



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:56 PM GMT

PDB ID : 4V7T
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-14
Resolution : 3.19 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

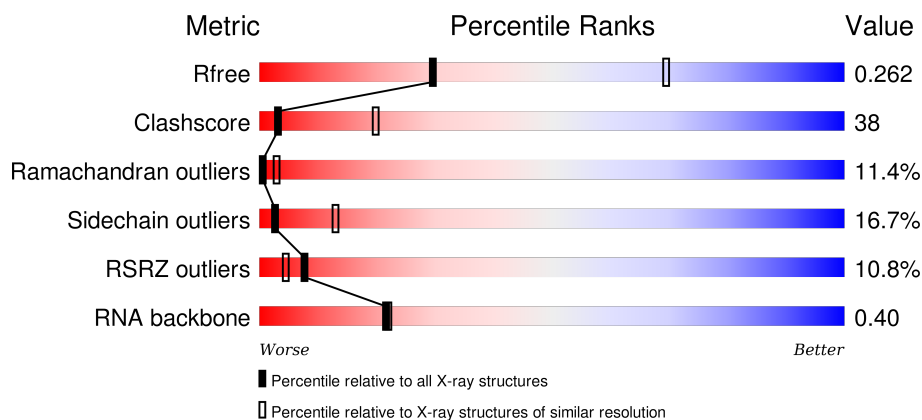
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1533	<div> <div>24%</div> <div>44%</div> <div>16%</div> <div>17%</div> </div>
2	AB	218	<div> <div>33%</div> <div>25%</div> <div>54%</div> <div>18%</div> <div>•</div> </div>
2	CB	218	<div> <div>20%</div> <div>30%</div> <div>54%</div> <div>14%</div> <div>•</div> </div>
3	AC	206	<div> <div>6%</div> <div>36%</div> <div>52%</div> <div>10%</div> <div>•</div> </div>



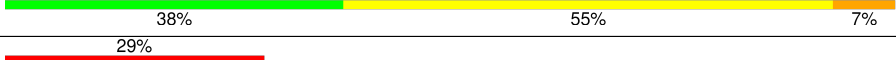

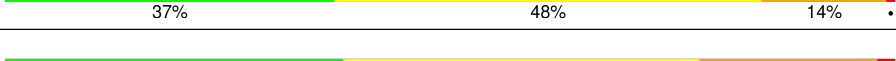
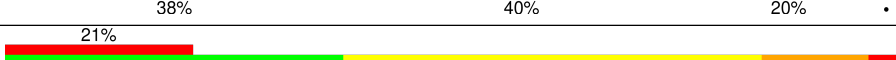
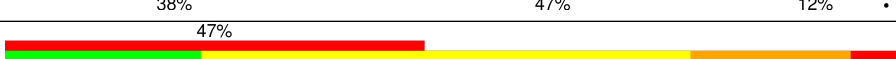
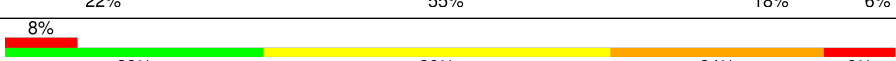
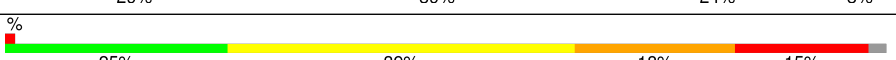
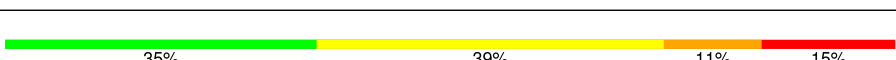
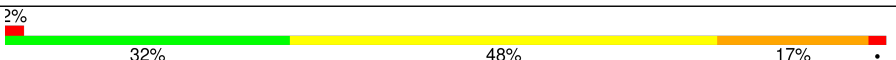
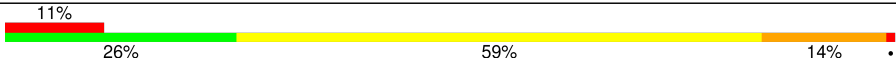
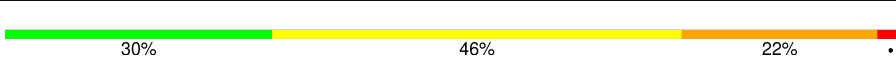
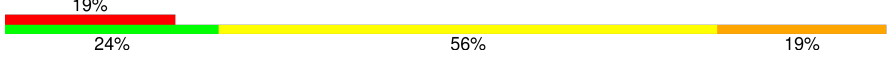
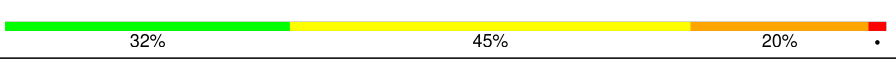
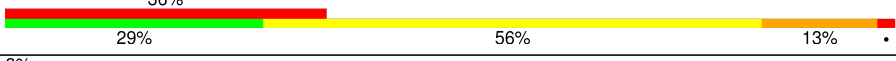

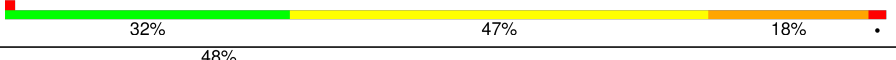

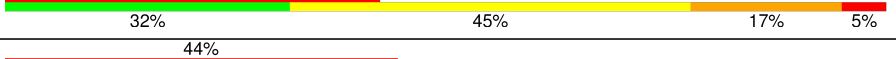



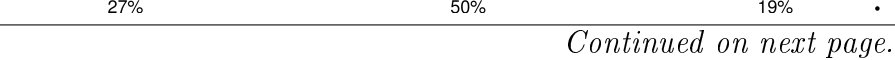

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Mol	Chain	Length	Quality of chain
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	

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Mol	Chain	Length	Quality of chain
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	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	

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Mol	Chain	Length	Quality of chain
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	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	

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Mol	Chain	Length	Quality of chain
44	BW	79	
44	DW	79	
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	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DA	2904	
58	DB	117	
59	DF	178	

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
60	MG	AA	1640	-	-	-	X
60	MG	BA	3013	-	-	-	X
60	MG	BA	3026	-	-	-	X
60	MG	BA	3039	-	-	-	X
60	MG	BA	3069	-	-	-	X
60	MG	BA	3082	-	-	-	X
60	MG	BA	3096	-	-	-	X
60	MG	BA	3100	-	-	-	X
60	MG	BA	3103	-	-	-	X
60	MG	BA	3104	-	-	-	X
60	MG	BA	3107	-	-	-	X
60	MG	BA	3115	-	-	-	X
60	MG	BA	3123	-	-	-	X
60	MG	BA	3130	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	CA	1628	-	-	-	X
60	MG	CA	1640	-	-	-	X
60	MG	DA	3002	-	-	-	X
60	MG	DA	3059	-	-	-	X
60	MG	DA	3074	-	-	-	X
60	MG	DA	3105	-	-	-	X
60	MG	DA	3114	-	-	-	X
60	MG	DA	3129	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 284499 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	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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			
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			

- 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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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			

- 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	S	0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O	S	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	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	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			
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			

- 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
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	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	0	0	0
			947	604	192	151			
38	DQ	117	Total	C	N	O	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			

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			449	281	87	79	2			
47	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- 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 RNA chain called 16S rRNA.

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

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 58 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 59 is a protein called 50S ribosomal protein L5.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

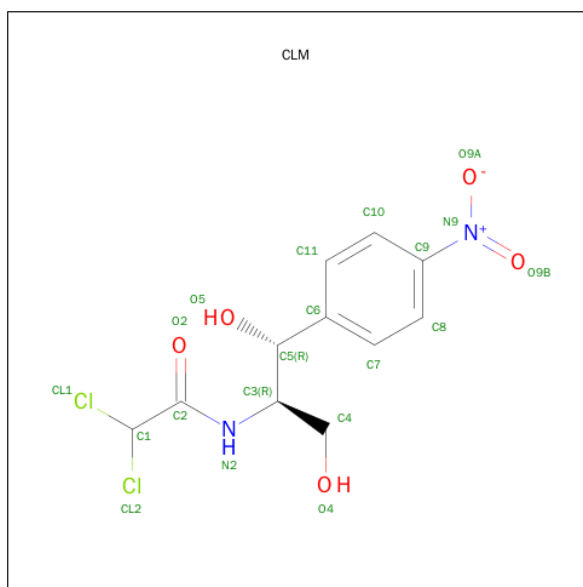
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	4	Total	Mg	0	0
			4	4		
60	DE	1	Total	Mg	0	0
			1	1		
60	BA	135	Total	Mg	0	0
			135	135		
60	CA	42	Total	Mg	0	0
			42	42		
60	DJ	1	Total	Mg	0	0
			1	1		
60	BL	1	Total	Mg	0	0
			1	1		
60	DA	133	Total	Mg	0	0
			133	133		
60	AA	42	Total	Mg	0	0
			42	42		
60	AN	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DC	1	Total	Mg	0	0
			1	1		
60	DB	1	Total	Mg	0	0
			1	1		

- Molecule 61 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	197	Total	O	0	0
			197	197		
63	AL	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AN	6	Total 6	O 6	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	1	Total 1	O 1	0	0
63	BA	608	Total 608	O 608	0	0
63	BB	19	Total 19	O 19	0	0
63	BC	8	Total 8	O 8	0	0
63	BD	2	Total 2	O 2	0	0
63	BE	1	Total 1	O 1	0	0
63	BL	4	Total 4	O 4	0	0
63	BN	2	Total 2	O 2	0	0
63	BQ	1	Total 1	O 1	0	0
63	BT	2	Total 2	O 2	0	0
63	BV	1	Total 1	O 1	0	0
63	B2	2	Total 2	O 2	0	0
63	B3	2	Total 2	O 2	0	0
63	B4	2	Total 2	O 2	0	0
63	CA	195	Total 195	O 195	0	0
63	CE	3	Total 3	O 3	0	0
63	CI	1	Total 1	O 1	0	0
63	CL	1	Total 1	O 1	0	0
63	CN	3	Total 3	O 3	0	0

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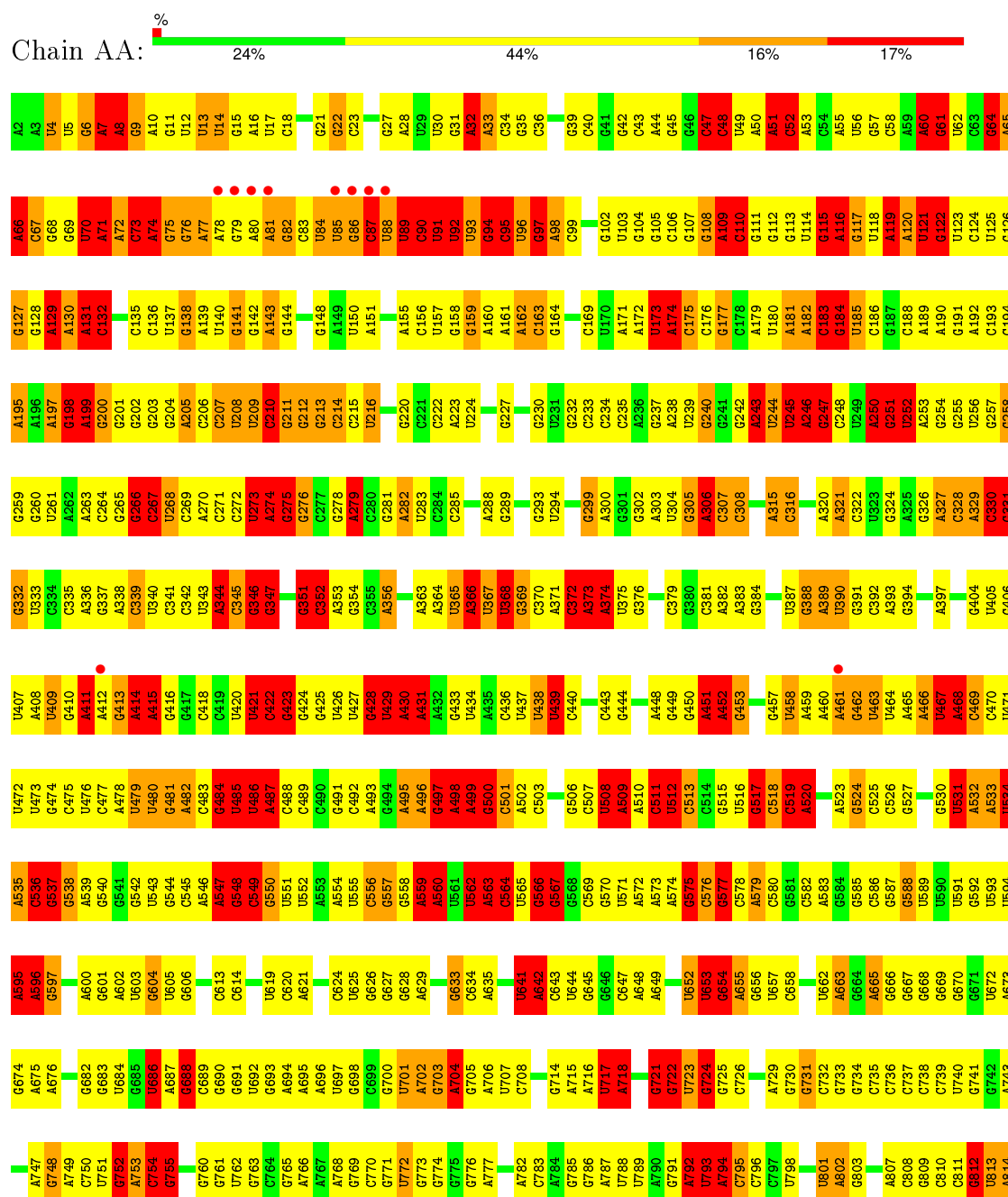
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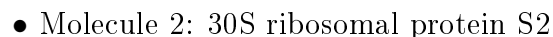
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63	CU	2	Total 2	O 2	0	0
63	DA	603	Total 603	O 603	0	0
63	DB	4	Total 4	O 4	0	0
63	DC	10	Total 10	O 10	0	0
63	DD	1	Total 1	O 1	0	0
63	DE	3	Total 3	O 3	0	0
63	DJ	4	Total 4	O 4	0	0
63	DL	5	Total 5	O 5	0	0
63	DN	2	Total 2	O 2	0	0
63	DT	2	Total 2	O 2	0	0
63	DU	2	Total 2	O 2	0	0
63	DV	1	Total 1	O 1	0	0
63	D2	1	Total 1	O 1	0	0
63	D3	1	Total 1	O 1	0	0
63	D4	4	Total 4	O 4	0	0

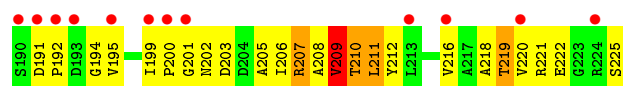
3 Residue-property plots

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

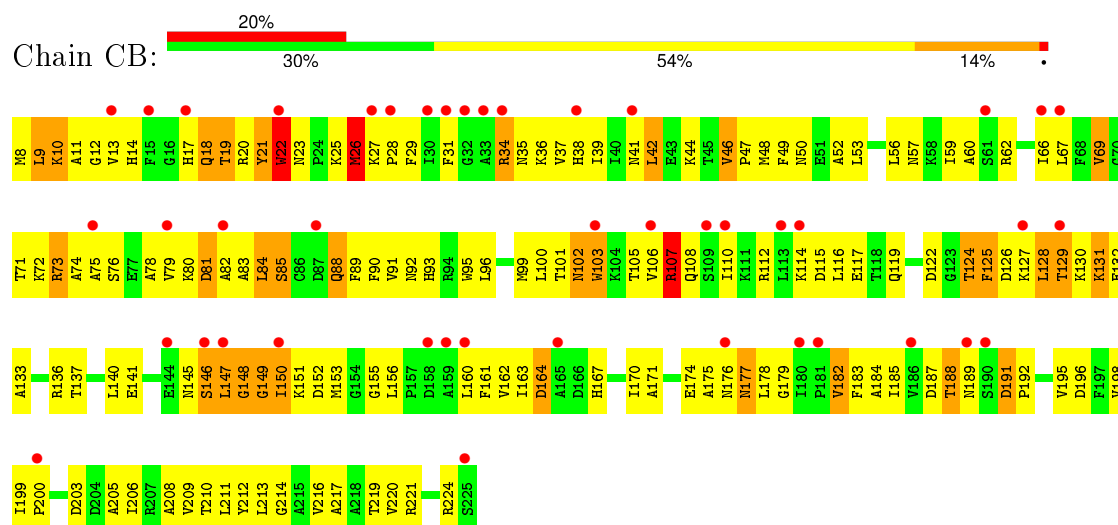
• Molecule 1: 16S rRNA



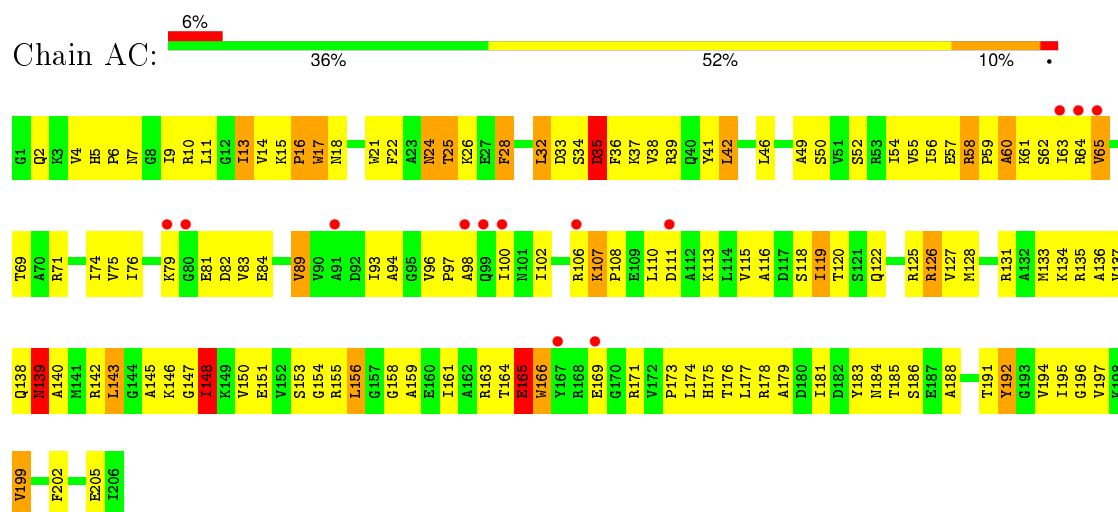




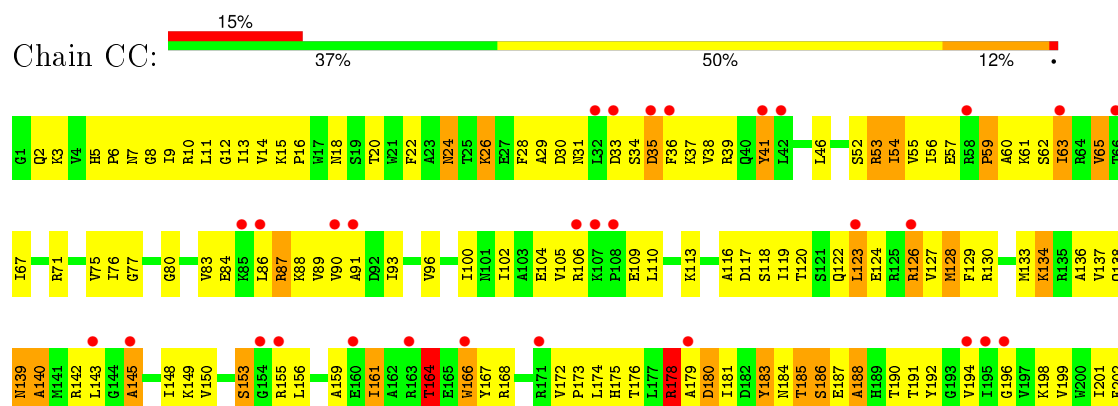
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



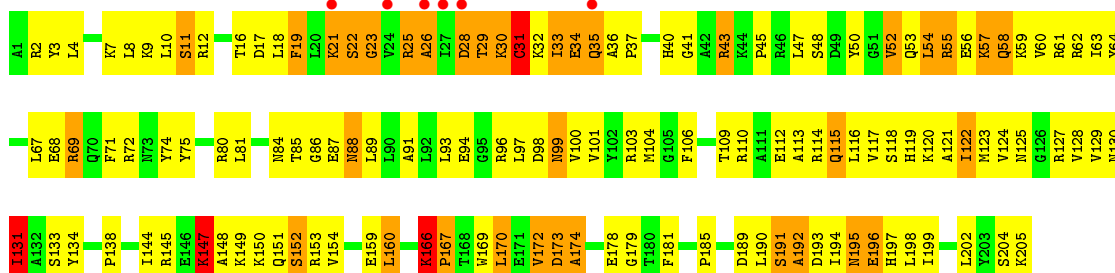
• Molecule 3: 30S ribosomal protein S3

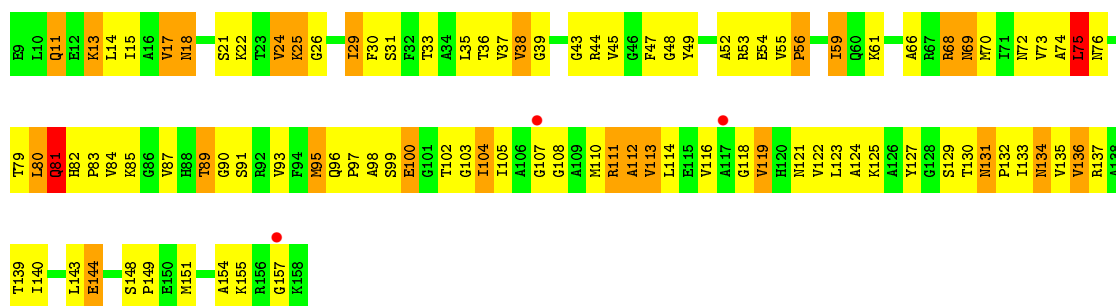


K203
E204
E205
I206

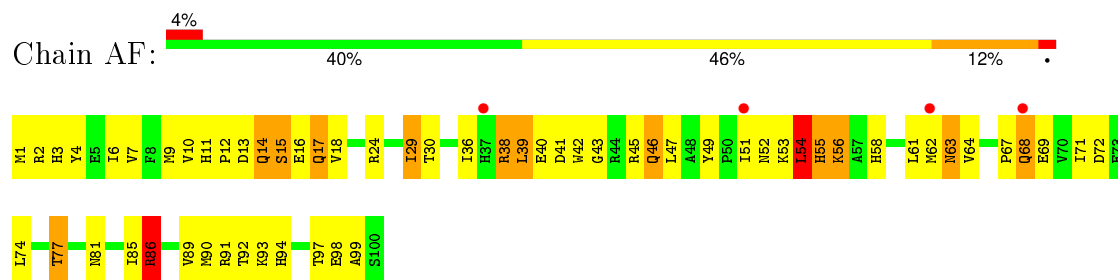
• Molecule 4: 30S ribosomal protein S4

Chain AD:  3% 34% 47% 17%

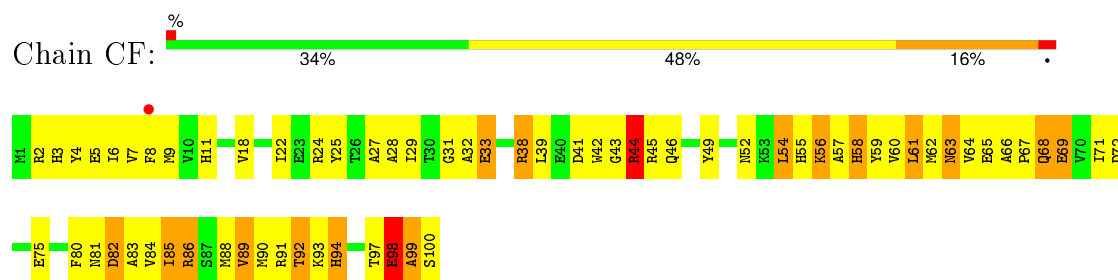




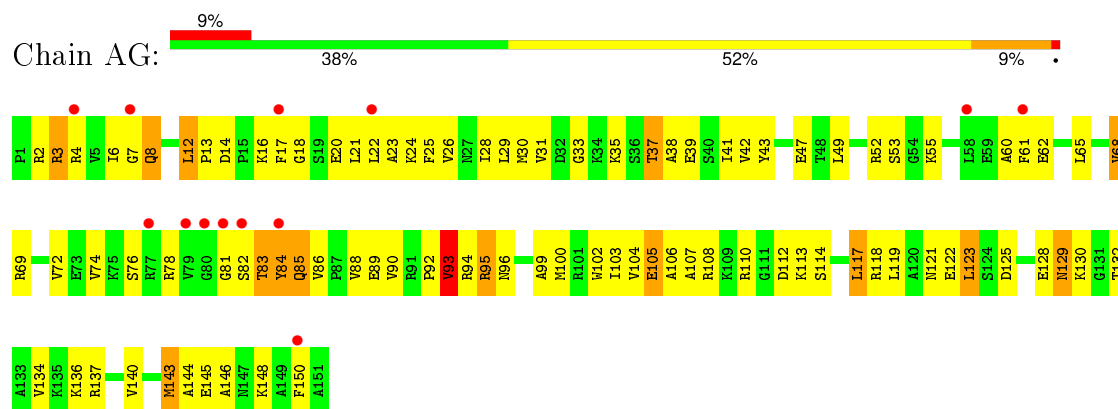
• Molecule 6: 30S ribosomal protein S6



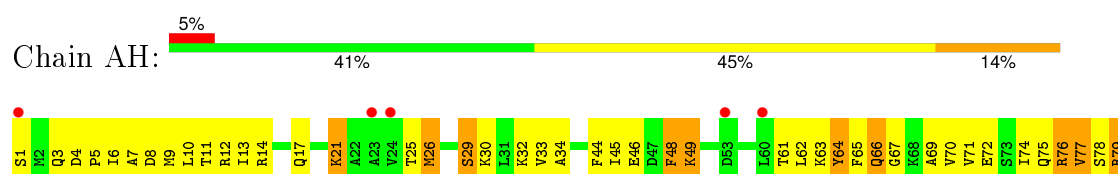
• Molecule 6: 30S ribosomal protein S6

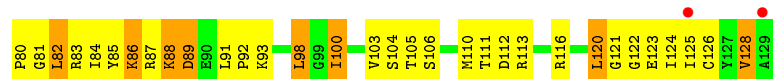


• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8





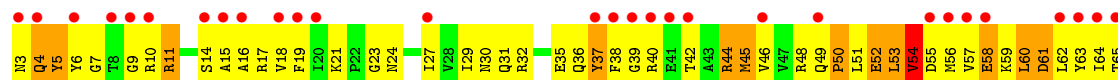
• Molecule 8: 30S ribosomal protein S8



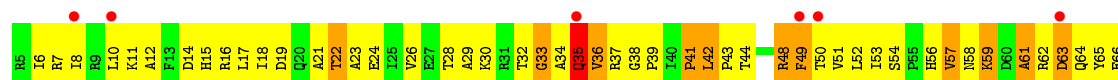
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

