



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:57 PM GMT

PDB ID : 4V7S
Title : Crystal structure of the E. coli ribosome bound to telithromycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-05
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

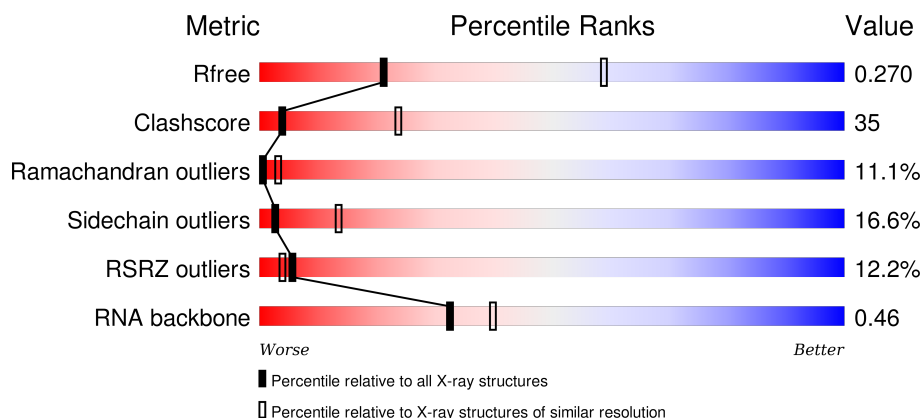
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



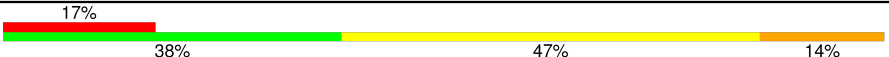

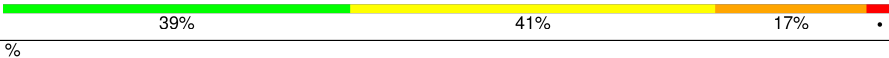
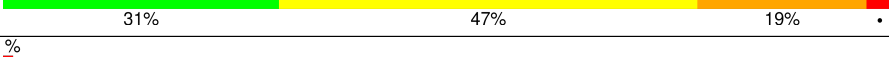

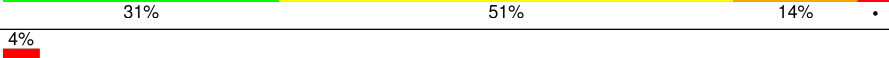
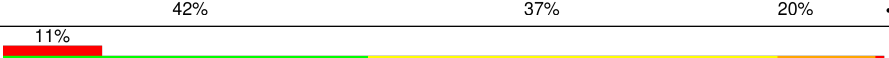
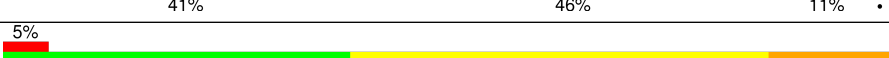
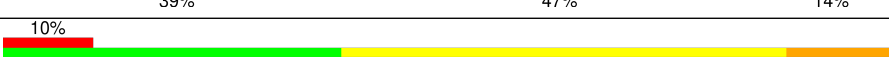
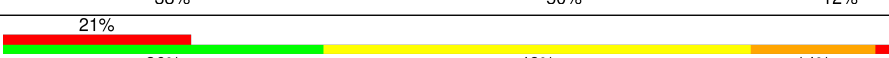
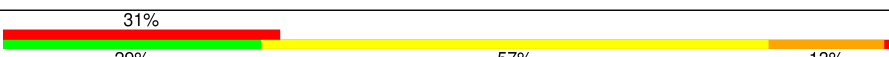
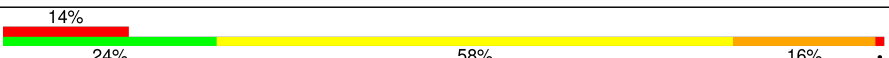


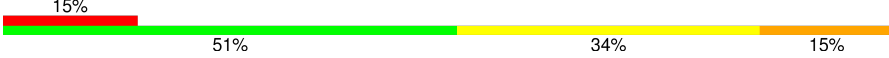

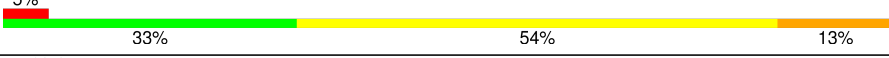
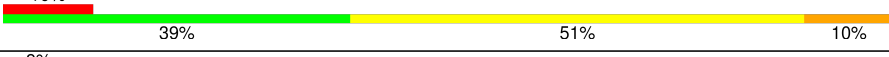
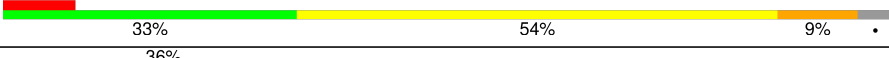
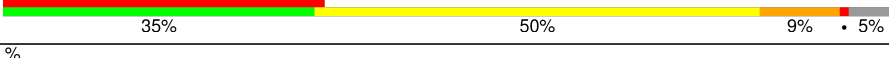

