



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2017 – 09:24 PM EDT

PDB ID : 4U1V
Title : Crystal structure of the E. coli ribosome bound to linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : unknown
Resolution : 3.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

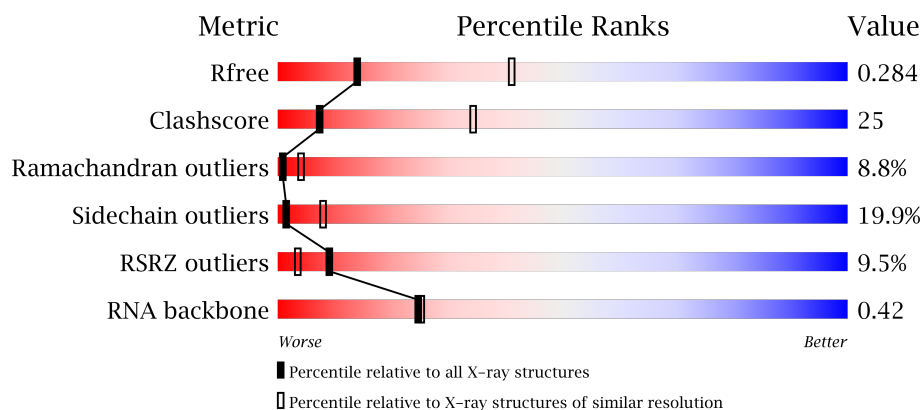
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>0.2%</div> <div>23% 58% 19%</div> </div>
1	CA	1539	<div> <div>2%</div> <div>29% 53% 17%</div> </div>
2	AB	218	<div> <div>24%</div> <div>22% 48% 25% 5%</div> </div>
2	CB	218	<div> <div>32%</div> <div>31% 44% 22%</div> </div>

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

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





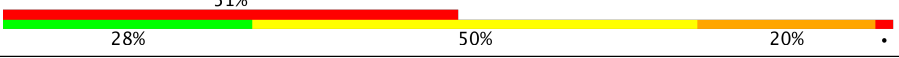
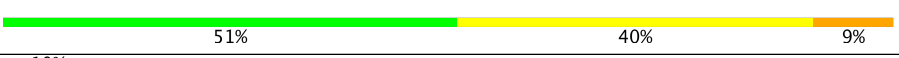

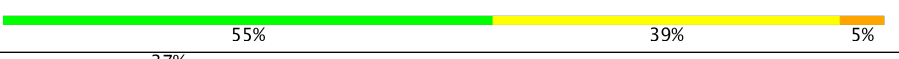
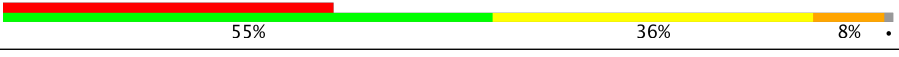
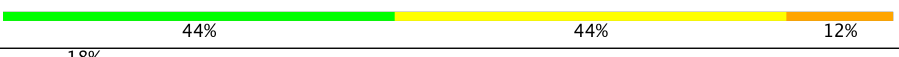
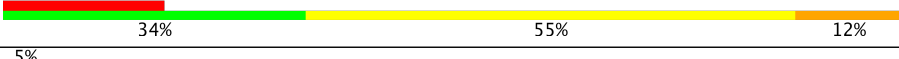
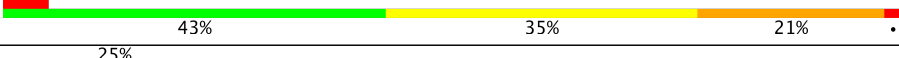
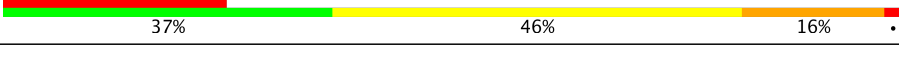

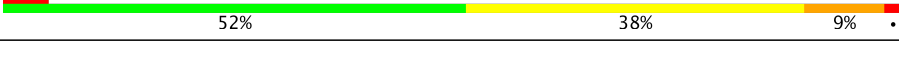
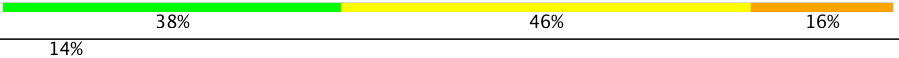

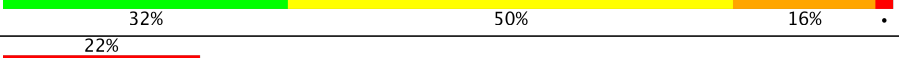

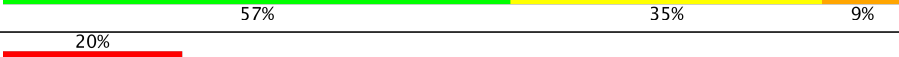
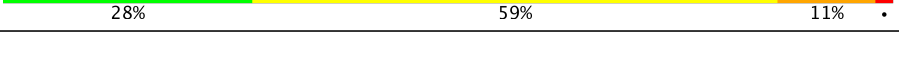
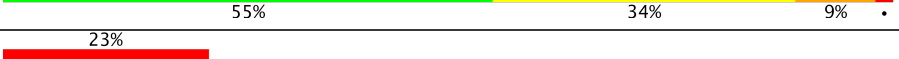

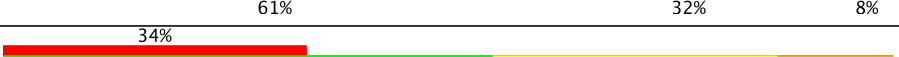

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP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

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

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	7	
54	D6	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MHW	B6	1	-	X	-	-
54	MHW	D6	1	-	X	X	-
55	MG	AA	1622	-	-	-	X
55	MG	AA	1669	-	-	-	X
55	MG	AA	1670	-	-	-	X
55	MG	AM	201	-	-	-	X
55	MG	BA	3005	-	-	-	X
55	MG	BA	3015	-	-	-	X
55	MG	BA	3027	-	-	-	X
55	MG	BA	3040	-	-	-	X
55	MG	BA	3055	-	-	-	X
55	MG	BA	3083	-	-	-	X
55	MG	BA	3104	-	-	-	X
55	MG	BA	3105	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3131	-	-	-	X
55	MG	BA	3136	-	-	-	X
55	MG	BA	3146	-	-	-	X
55	MG	BA	3152	-	-	-	X
55	MG	BA	3170	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3186	-	-	-	X
55	MG	CA	1615	-	-	-	X
55	MG	CA	1626	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3032	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3106	-	-	-	X
55	MG	DA	3110	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3113	-	-	-	X
55	MG	DA	3154	-	-	-	X
55	MG	DA	3158	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288320 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Linopristin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

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

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

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	615	Total O 615 615	0	0
57	BB	14	Total O 14 14	0	0
57	BC	10	Total O 10 10	0	0
57	BD	4	Total O 4 4	0	0
57	BE	4	Total O 4 4	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BJ	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	2	Total O 2 2	0	0
57	BS	1	Total O 1 1	0	0
57	BU	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0

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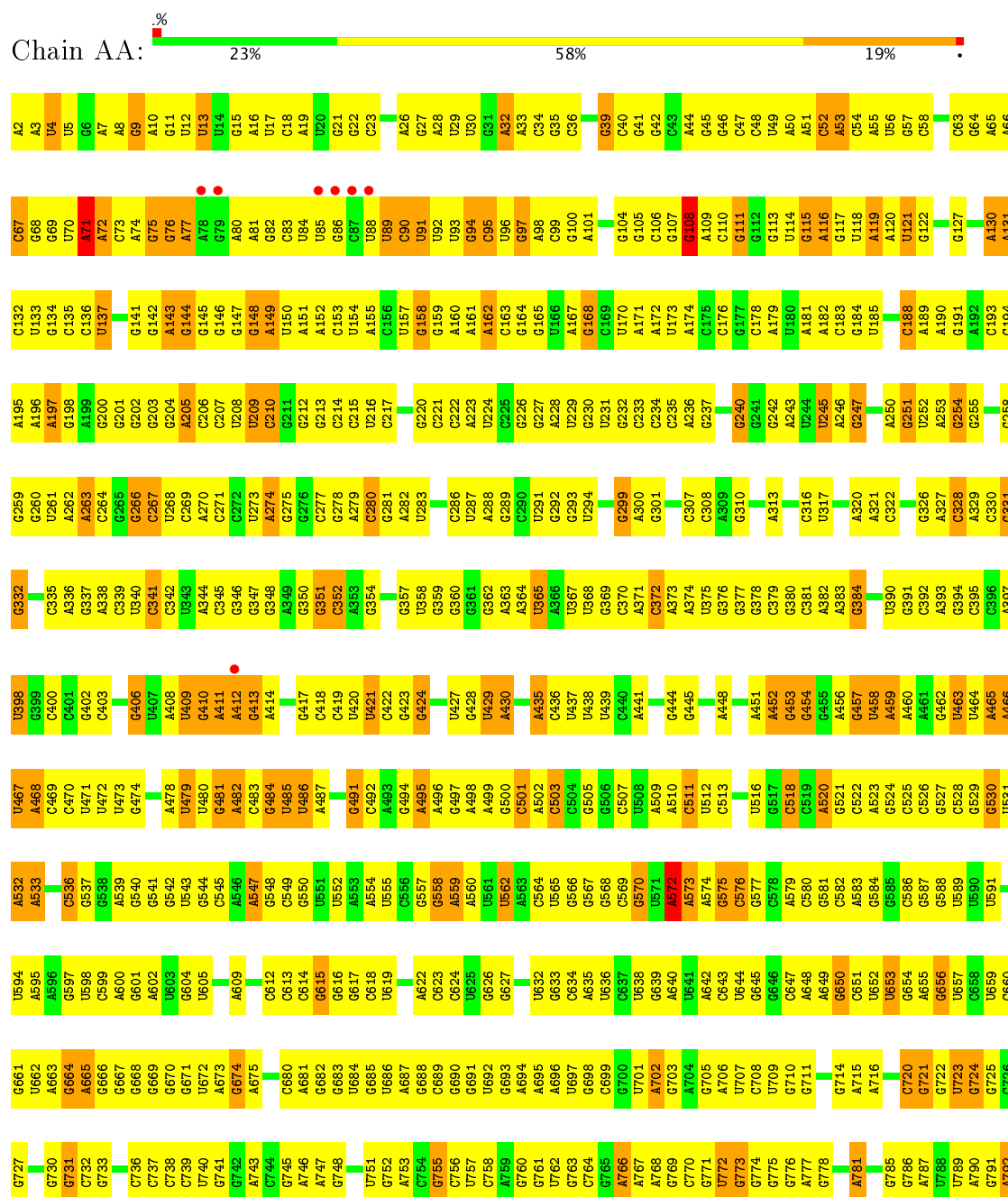
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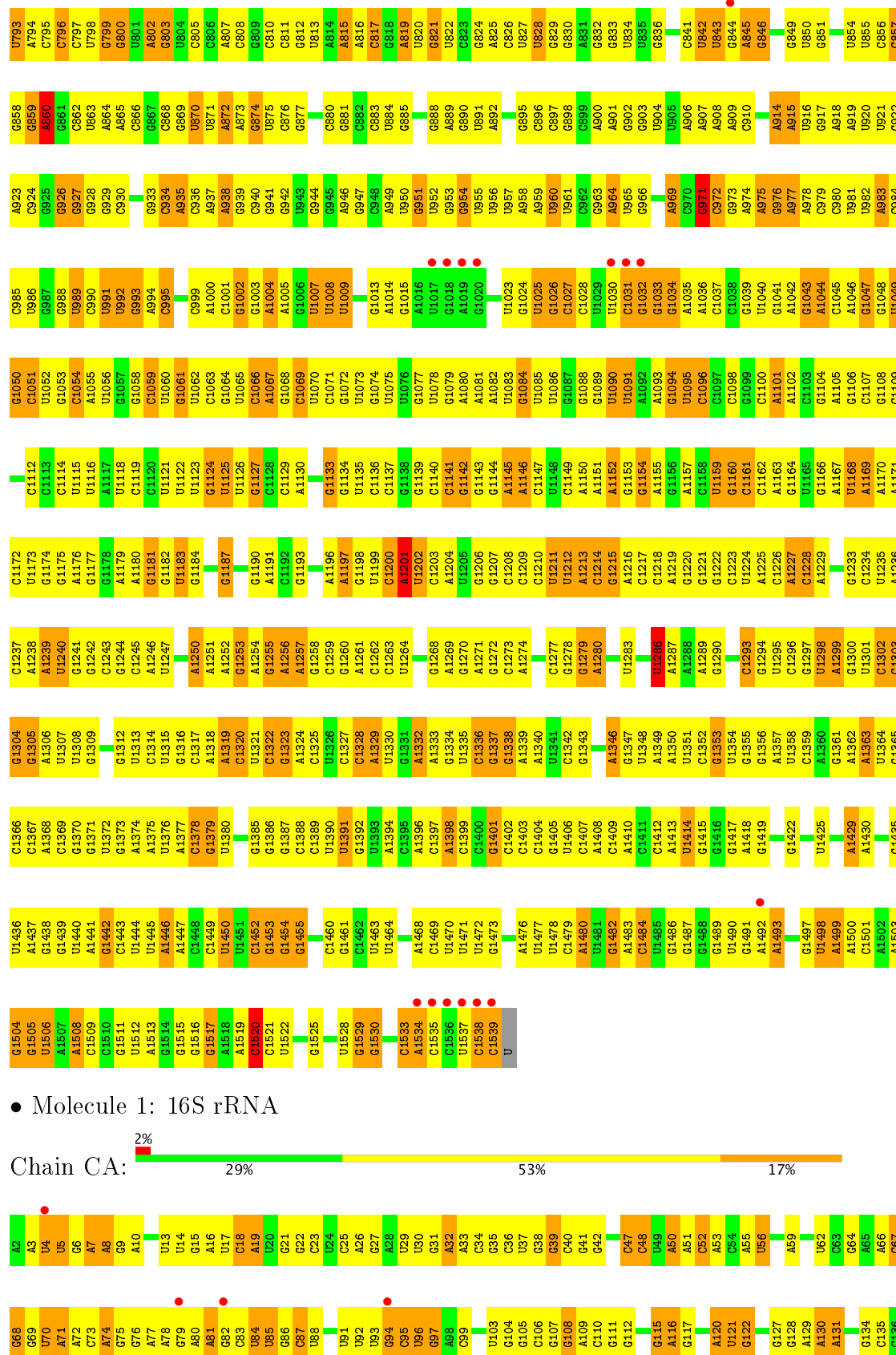
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57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

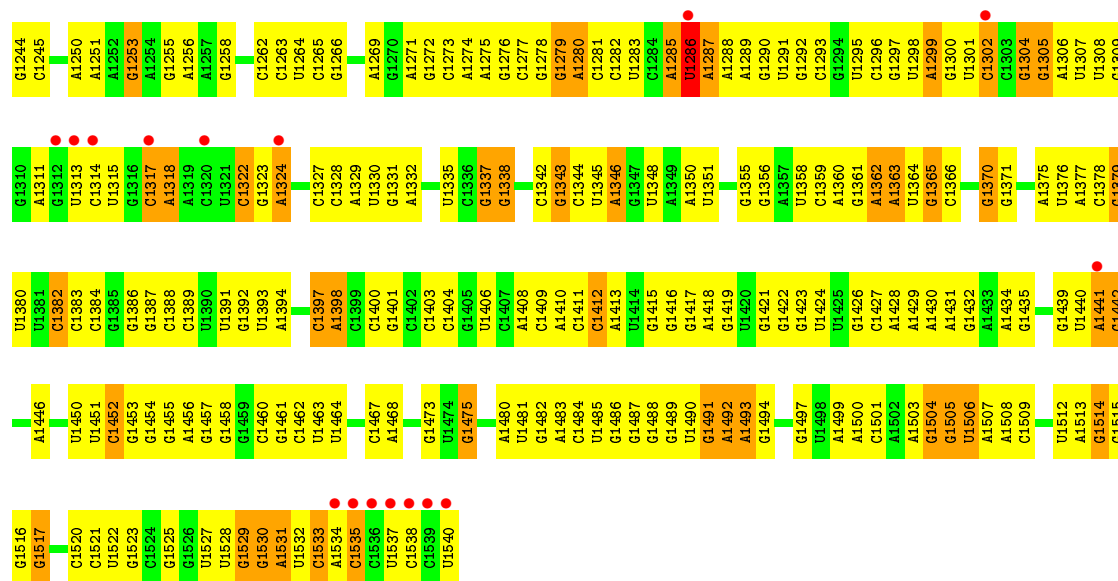
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

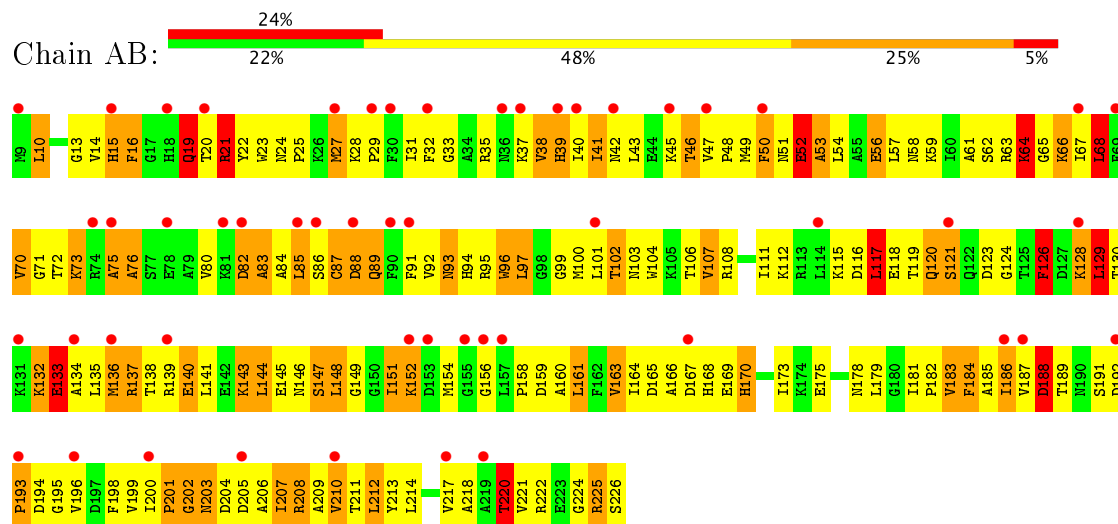




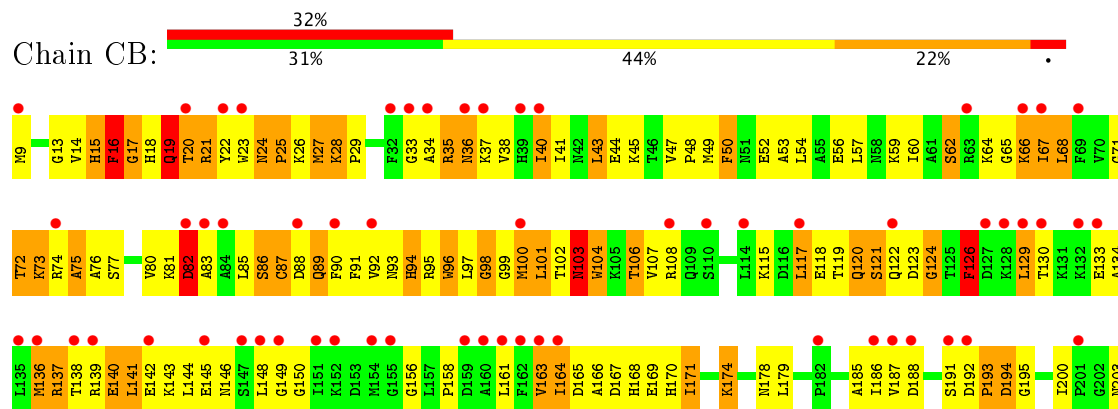


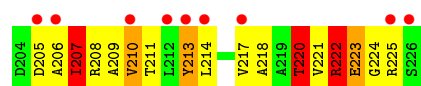


• Molecule 2: 30S ribosomal protein S2

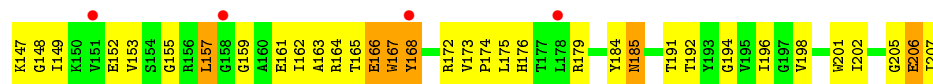
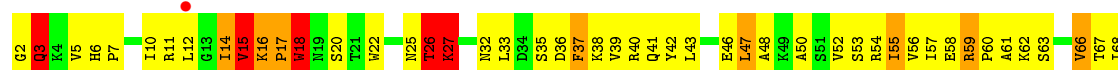
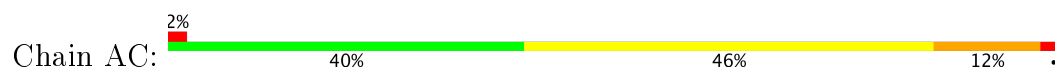


• Molecule 2: 30S ribosomal protein S2

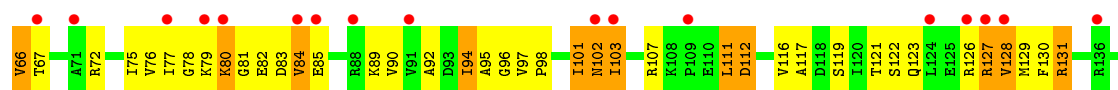
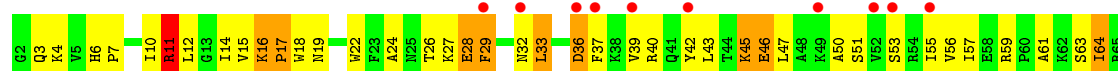
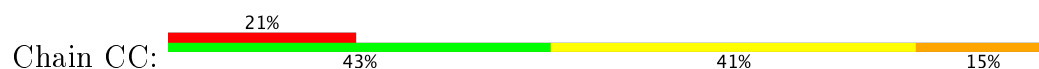




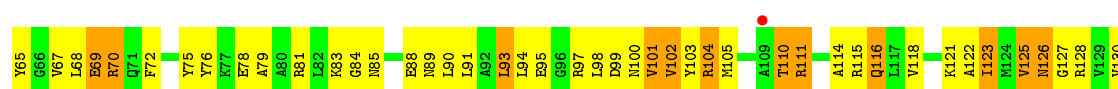
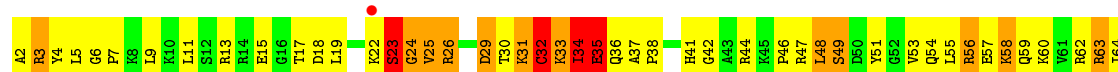
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

