C1164
U2182	G2122	C1914	A1689	A1610	U1532	G1451	G1380	A1243	A1243	A1165
A2183	G2123	U1915	U1692	G1613	C1533	G1452	G1381	A1244	A1244	G1166
G2184	G2124	G1916	G1693	A1616	A1534	C1453	A1383	A1245	G1245	C1167
C2185	G2125	U1917	G1694	A1617	A1535	U1456	A1384	A1246	A1246	G1168
G2186	A2126	A1918	G1695	A1618	G1537	U1457	A1385	A1247	A1247	A1169
U2187	G2127	U1919	G1696	G1619	G1546	G1458	A1386	G1248	G1248	G1170
U2188	A2127	G1920	A1697	G1620	C1547	U1459	U1394	G1251	G1251	G1171
U2189	G2128	A1921	A1698	G1621	C1548	U1460	A1395	C1252	C1252	U1172
G2190	U2130	U1922	G1699	A1626	A1549	U1461	U1400	G1253	A1253	U1173
A2191	U2131	G1923	A1700	A1627	U1554	C1462	G1401	A1254	A1254	U1174
U2192	U2132	C1924	A1701	G1627	U1555	U1463	G1402	U1255	U1255	G1175
G2193	G2133	U1925	G1702	G1632	A1553	U1464	U1403	G1256	G1256	U1176
A2194	A2134	U1926	G1703	A1632	U1554	U1465	A1404	G1332	G1259	U1177
U2195	G2135	G1927	C1706	G1633	G1555	U1466	U1405	G1333	U1263	G1178
C2196	A2136	A1928	G1707	A1634	C1557	U1467	U1406	G1334	A1264	U1182
C2197	G2137	U1929	G1708	A1637	C1558	U1468	G1407	U1335	U1183	U1183
U2197	U2137	G1930	U1709	G1637	U1559	U1469	G1408	G1336	A1265	U1184
A2198	G2138	U1931	U1710	C1644	G1560	G1470	U1409	G1337	G1266	G1185
G2201	U2139	G1932	A1783	U1647	U1563	U1471	G1410	G1338	U1267	G1186
U2202	G2140	U1933	A1784	U1648	U1564	U1472	U1411	G1339	A1268	G1187
G2203	A2141	G1934	A1785	U1649	C1565	U1473	U1412	U1340	U1269	U1188
G2204	G2142	U1935	G1707	G1649	U1566	U1474	A1413	G1341	A1269	U1189
A2205	U2143	A1936	U1708	A1650	A1567	U1475	G1414	A1342	G1270	G1190
G2206	U2144	U1937	U1709	A1651	G1568	U1476	U1415	G1343	G1271	G1191
G2207	A2145	G1938	G1710	A1652	G1569	U1477	U1416	U1344	A1272	G1192
U2208	G2146	U1939	U1711	U1653	A1570	U1478	C1417	G1345	U1273	G1193
A2209	U2147	A1940	U1712	U1654	A1571	G1482	G1418	C1349	A1275	C1196
G2210	A2148	G1941	U1713	A1655	U1570	U1483	A1419	G1350	G1277	G1197
A2211	G2149	U1942	U1714	G1656	U1571	U1484	U1420	U1351	U1278	G1198
U2212	U2150	U1943	U1715	U1657	U1572	U1485	U1421	U1352	U1279	G1199
G2213	G2151	U1944	U1716	U1658	U1573	U1486	U1422	U1353	G1280	G1200
U2214	U2152	U1945	U1717	U1659	U1574	U1487	U1423	U1354	G1281	G1201
G2215	G2153	U1946	U1718	U1660	U1575	U1488	U1424	U1355	G1282	G1202
G2216	U2154	U1947	U1719	U1661	U1576	U1489	U1425	U1356	G1283	G1203
G2217	A2155	U1948	U1720	U1662	U1577	U1490	U1426	U1357	G1284	G1204
		U1949	U1721	U1663	U1578	U1491	U1427	U1358	G1285	G1205
		U1950	U1722	U1664	U1579	U1492	U1428	U1359	G1286	G1206
		U1951	U1723	U1665	U1580	U1493	U1429	U1360	G1287	G1207
		U1952	U1724	U1666	U1581	U1494	U1430	U1361	G1288	G1208
		U1953	U1725	U1667	U1582	U1495	U1431	U1362	G1289	G1209
		U1954	U1726	U1668	U1583	U1496	U1432	U1363	G1290	G1210
		U1955	U1727	U1669	U1584	U1497	U1433	U1364	G1291	G1211
		U1956	U1728	U1670	U1585	U1498	U1434	U1365	G1292	G1212
		U1957	U1729	U1671	U1586	U1499	U1435	U1366	G1293	G1213
		U1958	U1730	U1672	U1587	U1500	U1436	U1367	G1294	G1214
		U1959	U1731	U1673	U1588	U1501	U1437	U1368	G1295	G1215
		U1960	U1732	U1674	U1589	U1502	U1438	U1369	G1296	G1216
		U1961	U1733	U1675	U1590	U1503	U1439	U1370	G1297	G1217
		U1962	U1734	U1676	U1591	U1504	U1440	U1371	G1298	G1218
		U1963	U1735	U1677	U1592	U1505	U1441	U1372	G1299	G1219
		U1964	U1736	U1678	U1593	U1506	U1442	U1373	G1300	G1220
		U1965	U1737	U1679	U1594	U1507	U1443	U1374	G1301	G1221
		U1966	U1738	U1680	U1595	U1508	U1444	U1375	G1302	G1222
		U1967	U1739	U1681	U1596	U1509	U1445	U1376	G1303	G1223
		U1968	U1740	U1682	U1597	U1510	U1446	U1377	G1304	G1224
		U1969	U1741	U1683	U1598	U1511	U1447	U1378	G1305	G1225
		U1970	U1742	U1684	U1599	U1512	U1448	U1379	G1306	G1226
		U1971	U1743	U1685	U1600	U1513	U1449	U1380	G1307	G1227
		U1972	U1744	U1686	U1601	U1514	U1450	G1308	G1308	G1228
		U1973	U1745	U1687	U1602	U1515	U1451	G1309	G1309	G1229
		U1974	U1746	U1688	U1603	U1516	U1452	G1310	G1310	G1230
		U1975	U1747	U1689	U1604	U1517	U1453	G1311	G1311	G1231
		U1976	U1748	U1690	U1605	U1518	U1454	G1312	G1312	G1232
		U1977	U1749	U1691	U1606	U1519	U1455	G1313	G1313	G1233
		U1978	U1750	U1692	U1607	U1520	U1456	G1314	G1314	G1234
		U1979	U1751	U1693	U1608	U1521	U1457	G1315	G1315	G1235
		U1980	U1752	U1694	U1609	U1522	U1458	G1316	G1316	G1236
		U1981	U1753	U1695	U1610	U1523	U1459	G1317	G1317	G1237
		U1982	U1754	U1696	U1611	U1524	U1460	G1318	G1318	G1238
		U1983	U1755	U1697	U1612	U1525	U1461	G1319	G1319	G1239
		U1984	U1756	U1698	U1613	U1526	U1462	G1320	G1320	G1240
		U1985	U1757	U1699	U1614	U1527	U1463	G1321	G1321	G1241
		U1986	U1758	U1700	U1615	U1528	U1464	G1322	G1322	G1242
		U1987	U1759	U1701	U1616	U1529	U1465	G1323	G1323	G1243
		U1988	U1760	U1702	U1617	U1530	U1466	G1324	G1324	G1244
		U1989	U1761	U1703	U1618	U1531	U1467	G1325	G1325	G1245
		U1990	U1762	U1704	U1619	U1532	U1468	G1326	G1326	G1246
		U1991	U1763	U1705	U1620	U1533	U1469	G1327	G1327	G1247
		U1992	U1764	U1706	U1621	U1534	U1470	G1328	G1328	G1248
		U1993	U1765	U1707	U1622	U1535	U1471	G1329	G1329	G1249
		U1994	U1766	U1708	U1623	U1536	U1472	G1330	G1330	G1250
		U1995	U1767	U1709	U1624	U1537	U1473	G1331	G1331	G1251
		U1996	U1768	U1710	U1625	U1538	U1474	G1332	G1332	G1252
		U1997	U1769	U1711	U1626	U1539	U1475	G1333	G1333	G1253
		U1998	U1770	U1712	U1627	U1540	U1476	G1334	G1334	G1254
		U1999	U1771	U1713	U1628	U1541	U1477	G1335	G1335	G1255
		U2000	U1772	U1714	U1629	U1542	U1478	G1336	G1336	G1256
		U2001	U1773	U1715	U1630	U1543	U1479	G1337	G1337	G1257
		U2002	U1774	U1716	U1631	U1544	U1480	G1338	G1338	G1258
		U2003	U1775	U1717	U1632	U1545	U1481	G1339	G1339	G1259
		U2004	U1776	U1718	U1633	U1546	U1482	G1340	G1340	G1260
		U2005	U1777	U1719	U1634	U1547	U1483	G1341	G134	

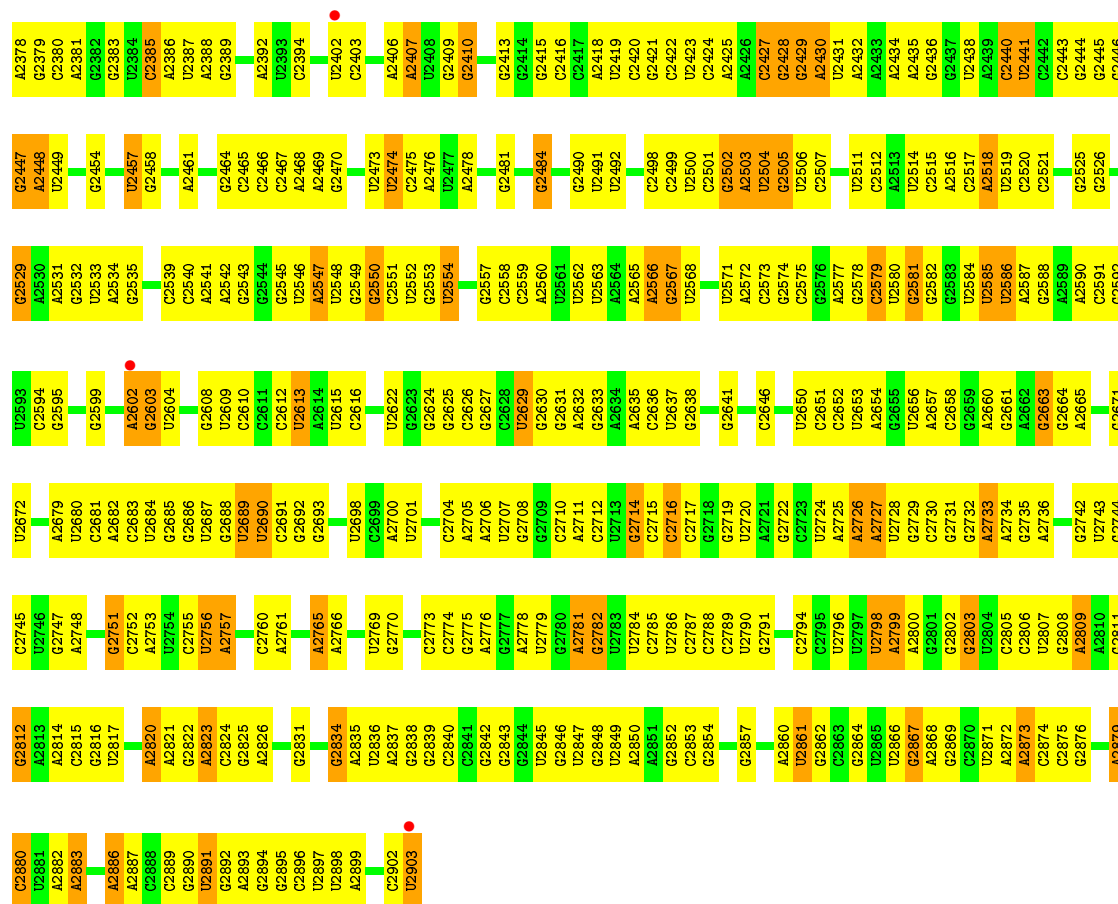


• Molecule 22: 23S rRNA



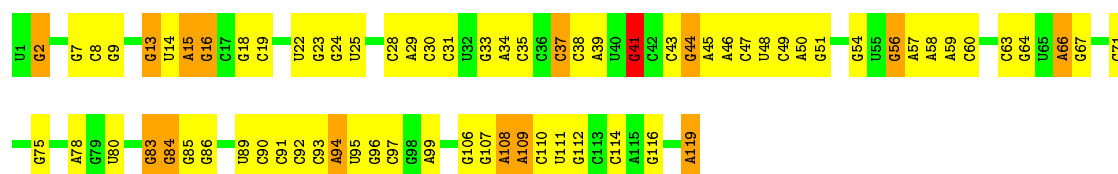
A1262	A1263	A1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	U1274	A1275	A1276	G1277	G1278	G1279	G1280	G1281	U1282		A1285	A1286	A1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	A1301		A1304	G1305	G1306	A1307	A1308	A1309	G1310	G1311	G1312	G1313	G1314	G1315	U1316	G1317	U1318	G1319	G1320	A1321	A1322	C1323							
G1197	U1198	U1199	C1200	U1203	A1204	A1268	A1269	U1205	U1206	G1207	C1208	U1209	G1211	G1212	A1213	A1214	G1215		U1219	G1220	G1221	U1222	G1223	U1224	G1225	A1226	G1227	G1228	G1229	A1230	U1231	G1232	C1233		G1236	A1237	G1238	G1239	U1240	A1241	U1242		G1245	A1246	A1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	G1257	U1258	G1259	A1321	A1322	C1261						
G1115	G1116	C1117	U1118	U1119	G1120	C1121	G1122	U1080	U1081	G1062	G1063	A1126	A1127	G1128		G1131	U1132	A1133	A1134	C1135	G1136		G1139	C1140	U1141	A1142		C1146	A1147		C1153	G1154	A1155	A1156		A1169	C1170	G1171	A1089	U1173	G1091	U1174	A1175	U1176		G1177	C1178	U1179	U1180	U1181	G1182	U1183	U1184	G1185	U1186	G1187	U1188	A1189	U1190		A1194	G1195	C1196			
C1052	C1053		G1056	A1057	U1058	U1059	U1060	U1061	G1062	G1063		A1064	U1065	U1066		G1121	A1067	G1068	A1069	A1070	G1071	C1072	A1073	C1074	C1075	C1076	A1077		U1078	G1079	A1080	U1081	U1082	U1083	A1085	A1086	G1087	A1088	A1089		G1092	G1093	U1094	A1095	A1096	U1097	U1098	U1099	U1100	U1101	C1102	A1103	C1104		G1107	U1108	U1109	G1110	A1111	G1112						
G1197	U1198	U1199	C1200	U1203	A1204	A1268	A1269	G1206	C1207	G1208	U1209	G1210	G1211	G1212	A1213	A1214	G1215		U1219	G1220	G1221	U1222	G1223	U1224	G1225	A1226	G1227	G1228	G1229	A1230	U1231	G1232	C1233		G1236	A1237	G1238	G1239	U1240	A1241	U1242		G1245	A1246	A1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	G1257	U1258	G1259	A1321	A1322	C1261						
A322	C323	A324		G327	U328	G329	A330	C331	A332	G333	C334	C335		G338		C341	A342	C343	A344	A345	A346	A347	A412	U416	C417	A418		A352	C353	A354	U355	G356	C357	U358	G359	U360	U427	A428	A429	A430	U431	A432	C433	C366	G367		G370	A371	G372	U373	A374		G377	C378	G379	C445	C446	G381	A447	U448	A449	C450	G386			
U387	G388	G389	U390	A391	U392		U395	G396	U397	C398	G399	G400	A401	A402	U403	A404	U405		G408	G409	G410	G411	A412	U416	C417	A418		A352	C353	A354	U355	G356	C357	U358	G359	U360	U427	A428	A429	A430	U431	A432	C433	C366	G367		G370	A371	G372	U373	A374		G377	C378	G379	C445	C446	G381	A447	U448	A449	C450	G386			
G452	A453	A454	C455	C456	A457	U458	U459	A460	C461	C462	G463	U464	G465	A466	G467	G468	G469	A470	A471	A472	G473	G474	G475	A476	A477	A478	A479	A480	A481	G482	A483	U484	C485	C486	C487	G488	A489	C490	G491	A492	C493	G494	G495	G496	A497	G498	U499	U500	A501	A502	A503	A504	A505	G506	A507	A508	C509	U510	U511							
G512	A513	A514	A515	C516	U517	G520	U521	A522	C523	G524	U525	A526	G527	A528	U529	G530	C531	A532	G533	U534	G535	G536	G537	A538	G539	G540	A541	C542	G543	U544	U545	U546	G548	G549	C550	G551	U552	G553	U554	G555		U556	G559	C560	G561	U562	A563	C564	A631	C565		U568	U569	C570	G571	A572	U573	A574								
A575	U576	G577	G578	G579	U580	C581	A582	G583	C584	G585	A586	C587	U588	U589	A590	U591	A592	U593	U594	C595		A599	G600	C601	A602	A603	G604	G605	U606	U607	A608	A609	U645	U646	C610		A613	A614	U615	A616	G617	G618	G619	G620	A621	G622		A626	A627	G628	G629	G630	A631	A632	A633	C634	G635	G636	A637	C638	U639					
U642	A643	A644	C645	U646	G647	G648	U649	G650	G651	A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702										
U703	G704		G705	G706	G707	G708		G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678	C679	C680	G681	U682	G683	U684	G685	A686	C687	G690	C691	U692	A693	U694	G695	U696	G697	C698	A699	G700	U701	U702
G778	U779	G780	A781	U782	A783			G712		A716	G717			G718	G719	U720	A721			A654	A655	G656	U657	U658	A659	U660	C661	A662	A663	G664	U665	U666	A667	A668	G669	A670	C671	C672	C673	U674	A675	A676	A677	C678																						