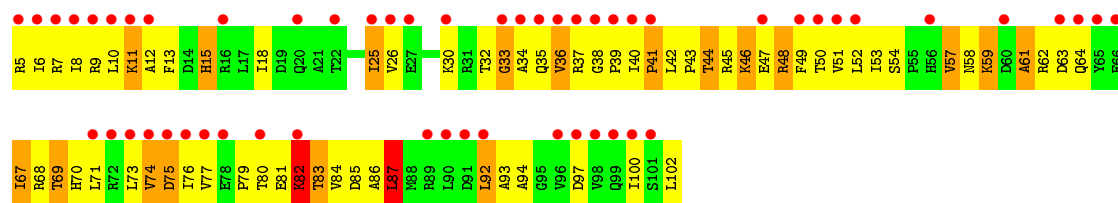


• Molecule 10: 30S ribosomal protein S10

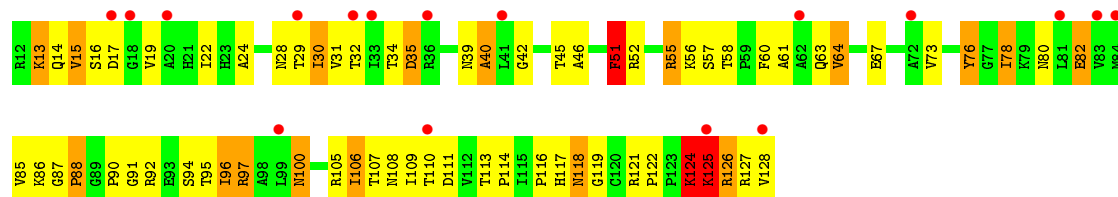
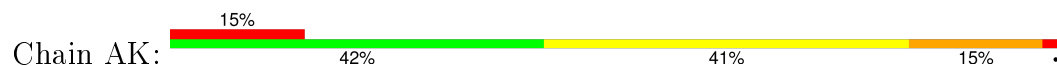


• Molecule 10: 30S ribosomal protein S10

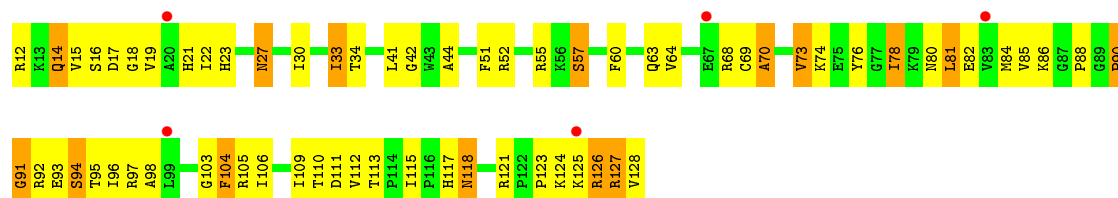




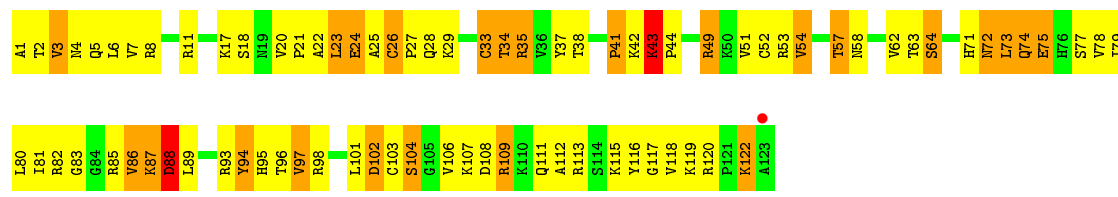
• Molecule 11: 30S ribosomal protein S11



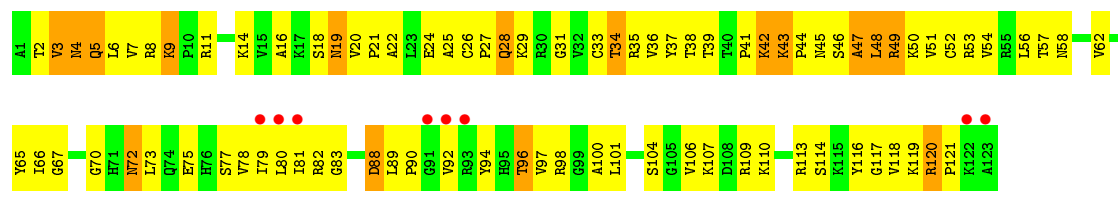
• Molecule 11: 30S ribosomal protein S11



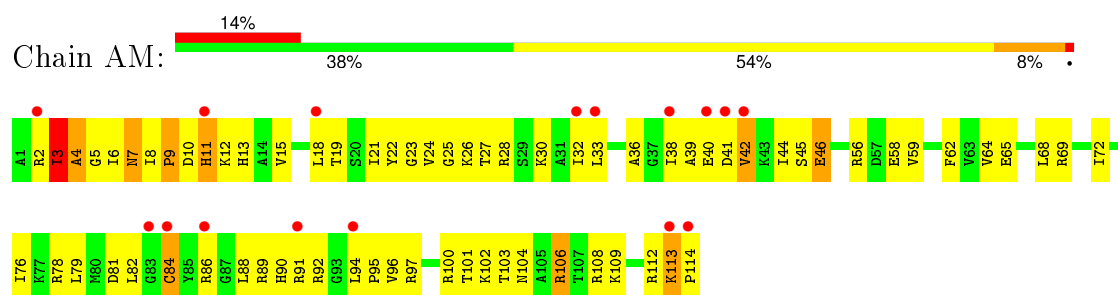
• Molecule 12: 30S ribosomal protein S12



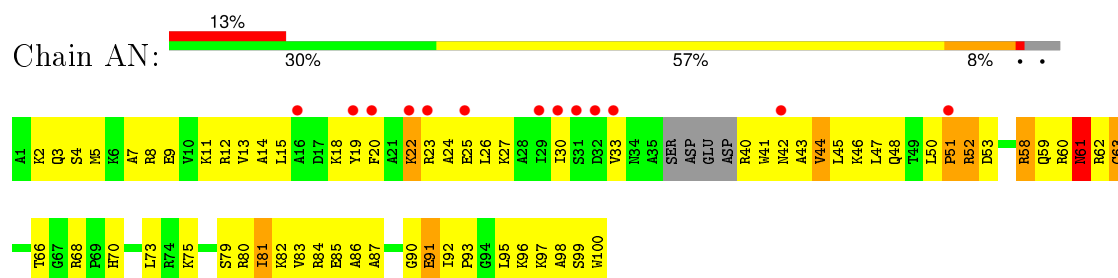
• Molecule 12: 30S ribosomal protein S12



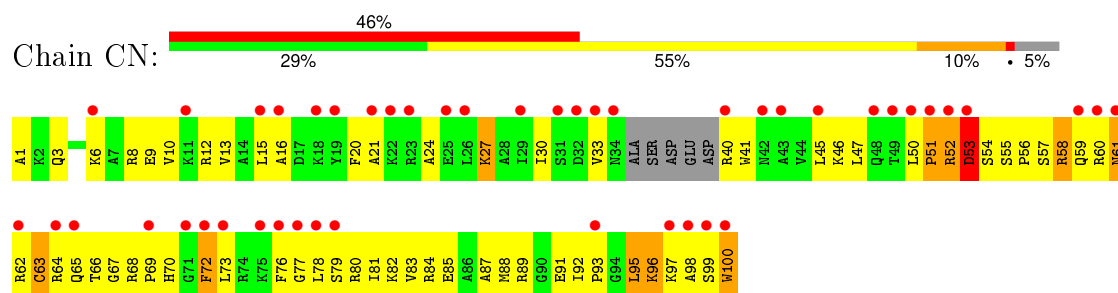
• Molecule 13: 30S ribosomal protein S13



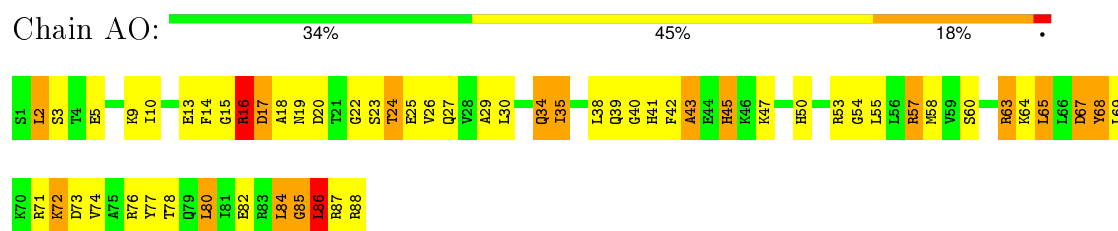
- Molecule 14: 30S ribosomal protein S14



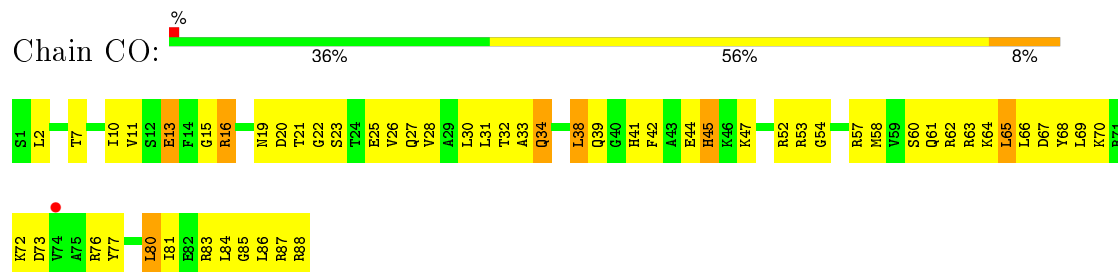
- Molecule 14: 30S ribosomal protein S14



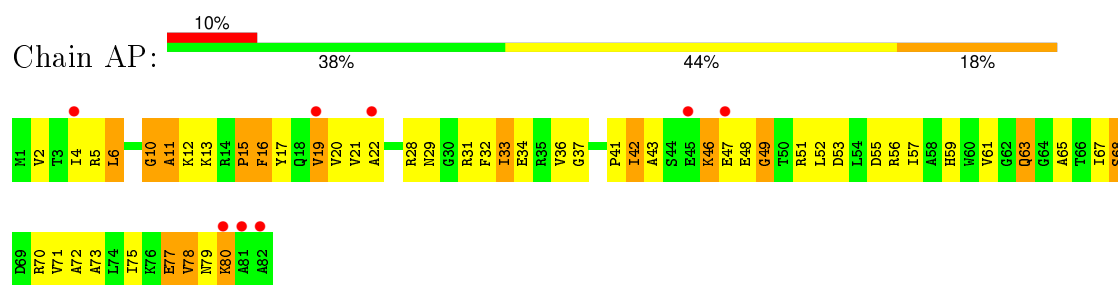
- Molecule 15: 30S ribosomal protein S15



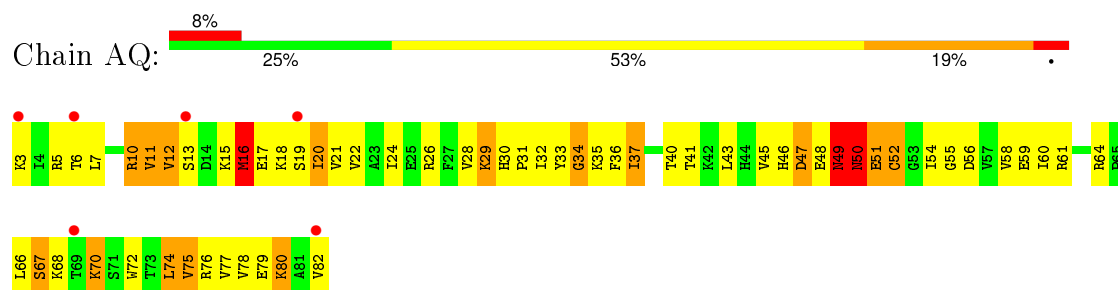
- Molecule 15: 30S ribosomal protein S15



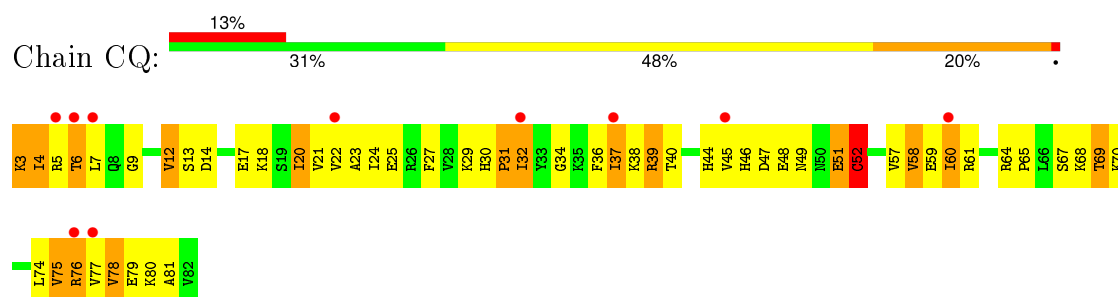
- Molecule 16: 30S ribosomal protein S16



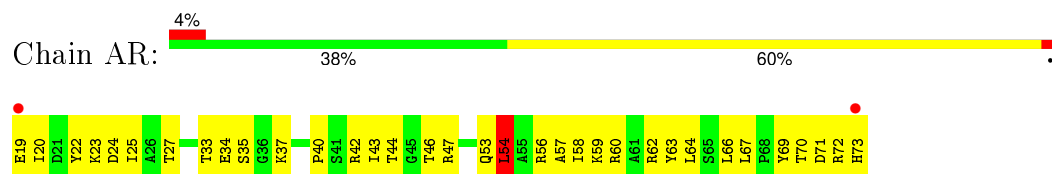
- Molecule 17: 30S ribosomal protein S17



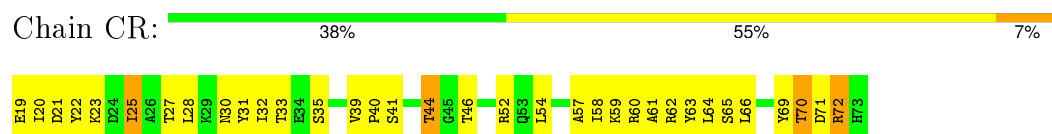
- Molecule 17: 30S ribosomal protein S17



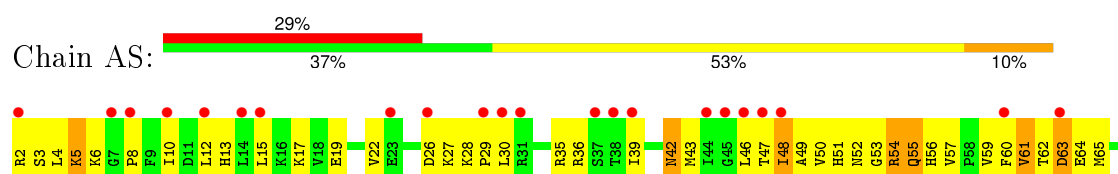
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

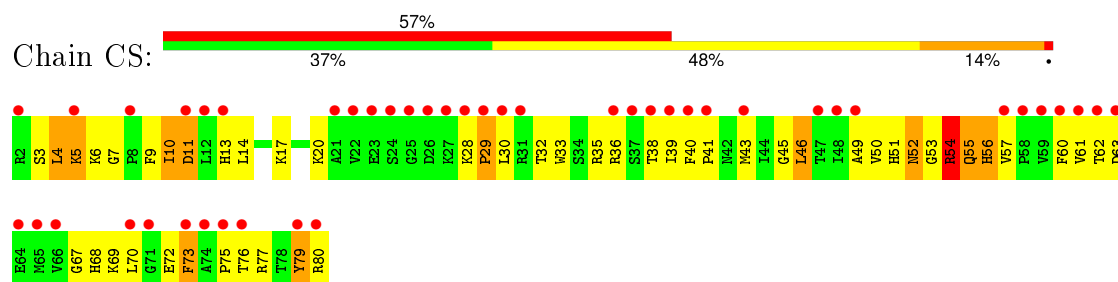


- Molecule 19: 30S ribosomal protein S19

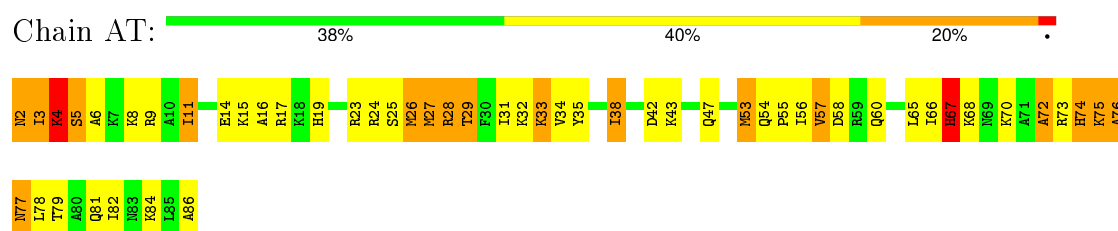




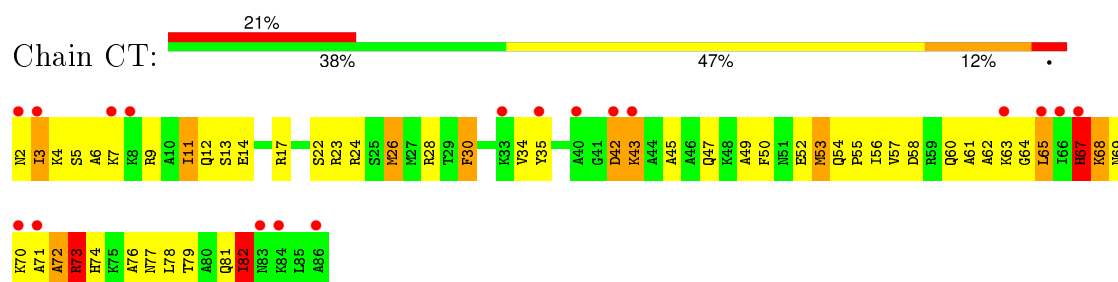
- Molecule 19: 30S ribosomal protein S19



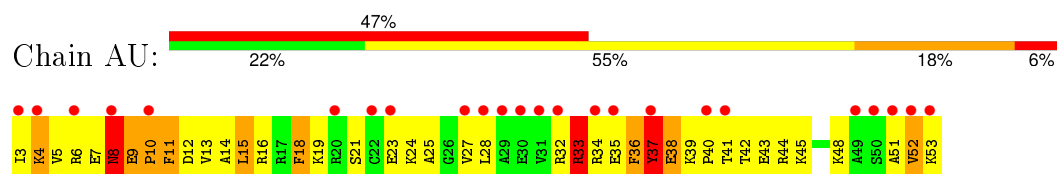
- Molecule 20: 30S ribosomal protein S20



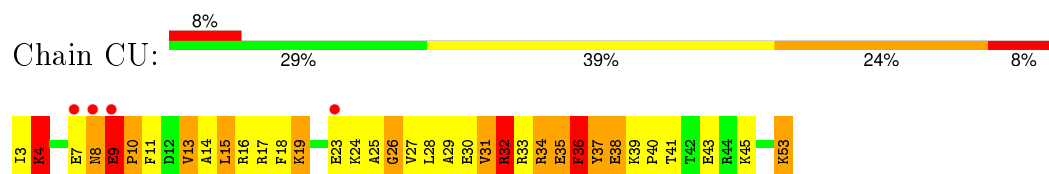
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA



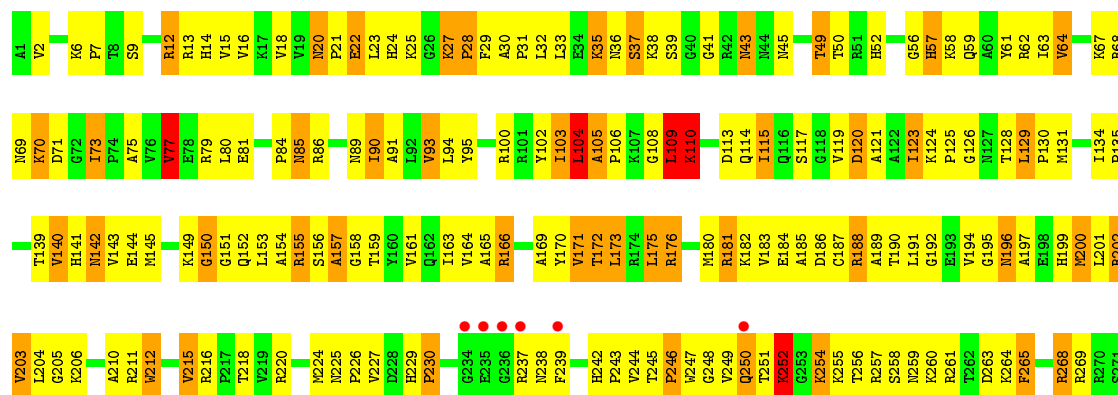


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U2026	C1957	A1885	C1816	U1680	U1748	C1748	C1615	A1552	G1483	U1415	A1347	U1282	C1221	A1155	A1090
G2027	G1958	A1886	G1817	G1681	G1753	G1682	C1616	U1554	U1484	C1417	C1348	G1283	U1222	G1156	G1091
U2028	G1959	A1887	U1818	G1682	G1753	G1682	C1617	U1555	U1485	G1418	C1349	A1286	U1224	G1157	C1092
G2029	A1960	A1889	A1919	U1683	A1754	U1683	G1618	G1555	U1486	G1419	C1350	A1287	U1225	U1159	G1093
A2030	G1961	A1890	U1820	C1684	G1684	C1685	G1619	G1557	U1487	A1420	C1351	G1288	A1226	U1160	U1094
A2031	G1962	A1891	A1821	G1685	G1756	C1685	G1622	C1558	C1488	G1421	U1352	G1289	G1227	A1095	A1096
G2032	G1963	U1898	G1822	U1688	A1757	U1688	G1623	U1559	C1489	G1422	A1353	G1290	G1228	C1161	U1097
A2033	A1964	A1899	G1823	U1758	U1758	A1689	U1624	G1560	A1490	G1423	A1354	C1291	G1229	G1162	G1098
U2034	C1965	A1900	U1824	A1759	A1759	A1690	C1625	G1561	G1491	G1424	G1355	G1292	A1230	G1163	A1099
G2035	A1966	A1901	U1825	G1696	G1764	G1696	G1626	U1562	G1492	G1425	G1356	G1293	U1231	A1165	G1099
C2036	G1967	C1902	G1826	U1693	G1761	U1693	A1826	U1563	G1493	G1426	G1357	U1232	U1231	A1103	A1103
A2037	G1968	U1827	U1827	G1694	A1762	G1694	G1627	U1564	C1494	A1427	C1357	G1294	G1232	G1166	A1104
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A2042	G1972	C1908	C1832	A1698	G1766	A1698	G1631	U1568	G1498	G1432	G1361	G1298	G1236	C1171	U1108
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G2046	G1980	A1913	C1836	C1706	A1773	C1706	A1637	G1502	A1502	G1436	G1370	G1303	G1243	U1177	U1113
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G2083	C2021	A1874	C1875	A1744	A1744	A1744	A1675	C1612	A1548	U1476	U1413	G1343	G1280	G1216	
C2084	U2022	G1953	G1876	U1745	U1745	U1745	A1676	G1613	C1550	G1478					
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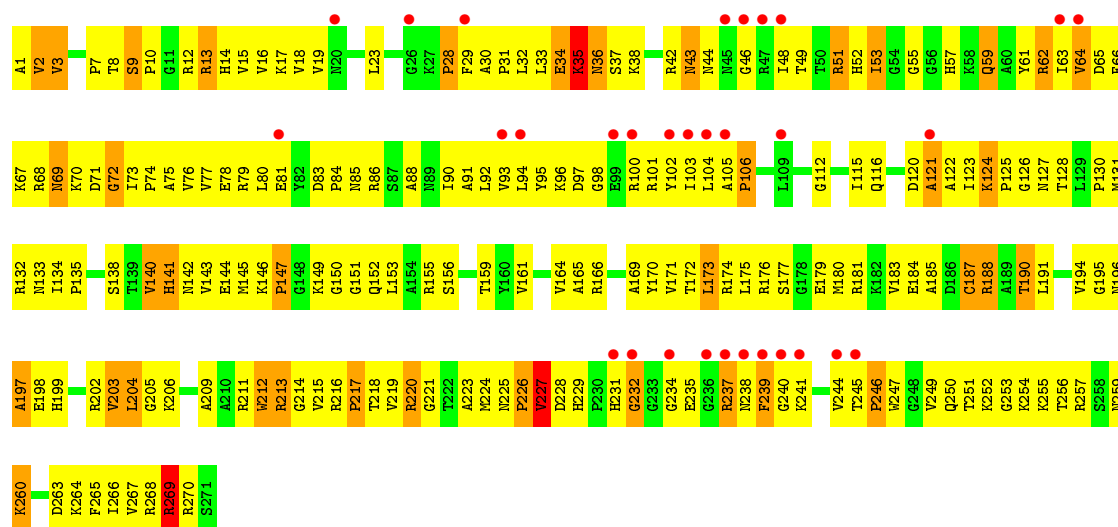