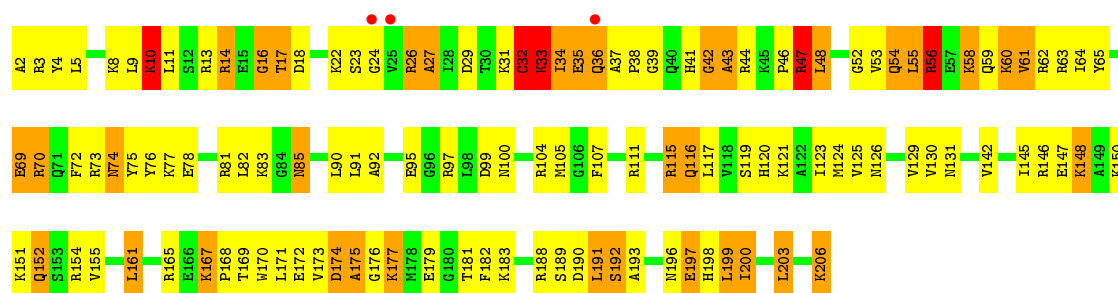


• Molecule 4: 30S ribosomal protein S4

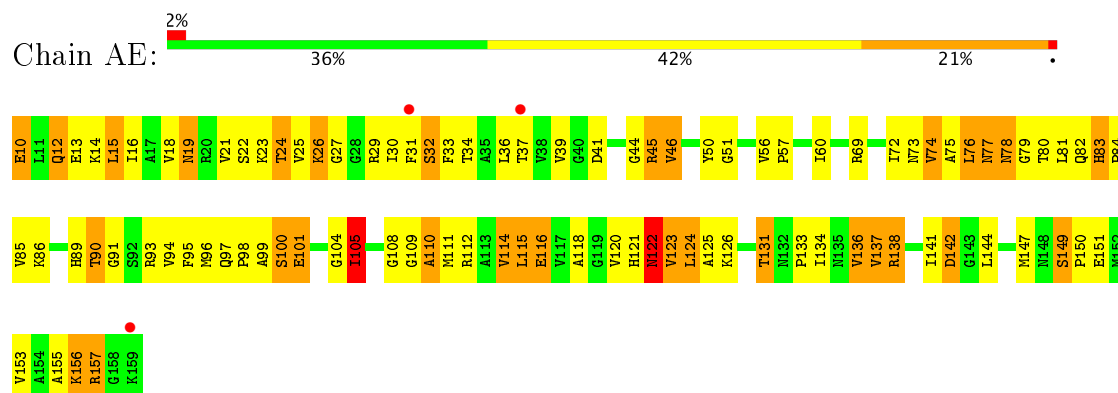


• Molecule 4: 30S ribosomal protein S4

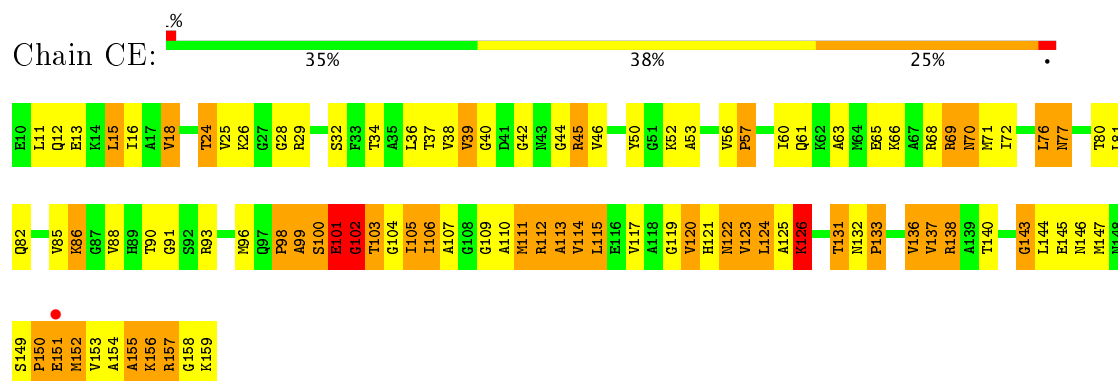




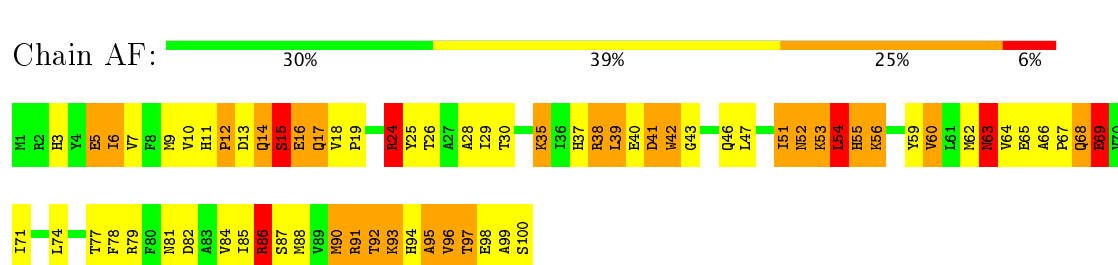
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

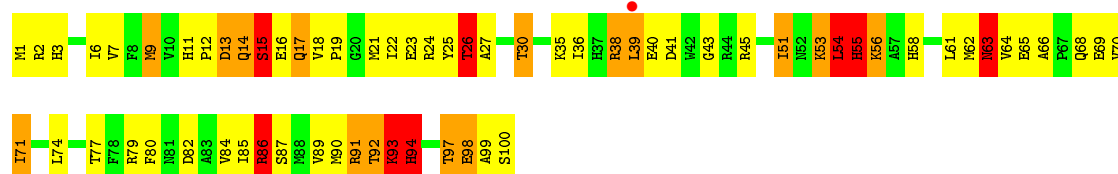


• Molecule 6: 30S ribosomal protein S6

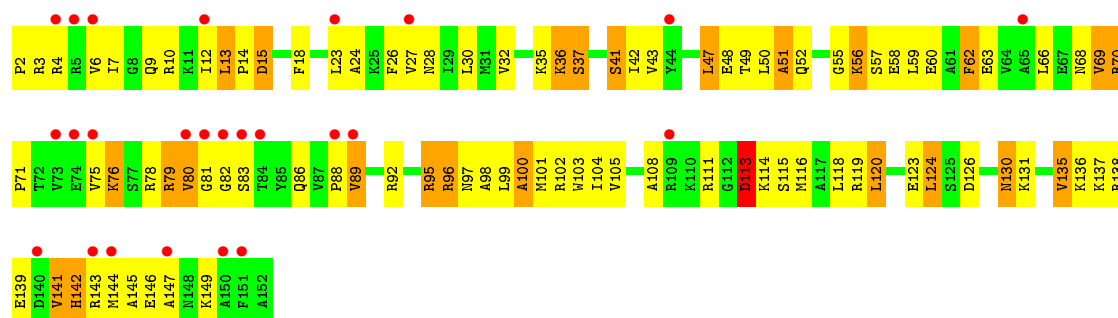
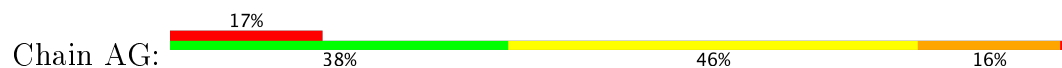


• Molecule 6: 30S ribosomal protein S6

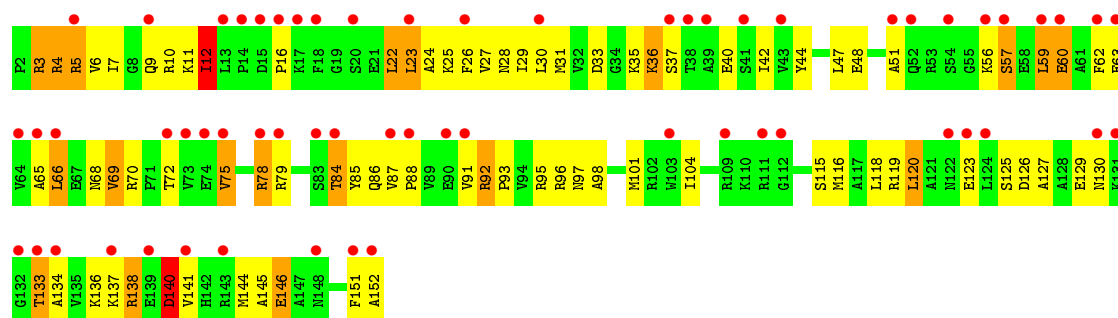
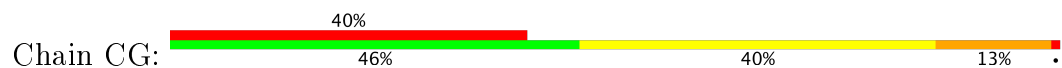




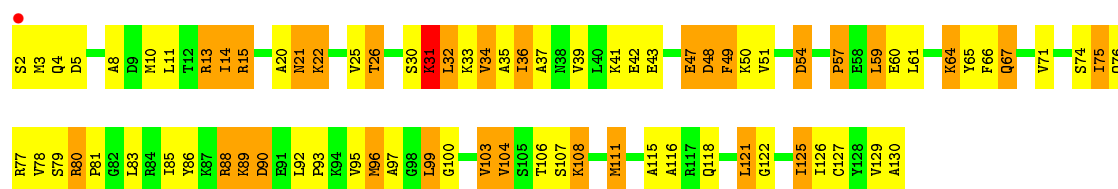
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

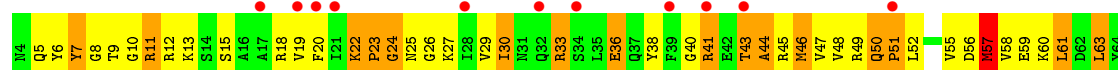


• Molecule 8: 30S ribosomal protein S8

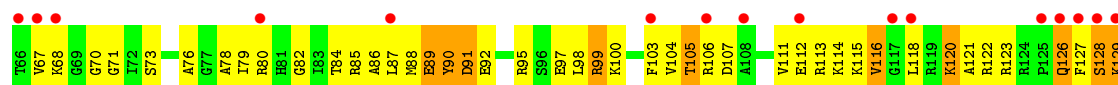
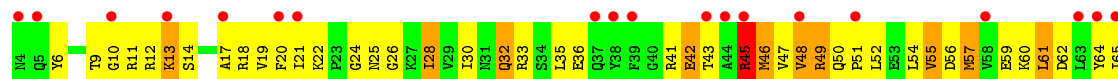




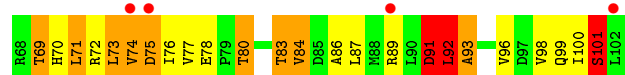
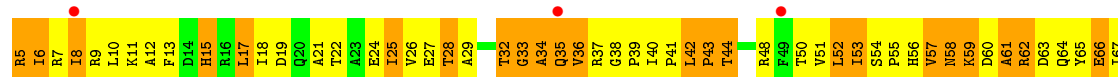
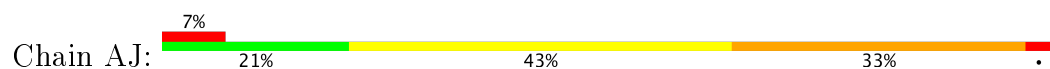
• Molecule 9: 30S ribosomal protein S9



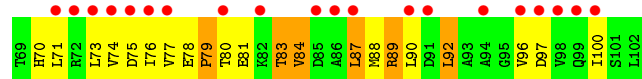
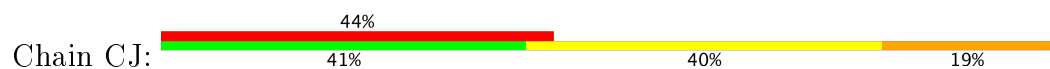
• Molecule 9: 30S ribosomal protein S9



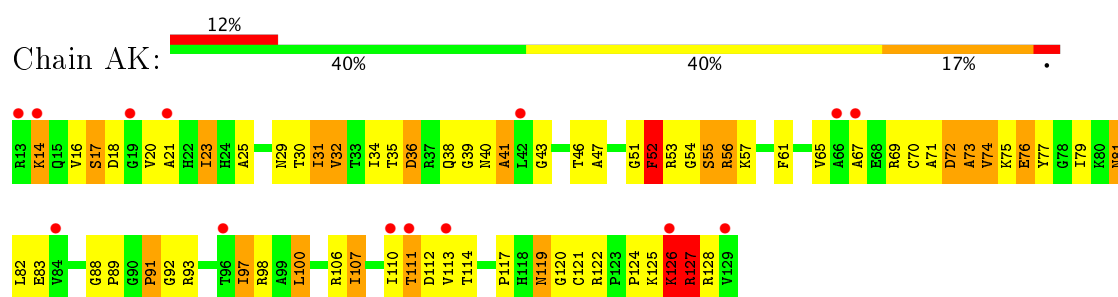
• Molecule 10: 30S ribosomal protein S10



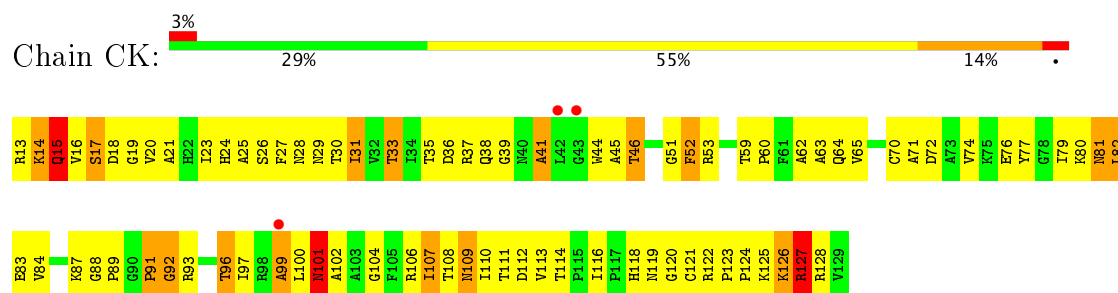
• Molecule 10: 30S ribosomal protein S10



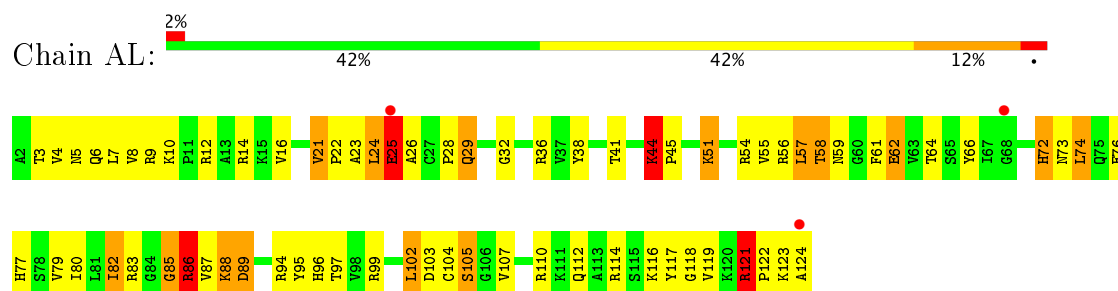
• Molecule 11: 30S ribosomal protein S11



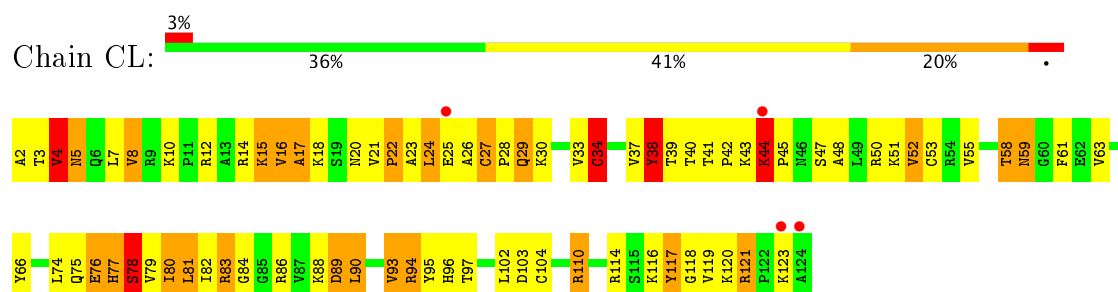
- Molecule 11: 30S ribosomal protein S11



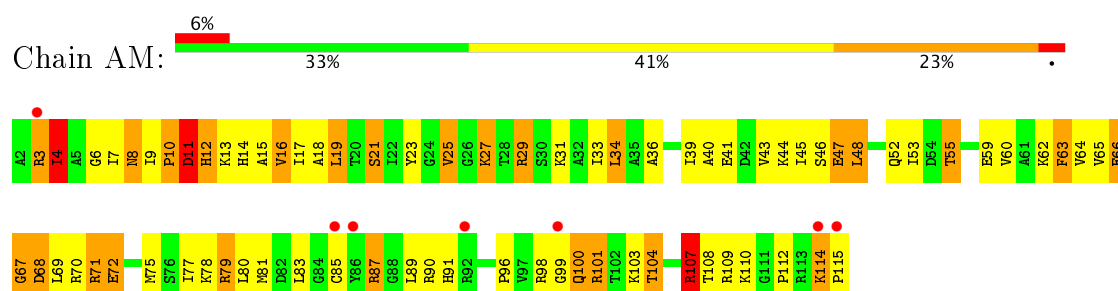
- Molecule 12: 30S ribosomal protein S12



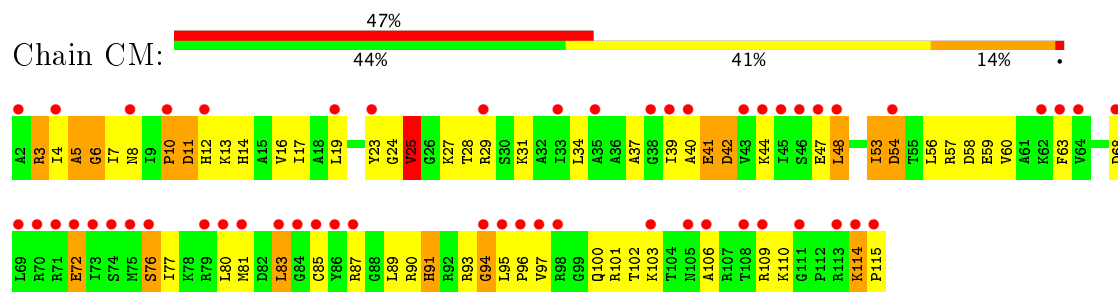
- Molecule 12: 30S ribosomal protein S12



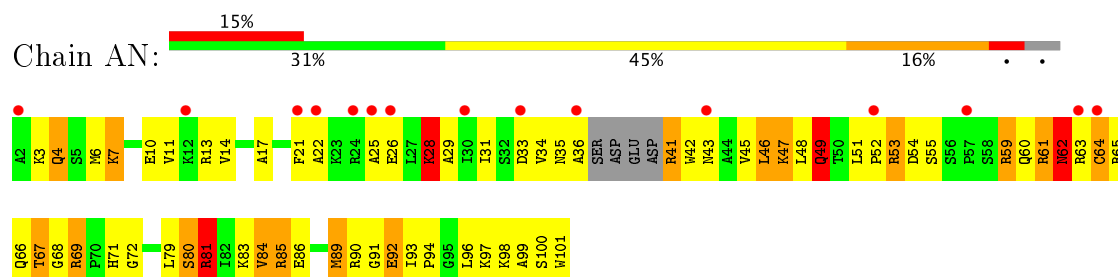
- Molecule 13: 30S ribosomal protein S13



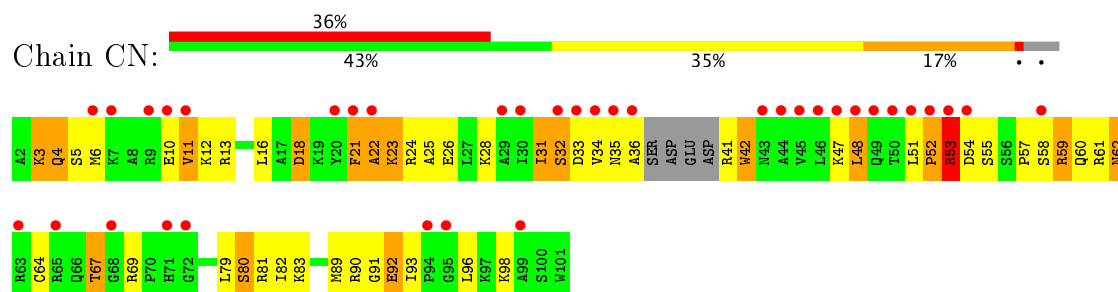
- Molecule 13: 30S ribosomal protein S13



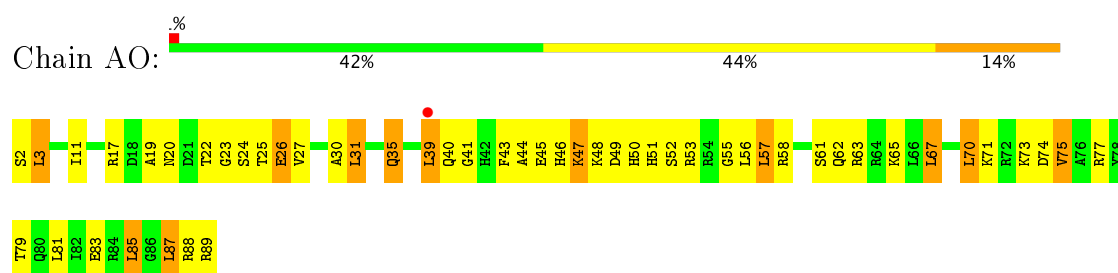
- Molecule 14: 30S ribosomal protein S14



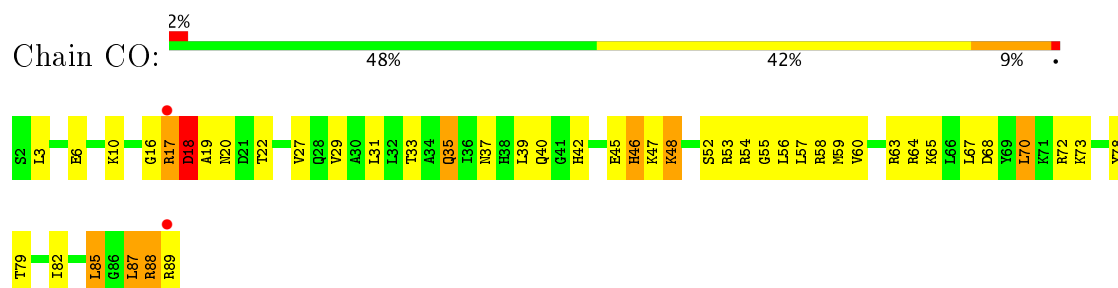
- Molecule 14: 30S ribosomal protein S14



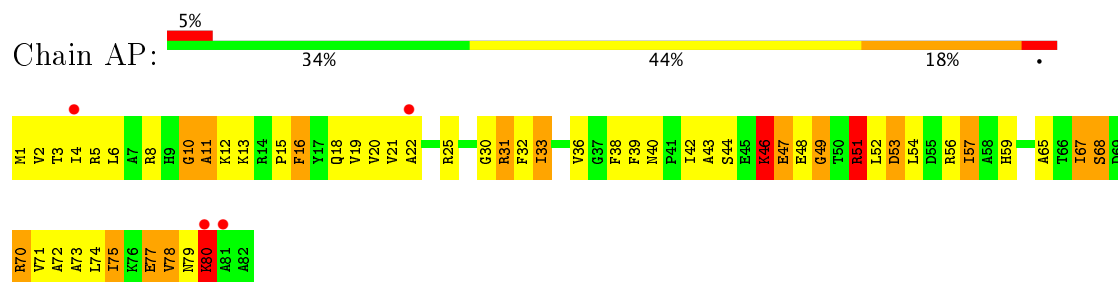
- Molecule 15: 30S ribosomal protein S15



