



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:22 PM GMT

PDB ID : 4U20
Title : Crystal structure of the E. coli ribosome bound to flopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-06-06
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

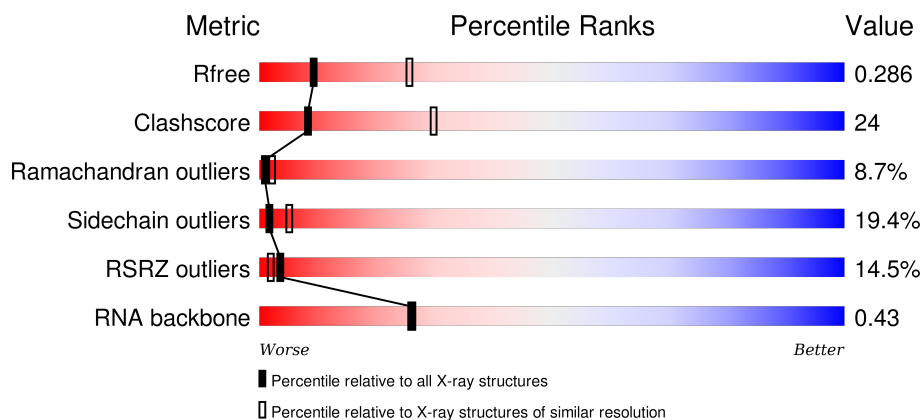
1 Overall quality at a glance

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>30% 52% 17%</div> </div>
1	CA	1539	<div> <div>5%</div> <div>31% 53% 16%</div> </div>
2	AB	218	<div> <div>20%</div> <div>16% 46% 30% 7%</div> </div>
2	CB	218	<div> <div>30%</div> <div>24% 48% 25%</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	1622	-	-	-	X
54	MG	AA	1644	-	-	-	X
54	MG	AA	1655	-	-	-	X
54	MG	BA	3029	-	-	-	X
54	MG	BA	3042	-	-	-	X
54	MG	BA	3051	-	-	-	X
54	MG	BA	3110	-	-	-	X
54	MG	BA	3133	-	-	-	X
54	MG	BA	3145	-	-	-	X
54	MG	BA	3162	-	-	-	X
54	MG	BA	3171	-	-	-	X
54	MG	BA	3176	-	-	-	X
54	MG	BA	3179	-	-	-	X
54	MG	BA	3187	-	-	-	X
54	MG	CA	1615	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3029	-	-	-	X
54	MG	DA	3042	-	-	-	X
54	MG	DA	3049	-	-	-	X
54	MG	DA	3059	-	-	-	X
54	MG	DA	3061	-	-	-	X
54	MG	DA	3065	-	-	-	X
54	MG	DA	3070	-	-	-	X
54	MG	DA	3073	-	-	-	X
54	MG	DA	3111	-	-	-	X
54	MG	DA	3125	-	-	-	X
54	MG	DA	3140	-	-	-	X
54	MG	DA	3154	-	-	-	X
55	VIF	BA	3001	-	-	-	X
56	ZN	B4	101	-	-	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			
			780	492	146	142	0	0	0

- 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		
			753	479	137	134	3	0	0
43	DV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- 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		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- 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		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

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

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

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

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

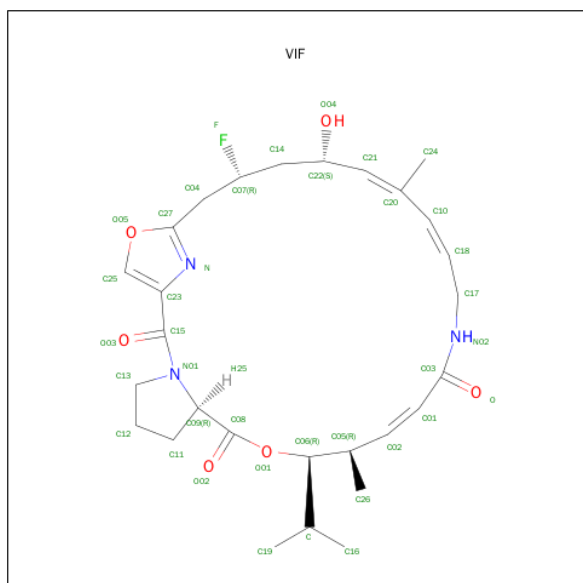
- Molecule 53 is a protein called 50S ribosomal protein L1.

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	194	Total	Mg	0	0
			194	194		
54	BN	1	Total	Mg	0	0
			1	1		
54	DQ	1	Total	Mg	0	0
			1	1		
54	CM	1	Total	Mg	0	0
			1	1		
54	D2	1	Total	Mg	0	0
			1	1		
54	AA	72	Total	Mg	0	0
			72	72		
54	DA	166	Total	Mg	0	0
			166	166		
54	DB	3	Total	Mg	0	0
			3	3		
54	CA	55	Total	Mg	0	0
			55	55		

- Molecule 55 is Flopristin (three-letter code: VIF) (formula: C₂₈H₃₈FN₃O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
55	DA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total	O	0	0
			195	195		
57	AL	1	Total	O	0	0
			1	1		
57	AN	5	Total	O	0	0
			5	5		
57	AT	1	Total	O	0	0
			1	1		
57	AU	1	Total	O	0	0
			1	1		
57	BA	620	Total	O	0	0
			620	620		
57	BB	13	Total	O	0	0
			13	13		
57	BC	6	Total	O	0	0
			6	6		
57	BD	3	Total	O	0	0
			3	3		
57	BE	4	Total	O	0	0
			4	4		
57	BF	1	Total	O	0	0
			1	1		
57	BG	1	Total	O	0	0
			1	1		
57	BL	8	Total	O	0	0
			8	8		
57	BN	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BS	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	1	Total 1	O 1	0	0
57	CA	189	Total 189	O 189	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	3	Total 3	O 3	0	0
57	CT	4	Total 4	O 4	0	0
57	CU	1	Total 1	O 1	0	0
57	DA	613	Total 613	O 613	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	2	Total 2	O 2	0	0
57	DJ	1	Total 1	O 1	0	0
57	DL	3	Total 3	O 3	0	0
57	DN	1	Total 1	O 1	0	0
57	DT	2	Total 2	O 2	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0

Continued on next page...

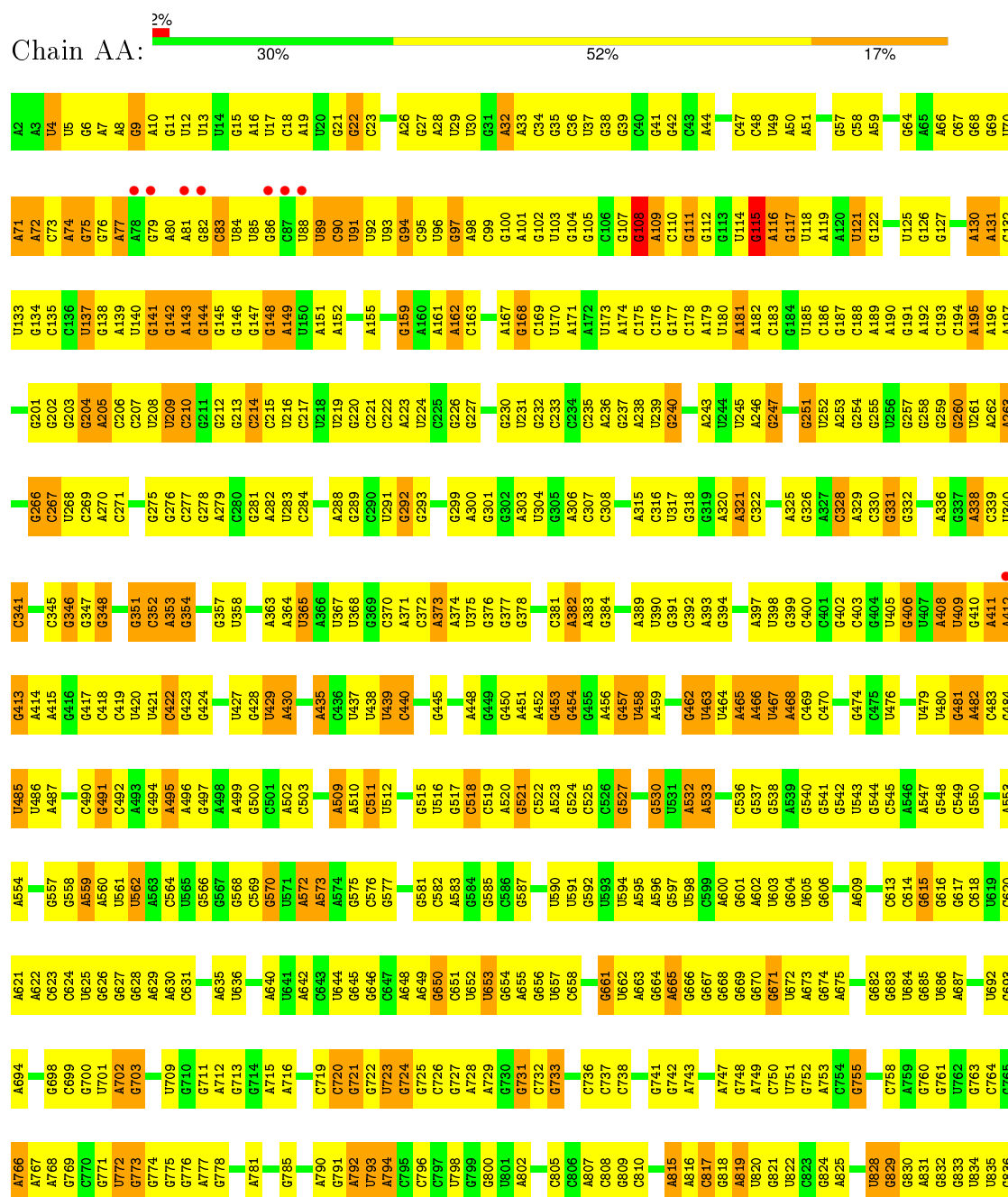
Continued from previous page...

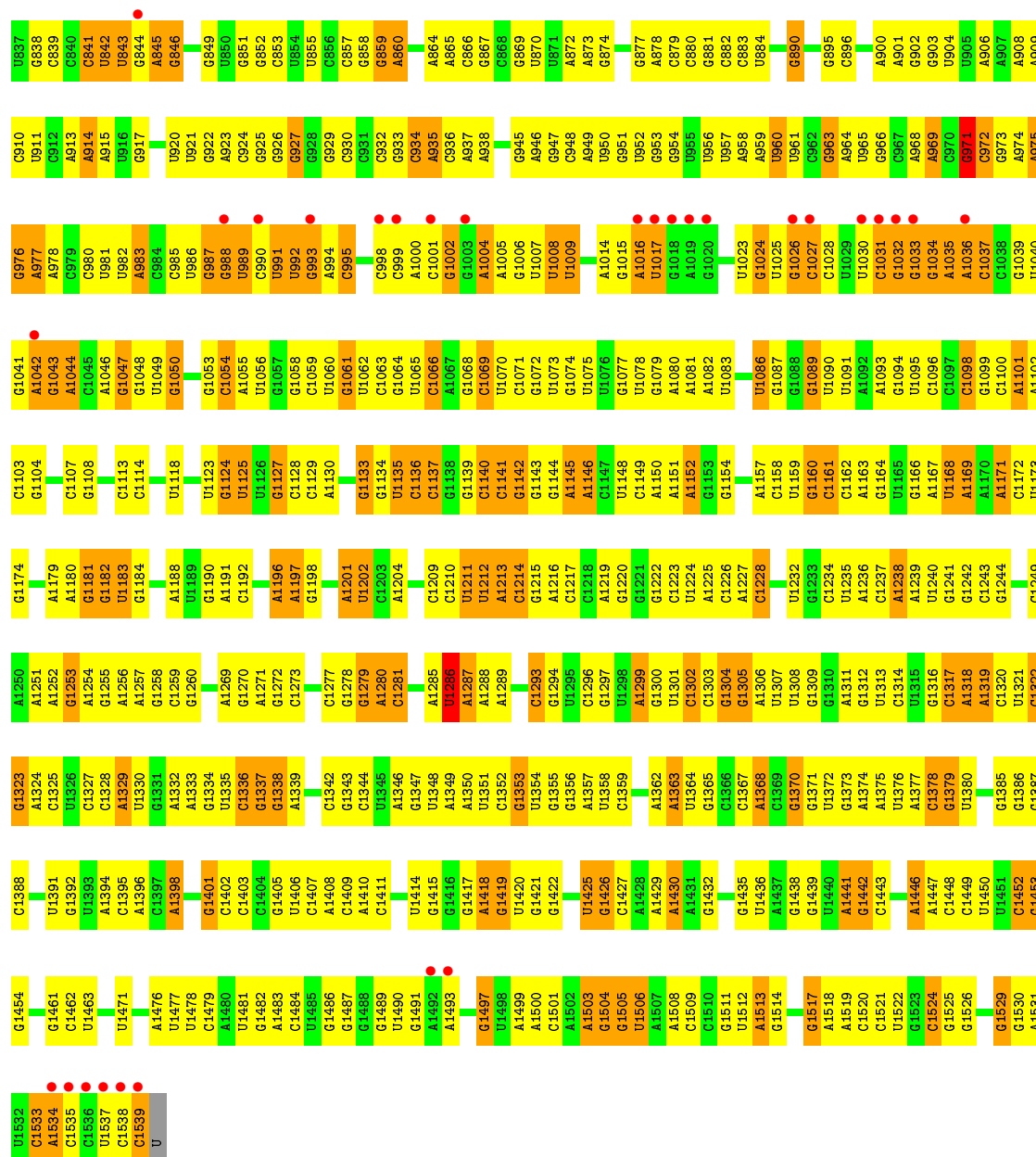
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D2	3	Total 3	O 3	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

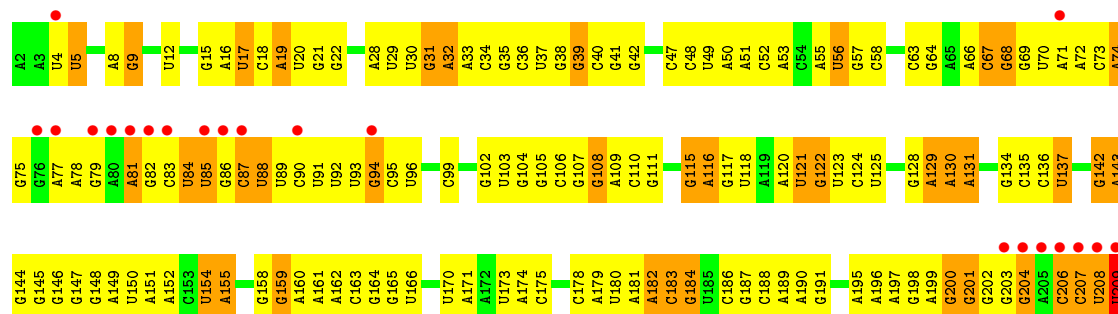
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

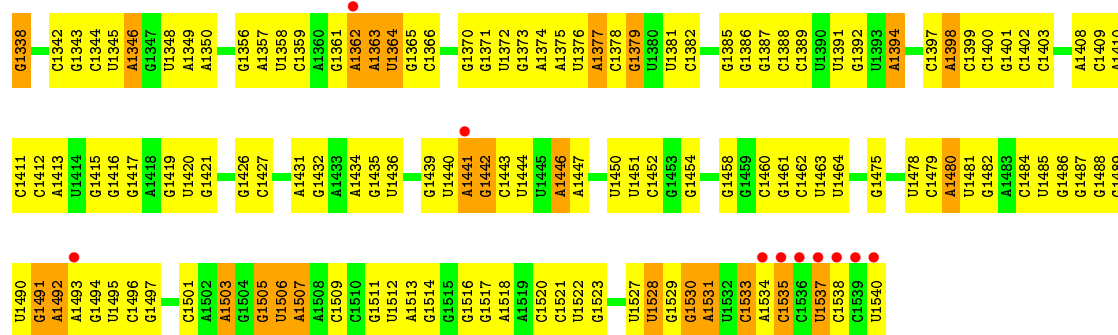




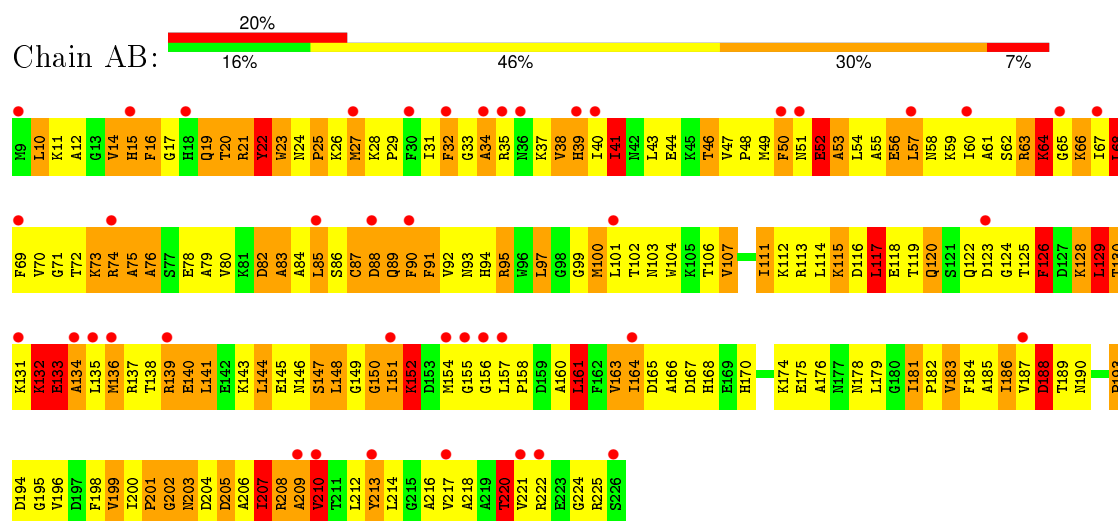
• Molecule 1: 16S rRNA



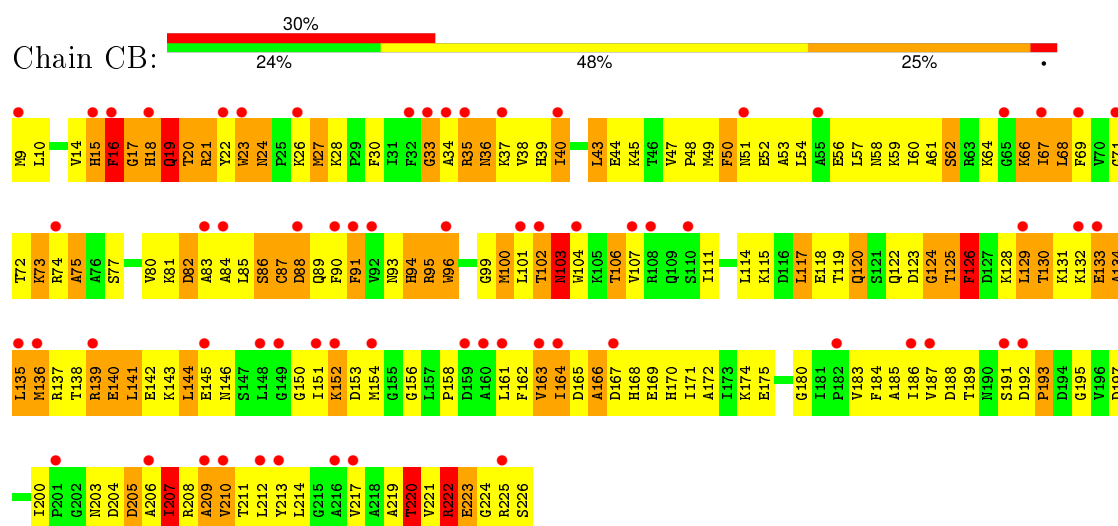
A1274	A1275	G1276	G1277	G1278	G1279	A1280	G1284	A1285	G1286	A1287	A1288	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	A1299	G1300	G1301	G1302	G1303	G1304	G1305	A1306	A1307	A1308	G1309	G1310	A1311	G1312	G1313	G1314	G1315	G1316	A1317	A1318	A1319	G1320	G1321	G1322	G1323	A1324	G1325	G1326	G1327	G1328	A1329	G1330	G1331	A1332	G1335	G1336	G1337			
U1205	G1206	U1211	U1212	A1213	G1214	G1215	G1216	G1217	G1218	A1219	G1220	G1221	G1222	G1223	A1224	A1225	A1226	A1227	G1231	G1232	A1233	G1234	U1235	A1238	A1239	A1240	G1241	G1242	G1243	G1244	A1245	G1246	G1247	A1248	A1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1260	A1261	G1262	G1263	G1264	G1265	G1266	A1267	G1268	A1269	G1270	A1271	G1272	G1273		
G1133	G1134	U1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	A1145	A1146	A1150	A1151	A1152	G1153	G1154	A1155	A1156	A1157	G1158	U1159	G1160	G1161	G1162	A1163	G1166	A1167	U1168	A1169	A1170	A1171	G1174	A1179	A1180	G1181	G1182	U1183	G1184	G1185	G1191	G1192	G1195	A1196	A1197	G1198	G1199	G1200	A1201	A1202	G1203	A1204						
A994	C995	A996	U997	G998	G999	A1000	C1001	G1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	G1013	A1014	G1015	A1016	U1017	G1018	A1019	G1020	A1021	A1022	G1023	G1024	U1025	G1026	C1027	G1028	U1029	C1030	G1031	G1032	G1033	A1034	A1035	A1036	C1037	G1038	G1039	A974	A975	G1041	A1042	G1043	A1044	C979	C980	A983	G987	G988	U989	C990	U991	U992	A1055	U1056
G846	G847	C848	G851	G852	C853	U854	U855	C856	C857	G858	G859	A860	G861	C862	U863	C866	G867	G868	G869	A872	G873	G874	C875	U876	G877	G878	C879	C880	G881	A885	C882	C883	U884	G885	G886	A887	C888	G889	U890	G891	G892	G893	G894	G895	G896	G897	C898	A900	A901	U905	A906	A909	C910	A913	A914	A919	U920		
U921	G922	A923	C924	G925	G926	G929	C930	C931	C932	G933	G934	A935	A938	G939	C940	G941	G942	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U965	G966	C967	A968	A969	C970	G971	C972	G973	G974	A975	G976	A977	A978	C979	C980	A983	G987	G988	U989	C990	U991	U992	G993						
G1061	U1062	U1065	G1066	A1067	G1068	G1069	U1070	C1071	G1072	U1073	G1074	U1075	U1076	G1077	U1078	G1079	A1080	A1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	G1112	U1118	G1124	U1125	U1126	U1127	G1128	C1129	A1130	G1131	C1132						
G1133	G1134	U1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	A1145	A1146	A1150	A1151	A1152	G1153	G1154	A1155	A1156	A1157	G1158	U1159	G1160	G1161	G1162	A1163	G1166	A1167	U1168	A1169	A1170	A1171	G1174	A1179	A1180	G1181	G1182	U1183	G1184	G1185	G1191	G1192	G1195	A1196	A1197	G1198	G1199	G1200	A1201	A1202	G1203	A1204						
U1205	G1206	U1211	U1212	A1213	G1214	G1215	G1216	G1217	G1218	A1219	G1220	G1221	G1222	G1223	A1224	A1225	A1226	A1227	G1231	G1232	A1233	G1234	U1235	A1238	A1239	A1240	G1241	G1242	G1243	G1244	A1245	G1246	G1247	A1248	A1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1260	A1261	G1262	G1263	G1264	G1265	G1266	A1267	G1268	A1269	G1270	A1271	G1272	G1273		
A1274	A1275	G1276	G1277	G1278	G1279	A1280	G1284	A1285	G1286	A1287	A1288	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	A1299	G1300	G1301	G1302	G1303	G1304	G1305	A1306	A1307	A1308	G1309	G1310	A1311	G1312	G1313	G1314	G1315	G1316	A1317	A1318	A1319	G1320	G1321	G1322	G1323	A1324	G1325	G1326	G1327	G1328	A1329	G1330	G1331	A1332	G1335	G1336	G1337			
C210	G211	G212	G213	C214	G215	U216	C217	G219	C220	G221	U222	G223	C224	G227	A228	U229	G230	C234	G237	A238	U239	G240	G241	G242	A243	U244	U245	A246	G247	C248	U249	G250	A251	U252	G253	G254	G255	G256	G257	G258	U261	A262	A263	C264	G265	G266	C267	A268	C269	A270	G271	G272	U273	G276	G277	G278			