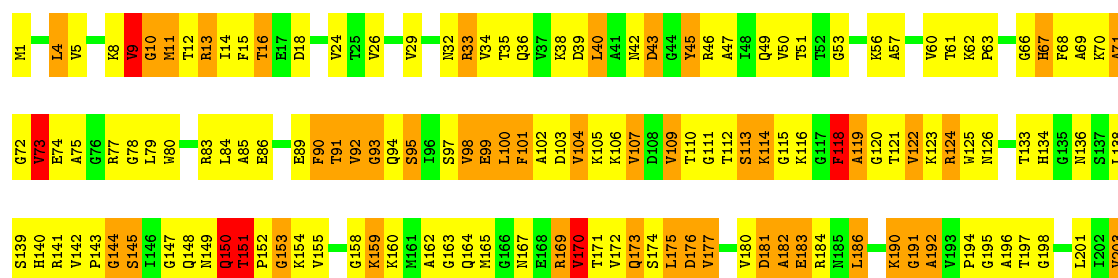
• Molecule 24: 50S ribosomal protein L2



• Molecule 24: 50S ribosomal protein L2

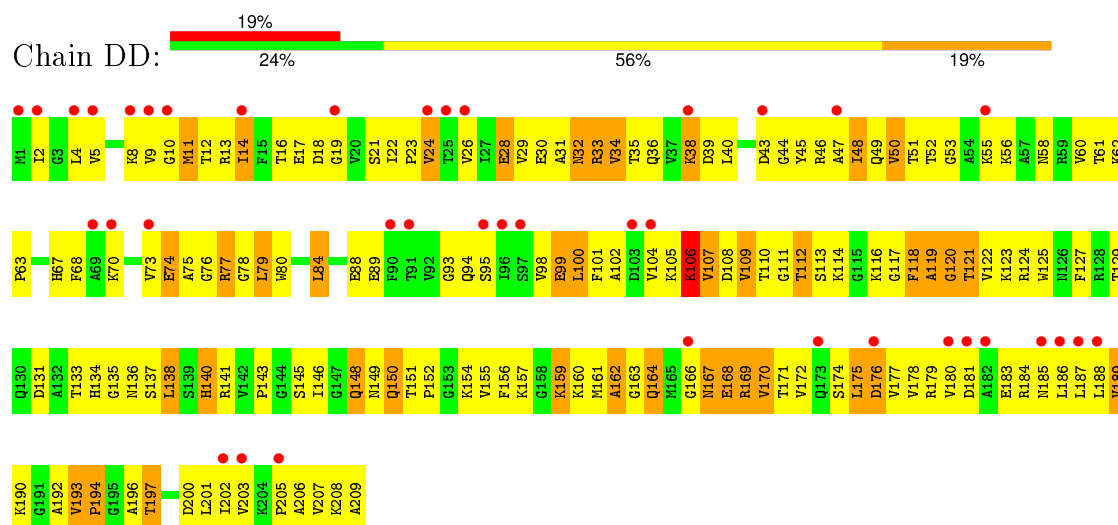


• Molecule 25: 50S ribosomal protein L3

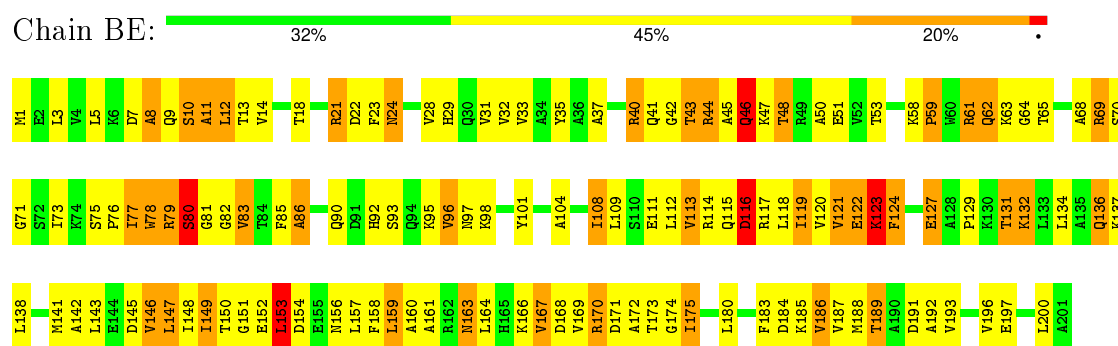




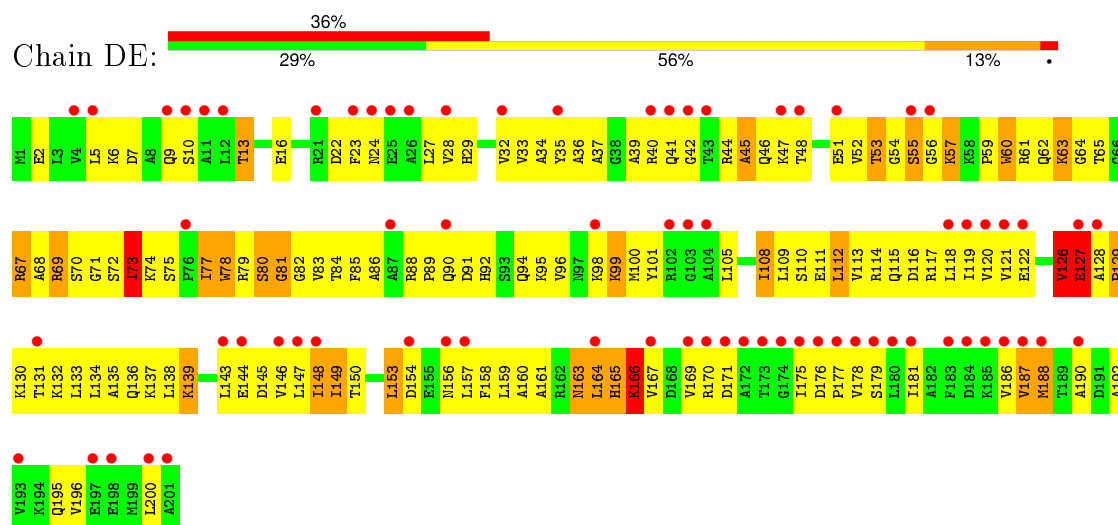
• Molecule 25: 50S ribosomal protein L3



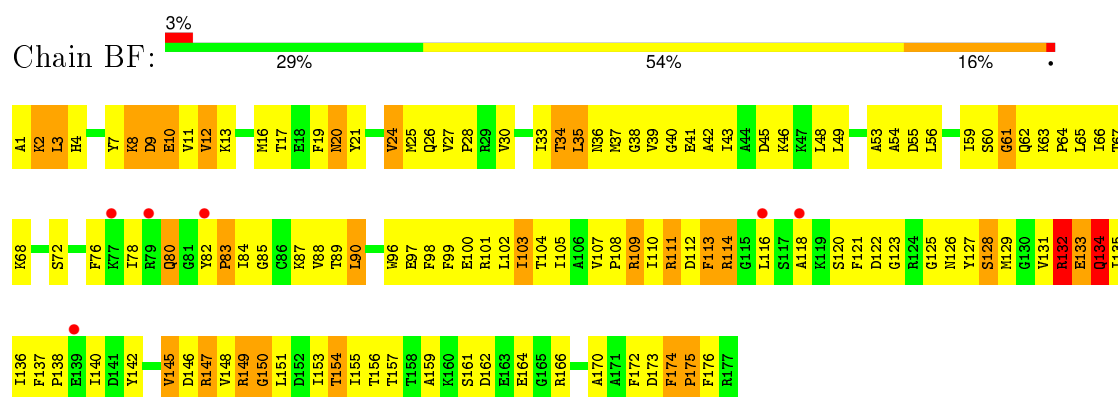
• Molecule 26: 50S ribosomal protein L4



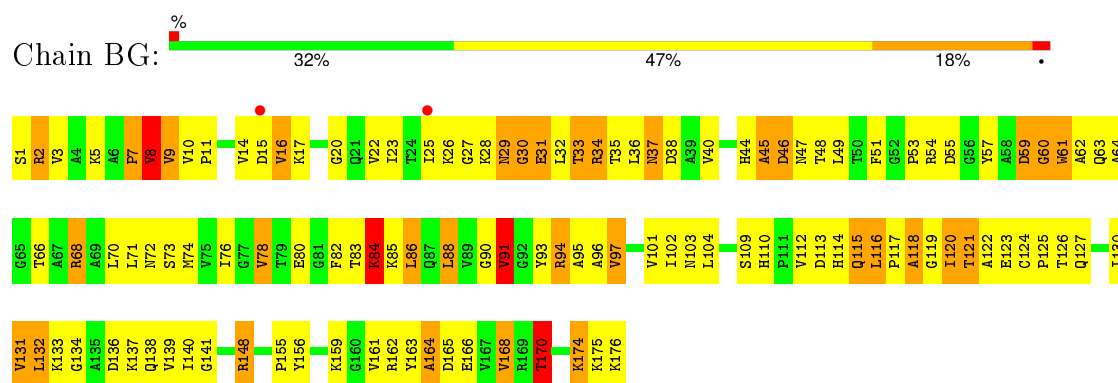
• Molecule 26: 50S ribosomal protein L4



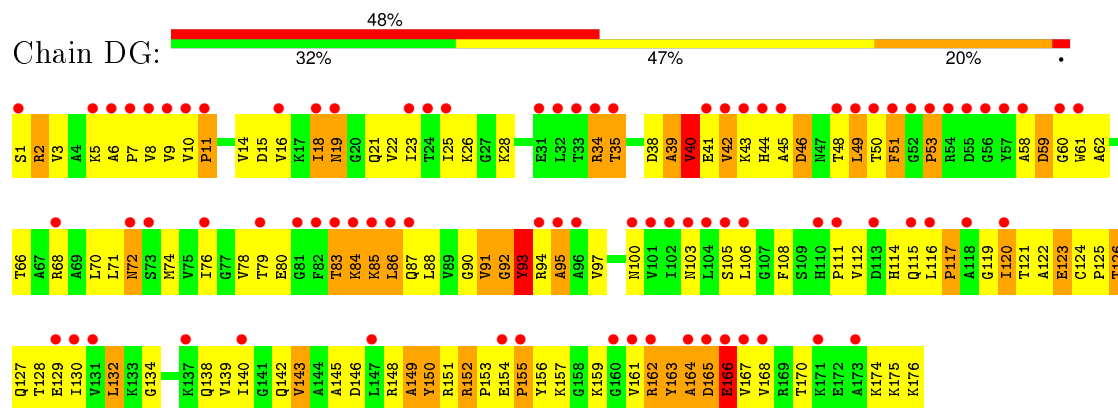
• Molecule 27: 50S ribosomal protein L5



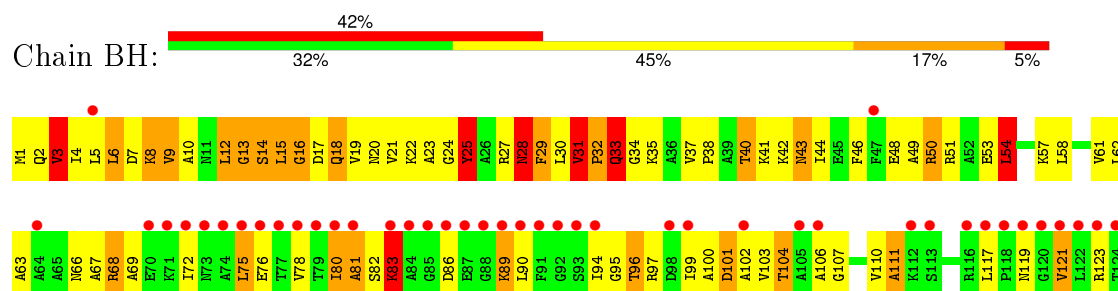
• Molecule 28: 50S ribosomal protein L6



• Molecule 28: 50S ribosomal protein L6

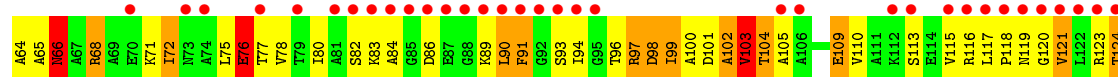
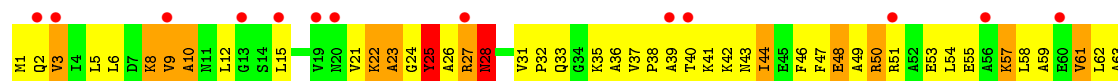


• Molecule 29: 50S ribosomal protein L9

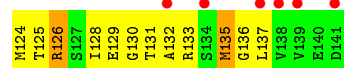
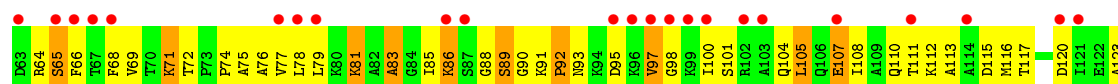
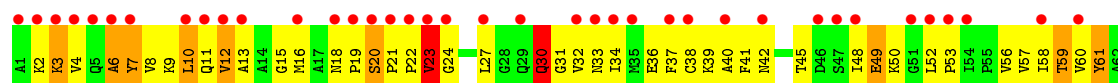




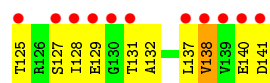
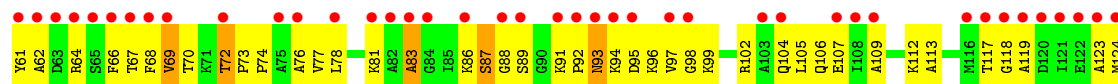
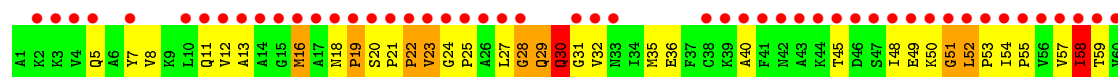
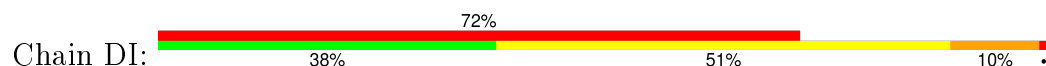
- Molecule 29: 50S ribosomal protein L9



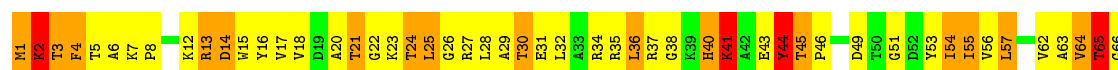
- Molecule 30: 50S ribosomal protein L11

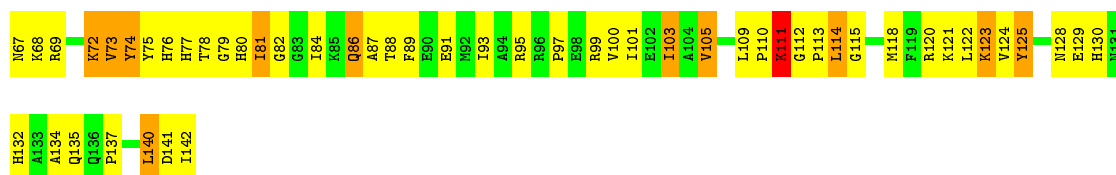


- Molecule 30: 50S ribosomal protein L11

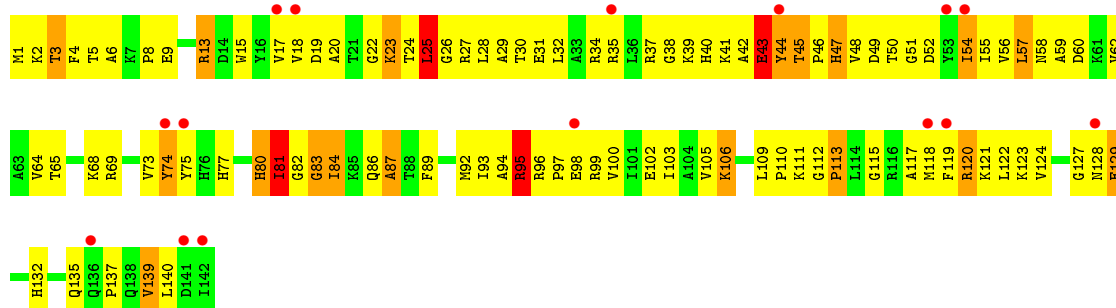


- Molecule 31: 50S ribosomal protein L13

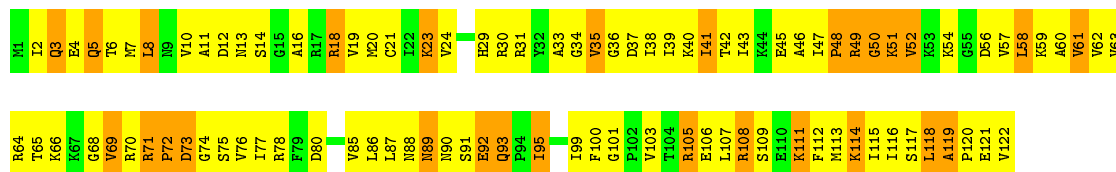




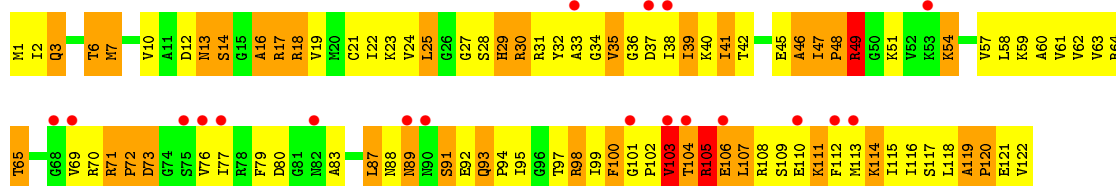
- Molecule 31: 50S ribosomal protein L13



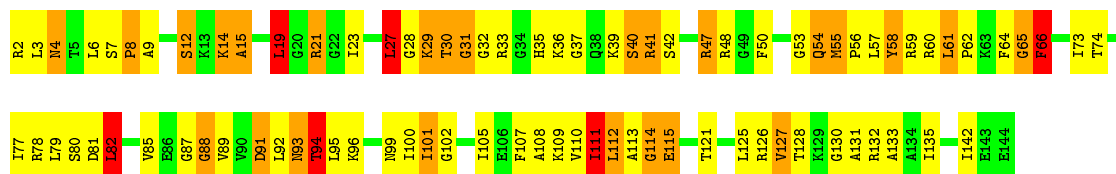
- Molecule 32: 50S ribosomal protein L14



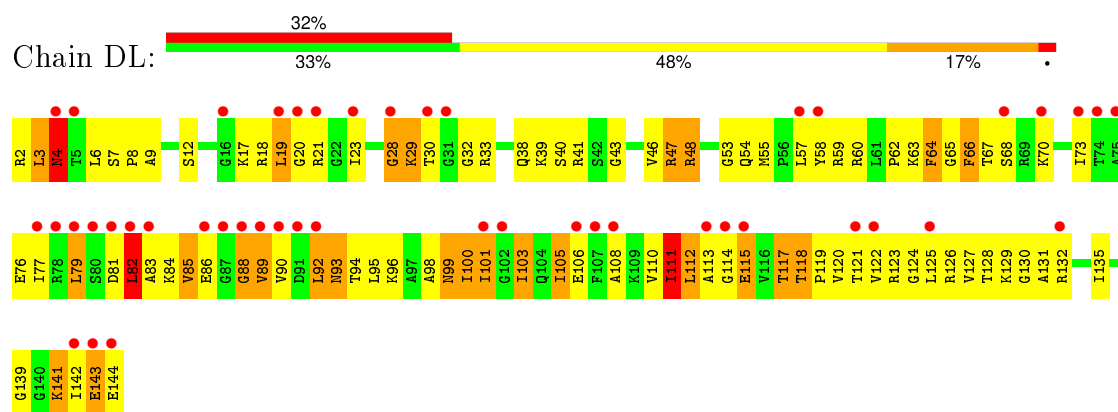
- Molecule 32: 50S ribosomal protein L14



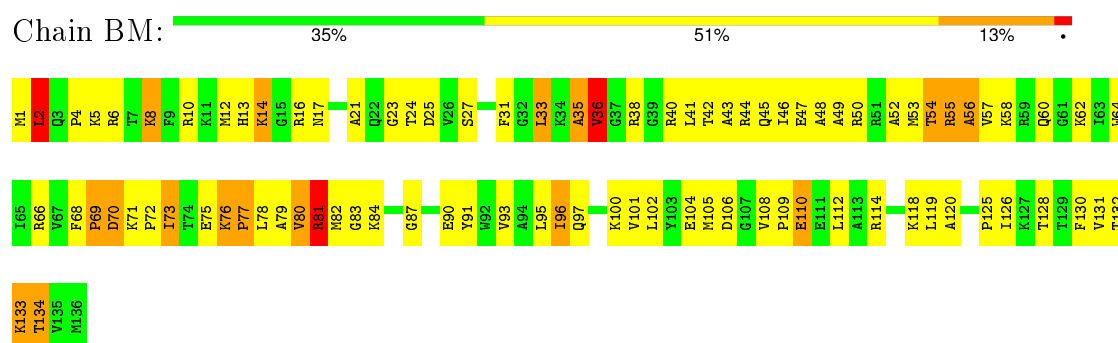
- Molecule 33: 50S ribosomal protein L15



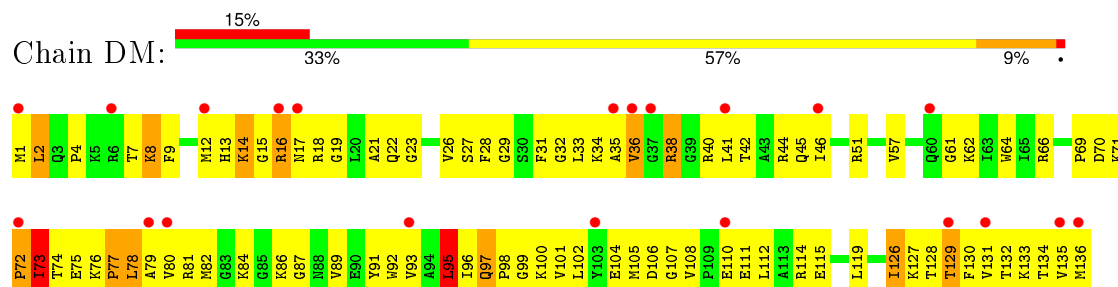
- Molecule 33: 50S ribosomal protein L15