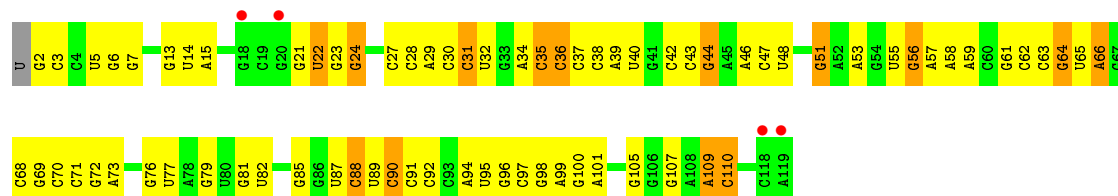
• Molecule 23: 5S rRNA

Chain BB: 39% 48% 12%



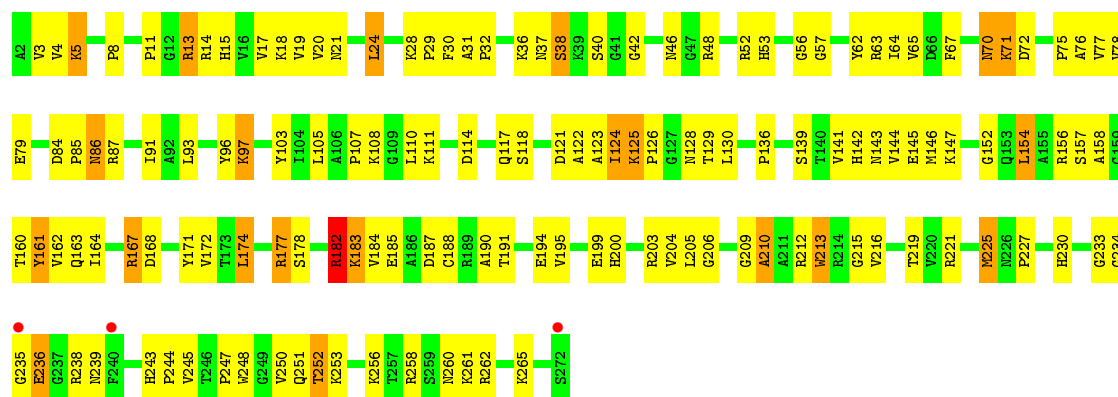
• Molecule 23: 5S rRNA

Chain DB: 3% 37% 50% 12%

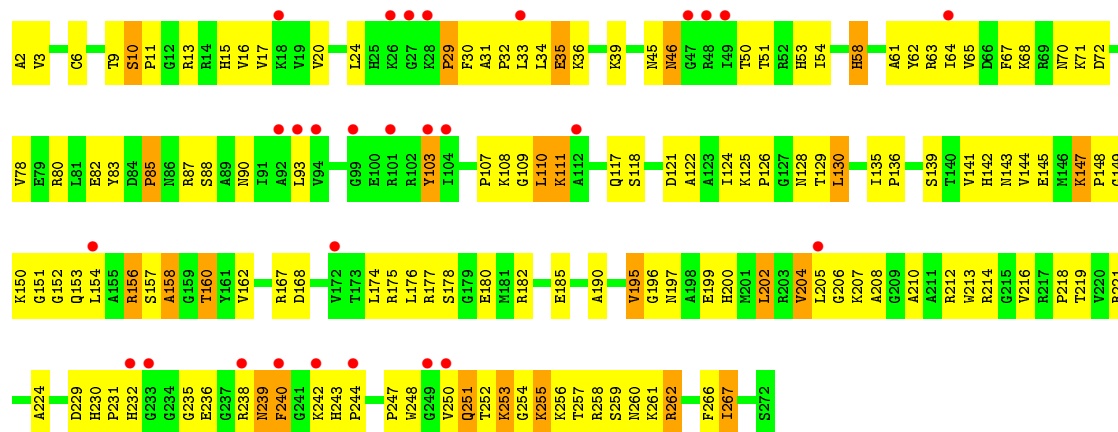


• Molecule 24: 50S ribosomal protein L2

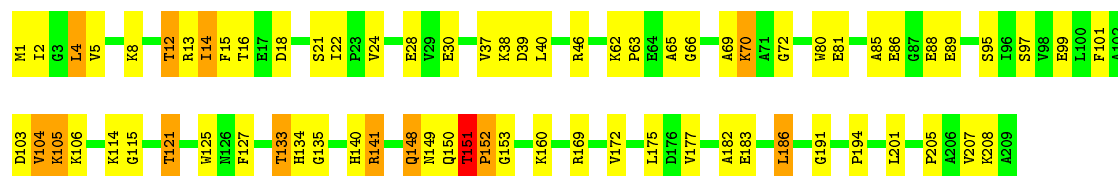
Chain BC: 47% 45% 8%



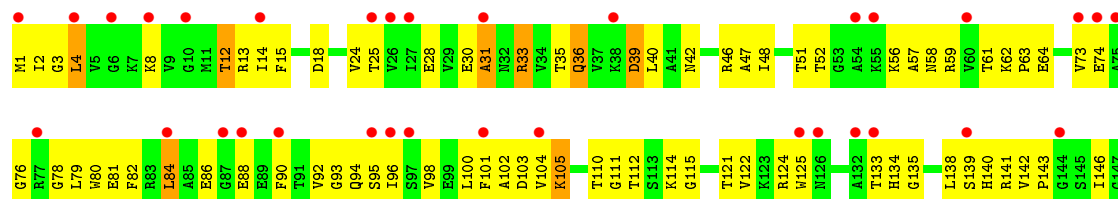
• Molecule 24: 50S ribosomal protein L2

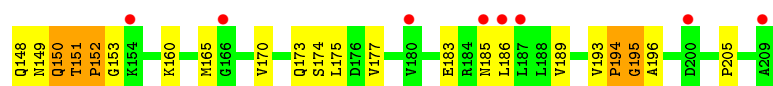


• Molecule 25: 50S ribosomal protein L3

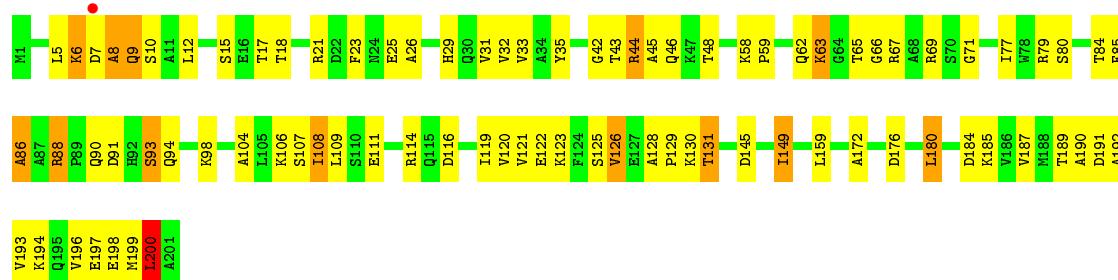


• Molecule 25: 50S ribosomal protein L3

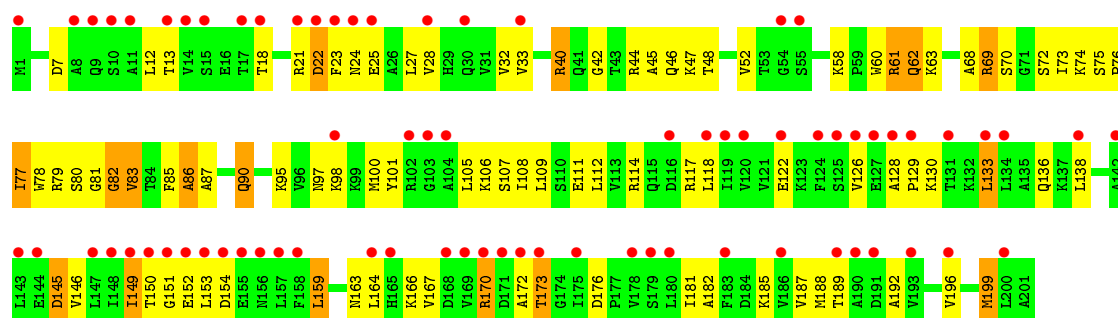
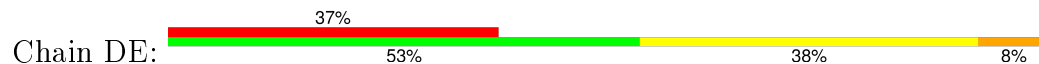




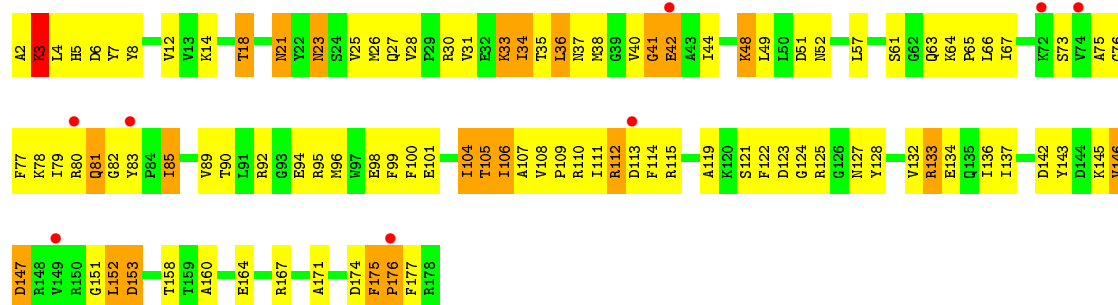
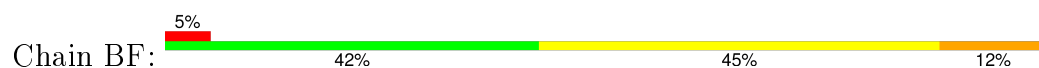
- Molecule 26: 50S ribosomal protein L4



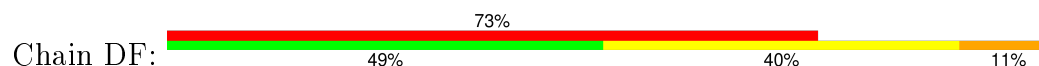
- Molecule 26: 50S ribosomal protein L4

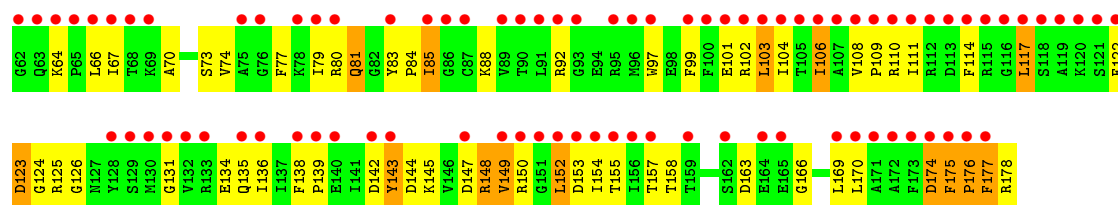


- Molecule 27: 50S ribosomal protein L5

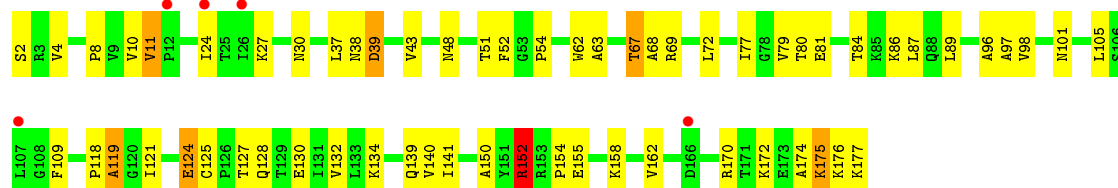


- Molecule 27: 50S ribosomal protein L5

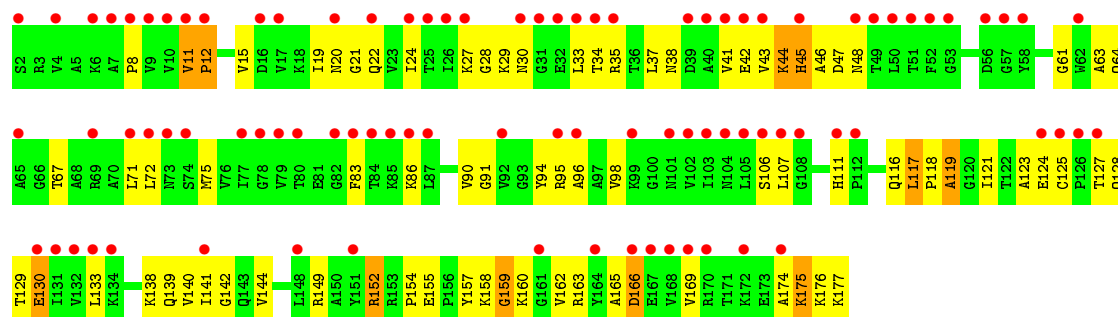




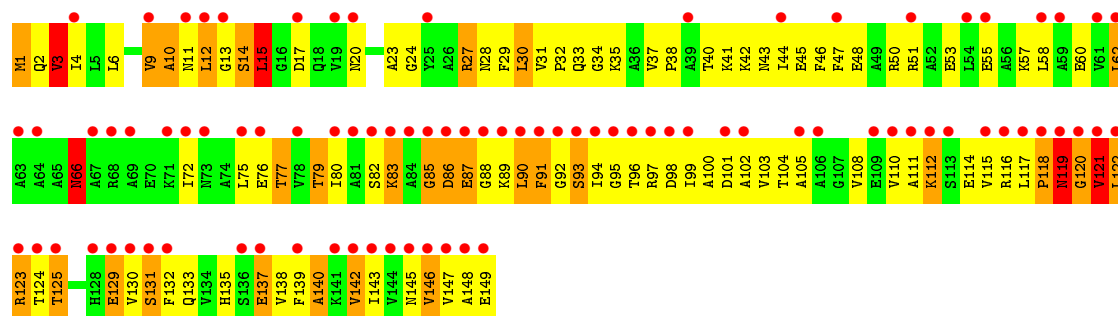
• Molecule 28: 50S ribosomal protein L6



• Molecule 28: 50S ribosomal protein L6

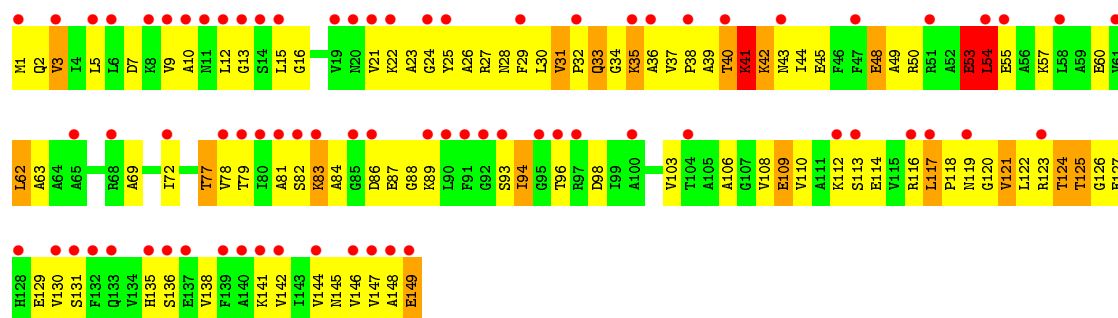


• Molecule 29: 50S ribosomal protein L9

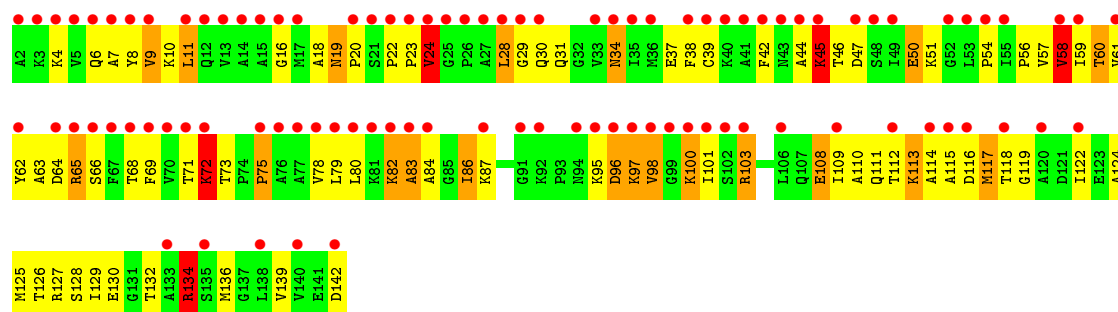


• Molecule 29: 50S ribosomal protein L9

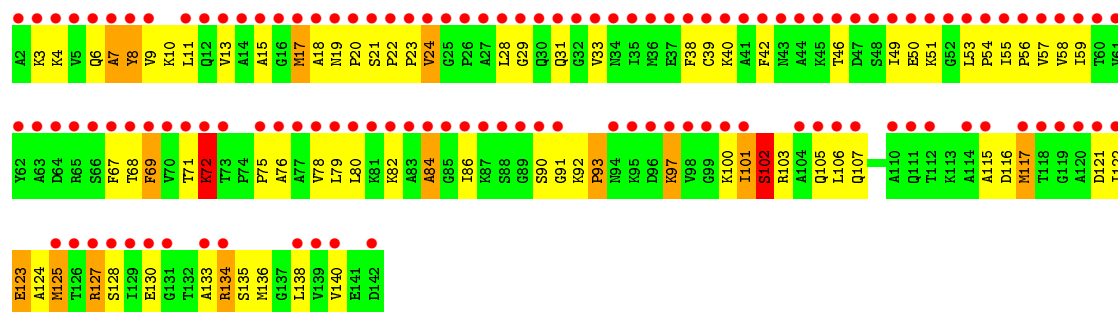
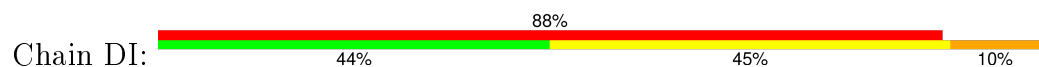




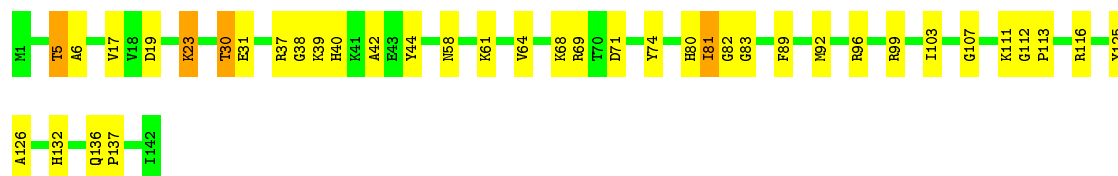
- Molecule 30: 50S ribosomal protein L11