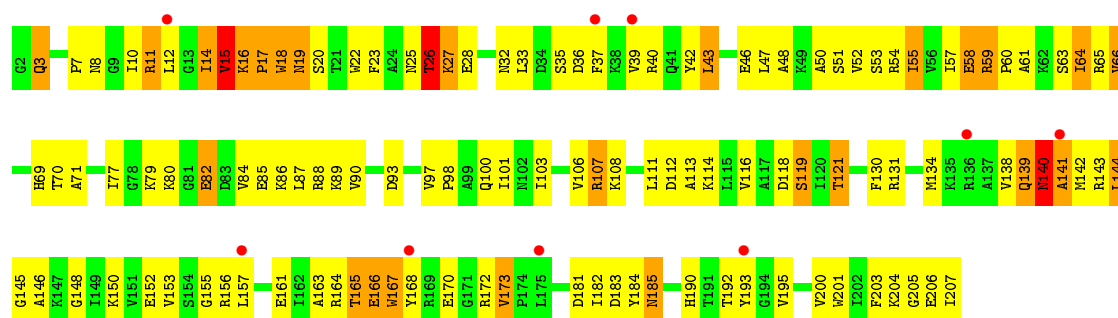


• Molecule 2: 30S ribosomal protein S2

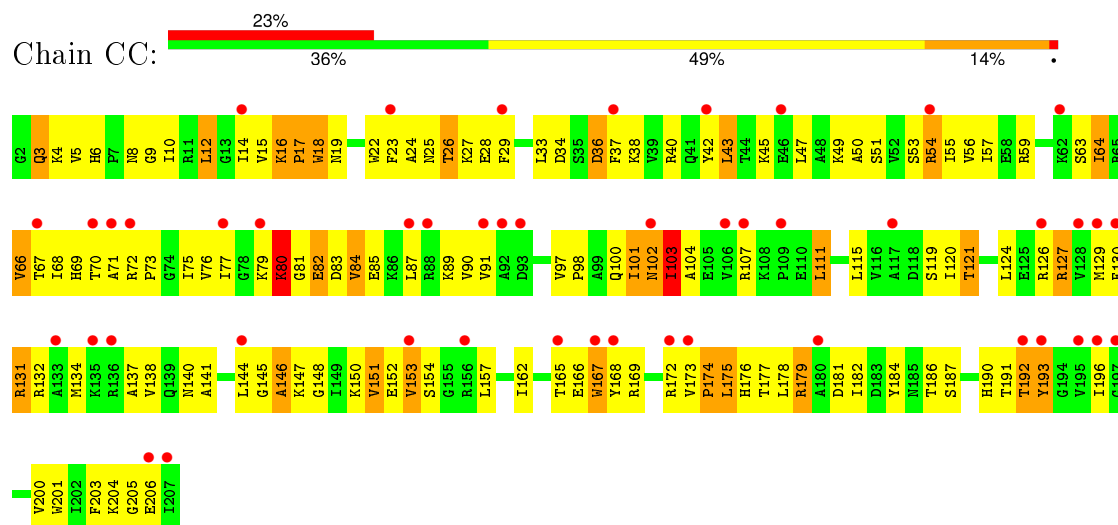


• Molecule 2: 30S ribosomal protein S2

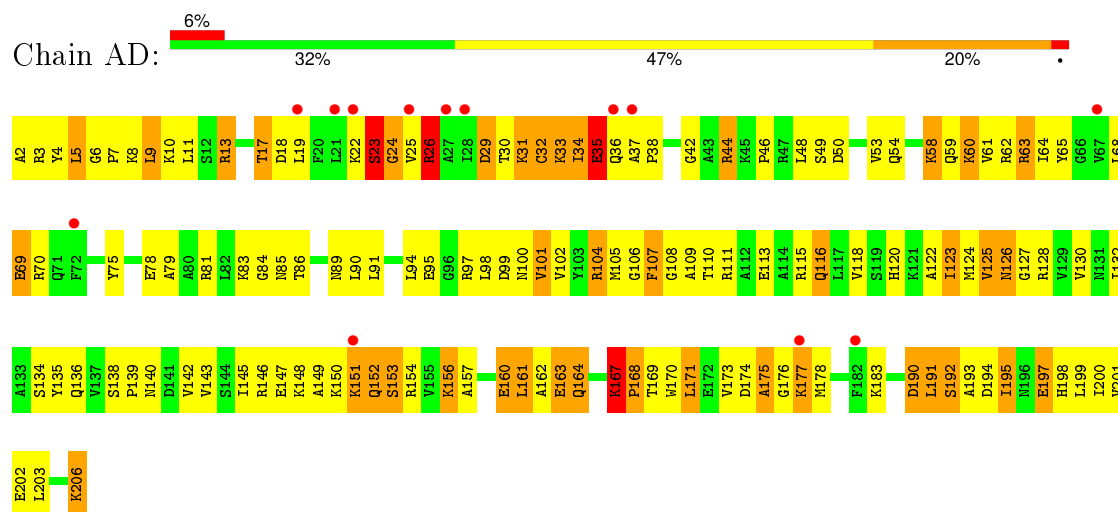




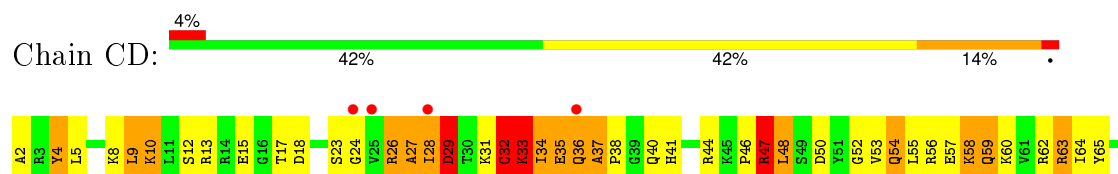
• Molecule 3: 30S ribosomal protein S3

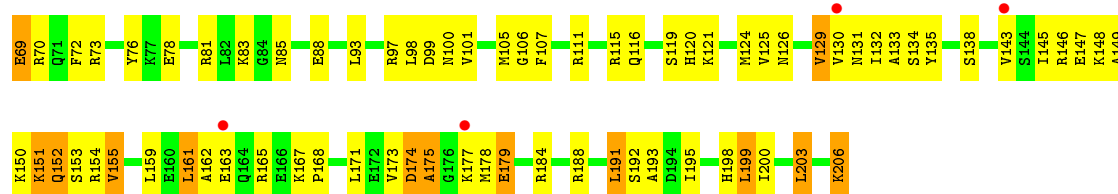


• Molecule 4: 30S ribosomal protein S4

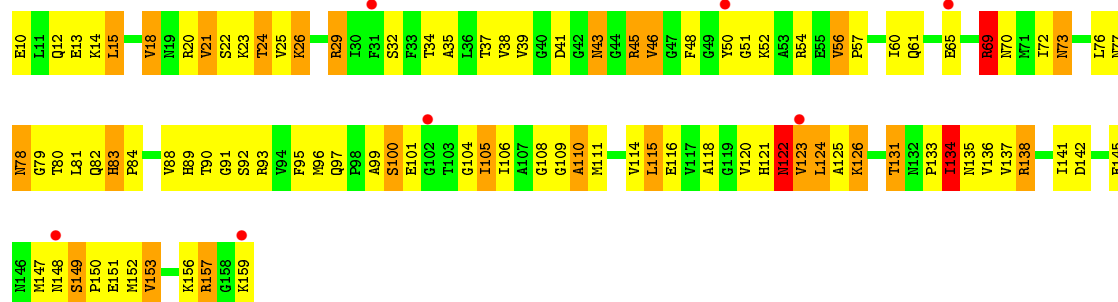


• Molecule 4: 30S ribosomal protein S4

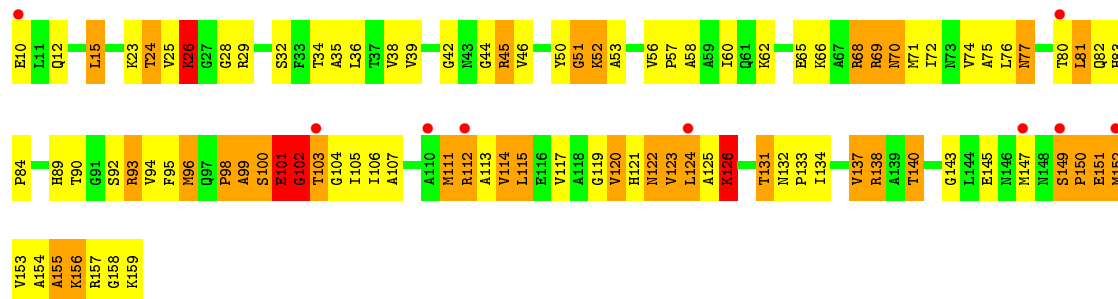




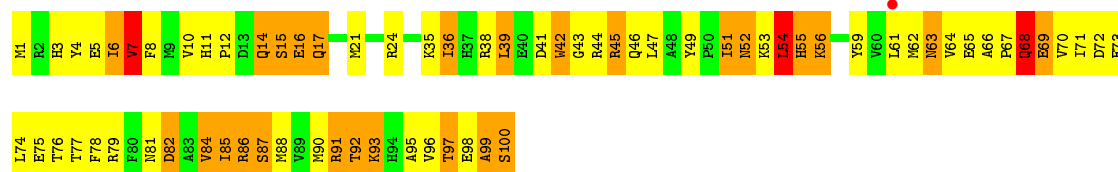
• Molecule 5: 30S ribosomal protein S5



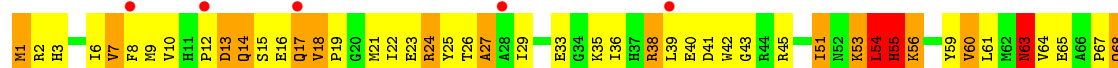
• Molecule 5: 30S ribosomal protein S5

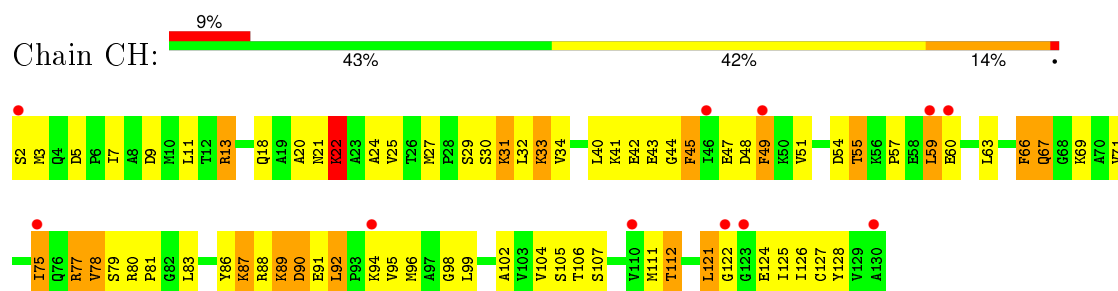
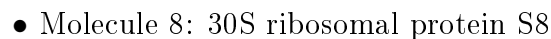
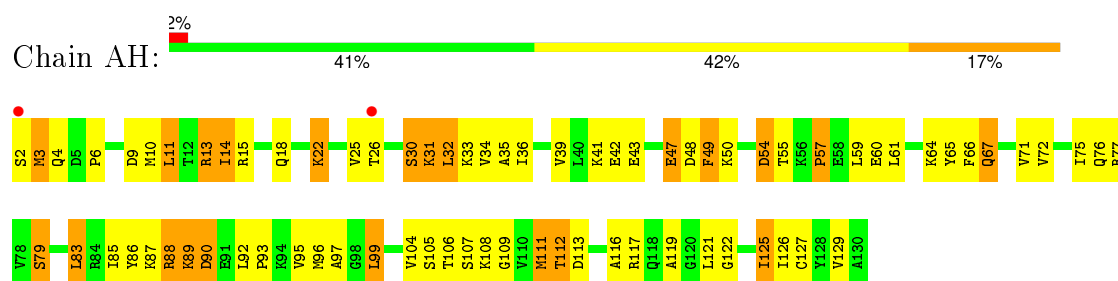
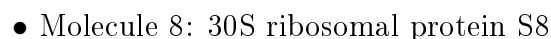
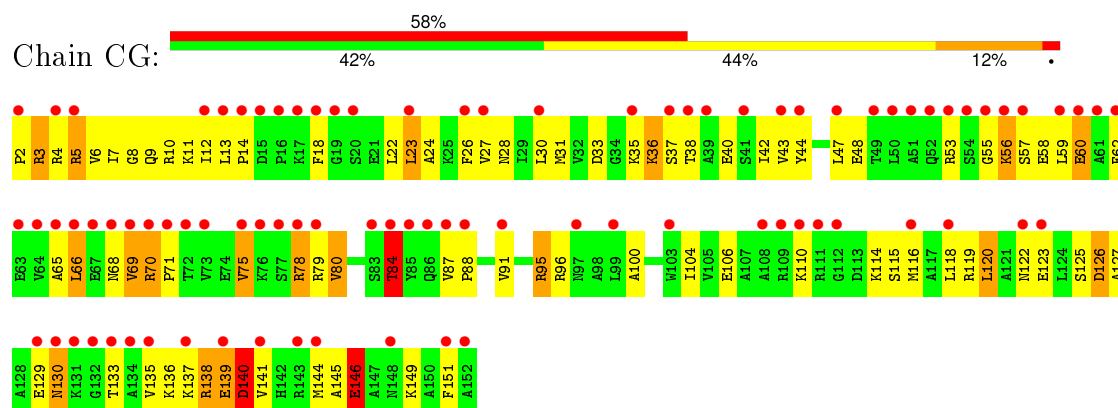
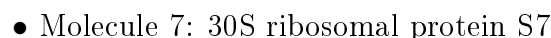
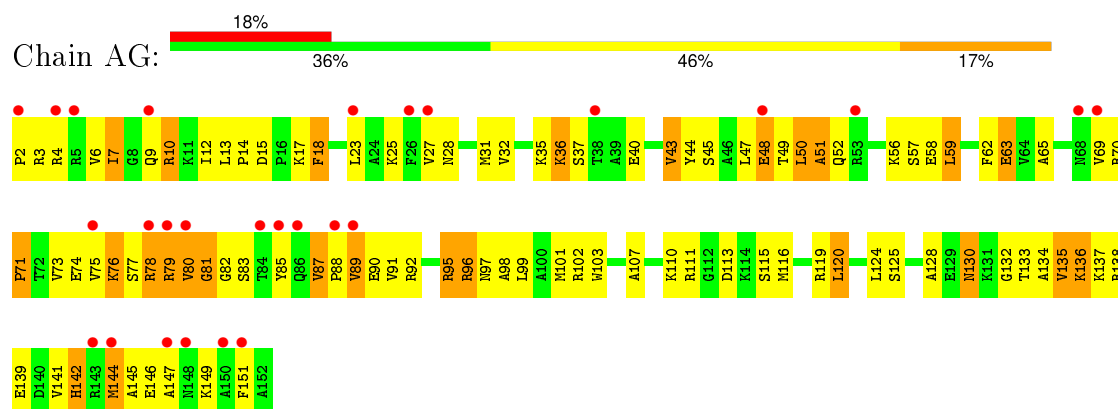
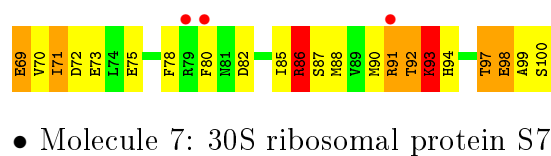


• Molecule 6: 30S ribosomal protein S6

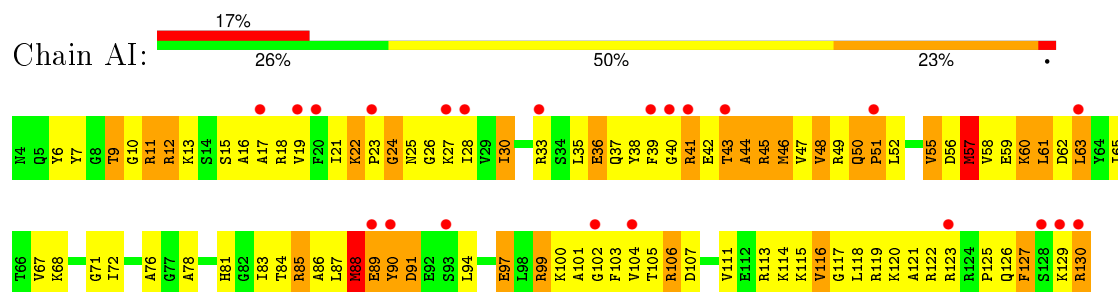


• Molecule 6: 30S ribosomal protein S6

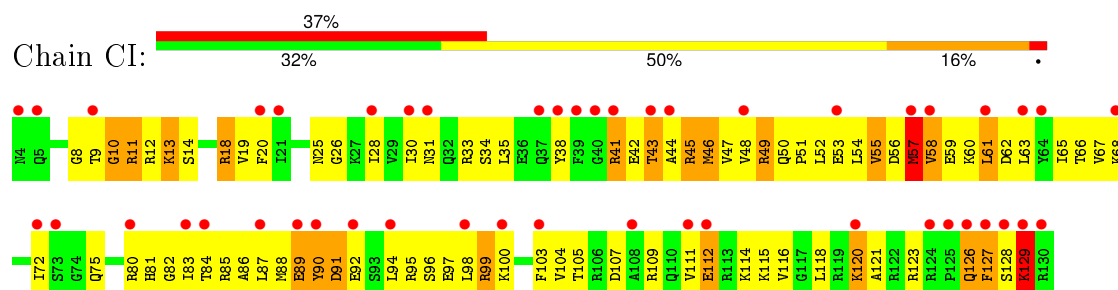




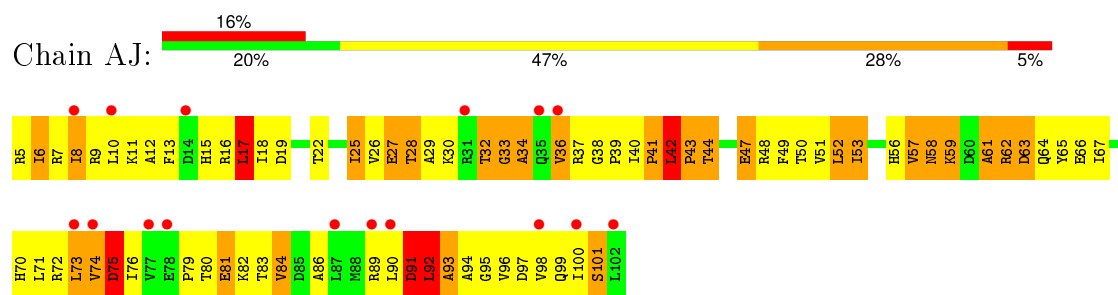
- Molecule 9: 30S ribosomal protein S9



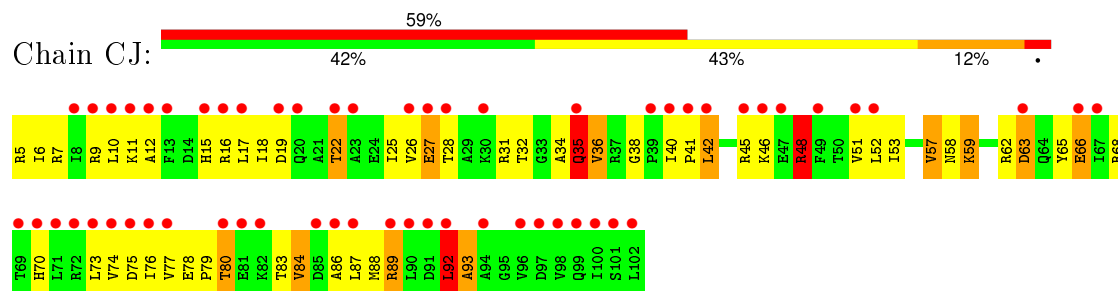
- Molecule 9: 30S ribosomal protein S9



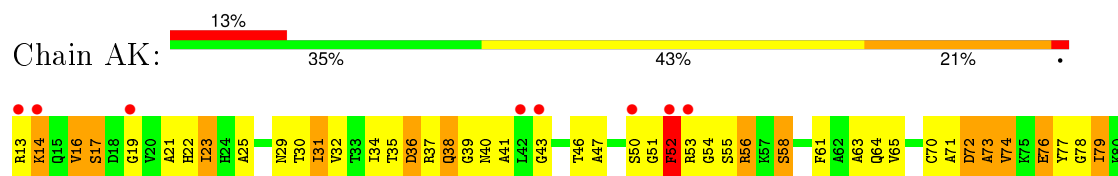
- Molecule 10: 30S ribosomal protein S10

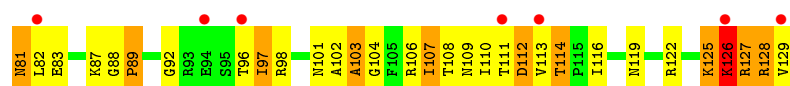


- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11





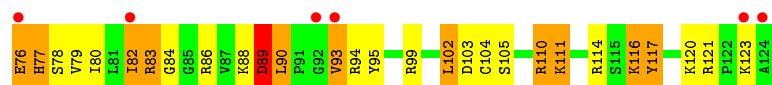
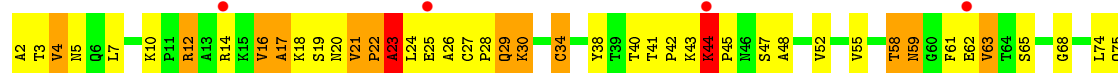
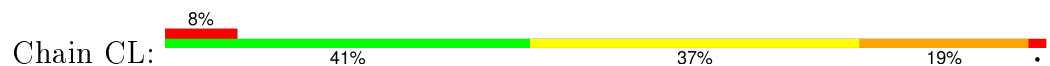
- Molecule 11: 30S ribosomal protein S11



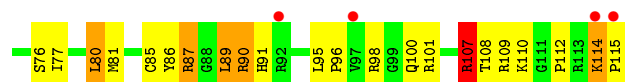
- Molecule 12: 30S ribosomal protein S12



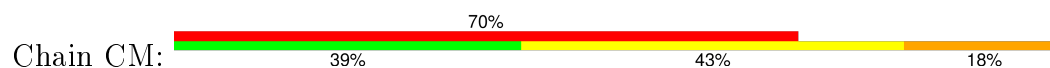
- Molecule 12: 30S ribosomal protein S12

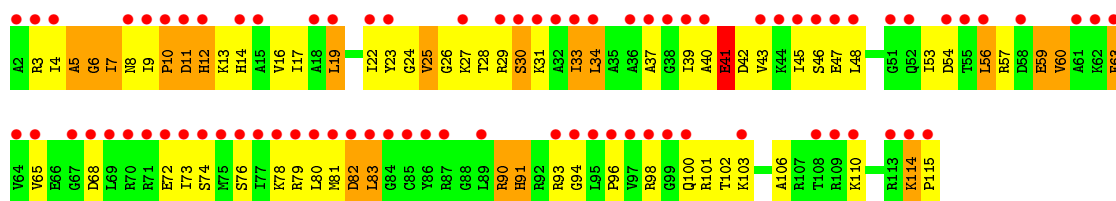


- Molecule 13: 30S ribosomal protein S13

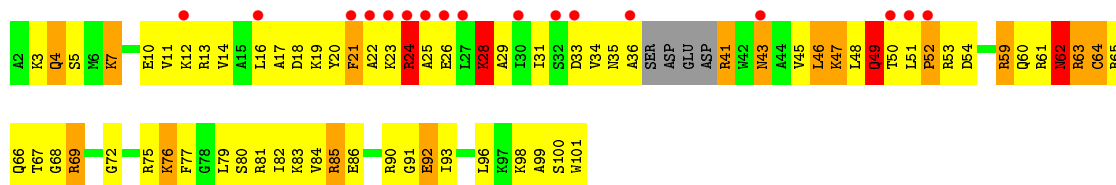


- Molecule 13: 30S ribosomal protein S13

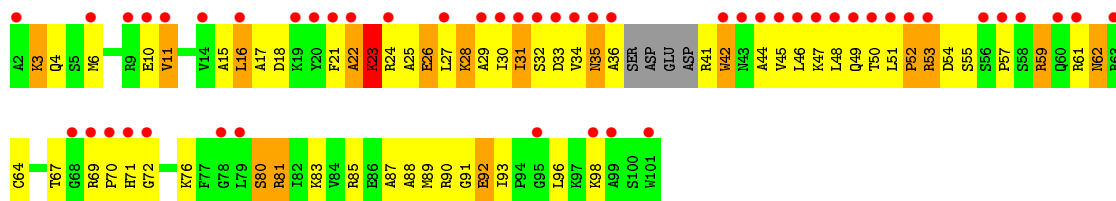




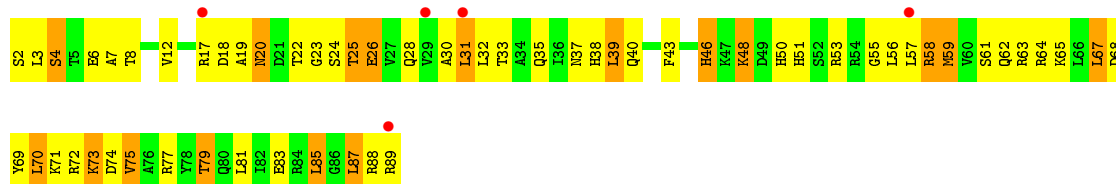
• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14



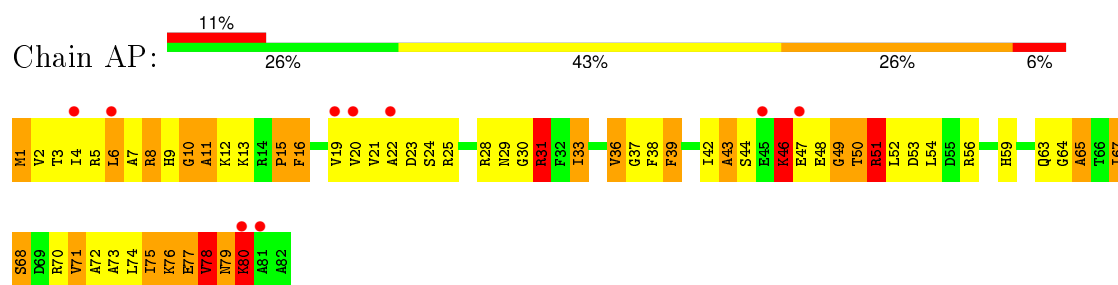
• Molecule 15: 30S ribosomal protein S15



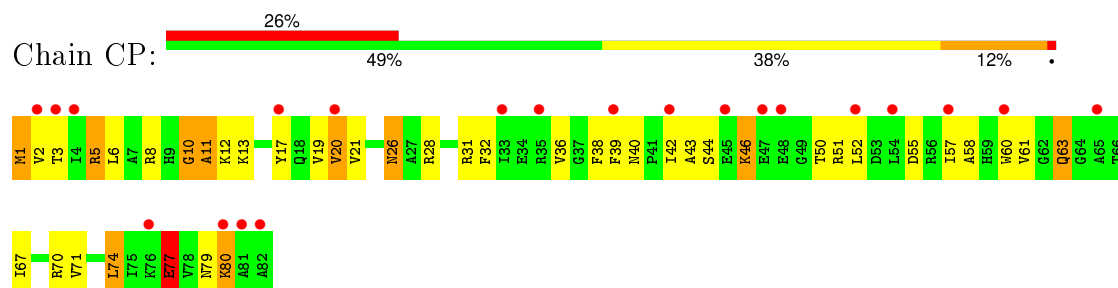
• Molecule 15: 30S ribosomal protein S15



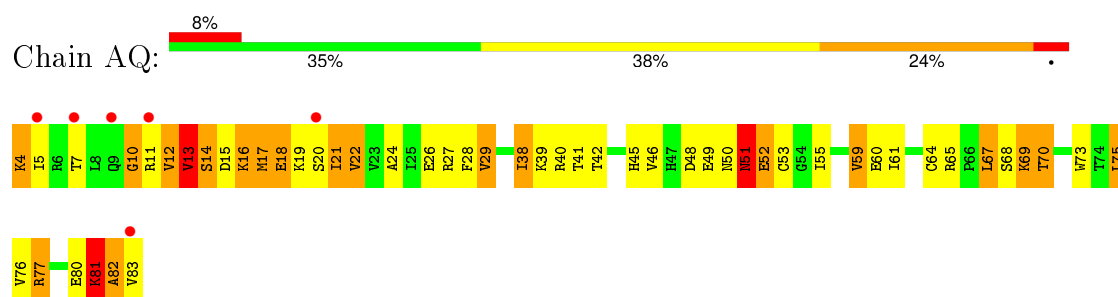
• Molecule 16: 30S ribosomal protein S16



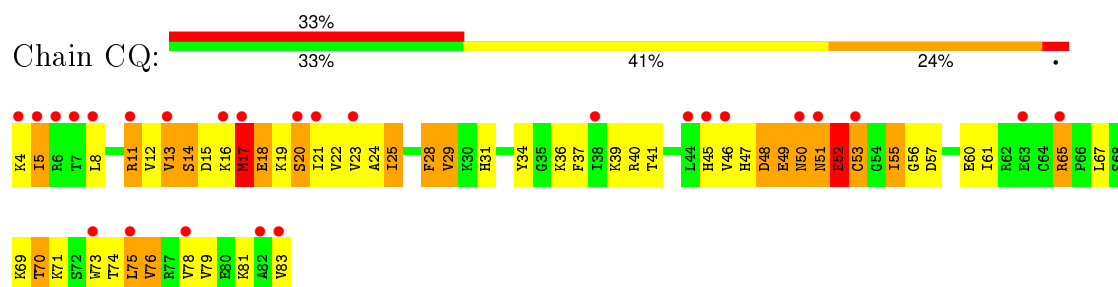
- Molecule 16: 30S ribosomal protein S16



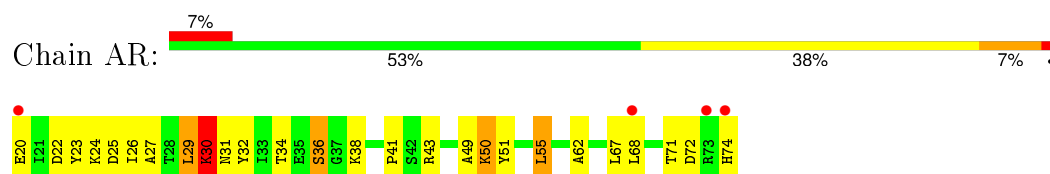
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