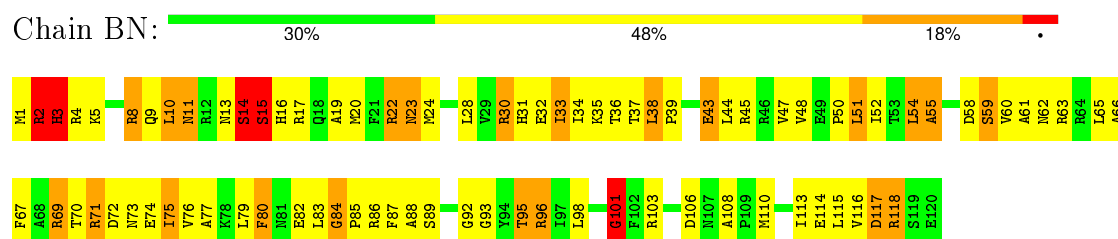
- Molecule 34: 50S ribosomal protein L16



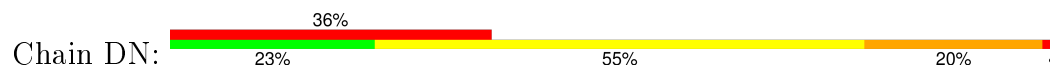
- Molecule 34: 50S ribosomal protein L16

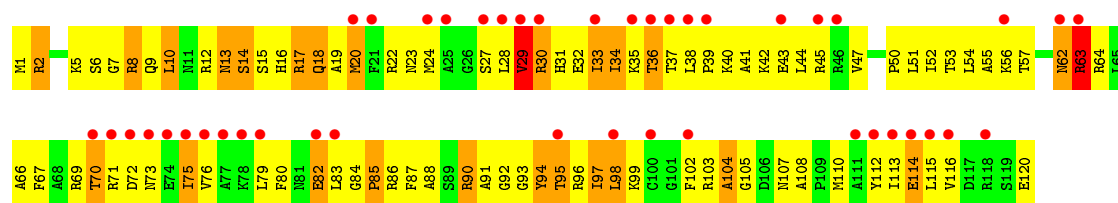


- Molecule 35: 50S ribosomal protein L17



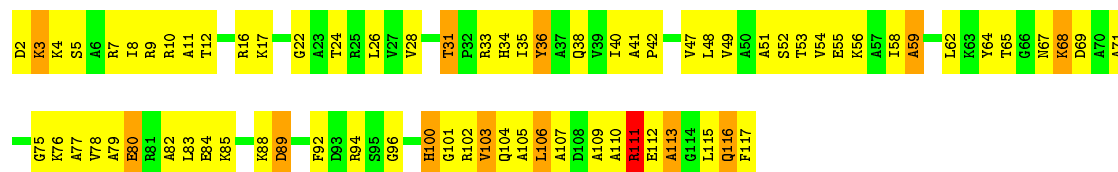
- Molecule 35: 50S ribosomal protein L17





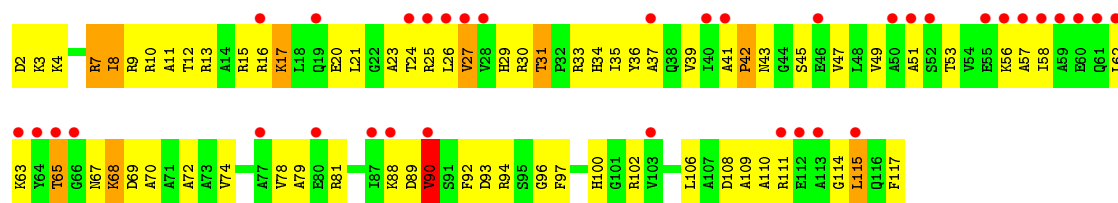
• Molecule 36: 50S ribosomal protein L18

Chain BO: 36% 53% 10% .



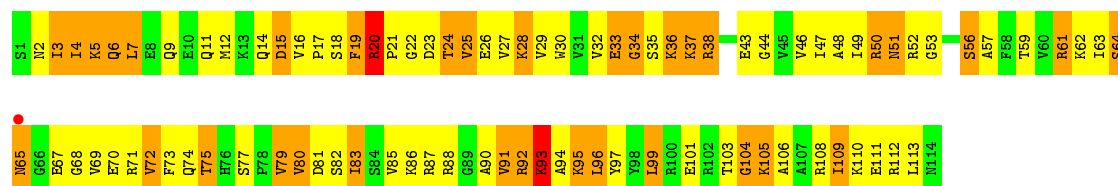
• Molecule 36: 50S ribosomal protein L18

Chain DO: 31% 40% 52% 8% .



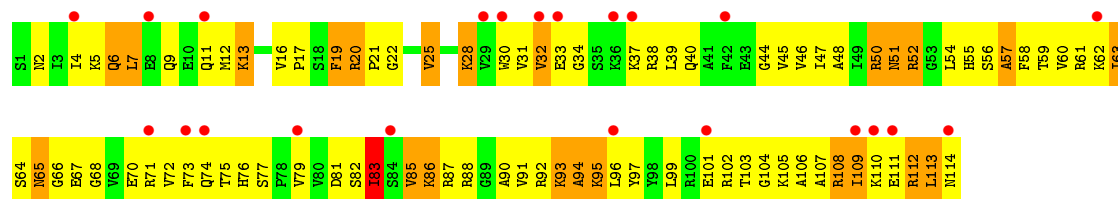
• Molecule 37: 50S ribosomal protein L19

Chain BP: 21% 47% 30% .



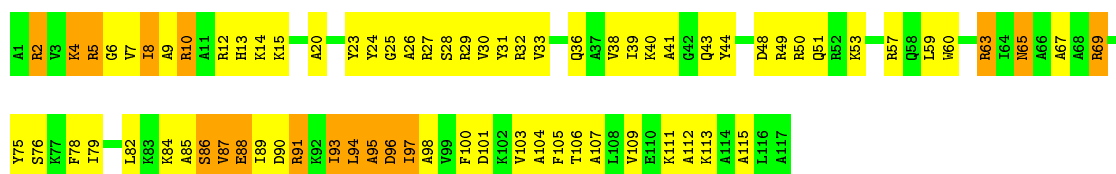
• Molecule 37: 50S ribosomal protein L19

Chain DP: 19% 23% 56% 20% .

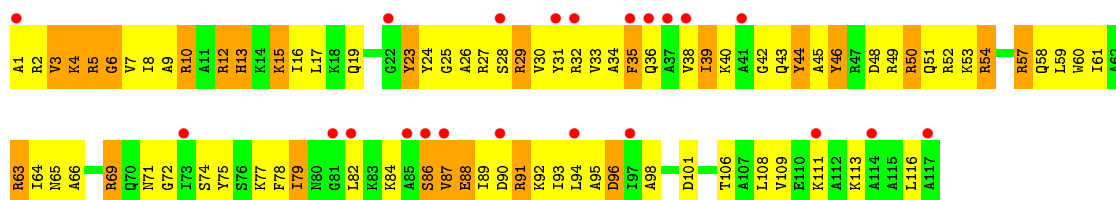


• Molecule 38: 50S ribosomal protein L20

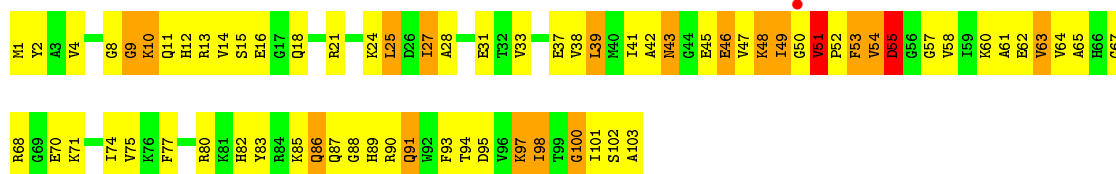
Chain BQ: 37% 49% 15%



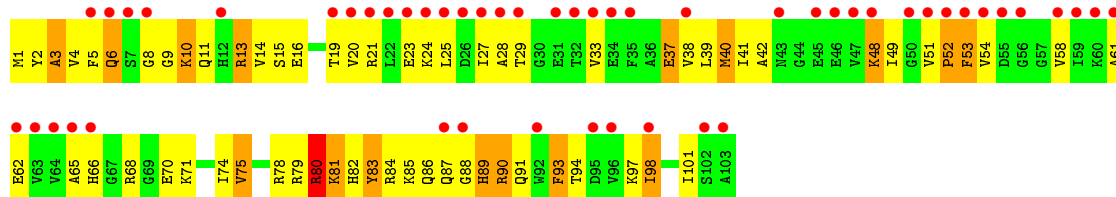
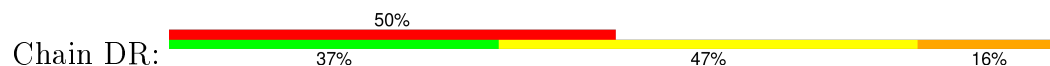
• Molecule 38: 50S ribosomal protein L20



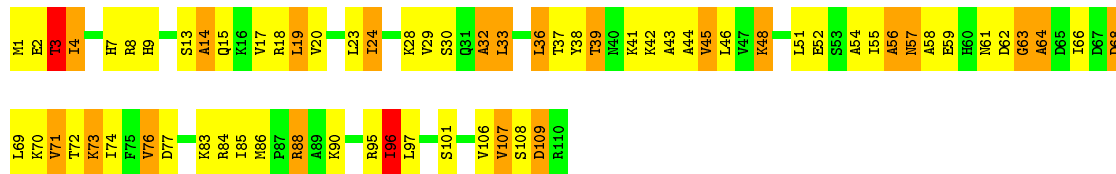
• Molecule 39: 50S ribosomal protein L21



• Molecule 39: 50S ribosomal protein L21

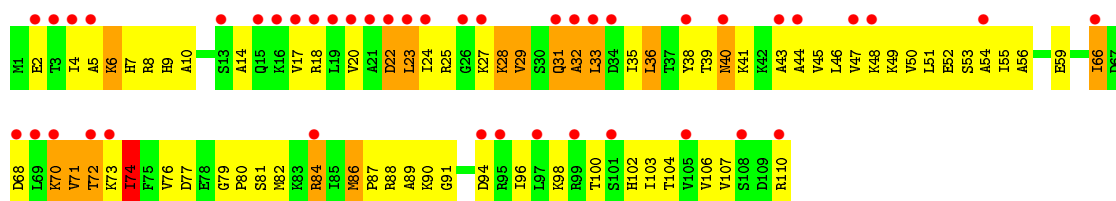


• Molecule 40: 50S ribosomal protein L22

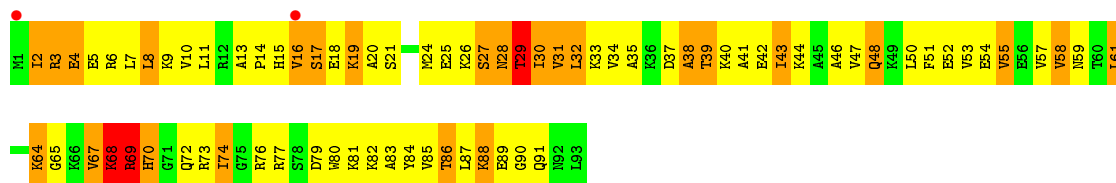
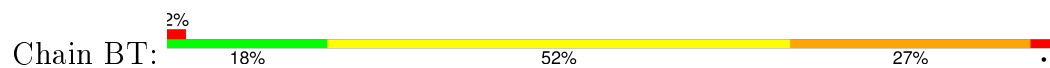


• Molecule 40: 50S ribosomal protein L22

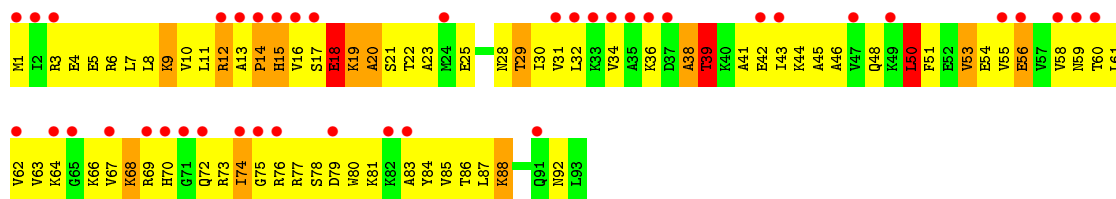




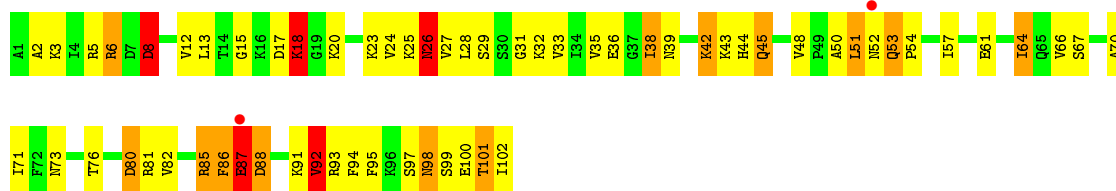
• Molecule 41: 50S ribosomal protein L23



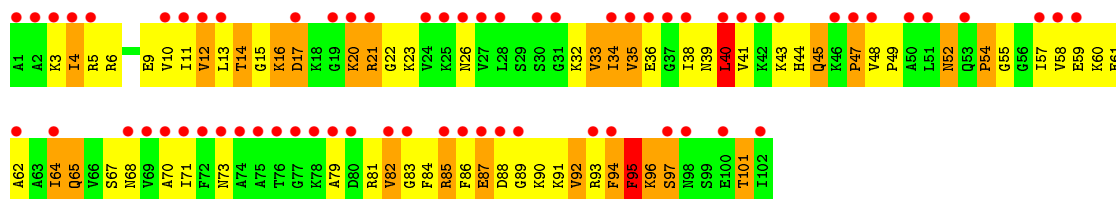
• Molecule 41: 50S ribosomal protein L23



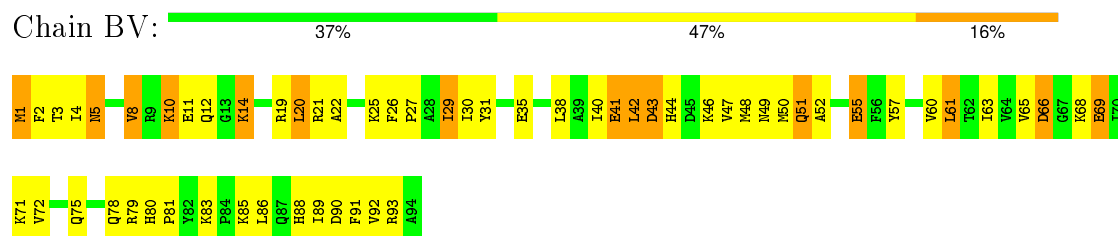
• Molecule 42: 50S ribosomal protein L24



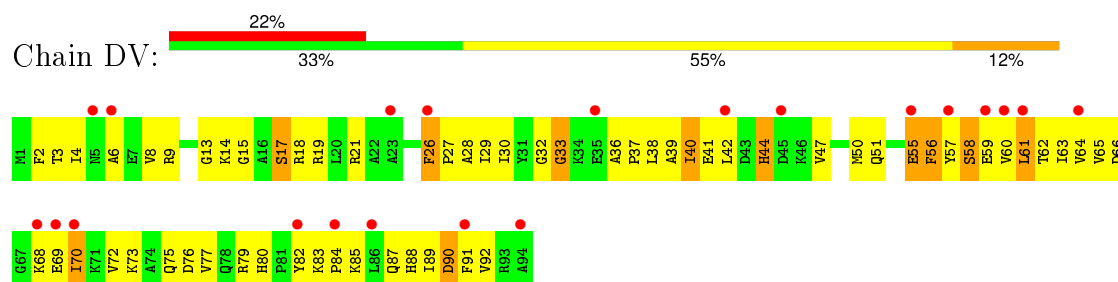
• Molecule 42: 50S ribosomal protein L24



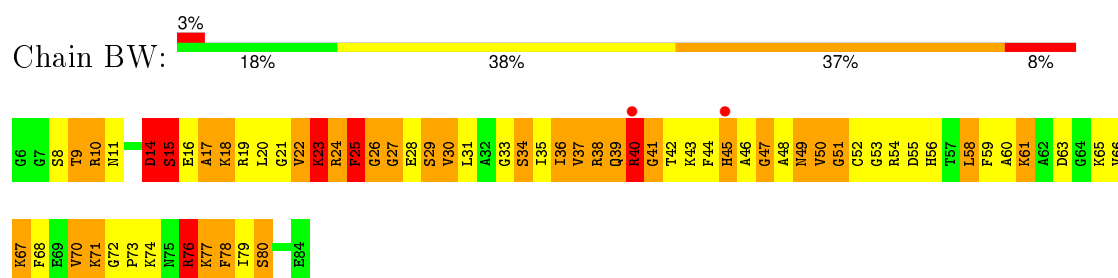
• Molecule 43: 50S ribosomal protein L25



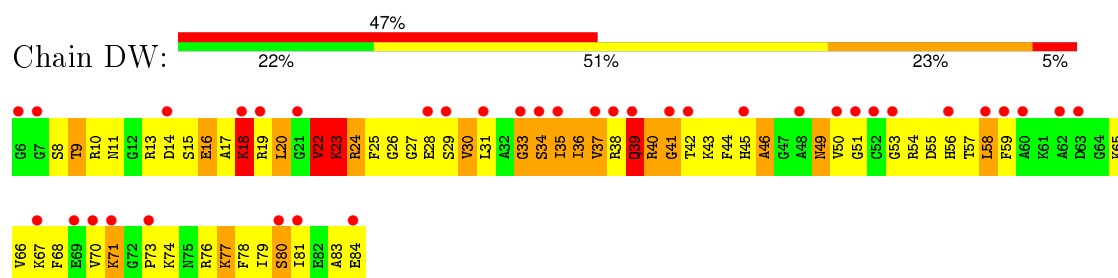
- Molecule 43: 50S ribosomal protein L25



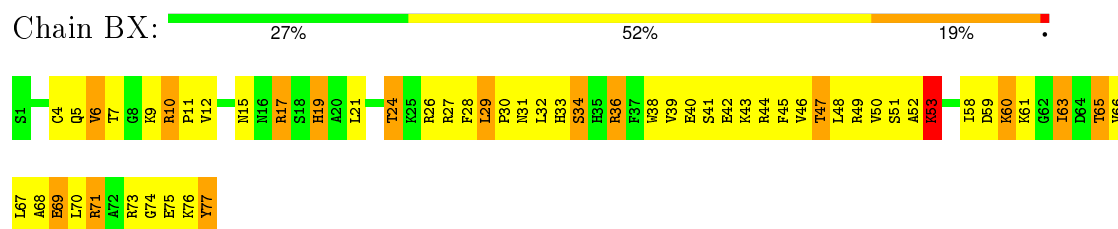
- Molecule 44: 50S ribosomal protein L27



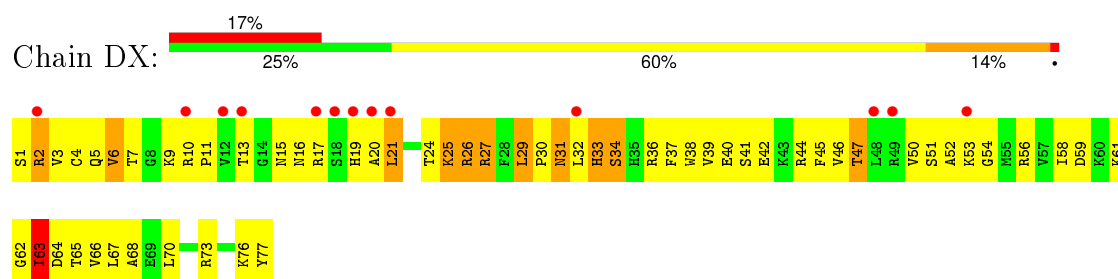
- Molecule 44: 50S ribosomal protein L27



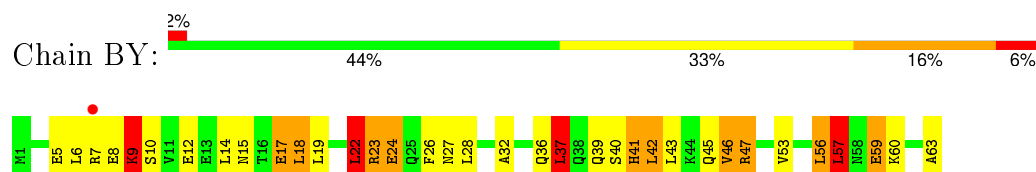
- Molecule 45: 50S ribosomal protein L28



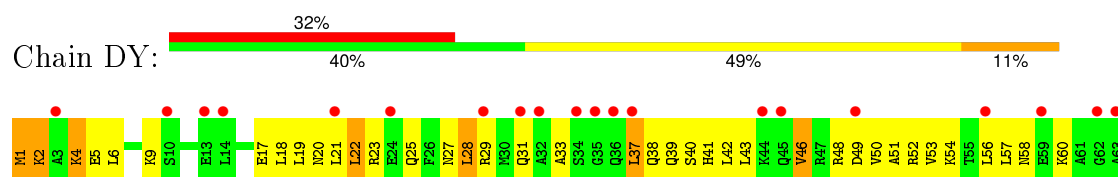
- Molecule 45: 50S ribosomal protein L28



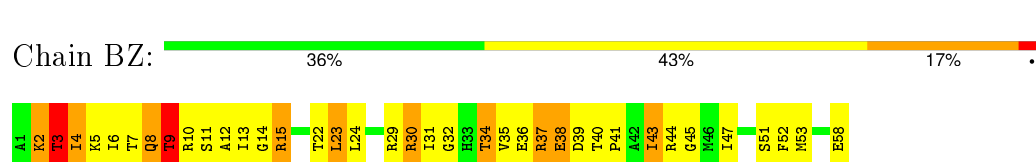
- Molecule 46: 50S ribosomal protein L29



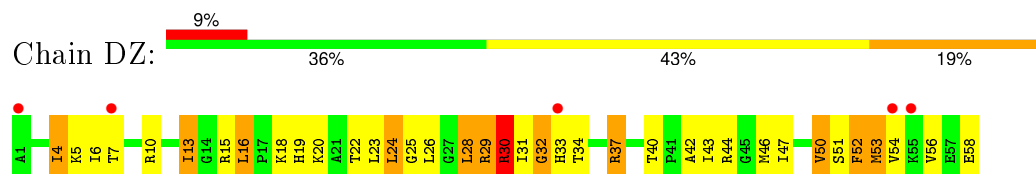
- Molecule 46: 50S ribosomal protein L29



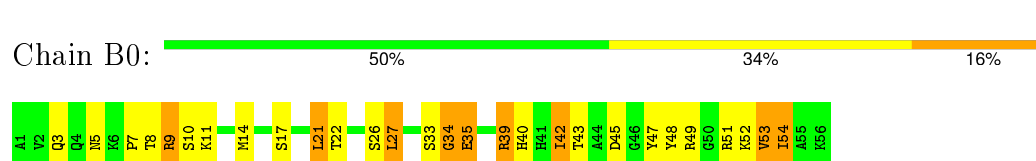
- Molecule 47: 50S ribosomal protein L30



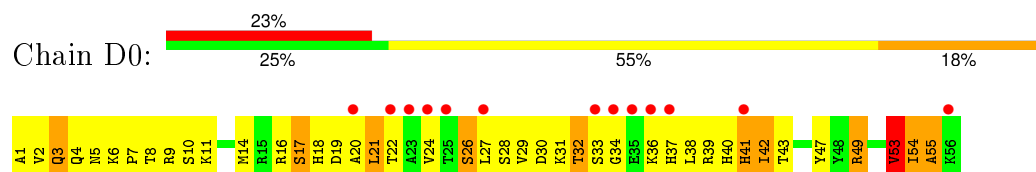
- Molecule 47: 50S ribosomal protein L30



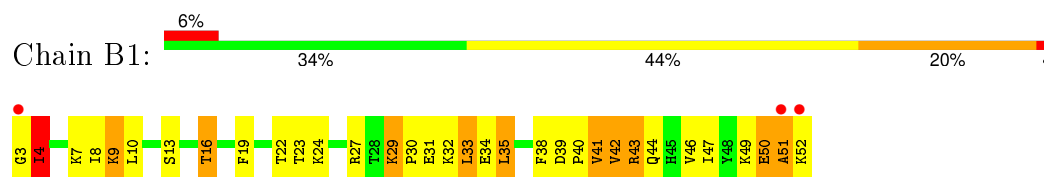
- Molecule 48: 50S ribosomal protein L32