- Molecule 30: 50S ribosomal protein L11

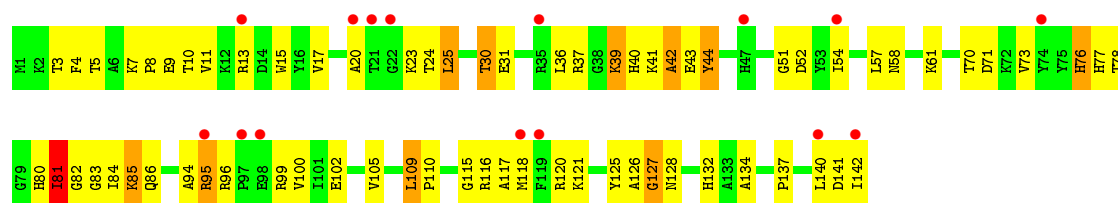


- Molecule 31: 50S ribosomal protein L13



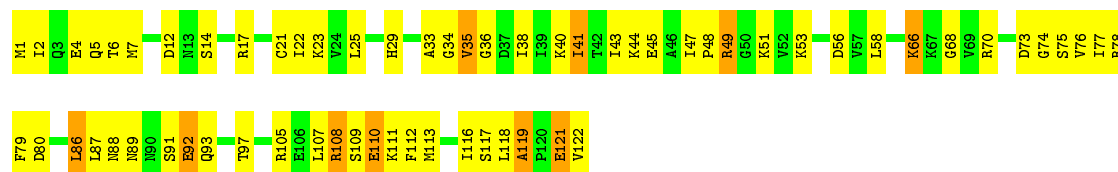
- Molecule 31: 50S ribosomal protein L13





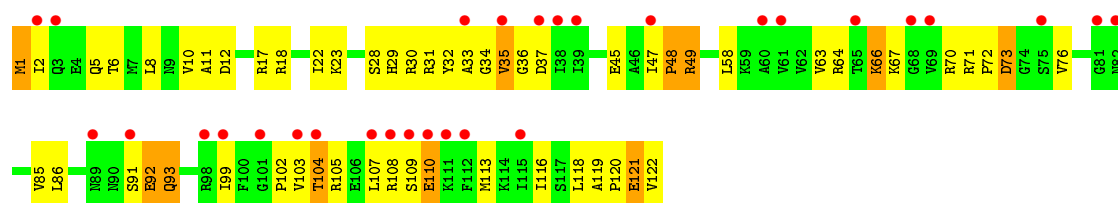
• Molecule 32: 50S ribosomal protein L14

Chain BK: 48% 44% 8%



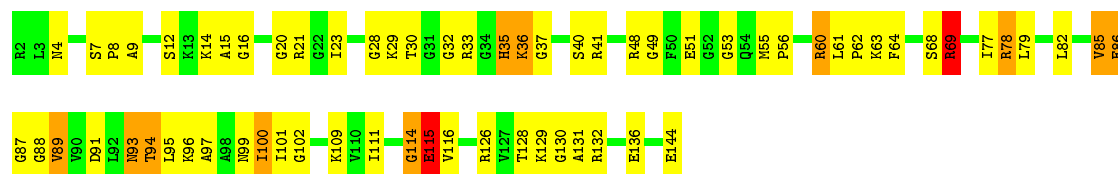
• Molecule 32: 50S ribosomal protein L14

Chain DK: 25% 53% 38% 9%



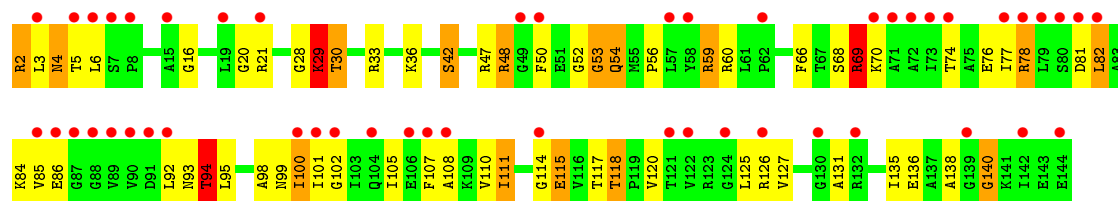
• Molecule 33: 50S ribosomal protein L15

Chain BL: 54% 37% 8%



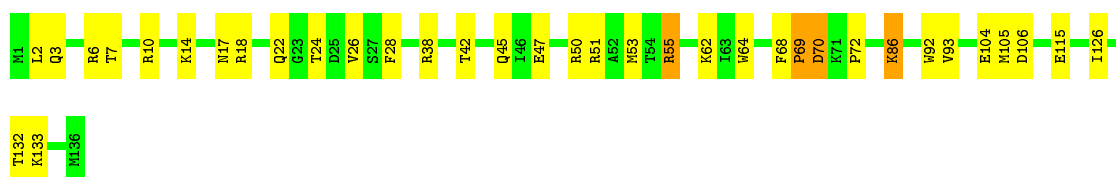
• Molecule 33: 50S ribosomal protein L15

Chain DL: 34% 56% 31% 10%

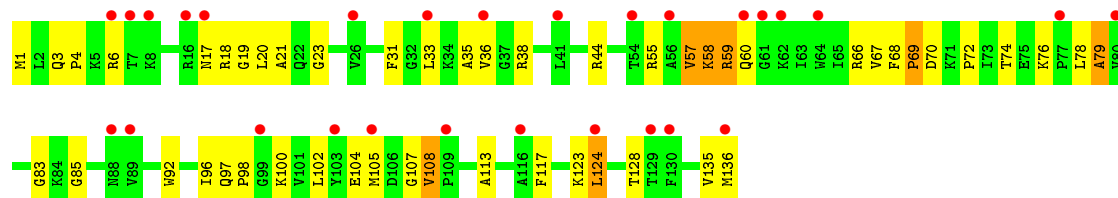


• Molecule 34: 50S ribosomal protein L16

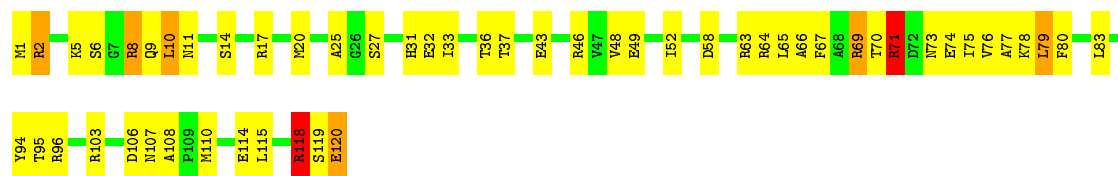
Chain BM: 74% 24% 2%



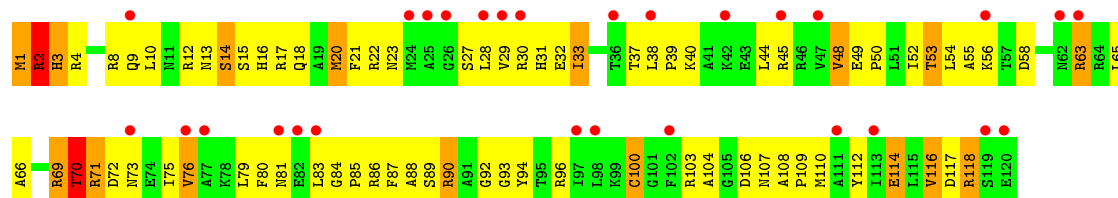
- Molecule 34: 50S ribosomal protein L16



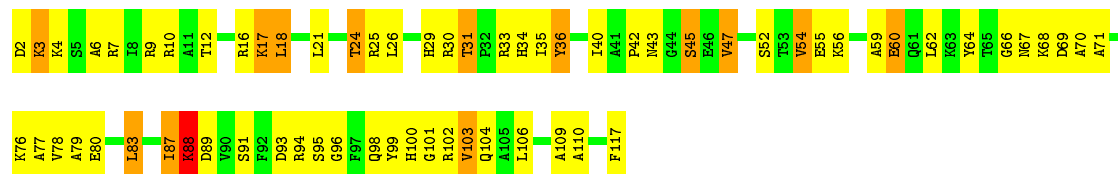
- Molecule 35: 50S ribosomal protein L17



- Molecule 35: 50S ribosomal protein L17

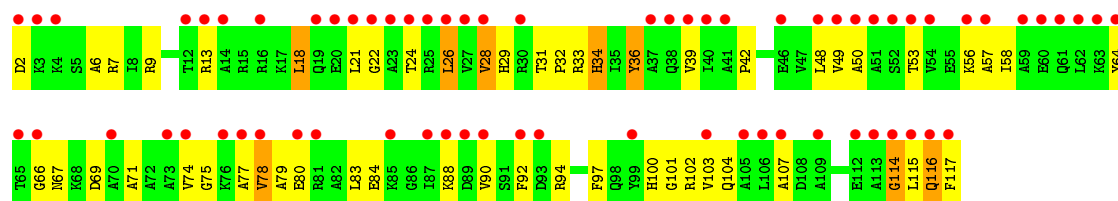


- Molecule 36: 50S ribosomal protein L18



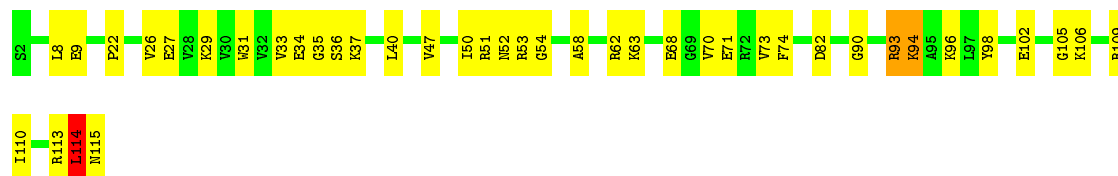
- Molecule 36: 50S ribosomal protein L18





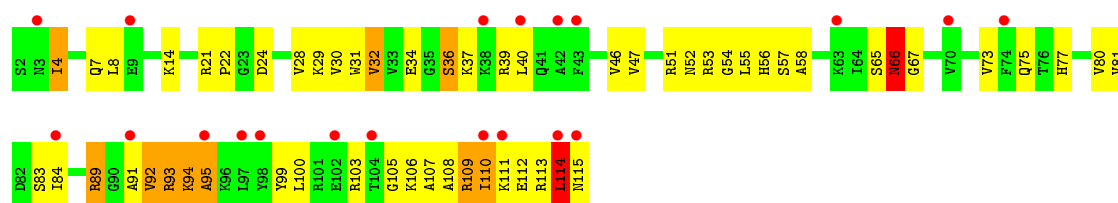
• Molecule 37: 50S ribosomal protein L19

Chain BP: 64% 33% ..



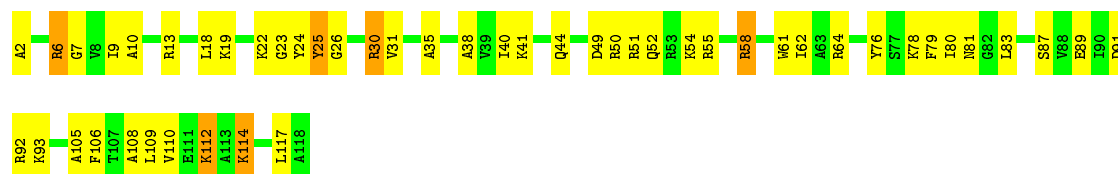
• Molecule 37: 50S ribosomal protein L19

Chain DP: 18% 50% 39% 9% .



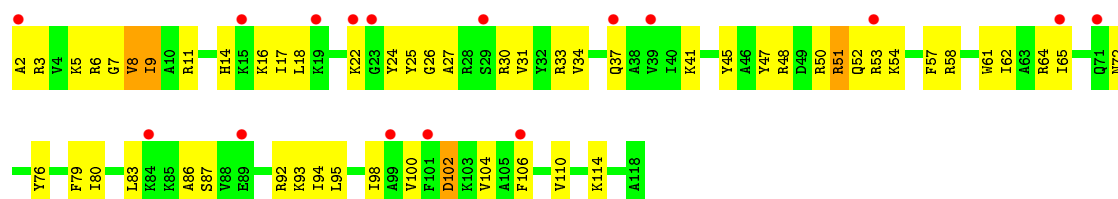
• Molecule 38: 50S ribosomal protein L20

Chain BQ: 58% 37% 5%



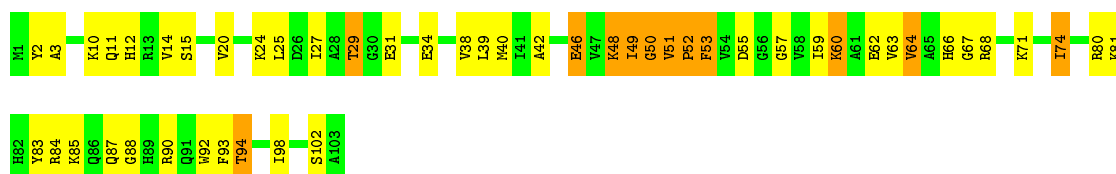
• Molecule 38: 50S ribosomal protein L20

Chain DQ: 14% 53% 44% .

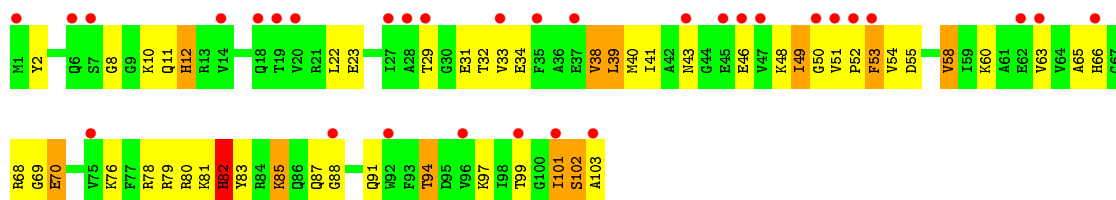


• Molecule 39: 50S ribosomal protein L21

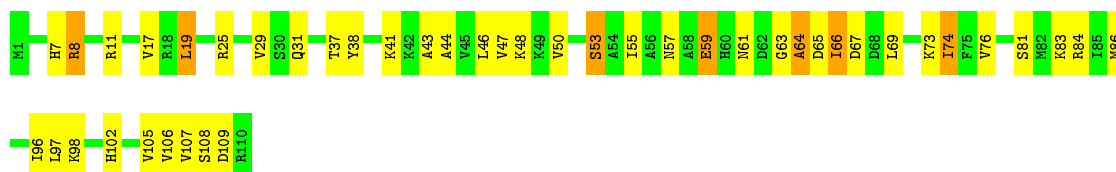
Chain BR: 51% 37% 12%



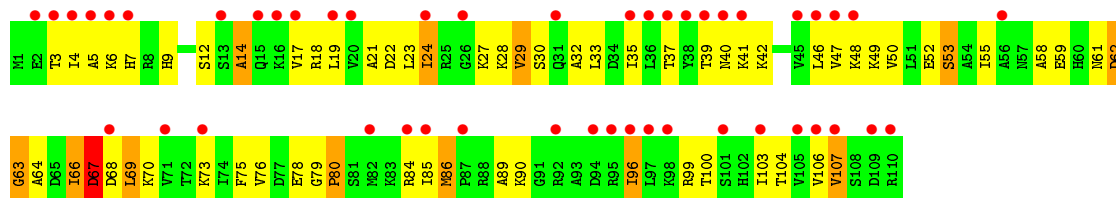
• Molecule 39: 50S ribosomal protein L21



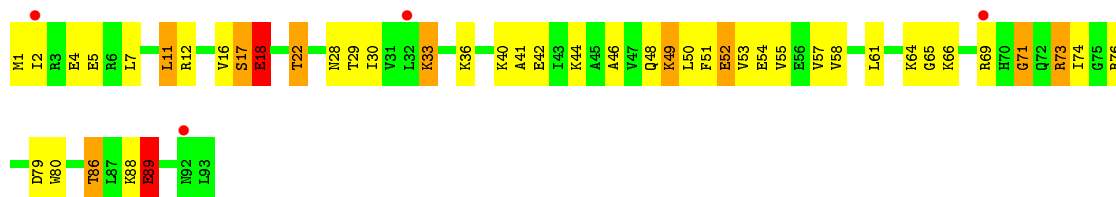
• Molecule 40: 50S ribosomal protein L22



• Molecule 40: 50S ribosomal protein L22

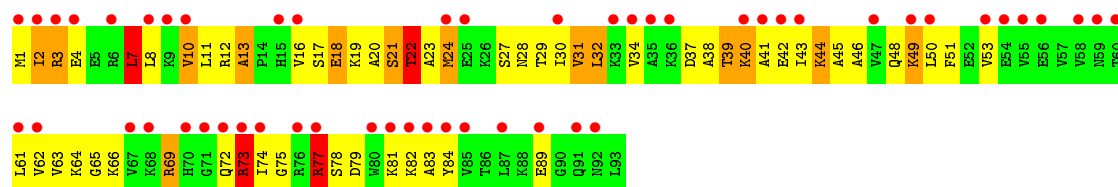


• Molecule 41: 50S ribosomal protein L23

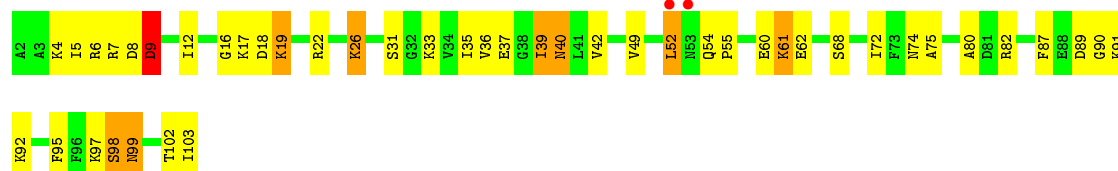


• Molecule 41: 50S ribosomal protein L23

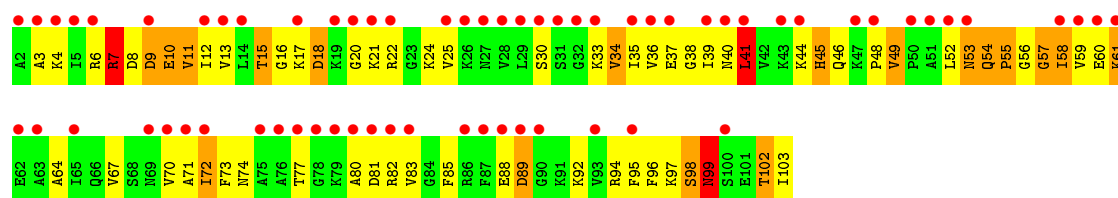




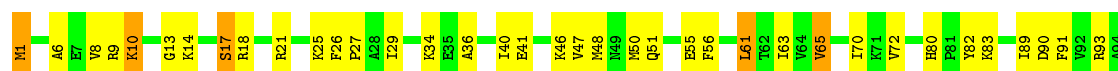
• Molecule 42: 50S ribosomal protein L24