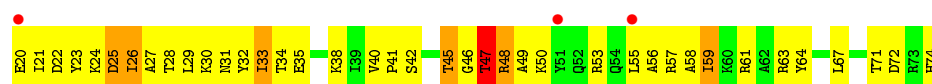


- Molecule 18: 30S ribosomal protein S18

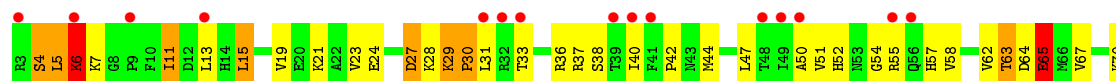


- Molecule 18: 30S ribosomal protein S18

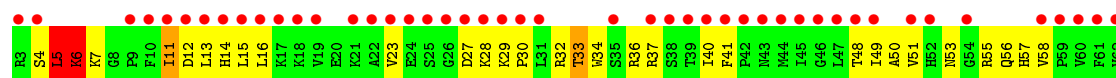
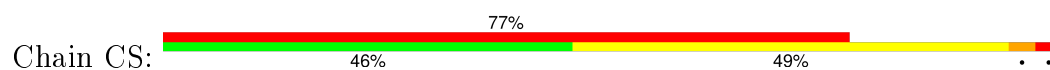




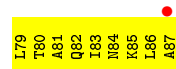
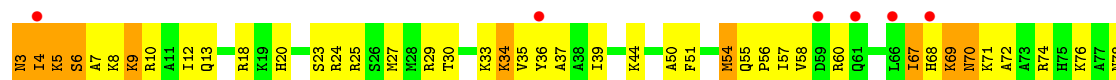
• Molecule 19: 30S ribosomal protein S19



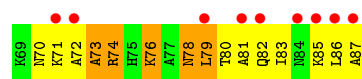
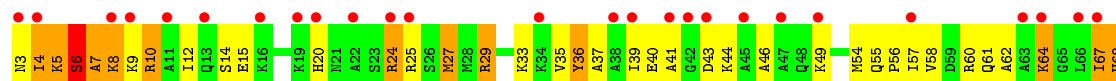
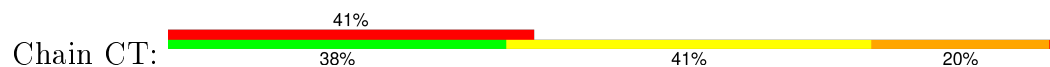
• Molecule 19: 30S ribosomal protein S19



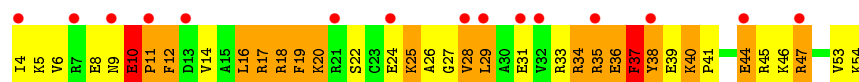
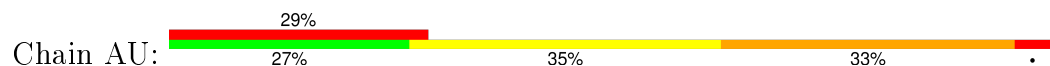
• Molecule 20: 30S ribosomal protein S20



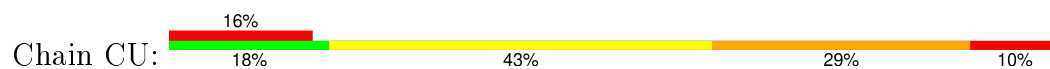
• Molecule 20: 30S ribosomal protein S20



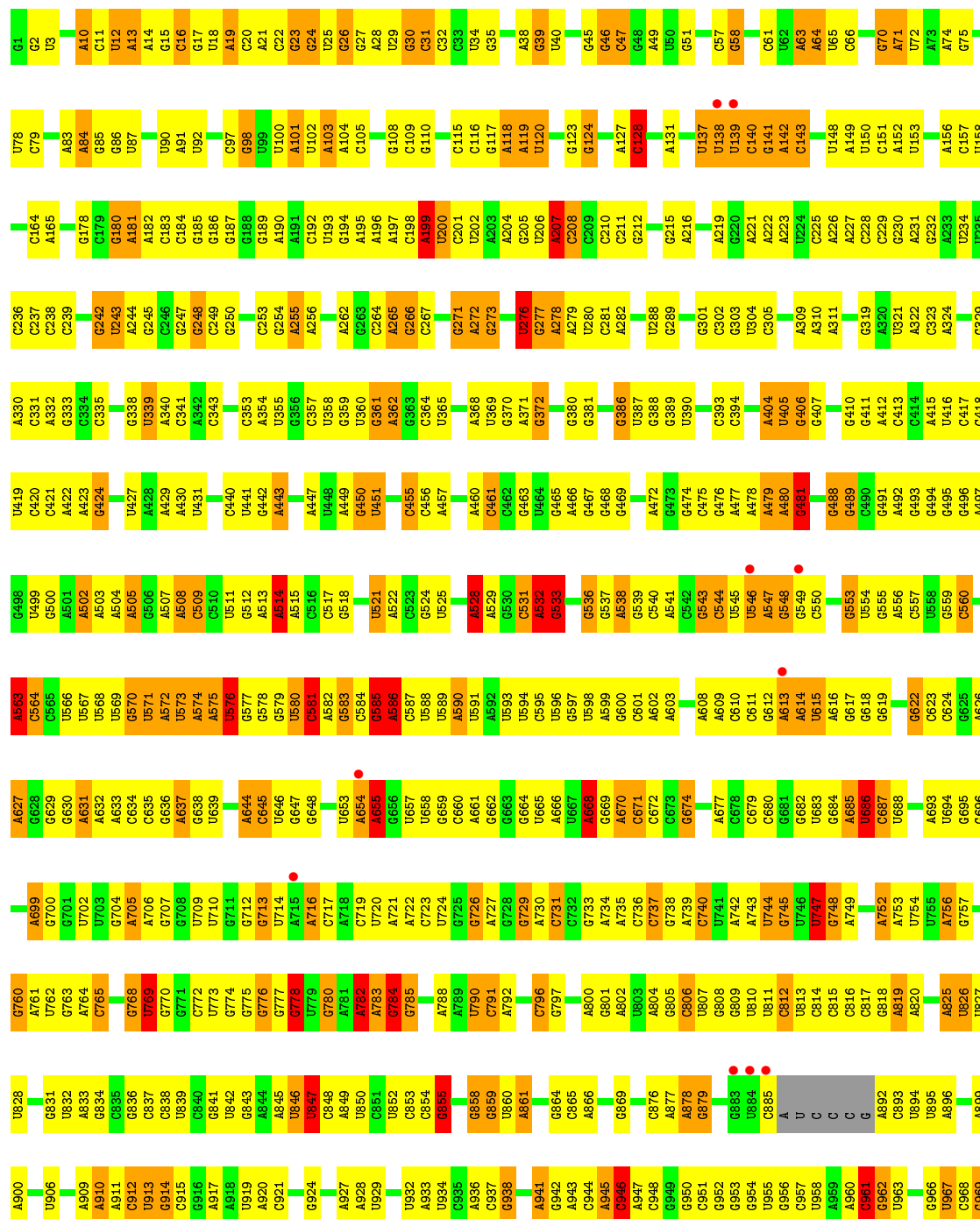
• Molecule 21: 30S ribosomal protein S21



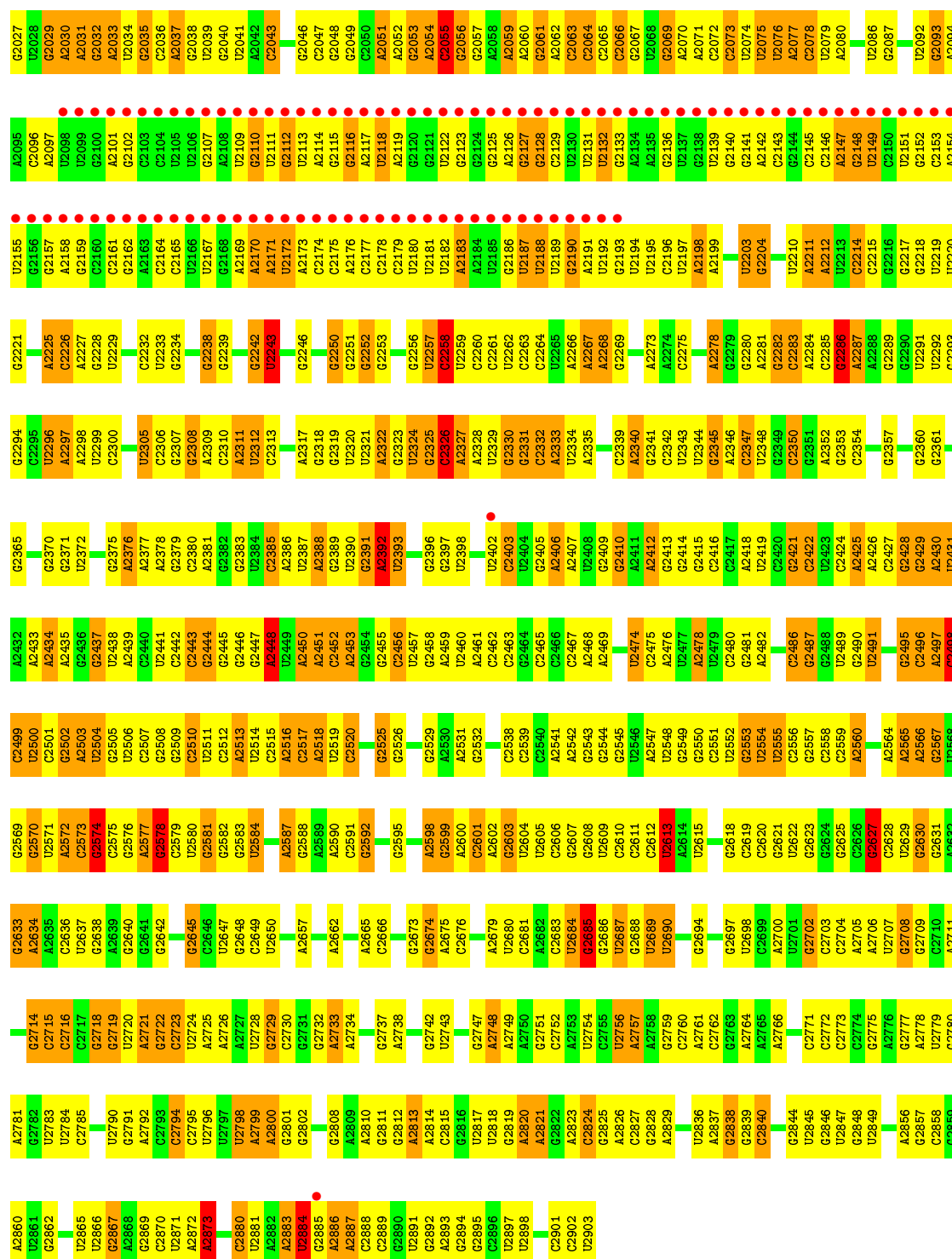
● Molecule 21: 30S ribosomal protein S21



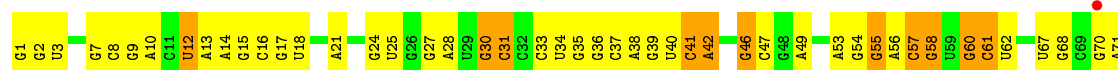
● Molecule 22: 23S rRNA



C1961	A1899	C1830	G1763	U1680	C1533	U1460	A1383	G1317	U1231	G1166	G1100	A1032	U970
C1962	A1900	G1891	C1764	G1681	U1534	U1460	A1384	U1318	A1237	C1167	U1101	U1033	G971
U1963	A1901	C1832		U1682	A1535	C1461	A1385	C1319	A1238	G1168	C1102		A972
C1964	C1902	C1833	G1767	U1683	C1536	C1461	C1386	C1320	G1239	A1169	A1040	A1040	A973
C1965	G1903		U1768	G1686	G1537	G1464	A1387	A1321	U1240	C1170	U1104	G1041	G974
A1966	G1904	C1837	C1769	U1687	G1538	G1465	A1392	A1322	U1241	C1171	U1105	G1042	A975
C1967	C1905	C1838	G1770	G1687		U1466	A1392	G1323	A1241	C1172	G1106	C1043	G976
C1968	G1906	C1839	C1771	U1688	G1546	U1467	A1393	G1324	U1242	U1173	G1107	G1044	G977
A1969	G1907	G1840	A1772	U1689	C1547	U1468	U1394	U1325	C1243	U1174	U1108	C1045	G978
A1970	C1908	U1841	A1773	G1692	A1548	A1469	A1395	U1326	A1244	A1175	C1109	A1046	A979
U1971	C1909	G1842	C1774	U1692	A1549	A1470		C1327	G1245	U1176	G1110	A980	A980
G1972	G1910	C1843	U1775	U1693	C1550		A1403	U1328	A1246	G1177	A1111	G1061	A981
G1973	U1911	G1844	G1776	C1694	A1626	U1474	A1404	U1329	A1247	C1178		G1061	C982
C1974	A1912	G1845	U1777	G1695	G1827	U1475	U1405	G1330	G1248	G1179	U1113		A983
	A1913	G1846	U1778	U1696	G1628	U1476	U1406	G1331	U1249	U1180	G1114	A1054	A984
	C1914	A1847	U1779	G1697		U1477	G1407	G1332	G1250	U1181	G1115	G1055	C985
	U1915	G1848	U1780	U1698				G1333	C1251	G1182	G1116	G1056	C986
G1982	A1916	G1849	U1781	C1699	C1558	U1487	U1411	G1334	A1253	U1183		A1057	C987
G1983	U1917	G1850	U1782	U1700	C1559	C1488	U1412	C1335	U1254	U1184	G1120	U1058	A988
G1984	G1918	U1851	A1783	A1701	C1561	C1483	A1413	C1336	U1255	G1185	C1121	G1059	G989
C1985	U1919	A1852	A1784		C1562	U1484	C1414	G1337	G1256	G1186	G1122	U1060	A990
C1986	C1920	A1853	U1785	U1712	U1563		U1415	U1340	C1257	U1188	G1123	U1061	C991
	G1921	A1854	A1786	U1713	C1638	U1487	G1416	G1341	U1258	G1189	G1125	G1062	C992
	U1922			U1714		C1488	C1417	G1342	A1259	A1190	G1126	C1064	G993
G1989	G1923			G1715	A1641	C1489	C1418	A1342	G1260	G1191	A1127	U1065	C994
C1990	U1924			U1716	G1642	U1490	A1419	G1343		G1192	G1128		C995
U1991	C1925			U1717	G1643	G1491	A1420	C1344	A1265	G1193		U1066	A996
G1992	U1926			G1718	A1644	G1492	A1421	C1345	G1266	A1194	G1131	A1067	G997
U1993	C1927			G1719	G1645	C1493	A1422	G1346	U1267	G1195	G1132	G1068	C998
C1994	G1928			U1720	A1572	A1494	G1423	A1347	A1268	G1196	A1133	A1070	U999
	U1929			G1721	C1572	A1495	G1424	C1348	A1269	G1197	A1134	G1071	A1000
G1987	G1930			U1722	C1575	A1496	G1425	C1349	U1270	G1198	G1138	C1075	C1005
A1998	U1931				G1649		G1426	G1350	C1271	G1200	G1139	C1076	C1006
C2000	A1932			U1729	U1576	C1499	A1427	C1351	A1274	U1203	G1140	A1077	G1007
C2001	C1933			C1730	U1577	G1500	A1428	C1352	A1275	A1204	U1141	U1078	A1008
G2002	G1934			G1731	U1578	G1501	G1429	G1356	G1276	A1205	A1142	C1079	A1009
G2003	C1935			C1732	C1582	A1502	G1430	G1357	G1277	G1206	A1143	A1080	A1010
A2004	G1936			G1733	A1583	A1503	A1431	G1358	C1278	C1207	A1144	U1081	G1011
C2005	A1937			G1734	U1584	A1504	G1432	G1359			G1145	U1082	U1012
A2006	C1938			A1735	C1585	A1505	A1433	G1364	G1283	C1211	G1146	U1083	G1013
U2007	G1875			U1736	U1586	U1506	A1434	A1365	A1284	G1212	A1147	A1084	A1014
A2009	C1941			G1737	G1587	C1507	G1435	A1366	A1285		U1148	A1085	
G2010	A1876			G1738	G1588	A1508	G1436	A1367	A1286	G1216	G1149	A1086	U1018
C2011	G1877			A1739	U1589	A1509	G1437	G1368	G1287	U1217	G1150	G1087	U1019
G2012	C1879			A1744	A1590	G1510	U1438	G1369	G1288	U1219	A1151	A1088	A1020
A2013	U1945			A1745	A1591	G1511	A1439	G1370	G1289	G1220	G1152	A1089	A1021
A2014	C1946			U1746	C1592	C1512	U1440	A1372	G1300	G1221	C1153	A1090	A1022
A2015	U1947			U1747	A1593	U1513	U1441	G1374	A1301	G1222	G1154	G1091	G1022
U2016	G1948			C1748	U1594	G1514	U1442	G1375	A1302	G1223	A1155	C1092	U1023
U2017	G1949					A1515	U1443	G1376	G1303	G1224	A1156	G1093	G1024
G2018	C2018			A1754	A1597		G1444	C1377	C1305	A1226	G1157	U1094	G1025
A2019	A1885			A1821	U1602	C1518	G1445	A1378	G1306	G1227	G1160	A1095	G1026
A2020	U1951			A1755	U1602	G1519	G1446	G1379	A1307	G1228	A1164	A1096	A1027
				G1756			C1447	U1375	G1303	G1229	C1164	A1098	A1028
				U1757	C1605	U1523	G1448	C1377	G1304				
U1955	U1956			A1758	G1606		G1449	A1378	C1305				
C2022	C1957			U1759	C1607	A1528	G1449	G1378	G1305				
C2023	G1958			A1760	C1608	G1529	G1450	A1379	G1311				
G2024	C1959			C1761	A1608	G1529	G1451	U1380	U1316				
C2025	G1959			A1762	A1610		A1452						
U2026	U1960					A1532	A1453						

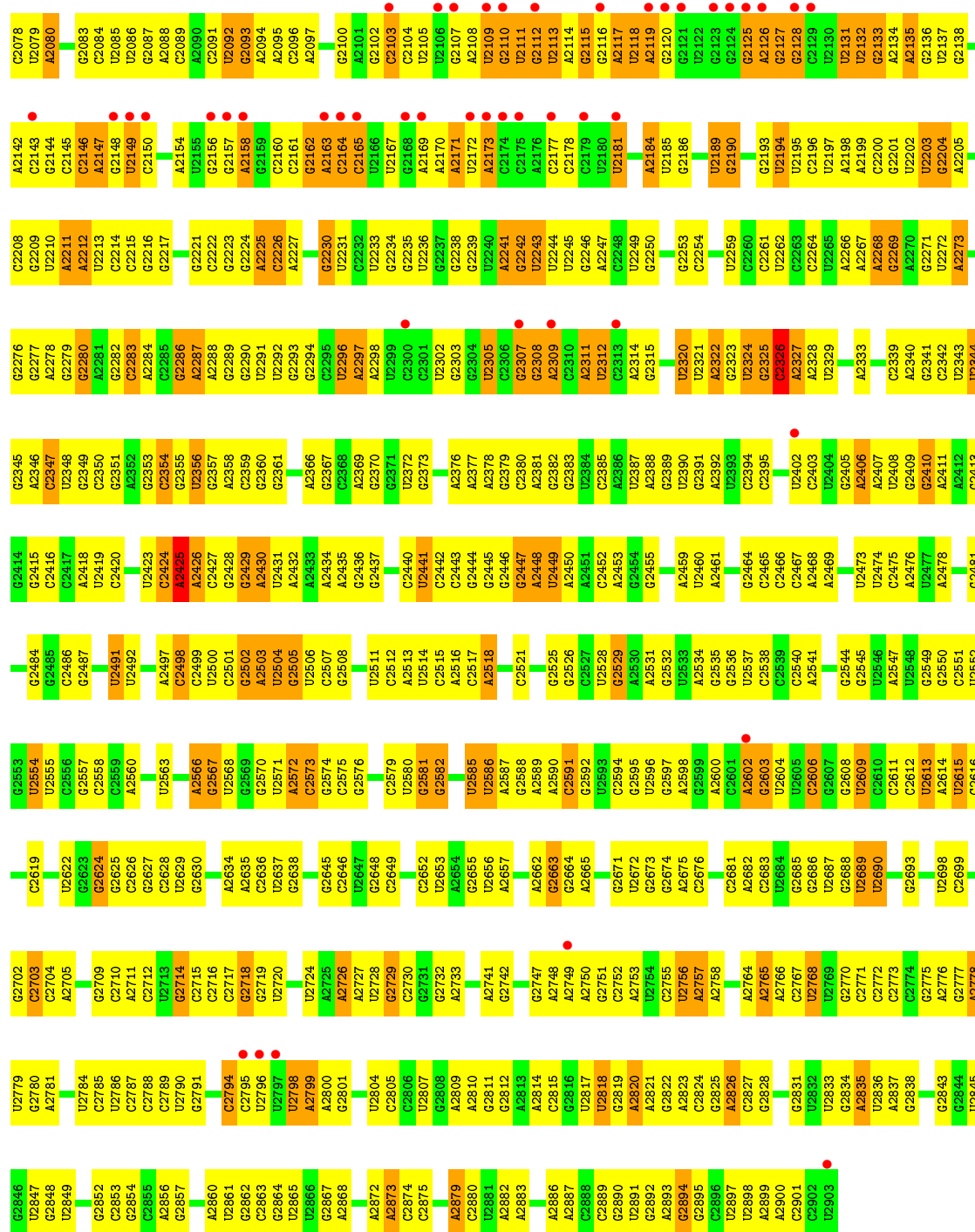


- Molecule 22: 23S rRNA



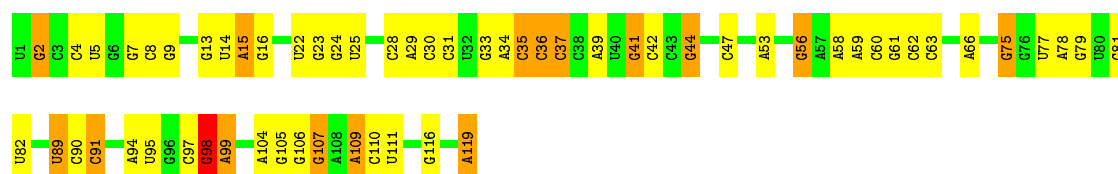
A1021	G953	G882	C806	C740	G674	C611	U546	G481	G411	A346	U280	A207	A142	U72
G1022	G954	G883	U810	U741	A675	G612	A547	A482	A412	A347	A482	C208	C143	A73
U1023	G955	U884	U811	A742	A676	A613	G548	A483	A413	A348	C209	C209	A74	A74
G1024	G956	C885	U812	A743	A677	A614	G549	C484	C414	U349	G285	C210	A146	G75
G1025	C957	A	U813	U746	C678	G615	C550	C485	A415	G351	U286	C211	C147	C76
A1027	A959	C	C814	U747	C680	G617	G555	C487	C417	A352	G287	G212	U148	G77
A1028	A960	C	C815	G748	G681	G618	G556	C488	C418	C353	G288	A213	A149	U78
A1029	C961	C	C816	A749	G682	G619	A556	C489	U419	C354	U290	G214	U150	C79
C1030		G	C817	A750	U683	G620	C557	C490	U420	U355	U291	A216	C151	
G1031		A892	G818	A751	U684	A621	U558	G491	C421	C356	U292	A217	U153	U82
A1032	G966	C893	A819	A752	A685	G622		A492	A422	C357	U293	A218	U154	A83
U1033		C894	A820	A753	U686	C623	U562	G493	A423		C294	A219	U155	A84
G1034	G969	U894	A821	U754	C687	C624	A563	G494	G424	U360	G295	A219	A156	A85
U1035	G970	A895	A821	U755	U688		C564	G495	G425	C361	U296	A221	C157	G86
	A972	C897	G822	U756	U689		C565	G496	C426	A362	G297	A222	C157	U87
A973		C898	U826	G757	G690	G628	C566	A497	U427	G363	C298	A223	U158	G88
G974	U827		U827	C758	C691	G629	U567	G498		C364	A299	U224	G159	A89
	U828		U828		G692		U568	U499	A432	U365	A300	C225	A160	U90
A975	A829	C903	A830	U761	G693	G630	U569	G500	A433	C366	G301	A226	A161	A91
G976	U831	G904	G831	A762	U694	A632	G570	A501	U434	G367	G302	A227	U162	U92
G1041	A905		G832	A763	G695	A633	U571	A502	C435	A368	G303	C228	C163	G93
G1042	U906		G833	C765	G696	C634	A572	A503	U436	U369	U304	C229	A94	A94
G1043	A833		A833	U766	C697	C635	U573	A504	U437	G370	C305	G230	A167	A95
C1044	G834		G834	U767	C698	C636	A574	A505	G438	A371	U306	G231	G168	G98
A981	G835		G835	U768	G699	A637	U575	G506		G372	G307	G232	G169	
C1045	A909		C937	U769	G700	G638	U576	A507	G442	U373	G308	A233		A101
G1047	C937		U837	G770	G701	U639	U577	A508	A443	A374	A309	U234	U174	U102
	U838		U838	C772	U702	C640	G579	C509	C444		A310	U235	U174	
A982	A844		A844		U703	U641	U580	C510	C445		A311	C236	G175	C105
C1048	A945		A945	G775	G704	U642	C581	U511	G446	G377	G312	C239	G176	C106
G1051	G989		U846	G775	A705	A643	A582	G512	A447	C379	G313		G177	C107
A1050	A990		U847	G776	A706	A644	G583	G513	U449	G380	G313		G178	C108
C1052			C948	G777	G707	C645	C584	A514	U449	G381	G317	G242	C179	C109
G1053	G993		U850	G778		U646	G585		G450	A382	C318	U243	G180	G110
U1060	C994		C951	G779	A715	G647	A866	C517	U451	C383	G319	A244	A181	A111
U1061	C995		A827	G780	A716	G648	C587		G452	A384	A320	G245	G182	U112
G1062	A996		A828	A781	C717	G649	C588		A453	C385	G321	C246	C183	C115
C1063	G997		G856	A782	A718	C650	U589	G520	A454	C386	A322	G247	C184	
U1064	C998		G857	A783	G719	G651	A590	A522	C455	U387	C323	G248	G185	
U1065	G999		G858	G784	U720	U652	U591	C523	C456	G388	A324	C249	G186	
A1067	A1000		G859	G785	A721	U653	A592	G524	A457	G389	C324	G250	G187	A118
G1068	A1001				A722	A654	U525	G524		U390	G327	A251	G187	A119
A1069	C935		G864	C786	C723	A655	U593	U526	A460	A391	U328	A251	G188	U120
C1070	G1003		C965	A788	U724	G656	C595	A527	C461	U392	G329	A255	G189	G121
G1071	U1004		A866	A789	G725	U657	U596	A528		C393	A330		A190	A125
C1072	C1005		C967	U790	G726	U658	G597	A529	A466	G396	G333	C264	C192	A126
A1073	C1006		U868	C791	A727	G659	U598	G530	G467		G334	A265	C192	A127
			G869	A792	G728	C660	A599	C531	G468		C334	G266	A195	C128
G1074	A1009		G869	A793	G729	A661	G600	A532	G469		C335	C267	A196	
C1075	C942		U870	A794	A730	G662	C901	A533	A470		C336	C268	A197	
C1076	A1010		U871	A795	A731	G663	A602	A534	A471		G337	C269	C198	G132
U1077	G1011		U872	C795	G732	G664	A603	U534	A472		G338	A270	C199	U133
A1078	U1012		C973	G796	G733		G604	G536			U339	G271	U200	G134
C1079	C1013		G874	G797	G733		G605	G537			A340	A272	G136	U135
A1080	U1014		G875	G798	A734		U606	A538			A341		C201	U137
U1081	G1015		A878	G799	A735		U607	G475			A342		U202	U137
U1082	G1016		G879	A802	C736		U608	A477			G343		A203	U138
C1083			G880	C737	G671		A608	A478			C343		A204	U139
A1084	U1019		G881	C738	C672		A609	A479			A344		A278	G140
	C982		C981	C739	A730		C810	U615			A345		G205	C141