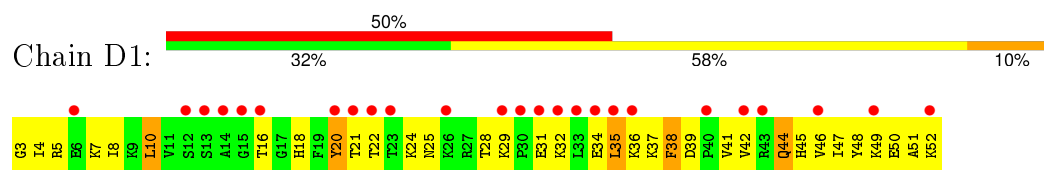
- Molecule 48: 50S ribosomal protein L32



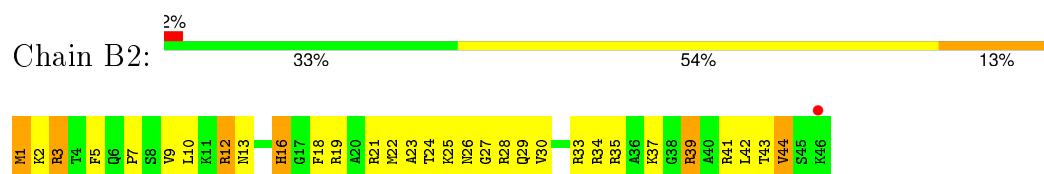
- Molecule 49: 50S ribosomal protein L33



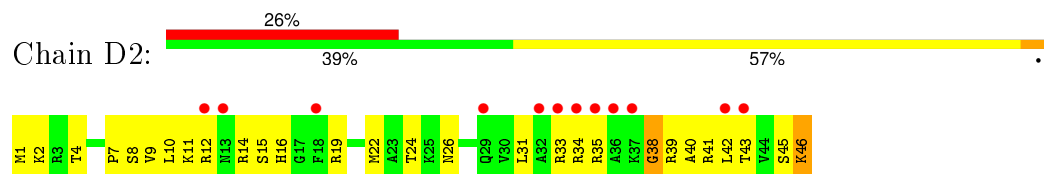
- Molecule 49: 50S ribosomal protein L33



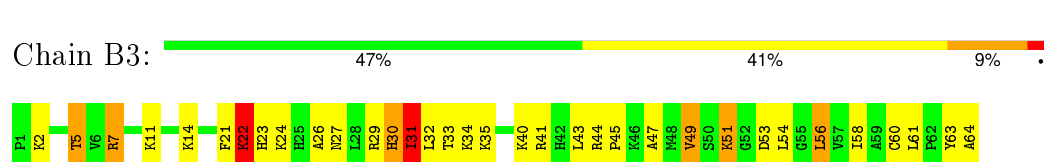
- Molecule 50: 50S ribosomal protein L34



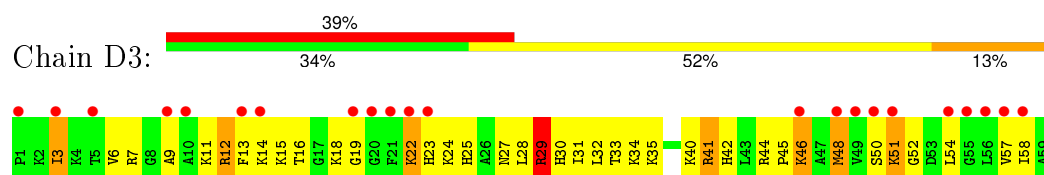
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

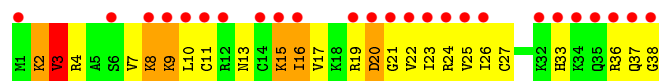


- Molecule 52: 50S ribosomal protein L36

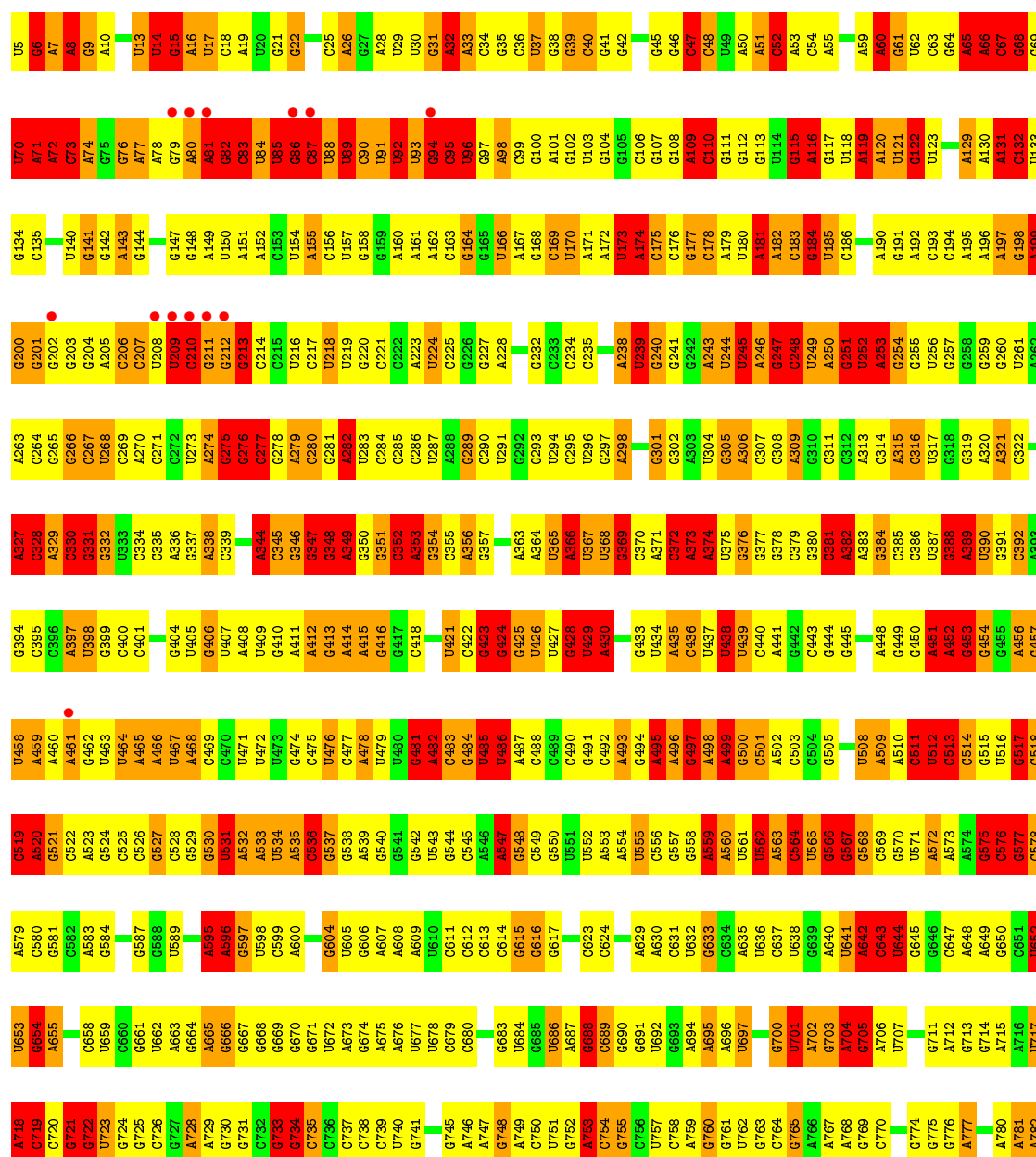
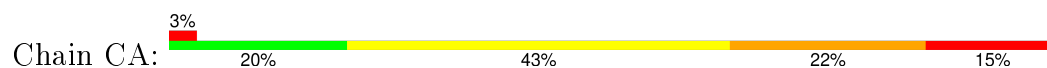


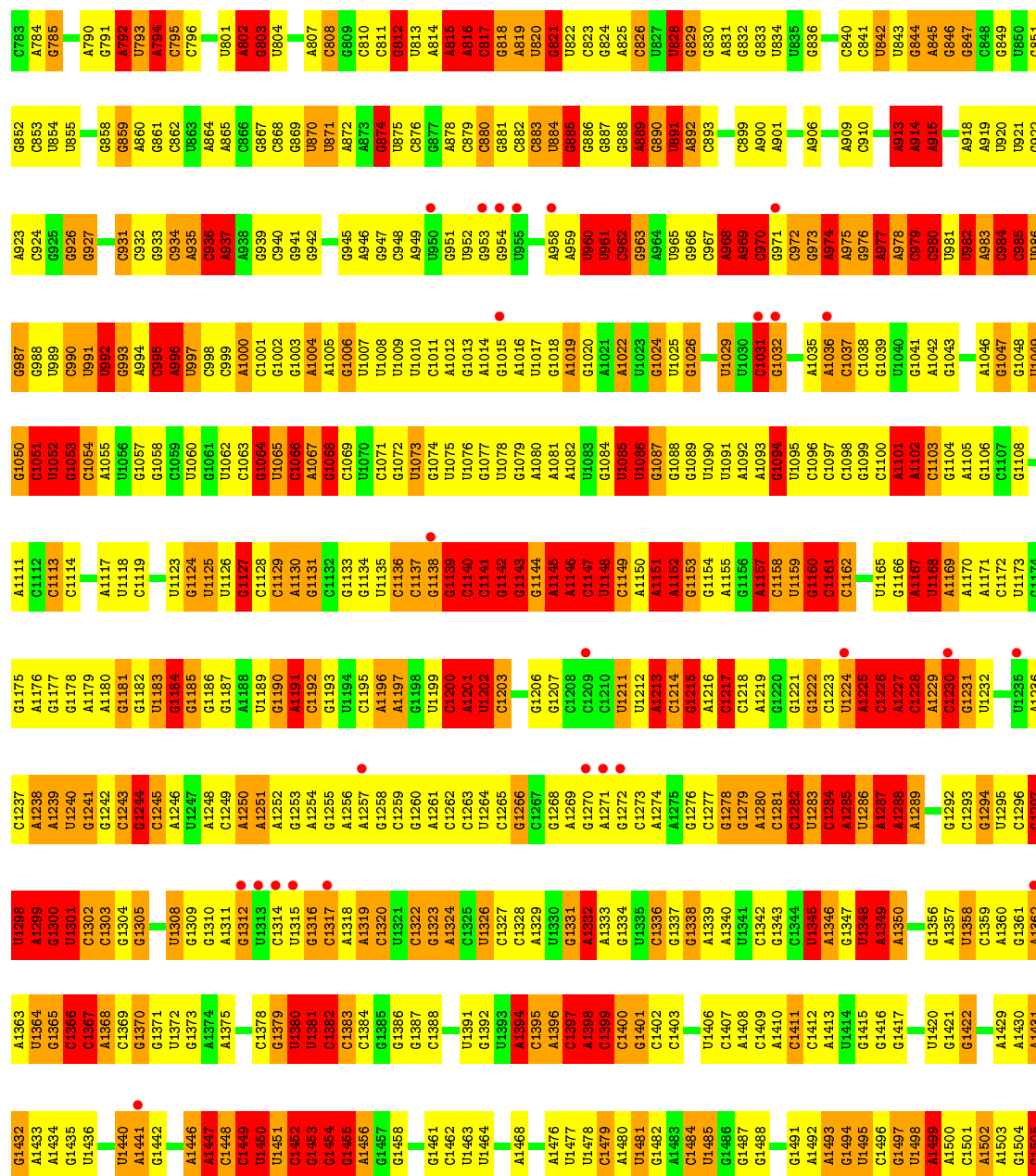


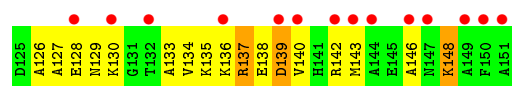
- Molecule 52: 50S ribosomal protein L36



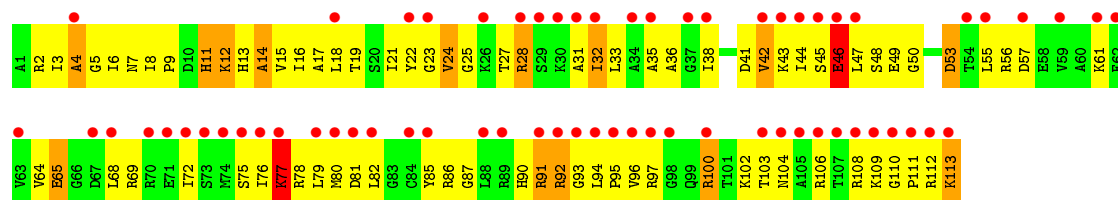
- Molecule 53: 16S rRNA



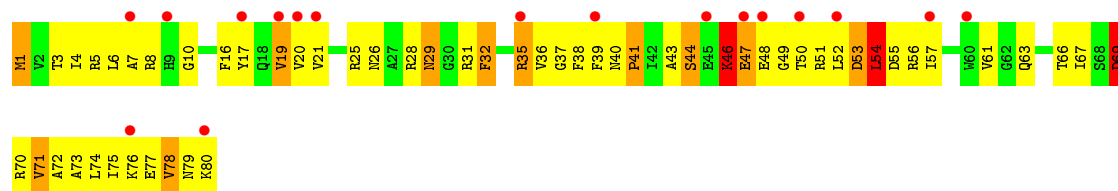




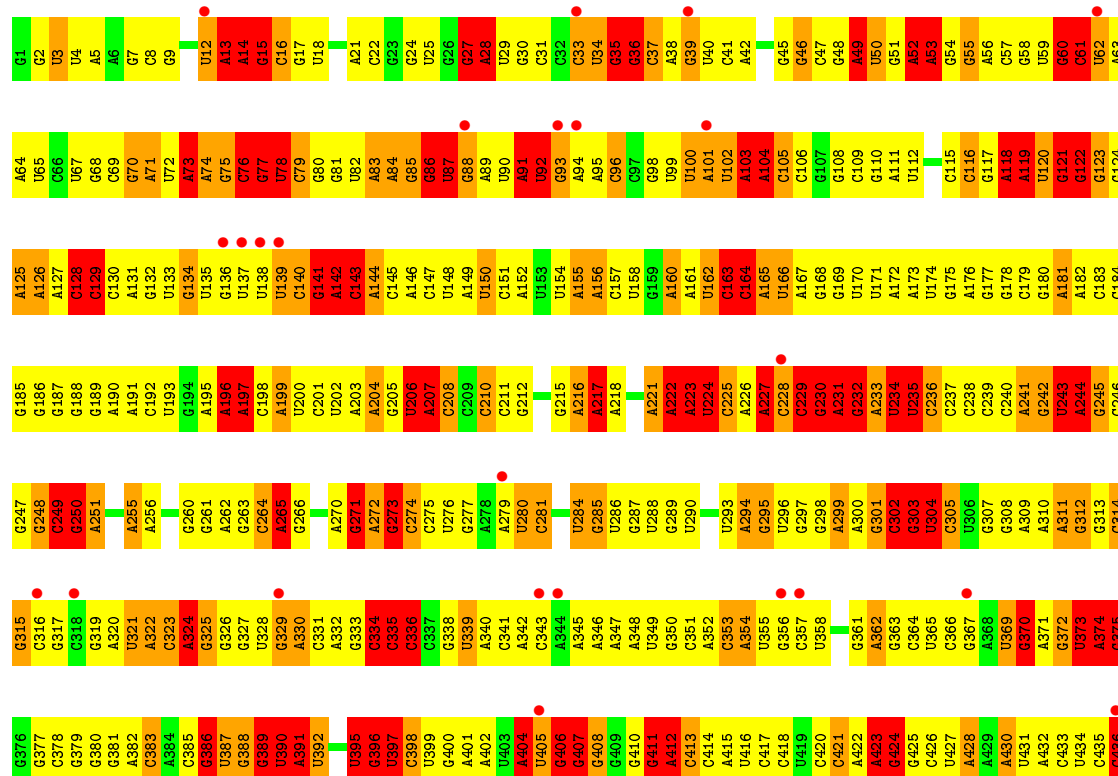
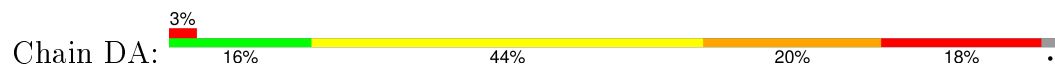
- Molecule 55: 30S ribosomal protein S13



- Molecule 56: 30S ribosomal protein S16

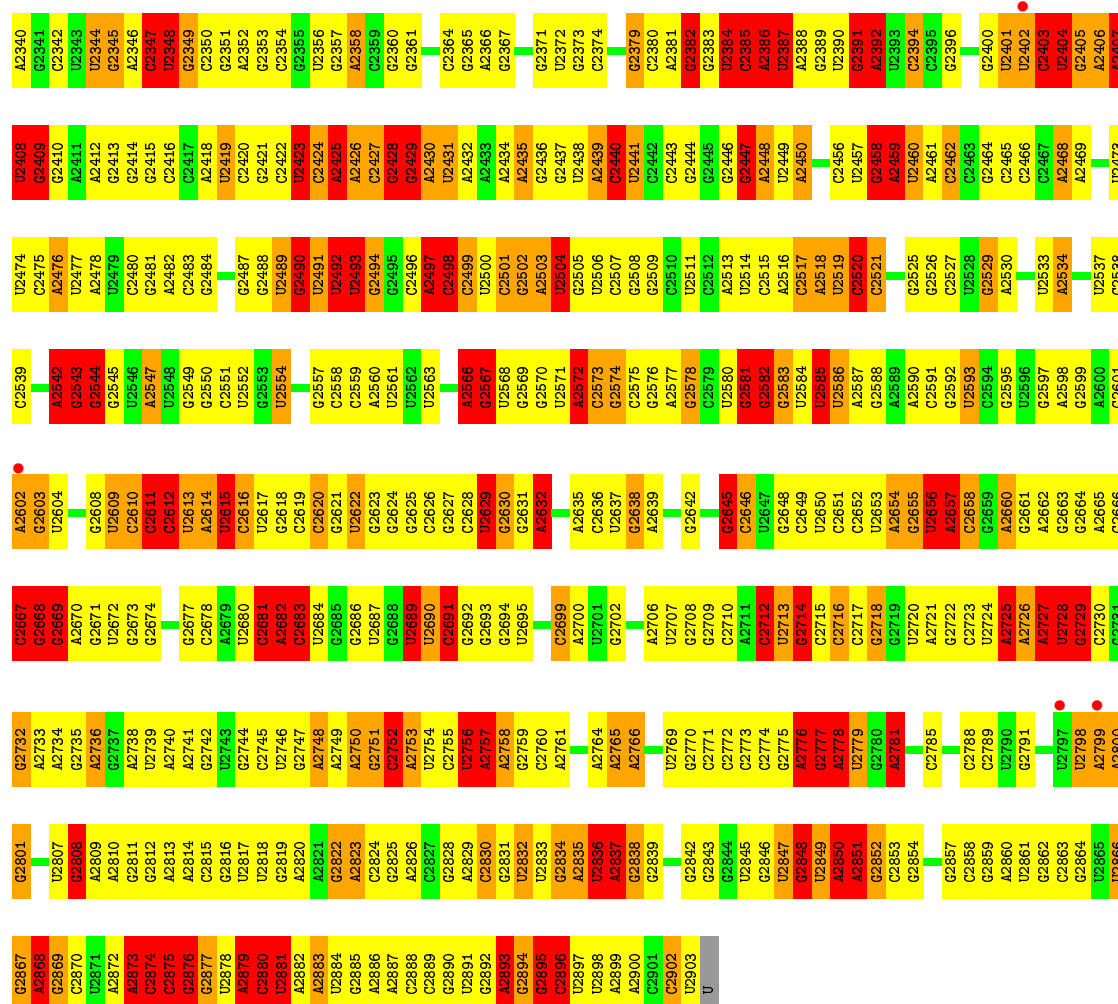


- Molecule 57: 23S rRNA



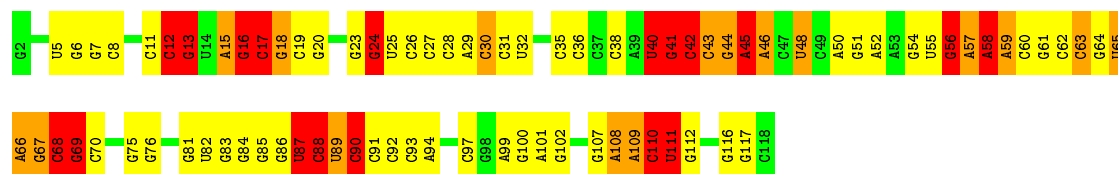
C1323	G1324	U1263	G1202	U1141	G1076	G1013	G949	A819	U755	G695	G629	U569	A497	U437
G1325	A1264	A1142	U1203	A1143	A1077	A1014	G950	A820	A756	G696	G630	G570	G498	G438
U1326	A1265	A1144	A1204	A1145	U1078	U1015	G951	A821	G757	G697	A632	A572	U499	A439
A1327	G1266	G1144	G1205	G1145	G1079	G1016	G952	G823	G762	G698	G633	U573	C440	C440
U1328	U1267	G1145	G1206	C1146	A1081	U1019	G953	G824	G763	A699	G634	A574	A502	U441
A1268	A1268	C1147	C1207	U1147	U1082	A1020	G956	G825	G764	G700	C635	A575	A503	G442
A1269	C1208	U1148	C1208	U1148	U1083	A1021	G957	G826	C765	G701	G636	U576	A504	A443
C1330	U1209	G1149	U1210	U1149	A1084	G1022	C958	U828	U766	U703	A637	G578	A507	C444
G1331	C1211	C1152	G1211	C1152	A1085	U1023	C959	U829	C766	G704	G638	G579	A508	G446
G1332	C1212	A1153	G1212	A1153	A1086	G1024	A960	A830	C767	G705	G639	G580	A509	A447
G1333	G1213	G1154	G1213	G1154	G1087	G1025	G961	G831	G770	A706	G640	U581	C509	U448
G1334	A1214	G1155	G1214	G1155	A1088	G1026	G962	G832	C771	G707	G641	C581	C510	A449
A1275	G1215	A1156	G1215	A1156	A1089	A1027	G963	U833	C772	G708	G642	A582	U511	G450
A1276	G1216	A1157	G1216	A1157	G1090	A1028	C964	A834	U773	G709	G643	G583	U512	G451
G1337	U1217	C1158	U1217	C1158	C1091	G1031	C965	G835	U774	U710	G644	C584	A513	G452
G1338	G1218	U1159	G1218	U1159	G1092	A1032	G966	C836	G775	G712	G645	A585	A514	A453
U1340	U1219	G1160	U1219	G1160	G1093	G1033	G969	C837	G776	G713	G646	A586	A515	A454
G1341	G1220	U1097	G1220	U1097	U1034	U1034	U970	C838	G777	U714	G647	C587	C516	A455
A1342	C1161	U1098	C1161	U1098	G1035	G1035	G971	C839	G778	U715	G648	U588	C517	C456
G1343	G1162	G1099	U1222	G1162	U1036	G1036	G972	C840	U779	A716	G649	A590	G518	A457
U1283	G1163	C1164	G1223	G1163	G1037	G1037	A973	C841	G780	G717	G650	U591	U519	G458
A1284	C1165	C1165	G1223	C1165	G1038	G1038	G974	C842	G781	G718	G651	A592	U459	U459
A1285	A1166	C1166	G1224	A1166	U1101	A1039	G975	A843	A782	G719	G652	U593	U525	A460
A1286	G1227	C1167	G1227	C1167	C1102	G1039	G976	A844	G783	G720	G653	U594	U526	C461
A1287	G1228	G1168	G1228	G1168	A1103	G1040	G977	A845	G784	U721	G655	U595	A527	G463
G1288	C1229	A1169	C1229	A1169	G1107	G1041	U971	U847	G785	A722	G656	U596	C527	U464
C1289	A1230	G1170	A1230	G1170	U108	G1042	A980	C848	G786	G723	G657	U597	A528	G465
C1290	U1231	G1171	U1231	G1171	C1109	G1043	A981	A849	C787	U724	G658	U598	A529	A466
G1292	G1232	C1172	G1232	C1172	G1110	G1044	C982	U850	A788	G725	G659	A599	C531	A467
C1293	U1233	U1173	U1233	U1173	G1111	A1046	A983	C851	U790	G726	G660	G600	A532	G468
U1294	U1234	U1174	U1234	U1174	A1112	G1047	A984	C852	A791	A727	G661	U599	C532	G469
C1295	G1235	A1175	G1235	A1175	C1113	A1048	C985	U853	G792	G728	G662	A602	U534	A470
G1356	A1236	U1176	A1236	U1176	U1113	C1049	G985	C854	A793	G729	G663	A603	G535	A471
G1357	G1237	G1177	G1237	G1177	C1114	A1050	A986	C855	A794	A730	G664	G604	A472	A472
G1358	U1238	C1178	U1238	C1178	G1115	G1051	U989	A856	C795	G731	G665	G605	A538	G473
G1299	G1239	G1179	G1239	G1179	G1116	G1052	A920	C857	C796	C732	A666	U606	C544	G474
A1300	U1240	U1180	U1240	U1180	C1117	C1053	A990	G858	G797	G733	G667	U607	C545	G475
A1301	A1241	U1181	A1241	U1181	C1118	A1054	C991	G859	G798	A734	A668	A608	U546	G476
A1302	U1242	G1182	U1242	G1182	U1119	G1055	G992	U860	G799	A735	G669	A609	A477	A477
G1303	C1243	U1183	C1243	U1183	G1120	G1056	G993	A861	A800	C736	G670	C610	U547	A478
A1304	A1244	G1184	A1244	G1184	G1121	A1057	C994	A862	G801	C737	C671	C611	G548	A479
C1305	G1245	U1185	G1245	U1185	G1122	U1058	C995	A863	A802	G738	C672	G612	G549	A480
G1306	A1246	G1186	A1246	G1186	G1123	U1059	A996	U864	U803	G739	C673	A613	C550	G481
A1307	U1247	G1187	U1247	G1187	G1125	U1060	G997	G865	C804	C740	G674	A614	G551	G482
A1308	G1248	A1126	G1248	A1126	A1126	U1061	C998	A866	A804	U741	A675	U615	G552	A483
G1309	U1249	U1188	U1249	U1188	A1127	G1062	U999	U867	C806	A742	A676	A616	G553	C484
C1310	G1250	A1189	G1250	A1189	G1128	G1063	A1000	U868	C807	A743	A677	G617	U554	C485
G1311	A1251	G1190	A1251	G1190	A1129	G1064	A1001	U869	U807	A744	C678	G618	G555	C486
U1312	G1252	G1191	G1252	G1191	U1130	U1065	G1002	C935	G808	U745	C679	G619	U558	C487
U1313	A1253	G1192	A1253	G1192	G1131	U1066	C936	U870	G809	G746	C680	G620	U559	G488
G1314	G1254	G1193	G1254	G1193	U1132	U1067	U1004	U871	U810	U747	G682	A621	U560	G489
C1315	U1255	A1194	U1255	A1194	A1133	G1068	C1005	U872	U811	G748	U683	G622	U561	C490
U1316	G1256	G1195	G1256	G1195	A1134	A1069	C1006	C873	C812	G749	G684	C623	A563	G491
G1317	C1257	G1196	C1257	G1196	A1070	G1070	U1007	G874	A750	A749	G685	C624	C564	A492
U1318	U1258	G1197	U1258	G1197	G1135	A1071	C944	G875	C814	A751	U686	G625	C565	G493
G1319	G1259	U1198	G1259	U1198	G1137	G1072	A1008	C876	C815	A752	U687	A626	U566	G494
C1320	U1260	U1199	U1260	U1199	G1138	A1073	A1009	A877	C816	A753	C687	G627	U567	G495
A1321	G1261	C1200	G1261	C1200	G1139	A1074	C946	A878	A754	U754	U688	A627	U568	G496
A1322	U1262	U1201	C1075	U1201	C1140	C1075	C948	G	G818		A689	G628	U569	