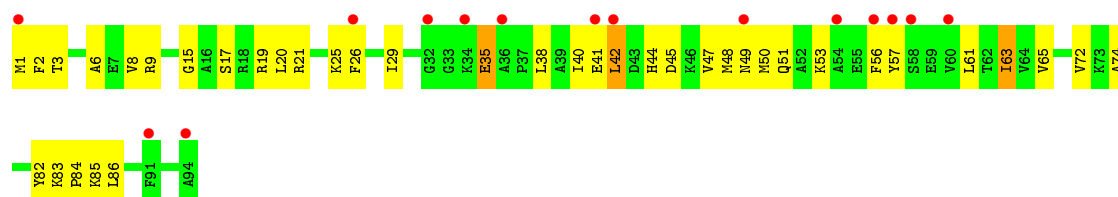
• Molecule 42: 50S ribosomal protein L24



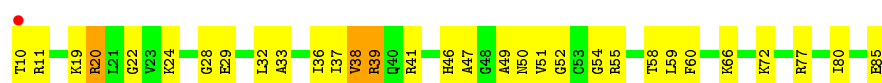
• Molecule 43: 50S ribosomal protein L25



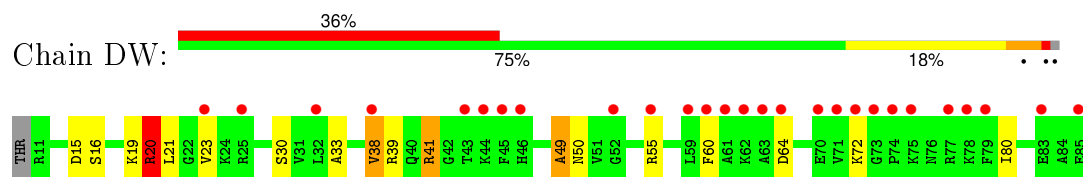
• Molecule 43: 50S ribosomal protein L25



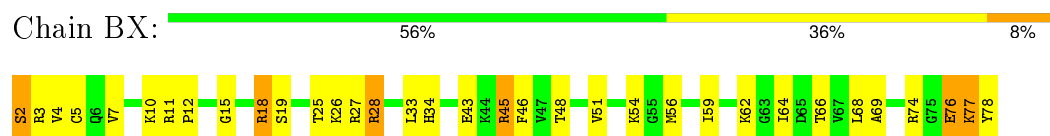
• Molecule 44: 50S ribosomal protein L27



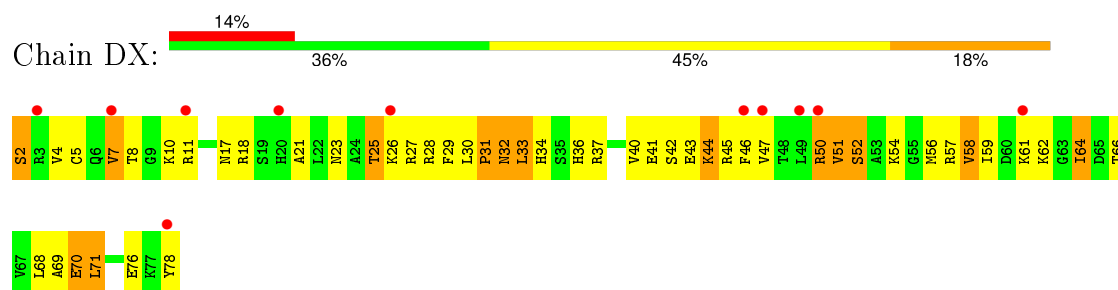
- Molecule 44: 50S ribosomal protein L27



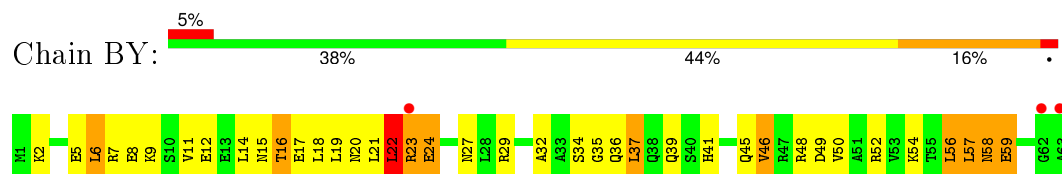
- Molecule 45: 50S ribosomal protein L28



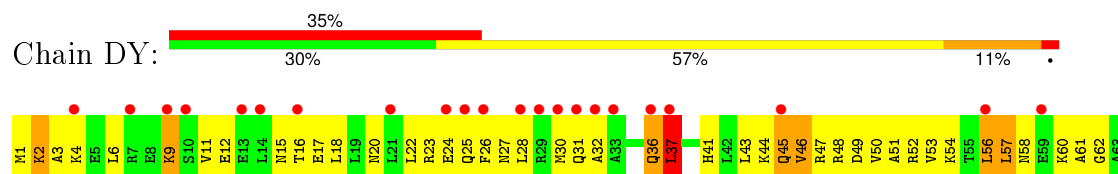
- Molecule 45: 50S ribosomal protein L28



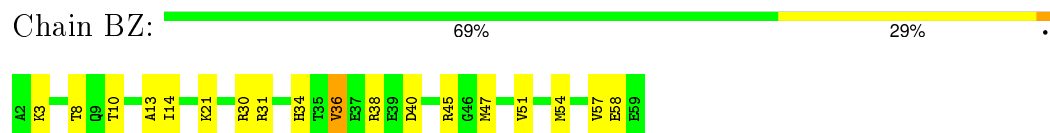
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29

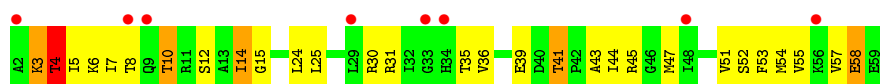


- Molecule 47: 50S ribosomal protein L30



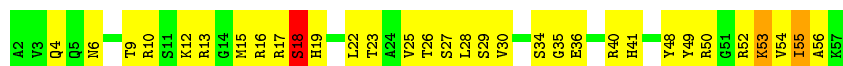
- Molecule 47: 50S ribosomal protein L30





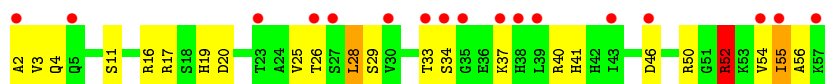
- Molecule 48: 50S ribosomal protein L32

Chain B0: 43% 52%



- Molecule 48: 50S ribosomal protein L32

Chain D0: 30% 59% 36%



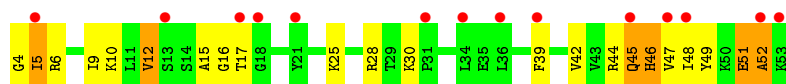
- Molecule 49: 50S ribosomal protein L33

Chain B1: 4% 42% 46% 10%



- Molecule 49: 50S ribosomal protein L33

Chain D1: 28% 56% 32% 12%



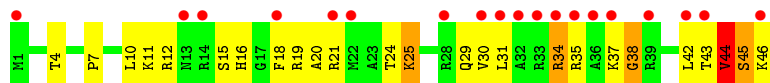
- Molecule 50: 50S ribosomal protein L34

Chain B2: 2% 63% 30% 7%



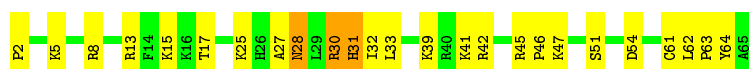
- Molecule 50: 50S ribosomal protein L34

Chain D2: 41% 46% 43% 9%

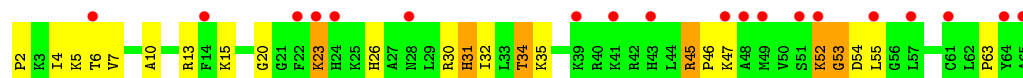


- Molecule 51: 50S ribosomal protein L35

Chain B3: 61% 34% 5%



- Molecule 51: 50S ribosomal protein L35



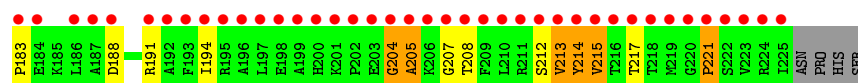
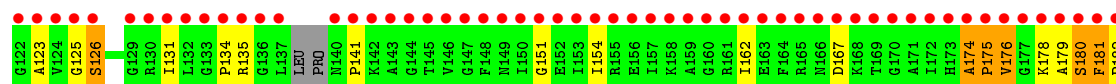
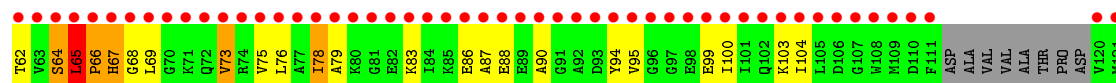
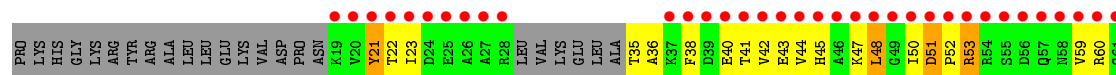
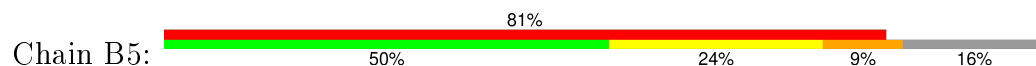
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.64Å 434.61Å 625.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.41 – 2.90 69.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (69.41-2.90) 90.0 (69.41-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.223 , 0.265 0.232 , 0.272	Depositor DCC
R_{free} test set	4560 reflections (0.41%)	DCC
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1126727 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	288258	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 1.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: VIR, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.48	0/36944	0.93	23/57632 (0.0%)
1	CA	0.41	0/36966	0.88	12/57666 (0.0%)
2	AB	0.34	0/1736	0.59	0/2338
2	CB	0.32	0/1736	0.55	0/2338
3	AC	0.35	0/1652	0.58	0/2225
3	CC	0.31	0/1652	0.51	0/2225
4	AD	0.36	0/1665	0.61	0/2227
4	CD	0.40	0/1665	0.63	0/2227
5	AE	0.38	0/1119	0.65	0/1504
5	CE	0.38	0/1119	0.69	0/1504
6	AF	0.40	0/836	0.66	1/1128 (0.1%)
6	CF	0.33	0/836	0.61	1/1128 (0.1%)
7	AG	0.34	0/1196	0.54	0/1602
7	CG	0.32	0/1196	0.51	0/1602
8	AH	0.40	0/989	0.59	0/1326
8	CH	0.31	0/989	0.54	0/1326
9	AI	0.32	0/1034	0.60	0/1375
9	CI	0.31	0/1034	0.56	0/1375
10	AJ	0.36	0/797	0.58	0/1077
10	CJ	0.32	0/797	0.55	0/1077
11	AK	0.33	0/893	0.58	0/1205
11	CK	0.35	0/893	0.60	0/1205
12	AL	0.40	0/969	0.68	0/1300
12	CL	0.37	0/969	0.66	0/1300
13	AM	0.33	0/893	0.61	0/1193
13	CM	0.32	0/893	0.56	0/1193
14	AN	0.37	0/785	0.59	0/1043
14	CN	0.30	0/785	0.49	0/1043
15	AO	0.33	0/718	0.60	0/959
15	CO	0.31	0/718	0.51	0/959
16	AP	0.38	0/659	0.62	0/884
16	CP	0.33	0/659	0.55	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.38	0/658	0.62	0/881
17	CQ	0.37	0/658	0.57	0/881
18	AR	0.33	0/463	0.54	0/621
18	CR	0.35	0/463	0.58	0/621
19	AS	0.35	0/653	0.60	0/877
19	CS	0.34	0/653	0.53	0/877
20	AT	0.39	0/671	0.60	0/888
20	CT	0.32	0/671	0.55	0/888
21	AU	0.43	0/431	0.65	0/570
21	CU	0.45	0/431	0.63	0/570
22	BA	0.82	19/69659 (0.0%)	1.28	469/108672 (0.4%)
22	DA	0.39	0/69659	0.88	19/108672 (0.0%)
23	BB	0.74	0/2850	1.25	7/4444 (0.2%)
23	DB	0.31	0/2828	0.81	0/4410
24	BC	0.52	0/2122	0.72	1/2852 (0.0%)
24	DC	0.35	0/2122	0.59	0/2852
25	BD	0.58	0/1586	0.75	1/2134 (0.0%)
25	DD	0.33	0/1586	0.55	0/2134
26	BE	0.51	0/1571	0.66	0/2113
26	DE	0.33	0/1571	0.54	0/2113
27	BF	0.41	0/1435	0.63	0/1926
27	DF	0.30	0/1435	0.48	0/1926
28	BG	0.41	0/1343	0.61	0/1816
28	DG	0.30	0/1343	0.48	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	0.36	0/1046	0.57	0/1410
30	DI	0.36	0/1046	0.53	0/1410
31	BJ	0.61	0/1152	0.73	0/1551
31	DJ	0.32	0/1152	0.55	0/1551
32	BK	0.57	0/948	0.76	1/1268 (0.1%)
32	DK	0.36	0/948	0.55	0/1268
33	BL	0.55	0/1054	0.77	0/1403
33	DL	0.32	0/1054	0.58	0/1403
34	BM	0.58	0/1093	0.75	0/1460
34	DM	0.31	0/1093	0.50	0/1460
35	BN	0.57	0/974	0.77	2/1301 (0.2%)
35	DN	0.33	0/974	0.55	0/1301
36	BO	0.48	0/902	0.67	0/1209
36	DO	0.30	0/902	0.49	0/1209
37	BP	0.54	0/929	0.67	0/1242
37	DP	0.34	0/929	0.55	0/1242
38	BQ	0.67	0/960	0.76	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.33	0/960	0.51	0/1278
39	BR	0.63	0/829	0.83	0/1107
39	DR	0.32	0/829	0.57	0/1107
40	BS	0.66	0/864	0.83	1/1156 (0.1%)
40	DS	0.33	0/864	0.56	0/1156
41	BT	0.48	0/745	0.65	0/994
41	DT	0.32	0/745	0.56	0/994
42	BU	0.46	0/788	0.68	0/1051
42	DU	0.37	0/788	0.56	0/1051
43	BV	0.51	0/766	0.69	0/1025
43	DV	0.28	0/766	0.45	0/1025
44	BW	0.56	0/587	0.70	0/776
44	DW	0.31	0/576	0.50	0/762
45	BX	0.46	0/635	0.65	0/848
45	DX	0.32	0/635	0.55	0/848
46	BY	0.42	0/510	0.66	0/677
46	DY	0.33	0/510	0.55	0/677
47	BZ	0.63	0/453	0.68	0/605
47	DZ	0.30	0/453	0.53	0/605
48	B0	0.58	0/450	0.72	0/599
48	D0	0.34	0/450	0.57	0/599
49	B1	0.45	0/417	0.62	0/554
49	D1	0.33	0/417	0.52	0/554
50	B2	0.57	0/380	0.80	0/498
50	D2	0.36	0/380	0.60	0/498
51	B3	0.52	0/513	0.70	0/676
51	D3	0.32	0/513	0.52	0/676
52	B4	0.57	0/303	0.74	0/397
52	D4	0.30	0/303	0.54	0/397
53	B5	0.33	0/1145	0.50	0/1556
All	All	0.54	19/310626 (0.0%)	0.94	539/464366 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	1
6	CF	0	1
11	AK	0	1
12	CL	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
21	AU	0	1
21	CU	0	1
25	BD	0	1
All	All	0	7

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-11.58	1.30	1.37
22	BA	984	A	N9-C4	-11.48	1.30	1.37
22	BA	1936	A	N9-C4	-9.61	1.32	1.37
22	BA	528	A	N7-C5	-6.85	1.35	1.39
22	BA	752	A	N9-C4	-6.64	1.33	1.37