U2011	U1939	G1790	G1649	G1577	A1504	C1438	G1361	C1297	A1230	G1149	A1086
G2012	U1940	A1791	A1650	U1578	A1509	G1429	C1362	G1298	U1231	G1149	G1087
A2013	G1862	G1792	A1651	G1651	A1510	G1430	C1363	G1299	C1232	C1152	A1088
A2015	G1863	G1793	A1652	G1652	A1510	A1431	C1364	G1300	G1233	C1153	A1089
	U1944	A1794	G1653	C1583	G1514	G1432	A1365	A1301	U1234	G1154	A1090
G2018	U1945	C1795	A1654	A1583	G1515	A1433	A1366	A1302	G1235	A1155	G1091
A2019	U1946	U1796	A1655	U1584	A1516	A1434	A1367	G1303	G1236	A1156	C1092
C1947	G1867	C1797	C1656	U1585	G1516	G1435	A1368	A1304	A1237		G1093
	C1868	G1798		A1586	G1519	G1436	G1369	C1305	G1237	G1162	U1094
A2020	U1951	C1799	G1659	G1587	G1520	G1437	C1370	C1306	G1238		A1095
C2021	G1869	G1799	G1660	G1588	G1521	G1438	G1371	C1307	U1240		A1096
U2022	C1870	G1732	G1661	U1589	G1522	A1439	U1372	A1308	A1241		U1097
C2023	A1801	G1733	G1662	C1592	U1523		G1373	G1309			A1098
G2024	A1802	G1734	G1663	G1593	G1524	G1445	G1374	G1310			G1099
C2025	A1803	U1736	G1664	A1594	G1525	G1446	U1375	G1311	A1247		G1100
C2026	G1874	G1737	A1665	U1595	A1526	G1447	C1376	U1312	G1248		U1101
G2027	A1875	G1738	A1666	C1596	C1526	G1448	G1377	U1313	U1249		C1102
U2028	A1876	A1739	G1666	A1596	G1527	G1449	A1378	C1314	G1250		A1103
G2029	G1877	G1740	G1667	A1597	A1528	G1450	U1379	C1315	G1251		C1104
A2030	U1880	C1741	A1668	A1598	G1529	G1451	G1380	C1316	A1252		U1105
A2031	C1881	A1809	A1669	C1599	G1530	G1452	G1381	U1317	A1253		G1106
A2032	U1882	G1743	C1670	A1600	A1531	G1453	G1382	U1318	U1254		U1107
U2033	U1883	A1744	A1671	G1601	A1532	G1454	A1383	C1319	G1256		G1108
A2034	G1884	A1745	A1672	G1602	C1533	U1455	U1384	C1320	C1257		U1109
		A1746	G1673	U1603	U1534	U1456	A1385		U1258		G1110
		U1747	G1674	A1604	A1535	C1457	C1386		U1181		A1111
A2037	A1889	G1814	C1675	C1605	C1536	C1458	A1387		G1259		G1112
G2038	C1893	C1816	A1676	C1606	G1537	G1459		G1324			U1113
U2039	C1894	U1750	A1677	G1607	G1538	G1460	U1390	U1325	A1262		G1114
G2040	C1895	G1751	G1678	C1608	U1539	G1461	U1391	U1326	U1263		G1115
C2043	A1899	A1819	G1679	A1609	G1540	U1462	A1392	A1327	A1264		U1116
C2044	U1903	U1820	U1680	A1609	C1541	U1463	A1393	U1328	U1265		G1117
C2045	G1903	A1821	G1681	A1610	G1542	A1464	A1394	U1329	G1266		C1118
G2046		G1822	G1682	U1613	A1543	G1471	A1395	C1330	U1267		U1119
C2047	G1906	U1758	U1683	A1614	A1544	G1472	U1396	G1332	A1268		G1120
G2048	G1907	U1759	U1688	A1615	A1545	U1473	U1397	G1333	G1270		C1121
		A1760	A1689	A1616	G1546	U1474		G1334	G1271		G1122
A2051	U1911	U1827	A1690	C1617	C1547	U1475	G1404	C1335	A1272		
A2052	A1912	G1828	C1691	A1618	A1548	A1476	U1405	C1336	U1273		G1125
G2053	C1913	U1829	U1692	G1619	C1549	G1477	U1406	G1337	A1274		A1126
A2054	U1915	C1830	U1693	G1620	C1550	G1478	U1407	G1338	U1275		A1127
C2055	A1916	G1831	C1694	U1621	A1551	U1480	G1408	G1339	A1276		G1128
G2056	U1917	C1832	G1695	G1622	A1552	G1482	U1409	U1340	G1277		A1129
C2057	A1918	U1833	G1696	U1623	U1553	G1483	G1410	G1341	G1278		G1206
A2058		U1834	A1698	G1624	U1554	U1484	U1411	A1342	G1279		C1207
A2059	C1994	G1835	C1699	C1625	G1555		U1412	G1343	G1280		U1132
G2060	U1995		G1702	A1626	C1556	A1490	A1413	U1344	G1281		A1133
G2061	C1996	C1838	G1703	U1636	U1562	G1491	A1414	C1345			G1135
A2062	C1997	G1839	G1704	A1637	U1563	G1492	U1415		A1285		G1136
C2063	U1926	C1843	A1705	C1638	C1564	C1493	G1416	C1351	A1286		G1137
	U1927		C1706	C1639	C1565	A1494	G1417	C1352	A1287		G1138
C2066	C2001		U1779	C1640	A1495	A1495	G1418	U1353	G1288		G1139
G2069		G1846	A1780	U1641	A1566	A1496	A1419	A1354	G1289		U1140
A2070		A1847	U1781	A1541	G1567	U1497	A1420	G1355	C1290		G1222
A2071		A1848	U1782	G1568	C1568	G1498	G1421	G1356	C1291		U1141
C2072		A1854	A1783	C1644	A1569	C1499	G1422	G1357	G1292		A1142
C2073		U1855	A1785	G1645	A1570	G1500	G1423	C1358	G1293		A1143
U2074		U1714	U1715	C1646	A1571	G1501	G1424	G1359	U1294		A1144
U2075		U1716	U1716	U1648	U1576	A1502	G1426	G1360	G1296		A1147
						A1503	A1427				U1148