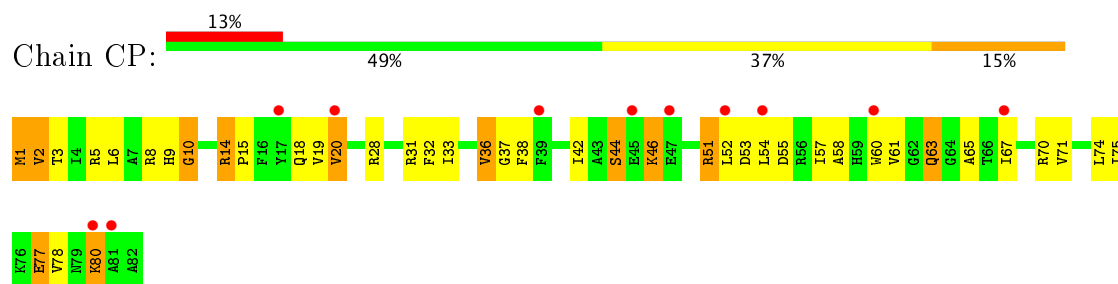
- Molecule 15: 30S ribosomal protein S15



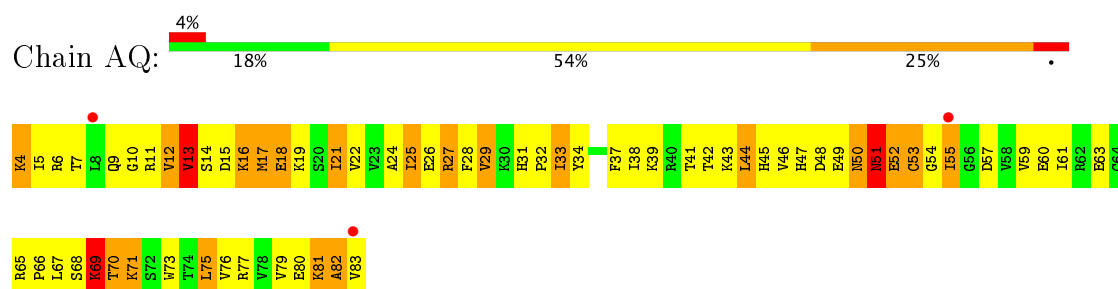
- Molecule 16: 30S ribosomal protein S16



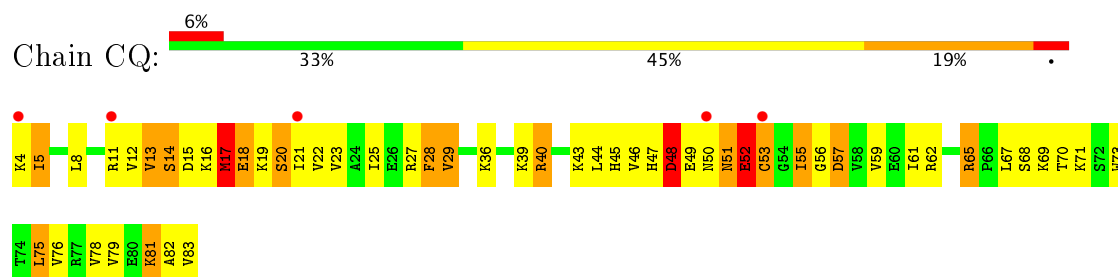
- Molecule 16: 30S ribosomal protein S16



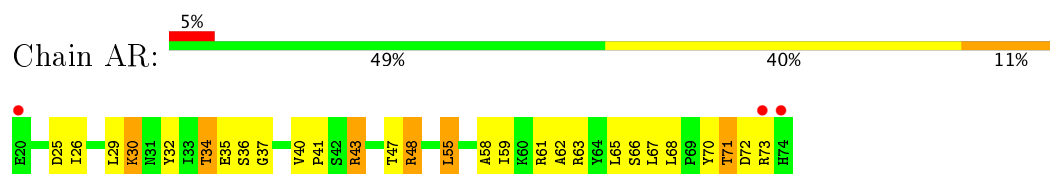
- Molecule 17: 30S ribosomal protein S17



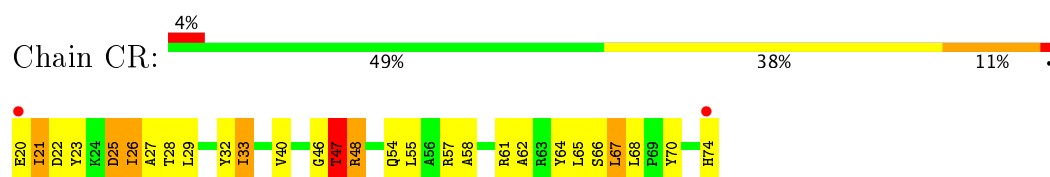
- Molecule 17: 30S ribosomal protein S17



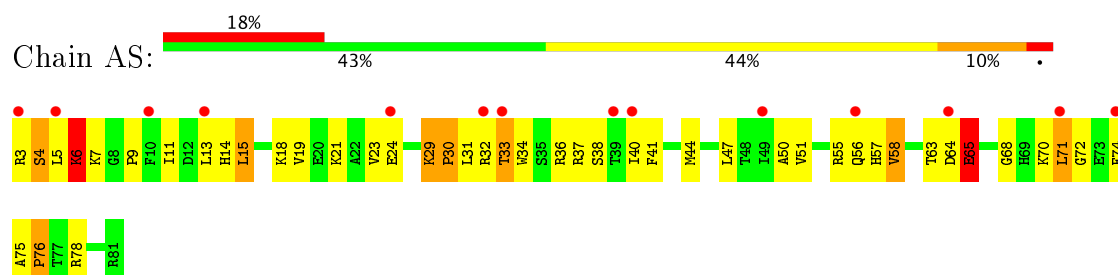
- Molecule 18: 30S ribosomal protein S18



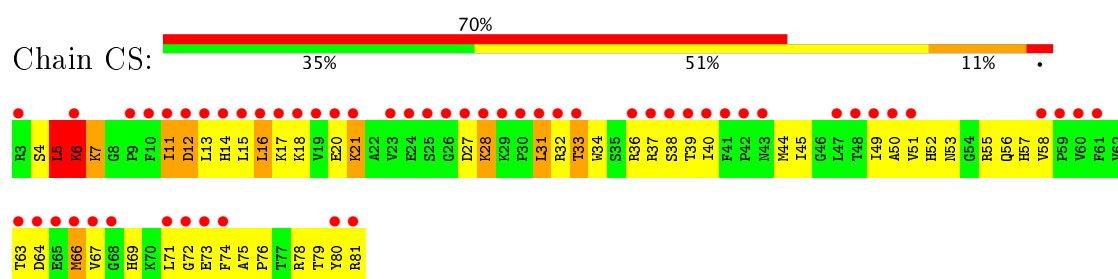
- Molecule 18: 30S ribosomal protein S18



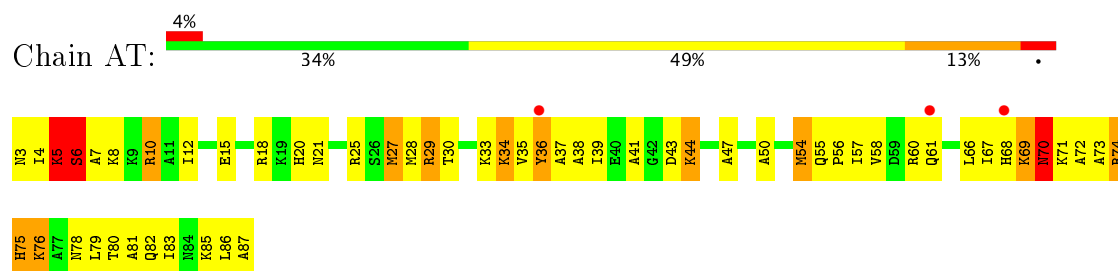
• Molecule 19: 30S ribosomal protein S19



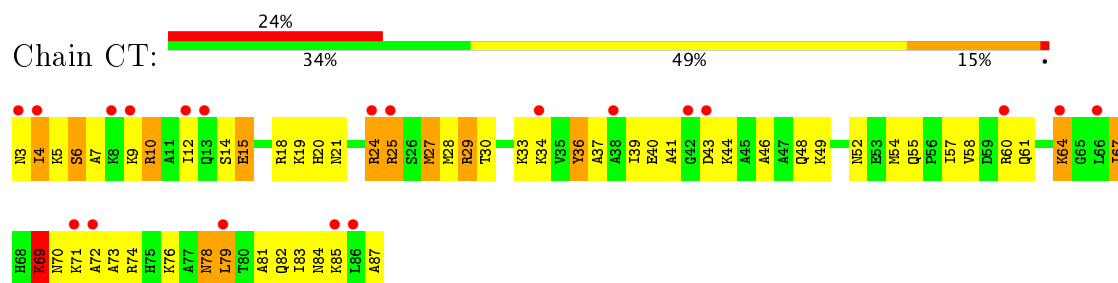
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

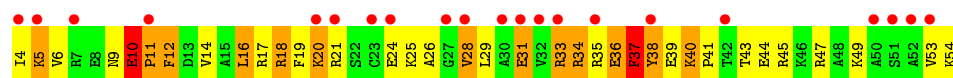


• Molecule 20: 30S ribosomal protein S20

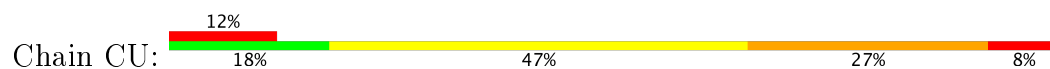


• Molecule 21: 30S ribosomal protein S21

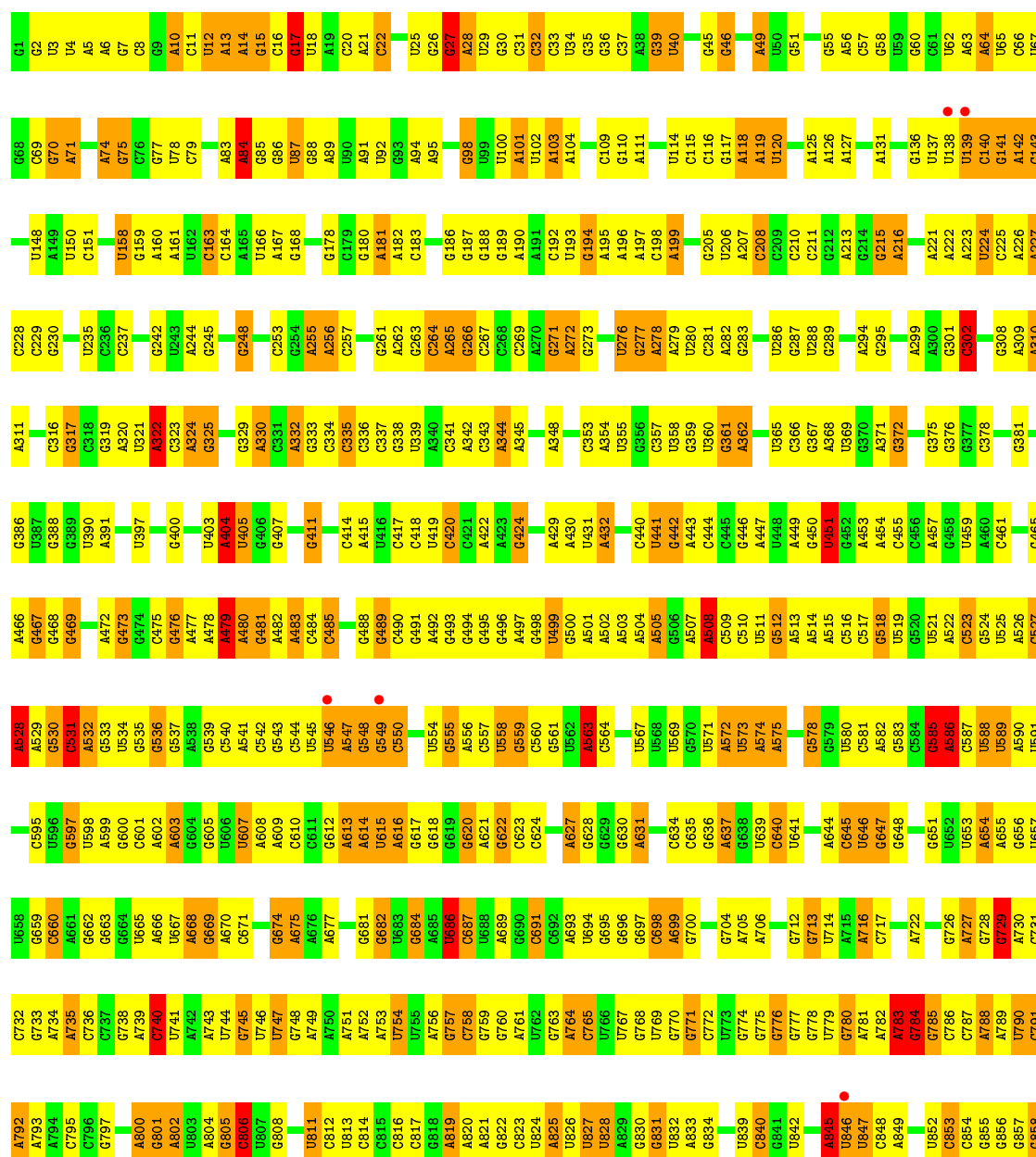




- Molecule 21: 30S ribosomal protein S21

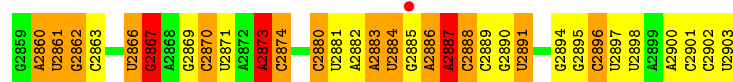


- Molecule 22: 23S rRNA

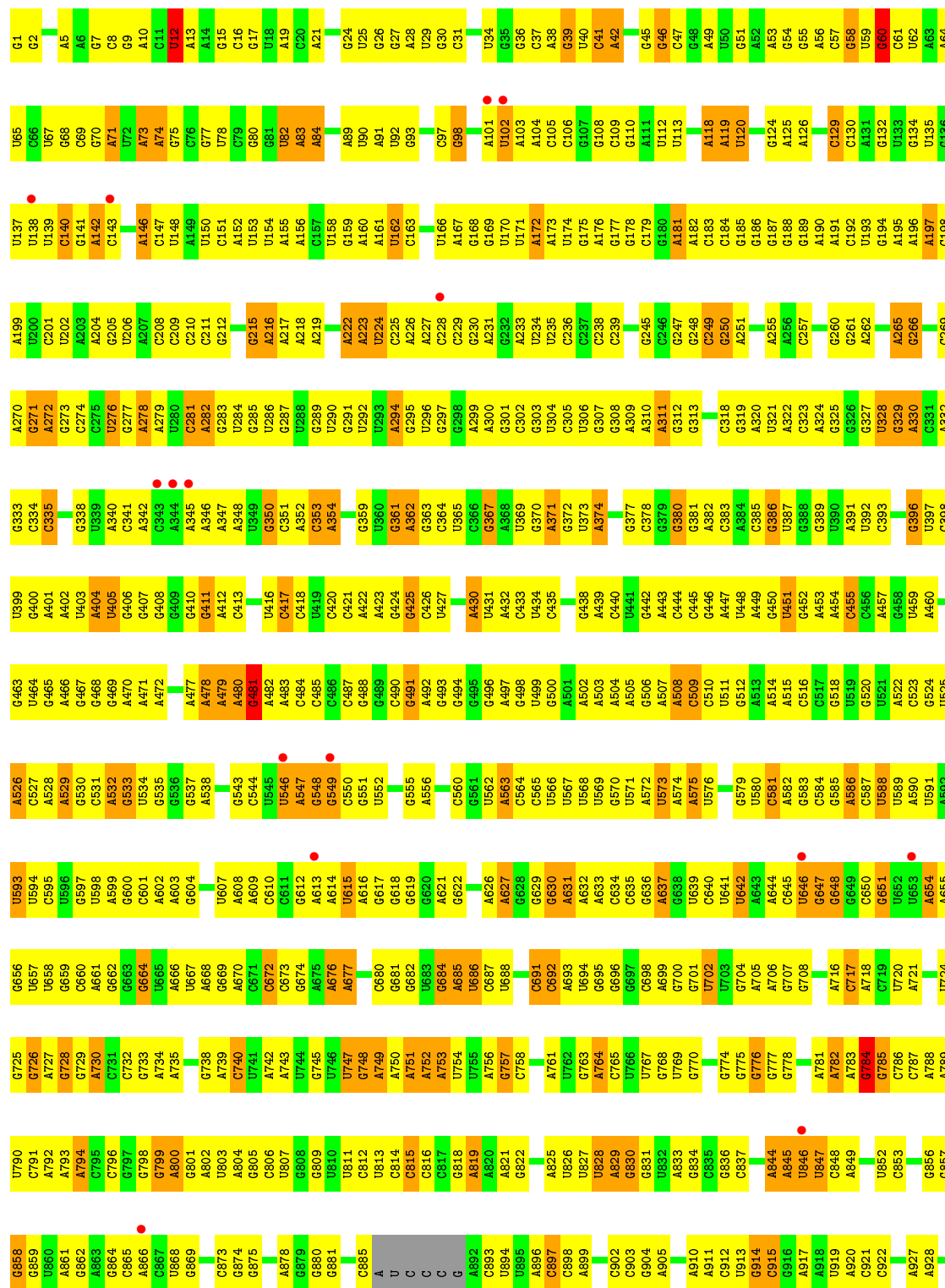


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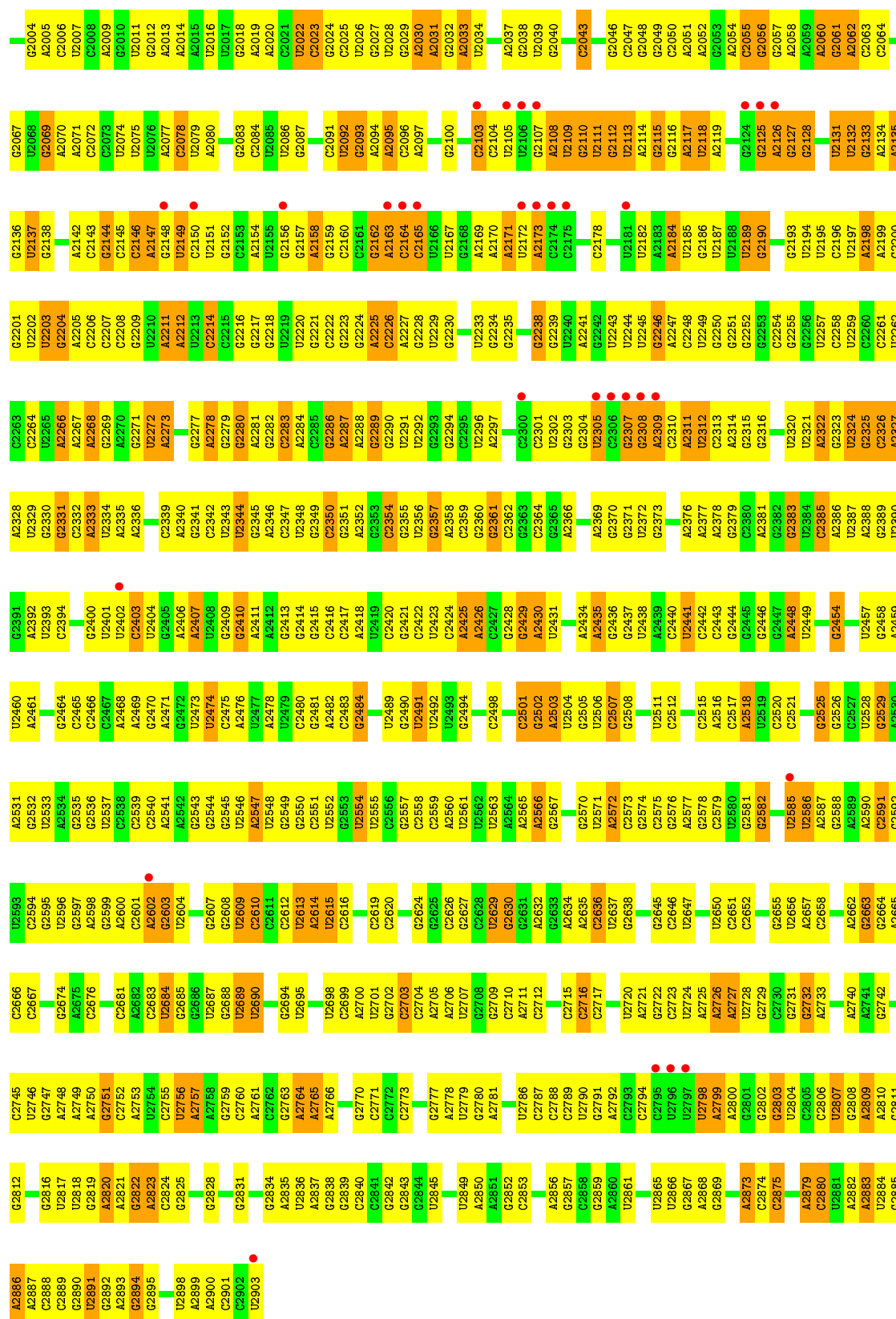
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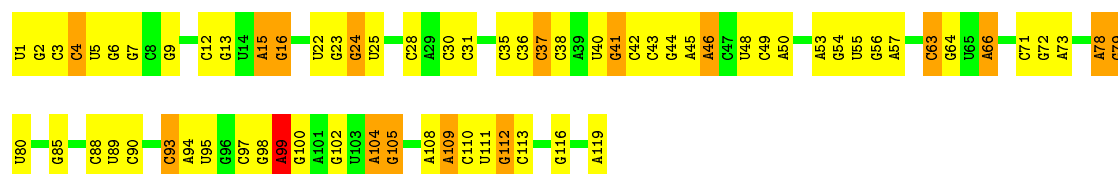


• Molecule 22: 23S rRNA



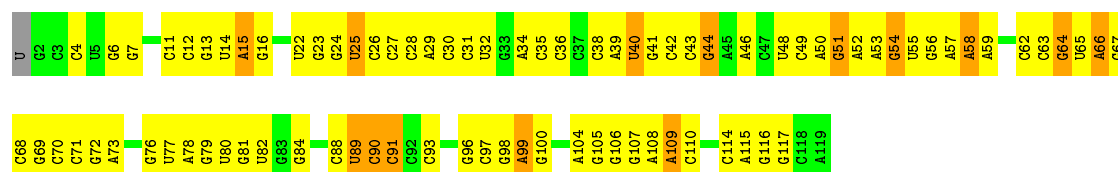






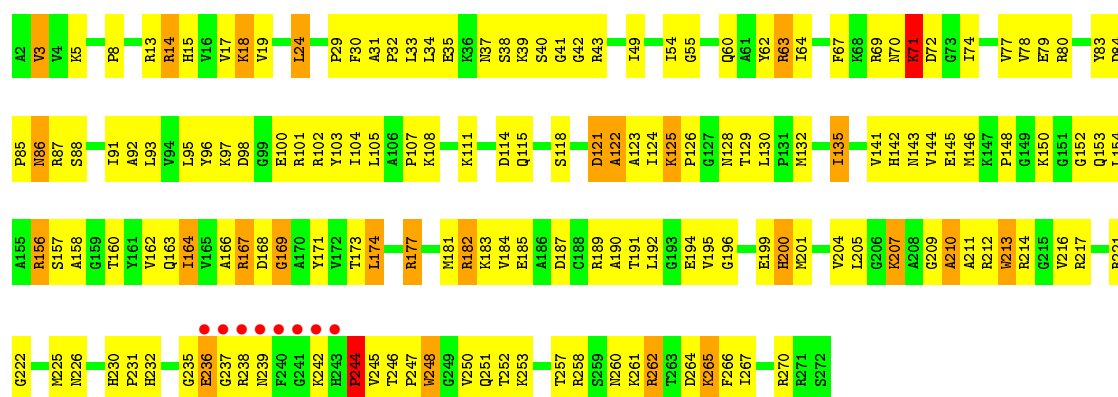
• Molecule 23: 5S rRNA

Chain DB: 29% 59% 12% .