The worst 5 of 539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	528	A	N1-C6-N6	15.09	127.66	118.60
22	BA	974	G	C4-C5-N7	14.38	116.55	110.80
22	BA	984	A	C2-N3-C4	-13.21	103.99	110.60
22	BA	984	A	N3-C4-C5	12.10	135.27	126.80
22	BA	1936	A	C2-N3-C4	-11.70	104.75	110.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
25	BD	151	THR	Peptide
5	CE	102	GLY	Peptide
6	CF	54	LEU	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	1123	4
1	CA	33015	0	16617	1084	0
2	AB	1705	0	1732	191	0
2	CB	1705	0	1732	131	0
3	AC	1625	0	1696	83	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	149	0
4	CD	1643	0	1707	119	0
5	AE	1106	0	1148	74	0
5	CE	1106	0	1148	112	0
6	AF	818	0	808	67	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	55	0
7	CG	1182	0	1238	65	0
8	AH	979	0	1031	68	0
8	CH	979	0	1031	41	0
9	AI	1022	0	1070	79	0
9	CI	1022	0	1070	63	0
10	AJ	787	0	828	80	0
10	CJ	787	0	828	50	0
11	AK	877	0	887	66	0
11	CK	877	0	887	67	0
12	AL	955	0	1016	66	0
12	CL	955	0	1016	77	0
13	AM	884	0	941	66	0
13	CM	884	0	941	47	0
14	AN	774	0	824	65	0
14	CN	774	0	824	48	0
15	AO	710	0	728	31	0
15	CO	710	0	728	42	0
16	AP	649	0	666	61	0
16	CP	649	0	666	28	0
17	AQ	649	0	691	70	0
17	CQ	649	0	691	53	0
18	AR	456	0	478	21	0
18	CR	456	0	478	33	0
19	AS	638	0	665	54	0
19	CS	638	0	665	36	0
20	AT	665	0	714	56	0
20	CT	665	0	714	43	0
21	AU	426	0	449	58	0
21	CU	426	0	449	54	0
22	BA	62195	0	31280	1616	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2231	0
23	BB	2549	0	1291	52	0
23	DB	2529	0	1281	62	0
24	BC	2083	0	2154	122	0
24	DC	2083	0	2154	127	0
25	BD	1565	0	1616	66	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	69	0
26	DE	1552	0	1619	78	0
27	BF	1411	0	1444	94	0
27	DF	1411	0	1444	62	0
28	BG	1323	0	1371	50	0
28	DG	1323	0	1371	52	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	120	4
30	BI	1032	0	1085	70	0
30	DI	1032	0	1085	67	0
31	BJ	1129	0	1162	37	0
31	DJ	1129	0	1162	54	0
32	BK	939	0	1012	46	0
32	DK	939	0	1012	50	0
33	BL	1045	0	1117	61	0
33	DL	1045	0	1117	66	0
34	BM	1074	0	1157	27	0
34	DM	1074	0	1157	30	0
35	BN	961	0	1000	44	0
35	DN	961	0	1000	70	0
36	BO	892	0	923	55	0
36	DO	892	0	923	44	0
37	BP	917	0	962	31	0
37	DP	917	0	962	45	0
38	BQ	947	0	1019	49	0
38	DQ	947	0	1019	50	0
39	BR	816	0	839	71	0
39	DR	816	0	839	47	0
40	BS	857	0	922	36	0
40	DS	857	0	922	46	0
41	BT	739	0	807	41	0
41	DT	739	0	807	59	0
42	BU	780	0	831	28	0
42	DU	780	0	831	73	0
43	BV	753	0	780	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	27	0
44	BW	580	0	594	17	0
44	DW	569	0	581	16	0
45	BX	625	0	652	24	0
45	DX	625	0	652	47	0
46	BY	509	0	543	33	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	10	0
47	DZ	449	0	488	18	0
48	B0	444	0	458	24	0
48	D0	444	0	458	18	0
49	B1	410	0	440	25	0
49	D1	410	0	440	16	0
50	B2	377	0	418	15	0
50	D2	377	0	418	24	0
51	B3	504	0	572	27	0
51	D3	504	0	572	20	0
52	B4	302	0	340	14	0
52	D4	302	0	342	15	0
53	B5	1142	0	865	48	0
54	AA	71	0	0	0	0
54	AN	1	0	0	0	0
54	BA	193	0	0	0	0
54	BB	4	0	0	0	0
54	BD	1	0	0	0	0
54	BQ	1	0	0	0	0
54	CA	56	0	0	0	0
54	D2	1	0	0	0	0
54	DA	166	0	0	0	0
54	DB	3	0	0	0	0
54	DQ	1	0	0	0	0
55	BA	38	0	35	5	0
55	DA	38	0	35	15	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	192	0	0	25	0
57	AL	2	0	0	0	0
57	AN	6	0	0	1	0
57	AT	2	0	0	0	0
57	AU	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	2	0	0	0	0
57	BA	620	0	0	65	0
57	BB	13	0	0	0	0
57	BC	7	0	0	1	0
57	BD	3	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BJ	1	0	0	0	0
57	BL	5	0	0	0	0
57	BN	3	0	0	0	0
57	BQ	1	0	0	0	0
57	BS	1	0	0	0	0
57	BT	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	191	0	0	26	0
57	CL	1	0	0	0	0
57	CN	2	0	0	0	0
57	CT	2	0	0	0	0
57	CU	2	0	0	1	0
57	D2	1	0	0	1	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	105	0
57	DB	13	0	0	0	0
57	DC	12	0	0	2	0
57	DD	4	0	0	2	0
57	DE	6	0	0	2	0
57	DJ	1	0	0	0	0
57	DL	4	0	0	1	0
57	DN	2	0	0	0	0
57	DT	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	288258	0	192859	10766	4

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 23.

The worst 5 of 10766 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)
22:BA:1153:C:OP2	57:BA:3360:HOH:O	1.56	1.23
22:BA:621:A:OP2	57:BA:3293:HOH:O	1.57	1.23
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:123:ARG:HH22	1:CA:367:U:P	1.69	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14

All (4) 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:OP1	29:DH:93:SER:OG[4_455]	1.70	0.50
1:AA:367:U:O5'	29:DH:123:ARG:NH2[4_455]	2.02	0.18
1:AA:368:U:O4	29:DH:83:LYS:CE[4_455]	2.03	0.17
1:AA:368:U:O4	29:DH:83:LYS:CB[4_455]	2.13	0.07

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%)	126 (58%)	40 (18%)	50 (23%)	0	0
2	CB	216/218 (99%)	133 (62%)	52 (24%)	31 (14%)	0	0
3	AC	204/206 (99%)	149 (73%)	38 (19%)	17 (8%)	1	2
3	CC	204/206 (99%)	153 (75%)	40 (20%)	11 (5%)	2	7
4	AD	203/205 (99%)	139 (68%)	33 (16%)	31 (15%)	0	0
4	CD	203/205 (99%)	150 (74%)	31 (15%)	22 (11%)	0	1
5	AE	148/150 (99%)	104 (70%)	31 (21%)	13 (9%)	1	2
5	CE	148/150 (99%)	98 (66%)	28 (19%)	22 (15%)	0	0
6	AF	98/100 (98%)	66 (67%)	19 (19%)	13 (13%)	0	1
6	CF	98/100 (98%)	66 (67%)	16 (16%)	16 (16%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	111 (74%)	28 (19%)	10 (7%)	1	4
7	CG	149/151 (99%)	121 (81%)	20 (13%)	8 (5%)	2	7
8	AH	127/129 (98%)	91 (72%)	21 (16%)	15 (12%)	0	1
8	CH	127/129 (98%)	95 (75%)	24 (19%)	8 (6%)	2	5
9	AI	125/127 (98%)	91 (73%)	21 (17%)	13 (10%)	1	1
9	CI	125/127 (98%)	86 (69%)	28 (22%)	11 (9%)	1	2
10	AJ	96/98 (98%)	60 (62%)	15 (16%)	21 (22%)	0	0
10	CJ	96/98 (98%)	71 (74%)	13 (14%)	12 (12%)	0	1
11	AK	115/117 (98%)	84 (73%)	19 (16%)	12 (10%)	1	1
11	CK	115/117 (98%)	81 (70%)	24 (21%)	10 (9%)	1	2
12	AL	121/123 (98%)	92 (76%)	22 (18%)	7 (6%)	2	6
12	CL	121/123 (98%)	94 (78%)	12 (10%)	15 (12%)	0	1
13	AM	112/114 (98%)	81 (72%)	20 (18%)	11 (10%)	1	2
13	CM	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1	3
14	AN	92/100 (92%)	62 (67%)	18 (20%)	12 (13%)	0	1
14	CN	92/100 (92%)	59 (64%)	18 (20%)	15 (16%)	0	0
15	AO	86/88 (98%)	65 (76%)	16 (19%)	5 (6%)	2	6
15	CO	86/88 (98%)	70 (81%)	12 (14%)	4 (5%)	3	11
16	AP	80/82 (98%)	53 (66%)	15 (19%)	12 (15%)	0	0
16	CP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	2	5
17	AQ	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	1
17	CQ	78/80 (98%)	56 (72%)	11 (14%)	11 (14%)	0	0
18	AR	53/55 (96%)	43 (81%)	10 (19%)	0	100	100
18	CR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	1
19	AS	77/79 (98%)	54 (70%)	12 (16%)	11 (14%)	0	0
19	CS	77/79 (98%)	60 (78%)	12 (16%)	5 (6%)	1	4
20	AT	83/85 (98%)	60 (72%)	15 (18%)	8 (10%)	1	2
20	CT	83/85 (98%)	64 (77%)	12 (14%)	7 (8%)	1	2
21	AU	49/51 (96%)	27 (55%)	9 (18%)	13 (26%)	0	0
21	CU	49/51 (96%)	26 (53%)	12 (24%)	11 (22%)	0	0
24	BC	269/271 (99%)	211 (78%)	47 (18%)	11 (4%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	204 (76%)	50 (19%)	15 (6%)	2	7
25	BD	207/209 (99%)	180 (87%)	20 (10%)	7 (3%)	5	19
25	DD	207/209 (99%)	168 (81%)	29 (14%)	10 (5%)	3	10
26	BE	199/201 (99%)	167 (84%)	26 (13%)	6 (3%)	5	22
26	DE	199/201 (99%)	160 (80%)	28 (14%)	11 (6%)	2	7
27	BF	175/177 (99%)	144 (82%)	24 (14%)	7 (4%)	4	15
27	DF	175/177 (99%)	137 (78%)	24 (14%)	14 (8%)	1	3
28	BG	174/176 (99%)	149 (86%)	20 (12%)	5 (3%)	6	23
28	DG	174/176 (99%)	136 (78%)	29 (17%)	9 (5%)	2	8
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	2
30	BI	139/141 (99%)	85 (61%)	36 (26%)	18 (13%)	0	1
30	DI	139/141 (99%)	82 (59%)	44 (32%)	13 (9%)	1	2
31	BJ	140/142 (99%)	129 (92%)	10 (7%)	1 (1%)	26	63
31	DJ	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	4	18
32	BK	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	3	9
32	DK	120/122 (98%)	100 (83%)	13 (11%)	7 (6%)	2	6
33	BL	141/143 (99%)	112 (79%)	22 (16%)	7 (5%)	3	9
33	DL	141/143 (99%)	99 (70%)	29 (21%)	13 (9%)	1	2
34	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	13	42
34	DM	134/136 (98%)	111 (83%)	15 (11%)	8 (6%)	2	6
35	BN	118/120 (98%)	104 (88%)	10 (8%)	4 (3%)	5	19
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	4
36	BO	114/116 (98%)	87 (76%)	21 (18%)	6 (5%)	2	8
36	DO	114/116 (98%)	85 (75%)	22 (19%)	7 (6%)	2	5
37	BP	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	4	18
37	DP	112/114 (98%)	84 (75%)	16 (14%)	12 (11%)	0	1
38	BQ	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	11	38
38	DQ	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	21	57
39	BR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	3
39	DR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	98 (91%)	7 (6%)	3 (3%)	6	24
40	DS	108/110 (98%)	88 (82%)	12 (11%)	8 (7%)	1	3
41	BT	91/93 (98%)	72 (79%)	13 (14%)	6 (7%)	1	4
41	DT	91/93 (98%)	52 (57%)	28 (31%)	11 (12%)	0	1
42	BU	100/102 (98%)	76 (76%)	16 (16%)	8 (8%)	1	3
42	DU	100/102 (98%)	71 (71%)	16 (16%)	13 (13%)	0	1
43	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
43	DV	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	17	51
44	BW	74/76 (97%)	68 (92%)	5 (7%)	1 (1%)	14	44
44	DW	73/76 (96%)	63 (86%)	8 (11%)	2 (3%)	6	25
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	15	46
45	DX	75/77 (97%)	55 (73%)	12 (16%)	8 (11%)	0	1
46	BY	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	1
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	2
47	BZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	DZ	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	7
48	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	4	17
48	D0	54/56 (96%)	39 (72%)	13 (24%)	2 (4%)	4	17
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	2
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	2	5
50	B2	44/46 (96%)	40 (91%)	3 (7%)	1 (2%)	8	30
50	D2	44/46 (96%)	33 (75%)	8 (18%)	3 (7%)	1	4
51	B3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	12	40
51	D3	62/64 (97%)	46 (74%)	13 (21%)	3 (5%)	3	10
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	24
53	B5	183/228 (80%)	97 (53%)	57 (31%)	29 (16%)	0	0
All	All	11418/11672 (98%)	8663 (76%)	1837 (16%)	918 (8%)	1	3

5 of 918 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	21	ARG
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	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%)	133 (74%)	47 (26%)	0	2
2	CB	180/180 (100%)	140 (78%)	40 (22%)	1	3
3	AC	170/170 (100%)	134 (79%)	36 (21%)	1	4
3	CC	170/170 (100%)	136 (80%)	34 (20%)	1	5
4	AD	172/172 (100%)	136 (79%)	36 (21%)	1	4
4	CD	172/172 (100%)	145 (84%)	27 (16%)	3	9
5	AE	113/113 (100%)	87 (77%)	26 (23%)	1	3
5	CE	113/113 (100%)	87 (77%)	26 (23%)	1	3
6	AF	87/87 (100%)	61 (70%)	26 (30%)	0	1
6	CF	87/87 (100%)	62 (71%)	25 (29%)	0	1
7	AG	124/124 (100%)	95 (77%)	29 (23%)	1	2
7	CG	124/124 (100%)	89 (72%)	35 (28%)	0	1
8	AH	104/104 (100%)	87 (84%)	17 (16%)	3	8
8	CH	104/104 (100%)	84 (81%)	20 (19%)	2	5
9	AI	105/105 (100%)	71 (68%)	34 (32%)	0	1
9	CI	105/105 (100%)	77 (73%)	28 (27%)	0	2
10	AJ	86/86 (100%)	69 (80%)	17 (20%)	1	5
10	CJ	86/86 (100%)	67 (78%)	19 (22%)	1	3
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	3
11	CK	90/90 (100%)	68 (76%)	22 (24%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	87 (84%)	16 (16%)	3	10
12	CL	103/103 (100%)	83 (81%)	20 (19%)	2	5
13	AM	92/92 (100%)	72 (78%)	20 (22%)	1	3
13	CM	92/92 (100%)	71 (77%)	21 (23%)	1	3
14	AN	79/83 (95%)	64 (81%)	15 (19%)	2	6
14	CN	79/83 (95%)	65 (82%)	14 (18%)	2	7
15	AO	75/76 (99%)	61 (81%)	14 (19%)	2	6
15	CO	75/76 (99%)	58 (77%)	17 (23%)	1	3
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	3
16	CP	65/65 (100%)	51 (78%)	14 (22%)	1	4
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	1
17	CQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
18	AR	48/48 (100%)	37 (77%)	11 (23%)	1	3
18	CR	48/48 (100%)	37 (77%)	11 (23%)	1	3
19	AS	70/70 (100%)	58 (83%)	12 (17%)	2	7
19	CS	70/70 (100%)	59 (84%)	11 (16%)	3	9
20	AT	65/65 (100%)	50 (77%)	15 (23%)	1	3
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	2
21	AU	44/44 (100%)	26 (59%)	18 (41%)	0	0
21	CU	44/44 (100%)	25 (57%)	19 (43%)	0	0
24	BC	216/216 (100%)	184 (85%)	32 (15%)	4	11
24	DC	216/216 (100%)	185 (86%)	31 (14%)	4	12
25	BD	164/164 (100%)	152 (93%)	12 (7%)	17	45
25	DD	164/164 (100%)	146 (89%)	18 (11%)	8	23
26	BE	165/165 (100%)	142 (86%)	23 (14%)	4	12
26	DE	165/165 (100%)	142 (86%)	23 (14%)	4	12
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	6
27	DF	148/148 (100%)	124 (84%)	24 (16%)	3	9
28	BG	137/137 (100%)	127 (93%)	10 (7%)	17	45
28	DG	137/137 (100%)	121 (88%)	16 (12%)	7	19
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	3
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	2
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	3
31	BJ	116/116 (100%)	111 (96%)	5 (4%)	35	71
31	DJ	116/116 (100%)	101 (87%)	15 (13%)	5	16
32	BK	103/103 (100%)	91 (88%)	12 (12%)	7	19
32	DK	103/103 (100%)	96 (93%)	7 (7%)	20	49
33	BL	102/102 (100%)	88 (86%)	14 (14%)	4	13
33	DL	102/102 (100%)	89 (87%)	13 (13%)	5	16
34	BM	109/109 (100%)	102 (94%)	7 (6%)	22	53
34	DM	109/109 (100%)	101 (93%)	8 (7%)	17	45
35	BN	100/100 (100%)	90 (90%)	10 (10%)	9	28
35	DN	100/100 (100%)	80 (80%)	20 (20%)	1	5
36	BO	86/86 (100%)	70 (81%)	16 (19%)	2	6
36	DO	86/86 (100%)	73 (85%)	13 (15%)	3	11
37	BP	99/99 (100%)	91 (92%)	8 (8%)	15	39
37	DP	99/99 (100%)	84 (85%)	15 (15%)	3	10
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	12	34
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	6	17
39	BR	84/84 (100%)	72 (86%)	12 (14%)	4	12
39	DR	84/84 (100%)	68 (81%)	16 (19%)	2	6
40	BS	93/93 (100%)	80 (86%)	13 (14%)	4	12
40	DS	93/93 (100%)	80 (86%)	13 (14%)	4	12
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	11
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	7
42	BU	83/83 (100%)	73 (88%)	10 (12%)	6	18
42	DU	83/83 (100%)	66 (80%)	17 (20%)	1	4
43	BV	78/78 (100%)	69 (88%)	9 (12%)	7	21
43	DV	78/78 (100%)	65 (83%)	13 (17%)	3	8
44	BW	57/58 (98%)	50 (88%)	7 (12%)	6	17
44	DW	56/58 (97%)	51 (91%)	5 (9%)	12	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	3	8
45	DX	67/67 (100%)	54 (81%)	13 (19%)	2	5
46	BY	55/55 (100%)	47 (86%)	8 (14%)	4	12
46	DY	55/55 (100%)	45 (82%)	10 (18%)	2	6
47	BZ	48/48 (100%)	44 (92%)	4 (8%)	14	38
47	DZ	48/48 (100%)	37 (77%)	11 (23%)	1	3
48	B0	47/47 (100%)	41 (87%)	6 (13%)	5	16
48	D0	47/47 (100%)	43 (92%)	4 (8%)	13	37
49	B1	45/45 (100%)	38 (84%)	7 (16%)	3	10
49	D1	45/45 (100%)	41 (91%)	4 (9%)	12	35
50	B2	38/38 (100%)	33 (87%)	5 (13%)	5	14
50	D2	38/38 (100%)	31 (82%)	7 (18%)	2	6
51	B3	51/51 (100%)	48 (94%)	3 (6%)	24	58
51	D3	51/51 (100%)	44 (86%)	7 (14%)	4	13
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	7
52	D4	34/34 (100%)	30 (88%)	4 (12%)	6	19
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	4
All	All	9386/9518 (99%)	7728 (82%)	1658 (18%)	2	7

5 of 1658 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BX	18	ARG
5	CE	115	LEU
39	DR	85	LYS
48	B0	18	SER
2	CB	163	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	CC	176	HIS
8	CH	18	GLN
46	DY	41	HIS
4	CD	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	CD	198	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	321 (20%)	13 (0%)
1	CA	1538/1539 (99%)	312 (20%)	8 (0%)
22	BA	2895/2903 (99%)	513 (17%)	22 (0%)
22	DA	2895/2903 (99%)	635 (21%)	23 (0%)
23	BB	118/119 (99%)	18 (15%)	0
23	DB	117/119 (98%)	22 (18%)	0
All	All	9100/9122 (99%)	1821 (20%)	66 (0%)