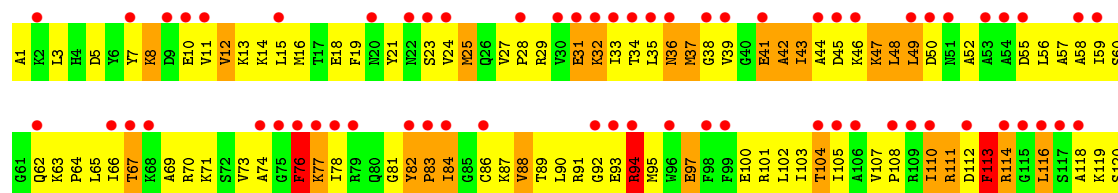
• Molecule 58: 5S rRNA

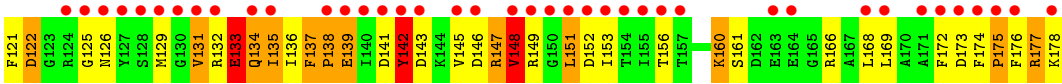
Chain DB: 29% 42% 14% 15%



• Molecule 59: 50S ribosomal protein L5

Chain DF: 26% 49% 21%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19 82.15 – 3.19	Depositor EDS
% Data completeness (in resolution range)	75.8 (82.15-3.19) 75.8 (82.15-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.252 0.204 , 0.262	Depositor DCC
R_{free} test set	15290 reflections (2.20%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 85.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 759111 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284499	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.50	6/36834 (0.0%)	1.27	532/57462 (0.9%)
2	AB	0.40	2/1736 (0.1%)	0.57	4/2338 (0.2%)
2	CB	0.37	2/1736 (0.1%)	0.54	4/2338 (0.2%)
3	AC	0.26	0/1652	0.50	0/2225
3	CC	0.23	0/1652	0.44	0/2225
4	AD	0.29	0/1665	0.52	0/2227
4	CD	0.34	0/1665	0.57	0/2227
5	AE	0.37	1/1119 (0.1%)	0.59	0/1504
5	CE	0.31	0/1119	0.55	0/1504
6	AF	0.28	0/836	0.49	0/1128
6	CF	0.27	0/836	0.50	0/1128
7	AG	0.23	0/1196	0.46	0/1602
8	AH	0.29	0/989	0.54	0/1326
8	CH	0.26	0/989	0.49	0/1326
9	AI	0.23	0/1034	0.47	0/1375
9	CI	0.22	0/1034	0.42	0/1375
10	AJ	0.24	0/797	0.49	0/1077
10	CJ	0.22	0/797	0.47	0/1077
11	AK	0.27	0/893	0.52	0/1205
11	CK	0.25	0/893	0.51	0/1205
12	AL	0.36	0/969	0.67	0/1300
12	CL	0.40	1/969 (0.1%)	0.56	0/1300
13	AM	0.22	0/893	0.47	0/1193
14	AN	0.25	0/785	0.49	0/1043
14	CN	0.21	0/780	0.39	0/1036
15	AO	0.27	0/722	0.47	0/964
15	CO	0.25	0/722	0.45	0/964
16	AP	0.28	0/659	0.49	0/884
17	AQ	0.35	0/658	0.56	0/881
17	CQ	0.27	0/658	0.51	0/881
18	AR	0.28	0/463	0.50	0/621
18	CR	0.28	0/463	0.46	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.23	0/653	0.47	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.30	0/671	0.57	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.28	0/431	0.49	0/570
21	CU	0.31	0/431	0.60	0/570
22	BA	0.71	8/68626 (0.0%)	1.50	1274/107056 (1.2%)
23	BB	0.64	0/2828	1.43	38/4410 (0.9%)
24	BC	0.41	0/2122	0.69	1/2852 (0.0%)
24	DC	0.29	0/2122	0.53	0/2852
25	BD	0.48	0/1586	0.76	2/2134 (0.1%)
25	DD	0.28	0/1586	0.57	0/2134
26	BE	0.40	0/1571	0.66	1/2113 (0.0%)
26	DE	0.25	0/1571	0.47	0/2113
27	BF	0.31	0/1435	0.54	0/1926
28	BG	0.33	0/1343	0.60	0/1816
28	DG	0.22	0/1343	0.46	0/1816
29	BH	0.30	0/1122	0.50	0/1515
29	DH	0.34	1/1122 (0.1%)	0.50	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.43	0/1410
31	BJ	0.51	0/1152	0.75	0/1551
31	DJ	0.26	0/1152	0.57	1/1551 (0.1%)
32	BK	0.46	0/948	0.78	0/1268
32	DK	0.29	0/948	0.55	0/1268
33	BL	0.42	0/1054	0.75	1/1403 (0.1%)
33	DL	0.24	0/1054	0.51	0/1403
34	BM	0.44	0/1093	0.67	0/1460
34	DM	0.27	0/1093	0.48	0/1460
35	BN	0.45	0/974	0.70	1/1301 (0.1%)
35	DN	0.27	0/974	0.51	0/1301
36	BO	0.38	0/902	0.60	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.43	0/929	0.71	0/1242
37	DP	0.28	0/929	0.49	0/1242
38	BQ	0.52	0/960	0.76	0/1278
38	DQ	0.26	0/960	0.44	0/1278
39	BR	0.54	0/829	0.77	1/1107 (0.1%)
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.50	0/864	0.73	0/1156
40	DS	0.27	0/864	0.51	0/1156
41	BT	0.43	0/745	0.71	0/994
41	DT	0.22	0/745	0.48	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	BU	0.39	0/788	0.70	0/1051
42	DU	0.23	0/788	0.46	0/1051
43	BV	0.39	0/766	0.61	0/1025
43	DV	0.23	0/766	0.43	0/1025
44	BW	0.53	0/603	0.82	0/797
44	DW	0.25	0/603	0.49	0/797
45	BX	0.37	0/635	0.66	0/848
45	DX	0.27	0/635	0.56	0/848
46	BY	0.33	0/510	0.62	0/677
46	DY	0.21	0/510	0.43	0/677
47	BZ	0.45	0/453	0.80	0/605
47	DZ	0.25	0/453	0.50	0/605
48	B0	0.43	0/450	0.71	0/599
48	D0	0.26	0/450	0.50	0/599
49	B1	0.31	0/417	0.57	0/554
49	D1	0.24	0/417	0.45	0/554
50	B2	0.41	0/380	0.71	0/498
50	D2	0.26	0/380	0.51	0/498
51	B3	0.43	0/513	0.66	0/676
51	D3	0.27	0/513	0.52	0/676
52	B4	0.39	0/303	0.69	0/397
52	D4	0.43	0/303	0.54	0/397
53	CA	0.47	6/36762 (0.0%)	1.24	525/57350 (0.9%)
54	CG	0.22	0/1188	0.44	0/1591
55	CM	0.19	0/885	0.41	0/1181
56	CP	0.28	0/649	0.52	0/870
57	DA	0.46	0/68314	1.28	1097/106569 (1.0%)
58	DB	0.51	1/2803 (0.0%)	1.21	38/4371 (0.9%)
59	DF	0.23	0/1444	0.48	0/1937
All	All	0.50	28/306773 (0.0%)	1.19	3520/458565 (0.8%)

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
25	BD	0	1
35	BN	0	1
All	All	0	3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DB	69	G	O3'-P	-16.79	1.41	1.61
1	AA	1047	G	O3'-P	-14.49	1.43	1.61
2	AB	107	ARG	C-N	11.33	1.60	1.34
53	CA	1396	A	O3'-P	-11.26	1.47	1.61
2	CB	146	SER	C-N	10.14	1.57	1.34

The worst 5 of 3520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	CA	1396	A	P-O3'-C3'	16.36	139.33	119.70
57	DA	2586	U	N1-C1'-C2'	-15.75	93.52	114.00
22	BA	2283	C	N1-C1'-C2'	-15.29	94.12	114.00
57	DA	1997	C	N1-C1'-C2'	-14.86	94.69	114.00
23	BB	90	C	N1-C1'-C2'	-14.66	94.94	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide
2	CB	107	ARG	Mainchain

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	32895	0	16553	1473	0
2	AB	1705	0	1732	195	0
2	CB	1705	0	1732	176	0
3	AC	1625	0	1699	121	0
3	CC	1625	0	1699	127	0
4	AD	1643	0	1710	166	0
4	CD	1643	0	1710	177	0
5	AE	1106	0	1147	146	0
5	CE	1106	0	1148	123	0
6	AF	818	0	808	76	0
6	CF	818	0	808	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	89	0
8	AH	979	0	1034	102	0
8	CH	979	0	1034	115	0
9	AI	1022	0	1070	91	0
9	CI	1022	0	1070	108	0
10	AJ	787	0	828	83	0
10	CJ	787	0	828	93	0
11	AK	877	0	887	91	0
11	CK	877	0	887	79	0
12	AL	955	0	1019	92	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	70	0
14	AN	774	0	827	81	0
14	CN	769	0	822	85	0
15	AO	714	0	737	59	0
15	CO	714	0	737	58	0
16	AP	649	0	666	62	0
17	AQ	649	0	691	81	0
17	CQ	649	0	691	70	0
18	AR	456	0	478	31	0
18	CR	456	0	478	47	0
19	AS	638	0	665	47	0
19	CS	638	0	665	64	0
20	AT	665	0	714	65	0
20	CT	665	0	714	61	0
21	AU	426	0	449	79	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	2356	0
23	BB	2529	0	1281	83	0
24	BC	2083	0	2157	223	0
24	DC	2083	0	2157	262	0
25	BD	1565	0	1616	223	0
25	DD	1565	0	1616	197	0
26	BE	1552	0	1619	152	0
26	DE	1552	0	1619	179	0
27	BF	1411	0	1447	140	0
28	BG	1323	0	1374	147	0
28	DG	1323	0	1374	131	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	115	0
30	BI	1032	0	1088	109	0
30	DI	1032	0	1088	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BJ	1129	0	1162	171	0
31	DJ	1129	0	1162	133	0
32	BK	939	0	1012	113	0
32	DK	939	0	1012	128	0
33	BL	1045	0	1117	122	0
33	DL	1045	0	1117	117	0
34	BM	1074	0	1157	99	0
34	DM	1074	0	1157	107	0
35	BN	961	0	1000	96	0
35	DN	961	0	1000	134	0
36	BO	892	0	923	75	0
36	DO	892	0	923	71	0
37	BP	917	0	965	139	0
37	DP	917	0	965	130	0
38	BQ	947	0	1022	153	0
38	DQ	947	0	1022	124	0
39	BR	816	0	839	116	0
39	DR	816	0	839	87	0
40	BS	857	0	922	81	0
40	DS	857	0	922	78	0
41	BT	739	0	807	112	0
41	DT	739	0	807	108	0
42	BU	780	0	834	52	0
42	DU	780	0	834	92	0
43	BV	753	0	780	70	0
43	DV	753	0	780	71	0
44	BW	596	0	610	201	0
44	DW	596	0	610	117	0
45	BX	625	0	655	67	0
45	DX	625	0	655	85	0
46	BY	509	0	543	44	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	39	0
47	DZ	449	0	491	42	0
48	B0	444	0	461	33	0
48	D0	444	0	461	64	0
49	B1	410	0	440	38	0
49	D1	410	0	440	38	0
50	B2	377	0	418	37	0
50	D2	377	0	418	31	0
51	B3	504	0	574	46	0
51	D3	504	0	574	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	302	0	340	39	0
52	D4	302	0	343	36	0
53	CA	32831	0	16521	1811	0
54	CG	1175	0	1230	125	0
55	CM	877	0	937	97	0
56	CP	639	0	656	71	0
57	DA	60995	0	30679	3815	0
58	DB	2507	0	1270	168	0
59	DF	1420	0	1460	194	0
60	AA	42	0	0	0	0
60	AN	1	0	0	0	0
60	BA	135	0	0	0	0
60	BB	4	0	0	0	0
60	BL	1	0	0	0	0
60	CA	42	0	0	0	0
60	DA	133	0	0	0	0
60	DB	1	0	0	0	0
60	DC	1	0	0	0	0
60	DE	1	0	0	0	0
60	DJ	1	0	0	0	0
61	BA	20	0	11	1	0
62	B4	1	0	0	0	0
62	D4	1	0	0	0	0
63	AA	197	0	0	11	0
63	AL	2	0	0	0	0
63	AN	6	0	0	1	0
63	AT	2	0	0	0	0
63	AU	1	0	0	0	0
63	B2	2	0	0	0	0
63	B3	2	0	0	0	0
63	B4	2	0	0	0	0
63	BA	608	0	0	43	0
63	BB	19	0	0	0	0
63	BC	8	0	0	0	0
63	BD	2	0	0	3	0
63	BE	1	0	0	0	0
63	BL	4	0	0	1	0
63	BN	2	0	0	0	0
63	BQ	1	0	0	0	0
63	BT	2	0	0	1	0
63	BV	1	0	0	1	0
63	CA	195	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CE	3	0	0	1	0
63	CI	1	0	0	0	0
63	CL	1	0	0	0	0
63	CN	3	0	0	0	0
63	CT	2	0	0	0	0
63	CU	2	0	0	0	0
63	D2	1	0	0	1	0
63	D3	1	0	0	0	0
63	D4	4	0	0	0	0
63	DA	603	0	0	19	0
63	DB	4	0	0	0	0
63	DC	10	0	0	0	0
63	DD	1	0	0	0	0
63	DE	3	0	0	0	0
63	DJ	4	0	0	0	0
63	DL	5	0	0	0	0
63	DN	2	0	0	0	0
63	DT	2	0	0	0	0
63	DU	2	0	0	0	0
63	DV	1	0	0	0	0
All	All	284499	0	190851	17927	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 17927 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)
57:DA:2092:U:H1'	57:DA:2093:G:C8	1.52	1.43
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.44	1.29
57:DA:2092:U:O2'	57:DA:2093:G:H5"	1.08	1.24
38:BQ:63:ARG:HH12	38:BQ:96:ASP:CA	1.55	1.20
28:BG:83:THR:HA	28:BG:84:LYS:NZ	1.57	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	55 (26%)	29 (13%)	0	1
2	CB	216/218 (99%)	149 (69%)	49 (23%)	18 (8%)	1	7
3	AC	204/206 (99%)	153 (75%)	34 (17%)	17 (8%)	1	7
3	CC	204/206 (99%)	145 (71%)	39 (19%)	20 (10%)	1	4
4	AD	203/205 (99%)	133 (66%)	43 (21%)	27 (13%)	0	1
4	CD	203/205 (99%)	138 (68%)	42 (21%)	23 (11%)	0	3
5	AE	148/150 (99%)	103 (70%)	28 (19%)	17 (12%)	0	3
5	CE	148/150 (99%)	106 (72%)	24 (16%)	18 (12%)	0	2
6	AF	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	10
6	CF	98/100 (98%)	68 (69%)	19 (19%)	11 (11%)	0	3
7	AG	149/151 (99%)	108 (72%)	35 (24%)	6 (4%)	4	27
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	3	22
8	CH	127/129 (98%)	89 (70%)	29 (23%)	9 (7%)	1	10
9	AI	125/127 (98%)	84 (67%)	30 (24%)	11 (9%)	1	5
9	CI	125/127 (98%)	90 (72%)	23 (18%)	12 (10%)	1	5
10	AJ	96/98 (98%)	70 (73%)	16 (17%)	10 (10%)	1	4
10	CJ	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	1
11	AK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	8
11	CK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	8
12	AL	121/123 (98%)	88 (73%)	16 (13%)	17 (14%)	0	1
12	CL	121/123 (98%)	83 (69%)	30 (25%)	8 (7%)	1	12
13	AM	112/114 (98%)	84 (75%)	19 (17%)	9 (8%)	1	7
14	AN	92/100 (92%)	58 (63%)	22 (24%)	12 (13%)	0	2
14	CN	91/100 (91%)	60 (66%)	26 (29%)	5 (6%)	2	18
15	AO	86/88 (98%)	62 (72%)	13 (15%)	11 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	4	31
16	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	3
17	AQ	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	CQ	78/80 (98%)	61 (78%)	8 (10%)	9 (12%)	0	3
18	AR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	4	28
18	CR	53/55 (96%)	42 (79%)	10 (19%)	1 (2%)	10	50
19	AS	77/79 (98%)	59 (77%)	12 (16%)	6 (8%)	1	8
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	5
20	AT	83/85 (98%)	65 (78%)	10 (12%)	8 (10%)	1	5
20	CT	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	0	3
21	AU	49/51 (96%)	26 (53%)	15 (31%)	8 (16%)	0	1
21	CU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
24	BC	269/271 (99%)	180 (67%)	61 (23%)	28 (10%)	1	4
24	DC	269/271 (99%)	164 (61%)	72 (27%)	33 (12%)	0	2
25	BD	207/209 (99%)	141 (68%)	37 (18%)	29 (14%)	0	1
25	DD	207/209 (99%)	134 (65%)	41 (20%)	32 (16%)	0	1
26	BE	199/201 (99%)	148 (74%)	31 (16%)	20 (10%)	1	4
26	DE	199/201 (99%)	120 (60%)	54 (27%)	25 (13%)	0	2
27	BF	175/177 (99%)	127 (73%)	29 (17%)	19 (11%)	0	3
28	BG	174/176 (99%)	116 (67%)	34 (20%)	24 (14%)	0	1
28	DG	174/176 (99%)	104 (60%)	39 (22%)	31 (18%)	0	0
29	BH	147/149 (99%)	63 (43%)	52 (35%)	32 (22%)	0	0
29	DH	147/149 (99%)	73 (50%)	53 (36%)	21 (14%)	0	1
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	4
30	DI	139/141 (99%)	83 (60%)	38 (27%)	18 (13%)	0	2
31	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	1	4
31	DJ	140/142 (99%)	92 (66%)	30 (21%)	18 (13%)	0	2
32	BK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	1
32	DK	120/122 (98%)	77 (64%)	21 (18%)	22 (18%)	0	0
33	BL	141/143 (99%)	95 (67%)	30 (21%)	16 (11%)	0	3
33	DL	141/143 (99%)	78 (55%)	42 (30%)	21 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	1	4
34	DM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	3
35	BN	118/120 (98%)	88 (75%)	20 (17%)	10 (8%)	1	6
35	DN	118/120 (98%)	67 (57%)	35 (30%)	16 (14%)	0	1
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	8
36	DO	114/116 (98%)	79 (69%)	27 (24%)	8 (7%)	1	10
37	BP	112/114 (98%)	74 (66%)	23 (20%)	15 (13%)	0	1
37	DP	112/114 (98%)	66 (59%)	28 (25%)	18 (16%)	0	1
38	BQ	115/117 (98%)	99 (86%)	9 (8%)	7 (6%)	2	15
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	0	3
39	BR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	8
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	1	4
40	BS	108/110 (98%)	83 (77%)	16 (15%)	9 (8%)	1	7
40	DS	108/110 (98%)	76 (70%)	24 (22%)	8 (7%)	1	9
41	BT	91/93 (98%)	58 (64%)	20 (22%)	13 (14%)	0	1
41	DT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
42	BU	100/102 (98%)	70 (70%)	16 (16%)	14 (14%)	0	1
42	DU	100/102 (98%)	51 (51%)	27 (27%)	22 (22%)	0	0
43	BV	92/94 (98%)	77 (84%)	14 (15%)	1 (1%)	17	62
43	DV	92/94 (98%)	65 (71%)	22 (24%)	5 (5%)	2	19
44	BW	77/79 (98%)	31 (40%)	18 (23%)	28 (36%)	0	0
44	DW	77/79 (98%)	32 (42%)	26 (34%)	19 (25%)	0	0
45	BX	75/77 (97%)	58 (77%)	13 (17%)	4 (5%)	2	19
45	DX	75/77 (97%)	48 (64%)	19 (25%)	8 (11%)	0	3
46	BY	61/63 (97%)	40 (66%)	13 (21%)	8 (13%)	0	2
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	7
47	BZ	56/58 (97%)	43 (77%)	10 (18%)	3 (5%)	2	19
47	DZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	3
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	5
48	D0	54/56 (96%)	40 (74%)	7 (13%)	7 (13%)	0	2
49	B1	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	1	4
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	8	44
50	D2	44/46 (96%)	30 (68%)	7 (16%)	7 (16%)	0	1
51	B3	62/64 (97%)	51 (82%)	8 (13%)	3 (5%)	3	22
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	7
52	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	7
52	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	1
54	CG	148/150 (99%)	98 (66%)	42 (28%)	8 (5%)	2	19
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	0	3
56	CP	78/80 (98%)	49 (63%)	19 (24%)	10 (13%)	0	2
59	DF	176/178 (99%)	98 (56%)	44 (25%)	34 (19%)	0	0
All	All	11238/11447 (98%)	7571 (67%)	2387 (21%)	1280 (11%)	0	3

5 of 1280 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	40	ILE
2	AB	72	LYS
2	AB	75	ALA
2	AB	119	GLN