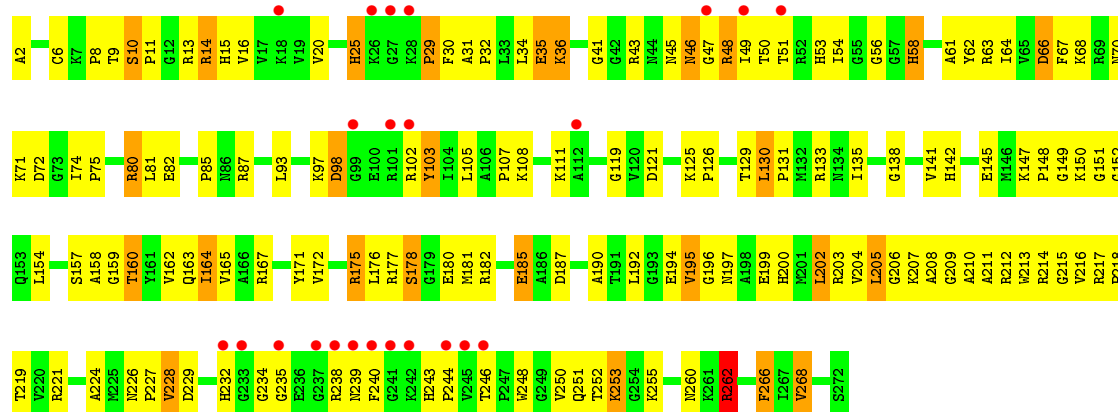
• Molecule 24: 50S ribosomal protein L2

Chain BC: 3% 40% 50% 9% .



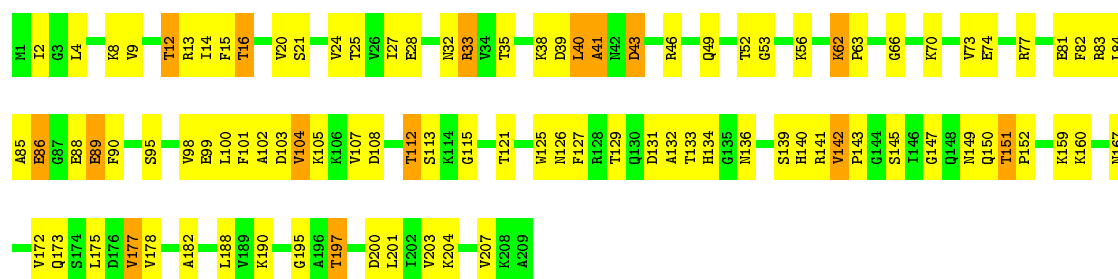
• Molecule 24: 50S ribosomal protein L2

Chain DC: 8% 45% 45% 10%



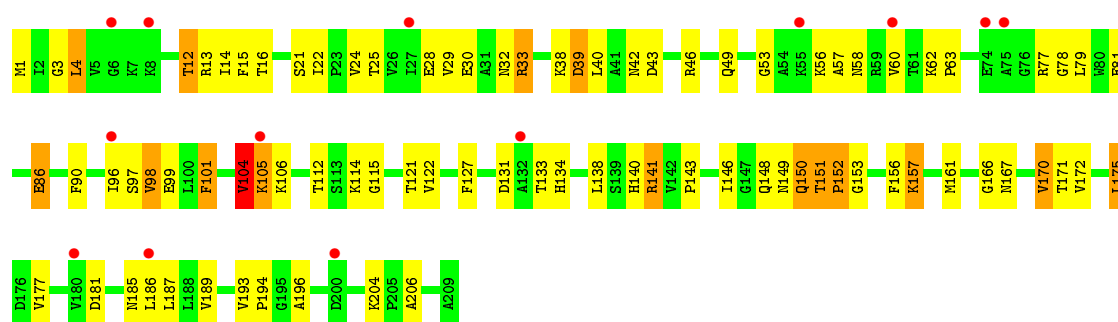
• Molecule 25: 50S ribosomal protein L3

Chain BD: 



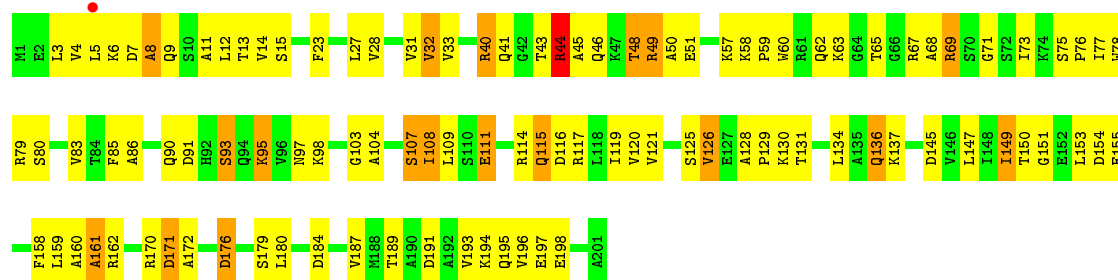
- Molecule 25: 50S ribosomal protein L3

Chain DD: 



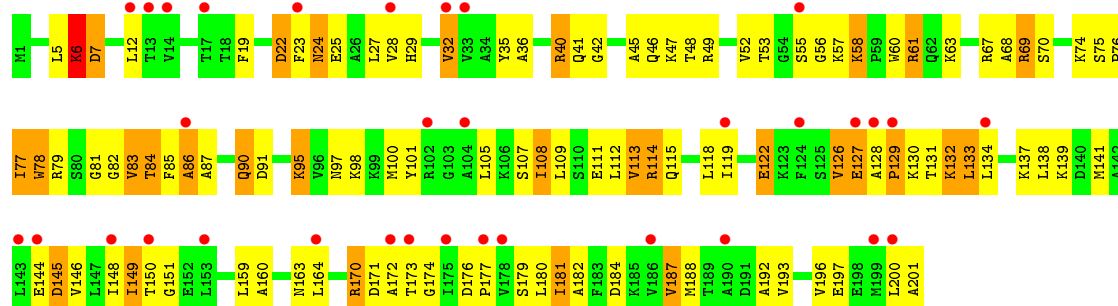
- Molecule 26: 50S ribosomal protein L4

Chain BE: 



- Molecule 26: 50S ribosomal protein L4

Chain DE: 



Chain BF:

Category	Percentage
Red	6%
Green	37%
Yellow	49%
Orange	13%

Chain DF:

Chain DF	Percentage
A2	53%
K3	53%
L4	53%
H5	53%
D6	53%
Y7	53%
Y8	53%
K9	53%
D10	53%
E11	53%
V12	53%
V13	53%
K14	53%
K15	53%
K16	53%
M17	53%
F20	49%
M21	49%
Y22	49%
M23	49%
S24	49%
V25	49%
M26	49%
Q27	49%
V28	49%
P29	49%
R30	49%
V31	49%
E32	49%
K33	49%
I34	49%
T35	49%
L36	49%
N37	49%
M38	49%
G39	49%
V40	49%
G41	49%
E42	49%
A43	49%
I44	49%
A45	49%
D46	49%
K47	49%
K48	49%
L49	49%
L50	49%
D51	49%
N52	49%
A53	49%
A54	49%
A55	49%
D56	49%
L57	49%
I60	49%
S61	49%
G62	49%
O63	49%
K64	11%
P65	11%
L66	11%
I67	11%
S73	11%
V74	11%
A75	11%
G76	11%
F77	11%
K78	11%
I79	11%
R80	11%
Q81	11%
G82	11%
Y83	11%
P84	11%
I85	11%
G86	11%
C87	11%
K88	11%
V89	11%
T90	11%
L91	11%
R92	11%
G93	11%
E94	11%
R95	11%
N96	11%
W97	11%
E98	11%
F99	11%
F100	11%
E101	11%
R102	11%
L103	11%
I104	11%
I106	11%
A107	11%
V108	11%
P109	11%
R110	11%
I111	11%
R112	11%
D113	11%
F114	11%
R115	11%
G116	11%
L117	11%
S118	11%
A119	11%
K120	11%
S121	11%
F122	11%
D123	11%
G124	11%
R125	11%
V126	11%
S129	11%
M130	11%
G131	11%
V132	11%
R133	11%
E134	11%
Q135	11%
I136	11%
P139	11%
E140	11%
I141	11%
D142	11%
V143	11%
D144	11%
K145	11%
V146	11%
D147	11%
R148	11%
V149	11%
R150	11%
G151	11%
L152	11%
D153	11%
I154	11%
I156	11%
T157	11%
T158	11%
K161	11%
S162	11%
D163	11%
E164	11%
E165	11%
L169	11%
L170	11%
D174	11%
F175	11%
P176	11%
F177	11%
R178	11%
V179	11%

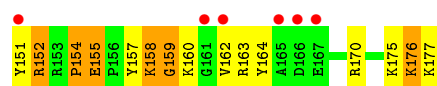
Chain BG: 55% 38% 7%

Chain DG:

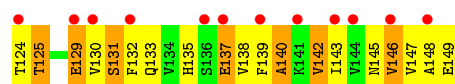
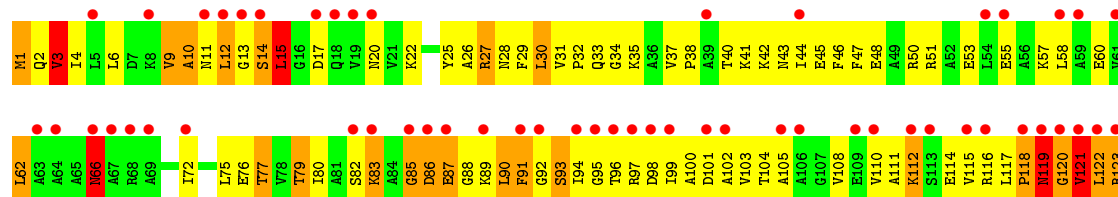
22% 54% 36% 9%

S2 R3 V4 V43 K44 L45 A46 D47 M48 L49 L50 T51 F52 G53 P54 V58 A59 D60 G61 A62 A63 Q64 T67 A68 R69 A70 L71 L72 L77

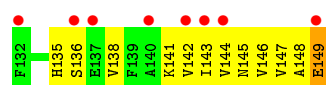
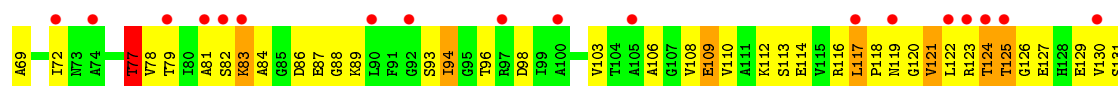
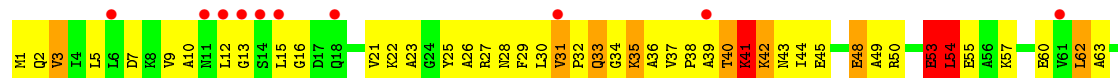
T80 E81 G82 F83 T84 K85 L89 G90 G91 V92 G93 Y94 R95 V98 V102 V103 T104 L105 G106 S106 L107 G108 F109 F110 H111 P112 P113 D114 H115 Q116 L117 P118 A119 G120 L121 T122 A123 E124 C125 P126 T127 T129 E130 I131 V132 L133 D137 V140 I141 V144 L148 R149 R150



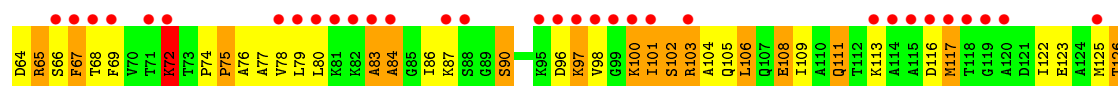
• Molecule 29: 50S ribosomal protein L9



• Molecule 29: 50S ribosomal protein L9

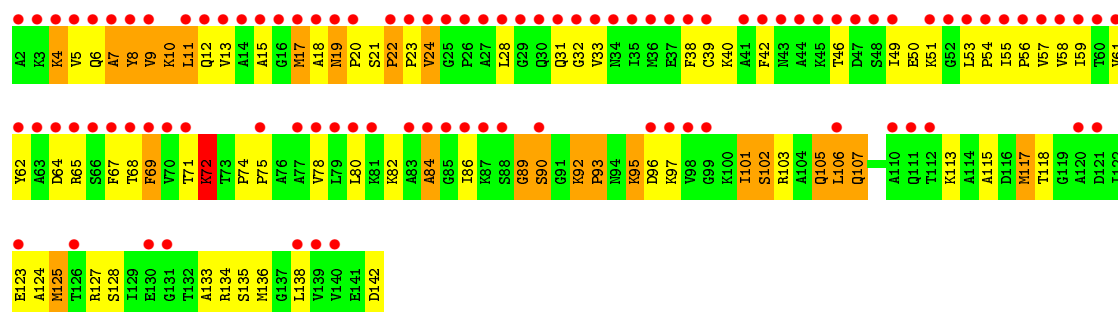


• Molecule 30: 50S ribosomal protein L11



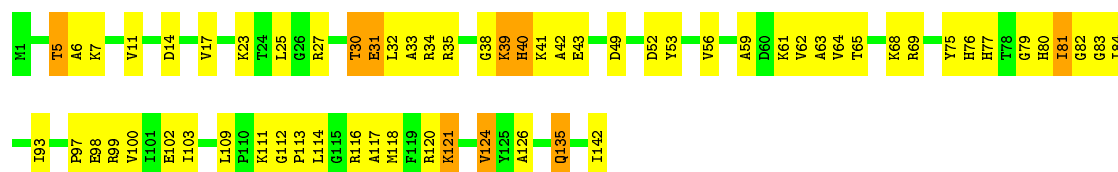
• Molecule 30: 50S ribosomal protein L11





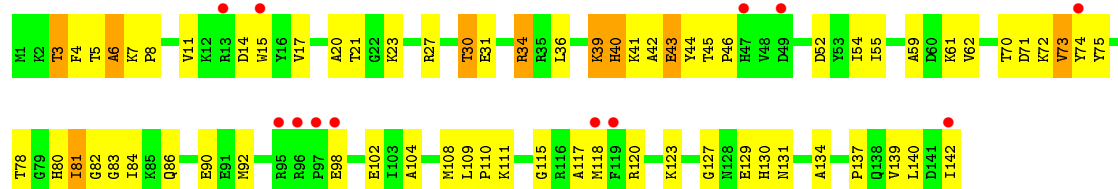
• Molecule 31: 50S ribosomal protein L13

Chain BJ: 56% 38% 6%



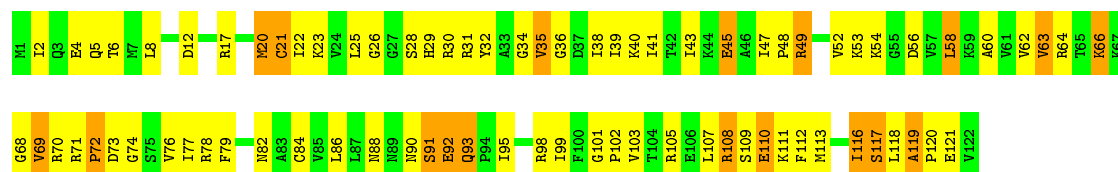
• Molecule 31: 50S ribosomal protein L13

Chain DJ: 8% 52% 42% 6%



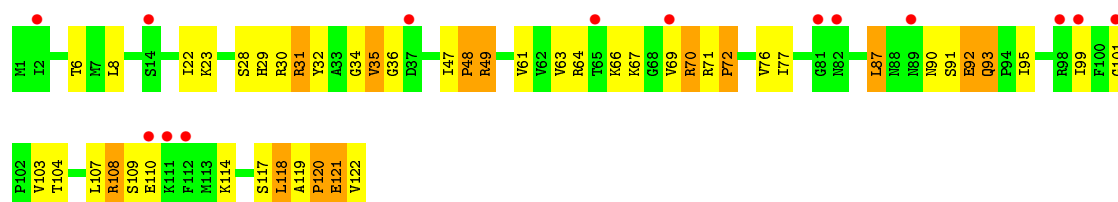
• Molecule 32: 50S ribosomal protein L14

Chain BK: 35% 50% 15%

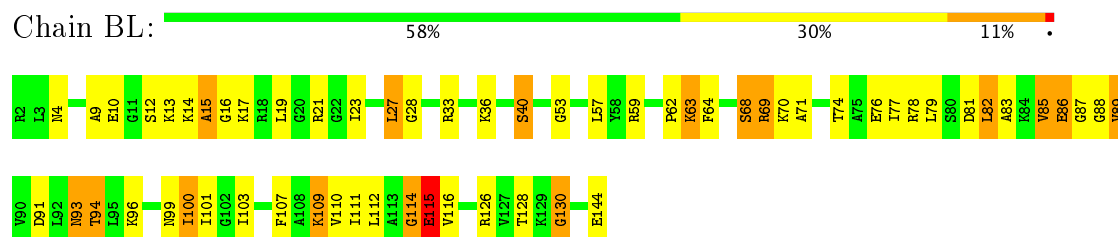


• Molecule 32: 50S ribosomal protein L14

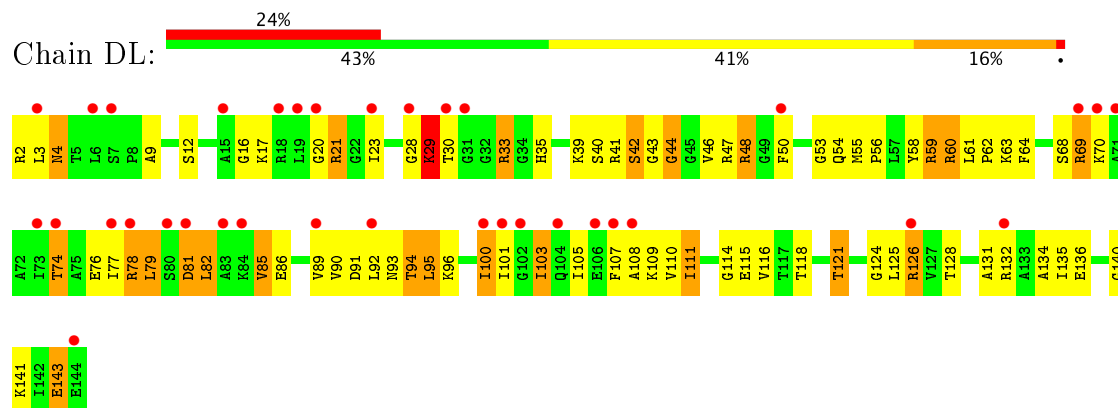
Chain DK: 11% 61% 28% 11%



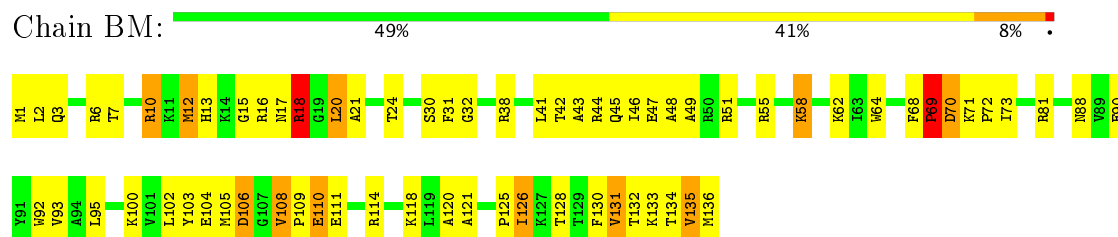
- Molecule 33: 50S ribosomal protein L15



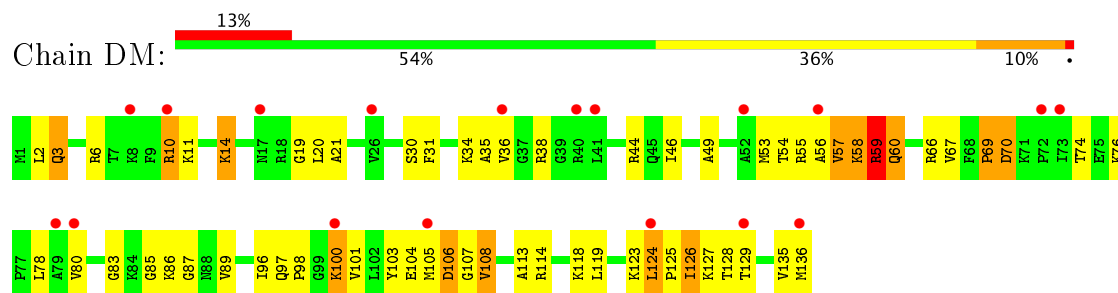
- Molecule 33: 50S ribosomal protein L15



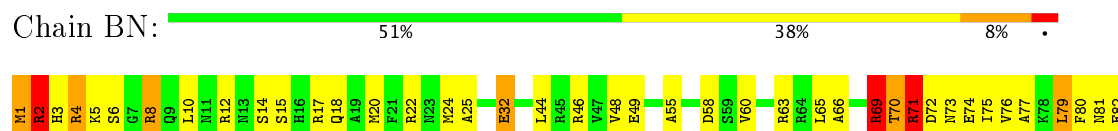
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

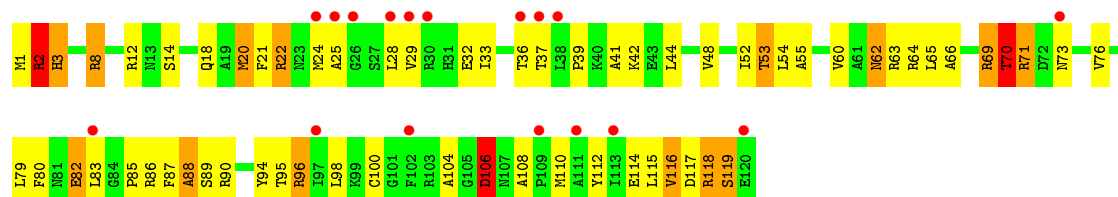


- Molecule 35: 50S ribosomal protein L17

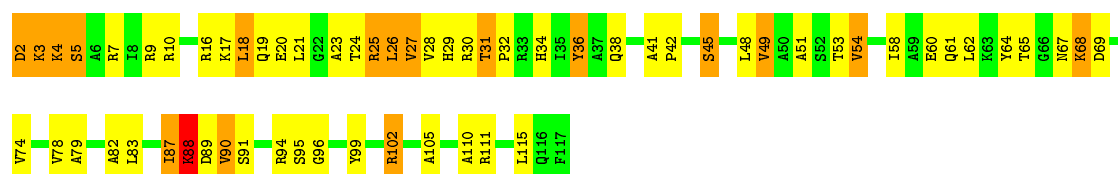




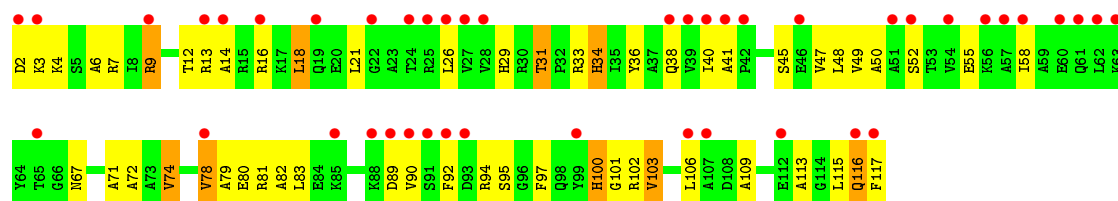
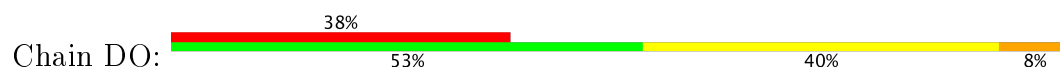
• Molecule 35: 50S ribosomal protein L17