5 of 1821 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	13	U

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2211	A
1	CA	115	G
22	DA	2286	G
22	BA	2282	G
22	BA	2756	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 502 ligands modelled in this entry, 500 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	VIR	BA	3001	-	34,40,40	3.41	10 (29%)	37,55,55	3.31	17 (45%)
55	VIR	DA	3001	-	34,40,40	3.37	10 (29%)	37,55,55	3.09	13 (35%)

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
55	VIR	BA	3001	-	-	0/42/58/58	0/1/3/3
55	VIR	DA	3001	-	-	1/42/58/58	0/1/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3001	VIR	C4-N5	-2.99	1.42	1.47
55	DA	3001	VIR	C4-N5	-2.92	1.42	1.47
55	BA	3001	VIR	C22-C20	2.01	1.50	1.45
55	DA	3001	VIR	C16-C14	2.18	1.54	1.51
55	DA	3001	VIR	C1-C37	2.42	1.56	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3001	VIR	C23-C22-C20	-9.33	111.52	125.75
55	BA	3001	VIR	C23-C22-C20	-8.73	112.42	125.75
55	BA	3001	VIR	C37-C1-N5	-8.06	113.59	122.91
55	DA	3001	VIR	C37-C1-N5	-7.46	114.29	122.91
55	BA	3001	VIR	C2-C1-C37	-6.10	112.31	128.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	DA	3001	VIR	C17-C19-C20-C21

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3001	VIR	5	0
55	DA	3001	VIR	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.12	24 (1%) 74 72	12, 51, 134, 181	0
1	CA	1539/1539 (100%)	0.19	61 (3%) 42 35	25, 70, 145, 177	0
2	AB	218/218 (100%)	1.03	32 (14%) 3 2	38, 75, 100, 123	0
2	CB	218/218 (100%)	1.25	60 (27%) 1 0	61, 87, 107, 126	0
3	AC	206/206 (100%)	0.26	11 (5%) 30 23	35, 57, 78, 93	0
3	CC	206/206 (100%)	1.64	76 (36%) 0 0	51, 80, 95, 105	0
4	AD	205/205 (100%)	0.33	6 (2%) 55 49	33, 56, 78, 104	0
4	CD	205/205 (100%)	0.03	6 (2%) 55 49	17, 38, 63, 87	0
5	AE	150/150 (100%)	0.09	2 (1%) 79 78	32, 48, 79, 101	0
5	CE	150/150 (100%)	0.26	5 (3%) 50 42	30, 56, 82, 103	0
6	AF	100/100 (100%)	-0.10	1 (1%) 84 82	34, 57, 73, 87	0
6	CF	100/100 (100%)	0.31	6 (6%) 25 18	45, 74, 94, 105	0
7	AG	151/151 (100%)	0.64	16 (10%) 8 5	54, 77, 96, 103	0
7	CG	151/151 (100%)	2.69	86 (56%) 0 0	82, 101, 110, 115	0
8	AH	129/129 (100%)	0.21	1 (0%) 87 86	31, 49, 66, 75	0
8	CH	129/129 (100%)	0.47	8 (6%) 24 17	50, 65, 81, 92	0
9	AI	127/127 (100%)	1.01	24 (18%) 2 1	44, 74, 96, 110	0
9	CI	127/127 (100%)	2.18	55 (43%) 0 0	73, 94, 111, 122	0
10	AJ	98/98 (100%)	0.73	12 (12%) 5 3	39, 66, 92, 122	0
10	CJ	98/98 (100%)	2.95	59 (60%) 0 0	71, 95, 111, 126	0
11	AK	117/117 (100%)	0.63	12 (10%) 9 5	26, 65, 92, 117	0
11	CK	117/117 (100%)	0.44	6 (5%) 32 25	38, 67, 80, 92	0
12	AL	123/123 (100%)	0.19	5 (4%) 41 34	21, 35, 64, 98	0
12	CL	123/123 (100%)	0.43	6 (4%) 33 27	36, 52, 78, 99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.51	8 (7%) 19 13	48, 69, 94, 103	0
13	CM	114/114 (100%)	3.06	81 (71%) 0 0	97, 109, 118, 119	0
14	AN	96/100 (96%)	0.75	14 (14%) 3 2	41, 61, 94, 103	0
14	CN	96/100 (96%)	2.60	52 (54%) 0 0	70, 95, 113, 120	0
15	AO	88/88 (100%)	0.25	3 (3%) 49 41	28, 51, 65, 89	0
15	CO	88/88 (100%)	0.28	3 (3%) 49 41	40, 63, 81, 98	0
16	AP	82/82 (100%)	0.70	7 (8%) 13 8	33, 47, 85, 101	0
16	CP	82/82 (100%)	1.21	16 (19%) 1 1	44, 61, 89, 106	0
17	AQ	80/80 (100%)	0.29	4 (5%) 32 26	28, 52, 77, 122	0
17	CQ	80/80 (100%)	1.12	16 (20%) 1 1	44, 76, 98, 103	0
18	AR	55/55 (100%)	0.13	3 (5%) 29 22	39, 52, 79, 108	0
18	CR	55/55 (100%)	0.37	4 (7%) 18 12	39, 55, 79, 111	0
19	AS	79/79 (100%)	1.01	20 (25%) 1 0	54, 69, 89, 101	0
19	CS	79/79 (100%)	4.50	62 (78%) 0 0	90, 110, 119, 125	0
20	AT	85/85 (100%)	0.58	4 (4%) 35 29	35, 48, 71, 101	0
20	CT	85/85 (100%)	1.62	29 (34%) 0 0	55, 74, 92, 99	0
21	AU	51/51 (100%)	1.07	9 (17%) 2 1	46, 75, 97, 106	0
21	CU	51/51 (100%)	0.68	7 (13%) 4 2	45, 72, 97, 105	0
22	BA	2897/2903 (99%)	0.09	110 (3%) 44 37	1, 15, 131, 195	0
22	DA	2897/2903 (99%)	0.32	111 (3%) 44 37	40, 82, 146, 181	0
23	BB	119/119 (100%)	-0.31	0 100 100	3, 25, 52, 85	0
23	DB	118/119 (99%)	0.17	4 (3%) 49 41	67, 112, 133, 144	0
24	BC	271/271 (100%)	-0.15	3 (1%) 82 80	5, 21, 36, 54	0
24	DC	271/271 (100%)	0.72	28 (10%) 9 5	43, 62, 77, 90	0
25	BD	209/209 (100%)	-0.25	0 100 100	1, 11, 35, 68	0
25	DD	209/209 (100%)	1.03	41 (19%) 1 1	49, 68, 84, 96	0
26	BE	201/201 (100%)	-0.26	1 (0%) 91 90	1, 23, 53, 91	0
26	DE	201/201 (100%)	1.67	74 (36%) 0 0	46, 85, 102, 109	0
27	BF	177/177 (100%)	0.32	8 (4%) 37 31	24, 43, 77, 90	0
27	DF	177/177 (100%)	3.33	129 (72%) 0 0	91, 108, 120, 126	0
28	BG	176/176 (100%)	0.13	5 (2%) 56 50	17, 38, 62, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.18	90 (51%) 0 0	72, 94, 106, 116	0
29	BH	149/149 (100%)	3.54	87 (58%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.18	75 (50%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.75	95 (67%) 0 0	90, 112, 122, 133	0
30	DI	141/141 (100%)	5.06	124 (87%) 0 0	102, 119, 129, 132	0
31	BJ	142/142 (100%)	-0.35	0 100 100	2, 7, 21, 37	0
31	DJ	142/142 (100%)	0.84	15 (10%) 8 5	50, 66, 79, 94	0
32	BK	122/122 (100%)	-0.36	0 100 100	4, 13, 32, 69	0
32	DK	122/122 (100%)	1.21	30 (24%) 1 0	47, 64, 83, 97	0
33	BL	143/143 (100%)	-0.19	0 100 100	1, 19, 44, 73	0
33	DL	143/143 (100%)	1.78	49 (34%) 0 0	46, 80, 95, 115	0
34	BM	136/136 (100%)	-0.30	0 100 100	2, 11, 31, 83	0
34	DM	136/136 (100%)	1.05	28 (20%) 1 1	42, 69, 82, 101	0
35	BN	120/120 (100%)	-0.33	0 100 100	3, 8, 19, 53	0
35	DN	120/120 (100%)	1.44	28 (23%) 1 0	56, 76, 89, 116	0
36	BO	116/116 (100%)	-0.17	0 100 100	12, 27, 45, 52	0
36	DO	116/116 (100%)	2.50	68 (58%) 0 0	81, 95, 105, 115	0
37	BP	114/114 (100%)	-0.29	0 100 100	7, 18, 43, 66	0
37	DP	114/114 (100%)	0.96	20 (17%) 2 1	58, 70, 85, 93	0
38	BQ	117/117 (100%)	-0.25	0 100 100	1, 4, 15, 30	0
38	DQ	117/117 (100%)	0.97	16 (13%) 4 2	54, 67, 79, 83	0
39	BR	103/103 (100%)	-0.34	0 100 100	1, 13, 33, 67	0
39	DR	103/103 (100%)	1.50	31 (30%) 1 0	52, 78, 88, 99	0
40	BS	110/110 (100%)	-0.28	0 100 100	1, 5, 24, 79	0
40	DS	110/110 (100%)	1.90	47 (42%) 0 0	57, 75, 89, 101	0
41	BT	93/93 (100%)	0.24	4 (4%) 39 32	8, 26, 75, 104	0
41	DT	93/93 (100%)	2.69	52 (55%) 0 0	68, 87, 103, 119	0
42	BU	102/102 (100%)	-0.19	2 (1%) 68 64	14, 29, 63, 92	0
42	DU	102/102 (100%)	3.34	65 (63%) 0 0	75, 92, 111, 120	0
43	BV	94/94 (100%)	-0.21	0 100 100	6, 20, 41, 55	0
43	DV	94/94 (100%)	0.91	15 (15%) 3 1	70, 85, 96, 104	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.14	1 (1%) 79 78	7, 13, 29, 53	0
44	DW	75/76 (98%)	1.81	27 (36%) 0 0	61, 80, 90, 104	0
45	BX	77/77 (100%)	-0.26	0 100 100	7, 23, 51, 72	0
45	DX	77/77 (100%)	0.93	11 (14%) 4 2	52, 70, 84, 88	0
46	BY	63/63 (100%)	0.16	3 (4%) 34 28	21, 39, 72, 94	0
46	DY	63/63 (100%)	1.60	22 (34%) 0 0	78, 95, 102, 106	0
47	BZ	58/58 (100%)	-0.20	0 100 100	1, 8, 24, 41	0
47	DZ	58/58 (100%)	0.73	8 (13%) 4 2	58, 71, 82, 95	0
48	B0	56/56 (100%)	-0.29	0 100 100	1, 12, 36, 69	0
48	D0	56/56 (100%)	1.52	17 (30%) 1 0	58, 79, 92, 102	0
49	B1	50/50 (100%)	-0.03	2 (4%) 42 35	18, 29, 48, 76	0
49	D1	50/50 (100%)	1.46	14 (28%) 1 0	70, 86, 94, 105	0
50	B2	46/46 (100%)	-0.19	1 (2%) 65 60	4, 9, 15, 86	0
50	D2	46/46 (100%)	1.97	19 (41%) 0 0	55, 69, 80, 102	0
51	B3	64/64 (100%)	-0.17	0 100 100	5, 10, 20, 33	0
51	D3	64/64 (100%)	1.40	19 (29%) 1 0	58, 71, 79, 82	0
52	B4	38/38 (100%)	-0.04	0 100 100	9, 18, 37, 53	0
52	D4	38/38 (100%)	2.14	18 (47%) 0 0	59, 75, 87, 101	0
53	B5	191/228 (83%)	6.88	184 (96%) 0 0	101, 117, 128, 136	0
All	All	20734/20794 (99%)	0.65	2723 (13%) 5 3	1, 63, 121, 195	0

The worst 5 of 2723 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	2	ALA	27.3
53	B5	208	THR	24.1
53	B5	207	GLY	21.9
53	B5	111	PHE	20.5
30	BI	53	LEU	18.0