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%)	142 (79%)	38 (21%)	1	7
2	CB	180/180 (100%)	156 (87%)	24 (13%)	5	23
3	AC	170/170 (100%)	142 (84%)	28 (16%)	3	13
3	CC	170/170 (100%)	152 (89%)	18 (11%)	8	34
4	AD	172/172 (100%)	146 (85%)	26 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	10
5	AE	113/113 (100%)	90 (80%)	23 (20%)	1	7
5	CE	113/113 (100%)	94 (83%)	19 (17%)	2	13
6	AF	87/87 (100%)	75 (86%)	12 (14%)	4	21
6	CF	87/87 (100%)	75 (86%)	12 (14%)	4	21
7	AG	124/124 (100%)	108 (87%)	16 (13%)	5	24
8	AH	104/104 (100%)	87 (84%)	17 (16%)	3	14
8	CH	104/104 (100%)	87 (84%)	17 (16%)	3	14
9	AI	105/105 (100%)	84 (80%)	21 (20%)	1	8
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	17
10	AJ	86/86 (100%)	72 (84%)	14 (16%)	3	14
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	8	35
11	AK	90/90 (100%)	73 (81%)	17 (19%)	2	10
11	CK	90/90 (100%)	77 (86%)	13 (14%)	4	19
12	AL	103/103 (100%)	82 (80%)	21 (20%)	1	7
12	CL	103/103 (100%)	86 (84%)	17 (16%)	3	13
13	AM	92/92 (100%)	87 (95%)	5 (5%)	27	68
14	AN	79/83 (95%)	72 (91%)	7 (9%)	12	44
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	17
15	AO	76/76 (100%)	67 (88%)	9 (12%)	6	29
15	CO	76/76 (100%)	69 (91%)	7 (9%)	11	41
16	AP	65/65 (100%)	57 (88%)	8 (12%)	6	27
17	AQ	74/74 (100%)	58 (78%)	16 (22%)	1	6
17	CQ	74/74 (100%)	61 (82%)	13 (18%)	2	11
18	AR	48/48 (100%)	46 (96%)	2 (4%)	36	75
18	CR	48/48 (100%)	44 (92%)	4 (8%)	14	49
19	AS	70/70 (100%)	61 (87%)	9 (13%)	5	24
19	CS	70/70 (100%)	62 (89%)	8 (11%)	7	31
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	53 (82%)	12 (18%)	2	10
21	AU	44/44 (100%)	33 (75%)	11 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	33 (75%)	11 (25%)	1	2
24	BC	216/216 (100%)	169 (78%)	47 (22%)	1	6
24	DC	216/216 (100%)	189 (88%)	27 (12%)	6	26
25	BD	164/164 (100%)	131 (80%)	33 (20%)	1	7
25	DD	164/164 (100%)	141 (86%)	23 (14%)	4	20
26	BE	165/165 (100%)	123 (74%)	42 (26%)	1	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	8	33
27	BF	148/148 (100%)	127 (86%)	21 (14%)	4	19
28	BG	137/137 (100%)	108 (79%)	29 (21%)	1	7
28	DG	137/137 (100%)	118 (86%)	19 (14%)	4	20
29	BH	114/114 (100%)	96 (84%)	18 (16%)	3	15
29	DH	114/114 (100%)	94 (82%)	20 (18%)	2	12
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	13
30	DI	109/109 (100%)	102 (94%)	7 (6%)	22	62
31	BJ	116/116 (100%)	87 (75%)	29 (25%)	1	2
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	6	28
32	BK	103/103 (100%)	86 (84%)	17 (16%)	3	13
32	DK	103/103 (100%)	81 (79%)	22 (21%)	1	6
33	BL	102/102 (100%)	77 (76%)	25 (24%)	1	3
33	DL	102/102 (100%)	87 (85%)	15 (15%)	4	18
34	BM	109/109 (100%)	85 (78%)	24 (22%)	1	6
34	DM	109/109 (100%)	97 (89%)	12 (11%)	8	33
35	BN	100/100 (100%)	77 (77%)	23 (23%)	1	4
35	DN	100/100 (100%)	82 (82%)	18 (18%)	2	11
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	8
36	DO	86/86 (100%)	79 (92%)	7 (8%)	15	51
37	BP	99/99 (100%)	69 (70%)	30 (30%)	0	1
37	DP	99/99 (100%)	88 (89%)	11 (11%)	8	32
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	3	15
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	3	15
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	71 (84%)	13 (16%)	3	15
40	BS	93/93 (100%)	71 (76%)	22 (24%)	1	4
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	12
41	BT	80/80 (100%)	59 (74%)	21 (26%)	0	2
41	DT	80/80 (100%)	74 (92%)	6 (8%)	17	55
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	7
42	DU	83/83 (100%)	72 (87%)	11 (13%)	5	23
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
43	DV	78/78 (100%)	67 (86%)	11 (14%)	4	20
44	BW	59/59 (100%)	42 (71%)	17 (29%)	0	1
44	DW	59/59 (100%)	46 (78%)	13 (22%)	1	6
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	3
45	DX	67/67 (100%)	58 (87%)	9 (13%)	5	22
46	BY	55/55 (100%)	42 (76%)	13 (24%)	1	4
46	DY	55/55 (100%)	52 (94%)	3 (6%)	27	68
47	BZ	48/48 (100%)	34 (71%)	14 (29%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	13
48	B0	47/47 (100%)	38 (81%)	9 (19%)	2	10
48	D0	47/47 (100%)	40 (85%)	7 (15%)	4	17
49	B1	45/45 (100%)	36 (80%)	9 (20%)	1	8
49	D1	45/45 (100%)	41 (91%)	4 (9%)	12	44
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	10
50	D2	38/38 (100%)	34 (90%)	4 (10%)	8	35
51	B3	51/51 (100%)	44 (86%)	7 (14%)	4	21
51	D3	51/51 (100%)	42 (82%)	9 (18%)	2	11
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	18
52	D4	34/34 (100%)	27 (79%)	7 (21%)	1	7
54	CG	123/123 (100%)	101 (82%)	22 (18%)	2	11
55	CM	91/91 (100%)	80 (88%)	11 (12%)	6	28
56	CP	65/65 (100%)	52 (80%)	13 (20%)	1	8
59	DF	149/149 (100%)	123 (83%)	26 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7772 (83%)	1559 (17%)	3 13

5 of 1559 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	25	LEU
49	B1	35	LEU
39	DR	13	ARG
40	BS	33	LEU
43	BV	43	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 333 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	72	GLN
3	CC	7	ASN
41	DT	48	GLN
43	BV	5	ASN
50	B2	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	478 (31%)	237 (15%)
22	BA	2850/2903 (98%)	829 (29%)	411 (14%)
23	BB	117/118 (99%)	31 (26%)	17 (14%)
53	CA	1529/1530 (99%)	540 (35%)	242 (15%)
57	DA	2838/2904 (97%)	1042 (36%)	504 (17%)
58	DB	116/117 (99%)	37 (31%)	17 (14%)
All	All	8982/9105 (98%)	2957 (32%)	1428 (15%)

5 of 2957 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 1428 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2880	C
53	CA	816	A
57	DA	2289	G
23	BB	109	A
53	CA	331	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 364 are monoatomic - leaving 1 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	$\# Z > 2$
61	CLM	BA	3136	-	18,20,20	2.42	4 (22%)	22,27,27	1.92	5 (22%)

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
61	CLM	BA	3136	-	-	0/22/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	3136	CLM	C8-C9	2.38	1.43	1.38
61	BA	3136	CLM	C2-N2	3.87	1.42	1.34
61	BA	3136	CLM	C11-C6	5.33	1.47	1.39
61	BA	3136	CLM	O9B-N9	6.62	1.35	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BA	3136	CLM	C3-N2-C2	-4.85	114.11	123.13
61	BA	3136	CLM	C4-C3-N2	2.64	114.10	109.29
61	BA	3136	CLM	O5-C5-C3	2.66	115.05	107.94
61	BA	3136	CLM	O4-C4-C3	2.71	118.37	111.12
61	BA	3136	CLM	C6-C5-C3	4.26	119.68	111.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BA	3136	CLM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.63	16 (1%) 84 75	28, 82, 201, 415	0
2	AB	218/218 (100%)	1.69	72 (33%) 0 0	117, 160, 233, 278	0
2	CB	218/218 (100%)	1.20	44 (20%) 1 1	121, 173, 237, 292	0
3	AC	206/206 (100%)	0.52	13 (6%) 23 13	64, 107, 164, 196	0
3	CC	206/206 (100%)	1.09	30 (14%) 3 2	79, 158, 229, 303	0
4	AD	205/205 (100%)	-0.05	6 (2%) 55 41	45, 89, 164, 275	0
4	CD	205/205 (100%)	-0.28	1 (0%) 91 87	39, 61, 122, 254	0
5	AE	150/150 (100%)	-0.15	1 (0%) 89 83	57, 81, 142, 210	0
5	CE	150/150 (100%)	0.36	3 (2%) 68 54	67, 99, 157, 252	0
6	AF	100/100 (100%)	0.10	4 (4%) 42 27	55, 103, 161, 189	0
6	CF	100/100 (100%)	-0.02	1 (1%) 84 75	72, 116, 176, 217	0
7	AG	151/151 (100%)	0.49	13 (8%) 13 7	88, 150, 218, 247	0
8	AH	129/129 (100%)	0.17	7 (5%) 29 17	44, 82, 127, 184	0
8	CH	129/129 (100%)	0.64	9 (6%) 19 11	68, 113, 170, 246	0
9	AI	127/127 (100%)	1.04	24 (18%) 2 1	72, 154, 248, 287	0
9	CI	127/127 (100%)	2.02	51 (40%) 0 0	116, 201, 289, 319	0
10	AJ	98/98 (100%)	0.77	16 (16%) 2 1	78, 127, 203, 244	0
10	CJ	98/98 (100%)	2.83	55 (56%) 0 0	114, 204, 278, 301	0
11	AK	117/117 (100%)	0.85	17 (14%) 3 2	47, 117, 196, 238	0
11	CK	117/117 (100%)	0.25	5 (4%) 39 25	68, 117, 175, 239	0
12	AL	123/123 (100%)	-0.16	1 (0%) 87 80	24, 57, 121, 180	0
12	CL	123/123 (100%)	0.48	8 (6%) 22 12	44, 89, 144, 226	0
13	AM	114/114 (100%)	0.67	16 (14%) 4 2	90, 158, 240, 281	0
14	AN	96/100 (96%)	0.48	13 (13%) 4 2	76, 122, 214, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	2.60	46 (48%) 0 0	123, 239, 369, 399	0
15	AO	88/88 (100%)	-0.40	0 100 100	40, 81, 123, 187	0
15	CO	88/88 (100%)	0.02	1 (1%) 82 72	76, 122, 190, 265	0
16	AP	82/82 (100%)	0.51	8 (9%) 10 5	46, 79, 155, 228	0
17	AQ	80/80 (100%)	0.42	6 (7%) 17 9	36, 79, 146, 244	0
17	CQ	80/80 (100%)	1.01	10 (12%) 5 3	61, 112, 163, 194	0
18	AR	55/55 (100%)	0.23	2 (3%) 46 31	60, 92, 174, 242	0
18	CR	55/55 (100%)	0.01	0 100 100	48, 91, 159, 236	0
19	AS	79/79 (100%)	1.28	23 (29%) 1 0	95, 156, 236, 256	0
19	CS	79/79 (100%)	2.94	45 (56%) 0 0	206, 416, 490, 515	0
20	AT	85/85 (100%)	-0.24	0 100 100	46, 83, 124, 174	0
20	CT	85/85 (100%)	1.11	18 (21%) 1 1	76, 142, 200, 234	0
21	AU	51/51 (100%)	1.90	24 (47%) 0 0	91, 152, 216, 243	0
21	CU	51/51 (100%)	0.54	4 (7%) 16 9	82, 115, 208, 290	0
22	BA	2854/2903 (98%)	-0.55	40 (1%) 78 65	7, 31, 162, 401	0
23	BB	118/118 (100%)	-0.69	0 100 100	20, 45, 78, 115	0
24	BC	271/271 (100%)	-0.35	6 (2%) 65 50	13, 41, 96, 201	0
24	DC	271/271 (100%)	0.65	31 (11%) 7 4	45, 101, 160, 200	0
25	BD	209/209 (100%)	-0.47	0 100 100	7, 29, 80, 144	0
25	DD	209/209 (100%)	0.97	39 (18%) 2 1	60, 123, 193, 270	0
26	BE	201/201 (100%)	-0.35	0 100 100	7, 42, 105, 189	0
26	DE	201/201 (100%)	1.92	73 (36%) 0 0	68, 254, 429, 475	0
27	BF	177/177 (100%)	0.05	6 (3%) 49 34	33, 78, 142, 205	0
28	BG	176/176 (100%)	-0.10	2 (1%) 82 72	23, 62, 124, 215	0
28	DG	176/176 (100%)	2.14	84 (47%) 0 0	79, 207, 297, 363	0
29	BH	149/149 (100%)	3.09	62 (41%) 0 0	41, 178, 274, 301	0
29	DH	149/149 (100%)	2.73	66 (44%) 0 0	93, 182, 270, 305	0
30	BI	141/141 (100%)	2.41	67 (47%) 0 0	171, 257, 316, 355	0
30	DI	141/141 (100%)	4.03	102 (72%) 0 0	227, 344, 382, 400	0
31	BJ	142/142 (100%)	-0.54	0 100 100	9, 23, 68, 127	0
31	DJ	142/142 (100%)	0.66	15 (10%) 8 4	63, 122, 184, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
32	BK	122/122 (100%)	-0.50	0 100 100	14, 31, 84, 254	0
32	DK	122/122 (100%)	0.83	19 (15%) 3 2	57, 106, 172, 204	0
33	BL	143/143 (100%)	-0.52	0 100 100	9, 37, 80, 126	0
33	DL	143/143 (100%)	1.60	46 (32%) 1 0	68, 176, 296, 329	0
34	BM	136/136 (100%)	-0.55	0 100 100	9, 29, 71, 133	0
34	DM	136/136 (100%)	0.89	21 (15%) 3 2	47, 126, 187, 223	0
35	BN	120/120 (100%)	-0.54	0 100 100	10, 25, 48, 123	0
35	DN	120/120 (100%)	1.62	43 (35%) 0 0	90, 149, 231, 305	0
36	BO	116/116 (100%)	-0.31	0 100 100	28, 49, 93, 126	0
36	DO	116/116 (100%)	1.57	36 (31%) 1 0	132, 176, 238, 280	0
37	BP	114/114 (100%)	-0.35	1 (0%) 85 78	17, 39, 95, 184	0
37	DP	114/114 (100%)	1.11	22 (19%) 2 1	63, 122, 187, 204	0
38	BQ	117/117 (100%)	-0.63	0 100 100	7, 20, 46, 100	0
38	DQ	117/117 (100%)	1.04	22 (18%) 2 1	78, 127, 221, 298	0
39	BR	103/103 (100%)	-0.50	1 (0%) 84 75	7, 34, 78, 139	0
39	DR	103/103 (100%)	2.49	51 (49%) 0 0	80, 157, 275, 306	0
40	BS	110/110 (100%)	-0.57	0 100 100	8, 23, 56, 172	0
40	DS	110/110 (100%)	1.77	43 (39%) 0 0	69, 142, 254, 323	0
41	BT	93/93 (100%)	-0.10	2 (2%) 65 50	22, 53, 135, 194	0
41	DT	93/93 (100%)	2.21	41 (44%) 0 0	125, 241, 359, 398	0
42	BU	102/102 (100%)	-0.09	2 (1%) 68 54	22, 54, 111, 237	0
42	DU	102/102 (100%)	3.95	66 (64%) 0 0	135, 334, 460, 561	0
43	BV	94/94 (100%)	-0.28	0 100 100	18, 47, 89, 149	0
43	DV	94/94 (100%)	1.14	21 (22%) 1 1	109, 156, 208, 233	0
44	BW	79/79 (100%)	-0.17	2 (2%) 61 47	13, 36, 90, 194	0
44	DW	79/79 (100%)	2.06	37 (46%) 0 0	99, 166, 250, 315	0
45	BX	77/77 (100%)	-0.41	0 100 100	17, 42, 87, 113	0
45	DX	77/77 (100%)	0.82	13 (16%) 2 1	72, 122, 190, 222	0
46	BY	63/63 (100%)	-0.15	1 (1%) 74 62	34, 73, 121, 155	0
46	DY	63/63 (100%)	1.72	20 (31%) 1 0	159, 374, 464, 494	0
47	BZ	58/58 (100%)	-0.54	0 100 100	7, 26, 61, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DZ	58/58 (100%)	0.64	5 (8%) 13 7	80, 142, 228, 257	0
48	B0	56/56 (100%)	-0.70	0 100 100	6, 26, 80, 127	0
48	D0	56/56 (100%)	1.34	13 (23%) 1 1	75, 148, 244, 284	0
49	B1	50/50 (100%)	0.77	3 (6%) 25 14	42, 66, 121, 173	0
49	D1	50/50 (100%)	2.17	25 (50%) 0 0	114, 179, 216, 264	0
50	B2	46/46 (100%)	-0.58	1 (2%) 65 50	11, 27, 56, 164	0
50	D2	46/46 (100%)	1.33	12 (26%) 1 0	79, 130, 179, 205	0
51	B3	64/64 (100%)	-0.58	0 100 100	11, 29, 53, 81	0
51	D3	64/64 (100%)	1.76	25 (39%) 0 0	85, 145, 232, 281	0
52	B4	38/38 (100%)	0.20	1 (2%) 59 45	29, 53, 95, 103	0
52	D4	38/38 (100%)	2.69	25 (65%) 0 0	87, 165, 229, 248	0
53	CA	1530/1530 (100%)	-0.08	40 (2%) 59 45	43, 110, 301, 420	0
54	CG	150/150 (100%)	2.30	70 (46%) 0 0	101, 233, 303, 344	0
55	CM	113/113 (100%)	2.58	65 (57%) 0 0	226, 447, 522, 562	0
56	CP	80/80 (100%)	0.96	17 (21%) 1 1	49, 105, 165, 226	0
57	DA	2841/2904 (97%)	0.20	89 (3%) 52 38	51, 132, 279, 491	0
58	DB	117/117 (100%)	-0.21	0 100 100	107, 180, 240, 264	0
59	DF	178/178 (100%)	2.46	104 (58%) 0 0	175, 239, 286, 345	0
All	All	20431/20552 (99%)	0.34	2211 (10%) 8 4	6, 103, 285, 562	0

The worst 5 of 2211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	22.2
14	CN	33	VAL	20.9
29	DH	124	THR	20.6
30	DI	51	GLY	20.1
29	DH	91	PHE	17.7