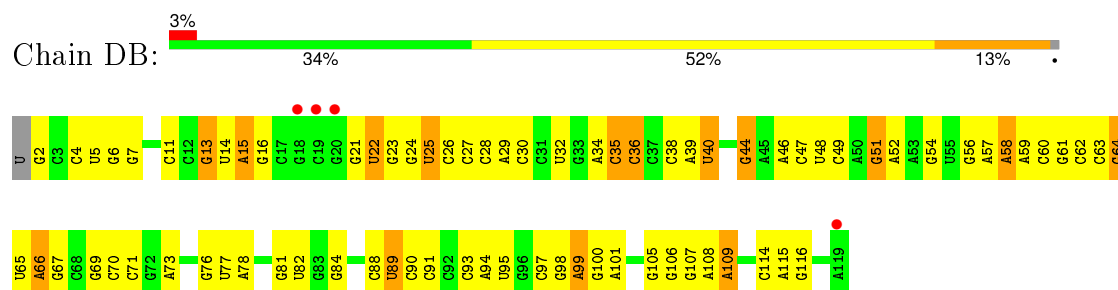


• Molecule 23: 5S rRNA

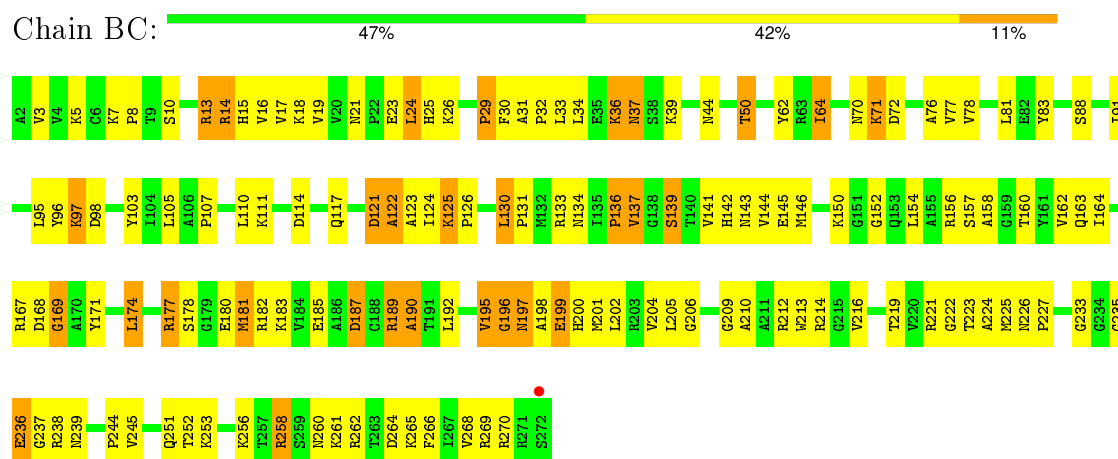
Chain BB: 50% 37% 13%



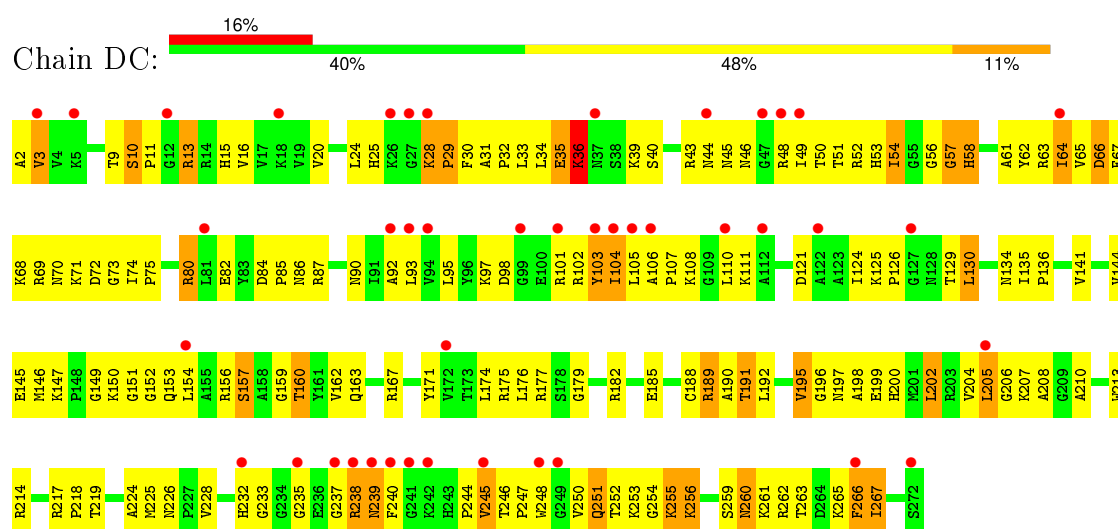
- Molecule 23: 5S rRNA



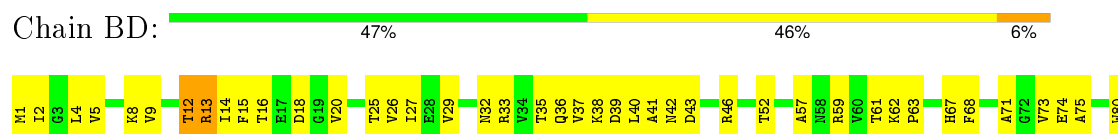
- Molecule 24: 50S ribosomal protein L2

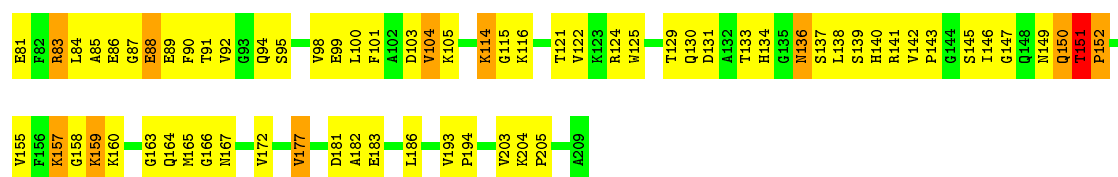


- Molecule 24: 50S ribosomal protein L2

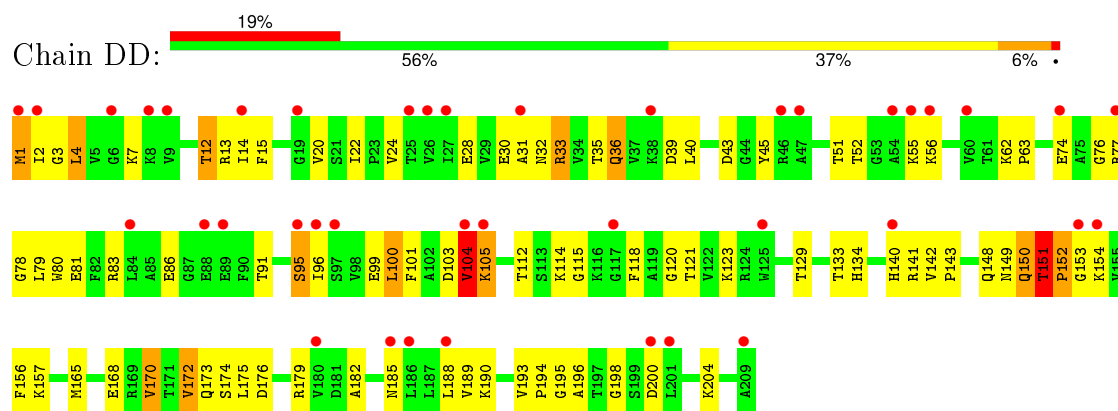


- Molecule 25: 50S ribosomal protein L3

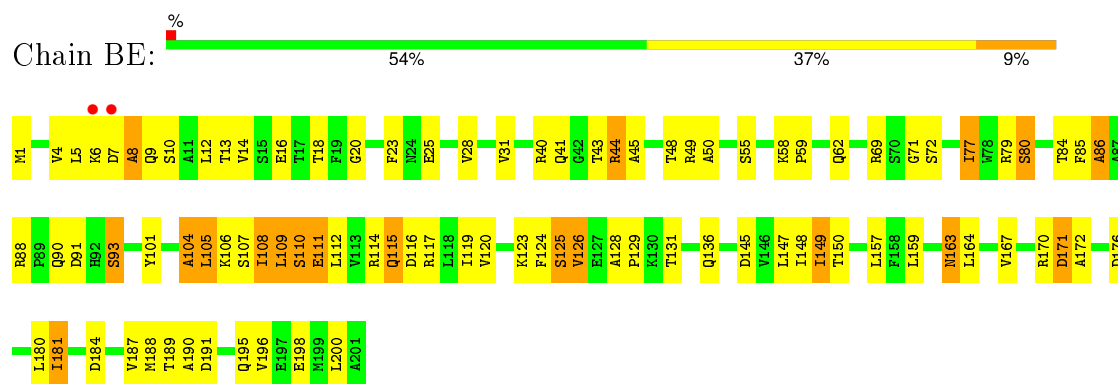




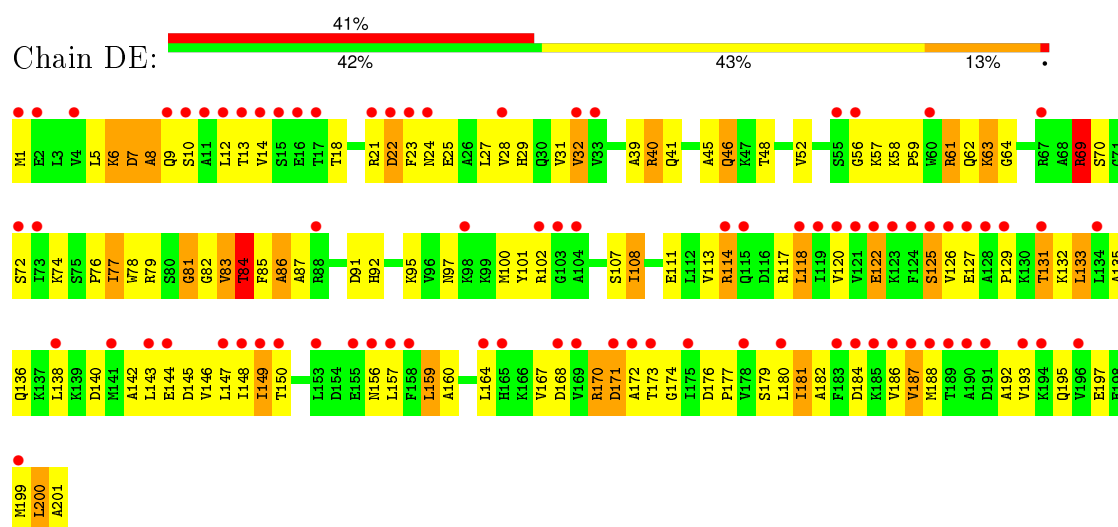
• Molecule 25: 50S ribosomal protein L3



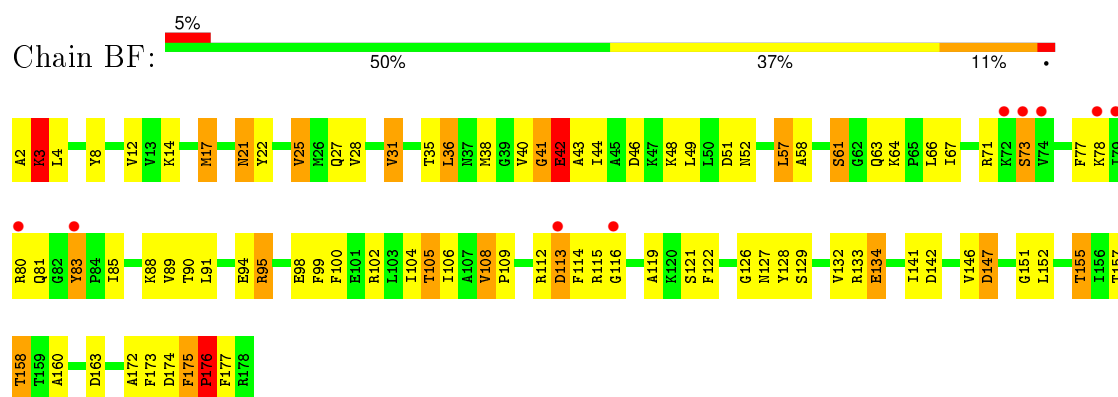
• Molecule 26: 50S ribosomal protein L4



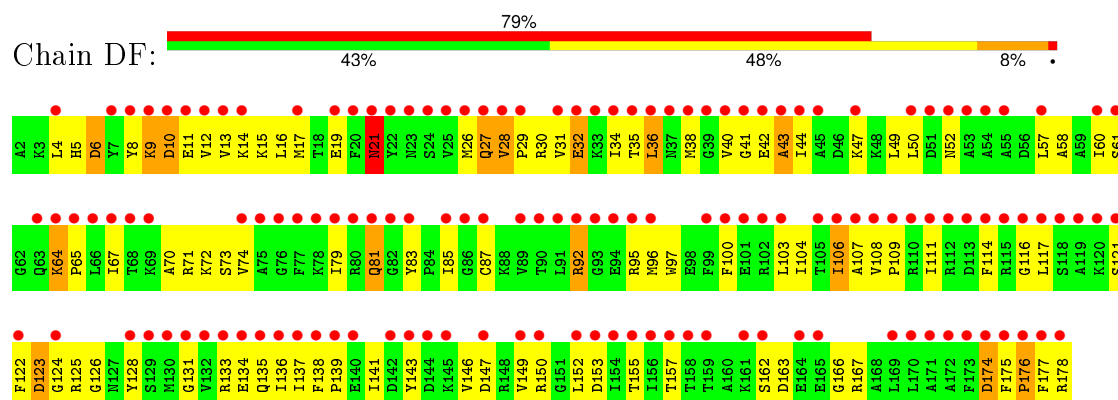
• Molecule 26: 50S ribosomal protein L4



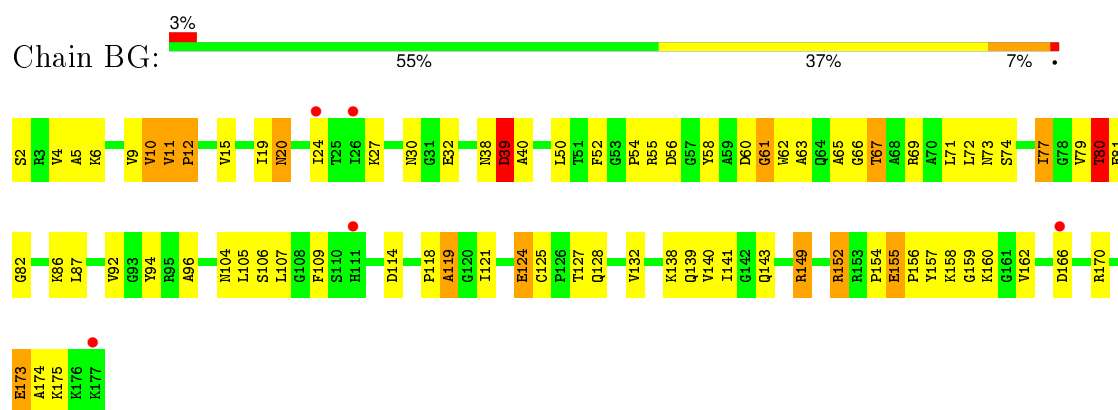
• Molecule 27: 50S ribosomal protein L5



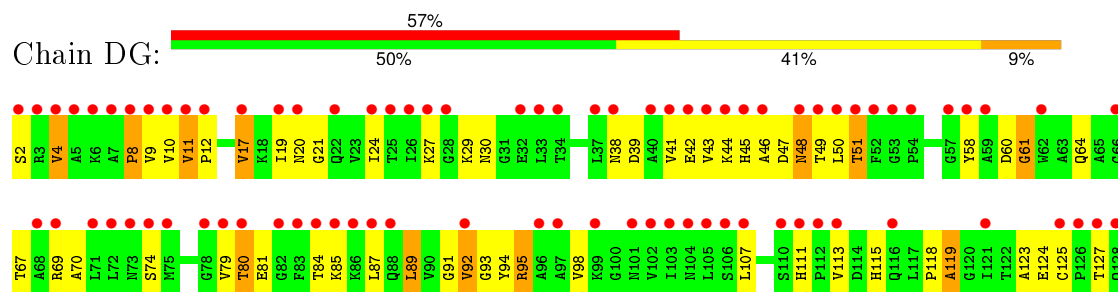
• Molecule 27: 50S ribosomal protein L5

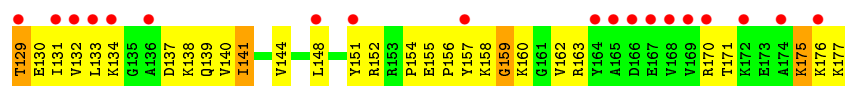


• Molecule 28: 50S ribosomal protein L6

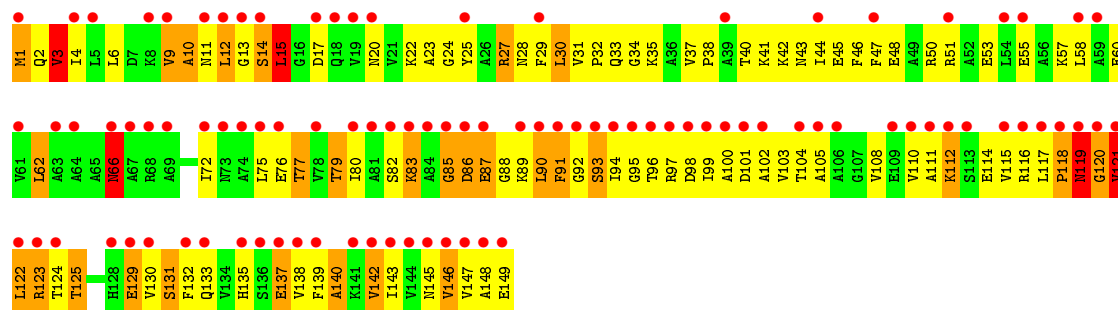


• Molecule 28: 50S ribosomal protein L6

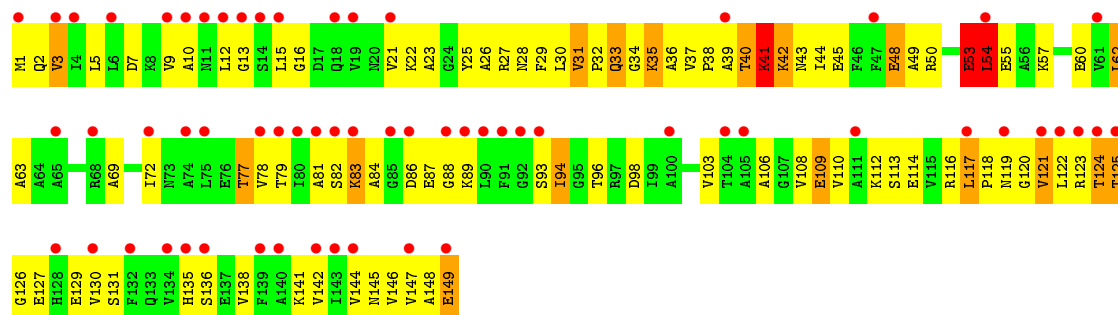




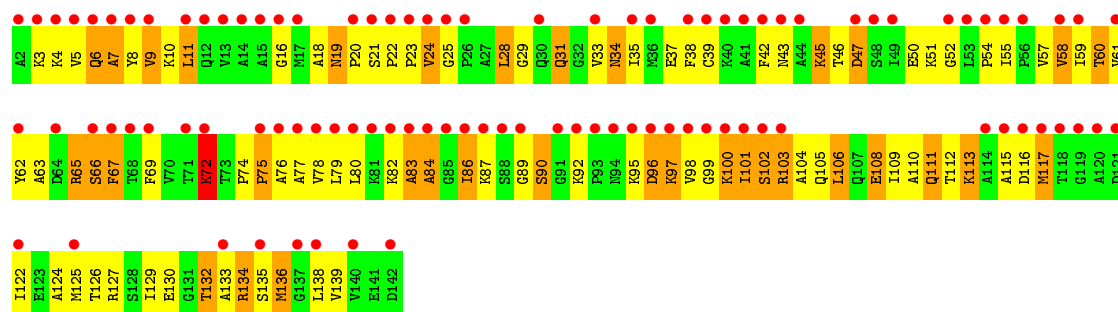
• Molecule 29: 50S ribosomal protein L9



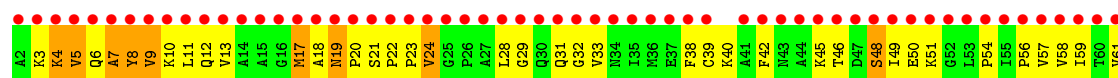
• Molecule 29: 50S ribosomal protein L9

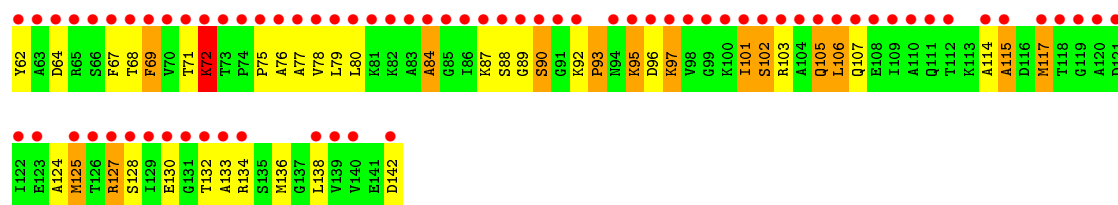


• Molecule 30: 50S ribosomal protein L11

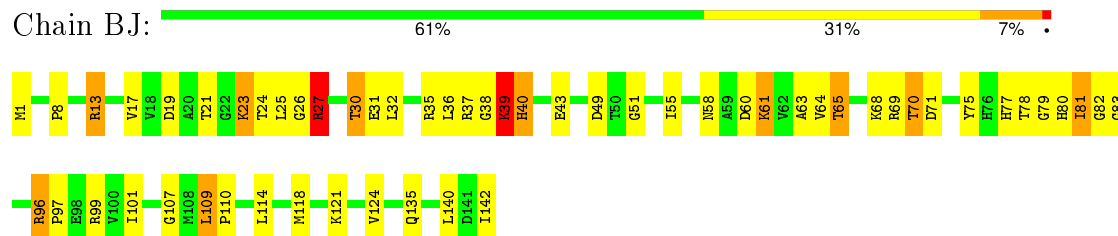


• Molecule 30: 50S ribosomal protein L11

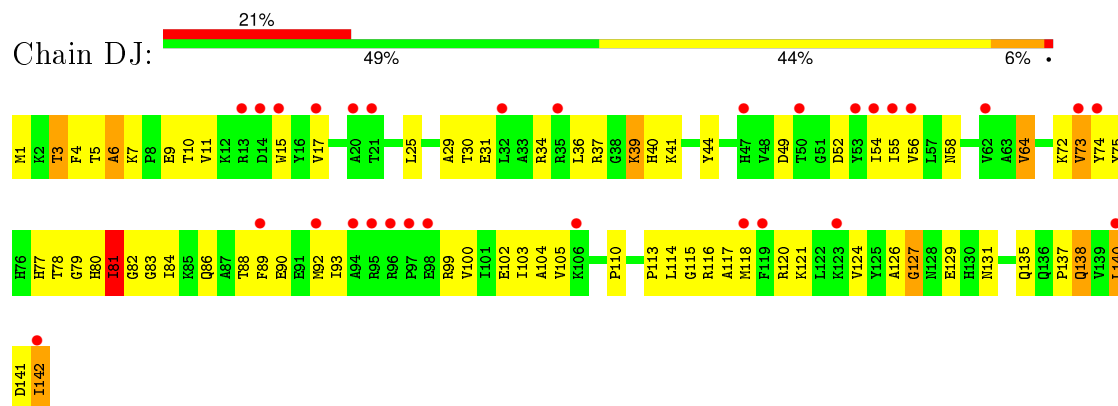




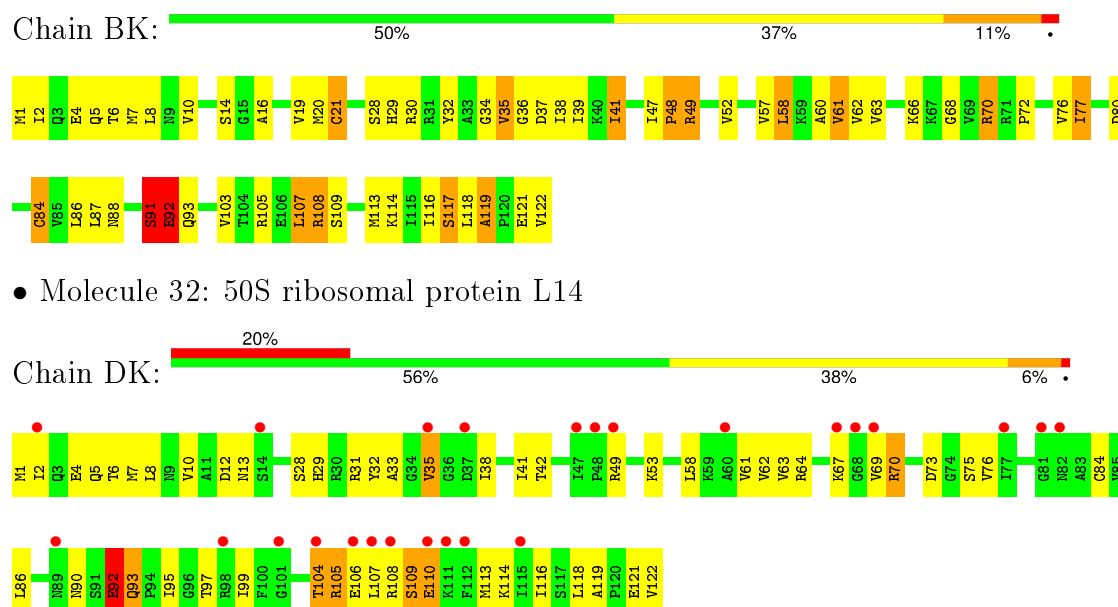
• Molecule 31: 50S ribosomal protein L13



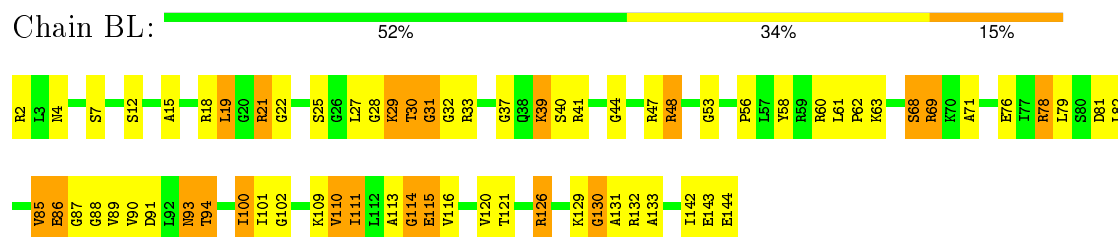
• Molecule 31: 50S ribosomal protein L13



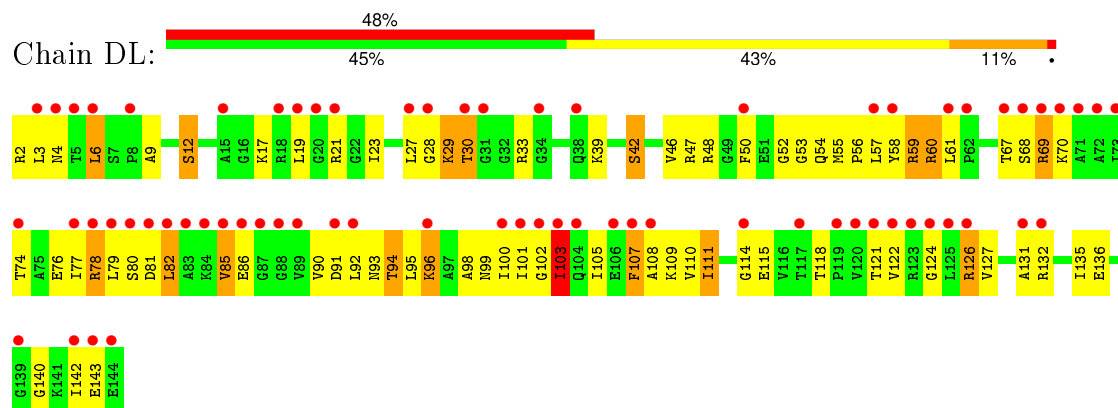
• Molecule 32: 50S ribosomal protein L14



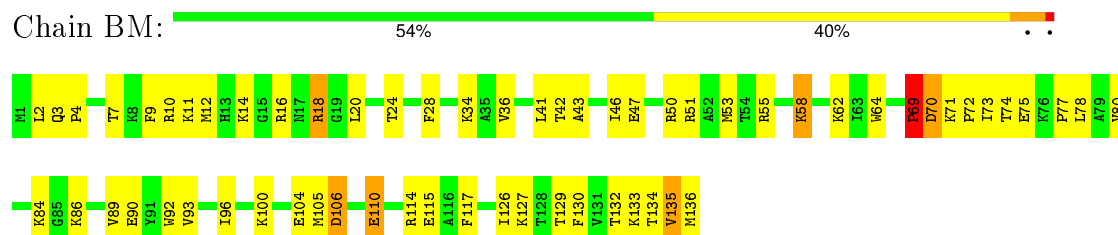
- Molecule 33: 50S ribosomal protein L15



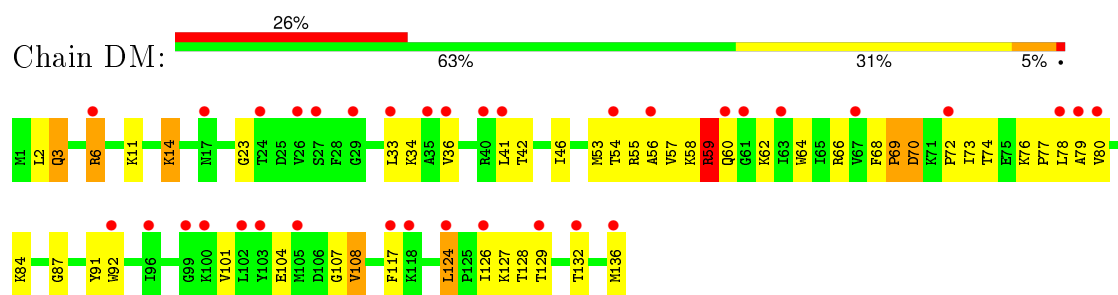
- Molecule 33: 50S ribosomal protein L15



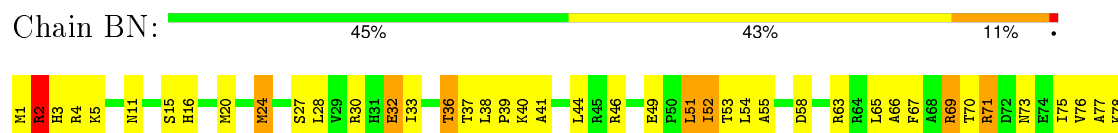
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

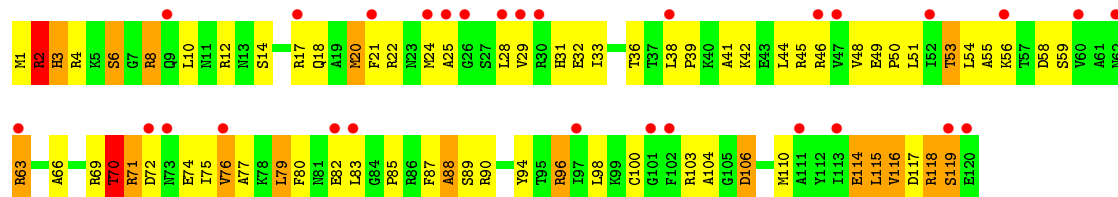


- Molecule 35: 50S ribosomal protein L17

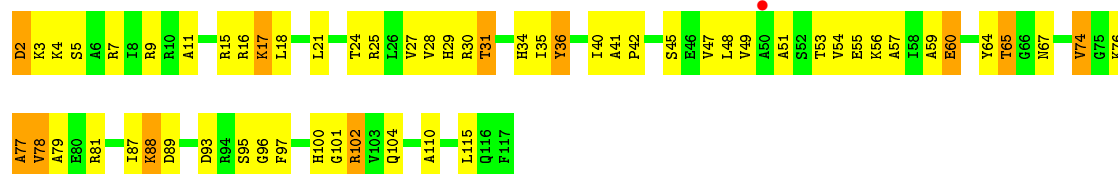




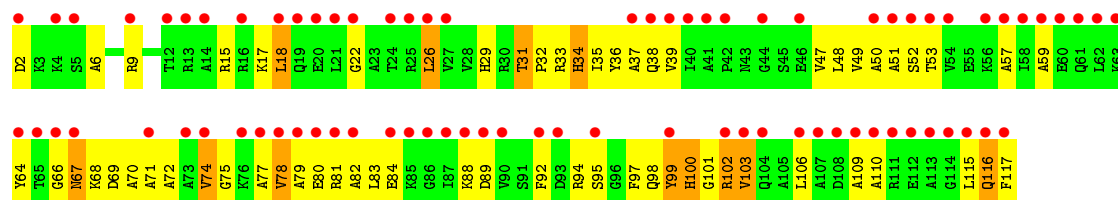
• Molecule 35: 50S ribosomal protein L17



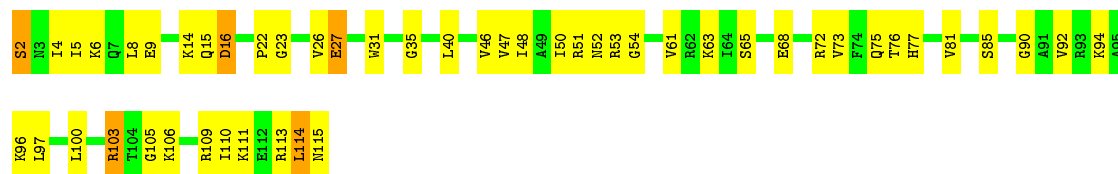
• Molecule 36: 50S ribosomal protein L18



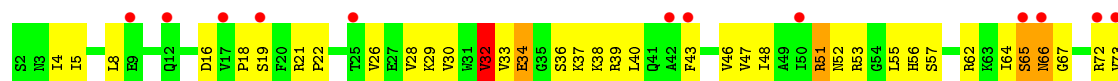
• Molecule 36: 50S ribosomal protein L18

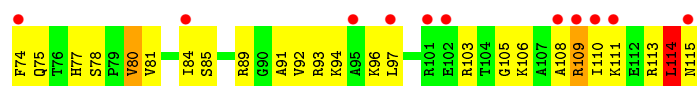


• Molecule 37: 50S ribosomal protein L19



• Molecule 37: 50S ribosomal protein L19

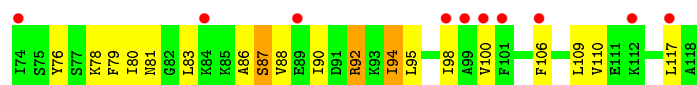
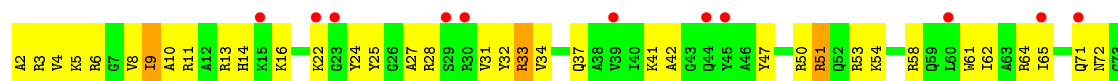




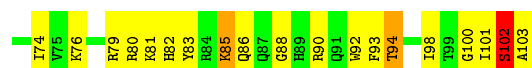
- Molecule 38: 50S ribosomal protein L20



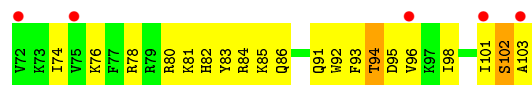
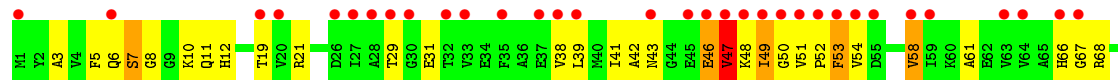
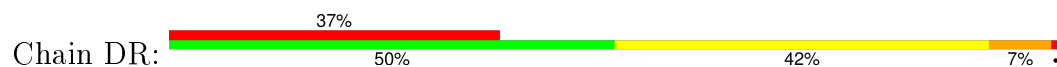
- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21

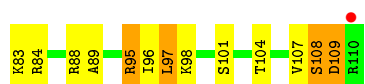


- Molecule 39: 50S ribosomal protein L21

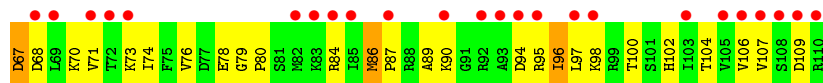
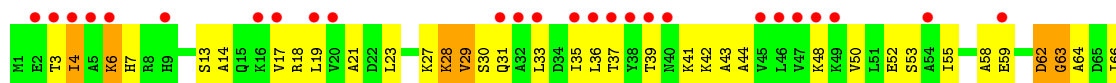


- Molecule 40: 50S ribosomal protein L22





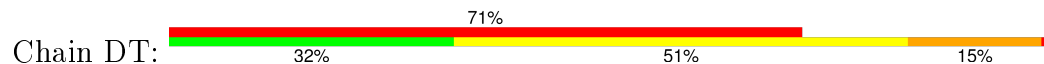
- Molecule 40: 50S ribosomal protein L22



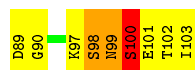
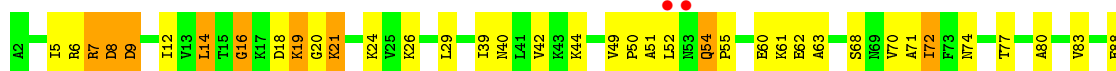
- Molecule 41: 50S ribosomal protein L23



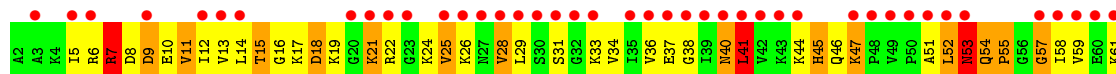
- Molecule 41: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L24

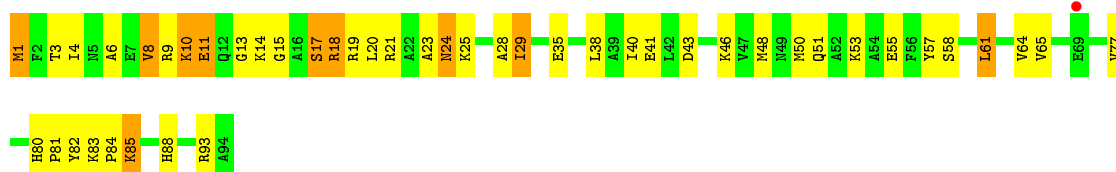


- Molecule 42: 50S ribosomal protein L24

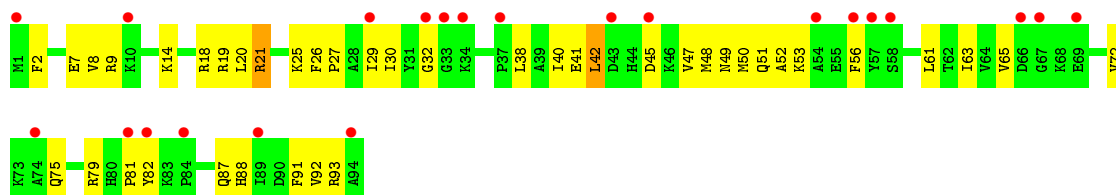




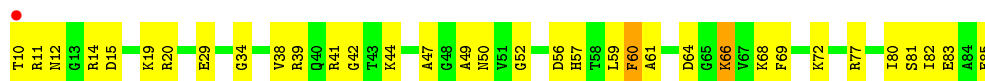
- Molecule 43: 50S ribosomal protein L25



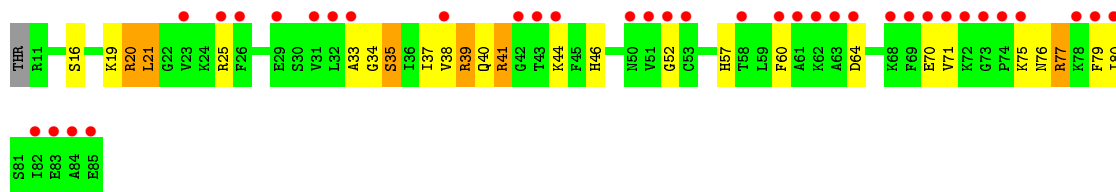
- Molecule 43: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L27



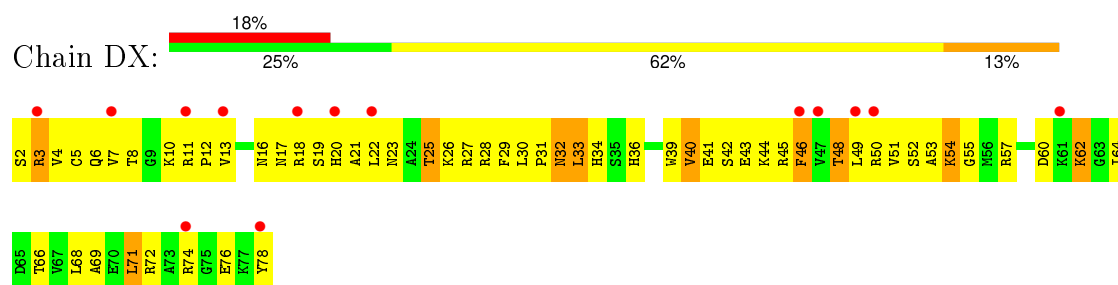
- Molecule 44: 50S ribosomal protein L27



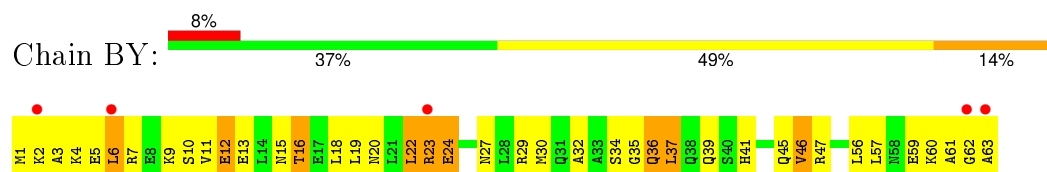
- Molecule 45: 50S ribosomal protein L28



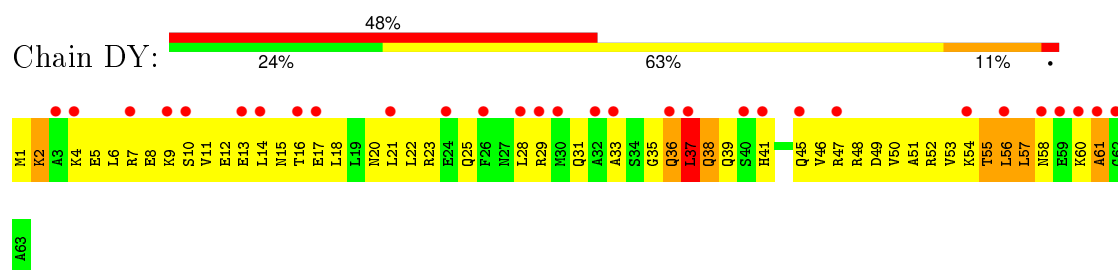
- Molecule 45: 50S ribosomal protein L28



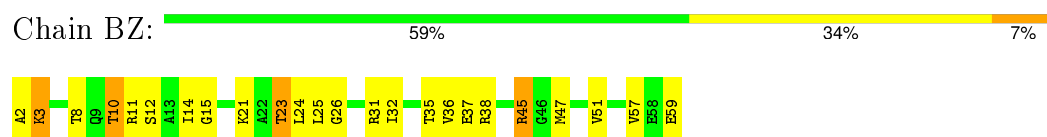
- Molecule 46: 50S ribosomal protein L29



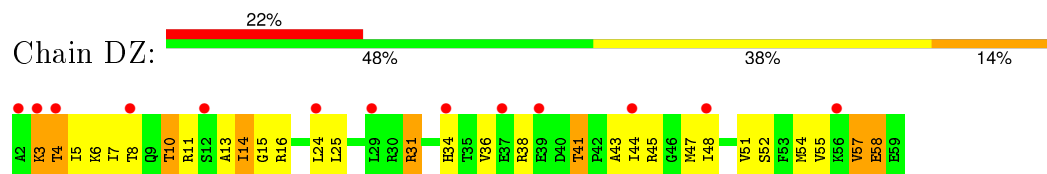
- Molecule 46: 50S ribosomal protein L29



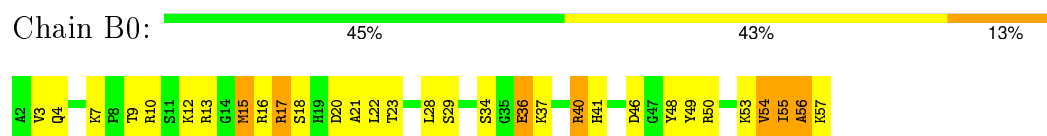
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

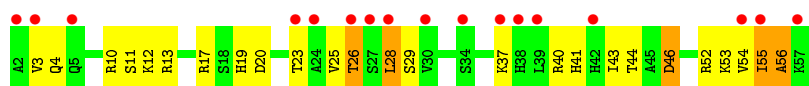


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

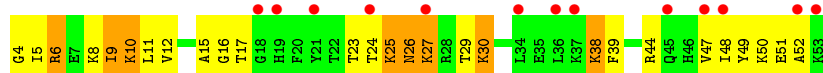




- Molecule 49: 50S ribosomal protein L33



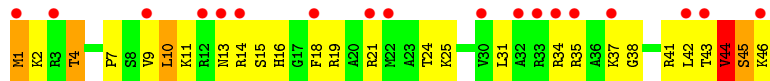
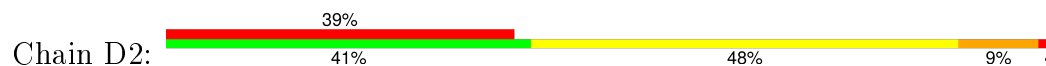
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



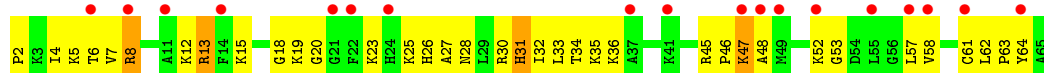
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35

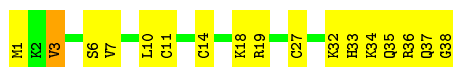


- Molecule 51: 50S ribosomal protein L35

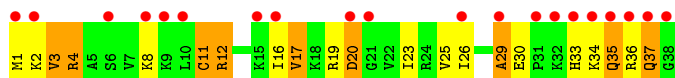


- Molecule 52: 50S ribosomal protein L36

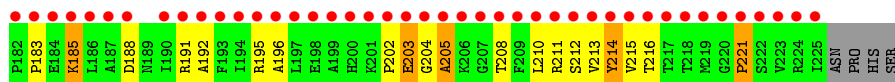
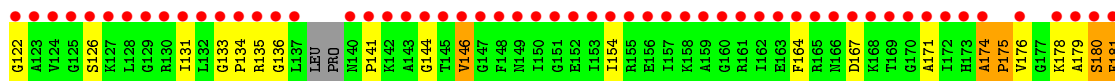
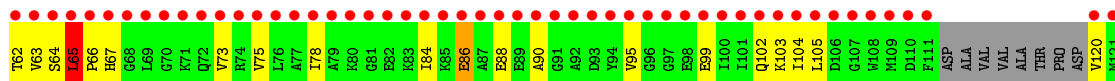
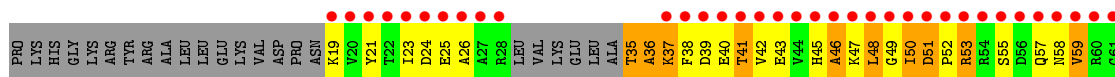
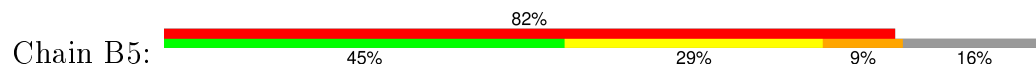




- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.79Å 433.06Å 623.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.33 – 2.90 69.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (69.33-2.90) 87.4 (69.33-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.235 , 0.279 0.245 , 0.286	Depositor DCC
R_{free} test set	4412 reflections (0.41%)	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 1093642 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	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 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, VIF, 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	0.47	0/36944	0.95	29/57632 (0.1%)
1	CA	0.40	0/36966	0.90	9/57666 (0.0%)
2	AB	0.36	0/1736	0.64	0/2338
2	CB	0.33	0/1736	0.60	0/2338
3	AC	0.35	0/1652	0.61	0/2225
3	CC	0.31	0/1652	0.57	0/2225
4	AD	0.35	0/1665	0.63	0/2227
4	CD	0.40	0/1665	0.66	0/2227
5	AE	0.39	0/1119	0.70	0/1504
5	CE	0.36	0/1119	0.70	0/1504
6	AF	0.39	0/836	0.65	0/1128
6	CF	0.33	0/836	0.63	1/1128 (0.1%)
7	AG	0.34	0/1196	0.59	0/1602
7	CG	0.32	0/1196	0.55	0/1602
8	AH	0.34	0/989	0.58	0/1326
8	CH	0.32	0/989	0.59	0/1326
9	AI	0.33	0/1034	0.62	0/1375
9	CI	0.32	0/1034	0.62	0/1375
10	AJ	0.34	0/797	0.61	0/1077
10	CJ	0.31	0/797	0.62	1/1077 (0.1%)
11	AK	0.35	0/893	0.60	0/1205
11	CK	0.34	0/893	0.60	0/1205
12	AL	0.39	0/969	0.65	0/1300
12	CL	0.36	0/969	0.70	0/1300
13	AM	0.33	0/893	0.71	1/1193 (0.1%)
13	CM	0.34	0/893	0.59	0/1193
14	AN	0.34	0/785	0.63	0/1043
14	CN	0.30	0/785	0.54	0/1043
15	AO	0.33	0/718	0.60	0/959
15	CO	0.32	0/718	0.56	0/959
16	AP	0.36	0/659	0.70	1/884 (0.1%)
16	CP	0.35	0/659	0.58	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.66	1/881 (0.1%)
17	CQ	0.36	0/658	0.61	0/881
18	AR	0.33	0/463	0.57	0/621
18	CR	0.32	0/463	0.58	0/621
19	AS	0.34	0/653	0.63	0/877
19	CS	0.33	0/653	0.54	0/877
20	AT	0.34	0/671	0.60	0/888
20	CT	0.32	0/671	0.57	0/888
21	AU	0.45	0/431	0.72	0/570
21	CU	0.45	0/431	0.73	0/570
22	BA	0.80	22/69659 (0.0%)	1.31	570/108672 (0.5%)
22	DA	0.40	0/69659	0.90	13/108672 (0.0%)
23	BB	0.68	0/2850	1.17	9/4444 (0.2%)
23	DB	0.35	0/2828	0.85	0/4410
24	BC	0.48	0/2122	0.72	0/2852
24	DC	0.34	0/2122	0.60	0/2852
25	BD	0.54	0/1586	0.78	1/2134 (0.0%)
25	DD	0.33	0/1586	0.57	0/2134
26	BE	0.46	0/1571	0.66	0/2113
26	DE	0.35	0/1571	0.59	0/2113
27	BF	0.37	0/1435	0.59	0/1926
27	DF	0.32	0/1435	0.52	0/1926
28	BG	0.37	0/1343	0.65	0/1816
28	DG	0.32	0/1343	0.53	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	0.37	0/1046	0.59	0/1410
30	DI	0.37	0/1046	0.61	0/1410
31	BJ	0.53	0/1152	0.74	1/1551 (0.1%)
31	DJ	0.32	0/1152	0.59	0/1551
32	BK	0.52	0/948	0.77	0/1268
32	DK	0.34	0/948	0.56	0/1268
33	BL	0.50	0/1054	0.81	1/1403 (0.1%)
33	DL	0.34	0/1054	0.61	0/1403
34	BM	0.53	0/1093	0.72	0/1460
34	DM	0.31	0/1093	0.54	0/1460
35	BN	0.54	0/974	0.75	0/1301
35	DN	0.35	0/974	0.58	0/1301
36	BO	0.40	0/902	0.64	0/1209
36	DO	0.30	0/902	0.51	0/1209
37	BP	0.49	0/929	0.72	1/1242 (0.1%)
37	DP	0.35	0/929	0.58	0/1242
38	BQ	0.65	0/960	0.83	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.33	0/960	0.53	0/1278
39	BR	0.60	0/829	0.79	1/1107 (0.1%)
39	DR	0.34	0/829	0.58	0/1107
40	BS	0.63	0/864	0.82	0/1156
40	DS	0.34	0/864	0.59	0/1156
41	BT	0.43	0/745	0.62	0/994
41	DT	0.35	0/745	0.60	0/994
42	BU	0.43	0/788	0.66	0/1051
42	DU	0.37	0/788	0.59	0/1051
43	BV	0.44	0/766	0.65	0/1025
43	DV	0.30	0/766	0.50	0/1025
44	BW	0.55	0/587	0.73	0/776
44	DW	0.31	0/576	0.49	0/762
45	BX	0.43	0/635	0.72	0/848
45	DX	0.34	0/635	0.60	0/848
46	BY	0.40	0/510	0.69	0/677
46	DY	0.34	0/510	0.58	0/677
47	BZ	0.55	0/453	0.82	0/605
47	DZ	0.31	0/453	0.55	0/605
48	B0	0.55	0/450	0.76	0/599
48	D0	0.35	0/450	0.61	0/599
49	B1	0.40	0/417	0.62	0/554
49	D1	0.34	0/417	0.56	0/554
50	B2	0.50	0/380	0.77	0/498
50	D2	0.36	0/380	0.59	0/498
51	B3	0.48	0/513	0.67	0/676
51	D3	0.31	0/513	0.54	0/676
52	B4	0.56	0/303	0.68	0/397
52	D4	0.46	0/303	0.64	0/397
53	B5	0.33	0/1145	0.55	0/1556
All	All	0.52	22/310626 (0.0%)	0.97	641/464366 (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
2	CB	0	1
5	CE	0	1
6	CF	0	1
11	AK	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
11	CK	0	1
12	CL	0	1
21	AU	0	2
21	CU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
47	BZ	0	1
All	All	0	13

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-9.47	1.32	1.37
22	BA	1977	A	N9-C4	-7.26	1.33	1.37
22	BA	1142	A	N9-C4	-7.11	1.33	1.37
22	BA	528	A	N7-C5	-7.06	1.35	1.39
22	BA	2071	A	N9-C4	-6.99	1.33	1.37

The worst 5 of 641 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	528	A	N1-C6-N6	13.66	126.80	118.60
25	BD	151	THR	C-N-CD	-12.30	93.53	120.60
22	BA	984	A	C2-N3-C4	-11.24	104.98	110.60
22	BA	532	A	O5'-P-OP1	-10.12	96.59	105.70
22	BA	528	A	C6-C5-N7	-9.92	125.36	132.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	Peptide
33	BL	110	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1173	4
1	CA	33015	0	16617	1168	1
2	AB	1705	0	1732	198	0
2	CB	1705	0	1732	149	0
3	AC	1625	0	1696	88	0
3	CC	1625	0	1696	94	0
4	AD	1643	0	1707	143	0
4	CD	1643	0	1707	130	0
5	AE	1106	0	1148	82	0
5	CE	1106	0	1148	115	0
6	AF	818	0	808	60	0
6	CF	818	0	808	65	0
7	AG	1182	0	1238	78	0
7	CG	1182	0	1238	57	0
8	AH	979	0	1031	64	0
8	CH	979	0	1031	54	0
9	AI	1022	0	1070	91	0
9	CI	1022	0	1070	67	0
10	AJ	787	0	828	97	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	87	0
11	CK	877	0	887	74	0
12	AL	955	0	1016	54	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	70	0
13	CM	884	0	941	56	0
14	AN	774	0	824	74	0
14	CN	774	0	824	55	0
15	AO	710	0	728	45	0
15	CO	710	0	728	46	0
16	AP	649	0	666	64	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	59	0
17	CQ	649	0	691	55	0
18	AR	456	0	478	22	0
18	CR	456	0	478	39	0
19	AS	638	0	665	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	30	0
20	AT	665	0	714	53	0
20	CT	665	0	714	48	0
21	AU	426	0	449	57	0
21	CU	426	0	449	54	0
22	BA	62195	0	31280	1960	0
22	DA	62195	0	31280	2094	1
23	BB	2549	0	1291	47	0
23	DB	2529	0	1281	64	0
24	BC	2083	0	2154	131	0
24	DC	2083	0	2154	140	0
25	BD	1565	0	1616	108	0
25	DD	1565	0	1616	85	0
26	BE	1552	0	1619	71	0
26	DE	1552	0	1619	108	0
27	BF	1411	0	1444	84	0
27	DF	1411	0	1444	53	0
28	BG	1323	0	1371	62	0
28	DG	1323	0	1371	62	0
29	BH	1110	0	1147	167	0
29	DH	1110	0	1148	93	4
30	BI	1032	0	1085	89	0
30	DI	1032	0	1085	76	0
31	BJ	1129	0	1162	45	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	48	0
32	DK	939	0	1012	35	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	71	0
34	BM	1074	0	1157	49	0
34	DM	1074	0	1157	31	0
35	BN	961	0	1000	68	0
35	DN	961	0	1000	69	0
36	BO	892	0	923	41	0
36	DO	892	0	923	48	0
37	BP	917	0	962	43	0
37	DP	917	0	962	49	0
38	BQ	947	0	1019	62	0
38	DQ	947	0	1019	56	0
39	BR	816	0	839	84	0
39	DR	816	0	839	52	0
40	BS	857	0	922	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	43	0
41	BT	739	0	807	34	0
41	DT	739	0	807	54	0
42	BU	780	0	831	35	0
42	DU	780	0	831	71	0
43	BV	753	0	780	35	0
43	DV	753	0	780	24	0
44	BW	580	0	594	21	0
44	DW	569	0	581	20	0
45	BX	625	0	652	26	0
45	DX	625	0	652	67	0
46	BY	509	0	543	36	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	20	0
47	DZ	449	0	488	16	0
48	B0	444	0	458	35	0
48	D0	444	0	458	26	0
49	B1	410	0	440	17	0
49	D1	410	0	440	19	0
50	B2	377	0	418	14	0
50	D2	377	0	418	28	0
51	B3	504	0	572	25	0
51	D3	504	0	572	31	0
52	B4	302	0	340	18	0
52	D4	302	0	342	21	0
53	B5	1142	0	865	58	0
54	AA	72	0	0	0	0
54	BA	194	0	0	0	0
54	BB	4	0	0	0	0
54	BN	1	0	0	0	0
54	CA	55	0	0	0	0
54	CM	1	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	38	5	0
55	DA	38	0	37	11	0
56	B4	1	0	0	2	0
56	D4	1	0	0	0	0
57	AA	195	0	0	29	0
57	AL	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AN	5	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	1	0
57	B3	2	0	0	0	0
57	B4	1	0	0	0	0
57	BA	620	0	0	101	0
57	BB	13	0	0	0	0
57	BC	6	0	0	4	0
57	BD	3	0	0	3	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	8	0	0	0	0
57	BN	4	0	0	0	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	19	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	0	0
57	D0	1	0	0	0	0
57	D2	3	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	613	0	0	87	0
57	DB	13	0	0	1	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	2	0	0	0	0
57	DJ	1	0	0	0	0
57	DL	3	0	0	1	0
57	DN	1	0	0	0	0
57	DT	2	0	0	0	0
57	DV	1	0	0	0	0
All	All	288258	0	192864	11506	5

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 24.

The worst 5 of 11506 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:123:ARG:NH2	1:CA:367:U:OP2	1.64	1.27
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:1153:C:OP2	57:BA:3357:HOH:O	1.59	1.19
15:AO:89:ARG:NH1	22:BA:716:A:OP2	1.75	1.19
22:BA:2574:G:OP1	57:BA:3713:HOH:O	1.61	1.18

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.71	0.49
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	1.89	0.31
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.04	0.16
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	2.10	0.10
1:CA:204:G:OP1	22:DA:289:G:O2'[3_545]	2.12	0.08

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%)	125 (58%)	36 (17%)	55 (26%)	0	0
2	CB	216/218 (99%)	126 (58%)	54 (25%)	36 (17%)	0	0
3	AC	204/206 (99%)	144 (71%)	48 (24%)	12 (6%)	2	6
3	CC	204/206 (99%)	146 (72%)	41 (20%)	17 (8%)	1	2
4	AD	203/205 (99%)	140 (69%)	38 (19%)	25 (12%)	0	1
4	CD	203/205 (99%)	148 (73%)	35 (17%)	20 (10%)	1	2
5	AE	148/150 (99%)	107 (72%)	24 (16%)	17 (12%)	0	1
5	CE	148/150 (99%)	100 (68%)	25 (17%)	23 (16%)	0	0
6	AF	98/100 (98%)	67 (68%)	17 (17%)	14 (14%)	0	0
6	CF	98/100 (98%)	65 (66%)	16 (16%)	17 (17%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	101 (68%)	33 (22%)	15 (10%)	1	2
7	CG	149/151 (99%)	120 (80%)	19 (13%)	10 (7%)	1	4
8	AH	127/129 (98%)	88 (69%)	29 (23%)	10 (8%)	1	3
8	CH	127/129 (98%)	101 (80%)	19 (15%)	7 (6%)	2	7
9	AI	125/127 (98%)	87 (70%)	23 (18%)	15 (12%)	0	1
9	CI	125/127 (98%)	91 (73%)	25 (20%)	9 (7%)	1	3
10	AJ	96/98 (98%)	63 (66%)	12 (12%)	21 (22%)	0	0
10	CJ	96/98 (98%)	72 (75%)	15 (16%)	9 (9%)	1	2
11	AK	115/117 (98%)	85 (74%)	17 (15%)	13 (11%)	0	1
11	CK	115/117 (98%)	83 (72%)	23 (20%)	9 (8%)	1	3
12	AL	121/123 (98%)	96 (79%)	15 (12%)	10 (8%)	1	2
12	CL	121/123 (98%)	92 (76%)	17 (14%)	12 (10%)	1	2
13	AM	112/114 (98%)	83 (74%)	17 (15%)	12 (11%)	0	1
13	CM	112/114 (98%)	80 (71%)	21 (19%)	11 (10%)	1	2
14	AN	92/100 (92%)	55 (60%)	25 (27%)	12 (13%)	0	1
14	CN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	0
15	AO	86/88 (98%)	63 (73%)	18 (21%)	5 (6%)	2	6
15	CO	86/88 (98%)	63 (73%)	19 (22%)	4 (5%)	3	11
16	AP	80/82 (98%)	44 (55%)	17 (21%)	19 (24%)	0	0
16	CP	80/82 (98%)	57 (71%)	18 (22%)	5 (6%)	2	5
17	AQ	78/80 (98%)	53 (68%)	16 (20%)	9 (12%)	0	1
17	CQ	78/80 (98%)	55 (70%)	14 (18%)	9 (12%)	0	1
18	AR	53/55 (96%)	44 (83%)	7 (13%)	2 (4%)	4	16
18	CR	53/55 (96%)	42 (79%)	7 (13%)	4 (8%)	1	3
19	AS	77/79 (98%)	53 (69%)	16 (21%)	8 (10%)	1	1
19	CS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	4	15
20	AT	83/85 (98%)	57 (69%)	20 (24%)	6 (7%)	1	3
20	CT	83/85 (98%)	62 (75%)	13 (16%)	8 (10%)	1	2
21	AU	49/51 (96%)	27 (55%)	10 (20%)	12 (24%)	0	0
21	CU	49/51 (96%)	24 (49%)	12 (24%)	13 (26%)	0	0
24	BC	269/271 (99%)	213 (79%)	39 (14%)	17 (6%)	2	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	200 (74%)	49 (18%)	20 (7%)	1	3
25	BD	207/209 (99%)	167 (81%)	33 (16%)	7 (3%)	5	19
25	DD	207/209 (99%)	165 (80%)	33 (16%)	9 (4%)	3	13
26	BE	199/201 (99%)	153 (77%)	39 (20%)	7 (4%)	4	18
26	DE	199/201 (99%)	146 (73%)	40 (20%)	13 (6%)	1	4
27	BF	175/177 (99%)	136 (78%)	30 (17%)	9 (5%)	2	9
27	DF	175/177 (99%)	136 (78%)	26 (15%)	13 (7%)	1	3
28	BG	174/176 (99%)	145 (83%)	19 (11%)	10 (6%)	2	6
28	DG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	2
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%)	71 (51%)	44 (32%)	24 (17%)	0	0
30	DI	139/141 (99%)	75 (54%)	49 (35%)	15 (11%)	0	1
31	BJ	140/142 (99%)	124 (89%)	12 (9%)	4 (3%)	6	23
31	DJ	140/142 (99%)	123 (88%)	12 (9%)	5 (4%)	4	18
32	BK	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	1	4
32	DK	120/122 (98%)	97 (81%)	16 (13%)	7 (6%)	2	6
33	BL	141/143 (99%)	106 (75%)	20 (14%)	15 (11%)	0	1
33	DL	141/143 (99%)	104 (74%)	27 (19%)	10 (7%)	1	3
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	13	42
34	DM	134/136 (98%)	111 (83%)	17 (13%)	6 (4%)	3	12
35	BN	118/120 (98%)	92 (78%)	19 (16%)	7 (6%)	2	6
35	DN	118/120 (98%)	91 (77%)	19 (16%)	8 (7%)	1	4
36	BO	114/116 (98%)	91 (80%)	19 (17%)	4 (4%)	4	18
36	DO	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	2	8
37	BP	112/114 (98%)	101 (90%)	6 (5%)	5 (4%)	3	12
37	DP	112/114 (98%)	89 (80%)	16 (14%)	7 (6%)	2	5
38	BQ	115/117 (98%)	93 (81%)	16 (14%)	6 (5%)	2	8
38	DQ	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	21	57
39	BR	101/103 (98%)	83 (82%)	9 (9%)	9 (9%)	1	2
39	DR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	83 (77%)	18 (17%)	7 (6%)	1	4
40	DS	108/110 (98%)	88 (82%)	13 (12%)	7 (6%)	1	4
41	BT	91/93 (98%)	69 (76%)	8 (9%)	14 (15%)	0	0
41	DT	91/93 (98%)	65 (71%)	14 (15%)	12 (13%)	0	1
42	BU	100/102 (98%)	75 (75%)	16 (16%)	9 (9%)	1	2
42	DU	100/102 (98%)	70 (70%)	19 (19%)	11 (11%)	0	1
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	17	51
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	8	31
44	BW	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
44	DW	73/76 (96%)	59 (81%)	11 (15%)	3 (4%)	3	14
45	BX	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	4	15
45	DX	75/77 (97%)	57 (76%)	14 (19%)	4 (5%)	2	8
46	BY	61/63 (97%)	35 (57%)	19 (31%)	7 (12%)	0	1
46	DY	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1	2
47	BZ	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4	18
48	B0	54/56 (96%)	44 (82%)	7 (13%)	3 (6%)	2	7
48	D0	54/56 (96%)	38 (70%)	12 (22%)	4 (7%)	1	3
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	2
49	D1	48/50 (96%)	40 (83%)	5 (10%)	3 (6%)	2	5
50	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	8	30
50	D2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	3	12
51	B3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	12	40
51	D3	62/64 (97%)	49 (79%)	10 (16%)	3 (5%)	3	10
52	B4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
52	D4	36/38 (95%)	28 (78%)	4 (11%)	4 (11%)	0	1
53	B5	183/228 (80%)	100 (55%)	49 (27%)	34 (19%)	0	0
All	All	11418/11672 (98%)	8486 (74%)	1941 (17%)	991 (9%)	1	2

5 of 991 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	16	PHE
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%)	117 (65%)	63 (35%)	0	0
2	CB	180/180 (100%)	130 (72%)	50 (28%)	0	1
3	AC	170/170 (100%)	134 (79%)	36 (21%)	1	4
3	CC	170/170 (100%)	134 (79%)	36 (21%)	1	4
4	AD	172/172 (100%)	135 (78%)	37 (22%)	1	4
4	CD	172/172 (100%)	136 (79%)	36 (21%)	1	4
5	AE	113/113 (100%)	86 (76%)	27 (24%)	1	2
5	CE	113/113 (100%)	85 (75%)	28 (25%)	1	2
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	1
6	CF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	94 (76%)	30 (24%)	1	2
7	CG	124/124 (100%)	91 (73%)	33 (27%)	0	2
8	AH	104/104 (100%)	81 (78%)	23 (22%)	1	3
8	CH	104/104 (100%)	81 (78%)	23 (22%)	1	3
9	AI	105/105 (100%)	75 (71%)	30 (29%)	0	1
9	CI	105/105 (100%)	76 (72%)	29 (28%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	2
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	4
11	AK	90/90 (100%)	67 (74%)	23 (26%)	0	2
11	CK	90/90 (100%)	71 (79%)	19 (21%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	81 (79%)	22 (21%)	1	4
12	CL	103/103 (100%)	76 (74%)	27 (26%)	0	2
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1	4
13	CM	92/92 (100%)	71 (77%)	21 (23%)	1	3
14	AN	79/83 (95%)	62 (78%)	17 (22%)	1	4
14	CN	79/83 (95%)	69 (87%)	10 (13%)	5	16
15	AO	75/76 (99%)	58 (77%)	17 (23%)	1	3
15	CO	75/76 (99%)	59 (79%)	16 (21%)	1	4
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0	1
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1	5
17	AQ	74/74 (100%)	49 (66%)	25 (34%)	0	0
17	CQ	74/74 (100%)	52 (70%)	22 (30%)	0	1
18	AR	48/48 (100%)	42 (88%)	6 (12%)	6	17
18	CR	48/48 (100%)	39 (81%)	9 (19%)	2	6
19	AS	70/70 (100%)	61 (87%)	9 (13%)	5	16
19	CS	70/70 (100%)	57 (81%)	13 (19%)	2	6
20	AT	65/65 (100%)	52 (80%)	13 (20%)	1	5
20	CT	65/65 (100%)	49 (75%)	16 (25%)	1	2
21	AU	44/44 (100%)	25 (57%)	19 (43%)	0	0
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	187 (87%)	29 (13%)	5	13
24	DC	216/216 (100%)	185 (86%)	31 (14%)	4	12
25	BD	164/164 (100%)	150 (92%)	14 (8%)	13	37
25	DD	164/164 (100%)	148 (90%)	16 (10%)	10	30
26	BE	165/165 (100%)	134 (81%)	31 (19%)	2	6
26	DE	165/165 (100%)	134 (81%)	31 (19%)	2	6
27	BF	148/148 (100%)	122 (82%)	26 (18%)	2	7
27	DF	148/148 (100%)	120 (81%)	28 (19%)	2	6
28	BG	137/137 (100%)	120 (88%)	17 (12%)	6	17
28	DG	137/137 (100%)	123 (90%)	14 (10%)	9	27
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%)	81 (74%)	28 (26%)	0	2
30	DI	109/109 (100%)	86 (79%)	23 (21%)	1	4
31	BJ	116/116 (100%)	97 (84%)	19 (16%)	3	8
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	13
32	BK	103/103 (100%)	86 (84%)	17 (16%)	3	8
32	DK	103/103 (100%)	91 (88%)	12 (12%)	7	19
33	BL	102/102 (100%)	83 (81%)	19 (19%)	2	6
33	DL	102/102 (100%)	78 (76%)	24 (24%)	1	2
34	BM	109/109 (100%)	96 (88%)	13 (12%)	6	19
34	DM	109/109 (100%)	98 (90%)	11 (10%)	9	28
35	BN	100/100 (100%)	85 (85%)	15 (15%)	3	11
35	DN	100/100 (100%)	82 (82%)	18 (18%)	2	6
36	BO	86/86 (100%)	68 (79%)	18 (21%)	1	4
36	DO	86/86 (100%)	70 (81%)	16 (19%)	2	6
37	BP	99/99 (100%)	91 (92%)	8 (8%)	15	39
37	DP	99/99 (100%)	82 (83%)	17 (17%)	2	7
38	BQ	89/89 (100%)	77 (86%)	12 (14%)	5	13
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	8
39	BR	84/84 (100%)	71 (84%)	13 (16%)	3	10
39	DR	84/84 (100%)	74 (88%)	10 (12%)	6	19
40	BS	93/93 (100%)	75 (81%)	18 (19%)	2	5
40	DS	93/93 (100%)	80 (86%)	13 (14%)	4	12
41	BT	80/80 (100%)	70 (88%)	10 (12%)	6	17
41	DT	80/80 (100%)	67 (84%)	13 (16%)	3	8
42	BU	83/83 (100%)	71 (86%)	12 (14%)	4	12
42	DU	83/83 (100%)	63 (76%)	20 (24%)	1	2
43	BV	78/78 (100%)	63 (81%)	15 (19%)	2	5
43	DV	78/78 (100%)	68 (87%)	10 (13%)	5	16
44	BW	57/58 (98%)	49 (86%)	8 (14%)	4	12
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%)	57 (85%)	10 (15%)	4	11
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	6
46	BY	55/55 (100%)	48 (87%)	7 (13%)	5	16
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3
47	BZ	48/48 (100%)	38 (79%)	10 (21%)	1	4
47	DZ	48/48 (100%)	37 (77%)	11 (23%)	1	3
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	11
48	D0	47/47 (100%)	41 (87%)	6 (13%)	5	16
49	B1	45/45 (100%)	41 (91%)	4 (9%)	12	35
49	D1	45/45 (100%)	37 (82%)	8 (18%)	2	6
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	6
50	D2	38/38 (100%)	31 (82%)	7 (18%)	2	6
51	B3	51/51 (100%)	45 (88%)	6 (12%)	6	19
51	D3	51/51 (100%)	45 (88%)	6 (12%)	6	19
52	B4	34/34 (100%)	31 (91%)	3 (9%)	12	35
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	4
All	All	9386/9518 (99%)	7568 (81%)	1818 (19%)	2	5

5 of 1818 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	29	LEU
4	CD	56	ARG
39	DR	46	GLU
44	BW	60	PHE
2	CB	18	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	CC	176	HIS
13	CM	91	HIS
46	DY	41	HIS
5	CE	89	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	CM	105	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	349 (22%)	15 (0%)
1	CA	1538/1539 (99%)	331 (21%)	9 (0%)
22	BA	2895/2903 (99%)	643 (22%)	30 (1%)
22	DA	2895/2903 (99%)	637 (22%)	29 (1%)
23	BB	118/119 (99%)	21 (17%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2006 (22%)	83 (0%)

5 of 2006 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 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2127	G
1	CA	209	U
22	DA	2308	G
22	BA	2211	A
22	BA	2326	C

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	VIF	BA	3001	-	35,40,40	2.57	13 (37%)	41,55,55	1.87	9 (21%)
55	VIF	DA	3001	-	35,40,40	2.53	11 (31%)	41,55,55	2.13	14 (34%)