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

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BA	3058	1/1	0.72	0.50	50.92	50,50,50,50	0
54	MG	BA	3145	1/1	0.91	0.61	48.56	37,37,37,37	0
54	MG	DA	3114	1/1	0.34	0.79	34.53	85,85,85,85	0
54	MG	AA	1643	1/1	0.79	1.28	30.45	61,61,61,61	0
54	MG	BA	3016	1/1	0.78	0.53	27.78	65,65,65,65	0
54	MG	DA	3003	1/1	0.84	0.49	25.94	95,95,95,95	0
54	MG	BA	3056	1/1	0.86	0.40	25.55	53,53,53,53	0
54	MG	DA	3117	1/1	0.88	0.47	24.52	73,73,73,73	0
54	MG	AA	1634	1/1	0.73	0.38	24.18	74,74,74,74	0
54	MG	BA	3139	1/1	0.98	0.41	23.88	3,3,3,3	0
54	MG	AA	1670	1/1	0.90	0.39	16.86	40,40,40,40	0
54	MG	BA	3035	1/1	0.98	0.34	11.74	44,44,44,44	0
54	MG	BA	3041	1/1	0.81	0.37	11.64	2,2,2,2	0
54	MG	BA	3151	1/1	0.94	0.27	11.61	33,33,33,33	0
54	MG	BA	3084	1/1	0.84	0.23	9.83	41,41,41,41	0
54	MG	BA	3155	1/1	0.93	0.29	9.69	18,18,18,18	0
54	MG	BA	3168	1/1	0.91	0.22	8.49	19,19,19,19	0
54	MG	AA	1654	1/1	0.96	0.21	8.48	42,42,42,42	0
54	MG	AA	1610	1/1	0.86	0.29	8.09	69,69,69,69	0
54	MG	DA	3125	1/1	0.76	0.58	8.04	92,92,92,92	0
54	MG	DA	3009	1/1	0.78	0.40	8.02	82,82,82,82	0
54	MG	BA	3185	1/1	0.99	0.20	7.71	13,13,13,13	0
54	MG	BA	3134	1/1	0.82	0.34	6.90	47,47,47,47	0
54	MG	DA	3042	1/1	0.75	0.39	6.73	64,64,64,64	0
54	MG	AA	1621	1/1	0.96	0.21	6.42	16,16,16,16	0
55	VIR	BA	3001	38/38	0.97	0.23	6.18	3,15,28,31	0
54	MG	BA	3147	1/1	0.94	0.19	5.92	42,42,42,42	0
54	MG	BA	3137	1/1	0.92	0.28	5.36	60,60,60,60	0
54	MG	AA	1662	1/1	0.97	0.25	4.82	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3110	1/1	0.79	0.29	4.51	46,46,46,46	0
54	MG	CA	1632	1/1	0.93	0.24	3.64	77,77,77,77	0
54	MG	DA	3029	1/1	0.81	0.37	3.59	74,74,74,74	0
54	MG	BA	3132	1/1	0.94	0.20	3.56	44,44,44,44	0
54	MG	DA	3050	1/1	0.85	0.31	3.39	89,89,89,89	0
54	MG	BA	3153	1/1	0.96	0.25	3.33	6,6,6,6	0
54	MG	DA	3072	1/1	0.70	0.27	3.32	81,81,81,81	0
54	MG	BA	3105	1/1	0.99	0.21	3.13	0,0,0,0	0
55	VIR	DA	3001	38/38	0.92	0.28	2.60	27,39,47,53	0
54	MG	BA	3110	1/1	0.96	0.20	2.11	2,2,2,2	0
54	MG	BA	3183	1/1	0.98	0.18	2.11	26,26,26,26	0
54	MG	BA	3109	1/1	0.94	0.19	2.04	1,1,1,1	0
54	MG	DA	3033	1/1	0.83	0.26	1.95	76,76,76,76	0
54	MG	DA	3133	1/1	0.83	0.34	1.92	72,72,72,72	0
54	MG	BA	3174	1/1	0.85	0.17	1.81	21,21,21,21	0
54	MG	DA	3158	1/1	0.81	0.25	1.59	56,56,56,56	0
54	MG	CA	1630	1/1	0.33	0.49	1.39	111,111,111,111	0
54	MG	DA	3111	1/1	0.87	0.19	1.28	41,41,41,41	0
54	MG	DA	3073	1/1	0.84	0.21	1.27	74,74,74,74	0
54	MG	BA	3106	1/1	0.96	0.18	1.07	0,0,0,0	0
54	MG	DA	3040	1/1	0.93	0.21	1.03	57,57,57,57	0
54	MG	BA	3131	1/1	0.95	0.18	1.03	2,2,2,2	0
54	MG	BA	3165	1/1	0.97	0.17	1.03	2,2,2,2	0
54	MG	DA	3154	1/1	0.94	0.23	0.96	42,42,42,42	0
54	MG	DA	3065	1/1	0.91	0.19	0.75	49,49,49,49	0
54	MG	DA	3095	1/1	0.91	0.26	0.74	84,84,84,84	0
54	MG	BA	3159	1/1	0.90	0.15	0.71	21,21,21,21	0
54	MG	BA	3050	1/1	0.98	0.18	0.67	4,4,4,4	0
54	MG	AN	201	1/1	0.88	0.18	0.15	60,60,60,60	0
54	MG	DA	3098	1/1	0.95	0.19	0.13	71,71,71,71	0
54	MG	DA	3109	1/1	0.87	0.17	0.04	48,48,48,48	0
54	MG	DA	3106	1/1	0.88	0.19	0.03	73,73,73,73	0
54	MG	DA	3019	1/1	0.93	0.20	-0.11	84,84,84,84	0
54	MG	BA	3022	1/1	0.96	0.17	-0.13	1,1,1,1	0
54	MG	BA	3014	1/1	0.94	0.17	-0.13	0,0,0,0	0
54	MG	BA	3163	1/1	0.95	0.16	-0.15	29,29,29,29	0
54	MG	BA	3009	1/1	0.94	0.16	-0.21	3,3,3,3	0
54	MG	BA	3064	1/1	0.99	0.16	-0.28	1,1,1,1	0
54	MG	AA	1631	1/1	0.89	0.12	-0.40	47,47,47,47	0
54	MG	CA	1615	1/1	0.76	0.14	-0.46	57,57,57,57	0
54	MG	DA	3130	1/1	0.97	0.18	-0.47	37,37,37,37	0
54	MG	CA	1603	1/1	0.95	0.14	-0.49	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	202	1/1	0.85	0.13	-0.52	61,61,61,61	0
54	MG	DA	3020	1/1	0.78	0.26	-0.54	87,87,87,87	0
54	MG	BA	3074	1/1	0.84	0.17	-0.61	22,22,22,22	0
54	MG	DA	3116	1/1	0.91	0.21	-0.64	95,95,95,95	0
54	MG	CA	1635	1/1	0.71	0.21	-0.66	123,123,123,123	0
54	MG	CA	1614	1/1	0.87	0.09	-0.96	48,48,48,48	0
54	MG	BA	3133	1/1	0.93	0.14	-1.03	27,27,27,27	0
54	MG	AA	1641	1/1	0.97	0.15	-1.05	22,22,22,22	0
54	MG	DA	3121	1/1	0.72	0.16	-1.07	83,83,83,83	0
54	MG	BA	3024	1/1	0.88	0.15	-1.10	1,1,1,1	0
54	MG	BA	3063	1/1	0.83	0.17	-1.14	9,9,9,9	0
54	MG	DA	3025	1/1	0.77	0.18	-1.14	54,54,54,54	0
56	ZN	D4	101	1/1	0.99	0.10	-1.16	84,84,84,84	0
54	MG	AA	1607	1/1	0.92	0.07	-1.45	51,51,51,51	0
54	MG	DA	3131	1/1	0.92	0.13	-1.50	69,69,69,69	0
54	MG	AA	1640	1/1	0.91	0.14	-1.50	21,21,21,21	0
54	MG	BA	3069	1/1	0.96	0.15	-1.52	7,7,7,7	0
54	MG	DA	3079	1/1	0.90	0.07	-1.56	96,96,96,96	0
54	MG	DB	201	1/1	0.80	0.12	-1.59	101,101,101,101	0
54	MG	CA	1616	1/1	0.96	0.14	-1.60	34,34,34,34	0
54	MG	BA	3013	1/1	0.98	0.16	-1.63	0,0,0,0	0
54	MG	BA	3029	1/1	0.98	0.16	-1.69	0,0,0,0	0
54	MG	CA	1612	1/1	0.97	0.07	-1.72	43,43,43,43	0
54	MG	DA	3099	1/1	0.74	0.12	-1.74	62,62,62,62	0
54	MG	BA	3078	1/1	0.95	0.10	-1.80	21,21,21,21	0
54	MG	DA	3070	1/1	0.77	0.13	-1.82	82,82,82,82	0
54	MG	BA	3051	1/1	0.96	0.12	-1.86	4,4,4,4	0
54	MG	BA	3019	1/1	0.98	0.11	-1.86	15,15,15,15	0
56	ZN	B4	101	1/1	0.99	0.12	-1.91	29,29,29,29	0
54	MG	BA	3108	1/1	0.96	0.15	-1.91	9,9,9,9	0
54	MG	BA	3117	1/1	0.97	0.14	-1.93	2,2,2,2	0
54	MG	DA	3137	1/1	0.80	0.11	-1.99	88,88,88,88	0
54	MG	BB	201	1/1	0.92	0.09	-2.07	36,36,36,36	0
54	MG	DA	3060	1/1	0.92	0.12	-2.18	41,41,41,41	0
54	MG	DA	3028	1/1	0.76	0.15	-2.22	87,87,87,87	0
54	MG	BA	3187	1/1	0.90	0.11	-2.24	30,30,30,30	0
54	MG	AA	1628	1/1	0.92	0.12	-2.26	53,53,53,53	0
54	MG	DA	3135	1/1	0.90	0.12	-2.28	54,54,54,54	0
54	MG	AA	1616	1/1	0.91	0.12	-2.31	47,47,47,47	0
54	MG	AA	1606	1/1	0.97	0.12	-2.41	35,35,35,35	0
54	MG	CA	1626	1/1	0.90	0.11	-2.52	52,52,52,52	0
54	MG	CA	1610	1/1	0.94	0.10	-2.52	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3065	1/1	0.97	0.14	-2.58	0,0,0,0	0
54	MG	DA	3044	1/1	0.92	0.08	-2.61	57,57,57,57	0
54	MG	BA	3037	1/1	0.77	0.13	-2.65	26,26,26,26	0
54	MG	DA	3048	1/1	0.85	0.13	-2.68	61,61,61,61	0
54	MG	BA	3080	1/1	0.89	0.13	-2.73	22,22,22,22	0
54	MG	CA	1601	1/1	0.91	0.12	-2.88	35,35,35,35	0
54	MG	BA	3135	1/1	0.93	0.13	-2.95	1,1,1,1	0
54	MG	BA	3025	1/1	0.96	0.12	-3.00	3,3,3,3	0
54	MG	DA	3081	1/1	0.93	0.11	-3.04	83,83,83,83	0
54	MG	AA	1639	1/1	0.88	0.09	-3.04	53,53,53,53	0
54	MG	DA	3129	1/1	0.87	0.11	-3.10	81,81,81,81	0
54	MG	CA	1640	1/1	0.95	0.11	-3.15	31,31,31,31	0
54	MG	AA	1617	1/1	0.97	0.09	-3.32	33,33,33,33	0
54	MG	DA	3080	1/1	0.75	0.07	-3.32	99,99,99,99	0
54	MG	CA	1617	1/1	0.86	0.11	-3.38	36,36,36,36	0
54	MG	BA	3098	1/1	0.96	0.10	-3.49	3,3,3,3	0
54	MG	CA	1634	1/1	0.95	0.10	-3.51	50,50,50,50	0
54	MG	DA	3064	1/1	0.87	0.12	-3.51	47,47,47,47	0
54	MG	DA	3024	1/1	0.83	0.07	-3.58	65,65,65,65	0
54	MG	DA	3075	1/1	0.77	0.13	-3.68	64,64,64,64	0
54	MG	AA	1604	1/1	0.91	0.05	-3.71	55,55,55,55	0
54	MG	DA	3018	1/1	0.80	0.11	-3.83	59,59,59,59	0
54	MG	DA	3066	1/1	0.91	0.10	-3.85	32,32,32,32	0
54	MG	BA	3054	1/1	0.98	0.12	-3.95	2,2,2,2	0
54	MG	DA	3013	1/1	0.91	0.13	-4.02	45,45,45,45	0
54	MG	BA	3097	1/1	0.98	0.12	-4.02	2,2,2,2	0
54	MG	BA	3023	1/1	0.97	0.14	-4.07	2,2,2,2	0
54	MG	BA	3130	1/1	0.98	0.14	-4.10	0,0,0,0	0
54	MG	DA	3051	1/1	0.93	0.07	-4.21	60,60,60,60	0
54	MG	BA	3186	1/1	0.97	0.09	-4.44	23,23,23,23	0
54	MG	BA	3028	1/1	0.92	0.11	-4.44	16,16,16,16	0
54	MG	AA	1629	1/1	0.79	0.11	-4.52	65,65,65,65	0
54	MG	DA	3023	1/1	0.96	0.08	-4.55	50,50,50,50	0
54	MG	CA	1622	1/1	0.77	0.10	-4.61	50,50,50,50	0
54	MG	BA	3033	1/1	0.96	0.15	-4.74	6,6,6,6	0
54	MG	DA	3055	1/1	0.90	0.10	-5.04	50,50,50,50	0
54	MG	BA	3152	1/1	0.96	0.10	-5.12	14,14,14,14	0
54	MG	CA	1607	1/1	0.95	0.09	-5.34	56,56,56,56	0
54	MG	DA	3107	1/1	0.86	0.11	-5.61	51,51,51,51	0
54	MG	AA	1609	1/1	0.94	0.07	-6.06	46,46,46,46	0
54	MG	CA	1619	1/1	0.86	0.11	-6.14	41,41,41,41	0
54	MG	BA	3018	1/1	0.94	0.12	-6.18	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3111	1/1	0.94	0.08	-6.43	24,24,24,24	0
54	MG	DA	3052	1/1	0.96	0.07	-6.45	35,35,35,35	0
54	MG	BA	3094	1/1	0.97	0.08	-6.48	21,21,21,21	0
54	MG	BA	3006	1/1	0.96	0.08	-6.81	47,47,47,47	0
54	MG	BA	3066	1/1	0.97	0.08	-6.93	3,3,3,3	0
54	MG	AA	1632	1/1	0.90	0.10	-7.13	39,39,39,39	0
54	MG	BA	3059	1/1	0.86	0.06	-7.43	17,17,17,17	0
54	MG	BA	3170	1/1	0.97	0.07	-7.82	23,23,23,23	0
54	MG	BA	3072	1/1	0.96	0.06	-8.21	13,13,13,13	0
54	MG	AA	1613	1/1	0.98	0.06	-8.47	26,26,26,26	0
54	MG	DA	3067	1/1	0.94	0.07	-8.50	48,48,48,48	0
54	MG	BA	3071	1/1	0.99	0.08	-8.64	6,6,6,6	0
54	MG	BA	3003	1/1	0.90	0.09	-9.94	23,23,23,23	0
54	MG	BA	3121	1/1	0.96	0.09	-10.60	4,4,4,4	0
54	MG	BA	3119	1/1	0.93	0.07	-10.78	12,12,12,12	0
54	MG	AA	1624	1/1	0.97	0.07	-11.45	32,32,32,32	0
54	MG	BA	3161	1/1	0.97	0.09	-13.62	11,11,11,11	0
54	MG	DA	3006	1/1	0.89	0.07	-24.48	99,99,99,99	0
54	MG	AA	1644	1/1	0.72	0.23	-	50,50,50,50	0
54	MG	CA	1649	1/1	0.82	0.11	-	68,68,68,68	0
54	MG	BA	3049	1/1	0.95	0.07	-	11,11,11,11	0
54	MG	DA	3108	1/1	0.92	0.08	-	74,74,74,74	0
54	MG	DA	3057	1/1	0.40	0.31	-	87,87,87,87	0
54	MG	DA	3035	1/1	0.98	0.06	-	43,43,43,43	0
54	MG	BA	3178	1/1	0.94	0.23	-	12,12,12,12	0
54	MG	DA	3061	1/1	0.48	0.54	-	85,85,85,85	0
54	MG	BA	3154	1/1	0.82	0.63	-	33,33,33,33	0
54	MG	CA	1651	1/1	0.90	0.38	-	50,50,50,50	0
54	MG	BA	3149	1/1	0.98	0.11	-	26,26,26,26	0
54	MG	DA	3127	1/1	0.80	0.24	-	81,81,81,81	0
54	MG	AA	1669	1/1	0.91	0.20	-	56,56,56,56	0
54	MG	AA	1614	1/1	0.47	0.14	-	66,66,66,66	0
54	MG	DA	3136	1/1	0.25	0.49	-	90,90,90,90	0
54	MG	CA	1613	1/1	0.96	0.16	-	15,15,15,15	0
54	MG	BA	3038	1/1	0.99	0.19	-	0,0,0,0	0
54	MG	BA	3031	1/1	0.93	0.14	-	3,3,3,3	0
54	MG	DA	3123	1/1	0.98	0.17	-	38,38,38,38	0
54	MG	BA	3060	1/1	0.90	0.13	-	19,19,19,19	0
54	MG	DA	3132	1/1	0.71	0.86	-	93,93,93,93	0
54	MG	DA	3162	1/1	0.82	0.25	-	67,67,67,67	0
54	MG	BB	204	1/1	0.98	0.33	-	6,6,6,6	0
54	MG	DA	3062	1/1	0.48	2.55	-	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1624	1/1	0.82	0.08	-	49,49,49,49	0
54	MG	DA	3017	1/1	0.56	0.50	-	90,90,90,90	0
54	MG	CA	1628	1/1	0.74	0.17	-	99,99,99,99	0
54	MG	AA	1661	1/1	0.83	0.45	-	43,43,43,43	0
54	MG	DA	3093	1/1	0.36	0.60	-	108,108,108,108	0
54	MG	DA	3115	1/1	0.92	0.11	-	48,48,48,48	0
54	MG	BA	3143	1/1	0.96	0.33	-	15,15,15,15	0
54	MG	AA	1653	1/1	0.96	0.18	-	21,21,21,21	0
54	MG	CA	1618	1/1	0.86	0.15	-	38,38,38,38	0
54	MG	BA	3055	1/1	0.87	0.13	-	13,13,13,13	0
54	MG	BA	3127	1/1	0.94	0.16	-	9,9,9,9	0
54	MG	CA	1609	1/1	0.75	0.13	-	82,82,82,82	0
54	MG	DA	3161	1/1	0.83	0.21	-	35,35,35,35	0
54	MG	AA	1651	1/1	0.83	0.36	-	52,52,52,52	0
54	MG	DA	3159	1/1	0.68	0.14	-	68,68,68,68	0
54	MG	BA	3103	1/1	0.91	0.11	-	8,8,8,8	0
54	MG	BA	3167	1/1	0.84	0.20	-	35,35,35,35	0
54	MG	CA	1642	1/1	0.89	0.20	-	26,26,26,26	0
54	MG	DA	3089	1/1	0.78	0.10	-	77,77,77,77	0
54	MG	AA	1630	1/1	0.93	0.17	-	53,53,53,53	0
54	MG	DA	3160	1/1	0.86	0.19	-	44,44,44,44	0
54	MG	BA	3150	1/1	0.89	0.22	-	41,41,41,41	0
54	MG	BA	3036	1/1	0.99	0.11	-	2,2,2,2	0
54	MG	DA	3002	1/1	0.88	0.19	-	64,64,64,64	0
54	MG	DA	3151	1/1	0.96	0.08	-	45,45,45,45	0
54	MG	DA	3088	1/1	0.92	0.03	-	61,61,61,61	0
54	MG	DA	3041	1/1	0.73	0.15	-	89,89,89,89	0
54	MG	DA	3086	1/1	0.90	0.18	-	83,83,83,83	0
54	MG	DA	3026	1/1	0.89	0.20	-	67,67,67,67	0
54	MG	DA	3077	1/1	0.97	0.11	-	62,62,62,62	0
54	MG	BA	3192	1/1	0.99	0.15	-	17,17,17,17	0
54	MG	BA	3164	1/1	0.95	0.29	-	15,15,15,15	0
54	MG	BA	3188	1/1	0.95	0.12	-	6,6,6,6	0
54	MG	DA	3043	1/1	0.77	0.18	-	84,84,84,84	0
54	MG	BB	202	1/1	0.95	0.07	-	8,8,8,8	0
54	MG	BA	3096	1/1	0.95	0.08	-	5,5,5,5	0
54	MG	BA	3081	1/1	0.75	0.11	-	19,19,19,19	0
54	MG	DA	3087	1/1	0.78	0.12	-	70,70,70,70	0
54	MG	AA	1623	1/1	0.81	0.11	-	39,39,39,39	0
54	MG	DA	3090	1/1	0.94	0.30	-	81,81,81,81	0
54	MG	DA	3149	1/1	0.57	0.24	-	63,63,63,63	0
54	MG	BA	3176	1/1	0.95	0.07	-	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3138	1/1	0.88	0.61	-	46,46,46,46	0
54	MG	CA	1629	1/1	0.74	0.12	-	85,85,85,85	0
54	MG	DA	3092	1/1	0.89	0.09	-	79,79,79,79	0
54	MG	AA	1608	1/1	0.97	0.13	-	18,18,18,18	0