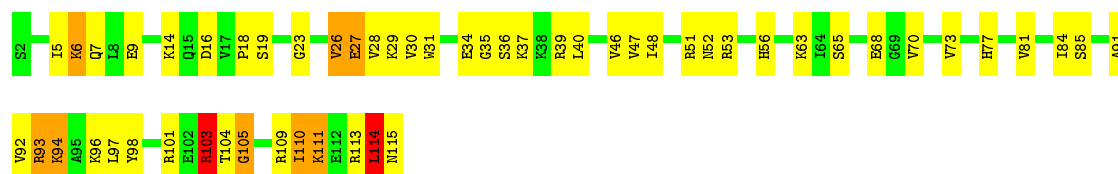
• Molecule 36: 50S ribosomal protein L18



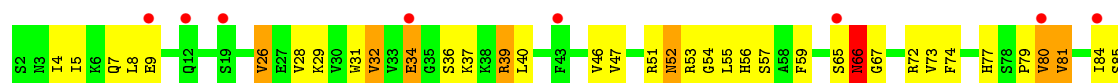
• Molecule 36: 50S ribosomal protein L18

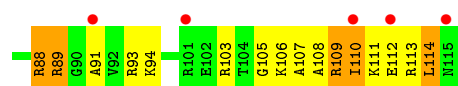


• Molecule 37: 50S ribosomal protein L19

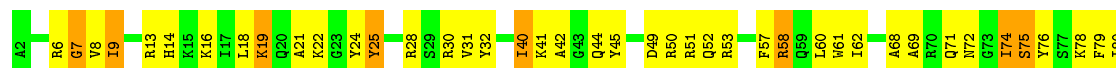


• Molecule 37: 50S ribosomal protein L19

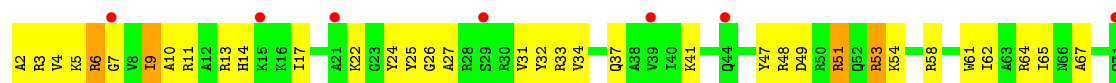




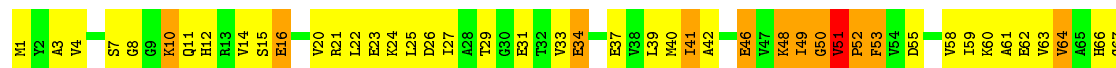
- Molecule 38: 50S ribosomal protein L20



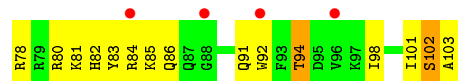
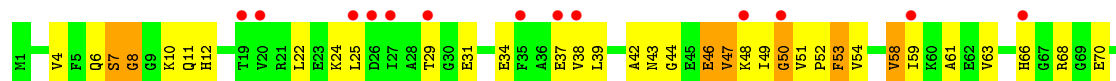
- Molecule 38: 50S ribosomal protein L20



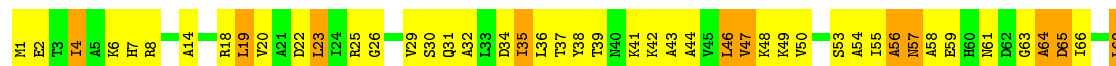
- Molecule 39: 50S ribosomal protein L21



- Molecule 39: 50S ribosomal protein L21

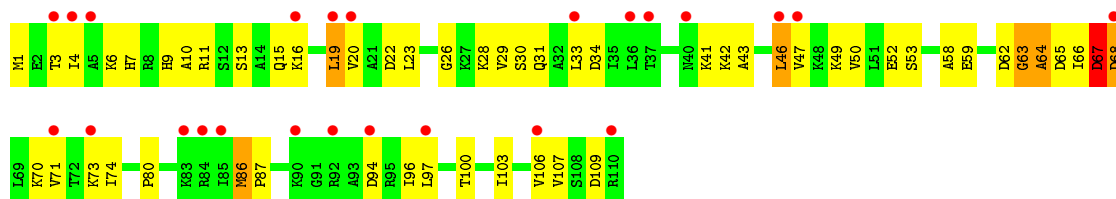


- Molecule 40: 50S ribosomal protein L22

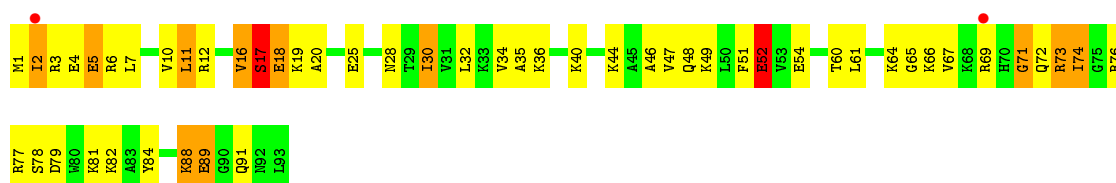
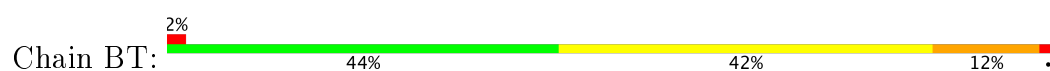




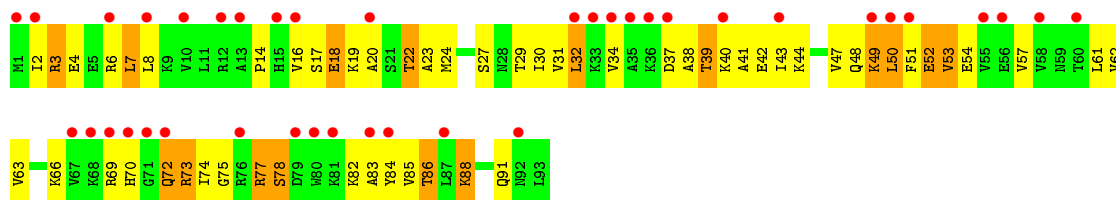
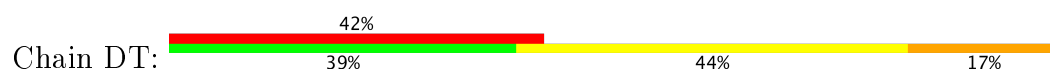
- Molecule 40: 50S ribosomal protein L22



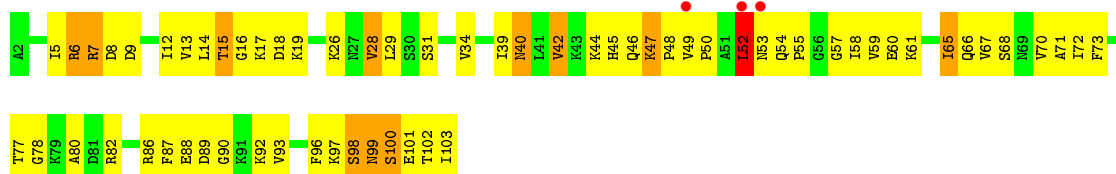
- Molecule 41: 50S ribosomal protein L23



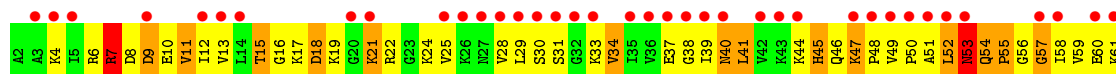
- Molecule 41: 50S ribosomal protein L23

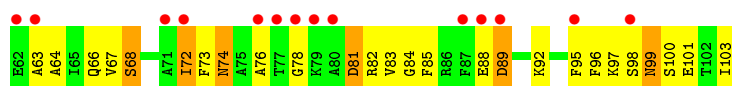


- Molecule 42: 50S ribosomal protein L24



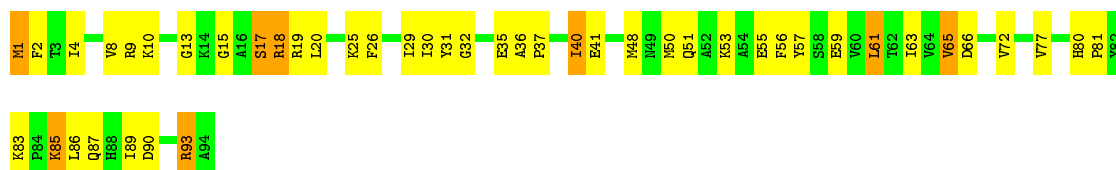
- Molecule 42: 50S ribosomal protein L24





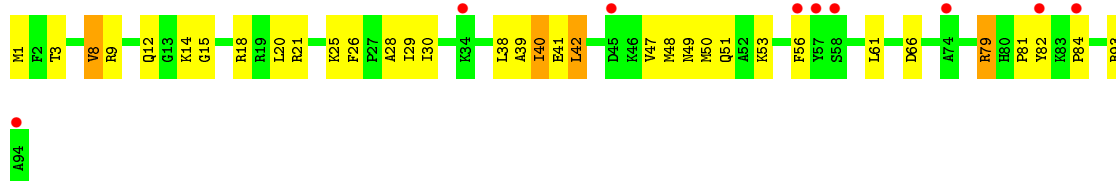
- Molecule 43: 50S ribosomal protein L25

Chain BV: 51% 40% 9%



- Molecule 43: 50S ribosomal protein L25

Chain DV: 10% 64% 32%



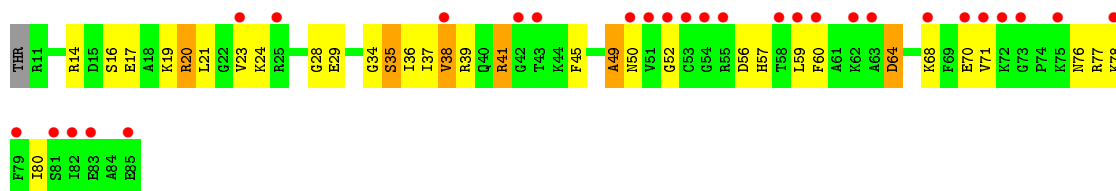
- Molecule 44: 50S ribosomal protein L27

Chain BW: 55% 39% 5%



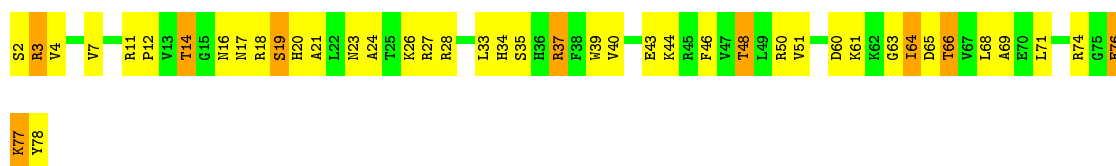
- Molecule 44: 50S ribosomal protein L27

Chain DW: 37% 55% 36% 8%

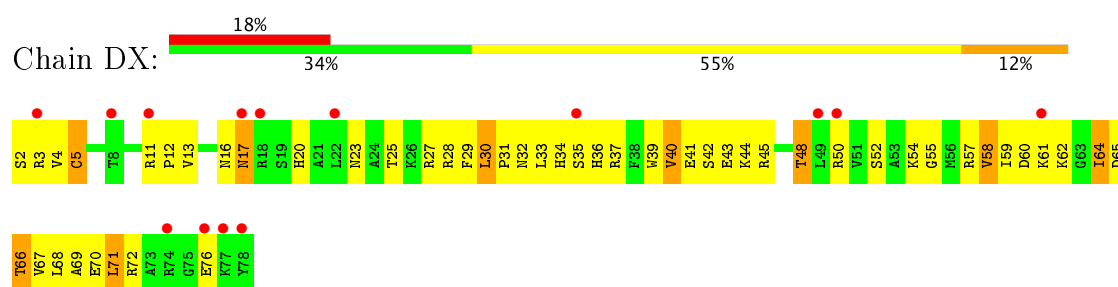


- Molecule 45: 50S ribosomal protein L28

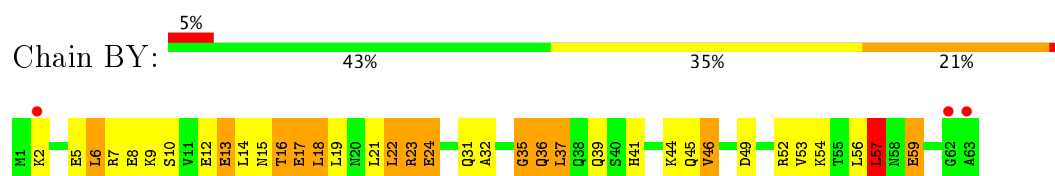
Chain BX: 44% 44% 12%



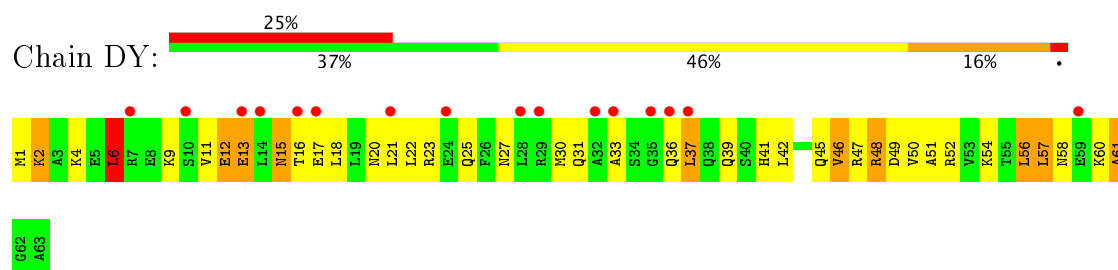
- Molecule 45: 50S ribosomal protein L28



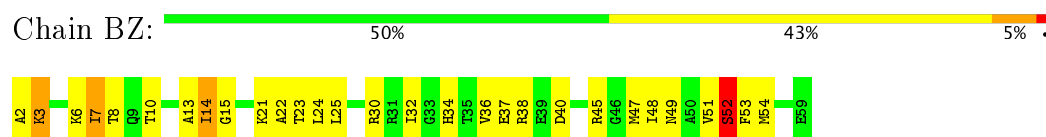
- Molecule 46: 50S ribosomal protein L29



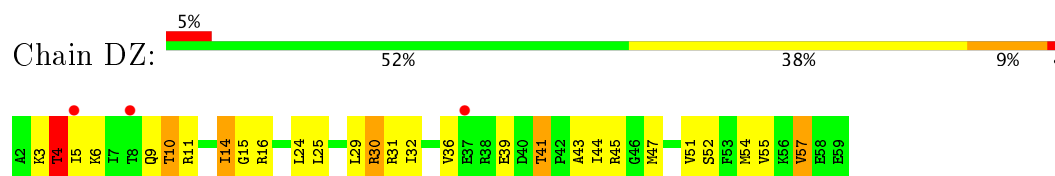
- Molecule 46: 50S ribosomal protein L29



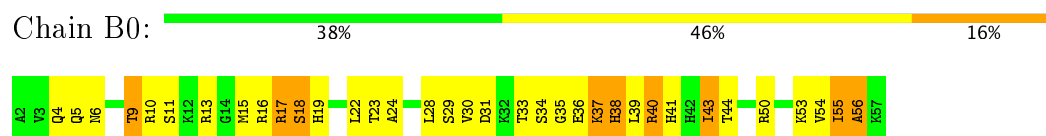
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

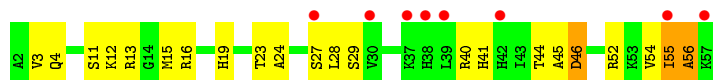


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

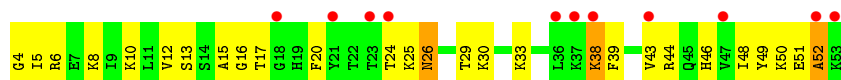




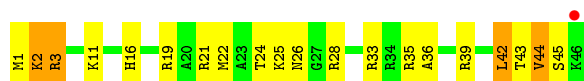
- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



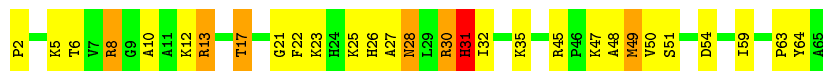
- Molecule 50: 50S ribosomal protein L34



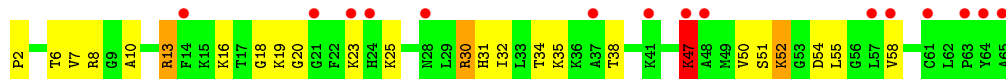
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

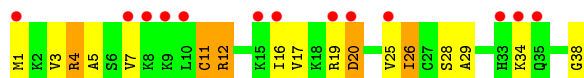


- Molecule 52: 50S ribosomal protein L36

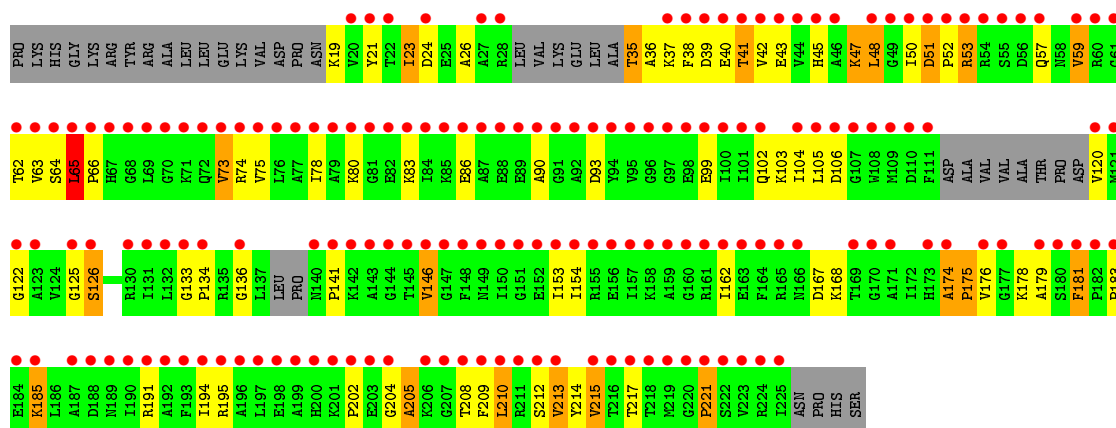
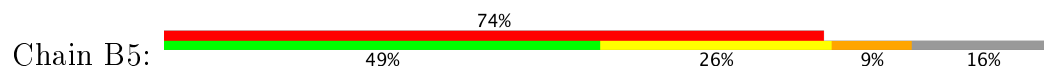




- Molecule 52: 50S ribosomal protein L36



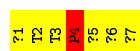
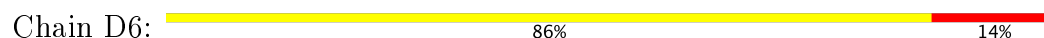
- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin



- Molecule 54: Linopristin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.49Å 433.90Å 621.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.15 – 3.00 69.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (69.15-3.00) 90.2 (69.15-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.225 , 0.274 0.235 , 0.284	Depositor DCC
R_{free} test set	4092 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288320	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DBB, MG, 04X, 004, MHW, MHU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.52	0/36944	1.02	48/57632 (0.1%)
1	CA	0.45	0/36966	0.96	27/57666 (0.0%)
2	AB	0.44	0/1736	0.65	0/2338
2	CB	0.38	0/1736	0.59	0/2338
3	AC	0.39	0/1652	0.61	0/2225
3	CC	0.37	0/1652	0.58	1/2225 (0.0%)
4	AD	0.39	0/1665	0.64	0/2227
4	CD	0.43	0/1665	0.65	0/2227
5	AE	0.41	0/1119	0.75	0/1504
5	CE	0.41	0/1119	0.73	0/1504
6	AF	0.41	0/836	0.77	2/1128 (0.2%)
6	CF	0.35	0/836	0.64	1/1128 (0.1%)
7	AG	0.37	0/1196	0.60	0/1602
7	CG	0.38	0/1196	0.54	0/1602
8	AH	0.40	0/989	0.63	0/1326
8	CH	0.34	0/989	0.57	0/1326
9	AI	0.39	0/1034	0.65	0/1375
9	CI	0.36	0/1034	0.59	0/1375
10	AJ	0.37	0/797	0.62	0/1077
10	CJ	0.36	0/797	0.61	0/1077
11	AK	0.38	0/893	0.63	0/1205
11	CK	0.37	0/893	0.61	0/1205
12	AL	0.41	0/969	0.71	0/1300
12	CL	0.41	0/969	0.73	0/1300
13	AM	0.38	0/893	0.70	1/1193 (0.1%)
13	CM	0.39	0/893	0.62	0/1193
14	AN	0.38	0/785	0.61	0/1043
14	CN	0.34	0/785	0.52	0/1043
15	AO	0.34	0/718	0.59	0/959
15	CO	0.32	0/718	0.57	0/959
16	AP	0.40	0/659	0.70	1/884 (0.1%)
16	CP	0.36	0/659	0.60	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.66	0/881
17	CQ	0.39	0/658	0.61	0/881
18	AR	0.37	0/463	0.61	0/621
18	CR	0.37	0/463	0.58	0/621
19	AS	0.43	0/653	0.66	0/877
19	CS	0.38	0/653	0.58	0/877
20	AT	0.43	0/671	0.63	0/888
20	CT	0.35	0/671	0.56	0/888
21	AU	0.50	0/431	0.71	0/570
21	CU	0.44	0/431	0.66	0/570
22	BA	0.90	44/69659 (0.1%)	1.39	725/108672 (0.7%)
22	DA	0.45	0/69659	0.95	28/108672 (0.0%)
23	BB	0.78	2/2850 (0.1%)	1.29	20/4444 (0.5%)
23	DB	0.39	0/2828	0.89	0/4410
24	BC	0.56	1/2122 (0.0%)	0.75	1/2852 (0.0%)
24	DC	0.37	0/2122	0.61	0/2852
25	BD	0.62	0/1586	0.80	1/2134 (0.0%)
25	DD	0.34	0/1586	0.55	0/2134
26	BE	0.54	0/1571	0.70	0/2113
26	DE	0.38	0/1571	0.60	0/2113
27	BF	0.41	0/1435	0.62	0/1926
27	DF	0.37	0/1435	0.53	0/1926
28	BG	0.45	0/1343	0.67	0/1816
28	DG	0.34	0/1343	0.52	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.44	0/1046	0.62	0/1410
30	DI	0.43	0/1046	0.59	0/1410
31	BJ	0.61	0/1152	0.75	1/1551 (0.1%)
31	DJ	0.35	0/1152	0.57	0/1551
32	BK	0.64	0/948	0.81	0/1268
32	DK	0.37	0/948	0.57	0/1268
33	BL	0.52	0/1054	0.75	0/1403
33	DL	0.38	0/1054	0.62	0/1403
34	BM	0.62	0/1093	0.80	1/1460 (0.1%)
34	DM	0.33	0/1093	0.56	0/1460
35	BN	0.61	0/974	0.88	3/1301 (0.2%)
35	DN	0.36	0/974	0.56	0/1301
36	BO	0.48	0/902	0.71	0/1209
36	DO	0.34	0/902	0.53	0/1209
37	BP	0.54	0/929	0.75	1/1242 (0.1%)
37	DP	0.37	0/929	0.58	0/1242
38	BQ	0.73	0/960	0.82	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.54	0/1278
39	BR	0.66	0/829	0.91	2/1107 (0.2%)
39	DR	0.36	0/829	0.59	0/1107
40	BS	0.72	0/864	0.81	0/1156
40	DS	0.36	0/864	0.63	0/1156
41	BT	0.49	0/745	0.68	0/994
41	DT	0.38	0/745	0.60	0/994
42	BU	0.48	0/788	0.72	0/1051
42	DU	0.43	0/788	0.61	0/1051
43	BV	0.52	0/766	0.70	0/1025
43	DV	0.32	0/766	0.48	0/1025
44	BW	0.64	0/587	0.79	0/776
44	DW	0.33	0/576	0.54	0/762
45	BX	0.45	0/635	0.73	0/848
45	DX	0.36	0/635	0.60	0/848
46	BY	0.46	0/510	0.71	0/677
46	DY	0.39	0/510	0.61	0/677
47	BZ	0.61	0/453	0.82	1/605 (0.2%)
47	DZ	0.32	0/453	0.58	0/605
48	B0	0.64	0/450	0.91	2/599 (0.3%)
48	D0	0.35	0/450	0.58	0/599
49	B1	0.46	0/417	0.67	0/554
49	D1	0.35	0/417	0.51	0/554
50	B2	0.55	0/380	0.83	0/498
50	D2	0.38	0/380	0.61	0/498
51	B3	0.58	0/513	0.75	0/676
51	D3	0.33	0/513	0.57	0/676
52	B4	0.60	0/303	0.71	0/397
52	D4	0.32	0/303	0.54	0/397
53	B5	0.39	0/1145	0.56	0/1556
54	B6	3.67	4/13 (30.8%)	4.12	3/15 (20.0%)
54	D6	3.86	3/13 (23.1%)	3.82	4/15 (26.7%)
All	All	0.59	54/310652 (0.0%)	1.02	876/464396 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	1
6	CF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	1
12	CL	0	2
21	AU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
48	B0	0	1
All	All	0	10