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

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3001	VIF	F-C07	-6.39	1.25	1.41
55	BA	3001	VIF	F-C07	-6.01	1.26	1.41
55	BA	3001	VIF	O01-C06	-4.79	1.37	1.44
55	BA	3001	VIF	C11-C09	-4.52	1.43	1.53
55	BA	3001	VIF	O01-C08	-4.28	1.24	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3001	VIF	C17-N02-C03	-5.55	115.49	121.76
55	BA	3001	VIF	C18-C10-C20	-4.82	118.40	125.75
55	DA	3001	VIF	C18-C10-C20	-4.36	119.09	125.75
55	DA	3001	VIF	C17-C18-C10	-4.19	113.05	125.31
55	DA	3001	VIF	O-C03-N02	-4.06	117.31	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3001	VIF	5	0
55	DA	3001	VIF	11	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.01	37 (2%) 62 57	13, 51, 135, 177	0
1	CA	1539/1539 (100%)	0.25	72 (4%) 35 29	27, 71, 143, 176	0
2	AB	218/218 (100%)	1.05	43 (19%) 1 1	40, 71, 99, 129	0
2	CB	218/218 (100%)	1.44	65 (29%) 1 0	57, 81, 107, 126	0
3	AC	206/206 (100%)	0.23	9 (4%) 38 32	36, 57, 81, 94	0
3	CC	206/206 (100%)	1.36	47 (22%) 1 0	53, 75, 93, 113	0
4	AD	205/205 (100%)	0.37	13 (6%) 23 17	33, 55, 79, 108	0
4	CD	205/205 (100%)	0.18	8 (3%) 43 36	21, 40, 74, 90	0
5	AE	150/150 (100%)	0.25	7 (4%) 35 29	28, 50, 82, 111	0
5	CE	150/150 (100%)	0.50	9 (6%) 25 18	33, 57, 84, 105	0
6	AF	100/100 (100%)	0.03	1 (1%) 84 82	33, 56, 75, 84	0
6	CF	100/100 (100%)	0.54	8 (8%) 15 10	47, 72, 95, 105	0
7	AG	151/151 (100%)	0.85	27 (17%) 2 1	49, 74, 98, 107	0
7	CG	151/151 (100%)	2.59	87 (57%) 0 0	77, 94, 106, 113	0
8	AH	129/129 (100%)	0.21	2 (1%) 74 72	29, 48, 71, 80	0
8	CH	129/129 (100%)	0.62	11 (8%) 13 8	47, 63, 82, 88	0
9	AI	127/127 (100%)	1.01	22 (17%) 2 1	45, 70, 95, 115	0
9	CI	127/127 (100%)	1.77	47 (37%) 0 0	68, 88, 106, 130	0
10	AJ	98/98 (100%)	0.89	16 (16%) 2 1	44, 64, 93, 121	0
10	CJ	98/98 (100%)	2.69	58 (59%) 0 0	68, 90, 109, 123	0
11	AK	117/117 (100%)	0.69	15 (12%) 5 3	27, 61, 87, 107	0
11	CK	117/117 (100%)	0.45	6 (5%) 32 25	37, 65, 83, 90	0
12	AL	123/123 (100%)	0.30	5 (4%) 41 34	24, 37, 71, 101	0
12	CL	123/123 (100%)	0.54	10 (8%) 15 9	38, 51, 79, 102	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%)	0.52	10 (8%) 12 8	46, 67, 90, 104	0
13	CM	114/114 (100%)	3.14	80 (70%) 0 0	84, 100, 114, 118	0
14	AN	96/100 (96%)	0.80	17 (17%) 2 1	41, 58, 92, 107	0
14	CN	96/100 (96%)	2.32	50 (52%) 0 0	64, 88, 107, 118	0
15	AO	88/88 (100%)	0.17	5 (5%) 27 21	31, 50, 66, 98	0
15	CO	88/88 (100%)	0.40	4 (4%) 37 31	39, 62, 84, 105	0
16	AP	82/82 (100%)	0.79	9 (10%) 7 4	33, 45, 80, 103	0
16	CP	82/82 (100%)	1.36	21 (25%) 1 0	44, 62, 89, 105	0
17	AQ	80/80 (100%)	0.56	6 (7%) 17 11	29, 54, 83, 123	0
17	CQ	80/80 (100%)	1.45	26 (32%) 1 0	41, 70, 96, 108	0
18	AR	55/55 (100%)	0.04	4 (7%) 18 12	37, 51, 76, 113	0
18	CR	55/55 (100%)	0.47	3 (5%) 29 22	39, 54, 82, 112	0
19	AS	79/79 (100%)	1.10	17 (21%) 1 0	46, 67, 92, 97	0
19	CS	79/79 (100%)	4.33	61 (77%) 0 0	82, 100, 113, 125	0
20	AT	85/85 (100%)	0.71	7 (8%) 14 9	33, 48, 72, 115	0
20	CT	85/85 (100%)	2.01	35 (41%) 0 0	53, 69, 91, 97	0
21	AU	51/51 (100%)	1.28	15 (29%) 1 0	45, 71, 92, 105	0
21	CU	51/51 (100%)	0.71	8 (15%) 3 1	42, 69, 92, 107	0
22	BA	2897/2903 (99%)	0.23	121 (4%) 40 33	2, 18, 128, 195	0
22	DA	2897/2903 (99%)	0.42	145 (5%) 32 26	44, 82, 142, 183	0
23	BB	119/119 (100%)	-0.25	0 100 100	5, 27, 53, 94	0
23	DB	118/119 (99%)	0.25	4 (3%) 49 41	68, 110, 132, 142	0
24	BC	271/271 (100%)	-0.04	1 (0%) 93 92	6, 24, 44, 62	0
24	DC	271/271 (100%)	0.95	43 (15%) 3 1	40, 61, 75, 83	0
25	BD	209/209 (100%)	-0.14	0 100 100	2, 14, 42, 69	0
25	DD	209/209 (100%)	1.06	40 (19%) 2 1	47, 65, 84, 98	0
26	BE	201/201 (100%)	-0.15	2 (0%) 84 82	4, 27, 55, 94	0
26	DE	201/201 (100%)	1.92	82 (40%) 0 0	38, 78, 97, 108	0
27	BF	177/177 (100%)	0.32	9 (5%) 32 25	23, 45, 85, 101	0
27	DF	177/177 (100%)	3.55	140 (79%) 0 0	80, 99, 114, 125	0
28	BG	176/176 (100%)	0.17	5 (2%) 56 50	21, 40, 66, 93	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%)	2.43	101 (57%) 0 0	68, 87, 103, 118	0
29	BH	149/149 (100%)	3.59	95 (63%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.85	61 (40%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.69	96 (68%) 0 0	82, 105, 120, 135	0
30	DI	141/141 (100%)	5.40	132 (93%) 0 0	95, 111, 121, 124	0
31	BJ	142/142 (100%)	-0.19	0 100 100	2, 11, 33, 52	0
31	DJ	142/142 (100%)	1.08	30 (21%) 1 1	50, 65, 81, 97	0
32	BK	122/122 (100%)	-0.26	0 100 100	6, 18, 37, 68	0
32	DK	122/122 (100%)	1.04	25 (20%) 1 1	46, 61, 80, 94	0
33	BL	143/143 (100%)	-0.06	0 100 100	3, 24, 50, 81	0
33	DL	143/143 (100%)	2.13	69 (48%) 0 0	45, 74, 91, 111	0
34	BM	136/136 (100%)	-0.22	0 100 100	3, 14, 33, 93	0
34	DM	136/136 (100%)	1.21	35 (25%) 1 0	44, 66, 82, 109	0
35	BN	120/120 (100%)	-0.22	0 100 100	6, 13, 25, 68	0
35	DN	120/120 (100%)	1.44	29 (24%) 1 0	53, 71, 88, 111	0
36	BO	116/116 (100%)	-0.03	1 (0%) 85 84	19, 29, 51, 57	0
36	DO	116/116 (100%)	3.12	78 (67%) 0 0	70, 88, 102, 113	0
37	BP	114/114 (100%)	-0.09	0 100 100	11, 21, 49, 73	0
37	DP	114/114 (100%)	1.08	23 (20%) 1 1	54, 67, 84, 91	0
38	BQ	117/117 (100%)	-0.18	0 100 100	3, 8, 19, 51	0
38	DQ	117/117 (100%)	0.92	21 (17%) 2 1	51, 65, 79, 82	0
39	BR	103/103 (100%)	-0.13	1 (0%) 84 82	3, 17, 36, 65	0
39	DR	103/103 (100%)	1.70	38 (36%) 0 0	52, 73, 87, 96	0
40	BS	110/110 (100%)	-0.11	1 (0%) 85 84	3, 8, 28, 88	0
40	DS	110/110 (100%)	2.06	50 (45%) 0 0	56, 70, 88, 96	0
41	BT	93/93 (100%)	0.33	2 (2%) 65 60	13, 30, 83, 101	0
41	DT	93/93 (100%)	3.00	66 (70%) 0 0	62, 81, 103, 109	0
42	BU	102/102 (100%)	-0.09	2 (1%) 68 64	13, 31, 60, 95	0
42	DU	102/102 (100%)	3.59	64 (62%) 0 0	66, 84, 105, 111	0
43	BV	94/94 (100%)	-0.12	1 (1%) 82 80	10, 24, 47, 58	0
43	DV	94/94 (100%)	1.15	22 (23%) 1 0	65, 79, 94, 97	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%)	-0.07	1 (1%) 79 78	9, 17, 38, 57	0
44	DW	75/76 (98%)	2.20	36 (48%) 0 0	51, 77, 88, 108	0
45	BX	77/77 (100%)	-0.19	1 (1%) 79 78	10, 26, 52, 79	0
45	DX	77/77 (100%)	1.01	14 (18%) 2 1	47, 67, 84, 89	0
46	BY	63/63 (100%)	0.41	5 (7%) 15 10	20, 44, 71, 96	0
46	DY	63/63 (100%)	2.10	30 (47%) 0 0	68, 88, 96, 103	0
47	BZ	58/58 (100%)	-0.13	0 100 100	6, 11, 36, 41	0
47	DZ	58/58 (100%)	0.99	13 (22%) 1 0	52, 70, 83, 88	0
48	B0	56/56 (100%)	-0.18	0 100 100	3, 14, 40, 75	0
48	D0	56/56 (100%)	1.41	17 (30%) 1 0	51, 71, 91, 105	0
49	B1	50/50 (100%)	-0.07	1 (2%) 68 64	20, 32, 58, 92	0
49	D1	50/50 (100%)	1.70	13 (26%) 1 0	64, 80, 92, 104	0
50	B2	46/46 (100%)	0.02	1 (2%) 65 60	7, 13, 20, 95	0
50	D2	46/46 (100%)	1.85	18 (39%) 0 0	51, 66, 79, 99	0
51	B3	64/64 (100%)	-0.08	0 100 100	9, 15, 25, 33	0
51	D3	64/64 (100%)	1.50	18 (28%) 1 0	54, 68, 79, 83	0
52	B4	38/38 (100%)	0.07	0 100 100	15, 22, 37, 55	0
52	D4	38/38 (100%)	2.24	20 (52%) 0 0	59, 72, 84, 97	0
53	B5	191/228 (83%)	6.59	186 (97%) 0 0	78, 108, 120, 133	0
All	All	20734/20794 (99%)	0.75	3012 (14%) 3 2	2, 62, 117, 195	0

The worst 5 of 3012 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	2	ALA	21.3
30	DI	3	LYS	19.1
22	BA	2104	C	18.1
30	BI	53	LEU	17.7
53	B5	111	PHE	17.6