54	MG	AA	1635	1/1	0.78	0.27	-	53,53,53,53	0
54	MG	AA	1652	1/1	0.89	0.15	-	55,55,55,55	0
54	MG	AA	1636	1/1	0.99	0.12	-	11,11,11,11	0
54	MG	AA	1671	1/1	0.76	0.89	-	56,56,56,56	0
54	MG	CA	1652	1/1	0.96	0.07	-	65,65,65,65	0
54	MG	DA	3140	1/1	0.95	0.34	-	34,34,34,34	0
54	MG	BA	3180	1/1	0.96	0.13	-	31,31,31,31	0
54	MG	DA	3134	1/1	-0.06	1.03	-	105,105,105,105	0
54	MG	CA	1656	1/1	0.42	0.54	-	55,55,55,55	0
54	MG	CA	1625	1/1	0.91	0.14	-	22,22,22,22	0
54	MG	DA	3148	1/1	0.47	0.46	-	58,58,58,58	0
54	MG	BA	3123	1/1	0.93	0.19	-	0,0,0,0	0
54	MG	AA	1601	1/1	0.89	0.14	-	56,56,56,56	0
54	MG	BA	3048	1/1	0.55	0.15	-	50,50,50,50	0
54	MG	DA	3164	1/1	0.82	0.67	-	67,67,67,67	0
54	MG	BA	3128	1/1	0.97	0.07	-	9,9,9,9	0
54	MG	DA	3032	1/1	0.91	0.12	-	61,61,61,61	0
54	MG	DA	3157	1/1	0.84	0.22	-	49,49,49,49	0
54	MG	BA	3100	1/1	0.94	0.08	-	8,8,8,8	0
54	MG	AA	1649	1/1	0.94	0.13	-	26,26,26,26	0
54	MG	DA	3007	1/1	0.83	0.20	-	104,104,104,104	0
54	MG	AA	1642	1/1	0.98	0.06	-	23,23,23,23	0
54	MG	AA	1645	1/1	0.98	0.19	-	58,58,58,58	0
54	MG	BA	3171	1/1	0.91	0.14	-	16,16,16,16	0
54	MG	CA	1604	1/1	0.92	0.12	-	88,88,88,88	0
54	MG	CA	1645	1/1	0.91	0.16	-	42,42,42,42	0
54	MG	BA	3116	1/1	0.92	0.15	-	48,48,48,48	0
54	MG	BA	3086	1/1	0.95	0.14	-	10,10,10,10	0
54	MG	DA	3046	1/1	0.76	0.12	-	78,78,78,78	0
54	MG	BA	3173	1/1	0.93	0.14	-	33,33,33,33	0
54	MG	CA	1646	1/1	0.43	0.35	-	66,66,66,66	0
54	MG	DA	3054	1/1	0.84	0.13	-	36,36,36,36	0
54	MG	DA	3010	1/1	0.93	0.09	-	71,71,71,71	0
54	MG	AA	1622	1/1	0.94	0.20	-	51,51,51,51	0
54	MG	BA	3040	1/1	0.96	0.15	-	0,0,0,0	0
54	MG	BA	3070	1/1	0.96	0.15	-	59,59,59,59	0
54	MG	DA	3144	1/1	0.94	0.15	-	63,63,63,63	0
54	MG	CA	1644	1/1	0.72	0.38	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3005	1/1	0.38	0.36	-	96,96,96,96	0
54	MG	DA	3047	1/1	0.78	0.14	-	78,78,78,78	0
54	MG	AA	1612	1/1	0.93	0.12	-	43,43,43,43	0
54	MG	BQ	201	1/1	0.98	0.17	-	0,0,0,0	0
54	MG	BA	3118	1/1	0.98	0.10	-	5,5,5,5	0
54	MG	AA	1660	1/1	0.87	0.14	-	51,51,51,51	0
54	MG	DA	3058	1/1	0.88	0.13	-	75,75,75,75	0
54	MG	BA	3043	1/1	0.86	0.15	-	2,2,2,2	0
54	MG	BD	301	1/1	0.94	0.11	-	34,34,34,34	0
54	MG	BA	3141	1/1	0.92	0.13	-	22,22,22,22	0
54	MG	CA	1639	1/1	0.90	0.11	-	52,52,52,52	0
54	MG	BA	3057	1/1	0.97	0.12	-	6,6,6,6	0
54	MG	CA	1621	1/1	0.70	0.09	-	69,69,69,69	0
54	MG	DA	3014	1/1	0.68	0.19	-	80,80,80,80	0
54	MG	BA	3002	1/1	0.94	0.06	-	15,15,15,15	0
54	MG	DA	3118	1/1	0.92	0.07	-	71,71,71,71	0
54	MG	DA	3071	1/1	0.66	0.11	-	97,97,97,97	0
54	MG	BA	3126	1/1	0.97	0.16	-	1,1,1,1	0
54	MG	DA	3150	1/1	0.89	0.23	-	42,42,42,42	0
54	MG	BA	3156	1/1	0.96	0.17	-	21,21,21,21	0
54	MG	BA	3007	1/1	0.97	0.08	-	17,17,17,17	0
54	MG	BA	3162	1/1	0.95	0.12	-	32,32,32,32	0
54	MG	DA	3143	1/1	0.97	0.10	-	32,32,32,32	0
54	MG	BA	3160	1/1	0.89	0.19	-	21,21,21,21	0
54	MG	AA	1638	1/1	0.89	0.08	-	61,61,61,61	0
54	MG	DA	3049	1/1	0.78	0.20	-	108,108,108,108	0
54	MG	BA	3194	1/1	0.98	0.06	-	28,28,28,28	0
54	MG	DA	3145	1/1	0.90	0.09	-	80,80,80,80	0
54	MG	DA	3021	1/1	0.96	0.19	-	56,56,56,56	0
54	MG	BA	3125	1/1	0.87	0.39	-	36,36,36,36	0
54	MG	DA	3076	1/1	0.80	0.10	-	65,65,65,65	0
54	MG	BA	3136	1/1	0.90	0.13	-	39,39,39,39	0
54	MG	DA	3063	1/1	0.63	0.61	-	95,95,95,95	0
54	MG	DA	3100	1/1	0.75	0.40	-	83,83,83,83	0
54	MG	BA	3114	1/1	0.89	0.17	-	0,0,0,0	0
54	MG	DA	3147	1/1	0.95	0.08	-	51,51,51,51	0
54	MG	DA	3034	1/1	0.90	0.06	-	64,64,64,64	0
54	MG	BA	3073	1/1	0.98	0.12	-	2,2,2,2	0
54	MG	BA	3052	1/1	0.99	0.12	-	8,8,8,8	0
54	MG	BA	3042	1/1	0.96	0.16	-	11,11,11,11	0
54	MG	BA	3010	1/1	0.98	0.10	-	0,0,0,0	0
54	MG	BA	3115	1/1	0.94	0.14	-	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	203	1/1	0.93	0.07	-	11,11,11,11	0
54	MG	AA	1655	1/1	0.95	0.15	-	37,37,37,37	0
54	MG	AA	1611	1/1	0.99	0.11	-	12,12,12,12	0
54	MG	CA	1655	1/1	0.85	0.12	-	44,44,44,44	0
54	MG	AA	1667	1/1	0.39	1.41	-	66,66,66,66	0
54	MG	AA	1656	1/1	0.99	0.11	-	37,37,37,37	0
54	MG	BA	3075	1/1	0.94	0.09	-	19,19,19,19	0
54	MG	BA	3107	1/1	0.98	0.23	-	1,1,1,1	0
54	MG	BA	3140	1/1	0.96	0.35	-	1,1,1,1	0
54	MG	DA	3156	1/1	0.87	0.25	-	64,64,64,64	0
54	MG	CA	1648	1/1	0.91	0.20	-	25,25,25,25	0
54	MG	DA	3083	1/1	0.94	0.07	-	54,54,54,54	0
54	MG	BA	3062	1/1	0.91	0.54	-	52,52,52,52	0
54	MG	AA	1615	1/1	0.97	0.04	-	63,63,63,63	0
54	MG	AA	1633	1/1	0.97	0.14	-	38,38,38,38	0
54	MG	BA	3039	1/1	0.98	0.15	-	0,0,0,0	0
54	MG	DA	3128	1/1	0.67	0.11	-	67,67,67,67	0
54	MG	BA	3088	1/1	0.87	0.12	-	35,35,35,35	0
54	MG	BA	3092	1/1	0.90	0.06	-	53,53,53,53	0
54	MG	DA	3139	1/1	0.91	0.42	-	49,49,49,49	0
54	MG	BA	3112	1/1	0.97	0.10	-	7,7,7,7	0
54	MG	AA	1618	1/1	0.89	0.40	-	54,54,54,54	0
54	MG	AA	1657	1/1	0.74	0.50	-	68,68,68,68	0
54	MG	CA	1627	1/1	0.88	0.18	-	80,80,80,80	0
54	MG	BA	3034	1/1	0.98	0.20	-	0,0,0,0	0
54	MG	BA	3089	1/1	0.84	0.15	-	28,28,28,28	0
54	MG	DA	3165	1/1	0.91	0.21	-	56,56,56,56	0
54	MG	BA	3026	1/1	0.77	0.22	-	35,35,35,35	0
54	MG	CA	1637	1/1	0.82	0.15	-	66,66,66,66	0
54	MG	DA	3152	1/1	0.89	0.27	-	60,60,60,60	0
54	MG	BA	3017	1/1	0.89	0.18	-	24,24,24,24	0
54	MG	DA	3119	1/1	0.92	0.07	-	50,50,50,50	0
54	MG	BA	3169	1/1	0.95	0.10	-	24,24,24,24	0
54	MG	DA	3091	1/1	0.89	0.08	-	78,78,78,78	0
54	MG	DA	3167	1/1	0.89	0.14	-	47,47,47,47	0
54	MG	AA	1625	1/1	0.95	0.16	-	19,19,19,19	0
54	MG	BA	3142	1/1	0.97	0.35	-	0,0,0,0	0
54	MG	DA	3096	1/1	0.51	0.33	-	86,86,86,86	0
54	MG	CA	1605	1/1	0.69	0.30	-	91,91,91,91	0
54	MG	BA	3045	1/1	0.89	0.12	-	20,20,20,20	0
54	MG	CA	1653	1/1	0.93	0.06	-	40,40,40,40	0
54	MG	BA	3005	1/1	0.91	0.06	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3084	1/1	0.82	0.11	-	68,68,68,68	0
54	MG	CA	1636	1/1	0.37	0.23	-	118,118,118,118	0
54	MG	CA	1608	1/1	0.84	0.11	-	61,61,61,61	0
54	MG	CA	1631	1/1	0.78	0.22	-	97,97,97,97	0
54	MG	BA	3157	1/1	0.91	0.20	-	20,20,20,20	0
54	MG	BA	3083	1/1	0.83	0.14	-	23,23,23,23	0
54	MG	BA	3181	1/1	0.96	0.20	-	31,31,31,31	0
54	MG	BA	3021	1/1	0.96	0.07	-	9,9,9,9	0
54	MG	CA	1641	1/1	0.60	0.37	-	69,69,69,69	0
54	MG	BA	3012	1/1	0.98	0.09	-	9,9,9,9	0
54	MG	AA	1626	1/1	0.90	0.28	-	56,56,56,56	0
54	MG	BA	3189	1/1	0.90	0.26	-	38,38,38,38	0
54	MG	BA	3091	1/1	0.96	0.11	-	21,21,21,21	0
54	MG	CA	1647	1/1	0.95	0.10	-	42,42,42,42	0
54	MG	DA	3037	1/1	0.89	0.14	-	59,59,59,59	0
54	MG	BA	3076	1/1	0.94	0.14	-	12,12,12,12	0
54	MG	BA	3124	1/1	0.83	0.15	-	18,18,18,18	0
54	MG	DA	3155	1/1	0.95	0.12	-	42,42,42,42	0
54	MG	DA	3153	1/1	0.83	0.34	-	61,61,61,61	0
54	MG	AA	1647	1/1	0.99	0.08	-	54,54,54,54	0
54	MG	DA	3074	1/1	0.82	0.29	-	66,66,66,66	0
54	MG	BA	3020	1/1	0.89	0.21	-	2,2,2,2	0
54	MG	BA	3104	1/1	0.91	0.09	-	12,12,12,12	0
54	MG	BA	3011	1/1	0.99	0.12	-	0,0,0,0	0
54	MG	CA	1650	1/1	0.75	0.19	-	46,46,46,46	0
54	MG	DA	3053	1/1	0.94	0.05	-	53,53,53,53	0
54	MG	BA	3158	1/1	0.96	0.14	-	16,16,16,16	0
54	MG	DA	3078	1/1	0.30	0.37	-	89,89,89,89	0
54	MG	AA	1650	1/1	0.93	0.21	-	42,42,42,42	0
54	MG	DA	3039	1/1	0.90	0.13	-	65,65,65,65	0
54	MG	AA	1620	1/1	0.89	0.07	-	37,37,37,37	0
54	MG	DA	3031	1/1	0.93	0.24	-	65,65,65,65	0
54	MG	DA	3012	1/1	0.80	0.14	-	74,74,74,74	0
54	MG	DA	3094	1/1	0.63	0.51	-	101,101,101,101	0
54	MG	DA	3124	1/1	0.90	0.11	-	54,54,54,54	0
54	MG	DA	3011	1/1	0.90	0.13	-	57,57,57,57	0
54	MG	DA	3004	1/1	0.88	0.09	-	69,69,69,69	0
54	MG	BA	3047	1/1	0.94	0.13	-	4,4,4,4	0
54	MG	DA	3082	1/1	0.91	0.09	-	62,62,62,62	0
54	MG	BA	3087	1/1	0.98	0.17	-	2,2,2,2	0
54	MG	CA	1654	1/1	0.90	0.14	-	56,56,56,56	0
54	MG	BA	3175	1/1	0.97	0.11	-	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3038	1/1	0.92	0.04	-	77,77,77,77	0
54	MG	AA	1668	1/1	0.91	0.08	-	36,36,36,36	0
54	MG	CA	1643	1/1	0.96	0.19	-	56,56,56,56	0
54	MG	BA	3068	1/1	0.98	0.21	-	0,0,0,0	0
54	MG	DA	3166	1/1	0.96	0.33	-	37,37,37,37	0
54	MG	AA	1646	1/1	0.84	0.28	-	53,53,53,53	0
54	MG	DA	3105	1/1	0.92	0.06	-	67,67,67,67	0
54	MG	BA	3184	1/1	0.98	0.21	-	11,11,11,11	0
54	MG	BA	3182	1/1	0.95	0.15	-	21,21,21,21	0
54	MG	BA	3008	1/1	0.91	0.11	-	32,32,32,32	0
54	MG	BA	3061	1/1	0.96	0.41	-	48,48,48,48	0
54	MG	CA	1602	1/1	0.71	0.08	-	79,79,79,79	0
54	MG	BA	3122	1/1	0.93	0.09	-	26,26,26,26	0
54	MG	BA	3015	1/1	0.89	0.08	-	14,14,14,14	0
54	MG	BA	3079	1/1	0.91	0.05	-	41,41,41,41	0
54	MG	DQ	201	1/1	0.67	0.33	-	53,53,53,53	0
54	MG	AA	1603	1/1	0.95	0.16	-	49,49,49,49	0
54	MG	DA	3085	1/1	0.86	0.16	-	83,83,83,83	0
54	MG	CA	1620	1/1	0.96	0.05	-	59,59,59,59	0
54	MG	DA	3036	1/1	0.77	0.15	-	78,78,78,78	0
54	MG	DA	3056	1/1	0.94	0.09	-	61,61,61,61	0
54	MG	DA	3112	1/1	0.86	0.13	-	73,73,73,73	0
54	MG	BA	3177	1/1	0.94	0.52	-	37,37,37,37	0
54	MG	CA	1606	1/1	0.85	0.09	-	68,68,68,68	0
54	MG	BA	3032	1/1	0.90	0.09	-	6,6,6,6	0
54	MG	D2	101	1/1	0.80	0.22	-	78,78,78,78	0
54	MG	CA	1638	1/1	0.65	0.21	-	83,83,83,83	0
54	MG	BA	3129	1/1	0.98	0.16	-	3,3,3,3	0
54	MG	BA	3190	1/1	0.90	0.21	-	43,43,43,43	0
54	MG	DA	3015	1/1	0.95	0.08	-	46,46,46,46	0
54	MG	BA	3120	1/1	0.85	0.18	-	39,39,39,39	0
54	MG	BA	3093	1/1	0.94	0.08	-	33,33,33,33	0
54	MG	BA	3144	1/1	0.99	0.18	-	12,12,12,12	0
54	MG	BA	3004	1/1	0.91	0.13	-	27,27,27,27	0
54	MG	AA	1602	1/1	0.85	0.31	-	55,55,55,55	0
54	MG	BA	3044	1/1	0.93	0.07	-	21,21,21,21	0
54	MG	DA	3016	1/1	0.78	0.34	-	75,75,75,75	0
54	MG	DA	3059	1/1	0.69	0.41	-	79,79,79,79	0
54	MG	BA	3027	1/1	0.98	0.10	-	3,3,3,3	0
54	MG	DA	3104	1/1	0.79	0.15	-	67,67,67,67	0
54	MG	BA	3095	1/1	0.88	0.12	-	30,30,30,30	0
54	MG	BA	3053	1/1	0.83	0.12	-	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3097	1/1	0.78	0.07	-	62,62,62,62	0
54	MG	BA	3085	1/1	0.80	0.21	-	30,30,30,30	0
54	MG	BA	3067	1/1	0.97	0.13	-	1,1,1,1	0
54	MG	BA	3077	1/1	0.59	0.64	-	74,74,74,74	0
54	MG	AA	1605	1/1	0.85	0.15	-	28,28,28,28	0
54	MG	DA	3101	1/1	0.58	0.21	-	81,81,81,81	0
54	MG	BA	3082	1/1	0.98	0.17	-	0,0,0,0	0
54	MG	BA	3030	1/1	0.97	0.12	-	14,14,14,14	0
54	MG	DA	3030	1/1	0.75	0.13	-	70,70,70,70	0
54	MG	DA	3022	1/1	0.96	0.20	-	56,56,56,56	0
54	MG	CA	1611	1/1	0.25	0.21	-	85,85,85,85	0
54	MG	AA	1619	1/1	0.83	0.07	-	61,61,61,61	0
54	MG	DA	3126	1/1	0.93	0.15	-	57,57,57,57	0
54	MG	AA	1627	1/1	0.96	0.07	-	39,39,39,39	0
54	MG	AA	1658	1/1	0.93	0.68	-	65,65,65,65	0
54	MG	CA	1633	1/1	0.64	0.30	-	81,81,81,81	0
54	MG	AA	1663	1/1	0.92	0.25	-	33,33,33,33	0
54	MG	BA	3172	1/1	0.96	0.09	-	26,26,26,26	0
54	MG	AA	1664	1/1	0.92	0.15	-	51,51,51,51	0
54	MG	BA	3166	1/1	0.87	0.25	-	40,40,40,40	0
54	MG	DA	3103	1/1	0.81	0.14	-	77,77,77,77	0
54	MG	BA	3102	1/1	0.94	0.10	-	9,9,9,9	0
54	MG	DA	3163	1/1	0.87	0.27	-	59,59,59,59	0
54	MG	AA	1666	1/1	0.89	0.27	-	43,43,43,43	0
54	MG	BA	3099	1/1	0.80	0.28	-	55,55,55,55	0
54	MG	DA	3045	1/1	0.12	0.40	-	102,102,102,102	0
54	MG	BA	3101	1/1	0.95	0.10	-	5,5,5,5	0
54	MG	AA	1665	1/1	0.88	0.25	-	37,37,37,37	0
54	MG	DA	3113	1/1	0.76	0.28	-	74,74,74,74	0
54	MG	DA	3122	1/1	0.94	0.10	-	39,39,39,39	0
54	MG	BA	3179	1/1	0.98	0.10	-	37,37,37,37	0
54	MG	DA	3069	1/1	0.92	0.17	-	53,53,53,53	0
54	MG	BA	3191	1/1	0.91	0.25	-	22,22,22,22	0
54	MG	BA	3090	1/1	0.95	0.07	-	3,3,3,3	0
54	MG	CA	1623	1/1	0.90	0.14	-	45,45,45,45	0
54	MG	AA	1648	1/1	0.80	0.37	-	49,49,49,49	0
54	MG	DA	3146	1/1	0.83	0.21	-	62,62,62,62	0
54	MG	DB	203	1/1	0.92	0.08	-	79,79,79,79	0
54	MG	DA	3142	1/1	0.87	0.24	-	41,41,41,41	0
54	MG	DA	3102	1/1	0.92	0.07	-	64,64,64,64	0
54	MG	DA	3141	1/1	0.80	0.37	-	40,40,40,40	0
54	MG	DA	3027	1/1	0.23	1.05	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3113	1/1	0.95	0.13	-	14,14,14,14	0
54	MG	BA	3146	1/1	0.96	0.19	-	6,6,6,6	0
54	MG	AA	1637	1/1	0.74	0.08	-	79,79,79,79	0
54	MG	DA	3068	1/1	0.92	0.08	-	51,51,51,51	0
54	MG	DA	3008	1/1	0.71	0.41	-	104,104,104,104	0
54	MG	AA	1659	1/1	0.33	2.11	-	77,77,77,77	0
54	MG	BA	3138	1/1	0.98	0.43	-	7,7,7,7	0
54	MG	BA	3148	1/1	0.98	0.48	-	28,28,28,28	0
54	MG	BA	3046	1/1	0.97	0.08	-	5,5,5,5	0
54	MG	BA	3193	1/1	0.93	0.18	-	34,34,34,34	0
54	MG	DA	3120	1/1	0.75	0.58	-	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.