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-12.83	1.30	1.37
22	BA	528	A	N9-C4	-10.27	1.31	1.37
22	BA	528	A	N3-C4	-8.70	1.29	1.34
22	BA	974	G	N9-C4	-8.12	1.31	1.38
22	BA	979	A	N9-C4	-7.80	1.33	1.37

The worst 5 of 876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	15.39	116.95	110.80
22	BA	974	G	C5-N7-C8	-15.02	96.79	104.30
22	BA	752	A	N1-C6-N6	14.90	127.54	118.60
22	BA	974	G	N1-C6-O6	14.51	128.61	119.90
22	BA	1779	U	N3-C4-O4	-13.09	110.24	119.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
48	B0	24	ALA	Peptide
25	BD	151	THR	Peptide
33	BL	28	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1338	4
1	CA	33015	0	16617	1198	0
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	121	0
3	AC	1625	0	1696	89	0
3	CC	1625	0	1696	80	0
4	AD	1643	0	1707	133	0
4	CD	1643	0	1707	144	0
5	AE	1106	0	1148	83	0
5	CE	1106	0	1148	104	0
6	AF	818	0	808	62	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	65	0
7	CG	1182	0	1238	59	0
8	AH	979	0	1031	67	0
8	CH	979	0	1031	47	0
9	AI	1022	0	1070	77	0
9	CI	1022	0	1070	69	0
10	AJ	787	0	828	87	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	79	0
11	CK	877	0	887	72	0
12	AL	955	0	1016	65	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	80	0
13	CM	884	0	941	46	0
14	AN	774	0	824	66	0
14	CN	774	0	824	44	0
15	AO	710	0	728	35	0
15	CO	710	0	728	42	0
16	AP	649	0	666	53	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	69	0
17	CQ	649	0	691	50	0
18	AR	456	0	478	22	0
18	CR	456	0	478	23	0
19	AS	638	0	665	48	0
19	CS	638	0	665	38	0
20	AT	665	0	714	54	0
20	CT	665	0	714	38	0
21	AU	426	0	449	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	426	0	449	37	0
22	BA	62195	0	31280	2134	0
22	DA	62195	0	31280	2174	0
23	BB	2549	0	1291	56	0
23	DB	2529	0	1281	72	0
24	BC	2083	0	2154	157	0
24	DC	2083	0	2154	123	0
25	BD	1565	0	1616	92	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	75	0
26	DE	1552	0	1619	103	0
27	BF	1411	0	1444	105	0
27	DF	1411	0	1444	63	0
28	BG	1323	0	1371	61	0
28	DG	1323	0	1371	56	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	90	4
30	BI	1032	0	1085	82	0
30	DI	1032	0	1085	72	0
31	BJ	1129	0	1162	64	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	75	0
32	DK	939	0	1012	38	0
33	BL	1045	0	1117	51	0
33	DL	1045	0	1117	81	0
34	BM	1074	0	1157	47	0
34	DM	1074	0	1157	43	0
35	BN	961	0	1000	51	0
35	DN	961	0	1000	55	0
36	BO	892	0	923	57	0
36	DO	892	0	923	50	0
37	BP	917	0	962	48	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	61	0
38	DQ	947	0	1019	55	0
39	BR	816	0	839	84	0
39	DR	816	0	839	47	0
40	BS	857	0	922	64	0
40	DS	857	0	922	39	0
41	BT	739	0	807	46	0
41	DT	739	0	807	44	0
42	BU	780	0	831	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DU	780	0	831	65	0
43	BV	753	0	780	31	0
43	DV	753	0	780	25	0
44	BW	580	0	594	23	0
44	DW	569	0	581	26	0
45	BX	625	0	652	35	0
45	DX	625	0	652	55	0
46	BY	509	0	543	29	0
46	DY	509	0	543	38	0
47	BZ	449	0	488	19	0
47	DZ	449	0	488	14	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	32	0
49	D1	410	0	440	19	0
50	B2	377	0	418	19	0
50	D2	377	0	418	34	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	12	0
52	D4	302	0	342	17	0
53	B5	1142	0	865	49	0
54	B6	69	0	60	5	0
54	D6	69	0	60	14	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	23	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	1	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	2	0	0	0	0
57	BA	615	0	0	101	0
57	BB	14	0	0	0	0
57	BC	10	0	0	0	0
57	BD	4	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BJ	1	0	0	0	0
57	BL	6	0	0	0	0
57	BN	2	0	0	0	0
57	BS	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	189	0	0	20	0
57	CL	1	0	0	0	0
57	CN	3	0	0	2	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D0	1	0	0	0	0
57	D2	2	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	82	0
57	DB	13	0	0	3	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	6	0	0	1	0
57	DL	5	0	0	1	0
57	DN	2	0	0	0	0
57	DT	2	0	0	0	0
57	DU	1	0	0	1	0
57	DV	1	0	0	0	0
All	All	288320	0	192909	11780	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 11780 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1006:C:OP2	57:BA:3781:HOH:O	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:2714:G:OP2	57:BA:3548:HOH:O	1.61	1.18
22:BA:1603:A:OP1	57:BA:3411:HOH:O	1.61	1.15
54:D6:4:PRO:HB2	54:D6:5:MHU:HM1	1.15	1.14

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.78	0.42
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.93	0.27
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	135 (62%)	36 (17%)	45 (21%)	0	0
2	CB	216/218 (99%)	143 (66%)	36 (17%)	37 (17%)	0	1
3	AC	204/206 (99%)	142 (70%)	42 (21%)	20 (10%)	1	3
3	CC	204/206 (99%)	145 (71%)	41 (20%)	18 (9%)	1	4
4	AD	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	1
4	CD	203/205 (99%)	129 (64%)	48 (24%)	26 (13%)	0	1
5	AE	148/150 (99%)	98 (66%)	33 (22%)	17 (12%)	0	2
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	1
6	AF	98/100 (98%)	61 (62%)	19 (19%)	18 (18%)	0	0
6	CF	98/100 (98%)	64 (65%)	18 (18%)	16 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	5
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	2	13
8	AH	127/129 (98%)	80 (63%)	29 (23%)	18 (14%)	0	1
8	CH	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	9
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	1	4
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	1	6
10	AJ	96/98 (98%)	68 (71%)	7 (7%)	21 (22%)	0	0
10	CJ	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	1	3
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	1	4
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	1	4
12	CL	121/123 (98%)	89 (74%)	17 (14%)	15 (12%)	0	1
13	AM	112/114 (98%)	79 (70%)	22 (20%)	11 (10%)	1	3
13	CM	112/114 (98%)	86 (77%)	15 (13%)	11 (10%)	1	3
14	AN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	1
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	1
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	2	11
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	4	23
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	1
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	1	6
17	AQ	78/80 (98%)	52 (67%)	16 (20%)	10 (13%)	0	1
17	CQ	78/80 (98%)	55 (70%)	13 (17%)	10 (13%)	0	1
18	AR	53/55 (96%)	40 (76%)	12 (23%)	1 (2%)	9	41
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	6
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	5
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	2	14
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	0	2
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	6
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	1
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	206 (77%)	42 (16%)	21 (8%)	1	5
25	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	3	18
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	3	20
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	3	17
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	2	10
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	1	4
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	1	9
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	3	16
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	2	14
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	3
30	BI	139/141 (99%)	79 (57%)	34 (24%)	26 (19%)	0	0
30	DI	139/141 (99%)	79 (57%)	42 (30%)	18 (13%)	0	1
31	BJ	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	8	38
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	3	18
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1	4
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	1	4
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	1	6
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	1	8
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	5	27
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	3	17
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	6	32
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	7
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	3	17
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	10	43
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	3	17
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	9
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	4	23
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	20	62
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	1	7
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	12
40	DS	108/110 (98%)	87 (81%)	14 (13%)	7 (6%)	1	8
41	BT	91/93 (98%)	69 (76%)	13 (14%)	9 (10%)	1	3
41	DT	91/93 (98%)	62 (68%)	19 (21%)	10 (11%)	0	2
42	BU	100/102 (98%)	75 (75%)	17 (17%)	8 (8%)	1	5
42	DU	100/102 (98%)	72 (72%)	15 (15%)	13 (13%)	0	1
43	BV	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
43	DV	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	3	18
44	BW	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
44	DW	73/76 (96%)	58 (80%)	10 (14%)	5 (7%)	1	7
45	BX	75/77 (97%)	64 (85%)	7 (9%)	4 (5%)	2	13
45	DX	75/77 (97%)	56 (75%)	15 (20%)	4 (5%)	2	13
46	BY	61/63 (97%)	38 (62%)	13 (21%)	10 (16%)	0	1
46	DY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	1	3
47	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	13
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	13
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	4
48	D0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	6
49	B1	48/50 (96%)	39 (81%)	4 (8%)	5 (10%)	0	3
49	D1	48/50 (96%)	39 (81%)	6 (12%)	3 (6%)	1	9
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	3	17
50	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	7
51	B3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	5	26
51	D3	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	2	16
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	6	29
53	B5	183/228 (80%)	100 (55%)	53 (29%)	30 (16%)	0	1
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	11422/11686 (98%)	8514 (74%)	1907 (17%)	1001 (9%)	1	4

5 of 1001 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	22	TYR
2	AB	64	LYS
2	AB	68	LEU
2	AB	73	LYS
2	AB	75	ALA

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%)	125 (69%)	55 (31%)	0	2
2	CB	180/180 (100%)	126 (70%)	54 (30%)	0	2
3	AC	170/170 (100%)	137 (81%)	33 (19%)	1	9
3	CC	170/170 (100%)	130 (76%)	40 (24%)	1	4
4	AD	172/172 (100%)	128 (74%)	44 (26%)	0	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	10
5	AE	113/113 (100%)	85 (75%)	28 (25%)	1	3
5	CE	113/113 (100%)	83 (74%)	30 (26%)	0	3
6	AF	87/87 (100%)	63 (72%)	24 (28%)	0	2
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	88 (71%)	36 (29%)	0	2
7	CG	124/124 (100%)	92 (74%)	32 (26%)	0	3
8	AH	104/104 (100%)	80 (77%)	24 (23%)	1	4
8	CH	104/104 (100%)	79 (76%)	25 (24%)	1	4
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	2
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	2
10	AJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
10	CJ	86/86 (100%)	70 (81%)	16 (19%)	2	10
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	5
11	CK	90/90 (100%)	67 (74%)	23 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	78 (76%)	25 (24%)	1	4
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	4
13	AM	92/92 (100%)	65 (71%)	27 (29%)	0	2
13	CM	92/92 (100%)	69 (75%)	23 (25%)	1	3
14	AN	79/83 (95%)	63 (80%)	16 (20%)	1	7
14	CN	79/83 (95%)	69 (87%)	10 (13%)	5	22
15	AO	75/76 (99%)	61 (81%)	14 (19%)	2	10
15	CO	75/76 (99%)	64 (85%)	11 (15%)	3	17
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	4
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1	8
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
17	CQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
18	AR	48/48 (100%)	40 (83%)	8 (17%)	2	13
18	CR	48/48 (100%)	43 (90%)	5 (10%)	8	31
19	AS	70/70 (100%)	59 (84%)	11 (16%)	3	14
19	CS	70/70 (100%)	53 (76%)	17 (24%)	1	4
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	49 (75%)	16 (25%)	1	3
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	1
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	1
24	BC	216/216 (100%)	182 (84%)	34 (16%)	3	14
24	DC	216/216 (100%)	189 (88%)	27 (12%)	5	23
25	BD	164/164 (100%)	145 (88%)	19 (12%)	6	26
25	DD	164/164 (100%)	145 (88%)	19 (12%)	6	26
26	BE	165/165 (100%)	137 (83%)	28 (17%)	2	12
26	DE	165/165 (100%)	131 (79%)	34 (21%)	1	7
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	10
27	DF	148/148 (100%)	116 (78%)	32 (22%)	1	6
28	BG	137/137 (100%)	118 (86%)	19 (14%)	4	18
28	DG	137/137 (100%)	119 (87%)	18 (13%)	5	21
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	5
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	3
30	DI	109/109 (100%)	85 (78%)	24 (22%)	1	5
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	12	42
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	7	28
32	BK	103/103 (100%)	90 (87%)	13 (13%)	5	23
32	DK	103/103 (100%)	93 (90%)	10 (10%)	9	35
33	BL	102/102 (100%)	86 (84%)	16 (16%)	3	14
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	6
34	BM	109/109 (100%)	92 (84%)	17 (16%)	3	15
34	DM	109/109 (100%)	93 (85%)	16 (15%)	3	17
35	BN	100/100 (100%)	83 (83%)	17 (17%)	2	12
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	4
36	BO	86/86 (100%)	63 (73%)	23 (27%)	0	3
36	DO	86/86 (100%)	71 (83%)	15 (17%)	2	11
37	BP	99/99 (100%)	84 (85%)	15 (15%)	3	16
37	DP	99/99 (100%)	83 (84%)	16 (16%)	3	14
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	3	14
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	17
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	11
39	DR	84/84 (100%)	73 (87%)	11 (13%)	5	21
40	BS	93/93 (100%)	75 (81%)	18 (19%)	1	9
40	DS	93/93 (100%)	80 (86%)	13 (14%)	4	18
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	16
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	8
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	7
42	DU	83/83 (100%)	60 (72%)	23 (28%)	0	2
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	7
43	DV	78/78 (100%)	67 (86%)	11 (14%)	4	18
44	BW	57/58 (98%)	50 (88%)	7 (12%)	5	24
44	DW	56/58 (97%)	51 (91%)	5 (9%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	2	13
45	DX	67/67 (100%)	57 (85%)	10 (15%)	3	16
46	BY	55/55 (100%)	47 (86%)	8 (14%)	4	17
46	DY	55/55 (100%)	45 (82%)	10 (18%)	2	10
47	BZ	48/48 (100%)	42 (88%)	6 (12%)	5	23
47	DZ	48/48 (100%)	35 (73%)	13 (27%)	0	2
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	16
48	D0	47/47 (100%)	43 (92%)	4 (8%)	12	43
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	11
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	20
50	B2	38/38 (100%)	33 (87%)	5 (13%)	5	20
50	D2	38/38 (100%)	32 (84%)	6 (16%)	3	14
51	B3	51/51 (100%)	40 (78%)	11 (22%)	1	6
51	D3	51/51 (100%)	47 (92%)	4 (8%)	15	47
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	17
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	17
53	B5	61/180 (34%)	47 (77%)	14 (23%)	1	4
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7518 (80%)	1872 (20%)	1	8

5 of 1872 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	15	THR
3	CC	185	ASN
38	DQ	51	ARG
43	BV	65	VAL
53	B5	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
37	BP	56	HIS

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Mol	Chain	Res	Type
51	B3	31	HIS
37	DP	41	GLN
48	B0	42	HIS
51	B3	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	361 (23%)	17 (1%)
1	CA	1538/1539 (99%)	335 (21%)	16 (1%)
22	BA	2895/2903 (99%)	672 (23%)	36 (1%)
22	DA	2895/2903 (99%)	609 (21%)	33 (1%)
23	BB	118/119 (99%)	27 (22%)	1 (0%)
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2029 (22%)	103 (1%)

5 of 2029 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	13	U
1	AA	32	A

5 of 103 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2428	G
1	CA	209	U
22	DA	2286	G
22	BA	2430	A
22	BA	2873	A

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MHW	B6	1	54	9,9,10	2.91	3 (33%)	9,11,13	3.68	7 (77%)
54	DBB	B6	3	54	5,5,6	0.76	0	3,5,7	4.97	2 (66%)
54	MHU	B6	5	54	15,15,16	2.76	7 (46%)	18,19,21	2.33	5 (27%)
54	04X	B6	6	54	15,16,17	1.76	3 (20%)	11,20,22	4.57	6 (54%)
54	004	B6	7	54	8,10,11	3.57	6 (75%)	11,12,14	1.98	3 (27%)
54	MHW	D6	1	54	9,9,10	3.18	4 (44%)	9,11,13	2.28	6 (66%)
54	DBB	D6	3	54	5,5,6	1.23	1 (20%)	3,5,7	4.94	1 (33%)
54	MHU	D6	5	54	15,15,16	2.75	6 (40%)	18,19,21	2.18	3 (16%)
54	04X	D6	6	54	15,16,17	1.50	4 (26%)	11,20,22	5.33	7 (63%)
54	004	D6	7	54	8,10,11	3.46	6 (75%)	11,12,14	2.22	3 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	B6	5	54	-	0/8/12/14	0/1/1/1
54	04X	B6	6	54	-	0/4/24/26	0/2/2/2
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	D6	5	54	-	0/8/12/14	0/1/1/1
54	04X	D6	6	54	-	0/4/24/26	0/2/2/2
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-5.96	1.45	1.52
54	D6	1	MHW	CA-N	-5.75	1.28	1.35
54	D6	7	004	CB-CA	-5.58	1.46	1.52
54	D6	1	MHW	CG2-CB	-5.50	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	1	MHW	CG2-CB	-5.43	1.29	1.39

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	3	DBB	O-C-CA	-8.36	101.93	125.02
54	B6	1	MHW	O-C-CA	-8.33	117.11	124.32
54	D6	5	MHU	O-C-CA	-7.58	107.48	125.15
54	B6	5	MHU	O-C-CA	-7.07	108.66	125.15
54	B6	3	DBB	O-C-CA	-6.58	106.86	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	B6	3	DBB	1	0
54	B6	5	MHU	2	0
54	B6	7	004	1	0
54	D6	1	MHW	4	0
54	D6	3	DBB	2	0
54	D6	5	MHU	5	0
54	D6	6	04X	1	0
54	D6	7	004	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.39	22 (1%) 75 49	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	-0.20	36 (2%) 61 31	27, 72, 145, 177	0
2	AB	218/218 (100%)	1.15	52 (23%) 1 0	43, 76, 100, 125	0
2	CB	218/218 (100%)	1.54	69 (31%) 0 0	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.09	5 (2%) 59 30	39, 61, 83, 96	0
3	CC	206/206 (100%)	1.23	44 (21%) 1 1	57, 79, 97, 109	0
4	AD	205/205 (100%)	0.03	3 (1%) 74 47	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.20	3 (1%) 74 47	21, 40, 71, 90	0
5	AE	150/150 (100%)	0.01	3 (2%) 65 36	27, 51, 82, 106	0
5	CE	150/150 (100%)	0.02	1 (0%) 87 67	34, 59, 87, 104	0
6	AF	100/100 (100%)	-0.31	0 100 100	38, 59, 76, 84	0
6	CF	100/100 (100%)	-0.14	1 (1%) 82 58	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.82	25 (16%) 2 1	54, 78, 98, 108	0
7	CG	151/151 (100%)	1.77	60 (39%) 0 0	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.07	1 (0%) 86 64	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.08	4 (3%) 49 22	45, 65, 81, 90	0
9	AI	127/127 (100%)	1.01	21 (16%) 2 1	51, 73, 97, 113	0
9	CI	127/127 (100%)	1.42	36 (28%) 1 0	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.44	7 (7%) 17 6	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.87	43 (43%) 0 0	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.58	14 (11%) 5 2	32, 64, 91, 110	0
11	CK	117/117 (100%)	0.11	3 (2%) 56 27	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.11	3 (2%) 59 30	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.07	4 (3%) 47 21	39, 52, 79, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.42	7 (6%) 22 8	49, 71, 92, 105	0
13	CM	114/114 (100%)	1.97	54 (47%) 0 0	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.81	15 (15%) 2 1	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.88	36 (37%) 0 0	69, 91, 110, 118	0
15	AO	88/88 (100%)	-0.01	1 (1%) 80 55	31, 51, 68, 98	0
15	CO	88/88 (100%)	-0.02	2 (2%) 61 31	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.47	4 (4%) 30 12	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.66	11 (13%) 4 1	45, 62, 88, 106	0
17	AQ	80/80 (100%)	-0.03	3 (3%) 41 17	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.49	5 (6%) 21 7	44, 72, 96, 105	0
18	AR	55/55 (100%)	-0.14	3 (5%) 26 10	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.01	2 (3%) 43 18	46, 56, 82, 111	0
19	AS	79/79 (100%)	1.01	14 (17%) 2 1	55, 72, 92, 101	0
19	CS	79/79 (100%)	3.07	55 (69%) 0 0	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.10	3 (3%) 44 19	35, 51, 74, 111	0
20	CT	85/85 (100%)	1.24	20 (23%) 1 0	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.68	21 (41%) 0 0	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.39	6 (11%) 5 2	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.14	103 (3%) 43 18	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	-0.07	71 (2%) 58 29	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.52	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	-0.36	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.24	8 (2%) 51 23	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.42	23 (8%) 11 4	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.45	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.37	13 (6%) 21 8	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.43	1 (0%) 90 74	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.93	33 (16%) 2 1	45, 81, 98, 106	0
27	BF	177/177 (100%)	0.25	11 (6%) 21 8	15, 46, 88, 97	0
27	DF	177/177 (100%)	2.38	93 (52%) 0 0	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.16	0 100 100	15, 38, 64, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.19	39 (22%) 1 0	71, 90, 104, 117	0
29	BH	149/149 (100%)	2.30	66 (44%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.16	36 (24%) 1 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.43	66 (46%) 0 0	84, 108, 121, 136	0
30	DI	141/141 (100%)	3.62	96 (68%) 0 0	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.46	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.41	12 (8%) 11 4	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.54	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.65	14 (11%) 5 2	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.35	0 100 100	0, 21, 48, 76	0
33	DL	143/143 (100%)	1.25	35 (24%) 1 0	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.49	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.80	18 (13%) 4 1	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.47	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.59	17 (14%) 3 1	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.26	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	1.68	44 (37%) 0 0	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.32	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.57	13 (11%) 6 2	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.45	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.41	9 (7%) 14 5	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.48	0 100 100	1, 9, 31, 63	0
39	DR	103/103 (100%)	0.86	17 (16%) 2 1	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.38	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	1.06	24 (21%) 1 0	56, 73, 89, 96	0
41	BT	93/93 (100%)	-0.02	2 (2%) 62 33	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.83	39 (41%) 0 0	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.11	3 (2%) 52 24	10, 30, 61, 92	0
42	DU	102/102 (100%)	2.59	52 (50%) 0 0	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.36	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.46	9 (9%) 9 3	65, 82, 94, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.42	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	1.51	28 (37%) 0 0	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.37	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.61	14 (18%) 1 1	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.04	3 (4%) 31 12	22, 44, 74, 96	0
46	DY	63/63 (100%)	1.25	16 (25%) 1 0	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.38	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.25	3 (5%) 28 11	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.53	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.85	8 (14%) 3 1	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.28	2 (4%) 39 16	13, 31, 54, 87	0
49	D1	50/50 (100%)	1.17	11 (22%) 1 0	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.31	1 (2%) 62 33	3, 9, 17, 90	0
50	D2	46/46 (100%)	1.17	9 (19%) 1 1	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.33	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	0.93	15 (23%) 1 0	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.08	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.58	13 (34%) 0 0	63, 74, 85, 99	0
53	B5	191/228 (83%)	4.42	168 (87%) 0 0	85, 111, 123, 134	0
54	B6	2/7 (28%)	0.27	0 100 100	5, 5, 5, 9	0
54	D6	2/7 (28%)	0.75	0 100 100	53, 53, 53, 62	0
All	All	20738/20808 (99%)	0.27	1980 (9%) 9 3	0, 64, 119, 195	0