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	3171	1/1	0.75	0.32	25.86	34,34,34,34	0
54	MG	DA	3059	1/1	0.82	0.48	16.92	63,63,63,63	0
54	MG	BA	3133	1/1	0.93	0.30	15.99	48,48,48,48	0
54	MG	BA	3145	1/1	0.82	0.37	15.65	37,37,37,37	0
54	MG	BA	3042	1/1	0.90	0.35	12.45	7,7,7,7	0
54	MG	DA	3003	1/1	0.81	0.40	11.03	65,65,65,65	0
54	MG	DA	3073	1/1	0.61	0.45	11.00	76,76,76,76	0
54	MG	DA	3154	1/1	0.77	0.58	10.23	63,63,63,63	0
54	MG	BA	3187	1/1	0.93	0.27	8.62	16,16,16,16	0
54	MG	BA	3176	1/1	0.96	0.30	8.20	15,15,15,15	0
54	MG	DA	3070	1/1	0.79	0.27	6.58	69,69,69,69	0
54	MG	DA	3061	1/1	0.85	0.35	5.75	69,69,69,69	0
54	MG	BA	3110	1/1	0.91	0.24	5.49	4,4,4,4	0
54	MG	DA	3140	1/1	0.98	0.30	5.07	36,36,36,36	0
54	MG	AA	1622	1/1	0.97	0.22	4.92	17,17,17,17	0
54	MG	AA	1644	1/1	0.94	0.30	4.91	41,41,41,41	0
54	MG	AA	1655	1/1	0.90	0.22	4.89	50,50,50,50	0
54	MG	DA	3029	1/1	0.39	0.32	3.48	63,63,63,63	0
54	MG	BA	3162	1/1	0.94	0.23	3.43	17,17,17,17	0
55	VIF	BA	3001	38/38	0.96	0.21	3.27	3,9,14,18	0
54	MG	DA	3125	1/1	0.58	0.43	3.24	76,76,76,76	0
54	MG	DA	3065	1/1	0.91	0.23	3.10	46,46,46,46	0
54	MG	BA	3029	1/1	0.90	0.26	3.04	38,38,38,38	0
54	MG	DA	3049	1/1	0.56	0.35	3.03	84,84,84,84	0
54	MG	CA	1615	1/1	0.72	0.19	3.00	38,38,38,38	0
54	MG	BA	3051	1/1	0.97	0.22	2.78	11,11,11,11	0
54	MG	DA	3111	1/1	0.89	0.23	2.66	45,45,45,45	0
54	MG	DA	3042	1/1	0.59	0.27	2.21	67,67,67,67	0
54	MG	BA	3179	1/1	0.98	0.21	2.10	7,7,7,7	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	3152	1/1	0.82	0.35	1.99	54,54,54,54	0
54	MG	DA	3155	1/1	0.92	0.17	1.68	43,43,43,43	0
54	MG	DA	3106	1/1	0.79	0.22	1.65	61,61,61,61	0
54	MG	BA	3085	1/1	0.85	0.17	1.29	29,29,29,29	0
54	MG	BA	3160	1/1	0.98	0.18	1.22	16,16,16,16	0
54	MG	DA	3072	1/1	0.61	0.23	1.20	63,63,63,63	0
55	VIF	DA	3001	38/38	0.92	0.26	1.09	40,51,59,60	0
54	MG	CM	201	1/1	0.93	0.29	0.91	50,50,50,50	0
54	MG	BA	3065	1/1	0.90	0.19	0.90	2,2,2,2	0
54	MG	DA	3112	1/1	0.93	0.18	0.83	67,67,67,67	0
54	MG	CA	1640	1/1	0.92	0.17	0.78	22,22,22,22	0
54	MG	CA	1612	1/1	0.94	0.12	0.71	43,43,43,43	0
54	MG	DA	3051	1/1	0.95	0.19	0.66	43,43,43,43	0
54	MG	BA	3118	1/1	0.96	0.19	0.64	7,7,7,7	0
54	MG	DA	3130	1/1	0.96	0.18	0.59	35,35,35,35	0
54	MG	CA	1630	1/1	0.75	0.36	0.53	81,81,81,81	0
54	MG	DA	3158	1/1	0.94	0.22	0.51	46,46,46,46	0
54	MG	DA	3110	1/1	0.98	0.19	0.20	36,36,36,36	0
54	MG	BA	3075	1/1	0.83	0.19	-0.01	3,3,3,3	0
54	MG	DA	3009	1/1	0.83	0.19	-0.04	62,62,62,62	0
54	MG	BA	3014	1/1	0.94	0.18	-0.13	0,0,0,0	0
54	MG	DA	3146	1/1	0.85	0.17	-0.17	54,54,54,54	0
54	MG	BA	3132	1/1	0.95	0.18	-0.26	2,2,2,2	0
54	MG	AA	1617	1/1	0.79	0.18	-0.28	55,55,55,55	0
54	MG	DA	3019	1/1	0.76	0.20	-0.30	66,66,66,66	0
54	MG	DA	3013	1/1	0.95	0.20	-0.44	40,40,40,40	0
54	MG	DA	3116	1/1	0.87	0.24	-0.49	64,64,64,64	0
54	MG	AA	1663	1/1	0.84	0.15	-0.63	51,51,51,51	0
54	MG	BA	3064	1/1	0.93	0.17	-0.70	0,0,0,0	0
54	MG	BA	3116	1/1	0.84	0.17	-0.70	29,29,29,29	0
54	MG	DA	3014	1/1	0.58	0.16	-0.74	59,59,59,59	0
54	MG	DA	3117	1/1	0.95	0.14	-0.75	54,54,54,54	0
54	MG	BA	3164	1/1	0.95	0.14	-0.90	27,27,27,27	0
54	MG	AA	1636	1/1	0.93	0.12	-0.91	31,31,31,31	0
54	MG	DA	3079	1/1	0.78	0.12	-0.92	74,74,74,74	0
54	MG	DA	3133	1/1	0.89	0.13	-0.93	51,51,51,51	0
54	MG	DA	3048	1/1	0.69	0.17	-0.99	59,59,59,59	0
54	MG	CA	1614	1/1	0.85	0.08	-1.02	45,45,45,45	0
54	MG	BA	3006	1/1	0.96	0.13	-1.03	46,46,46,46	0
54	MG	BA	3081	1/1	0.94	0.14	-1.05	28,28,28,28	0
54	MG	DA	3137	1/1	0.34	0.14	-1.15	69,69,69,69	0
54	MG	DA	3040	1/1	0.92	0.16	-1.15	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	ZN	B4	101	1/1	0.98	0.14	-1.17	102,102,102,102	0
54	MG	DA	3064	1/1	0.96	0.15	-1.23	43,43,43,43	0
54	MG	BA	3134	1/1	0.85	0.11	-1.29	32,32,32,32	0
54	MG	CA	1632	1/1	0.93	0.14	-1.31	66,66,66,66	0
54	MG	DB	201	1/1	0.84	0.12	-1.32	83,83,83,83	0
56	ZN	D4	101	1/1	0.98	0.10	-1.35	78,78,78,78	0
54	MG	AA	1607	1/1	0.94	0.10	-1.37	47,47,47,47	0
54	MG	BA	3152	1/1	0.93	0.15	-1.46	27,27,27,27	0
54	MG	BA	3098	1/1	0.97	0.15	-1.49	5,5,5,5	0
54	MG	DA	3129	1/1	0.70	0.10	-1.52	65,65,65,65	0
54	MG	BA	3013	1/1	0.97	0.16	-1.67	3,3,3,3	0
54	MG	DA	3033	1/1	0.83	0.15	-1.80	53,53,53,53	0
54	MG	DA	3023	1/1	0.95	0.13	-2.00	36,36,36,36	0
54	MG	DA	3099	1/1	0.93	0.09	-2.10	37,37,37,37	0
54	MG	BA	3070	1/1	0.97	0.16	-2.10	0,0,0,0	0
54	MG	BA	3099	1/1	0.97	0.14	-2.15	5,5,5,5	0
54	MG	BA	3073	1/1	0.88	0.16	-2.17	30,30,30,30	0
54	MG	DA	3135	1/1	0.68	0.12	-2.22	41,41,41,41	0
54	MG	CA	1621	1/1	0.81	0.12	-2.22	63,63,63,63	0
54	MG	BB	201	1/1	0.96	0.09	-2.23	20,20,20,20	0
54	MG	AA	1629	1/1	0.93	0.12	-2.34	42,42,42,42	0
54	MG	BA	3049	1/1	0.82	0.10	-2.34	37,37,37,37	0
54	MG	AA	1616	1/1	0.86	0.10	-2.39	57,57,57,57	0
54	MG	BA	3185	1/1	0.96	0.14	-2.41	16,16,16,16	0
54	MG	DA	3098	1/1	0.96	0.08	-2.61	46,46,46,46	0
54	MG	DA	3024	1/1	0.89	0.08	-2.63	63,63,63,63	0
54	MG	DA	3044	1/1	0.90	0.10	-2.70	54,54,54,54	0
54	MG	CA	1616	1/1	0.86	0.12	-2.82	31,31,31,31	0
54	MG	BA	3055	1/1	0.98	0.14	-2.83	5,5,5,5	0
54	MG	DA	3026	1/1	0.90	0.09	-2.88	43,43,43,43	0
54	MG	CA	1635	1/1	0.23	0.15	-2.90	91,91,91,91	0
54	MG	CA	1603	1/1	0.95	0.12	-2.97	43,43,43,43	0
54	MG	BA	3137	1/1	0.87	0.14	-3.02	44,44,44,44	0
54	MG	BA	3111	1/1	0.96	0.13	-3.03	0,0,0,0	0
54	MG	BA	3018	1/1	0.87	0.15	-3.08	4,4,4,4	0
54	MG	BA	3038	1/1	0.90	0.13	-3.11	30,30,30,30	0
54	MG	BA	3009	1/1	0.90	0.16	-3.11	10,10,10,10	0
54	MG	DA	3018	1/1	0.93	0.14	-3.15	53,53,53,53	0
54	MG	BA	3026	1/1	0.96	0.11	-3.22	9,9,9,9	0
54	MG	BA	3136	1/1	0.96	0.14	-3.27	1,1,1,1	0
54	MG	BA	3024	1/1	0.98	0.13	-3.30	5,5,5,5	0
54	MG	BA	3025	1/1	0.89	0.11	-3.33	4,4,4,4	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	AA	1641	1/1	0.90	0.11	-3.36	16,16,16,16	0
54	MG	DA	3060	1/1	0.94	0.10	-3.36	43,43,43,43	0
54	MG	DA	3081	1/1	0.93	0.09	-3.41	67,67,67,67	0
54	MG	BA	3103	1/1	0.96	0.15	-3.41	0,0,0,0	0
54	MG	AA	1630	1/1	0.87	0.11	-3.41	53,53,53,53	0
54	MG	DA	3107	1/1	0.81	0.12	-3.50	47,47,47,47	0
54	MG	BA	3189	1/1	0.95	0.09	-3.58	25,25,25,25	0
54	MG	CA	1610	1/1	0.89	0.10	-3.58	57,57,57,57	0
54	MG	AA	1642	1/1	0.94	0.10	-3.59	21,21,21,21	0
54	MG	DA	3025	1/1	0.64	0.10	-3.72	40,40,40,40	0
54	MG	AA	1633	1/1	0.97	0.14	-3.78	29,29,29,29	0
54	MG	BA	3115	1/1	0.95	0.16	-3.85	11,11,11,11	0
54	MG	BA	3010	1/1	0.97	0.12	-3.93	3,3,3,3	0
54	MG	BA	3068	1/1	0.90	0.14	-3.94	8,8,8,8	0
54	MG	DA	3006	1/1	0.57	0.12	-3.96	76,76,76,76	0
54	MG	DA	3097	1/1	0.93	0.06	-4.00	49,49,49,49	0
54	MG	BA	3107	1/1	0.82	0.15	-4.02	1,1,1,1	0
54	MG	CA	1607	1/1	0.94	0.10	-4.33	46,46,46,46	0
54	MG	BA	3037	1/1	0.98	0.14	-4.36	1,1,1,1	0
54	MG	BA	3109	1/1	0.99	0.12	-4.37	20,20,20,20	0
54	MG	CA	1626	1/1	0.76	0.08	-4.37	48,48,48,48	0
54	MG	DA	3052	1/1	0.95	0.08	-4.51	32,32,32,32	0
54	MG	DA	3055	1/1	0.97	0.10	-4.56	48,48,48,48	0
54	MG	AA	1606	1/1	0.93	0.08	-4.62	36,36,36,36	0
54	MG	CA	1601	1/1	0.95	0.09	-4.66	34,34,34,34	0
54	MG	BA	3156	1/1	0.96	0.10	-4.69	17,17,17,17	0
54	MG	AA	1612	1/1	0.84	0.13	-4.81	33,33,33,33	0
54	MG	DA	3028	1/1	0.76	0.08	-4.96	62,62,62,62	0
54	MG	BA	3030	1/1	0.94	0.11	-5.09	4,4,4,4	0
54	MG	BA	3153	1/1	0.97	0.13	-5.09	15,15,15,15	0
54	MG	DA	3121	1/1	0.93	0.07	-5.21	54,54,54,54	0
54	MG	DA	3067	1/1	0.89	0.08	-5.38	48,48,48,48	0
54	MG	AA	1618	1/1	0.89	0.08	-5.38	41,41,41,41	0
54	MG	BA	3040	1/1	0.95	0.14	-5.40	3,3,3,3	0
54	MG	CA	1617	1/1	0.81	0.08	-5.47	33,33,33,33	0
54	MG	BA	3114	1/1	0.99	0.06	-5.64	18,18,18,18	0
54	MG	BA	3166	1/1	0.94	0.09	-5.73	6,6,6,6	0
54	MG	BA	3052	1/1	0.96	0.07	-5.96	8,8,8,8	0
54	MG	BA	3122	1/1	0.95	0.11	-6.41	10,10,10,10	0
54	MG	AA	1613	1/1	0.95	0.08	-6.44	25,25,25,25	0
54	MG	BA	3060	1/1	0.97	0.06	-6.50	16,16,16,16	0
54	MG	BA	3067	1/1	0.92	0.11	-6.64	4,4,4,4	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	1622	1/1	0.86	0.06	-6.69	53,53,53,53	0
54	MG	CA	1619	1/1	0.92	0.07	-7.36	30,30,30,30	0
54	MG	BA	3131	1/1	0.97	0.14	-7.70	0,0,0,0	0
54	MG	DA	3075	1/1	0.90	0.05	-8.35	47,47,47,47	0
54	MG	AA	1609	1/1	0.96	0.06	-8.51	28,28,28,28	0
54	MG	AA	1604	1/1	0.82	0.07	-9.60	43,43,43,43	0
54	MG	BA	3072	1/1	0.92	0.08	-11.63	6,6,6,6	0
54	MG	BA	3112	1/1	0.95	0.08	-11.99	16,16,16,16	0
54	MG	AA	1625	1/1	0.90	0.06	-12.61	35,35,35,35	0
54	MG	BA	3003	1/1	0.98	0.04	-21.02	19,19,19,19	0
54	MG	DA	3036	1/1	0.89	0.18	-	65,65,65,65	0
54	MG	AA	1648	1/1	0.98	0.16	-	54,54,54,54	0
54	MG	BA	3170	1/1	0.89	0.15	-	29,29,29,29	0
54	MG	DA	3016	1/1	0.88	0.76	-	65,65,65,65	0
54	MG	BA	3015	1/1	0.72	0.15	-	22,22,22,22	0
54	MG	BA	3090	1/1	0.97	0.12	-	28,28,28,28	0
54	MG	BA	3084	1/1	0.96	0.06	-	10,10,10,10	0
54	MG	BA	3108	1/1	0.97	0.16	-	0,0,0,0	0
54	MG	DA	3087	1/1	0.94	0.12	-	48,48,48,48	0
54	MG	DA	3094	1/1	0.48	0.40	-	78,78,78,78	0
54	MG	CA	1644	1/1	0.83	0.17	-	38,38,38,38	0
54	MG	AA	1602	1/1	0.85	0.15	-	40,40,40,40	0
54	MG	BA	3086	1/1	0.96	0.10	-	10,10,10,10	0
54	MG	DA	3131	1/1	0.93	0.12	-	58,58,58,58	0
54	MG	BA	3088	1/1	0.93	0.21	-	8,8,8,8	0
54	MG	CA	1638	1/1	0.78	0.10	-	54,54,54,54	0
54	MG	BA	3007	1/1	0.92	0.15	-	17,17,17,17	0
54	MG	BA	3039	1/1	0.96	0.20	-	2,2,2,2	0
54	MG	DA	3054	1/1	0.95	0.16	-	40,40,40,40	0
54	MG	AA	1623	1/1	0.79	0.06	-	42,42,42,42	0
54	MG	BA	3172	1/1	0.91	0.14	-	22,22,22,22	0
54	MG	DA	3120	1/1	0.66	0.56	-	80,80,80,80	0
54	MG	BA	3139	1/1	0.92	0.34	-	0,0,0,0	0
54	MG	BA	3101	1/1	0.86	0.10	-	8,8,8,8	0
54	MG	CA	1642	1/1	0.91	0.19	-	31,31,31,31	0
54	MG	AA	1672	1/1	0.76	0.33	-	40,40,40,40	0
54	MG	CA	1631	1/1	0.70	0.17	-	76,76,76,76	0
54	MG	BA	3161	1/1	0.91	0.18	-	19,19,19,19	0
54	MG	DA	3050	1/1	0.86	0.23	-	58,58,58,58	0
54	MG	BA	3149	1/1	0.97	0.15	-	26,26,26,26	0
54	MG	BA	3168	1/1	0.93	0.17	-	32,32,32,32	0
54	MG	BA	3091	1/1	0.97	0.10	-	4,4,4,4	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	1655	1/1	0.86	0.30	-	53,53,53,53	0
54	MG	BA	3180	1/1	0.92	0.17	-	10,10,10,10	0
54	MG	CA	1636	1/1	0.74	0.27	-	92,92,92,92	0
54	MG	BA	3063	1/1	0.96	0.20	-	41,41,41,41	0
54	MG	CA	1648	1/1	0.92	0.20	-	45,45,45,45	0
54	MG	BA	3020	1/1	0.95	0.09	-	24,24,24,24	0
54	MG	DA	3022	1/1	0.83	0.18	-	50,50,50,50	0
54	MG	CA	1628	1/1	0.72	0.29	-	70,70,70,70	0
54	MG	AA	1615	1/1	0.94	0.07	-	43,43,43,43	0
54	MG	BA	3117	1/1	0.94	0.28	-	40,40,40,40	0
54	MG	AA	1626	1/1	0.88	0.11	-	24,24,24,24	0
54	MG	AA	1634	1/1	0.94	0.11	-	40,40,40,40	0
54	MG	BA	3102	1/1	0.92	0.12	-	10,10,10,10	0
54	MG	BA	3048	1/1	0.92	0.09	-	25,25,25,25	0
54	MG	BA	3008	1/1	0.94	0.09	-	29,29,29,29	0
54	MG	AA	1646	1/1	0.99	0.10	-	39,39,39,39	0
54	MG	DA	3012	1/1	0.82	0.24	-	54,54,54,54	0
54	MG	DA	3062	1/1	0.86	1.26	-	73,73,73,73	0
54	MG	BA	3050	1/1	0.78	0.08	-	15,15,15,15	0
54	MG	DA	3167	1/1	0.92	0.12	-	39,39,39,39	0
54	MG	DA	3091	1/1	0.88	0.07	-	55,55,55,55	0
54	MG	BA	3096	1/1	0.99	0.06	-	17,17,17,17	0
54	MG	DA	3030	1/1	0.80	0.26	-	61,61,61,61	0
54	MG	DA	3126	1/1	0.91	0.17	-	51,51,51,51	0
54	MG	DB	203	1/1	0.86	0.05	-	70,70,70,70	0
54	MG	AA	1654	1/1	0.96	0.21	-	25,25,25,25	0
54	MG	CA	1606	1/1	0.94	0.08	-	49,49,49,49	0
54	MG	BA	3059	1/1	0.90	0.30	-	23,23,23,23	0
54	MG	DA	3165	1/1	0.97	0.05	-	46,46,46,46	0
54	MG	BA	3150	1/1	0.98	0.26	-	0,0,0,0	0
54	MG	DA	3166	1/1	0.95	0.31	-	41,41,41,41	0
54	MG	DA	3143	1/1	0.96	0.18	-	28,28,28,28	0
54	MG	CA	1641	1/1	0.78	0.49	-	59,59,59,59	0
54	MG	DA	3088	1/1	0.78	0.07	-	53,53,53,53	0
54	MG	DA	3104	1/1	0.79	0.34	-	59,59,59,59	0
54	MG	BA	3167	1/1	0.85	0.27	-	35,35,35,35	0
54	MG	DA	3100	1/1	0.77	0.53	-	68,68,68,68	0
54	MG	DA	3043	1/1	0.64	0.34	-	68,68,68,68	0
54	MG	CA	1618	1/1	0.82	0.16	-	38,38,38,38	0
54	MG	DA	3102	1/1	0.75	0.08	-	49,49,49,49	0
54	MG	BA	3017	1/1	0.94	0.10	-	9,9,9,9	0
54	MG	AA	1621	1/1	0.93	0.06	-	30,30,30,30	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	3045	1/1	0.99	0.07	-	14,14,14,14	0
54	MG	DA	3149	1/1	0.85	0.22	-	53,53,53,53	0
54	MG	BA	3142	1/1	0.97	0.30	-	1,1,1,1	0
54	MG	DA	3082	1/1	0.93	0.09	-	42,42,42,42	0
54	MG	AA	1639	1/1	0.94	0.06	-	56,56,56,56	0
54	MG	AA	1631	1/1	0.80	0.08	-	39,39,39,39	0
54	MG	DA	3056	1/1	0.86	0.10	-	52,52,52,52	0
54	MG	BA	3074	1/1	0.90	0.14	-	3,3,3,3	0
54	MG	BA	3036	1/1	0.94	0.18	-	9,9,9,9	0
54	MG	BA	3016	1/1	0.79	0.38	-	67,67,67,67	0
54	MG	DA	3034	1/1	0.93	0.06	-	54,54,54,54	0
54	MG	DA	3045	1/1	0.71	0.19	-	68,68,68,68	0
54	MG	DA	3004	1/1	0.88	0.08	-	58,58,58,58	0
54	MG	BA	3177	1/1	0.92	0.14	-	13,13,13,13	0
54	MG	BA	3163	1/1	0.88	0.18	-	31,31,31,31	0
54	MG	BA	3158	1/1	0.98	0.25	-	17,17,17,17	0
54	MG	BA	3165	1/1	0.97	0.23	-	9,9,9,9	0
54	MG	DA	3151	1/1	0.90	0.33	-	53,53,53,53	0
54	MG	DA	3103	1/1	0.90	0.09	-	45,45,45,45	0
54	MG	AA	1624	1/1	0.92	0.05	-	30,30,30,30	0
54	MG	BA	3129	1/1	0.90	0.09	-	7,7,7,7	0
54	MG	AA	1643	1/1	0.98	0.13	-	12,12,12,12	0
54	MG	DA	3138	1/1	0.91	0.28	-	42,42,42,42	0
54	MG	BA	3077	1/1	0.96	0.18	-	11,11,11,11	0
54	MG	BA	3069	1/1	0.94	0.17	-	2,2,2,2	0
54	MG	DA	3039	1/1	0.81	0.13	-	54,54,54,54	0
54	MG	BA	3105	1/1	0.96	0.11	-	9,9,9,9	0
54	MG	DA	3108	1/1	0.93	0.07	-	60,60,60,60	0
54	MG	BB	203	1/1	0.88	0.07	-	6,6,6,6	0
54	MG	DA	3153	1/1	0.86	0.11	-	56,56,56,56	0
54	MG	CA	1627	1/1	0.80	0.29	-	69,69,69,69	0
54	MG	AA	1649	1/1	0.95	0.11	-	34,34,34,34	0
54	MG	DA	3142	1/1	0.91	0.19	-	30,30,30,30	0
54	MG	DA	3096	1/1	0.94	0.22	-	62,62,62,62	0
54	MG	BA	3066	1/1	0.94	0.12	-	6,6,6,6	0
54	MG	DA	3010	1/1	0.94	0.13	-	57,57,57,57	0
54	MG	AA	1637	1/1	0.98	0.10	-	17,17,17,17	0
54	MG	BA	3071	1/1	0.98	0.11	-	45,45,45,45	0
54	MG	DA	3163	1/1	0.77	0.35	-	49,49,49,49	0
54	MG	BA	3147	1/1	0.96	0.23	-	25,25,25,25	0
54	MG	BA	3094	1/1	0.96	0.23	-	23,23,23,23	0
54	MG	BA	3157	1/1	0.96	0.14	-	7,7,7,7	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	AA	1614	1/1	0.80	0.18	-	52,52,52,52	0
54	MG	DA	3063	1/1	0.96	0.46	-	52,52,52,52	0
54	MG	BA	3044	1/1	0.95	0.14	-	4,4,4,4	0
54	MG	BA	3054	1/1	0.95	0.15	-	6,6,6,6	0
54	MG	BA	3113	1/1	0.91	0.14	-	30,30,30,30	0
54	MG	BA	3138	1/1	0.96	0.39	-	8,8,8,8	0
54	MG	BA	3021	1/1	0.92	0.21	-	0,0,0,0	0
54	MG	BA	3046	1/1	0.89	0.13	-	13,13,13,13	0
54	MG	AA	1666	1/1	0.98	0.37	-	25,25,25,25	0
54	MG	DA	3144	1/1	0.76	1.42	-	57,57,57,57	0
54	MG	BA	3192	1/1	0.94	0.17	-	22,22,22,22	0
54	MG	DQ	201	1/1	0.96	0.34	-	36,36,36,36	0
54	MG	CA	1646	1/1	0.87	0.17	-	40,40,40,40	0
54	MG	DA	3160	1/1	0.95	0.15	-	47,47,47,47	0
54	MG	DA	3084	1/1	0.95	0.06	-	50,50,50,50	0
54	MG	DA	3105	1/1	0.63	0.09	-	57,57,57,57	0
54	MG	BA	3127	1/1	0.85	0.17	-	7,7,7,7	0
54	MG	DA	3134	1/1	0.12	0.63	-	75,75,75,75	0
54	MG	AA	1670	1/1	0.86	0.31	-	50,50,50,50	0
54	MG	DA	3027	1/1	0.70	0.44	-	60,60,60,60	0
54	MG	AA	1668	1/1	0.88	0.21	-	41,41,41,41	0
54	MG	CA	1629	1/1	0.95	0.07	-	67,67,67,67	0
54	MG	BA	3082	1/1	0.86	0.10	-	12,12,12,12	0
54	MG	AA	1669	1/1	0.92	0.15	-	28,28,28,28	0
54	MG	DA	3058	1/1	0.73	0.30	-	65,65,65,65	0
54	MG	BA	3093	1/1	0.90	0.06	-	43,43,43,43	0
54	MG	CA	1651	1/1	0.95	0.05	-	54,54,54,54	0
54	MG	DA	3090	1/1	0.85	0.41	-	66,66,66,66	0
54	MG	BA	3047	1/1	0.81	0.15	-	19,19,19,19	0
54	MG	DA	3124	1/1	0.93	0.12	-	52,52,52,52	0
54	MG	CA	1609	1/1	0.96	0.04	-	57,57,57,57	0
54	MG	BA	3141	1/1	0.94	0.17	-	8,8,8,8	0
54	MG	BA	3011	1/1	0.99	0.11	-	3,3,3,3	0
54	MG	BA	3005	1/1	0.96	0.05	-	32,32,32,32	0
54	MG	DA	3101	1/1	0.90	0.18	-	54,54,54,54	0
54	MG	BA	3169	1/1	0.71	0.34	-	25,25,25,25	0
54	MG	DA	3089	1/1	0.66	0.10	-	57,57,57,57	0
54	MG	BA	3135	1/1	0.85	0.21	-	46,46,46,46	0
54	MG	BA	3155	1/1	0.91	0.18	-	37,37,37,37	0
54	MG	BA	3148	1/1	0.96	0.23	-	0,0,0,0	0
54	MG	AA	1601	1/1	0.84	0.15	-	53,53,53,53	0
54	MG	DA	3127	1/1	0.83	0.13	-	59,59,59,59	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	3068	1/1	0.94	0.10	-	43,43,43,43	0
54	MG	AA	1608	1/1	0.91	0.15	-	20,20,20,20	0
54	MG	CA	1652	1/1	0.87	0.10	-	45,45,45,45	0
54	MG	DA	3066	1/1	0.91	0.11	-	40,40,40,40	0
54	MG	BA	3106	1/1	0.96	0.18	-	3,3,3,3	0
54	MG	BA	3053	1/1	0.97	0.15	-	6,6,6,6	0
54	MG	DA	3122	1/1	0.94	0.07	-	42,42,42,42	0
54	MG	BA	3195	1/1	0.81	0.16	-	31,31,31,31	0
54	MG	BA	3190	1/1	0.93	0.20	-	19,19,19,19	0
54	MG	CA	1649	1/1	0.79	0.28	-	48,48,48,48	0
54	MG	DA	3015	1/1	0.65	0.12	-	57,57,57,57	0
54	MG	DA	3053	1/1	0.94	0.07	-	44,44,44,44	0
54	MG	BA	3056	1/1	0.97	0.12	-	7,7,7,7	0
54	MG	CA	1637	1/1	0.93	0.26	-	52,52,52,52	0
54	MG	CA	1602	1/1	0.74	0.10	-	69,69,69,69	0
54	MG	DA	3035	1/1	0.58	0.20	-	52,52,52,52	0
54	MG	CA	1611	1/1	0.20	0.21	-	68,68,68,68	0
54	MG	AA	1653	1/1	0.90	0.15	-	40,40,40,40	0
54	MG	BA	3182	1/1	0.94	0.12	-	26,26,26,26	0
54	MG	CA	1650	1/1	0.80	0.31	-	45,45,45,45	0
54	MG	AA	1645	1/1	0.72	0.48	-	41,41,41,41	0
54	MG	AA	1652	1/1	0.96	0.24	-	28,28,28,28	0
54	MG	AA	1658	1/1	0.70	0.50	-	47,47,47,47	0
54	MG	AA	1620	1/1	0.92	0.04	-	51,51,51,51	0
54	MG	DA	3047	1/1	0.65	0.12	-	60,60,60,60	0
54	MG	CA	1645	1/1	0.94	0.12	-	50,50,50,50	0
54	MG	DA	3041	1/1	0.75	0.13	-	62,62,62,62	0
54	MG	BA	3123	1/1	0.97	0.10	-	17,17,17,17	0
54	MG	BA	3062	1/1	0.90	0.43	-	36,36,36,36	0
54	MG	BA	3174	1/1	0.82	0.22	-	24,24,24,24	0
54	MG	CA	1654	1/1	0.85	0.23	-	40,40,40,40	0
54	MG	CA	1633	1/1	0.83	0.48	-	61,61,61,61	0
54	MG	DA	3038	1/1	0.80	0.17	-	74,74,74,74	0
54	MG	BA	3043	1/1	0.97	0.14	-	11,11,11,11	0
54	MG	DA	3161	1/1	0.88	0.22	-	39,39,39,39	0
54	MG	DA	3007	1/1	0.36	0.19	-	84,84,84,84	0
54	MG	BA	3027	1/1	0.83	0.15	-	47,47,47,47	0
54	MG	BA	3089	1/1	0.95	0.07	-	13,13,13,13	0
54	MG	AA	1667	1/1	0.86	0.27	-	47,47,47,47	0
54	MG	AA	1671	1/1	0.94	0.32	-	37,37,37,37	0
54	MG	AA	1619	1/1	0.97	0.19	-	44,44,44,44	0
54	MG	BA	3019	1/1	0.98	0.10	-	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	3113	1/1	0.91	0.27	-	56,56,56,56	0
54	MG	AA	1651	1/1	0.96	0.44	-	36,36,36,36	0
54	MG	CA	1647	1/1	0.95	0.20	-	19,19,19,19	0
54	MG	AA	1665	1/1	0.93	0.15	-	48,48,48,48	0
54	MG	CA	1608	1/1	0.93	0.26	-	56,56,56,56	0
54	MG	AA	1640	1/1	0.93	0.08	-	41,41,41,41	0
54	MG	AA	1662	1/1	0.94	0.14	-	25,25,25,25	0
54	MG	BB	204	1/1	0.88	0.35	-	15,15,15,15	0
54	MG	DA	3114	1/1	0.83	0.14	-	57,57,57,57	0
54	MG	CA	1634	1/1	0.93	0.12	-	55,55,55,55	0
54	MG	AA	1647	1/1	0.79	0.30	-	40,40,40,40	0
54	MG	DA	3159	1/1	0.92	0.14	-	57,57,57,57	0
54	MG	DA	3086	1/1	0.88	0.12	-	61,61,61,61	0
54	MG	BA	3146	1/1	0.91	0.23	-	12,12,12,12	0
54	MG	DA	3128	1/1	0.92	0.10	-	61,61,61,61	0
54	MG	BA	3022	1/1	0.97	0.12	-	3,3,3,3	0
54	MG	CA	1613	1/1	0.90	0.14	-	16,16,16,16	0
54	MG	BA	3058	1/1	0.95	0.11	-	11,11,11,11	0
54	MG	BA	3032	1/1	0.98	0.25	-	6,6,6,6	0
54	MG	BA	3144	1/1	0.94	0.27	-	14,14,14,14	0
54	MG	BA	3092	1/1	0.84	0.11	-	20,20,20,20	0
54	MG	AA	1656	1/1	0.85	0.26	-	43,43,43,43	0
54	MG	AA	1610	1/1	0.96	0.18	-	53,53,53,53	0
54	MG	DA	3069	1/1	0.98	0.08	-	56,56,56,56	0
54	MG	BA	3100	1/1	0.83	0.18	-	52,52,52,52	0
54	MG	DA	3109	1/1	0.88	0.11	-	54,54,54,54	0
54	MG	BA	3012	1/1	0.94	0.06	-	17,17,17,17	0
54	MG	BA	3078	1/1	0.92	0.21	-	26,26,26,26	0
54	MG	AA	1603	1/1	0.90	0.18	-	48,48,48,48	0
54	MG	BA	3083	1/1	0.98	0.15	-	0,0,0,0	0
54	MG	DA	3017	1/1	0.65	0.36	-	65,65,65,65	0
54	MG	DA	3147	1/1	0.83	0.17	-	45,45,45,45	0
54	MG	DA	3078	1/1	0.81	0.17	-	64,64,64,64	0
54	MG	DA	3145	1/1	0.81	0.07	-	60,60,60,60	0
54	MG	BA	3181	1/1	0.87	0.25	-	8,8,8,8	0
54	MG	BA	3004	1/1	0.92	0.11	-	24,24,24,24	0
54	MG	CA	1605	1/1	0.77	0.16	-	57,57,57,57	0
54	MG	BB	202	1/1	0.95	0.09	-	12,12,12,12	0
54	MG	BA	3061	1/1	0.94	0.20	-	22,22,22,22	0
54	MG	BA	3057	1/1	0.84	0.40	-	37,37,37,37	0
54	MG	DA	3083	1/1	0.89	0.11	-	52,52,52,52	0
54	MG	DA	3141	1/1	0.95	0.40	-	39,39,39,39	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	AA	1661	1/1	0.90	0.16	-	49,49,49,49	0
54	MG	BA	3193	1/1	0.74	0.50	-	10,10,10,10	0
54	MG	CA	1625	1/1	0.91	0.15	-	26,26,26,26	0
54	MG	BA	3031	1/1	0.77	0.13	-	10,10,10,10	0
54	MG	BA	3095	1/1	0.96	0.07	-	26,26,26,26	0
54	MG	BA	3194	1/1	0.96	0.15	-	4,4,4,4	0
54	MG	DA	3132	1/1	0.34	0.92	-	83,83,83,83	0
54	MG	DA	3032	1/1	0.92	0.12	-	46,46,46,46	0
54	MG	CA	1639	1/1	0.89	0.12	-	32,32,32,32	0
54	MG	BA	3140	1/1	0.96	0.27	-	0,0,0,0	0
54	MG	BA	3028	1/1	0.97	0.11	-	4,4,4,4	0
54	MG	BA	3151	1/1	0.91	0.32	-	44,44,44,44	0
54	MG	DA	3071	1/1	0.94	0.13	-	75,75,75,75	0
54	MG	DA	3164	1/1	0.90	0.22	-	50,50,50,50	0
54	MG	DA	3076	1/1	0.88	0.10	-	55,55,55,55	0
54	MG	BA	3034	1/1	0.94	0.14	-	20,20,20,20	0
54	MG	CA	1604	1/1	0.62	0.22	-	80,80,80,80	0
54	MG	AA	1638	1/1	0.71	0.13	-	57,57,57,57	0
54	MG	DA	3031	1/1	0.91	0.26	-	49,49,49,49	0
54	MG	DA	3119	1/1	0.85	0.09	-	52,52,52,52	0
54	MG	DA	3005	1/1	0.76	0.43	-	76,76,76,76	0
54	MG	DA	3011	1/1	0.79	0.08	-	65,65,65,65	0
54	MG	DA	3118	1/1	0.91	0.06	-	56,56,56,56	0
54	MG	BA	3079	1/1	0.87	0.06	-	30,30,30,30	0
54	MG	CA	1620	1/1	0.94	0.07	-	49,49,49,49	0
54	MG	DA	3046	1/1	0.78	0.12	-	72,72,72,72	0
54	MG	BA	3173	1/1	0.86	0.27	-	24,24,24,24	0
54	MG	BA	3124	1/1	0.95	0.22	-	0,0,0,0	0
54	MG	DA	3162	1/1	0.96	0.09	-	56,56,56,56	0
54	MG	BA	3184	1/1	0.94	0.20	-	21,21,21,21	0
54	MG	DA	3008	1/1	0.79	0.46	-	70,70,70,70	0
54	MG	AA	1664	1/1	0.91	0.19	-	30,30,30,30	0
54	MG	DA	3021	1/1	0.92	0.16	-	50,50,50,50	0
54	MG	BA	3125	1/1	0.97	0.21	-	6,6,6,6	0
54	MG	DA	3093	1/1	0.48	0.46	-	79,79,79,79	0
54	MG	DA	3157	1/1	0.83	0.21	-	42,42,42,42	0
54	MG	CA	1623	1/1	0.97	0.15	-	42,42,42,42	0
54	MG	DA	3095	1/1	0.74	0.13	-	75,75,75,75	0
54	MG	BA	3002	1/1	0.93	0.08	-	15,15,15,15	0
54	MG	DA	3148	1/1	0.75	0.20	-	47,47,47,47	0
54	MG	DA	3150	1/1	0.89	0.27	-	41,41,41,41	0
54	MG	BA	3104	1/1	0.82	0.14	-	16,16,16,16	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	3085	1/1	0.71	0.20	-	72,72,72,72	0
54	MG	AA	1611	1/1	0.96	0.09	-	25,25,25,25	0
54	MG	AA	1605	1/1	0.91	0.19	-	36,36,36,36	0
54	MG	BA	3023	1/1	0.97	0.15	-	0,0,0,0	0
54	MG	DA	3139	1/1	0.94	0.46	-	35,35,35,35	0
54	MG	DA	3020	1/1	0.83	0.24	-	75,75,75,75	0
54	MG	DA	3057	1/1	0.97	0.31	-	62,62,62,62	0
54	MG	DA	3115	1/1	0.87	0.14	-	45,45,45,45	0
54	MG	BA	3033	1/1	0.96	0.10	-	15,15,15,15	0
54	MG	BA	3076	1/1	0.93	0.06	-	29,29,29,29	0
54	MG	BA	3087	1/1	0.93	0.14	-	0,0,0,0	0
54	MG	BA	3143	1/1	0.93	0.20	-	7,7,7,7	0
54	MG	DA	3156	1/1	0.88	0.30	-	44,44,44,44	0
54	MG	BA	3128	1/1	0.97	0.15	-	5,5,5,5	0
54	MG	BA	3154	1/1	0.76	0.28	-	11,11,11,11	0
54	MG	DA	3037	1/1	0.95	0.12	-	46,46,46,46	0
54	MG	BA	3178	1/1	0.95	0.09	-	27,27,27,27	0
54	MG	AA	1635	1/1	0.92	0.14	-	49,49,49,49	0
54	MG	AA	1659	1/1	0.93	0.15	-	43,43,43,43	0
54	MG	BA	3159	1/1	0.97	0.15	-	25,25,25,25	0
54	MG	BA	3130	1/1	0.97	0.20	-	4,4,4,4	0
54	MG	AA	1657	1/1	0.99	0.07	-	28,28,28,28	0
54	MG	DA	3092	1/1	0.80	0.09	-	60,60,60,60	0
54	MG	BA	3041	1/1	0.98	0.15	-	7,7,7,7	0
54	MG	BA	3097	1/1	0.94	0.06	-	18,18,18,18	0
54	MG	BA	3186	1/1	0.93	0.15	-	10,10,10,10	0
54	MG	CA	1624	1/1	0.88	0.11	-	33,33,33,33	0
54	MG	AA	1650	1/1	0.91	0.15	-	31,31,31,31	0
54	MG	D2	101	1/1	0.70	0.16	-	63,63,63,63	0
54	MG	BA	3120	1/1	0.88	0.08	-	24,24,24,24	0
54	MG	AA	1628	1/1	0.85	0.10	-	45,45,45,45	0
54	MG	DA	3077	1/1	0.98	0.13	-	56,56,56,56	0
54	MG	DA	3136	1/1	0.30	0.25	-	67,67,67,67	0
54	MG	BA	3191	1/1	0.78	0.23	-	43,43,43,43	0
54	MG	AA	1632	1/1	0.94	0.11	-	41,41,41,41	0
54	MG	BA	3121	1/1	0.91	0.23	-	50,50,50,50	0
54	MG	BA	3126	1/1	0.86	0.26	-	25,25,25,25	0
54	MG	BN	201	1/1	0.97	0.06	-	6,6,6,6	0
54	MG	CA	1653	1/1	0.80	0.25	-	48,48,48,48	0
54	MG	DA	3002	1/1	0.83	0.09	-	52,52,52,52	0
54	MG	BA	3035	1/1	0.83	0.14	-	4,4,4,4	0
54	MG	DA	3074	1/1	0.85	0.11	-	49,49,49,49	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	3080	1/1	0.78	0.11	-	79,79,79,79	0
54	MG	AA	1660	1/1	0.87	0.54	-	38,38,38,38	0
54	MG	BA	3188	1/1	0.92	0.21	-	19,19,19,19	0
54	MG	BA	3183	1/1	0.97	0.13	-	20,20,20,20	0
54	MG	CA	1643	1/1	0.92	0.39	-	54,54,54,54	0
54	MG	BA	3119	1/1	0.95	0.07	-	9,9,9,9	0
54	MG	AA	1627	1/1	0.49	0.22	-	50,50,50,50	0
54	MG	BA	3080	1/1	0.83	0.06	-	50,50,50,50	0
54	MG	BA	3175	1/1	0.96	0.11	-	11,11,11,11	0
54	MG	DB	202	1/1	0.94	0.08	-	49,49,49,49	0
54	MG	DA	3123	1/1	0.98	0.16	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.