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

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

6.3 Carbohydrates ⓘ

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
60	MG	BA	3130	1/1	0.98	0.44	20.61	257,257,257,257	0
60	MG	DA	3059	1/1	0.94	0.38	15.13	241,241,241,241	0
60	MG	AA	1640	1/1	0.98	0.25	11.81	189,189,189,189	0
60	MG	CA	1640	1/1	0.89	0.29	10.84	171,171,171,171	0
60	MG	BA	3123	1/1	0.95	0.56	10.48	112,112,112,112	0
60	MG	DA	3074	1/1	0.88	0.45	8.03	239,239,239,239	0
60	MG	BA	3135	1/1	0.79	0.38	7.74	204,204,204,204	0
60	MG	BA	3107	1/1	0.97	0.19	4.67	8,8,8,8	0
60	MG	DA	3002	1/1	0.67	0.39	4.57	229,229,229,229	0
60	MG	BA	3082	1/1	0.95	0.17	4.13	98,98,98,98	0
60	MG	BA	3104	1/1	0.95	0.18	3.86	27,27,27,27	0
60	MG	BA	3039	1/1	0.98	0.20	3.64	9,9,9,9	0
60	MG	BA	3103	1/1	0.90	0.20	3.39	8,8,8,8	0
60	MG	BA	3115	1/1	0.96	0.18	3.28	8,8,8,8	0
60	MG	BA	3069	1/1	0.89	0.19	2.94	223,223,223,223	0
60	MG	BA	3026	1/1	0.99	0.18	2.80	122,122,122,122	0
60	MG	CA	1628	1/1	0.81	0.34	2.68	259,259,259,259	0
60	MG	DA	3114	1/1	0.97	0.24	2.47	166,166,166,166	0
60	MG	BA	3013	1/1	0.99	0.18	2.42	6,6,6,6	0
60	MG	BA	3096	1/1	0.98	0.17	2.29	59,59,59,59	0
60	MG	BA	3100	1/1	0.96	0.17	2.12	26,26,26,26	0
60	MG	DA	3105	1/1	0.54	0.23	2.06	305,305,305,305	0
60	MG	DA	3129	1/1	0.91	0.62	1.99	271,271,271,271	0
60	MG	CA	1625	1/1	0.95	0.21	1.34	160,160,160,160	0
60	MG	BA	3108	1/1	0.98	0.17	1.28	6,6,6,6	0
60	MG	CA	1607	1/1	0.91	0.21	1.14	222,222,222,222	0
60	MG	DA	3068	1/1	0.86	0.28	1.04	225,225,225,225	0
60	MG	DA	3043	1/1	0.91	0.22	0.82	112,112,112,112	0
60	MG	CA	1641	1/1	0.95	0.18	0.80	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1616	1/1	0.81	0.35	0.75	279,279,279,279	0
60	MG	DA	3056	1/1	0.84	0.37	0.74	243,243,243,243	0
60	MG	BA	3008	1/1	0.96	0.16	0.72	29,29,29,29	0
61	CLM	BA	3136	20/20	0.97	0.20	0.64	2,26,77,92	0
60	MG	BA	3129	1/1	0.99	0.15	0.48	15,15,15,15	0
60	MG	AA	1641	1/1	0.98	0.16	0.45	27,27,27,27	0
60	MG	AA	1630	1/1	0.95	0.14	0.44	209,209,209,209	0
60	MG	DA	3100	1/1	0.92	0.24	0.39	149,149,149,149	0
60	MG	DA	3133	1/1	0.74	0.26	0.38	241,241,241,241	0
60	MG	DA	3109	1/1	0.77	0.34	0.24	169,169,169,169	0
60	MG	DA	3026	1/1	0.62	0.21	0.23	139,139,139,139	0
60	MG	CA	1611	1/1	0.91	0.18	0.21	116,116,116,116	0
60	MG	AN	201	1/1	0.76	0.20	0.10	219,219,219,219	0
60	MG	AA	1621	1/1	0.99	0.14	-0.08	35,35,35,35	0
60	MG	CA	1631	1/1	0.92	0.20	-0.09	111,111,111,111	0
60	MG	DA	3128	1/1	0.94	0.26	-0.15	138,138,138,138	0
60	MG	BA	3072	1/1	0.99	0.16	-0.20	81,81,81,81	0
60	MG	CA	1618	1/1	0.78	0.17	-0.20	141,141,141,141	0
60	MG	DA	3094	1/1	0.91	0.21	-0.22	98,98,98,98	0
60	MG	CA	1637	1/1	0.92	0.19	-0.23	140,140,140,140	0
60	MG	DA	3041	1/1	0.77	0.20	-0.30	133,133,133,133	0
60	MG	CA	1629	1/1	0.77	0.20	-0.31	214,214,214,214	0
60	MG	CA	1621	1/1	0.97	0.16	-0.43	60,60,60,60	0
60	MG	DA	3050	1/1	0.84	0.17	-0.45	89,89,89,89	0
60	MG	BA	3106	1/1	0.96	0.14	-0.67	13,13,13,13	0
60	MG	DB	201	1/1	0.90	0.12	-0.68	109,109,109,109	0
60	MG	DC	301	1/1	0.91	0.15	-0.83	134,134,134,134	0
60	MG	BA	3131	1/1	0.98	0.09	-0.85	96,96,96,96	0
60	MG	DA	3082	1/1	0.79	0.11	-0.91	214,214,214,214	0
60	MG	BA	3046	1/1	0.95	0.12	-0.93	142,142,142,142	0
60	MG	CA	1617	1/1	0.80	0.15	-0.94	205,205,205,205	0
60	MG	AA	1632	1/1	0.97	0.10	-0.94	53,53,53,53	0
60	MG	DA	3102	1/1	0.94	0.16	-0.95	105,105,105,105	0
60	MG	BA	3120	1/1	0.99	0.06	-1.00	44,44,44,44	0
60	MG	BA	3048	1/1	0.97	0.14	-1.13	18,18,18,18	0
60	MG	BA	3133	1/1	0.99	0.14	-1.18	5,5,5,5	0
60	MG	DA	3022	1/1	0.90	0.17	-1.21	118,118,118,118	0
60	MG	CA	1606	1/1	0.88	0.14	-1.24	77,77,77,77	0
60	MG	BA	3049	1/1	0.97	0.12	-1.37	72,72,72,72	0
60	MG	AA	1616	1/1	0.97	0.13	-1.44	123,123,123,123	0
60	MG	BA	3119	1/1	0.98	0.14	-1.45	15,15,15,15	0
60	MG	DA	3047	1/1	0.96	0.14	-1.51	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3111	1/1	0.96	0.11	-1.53	89,89,89,89	0
60	MG	DA	3024	1/1	0.82	0.14	-1.56	147,147,147,147	0
60	MG	DA	3099	1/1	0.96	0.15	-1.59	96,96,96,96	0
60	MG	DA	3032	1/1	0.84	0.19	-1.59	193,193,193,193	0
60	MG	BA	3113	1/1	0.98	0.10	-1.62	34,34,34,34	0
60	MG	DA	3023	1/1	0.78	0.18	-1.70	90,90,90,90	0
60	MG	DA	3083	1/1	0.55	0.10	-1.72	176,176,176,176	0
60	MG	BA	3056	1/1	0.96	0.12	-1.74	86,86,86,86	0
60	MG	DA	3038	1/1	0.94	0.18	-1.85	163,163,163,163	0
60	MG	CA	1634	1/1	0.90	0.16	-2.04	200,200,200,200	0
60	MG	AA	1604	1/1	0.94	0.10	-2.19	112,112,112,112	0
60	MG	BB	202	1/1	0.93	0.09	-2.20	54,54,54,54	0
60	MG	DA	3065	1/1	0.98	0.12	-2.38	40,40,40,40	0
60	MG	DA	3054	1/1	0.98	0.13	-2.44	125,125,125,125	0
60	MG	DA	3064	1/1	0.96	0.13	-2.48	65,65,65,65	0
60	MG	AA	1611	1/1	0.98	0.10	-2.49	81,81,81,81	0
60	MG	DA	3071	1/1	0.90	0.09	-2.52	136,136,136,136	0
60	MG	BA	3128	1/1	0.99	0.13	-2.62	6,6,6,6	0
60	MG	DA	3131	1/1	0.92	0.10	-2.64	104,104,104,104	0
62	ZN	D4	101	1/1	0.92	0.09	-2.74	197,197,197,197	0
60	MG	BA	3027	1/1	0.98	0.12	-2.75	34,34,34,34	0
60	MG	DA	3012	1/1	0.89	0.12	-2.78	57,57,57,57	0
60	MG	AA	1609	1/1	0.95	0.10	-2.86	47,47,47,47	0
60	MG	DA	3103	1/1	0.87	0.16	-2.87	36,36,36,36	0
60	MG	AA	1607	1/1	0.94	0.10	-2.93	98,98,98,98	0
60	MG	DA	3049	1/1	0.92	0.14	-2.99	150,150,150,150	0
60	MG	DA	3104	1/1	0.96	0.15	-2.99	48,48,48,48	0
60	MG	BA	3022	1/1	0.91	0.11	-3.02	20,20,20,20	0
60	MG	BA	3052	1/1	0.99	0.09	-3.07	12,12,12,12	0
60	MG	DA	3051	1/1	0.95	0.09	-3.07	49,49,49,49	0
60	MG	DA	3039	1/1	0.97	0.15	-3.10	59,59,59,59	0
60	MG	BA	3023	1/1	0.99	0.12	-3.15	8,8,8,8	0
60	MG	AA	1606	1/1	0.98	0.10	-3.19	58,58,58,58	0
60	MG	CA	1642	1/1	0.88	0.07	-3.34	121,121,121,121	0
60	MG	BA	3062	1/1	1.00	0.13	-3.40	9,9,9,9	0
60	MG	DA	3123	1/1	0.95	0.14	-3.43	65,65,65,65	0
60	MG	BA	3012	1/1	0.93	0.13	-3.43	5,5,5,5	0
60	MG	BA	3109	1/1	0.98	0.10	-3.48	105,105,105,105	0
60	MG	BA	3021	1/1	0.98	0.11	-3.77	15,15,15,15	0
60	MG	BA	3002	1/1	0.94	0.09	-3.79	60,60,60,60	0
60	MG	BA	3095	1/1	0.99	0.12	-3.93	13,13,13,13	0
62	ZN	B4	101	1/1	0.96	0.05	-3.95	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1613	1/1	0.96	0.09	-4.10	56,56,56,56	0
60	MG	BA	3067	1/1	0.99	0.11	-4.26	22,22,22,22	0
60	MG	DA	3078	1/1	0.92	0.11	-4.31	95,95,95,95	0
60	MG	CA	1639	1/1	0.94	0.06	-4.50	148,148,148,148	0
60	MG	DA	3016	1/1	0.95	0.12	-4.55	75,75,75,75	0
60	MG	DA	3060	1/1	0.93	0.07	-4.77	144,144,144,144	0
60	MG	BA	3005	1/1	0.96	0.07	-4.78	60,60,60,60	0
60	MG	CA	1604	1/1	0.95	0.04	-4.79	65,65,65,65	0
60	MG	BA	3020	1/1	0.99	0.11	-4.85	21,21,21,21	0
60	MG	AA	1628	1/1	0.97	0.06	-5.14	70,70,70,70	0
60	MG	BA	3117	1/1	0.90	0.09	-5.63	79,79,79,79	0
60	MG	CA	1609	1/1	0.97	0.13	-5.63	71,71,71,71	0
60	MG	CA	1613	1/1	0.95	0.08	-5.74	116,116,116,116	0
60	MG	BA	3092	1/1	0.86	0.07	-5.96	30,30,30,30	0
60	MG	BA	3061	1/1	0.97	0.12	-6.37	11,11,11,11	0
60	MG	BA	3064	1/1	0.98	0.08	-6.68	8,8,8,8	0
60	MG	AA	1633	1/1	0.96	0.09	-6.74	52,52,52,52	0
60	MG	AA	1624	1/1	0.98	0.06	-7.28	139,139,139,139	0
60	MG	BA	3070	1/1	0.99	0.11	-7.65	76,76,76,76	0
60	MG	BA	3016	1/1	0.99	0.07	-7.67	5,5,5,5	0
60	MG	BA	3057	1/1	0.95	0.06	-7.86	43,43,43,43	0
60	MG	AA	1642	1/1	0.99	0.09	-7.86	42,42,42,42	0
60	MG	BA	3078	1/1	0.96	0.07	-8.31	49,49,49,49	0
60	MG	DA	3061	1/1	0.49	0.61	-	210,210,210,210	0
60	MG	BA	3075	1/1	0.94	0.19	-	74,74,74,74	0
60	MG	DA	3076	1/1	0.95	0.08	-	110,110,110,110	0
60	MG	DA	3063	1/1	0.27	0.97	-	305,305,305,305	0
60	MG	BA	3010	1/1	0.96	0.09	-	48,48,48,48	0
60	MG	BA	3001	1/1	0.94	0.07	-	84,84,84,84	0
60	MG	BA	3132	1/1	0.90	0.40	-	145,145,145,145	0
60	MG	BB	201	1/1	0.81	0.22	-	246,246,246,246	0
60	MG	DA	3057	1/1	0.88	0.40	-	257,257,257,257	0
60	MG	BA	3094	1/1	0.92	0.07	-	42,42,42,42	0
60	MG	DA	3067	1/1	0.93	0.11	-	95,95,95,95	0
60	MG	CA	1626	1/1	0.98	0.22	-	27,27,27,27	0
60	MG	BA	3017	1/1	0.98	0.07	-	27,27,27,27	0
60	MG	DE	301	1/1	0.58	0.31	-	191,191,191,191	0
60	MG	BA	3112	1/1	0.98	0.16	-	33,33,33,33	0
60	MG	BA	3099	1/1	0.99	0.10	-	32,32,32,32	0
60	MG	DA	3081	1/1	0.94	0.22	-	143,143,143,143	0
60	MG	BA	3033	1/1	0.95	0.16	-	89,89,89,89	0
60	MG	BA	3101	1/1	0.98	0.06	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3084	1/1	0.97	0.13	-	9,9,9,9	0
60	MG	DA	3118	1/1	0.97	0.06	-	75,75,75,75	0
60	MG	AA	1626	1/1	0.97	0.19	-	185,185,185,185	0
60	MG	DA	3011	1/1	0.63	0.27	-	215,215,215,215	0
60	MG	DA	3058	1/1	0.91	0.10	-	204,204,204,204	0
60	MG	DA	3069	1/1	0.90	0.12	-	93,93,93,93	0
60	MG	AA	1623	1/1	0.93	0.07	-	104,104,104,104	0
60	MG	CA	1627	1/1	0.93	0.33	-	220,220,220,220	0
60	MG	AA	1622	1/1	0.94	0.15	-	185,185,185,185	0
60	MG	BA	3080	1/1	0.98	0.14	-	25,25,25,25	0
60	MG	DA	3106	1/1	0.95	0.10	-	55,55,55,55	0
60	MG	BA	3097	1/1	0.85	0.15	-	182,182,182,182	0
60	MG	DA	3007	1/1	0.74	0.50	-	188,188,188,188	0
60	MG	BA	3055	1/1	0.94	0.36	-	240,240,240,240	0
60	MG	BA	3036	1/1	0.99	0.15	-	30,30,30,30	0
60	MG	BA	3091	1/1	0.95	0.14	-	131,131,131,131	0
60	MG	DA	3089	1/1	0.98	0.06	-	81,81,81,81	0
60	MG	BA	3134	1/1	0.93	0.11	-	145,145,145,145	0
60	MG	DA	3110	1/1	0.76	0.24	-	174,174,174,174	0
60	MG	AA	1636	1/1	0.96	0.18	-	149,149,149,149	0
60	MG	DA	3113	1/1	0.96	0.06	-	123,123,123,123	0
60	MG	DA	3095	1/1	0.91	0.15	-	110,110,110,110	0
60	MG	DA	3010	1/1	0.89	0.66	-	261,261,261,261	0
60	MG	DA	3075	1/1	0.63	0.51	-	229,229,229,229	0
60	MG	DA	3046	1/1	0.84	0.17	-	152,152,152,152	0
60	MG	BA	3083	1/1	0.96	0.10	-	52,52,52,52	0
60	MG	DA	3091	1/1	0.87	0.16	-	167,167,167,167	0
60	MG	DA	3122	1/1	0.72	0.11	-	155,155,155,155	0
60	MG	BA	3035	1/1	0.97	0.20	-	241,241,241,241	0
60	MG	DA	3035	1/1	0.96	0.36	-	228,228,228,228	0
60	MG	DA	3126	1/1	0.86	0.17	-	129,129,129,129	0
60	MG	BB	204	1/1	0.96	0.11	-	30,30,30,30	0
60	MG	BA	3077	1/1	0.98	0.13	-	151,151,151,151	0
60	MG	CA	1602	1/1	0.54	0.17	-	131,131,131,131	0
60	MG	DA	3013	1/1	0.78	0.36	-	209,209,209,209	0
60	MG	BA	3111	1/1	0.96	0.13	-	93,93,93,93	0
60	MG	BA	3041	1/1	0.95	0.14	-	12,12,12,12	0
60	MG	BA	3053	1/1	0.99	0.10	-	35,35,35,35	0
60	MG	DA	3107	1/1	0.73	0.60	-	201,201,201,201	0
60	MG	DA	3090	1/1	0.70	0.20	-	209,209,209,209	0
60	MG	DA	3088	1/1	0.97	0.21	-	102,102,102,102	0
60	MG	AA	1614	1/1	0.90	0.54	-	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3040	1/1	0.99	0.12	-	11,11,11,11	0
60	MG	AA	1637	1/1	0.97	0.11	-	34,34,34,34	0
60	MG	BA	3088	1/1	0.97	0.10	-	22,22,22,22	0
60	MG	BA	3030	1/1	0.97	0.14	-	34,34,34,34	0
60	MG	DA	3019	1/1	0.48	0.88	-	252,252,252,252	0
60	MG	BA	3063	1/1	1.00	0.12	-	11,11,11,11	0
60	MG	BA	3118	1/1	0.95	0.29	-	136,136,136,136	0
60	MG	DA	3027	1/1	0.80	0.54	-	277,277,277,277	0
60	MG	BA	3015	1/1	0.97	0.07	-	30,30,30,30	0
60	MG	BA	3093	1/1	0.99	0.10	-	68,68,68,68	0
60	MG	CA	1614	1/1	0.89	0.64	-	271,271,271,271	0
60	MG	DA	3077	1/1	0.71	0.78	-	259,259,259,259	0
60	MG	BA	3037	1/1	0.99	0.16	-	7,7,7,7	0
60	MG	DA	3055	1/1	0.98	0.10	-	121,121,121,121	0
60	MG	BA	3098	1/1	0.97	0.12	-	46,46,46,46	0
60	MG	AA	1605	1/1	0.99	0.12	-	30,30,30,30	0
60	MG	AA	1620	1/1	0.92	0.08	-	120,120,120,120	0
60	MG	BA	3011	1/1	0.98	0.08	-	149,149,149,149	0
60	MG	DA	3070	1/1	0.85	0.20	-	61,61,61,61	0
60	MG	DA	3044	1/1	0.65	0.13	-	230,230,230,230	0
60	MG	DA	3073	1/1	0.74	1.20	-	276,276,276,276	0
60	MG	BA	3110	1/1	0.99	0.09	-	65,65,65,65	0
60	MG	BA	3043	1/1	0.99	0.25	-	19,19,19,19	0
60	MG	BA	3019	1/1	0.99	0.15	-	50,50,50,50	0
60	MG	BA	3066	1/1	0.99	0.11	-	14,14,14,14	0
60	MG	DA	3006	1/1	0.76	0.12	-	149,149,149,149	0
60	MG	CA	1612	1/1	0.85	0.26	-	133,133,133,133	0
60	MG	DA	3045	1/1	0.88	0.14	-	76,76,76,76	0
60	MG	BA	3086	1/1	0.83	0.20	-	144,144,144,144	0
60	MG	AA	1602	1/1	0.99	0.08	-	117,117,117,117	0
60	MG	AA	1608	1/1	0.95	0.14	-	38,38,38,38	0
60	MG	DA	3048	1/1	0.63	0.16	-	243,243,243,243	0
60	MG	DA	3116	1/1	0.97	0.10	-	59,59,59,59	0
60	MG	BA	3014	1/1	0.96	0.17	-	75,75,75,75	0
60	MG	CA	1624	1/1	0.91	0.31	-	123,123,123,123	0
60	MG	BA	3089	1/1	0.91	0.08	-	39,39,39,39	0
60	MG	DA	3001	1/1	0.86	0.12	-	149,149,149,149	0
60	MG	DA	3030	1/1	0.72	0.20	-	66,66,66,66	0
60	MG	AA	1639	1/1	0.92	0.06	-	92,92,92,92	0
60	MG	BA	3009	1/1	0.97	0.15	-	12,12,12,12	0
60	MG	DA	3036	1/1	0.96	0.15	-	111,111,111,111	0
60	MG	AA	1618	1/1	0.85	0.68	-	217,217,217,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3127	1/1	0.56	1.91	-	274,274,274,274	0
60	MG	BA	3079	1/1	0.97	0.11	-	20,20,20,20	0
60	MG	DA	3120	1/1	0.93	0.14	-	84,84,84,84	0
60	MG	DA	3096	1/1	0.91	0.29	-	180,180,180,180	0
60	MG	BA	3071	1/1	0.97	0.11	-	8,8,8,8	0
60	MG	CA	1638	1/1	0.95	0.11	-	106,106,106,106	0
60	MG	CA	1622	1/1	0.77	0.12	-	196,196,196,196	0
60	MG	DA	3101	1/1	0.89	0.12	-	73,73,73,73	0
60	MG	DA	3029	1/1	0.90	0.17	-	135,135,135,135	0
60	MG	BA	3060	1/1	0.96	0.26	-	257,257,257,257	0
60	MG	BA	3050	1/1	0.98	0.10	-	12,12,12,12	0
60	MG	BA	3034	1/1	0.99	0.09	-	9,9,9,9	0
60	MG	DA	3028	1/1	0.84	0.40	-	195,195,195,195	0
60	MG	AA	1635	1/1	0.96	0.21	-	198,198,198,198	0
60	MG	CA	1623	1/1	0.80	0.12	-	79,79,79,79	0
60	MG	DA	3093	1/1	0.95	0.30	-	166,166,166,166	0
60	MG	BA	3029	1/1	0.98	0.20	-	10,10,10,10	0
60	MG	AA	1638	1/1	0.92	0.11	-	139,139,139,139	0
60	MG	DA	3033	1/1	0.96	0.07	-	91,91,91,91	0
60	MG	BA	3024	1/1	0.82	0.34	-	206,206,206,206	0
60	MG	AA	1612	1/1	0.97	0.14	-	103,103,103,103	0
60	MG	DA	3124	1/1	0.10	0.49	-	211,211,211,211	0
60	MG	BA	3068	1/1	0.73	0.11	-	174,174,174,174	0
60	MG	DA	3053	1/1	0.93	0.10	-	78,78,78,78	0
60	MG	DA	3117	1/1	0.61	0.12	-	99,99,99,99	0
60	MG	CA	1615	1/1	0.78	0.18	-	243,243,243,243	0
60	MG	DA	3009	1/1	0.95	0.11	-	75,75,75,75	0
60	MG	CA	1605	1/1	0.97	0.17	-	47,47,47,47	0
60	MG	DA	3021	1/1	0.96	0.16	-	169,169,169,169	0
60	MG	BA	3076	1/1	0.97	0.06	-	31,31,31,31	0
60	MG	BA	3065	1/1	0.99	0.15	-	27,27,27,27	0
60	MG	BA	3003	1/1	0.94	0.13	-	44,44,44,44	0
60	MG	BA	3042	1/1	0.99	0.13	-	34,34,34,34	0
60	MG	AA	1603	1/1	0.89	0.10	-	131,131,131,131	0
60	MG	DA	3085	1/1	0.62	0.16	-	127,127,127,127	0
60	MG	DJ	201	1/1	0.65	1.44	-	331,331,331,331	0
60	MG	DA	3004	1/1	0.89	0.16	-	86,86,86,86	0
60	MG	BA	3054	1/1	0.72	0.21	-	214,214,214,214	0
60	MG	CA	1636	1/1	0.95	0.10	-	130,130,130,130	0
60	MG	DA	3115	1/1	0.98	0.19	-	69,69,69,69	0
60	MG	DA	3086	1/1	0.91	0.10	-	185,185,185,185	0
60	MG	CA	1610	1/1	0.83	0.09	-	220,220,220,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3072	1/1	0.73	0.12	-	193,193,193,193	0
60	MG	AA	1615	1/1	0.98	0.04	-	127,127,127,127	0
60	MG	BA	3085	1/1	0.97	0.13	-	24,24,24,24	0
60	MG	DA	3031	1/1	0.91	0.10	-	121,121,121,121	0
60	MG	BA	3045	1/1	0.97	0.12	-	13,13,13,13	0
60	MG	CA	1635	1/1	0.97	0.09	-	85,85,85,85	0
60	MG	BA	3073	1/1	0.95	0.09	-	116,116,116,116	0
60	MG	BA	3102	1/1	0.98	0.10	-	14,14,14,14	0
60	MG	BA	3006	1/1	0.98	0.05	-	47,47,47,47	0
60	MG	DA	3080	1/1	0.96	0.25	-	70,70,70,70	0
60	MG	BA	3047	1/1	0.92	0.13	-	112,112,112,112	0
60	MG	BA	3007	1/1	0.95	0.10	-	84,84,84,84	0
60	MG	DA	3005	1/1	0.82	0.44	-	280,280,280,280	0
60	MG	AA	1629	1/1	0.94	0.14	-	227,227,227,227	0
60	MG	BA	3058	1/1	0.83	0.18	-	106,106,106,106	0
60	MG	DA	3062	1/1	0.27	2.37	-	262,262,262,262	0
60	MG	DA	3025	1/1	0.12	1.44	-	253,253,253,253	0
60	MG	DA	3130	1/1	0.41	1.45	-	305,305,305,305	0
60	MG	DA	3079	1/1	0.89	0.13	-	149,149,149,149	0
60	MG	BA	3031	1/1	0.99	0.12	-	15,15,15,15	0
60	MG	BA	3051	1/1	0.95	0.10	-	48,48,48,48	0
60	MG	DA	3092	1/1	0.95	0.12	-	209,209,209,209	0
60	MG	DA	3042	1/1	0.91	0.14	-	166,166,166,166	0
60	MG	BA	3018	1/1	1.00	0.30	-	10,10,10,10	0
60	MG	DA	3121	1/1	0.91	0.15	-	114,114,114,114	0
60	MG	DA	3084	1/1	0.91	0.26	-	157,157,157,157	0
60	MG	BA	3028	1/1	0.98	0.07	-	45,45,45,45	0
60	MG	BA	3059	1/1	0.98	0.16	-	147,147,147,147	0
60	MG	DA	3017	1/1	0.76	0.23	-	147,147,147,147	0
60	MG	BA	3122	1/1	0.96	0.12	-	25,25,25,25	0
60	MG	AA	1627	1/1	0.91	0.17	-	165,165,165,165	0
60	MG	CA	1630	1/1	0.69	0.12	-	176,176,176,176	0
60	MG	BA	3004	1/1	0.90	0.13	-	150,150,150,150	0
60	MG	AA	1601	1/1	0.96	0.15	-	93,93,93,93	0
60	MG	DA	3008	1/1	0.72	0.23	-	153,153,153,153	0
60	MG	BA	3081	1/1	0.98	0.04	-	41,41,41,41	0
60	MG	AA	1617	1/1	0.90	0.12	-	111,111,111,111	0
60	MG	BA	3090	1/1	0.93	0.14	-	93,93,93,93	0
60	MG	DA	3098	1/1	0.83	0.22	-	218,218,218,218	0
60	MG	BA	3044	1/1	0.89	0.16	-	56,56,56,56	0
60	MG	BA	3032	1/1	0.99	0.16	-	6,6,6,6	0
60	MG	DA	3034	1/1	0.93	0.21	-	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3025	1/1	0.98	0.10	-	38,38,38,38	0
60	MG	BA	3121	1/1	0.99	0.14	-	5,5,5,5	0
60	MG	CA	1603	1/1	0.96	0.16	-	140,140,140,140	0
60	MG	CA	1633	1/1	0.96	0.07	-	82,82,82,82	0
60	MG	DA	3040	1/1	0.86	0.21	-	120,120,120,120	0
60	MG	BB	203	1/1	0.99	0.10	-	16,16,16,16	0
60	MG	BL	201	1/1	0.98	0.07	-	34,34,34,34	0
60	MG	DA	3015	1/1	0.96	0.26	-	277,277,277,277	0
60	MG	CA	1619	1/1	0.96	0.26	-	243,243,243,243	0
60	MG	DA	3097	1/1	0.92	0.20	-	143,143,143,143	0
60	MG	BA	3087	1/1	0.93	0.12	-	182,182,182,182	0
60	MG	CA	1601	1/1	0.82	0.08	-	123,123,123,123	0
60	MG	CA	1620	1/1	0.94	0.20	-	209,209,209,209	0
60	MG	DA	3037	1/1	0.51	0.18	-	203,203,203,203	0
60	MG	DA	3020	1/1	0.98	0.19	-	36,36,36,36	0
60	MG	BA	3116	1/1	0.99	0.06	-	14,14,14,14	0
60	MG	DA	3119	1/1	0.88	0.22	-	84,84,84,84	0
60	MG	BA	3114	1/1	0.95	0.15	-	148,148,148,148	0
60	MG	BA	3125	1/1	0.98	0.11	-	26,26,26,26	0
60	MG	DA	3125	1/1	0.83	0.10	-	132,132,132,132	0
60	MG	DA	3014	1/1	0.90	0.40	-	177,177,177,177	0
60	MG	DA	3132	1/1	0.75	0.24	-	225,225,225,225	0
60	MG	AA	1625	1/1	0.97	0.22	-	31,31,31,31	0
60	MG	CA	1608	1/1	0.89	0.22	-	82,82,82,82	0
60	MG	AA	1610	1/1	0.79	0.08	-	200,200,200,200	0
60	MG	DA	3018	1/1	0.94	0.21	-	225,225,225,225	0
60	MG	DA	3052	1/1	0.93	0.20	-	105,105,105,105	0
60	MG	DA	3108	1/1	0.74	0.31	-	123,123,123,123	0
60	MG	DA	3087	1/1	0.88	0.15	-	178,178,178,178	0
60	MG	BA	3105	1/1	0.99	0.15	-	11,11,11,11	0
60	MG	DA	3003	1/1	0.87	0.98	-	253,253,253,253	0
60	MG	BA	3124	1/1	0.95	0.16	-	22,22,22,22	0
60	MG	BA	3038	1/1	0.99	0.17	-	21,21,21,21	0
60	MG	DA	3112	1/1	0.89	0.08	-	114,114,114,114	0
60	MG	AA	1634	1/1	0.98	0.07	-	58,58,58,58	0
60	MG	AA	1631	1/1	0.99	0.13	-	95,95,95,95	0
60	MG	BA	3126	1/1	0.99	0.14	-	32,32,32,32	0
60	MG	DA	3066	1/1	0.96	0.12	-	65,65,65,65	0
60	MG	AA	1619	1/1	0.96	0.06	-	165,165,165,165	0
60	MG	BA	3074	1/1	0.98	0.18	-	15,15,15,15	0
60	MG	CA	1632	1/1	0.88	0.17	-	143,143,143,143	0
60	MG	BA	3127	1/1	0.98	0.10	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.