The worst 5 of 1980 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	16.2
30	DI	6	GLN	16.2
22	BA	2100	G	15.8
30	DI	2	ALA	15.2
22	BA	2104	C	14.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	DBB	D6	3	6/7	0.88	0.50	-	45,50,65,70	0
54	004	D6	7	10/11	0.95	0.23	-	47,52,61,64	0
54	MHU	D6	5	15/16	0.82	0.38	-	45,58,69,72	0
54	DBB	B6	3	6/7	0.94	0.28	-	8,14,20,33	0
54	04X	B6	6	15/16	0.97	0.19	-	6,11,15,20	0
54	MHU	B6	5	15/16	0.93	0.24	-	3,7,15,15	0
54	MHW	B6	1	9/10	0.97	0.20	-	8,13,21,30	0
54	04X	D6	6	15/16	0.90	0.27	-	47,59,67,73	0
54	004	B6	7	10/11	0.97	0.28	-	2,4,6,6	0
54	MHW	D6	1	9/10	0.94	0.18	-	55,59,63,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
55	MG	BA	3015	1/1	0.79	0.40	22.56	61,61,61,61	0
55	MG	BA	3186	1/1	0.96	0.23	20.31	12,12,12,12	0
55	MG	BA	3170	1/1	0.96	0.25	19.57	22,22,22,22	0
55	MG	DA	3113	1/1	0.89	0.45	17.52	75,75,75,75	0
55	MG	BA	3040	1/1	0.91	0.38	16.33	2,2,2,2	0
55	MG	DA	3002	1/1	0.77	0.52	15.16	81,81,81,81	0
55	MG	BA	3178	1/1	0.92	0.35	14.57	12,12,12,12	0
55	MG	AA	1670	1/1	0.74	0.40	13.74	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1615	1/1	0.85	0.23	13.71	56,56,56,56	0
55	MG	BA	3027	1/1	0.93	0.34	13.17	36,36,36,36	0
55	MG	DA	3072	1/1	0.23	0.51	12.25	89,89,89,89	0
55	MG	BA	3136	1/1	0.92	0.57	11.95	43,43,43,43	0
55	MG	DA	3071	1/1	0.19	0.59	11.68	93,93,93,93	0
55	MG	BA	3131	1/1	0.97	0.32	10.85	37,37,37,37	0
55	MG	DA	3041	1/1	0.46	0.42	10.25	66,66,66,66	0
55	MG	AM	201	1/1	0.94	0.62	8.94	50,50,50,50	0
55	MG	DA	3158	1/1	0.78	0.46	8.39	58,58,58,58	0
55	MG	BA	3146	1/1	0.96	0.21	5.57	22,22,22,22	0
55	MG	DA	3028	1/1	0.69	0.56	5.30	86,86,86,86	0
55	MG	DA	3106	1/1	0.78	0.31	4.98	70,70,70,70	0
55	MG	BA	3083	1/1	0.96	0.22	4.58	34,34,34,34	0
55	MG	CA	1626	1/1	0.78	0.26	4.56	66,66,66,66	0
55	MG	BA	3104	1/1	0.95	0.26	4.43	0,0,0,0	0
55	MG	BA	3055	1/1	0.58	0.25	4.05	50,50,50,50	0
55	MG	DA	3154	1/1	0.82	0.24	4.00	40,40,40,40	0
55	MG	DA	3110	1/1	0.96	0.24	3.67	45,45,45,45	0
55	MG	AA	1622	1/1	0.97	0.22	3.31	21,21,21,21	0
55	MG	BA	3005	1/1	0.96	0.17	2.52	43,43,43,43	0
55	MG	BA	3109	1/1	0.85	0.21	2.52	1,1,1,1	0
55	MG	DA	3032	1/1	0.67	0.20	2.32	78,78,78,78	0
55	MG	BA	3105	1/1	0.95	0.22	2.24	0,0,0,0	0
55	MG	AA	1669	1/1	0.92	0.27	2.20	34,34,34,34	0
55	MG	BA	3152	1/1	0.91	0.27	2.08	8,8,8,8	0
55	MG	AA	1662	1/1	0.83	0.27	1.81	49,49,49,49	0
55	MG	BA	3144	1/1	0.92	0.25	1.76	24,24,24,24	0
55	MG	BA	3053	1/1	0.94	0.18	1.69	0,0,0,0	0
55	MG	DA	3137	1/1	0.70	0.27	1.52	84,84,84,84	0
55	MG	DA	3140	1/1	0.97	0.22	1.50	42,42,42,42	0
55	MG	DA	3069	1/1	0.87	0.20	1.40	77,77,77,77	0
55	MG	DA	3060	1/1	0.85	0.22	1.09	72,72,72,72	0
55	MG	BA	3096	1/1	0.96	0.18	1.09	2,2,2,2	0
55	MG	DA	3058	1/1	0.83	0.17	0.97	70,70,70,70	0
55	MG	DA	3152	1/1	0.88	0.32	0.86	55,55,55,55	0
55	MG	BA	3187	1/1	0.98	0.21	0.85	3,3,3,3	0
55	MG	AA	1629	1/1	0.93	0.17	0.84	54,54,54,54	0
55	MG	DA	3064	1/1	0.92	0.19	0.83	48,48,48,48	0
55	MG	DA	3130	1/1	0.90	0.18	0.83	43,43,43,43	0
55	MG	DA	3048	1/1	0.78	0.22	0.67	93,93,93,93	0
55	MG	BA	3116	1/1	0.97	0.19	0.45	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1603	1/1	0.95	0.15	0.40	45,45,45,45	0
55	MG	DB	202	1/1	0.90	0.13	0.25	57,57,57,57	0
55	MG	DA	3109	1/1	0.97	0.19	0.06	30,30,30,30	0
55	MG	CA	1640	1/1	0.93	0.15	-0.05	36,36,36,36	0
55	MG	DA	3078	1/1	0.71	0.20	-0.32	95,95,95,95	0
55	MG	DA	3094	1/1	0.75	0.19	-0.41	83,83,83,83	0
55	MG	DA	3133	1/1	0.81	0.19	-0.44	55,55,55,55	0
55	MG	BA	3023	1/1	0.93	0.17	-0.45	0,0,0,0	0
55	MG	AA	1636	1/1	0.88	0.18	-0.55	42,42,42,42	0
55	MG	BA	3151	1/1	0.93	0.14	-0.58	23,23,23,23	0
55	MG	DA	3097	1/1	0.95	0.15	-0.61	67,67,67,67	0
55	MG	BA	3132	1/1	0.97	0.20	-0.65	32,32,32,32	0
55	MG	AA	1630	1/1	0.83	0.15	-0.70	67,67,67,67	0
55	MG	AA	1639	1/1	0.88	0.10	-0.74	67,67,67,67	0
55	MG	DA	3024	1/1	0.73	0.17	-0.78	45,45,45,45	0
55	MG	AA	1617	1/1	0.85	0.12	-0.82	62,62,62,62	0
55	MG	DA	3129	1/1	0.92	0.13	-0.84	70,70,70,70	0
55	MG	DA	3047	1/1	0.90	0.14	-0.84	71,71,71,71	0
55	MG	DA	3121	1/1	0.74	0.16	-0.85	60,60,60,60	0
55	MG	AA	1607	1/1	0.88	0.12	-0.99	48,48,48,48	0
55	MG	DA	3018	1/1	0.86	0.11	-1.10	68,68,68,68	0
55	MG	DA	3117	1/1	0.96	0.12	-1.22	55,55,55,55	0
55	MG	BA	3036	1/1	0.90	0.15	-1.25	23,23,23,23	0
55	MG	BA	3022	1/1	0.96	0.15	-1.30	0,0,0,0	0
55	MG	DA	3008	1/1	0.70	0.16	-1.30	80,80,80,80	0
56	ZN	D4	101	1/1	0.97	0.07	-1.32	74,74,74,74	0
55	MG	BA	3163	1/1	0.96	0.14	-1.35	27,27,27,27	0
55	MG	DA	3115	1/1	0.84	0.08	-1.35	79,79,79,79	0
55	MG	BA	3155	1/1	0.94	0.18	-1.35	2,2,2,2	0
55	MG	BA	3068	1/1	0.95	0.18	-1.43	1,1,1,1	0
55	MG	CA	1601	1/1	0.92	0.17	-1.49	52,52,52,52	0
56	ZN	B4	101	1/1	1.00	0.08	-1.49	76,76,76,76	0
55	MG	BA	3121	1/1	0.96	0.06	-1.52	14,14,14,14	0
55	MG	DA	3046	1/1	0.85	0.11	-1.60	62,62,62,62	0
55	MG	DA	3012	1/1	0.95	0.14	-1.63	39,39,39,39	0
55	MG	BA	3017	1/1	0.98	0.16	-1.66	0,0,0,0	0
55	MG	DA	3017	1/1	0.98	0.18	-1.70	39,39,39,39	0
55	MG	DA	3063	1/1	0.87	0.12	-1.70	53,53,53,53	0
55	MG	CA	1614	1/1	0.94	0.05	-1.72	52,52,52,52	0
55	MG	BA	3107	1/1	0.99	0.14	-1.76	3,3,3,3	0
55	MG	CA	1635	1/1	0.75	0.11	-1.78	94,94,94,94	0
55	MG	BA	3118	1/1	0.90	0.14	-1.80	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3037	1/1	0.95	0.08	-1.82	76,76,76,76	0
55	MG	DA	3135	1/1	0.87	0.08	-1.84	46,46,46,46	0
55	MG	DA	3050	1/1	0.98	0.12	-1.84	52,52,52,52	0
55	MG	DA	3005	1/1	0.43	0.12	-1.86	90,90,90,90	0
55	MG	BA	3063	1/1	0.99	0.13	-2.04	2,2,2,2	0
55	MG	DA	3023	1/1	0.96	0.11	-2.08	60,60,60,60	0
55	MG	DA	3025	1/1	0.88	0.12	-2.08	65,65,65,65	0
55	MG	CA	1607	1/1	0.96	0.14	-2.10	55,55,55,55	0
55	MG	AA	1618	1/1	0.95	0.09	-2.11	34,34,34,34	0
55	MG	BA	3161	1/1	0.85	0.16	-2.11	15,15,15,15	0
55	MG	DA	3098	1/1	0.82	0.08	-2.21	50,50,50,50	0
55	MG	BA	3013	1/1	0.96	0.17	-2.27	0,0,0,0	0
55	MG	BA	3159	1/1	0.94	0.14	-2.32	24,24,24,24	0
55	MG	BA	3077	1/1	0.90	0.07	-2.34	38,38,38,38	0
55	MG	DA	3079	1/1	0.67	0.08	-2.37	94,94,94,94	0
55	MG	BA	3108	1/1	0.94	0.16	-2.38	5,5,5,5	0
55	MG	CA	1622	1/1	0.88	0.13	-2.48	57,57,57,57	0
55	MG	BA	3049	1/1	0.96	0.14	-2.50	3,3,3,3	0
55	MG	BB	201	1/1	0.94	0.08	-2.52	28,28,28,28	0
55	MG	DA	3105	1/1	0.97	0.11	-2.64	52,52,52,52	0
55	MG	DA	3027	1/1	0.55	0.12	-2.69	82,82,82,82	0
55	MG	BA	3073	1/1	0.91	0.15	-2.71	9,9,9,9	0
55	MG	CA	1612	1/1	0.95	0.05	-2.72	43,43,43,43	0
55	MG	AA	1634	1/1	0.75	0.09	-2.75	49,49,49,49	0
55	MG	DA	3066	1/1	0.95	0.12	-2.79	45,45,45,45	0
55	MG	AA	1640	1/1	0.94	0.10	-2.88	57,57,57,57	0
55	MG	DA	3080	1/1	0.91	0.10	-2.95	91,91,91,91	0
55	MG	DA	3082	1/1	0.72	0.11	-3.11	65,65,65,65	0
55	MG	AA	1604	1/1	0.92	0.08	-3.16	48,48,48,48	0
55	MG	BA	3008	1/1	0.98	0.13	-3.18	0,0,0,0	0
55	MG	BA	3018	1/1	0.97	0.08	-3.33	10,10,10,10	0
55	MG	DA	3059	1/1	0.91	0.09	-3.34	42,42,42,42	0
55	MG	CA	1632	1/1	0.90	0.07	-3.42	75,75,75,75	0
55	MG	CA	1610	1/1	0.94	0.07	-3.46	58,58,58,58	0
55	MG	BA	3112	1/1	0.91	0.09	-3.47	20,20,20,20	0
55	MG	BA	3165	1/1	0.96	0.12	-3.59	3,3,3,3	0
55	MG	DA	3049	1/1	0.90	0.10	-3.61	69,69,69,69	0
55	MG	CA	1619	1/1	0.93	0.12	-3.65	27,27,27,27	0
55	MG	BA	3175	1/1	0.94	0.10	-3.68	9,9,9,9	0
55	MG	BA	3079	1/1	0.94	0.09	-3.68	21,21,21,21	0
55	MG	AA	1612	1/1	0.98	0.13	-3.72	38,38,38,38	0
55	MG	DA	3013	1/1	0.83	0.11	-3.72	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	201	1/1	0.76	0.05	-3.79	96,96,96,96	0
55	MG	BA	3065	1/1	0.94	0.12	-3.80	1,1,1,1	0
55	MG	BA	3097	1/1	0.94	0.12	-3.93	0,0,0,0	0
55	MG	DA	3096	1/1	0.92	0.09	-4.02	54,54,54,54	0
55	MG	BA	3101	1/1	0.95	0.09	-4.13	11,11,11,11	0
55	MG	DA	3022	1/1	0.94	0.13	-4.15	43,43,43,43	0
55	MG	CA	1616	1/1	0.94	0.10	-4.17	38,38,38,38	0
55	MG	AA	1616	1/1	0.92	0.09	-4.28	62,62,62,62	0
55	MG	DA	3054	1/1	0.87	0.08	-4.31	62,62,62,62	0
55	MG	BA	3012	1/1	0.96	0.16	-4.41	0,0,0,0	0
55	MG	AA	1625	1/1	0.94	0.09	-4.41	51,51,51,51	0
55	MG	BA	3093	1/1	0.87	0.10	-4.55	26,26,26,26	0
55	MG	BA	3032	1/1	0.93	0.12	-4.56	2,2,2,2	0
55	MG	AA	1641	1/1	0.97	0.12	-4.66	7,7,7,7	0
55	MG	BA	3110	1/1	0.96	0.11	-4.79	26,26,26,26	0
55	MG	AA	1609	1/1	0.92	0.08	-4.96	33,33,33,33	0
55	MG	BA	3002	1/1	0.88	0.09	-5.04	18,18,18,18	0
55	MG	BA	3028	1/1	0.87	0.10	-5.09	3,3,3,3	0
55	MG	BA	3021	1/1	0.99	0.15	-5.19	2,2,2,2	0
55	MG	CA	1617	1/1	0.97	0.09	-5.33	41,41,41,41	0
55	MG	AA	1633	1/1	0.96	0.08	-5.73	35,35,35,35	0
55	MG	BA	3130	1/1	0.97	0.16	-5.80	2,2,2,2	0
55	MG	BA	3024	1/1	0.95	0.07	-6.08	3,3,3,3	0
55	MG	BA	3058	1/1	0.97	0.07	-6.50	15,15,15,15	0
55	MG	BA	3050	1/1	0.92	0.07	-6.51	7,7,7,7	0
55	MG	AA	1642	1/1	0.99	0.07	-6.51	25,25,25,25	0
55	MG	AA	1613	1/1	0.94	0.07	-6.60	23,23,23,23	0
55	MG	DA	3043	1/1	0.90	0.07	-6.79	67,67,67,67	0
55	MG	BA	3120	1/1	0.93	0.12	-6.82	11,11,11,11	0
55	MG	BA	3071	1/1	0.93	0.15	-7.58	17,17,17,17	0
55	MG	BA	3134	1/1	0.97	0.09	-8.26	3,3,3,3	0
55	MG	AA	1606	1/1	0.93	0.06	-8.45	58,58,58,58	0
55	MG	BA	3129	1/1	0.86	0.13	-8.83	0,0,0,0	0
55	MG	DA	3039	1/1	0.95	0.10	-9.16	53,53,53,53	0
55	MG	BA	3009	1/1	0.97	0.08	-9.90	2,2,2,2	0
55	MG	AA	1611	1/1	0.97	0.07	-17.05	21,21,21,21	0
55	MG	BA	3177	1/1	0.94	0.10	-	9,9,9,9	0
55	MG	BA	3016	1/1	0.71	0.22	-	31,31,31,31	0
55	MG	BA	3169	1/1	0.95	0.10	-	4,4,4,4	0
55	MG	AA	1627	1/1	0.18	0.55	-	76,76,76,76	0
55	MG	DA	3124	1/1	0.95	0.16	-	41,41,41,41	0
55	MG	DA	3053	1/1	0.91	0.13	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1637	1/1	0.96	0.14	-	16,16,16,16	0
55	MG	BA	3173	1/1	0.91	0.29	-	30,30,30,30	0
55	MG	CA	1605	1/1	0.75	0.25	-	78,78,78,78	0
55	MG	BA	3067	1/1	0.96	0.20	-	0,0,0,0	0
55	MG	DA	3074	1/1	0.98	0.08	-	47,47,47,47	0
55	MG	DA	3139	1/1	0.90	0.56	-	47,47,47,47	0
55	MG	DA	3040	1/1	0.80	0.20	-	66,66,66,66	0
55	MG	AA	1628	1/1	0.97	0.04	-	39,39,39,39	0
55	MG	AA	1666	1/1	0.95	0.24	-	32,32,32,32	0
55	MG	DA	3011	1/1	0.41	0.31	-	74,74,74,74	0
55	MG	CA	1613	1/1	0.96	0.14	-	17,17,17,17	0
55	MG	BA	3047	1/1	0.74	0.11	-	40,40,40,40	0
55	MG	BA	3069	1/1	0.96	0.15	-	64,64,64,64	0
55	MG	DA	3116	1/1	0.44	0.33	-	92,92,92,92	0
55	MG	BA	3128	1/1	0.98	0.19	-	3,3,3,3	0
55	MG	CA	1642	1/1	0.95	0.19	-	25,25,25,25	0
55	MG	BA	3099	1/1	0.90	0.16	-	21,21,21,21	0
55	MG	AA	1653	1/1	0.97	0.18	-	34,34,34,34	0
55	MG	BA	3195	1/1	0.95	0.14	-	36,36,36,36	0
55	MG	BA	3038	1/1	0.93	0.14	-	1,1,1,1	0
55	MG	DA	3099	1/1	0.83	0.42	-	82,82,82,82	0
55	MG	BA	3106	1/1	0.98	0.24	-	0,0,0,0	0
55	MG	DA	3034	1/1	0.95	0.20	-	58,58,58,58	0
55	MG	BA	3194	1/1	0.95	0.18	-	22,22,22,22	0
55	MG	BA	3158	1/1	0.97	0.12	-	15,15,15,15	0
55	MG	DA	3091	1/1	0.77	0.13	-	79,79,79,79	0
55	MG	CA	1648	1/1	0.89	0.14	-	51,51,51,51	0
55	MG	BA	3034	1/1	0.92	0.13	-	5,5,5,5	0
55	MG	DA	3089	1/1	0.88	0.62	-	91,91,91,91	0
55	MG	DA	3162	1/1	0.97	0.11	-	48,48,48,48	0
55	MG	DA	3151	1/1	0.75	0.46	-	40,40,40,40	0
55	MG	DA	3153	1/1	0.70	0.12	-	68,68,68,68	0
55	MG	DA	3164	1/1	0.76	0.77	-	56,56,56,56	0
55	MG	BA	3191	1/1	0.96	0.17	-	26,26,26,26	0
55	MG	DA	3122	1/1	0.74	0.08	-	64,64,64,64	0
55	MG	BA	3154	1/1	0.75	0.24	-	21,21,21,21	0
55	MG	AA	1605	1/1	0.93	0.20	-	29,29,29,29	0
55	MG	BA	3189	1/1	0.97	0.20	-	0,0,0,0	0
55	MG	BA	3166	1/1	0.88	0.20	-	37,37,37,37	0
55	MG	BA	3171	1/1	0.93	0.17	-	20,20,20,20	0
55	MG	BA	3062	1/1	0.97	0.11	-	4,4,4,4	0
55	MG	BA	3137	1/1	0.95	0.29	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3192	1/1	0.96	0.23	-	11,11,11,11	0
55	MG	BA	3011	1/1	0.72	0.16	-	30,30,30,30	0
55	MG	AA	1621	1/1	0.98	0.09	-	37,37,37,37	0
55	MG	BA	3102	1/1	0.93	0.17	-	17,17,17,17	0
55	MG	DA	3001	1/1	0.95	0.08	-	37,37,37,37	0
55	MG	CA	1644	1/1	0.96	0.38	-	36,36,36,36	0
55	MG	BA	3037	1/1	0.98	0.19	-	0,0,0,0	0
55	MG	DA	3067	1/1	0.99	0.18	-	43,43,43,43	0
55	MG	BA	3162	1/1	0.97	0.13	-	23,23,23,23	0
55	MG	BA	3035	1/1	0.98	0.07	-	0,0,0,0	0
55	MG	BA	3089	1/1	0.94	0.14	-	1,1,1,1	0
55	MG	BA	3087	1/1	0.94	0.09	-	27,27,27,27	0
55	MG	CA	1638	1/1	0.84	0.16	-	74,74,74,74	0
55	MG	DA	3093	1/1	0.25	0.35	-	99,99,99,99	0
55	MG	BA	3113	1/1	0.85	0.12	-	2,2,2,2	0
55	MG	BA	3138	1/1	0.94	0.30	-	0,0,0,0	0
55	MG	AA	1664	1/1	0.97	0.13	-	51,51,51,51	0
55	MG	CA	1652	1/1	0.81	0.11	-	62,62,62,62	0
55	MG	AA	1610	1/1	0.92	0.15	-	51,51,51,51	0
55	MG	DA	3100	1/1	0.85	0.31	-	73,73,73,73	0
55	MG	CA	1649	1/1	0.97	0.21	-	24,24,24,24	0
55	MG	BA	3095	1/1	0.92	0.07	-	14,14,14,14	0
55	MG	AA	1658	1/1	0.90	0.17	-	35,35,35,35	0
55	MG	DA	3131	1/1	0.98	0.14	-	50,50,50,50	0
55	MG	DA	3029	1/1	0.77	0.36	-	66,66,66,66	0
55	MG	BA	3090	1/1	0.73	0.20	-	33,33,33,33	0
55	MG	DA	3021	1/1	0.70	0.33	-	62,62,62,62	0
55	MG	BA	3025	1/1	0.78	0.18	-	40,40,40,40	0
55	MG	BA	3020	1/1	0.88	0.13	-	5,5,5,5	0
55	MG	BA	3123	1/1	0.93	0.13	-	11,11,11,11	0
55	MG	DA	3163	1/1	0.91	0.21	-	47,47,47,47	0
55	MG	BA	3190	1/1	0.79	0.53	-	42,42,42,42	0
55	MG	AA	1649	1/1	0.97	0.12	-	28,28,28,28	0
55	MG	AA	1656	1/1	0.99	0.07	-	32,32,32,32	0
55	MG	DA	3015	1/1	0.79	0.57	-	77,77,77,77	0
55	MG	BA	3160	1/1	0.88	0.20	-	5,5,5,5	0
55	MG	DA	3149	1/1	0.76	0.19	-	49,49,49,49	0
55	MG	BA	3072	1/1	0.97	0.19	-	2,2,2,2	0
55	MG	BA	3133	1/1	0.88	0.34	-	57,57,57,57	0
55	MG	DA	3061	1/1	0.26	1.78	-	97,97,97,97	0
55	MG	BA	3075	1/1	0.91	0.14	-	6,6,6,6	0
55	MG	BA	3003	1/1	0.88	0.10	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3095	1/1	0.92	0.24	-	69,69,69,69	0
55	MG	AA	1614	1/1	0.89	0.19	-	66,66,66,66	0
55	MG	DA	3004	1/1	0.86	0.47	-	87,87,87,87	0
55	MG	BA	3046	1/1	0.94	0.17	-	3,3,3,3	0
55	MG	AA	1632	1/1	0.97	0.13	-	40,40,40,40	0
55	MG	BA	3111	1/1	0.92	0.07	-	27,27,27,27	0
55	MG	BA	3085	1/1	0.96	0.17	-	11,11,11,11	0
55	MG	BA	3078	1/1	0.98	0.04	-	38,38,38,38	0
55	MG	AA	1620	1/1	0.94	0.06	-	55,55,55,55	0
55	MG	DA	3118	1/1	0.88	0.11	-	73,73,73,73	0
55	MG	CA	1641	1/1	0.94	0.40	-	58,58,58,58	0
55	MG	DA	3077	1/1	0.62	0.26	-	76,76,76,76	0
55	MG	CA	1650	1/1	0.88	0.64	-	50,50,50,50	0
55	MG	DA	3134	1/1	0.58	0.57	-	87,87,87,87	0
55	MG	AA	1635	1/1	0.63	0.27	-	76,76,76,76	0
55	MG	BA	3149	1/1	0.97	0.23	-	0,0,0,0	0
55	MG	BA	3125	1/1	0.95	0.17	-	2,2,2,2	0
55	MG	AA	1602	1/1	0.92	0.37	-	53,53,53,53	0
55	MG	CA	1633	1/1	0.89	0.80	-	82,82,82,82	0
55	MG	BA	3091	1/1	0.90	0.05	-	48,48,48,48	0
55	MG	BB	203	1/1	0.90	0.09	-	7,7,7,7	0
55	MG	DA	3085	1/1	0.58	0.19	-	78,78,78,78	0
55	MG	CA	1623	1/1	0.93	0.17	-	66,66,66,66	0
55	MG	BA	3014	1/1	0.93	0.20	-	26,26,26,26	0
55	MG	CA	1624	1/1	0.90	0.07	-	52,52,52,52	0
55	MG	BA	3122	1/1	0.94	0.17	-	0,0,0,0	0
55	MG	BA	3064	1/1	0.95	0.15	-	0,0,0,0	0
55	MG	DA	3120	1/1	0.59	0.56	-	95,95,95,95	0
55	MG	DA	3086	1/1	0.98	0.12	-	61,61,61,61	0
55	MG	DA	3167	1/1	0.94	0.13	-	30,30,30,30	0
55	MG	BA	3056	1/1	0.89	0.19	-	22,22,22,22	0
55	MG	CA	1647	1/1	0.95	0.31	-	35,35,35,35	0
55	MG	BA	3019	1/1	0.81	0.26	-	1,1,1,1	0
55	MG	AA	1645	1/1	0.99	0.09	-	42,42,42,42	0
55	MG	CA	1620	1/1	0.86	0.13	-	81,81,81,81	0
55	MG	DA	3107	1/1	0.91	0.19	-	56,56,56,56	0
55	MG	DQ	201	1/1	0.89	0.29	-	40,40,40,40	0
55	MG	DA	3020	1/1	0.97	0.19	-	44,44,44,44	0
55	MG	AA	1660	1/1	0.95	0.09	-	41,41,41,41	0
55	MG	DA	3006	1/1	0.83	0.22	-	98,98,98,98	0
55	MG	BA	3029	1/1	0.82	0.12	-	35,35,35,35	0
55	MG	BA	3086	1/1	0.99	0.20	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3166	1/1	0.84	0.19	-	44,44,44,44	0
55	MG	BA	3080	1/1	0.87	0.09	-	24,24,24,24	0
55	MG	BA	3094	1/1	0.96	0.12	-	20,20,20,20	0
55	MG	BA	3103	1/1	0.96	0.07	-	7,7,7,7	0
55	MG	DA	3044	1/1	0.80	0.22	-	83,83,83,83	0
55	MG	DA	3030	1/1	0.94	0.26	-	61,61,61,61	0
55	MG	BA	3004	1/1	0.82	0.14	-	52,52,52,52	0
55	MG	BB	202	1/1	0.89	0.10	-	4,4,4,4	0
55	MG	CA	1645	1/1	0.91	0.13	-	32,32,32,32	0
55	MG	DA	3019	1/1	0.77	0.15	-	84,84,84,84	0
55	MG	AA	1651	1/1	0.70	0.34	-	55,55,55,55	0
55	MG	BA	3141	1/1	0.99	0.40	-	0,0,0,0	0
55	MG	DA	3142	1/1	0.91	0.39	-	39,39,39,39	0
55	MG	BA	3127	1/1	0.97	0.10	-	2,2,2,2	0
55	MG	DA	3155	1/1	0.74	0.28	-	37,37,37,37	0
55	MG	BA	3074	1/1	0.93	0.21	-	32,32,32,32	0
55	MG	DA	3003	1/1	0.96	0.13	-	66,66,66,66	0
55	MG	CA	1609	1/1	0.67	0.09	-	78,78,78,78	0
55	MG	AA	1644	1/1	0.23	0.69	-	49,49,49,49	0
55	MG	DA	3112	1/1	0.86	0.13	-	64,64,64,64	0
55	MG	BA	3033	1/1	0.99	0.20	-	0,0,0,0	0
55	MG	DA	3087	1/1	0.90	0.05	-	58,58,58,58	0
55	MG	BA	3088	1/1	0.90	0.08	-	29,29,29,29	0
55	MG	AA	1638	1/1	0.94	0.11	-	63,63,63,63	0
55	MG	BA	3031	1/1	0.78	0.11	-	7,7,7,7	0
55	MG	DA	3088	1/1	0.88	0.08	-	69,69,69,69	0
55	MG	DA	3132	1/1	0.53	0.79	-	85,85,85,85	0
55	MG	DA	3102	1/1	0.86	0.31	-	72,72,72,72	0
55	MG	BA	3172	1/1	0.96	0.12	-	16,16,16,16	0
55	MG	AA	1603	1/1	0.97	0.21	-	57,57,57,57	0
55	MG	DA	3045	1/1	0.89	0.21	-	61,61,61,61	0
55	MG	CM	201	1/1	0.85	0.38	-	50,50,50,50	0
55	MG	BA	3043	1/1	0.97	0.06	-	23,23,23,23	0
55	MG	DA	3157	1/1	0.89	0.14	-	29,29,29,29	0
55	MG	DA	3010	1/1	0.76	0.10	-	64,64,64,64	0
55	MG	AA	1643	1/1	0.90	0.15	-	23,23,23,23	0
55	MG	DA	3055	1/1	0.84	0.07	-	57,57,57,57	0
55	MG	DA	3108	1/1	0.92	0.14	-	55,55,55,55	0
55	MG	BA	3026	1/1	0.90	0.10	-	6,6,6,6	0
55	MG	AA	1647	1/1	0.99	0.17	-	44,44,44,44	0
55	MG	DA	3073	1/1	0.87	0.10	-	35,35,35,35	0
55	MG	AA	1657	1/1	0.83	0.34	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3066	1/1	0.92	0.14	-	2,2,2,2	0
55	MG	DA	3160	1/1	0.79	0.20	-	47,47,47,47	0
55	MG	BA	3082	1/1	0.96	0.07	-	6,6,6,6	0
55	MG	CA	1634	1/1	0.96	0.07	-	58,58,58,58	0
55	MG	BA	3098	1/1	0.73	0.59	-	73,73,73,73	0
55	MG	DA	3138	1/1	0.90	0.36	-	37,37,37,37	0
55	MG	DA	3081	1/1	0.88	0.12	-	62,62,62,62	0
55	MG	DA	3156	1/1	0.96	0.13	-	58,58,58,58	0
55	MG	BA	3156	1/1	0.95	0.15	-	9,9,9,9	0
55	MG	DA	3062	1/1	0.69	0.78	-	70,70,70,70	0
55	MG	AA	1626	1/1	0.96	0.21	-	26,26,26,26	0
55	MG	BA	3060	1/1	0.98	0.13	-	29,29,29,29	0
55	MG	BA	3147	1/1	0.97	0.14	-	11,11,11,11	0
55	MG	BA	3183	1/1	0.94	0.26	-	22,22,22,22	0
55	MG	AA	1650	1/1	0.94	0.25	-	20,20,20,20	0
55	MG	DA	3009	1/1	0.84	0.09	-	69,69,69,69	0
55	MG	CA	1611	1/1	0.84	0.17	-	69,69,69,69	0
55	MG	DA	3103	1/1	0.88	0.28	-	67,67,67,67	0
55	MG	CA	1627	1/1	0.61	0.29	-	88,88,88,88	0
55	MG	BA	3185	1/1	0.96	0.14	-	5,5,5,5	0
55	MG	BA	3114	1/1	0.98	0.09	-	28,28,28,28	0
55	MG	DA	3026	1/1	0.94	0.69	-	75,75,75,75	0
55	MG	DA	3065	1/1	0.91	0.07	-	41,41,41,41	0
55	MG	DA	3111	1/1	0.69	0.12	-	81,81,81,81	0
55	MG	BA	3153	1/1	0.97	0.16	-	2,2,2,2	0
55	MG	BA	3176	1/1	0.95	0.27	-	24,24,24,24	0
55	MG	BA	3042	1/1	0.97	0.14	-	1,1,1,1	0
55	MG	CA	1631	1/1	0.34	0.26	-	98,98,98,98	0
55	MG	CA	1625	1/1	0.98	0.17	-	18,18,18,18	0
55	MG	BA	3048	1/1	0.73	0.08	-	26,26,26,26	0
55	MG	DA	3161	1/1	0.79	0.33	-	48,48,48,48	0
55	MG	BA	3052	1/1	0.90	0.09	-	21,21,21,21	0
55	MG	DA	3075	1/1	0.96	0.26	-	61,61,61,61	0
55	MG	AA	1601	1/1	0.76	0.11	-	61,61,61,61	0
55	MG	BA	3044	1/1	0.90	0.21	-	8,8,8,8	0
55	MG	AA	1663	1/1	0.92	0.23	-	49,49,49,49	0
55	MG	BA	3100	1/1	0.96	0.10	-	9,9,9,9	0
55	MG	AA	1655	1/1	0.93	0.14	-	20,20,20,20	0
55	MG	DA	3127	1/1	0.85	0.13	-	88,88,88,88	0
55	MG	AA	1624	1/1	0.87	0.10	-	50,50,50,50	0
55	MG	DA	3144	1/1	0.85	0.30	-	58,58,58,58	0
55	MG	AA	1652	1/1	0.83	0.13	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3081	1/1	0.98	0.10	-	0,0,0,0	0
55	MG	BA	3184	1/1	0.95	0.13	-	8,8,8,8	0
55	MG	CA	1618	1/1	0.91	0.21	-	35,35,35,35	0
55	MG	BA	3054	1/1	0.91	0.08	-	7,7,7,7	0
55	MG	CA	1621	1/1	0.50	0.09	-	67,67,67,67	0
55	MG	DA	3038	1/1	0.78	0.14	-	63,63,63,63	0
55	MG	AA	1615	1/1	0.94	0.13	-	63,63,63,63	0
55	MG	BA	3039	1/1	0.96	0.22	-	1,1,1,1	0
55	MG	AA	1608	1/1	0.94	0.15	-	20,20,20,20	0
55	MG	DA	3068	1/1	0.94	0.07	-	60,60,60,60	0
55	MG	CA	1604	1/1	0.85	0.07	-	78,78,78,78	0
55	MG	CA	1651	1/1	0.95	0.25	-	72,72,72,72	0
55	MG	DA	3150	1/1	0.75	0.21	-	50,50,50,50	0
55	MG	BA	3007	1/1	0.90	0.09	-	32,32,32,32	0
55	MG	BA	3181	1/1	0.93	0.12	-	26,26,26,26	0
55	MG	BA	3124	1/1	0.88	0.09	-	9,9,9,9	0
55	MG	CA	1606	1/1	0.88	0.25	-	76,76,76,76	0
55	MG	DA	3123	1/1	0.95	0.15	-	44,44,44,44	0
55	MG	BA	3001	1/1	0.93	0.05	-	21,21,21,21	0
55	MG	DA	3128	1/1	0.92	0.07	-	74,74,74,74	0
55	MG	BA	3140	1/1	0.94	0.15	-	7,7,7,7	0
55	MG	AA	1631	1/1	0.91	0.16	-	52,52,52,52	0
55	MG	BA	3059	1/1	0.92	0.12	-	5,5,5,5	0
55	MG	AA	1623	1/1	0.79	0.17	-	49,49,49,49	0
55	MG	DA	3016	1/1	0.60	0.42	-	84,84,84,84	0
55	MG	DA	3090	1/1	0.82	0.08	-	59,59,59,59	0
55	MG	DA	3145	1/1	0.76	0.10	-	68,68,68,68	0
55	MG	DA	3035	1/1	0.91	0.14	-	71,71,71,71	0
55	MG	CA	1628	1/1	0.59	0.27	-	100,100,100,100	0
55	MG	BA	3119	1/1	0.64	0.36	-	49,49,49,49	0
55	MG	DA	3119	1/1	0.94	0.07	-	58,58,58,58	0
55	MG	BA	3157	1/1	0.83	0.33	-	34,34,34,34	0
55	MG	BA	3150	1/1	0.87	0.20	-	37,37,37,37	0
55	MG	DA	3092	1/1	0.79	0.44	-	94,94,94,94	0
55	MG	CA	1636	1/1	0.70	0.30	-	97,97,97,97	0
55	MG	BA	3070	1/1	0.80	0.11	-	37,37,37,37	0
55	MG	AA	1646	1/1	0.77	0.21	-	50,50,50,50	0
55	MG	BA	3045	1/1	0.85	0.12	-	4,4,4,4	0
55	MG	DA	3056	1/1	0.67	0.28	-	80,80,80,80	0
55	MG	BA	3030	1/1	0.97	0.16	-	3,3,3,3	0
55	MG	DA	3136	1/1	0.81	0.42	-	81,81,81,81	0
55	MG	BA	3061	1/1	0.89	0.64	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3174	1/1	0.94	0.14	-	5,5,5,5	0
55	MG	DB	203	1/1	0.82	0.09	-	90,90,90,90	0
55	MG	BA	3145	1/1	0.90	0.16	-	26,26,26,26	0
55	MG	DA	3146	1/1	0.93	0.10	-	41,41,41,41	0
55	MG	AA	1619	1/1	0.94	0.16	-	65,65,65,65	0
55	MG	BA	3092	1/1	0.91	0.19	-	42,42,42,42	0
55	MG	AA	1668	1/1	0.92	0.38	-	33,33,33,33	0
55	MG	BA	3143	1/1	0.96	0.32	-	3,3,3,3	0
55	MG	BA	3167	1/1	0.88	0.17	-	22,22,22,22	0
55	MG	BA	3164	1/1	0.98	0.30	-	6,6,6,6	0
55	MG	DA	3042	1/1	0.78	0.14	-	69,69,69,69	0
55	MG	BA	3148	1/1	0.97	0.14	-	13,13,13,13	0
55	MG	AA	1671	1/1	0.85	0.35	-	54,54,54,54	0
55	MG	BA	3051	1/1	0.98	0.14	-	4,4,4,4	0
55	MG	AA	1648	1/1	0.77	0.25	-	39,39,39,39	0
55	MG	CA	1643	1/1	0.97	0.37	-	41,41,41,41	0
55	MG	DA	3159	1/1	0.93	0.26	-	57,57,57,57	0
55	MG	BA	3041	1/1	0.94	0.10	-	11,11,11,11	0
55	MG	BA	3076	1/1	0.85	0.28	-	56,56,56,56	0
55	MG	DA	3101	1/1	0.91	0.08	-	63,63,63,63	0
55	MG	BA	3139	1/1	0.98	0.27	-	0,0,0,0	0
55	MG	CA	1602	1/1	0.78	0.12	-	69,69,69,69	0
55	MG	BA	3179	1/1	0.93	0.34	-	30,30,30,30	0
55	MG	AA	1654	1/1	0.96	0.14	-	41,41,41,41	0
55	MG	BA	3057	1/1	0.93	0.21	-	20,20,20,20	0
55	MG	BA	3182	1/1	0.95	0.22	-	14,14,14,14	0
55	MG	BA	3180	1/1	0.88	0.62	-	25,25,25,25	0
55	MG	CA	1646	1/1	0.88	0.23	-	36,36,36,36	0
55	MG	CA	1655	1/1	0.75	1.01	-	67,67,67,67	0
55	MG	DA	3125	1/1	0.88	0.17	-	86,86,86,86	0
55	MG	DA	3033	1/1	0.82	0.09	-	54,54,54,54	0
55	MG	DA	3057	1/1	0.42	0.29	-	82,82,82,82	0
55	MG	BA	3084	1/1	0.95	0.10	-	7,7,7,7	0
55	MG	BA	3126	1/1	0.96	0.15	-	3,3,3,3	0
55	MG	DA	3076	1/1	0.96	0.13	-	59,59,59,59	0
55	MG	DA	3007	1/1	0.92	0.37	-	80,80,80,80	0
55	MG	CA	1637	1/1	0.52	0.37	-	80,80,80,80	0
55	MG	BA	3006	1/1	0.97	0.07	-	13,13,13,13	0
55	MG	DA	3148	1/1	0.92	0.22	-	51,51,51,51	0
55	MG	CA	1629	1/1	0.50	0.10	-	84,84,84,84	0
55	MG	DA	3070	1/1	0.60	0.11	-	93,93,93,93	0
55	MG	BA	3188	1/1	0.96	0.11	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3104	1/1	0.57	0.18	-	76,76,76,76	0
55	MG	BA	3135	1/1	0.66	0.26	-	48,48,48,48	0
55	MG	BA	3117	1/1	0.96	0.16	-	1,1,1,1	0
55	MG	DA	3141	1/1	0.94	0.42	-	45,45,45,45	0
55	MG	BB	204	1/1	0.97	0.36	-	0,0,0,0	0
55	MG	CA	1630	1/1	0.90	0.65	-	102,102,102,102	0
55	MG	AA	1665	1/1	0.63	0.74	-	53,53,53,53	0
55	MG	DA	3014	1/1	0.79	0.35	-	73,73,73,73	0
55	MG	DA	3147	1/1	0.91	0.15	-	35,35,35,35	0
55	MG	BA	3168	1/1	0.84	0.24	-	21,21,21,21	0
55	MG	DA	3083	1/1	0.89	0.23	-	65,65,65,65	0
55	MG	CA	1639	1/1	0.93	0.13	-	43,43,43,43	0
55	MG	DA	3084	1/1	0.78	0.16	-	75,75,75,75	0
55	MG	BA	3115	1/1	0.73	0.51	-	76,76,76,76	0
55	MG	DA	3051	1/1	0.95	0.05	-	33,33,33,33	0
55	MG	CA	1654	1/1	0.88	0.21	-	26,26,26,26	0
55	MG	CA	1608	1/1	0.89	0.12	-	65,65,65,65	0
55	MG	DA	3165	1/1	0.74	0.39	-	43,43,43,43	0
55	MG	BA	3010	1/1	0.98	0.09	-	1,1,1,1	0
55	MG	BA	3142	1/1	0.97	0.21	-	0,0,0,0	0
55	MG	DA	3114	1/1	0.95	0.09	-	52,52,52,52	0
55	MG	AA	1659	1/1	0.85	0.47	-	32,32,32,32	0
55	MG	DA	3126	1/1	0.80	0.17	-	61,61,61,61	0
55	MG	AA	1667	1/1	0.73	0.69	-	54,54,54,54	0
55	MG	CA	1653	1/1	0.91	0.39	-	48,48,48,48	0
55	MG	DA	3031	1/1	0.92	0.14	-	59,59,59,59	0
55	MG	DA	3052	1/1	0.95	0.06	-	47,47,47,47	0
55	MG	AA	1661	1/1	0.92	0.36	-	23,23,23,23	0
55	MG	DA	3036	1/1	0.93	0.12	-	57,57,57,57	0
55	MG	BA	3193	1/1	0.94	0.16	-	12,12,12,12	0
55	MG	DA	3143	1/1	0.95	0.18	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.