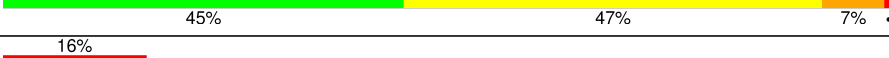

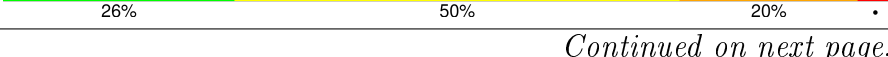

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)
RNA backbone	2183	1001 (3.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	AA	1533	<div> <div>10%</div> <div>31%</div> <div>49%</div> <div>19%</div> <div>•</div> </div>
2	AB	218	<div> <div>33%</div> <div>26%</div> <div>51%</div> <div>20%</div> <div>•</div> </div>
2	CB	218	<div> <div>39%</div> <div>35%</div> <div>50%</div> <div>14%</div> </div>
3	AC	206	<div> <div>10%</div> <div>44%</div> <div>42%</div> <div>12%</div> <div>•</div> </div>

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



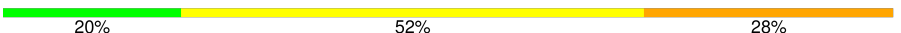
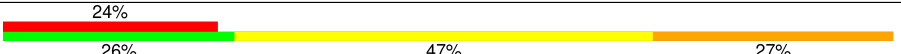

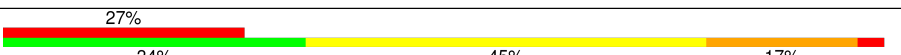
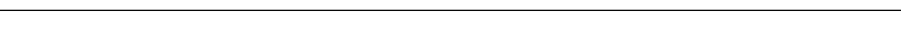
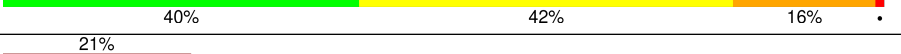



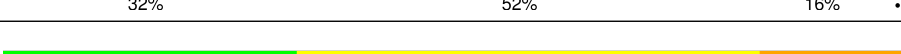
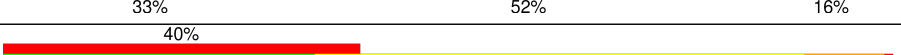
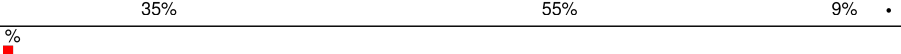
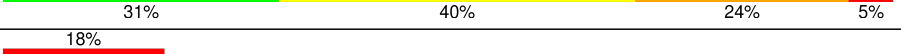
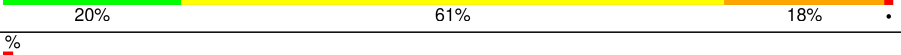
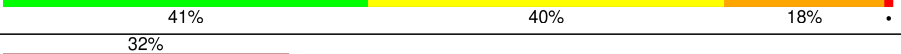
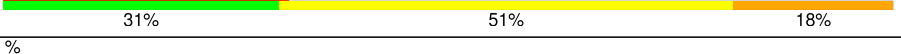
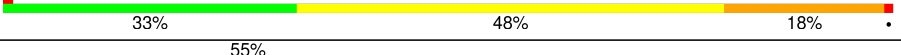



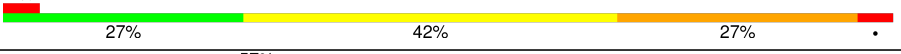
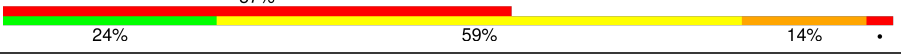

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Mol	Chain	Length	Quality of chain
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	

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

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Mol	Chain	Length	Quality of chain
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DB	117	
58	DF	178	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1641	-	-	-	X
59	MG	BA	3013	-	-	-	X
59	MG	BA	3021	-	-	-	X
59	MG	BA	3040	-	-	-	X
59	MG	BA	3070	-	-	-	X
59	MG	BA	3081	-	-	-	X
59	MG	BA	3095	-	-	-	X
59	MG	BA	3099	-	-	-	X
59	MG	BA	3102	-	-	-	X
59	MG	BA	3105	-	-	-	X
59	MG	BA	3106	-	-	-	X
59	MG	BA	3122	-	-	-	X
59	MG	BA	3129	-	-	-	X
59	MG	BA	3134	-	-	-	X
59	MG	CA	1612	-	-	-	X
59	MG	CA	1618	-	-	-	X
59	MG	CA	1624	-	-	-	X
59	MG	CA	1627	-	-	-	X
59	MG	CA	1636	-	-	-	X
59	MG	CA	1639	-	-	-	X
59	MG	DA	3002	-	-	-	X
59	MG	DA	3069	-	-	-	X
59	MG	DA	3075	-	-	-	X
59	MG	DA	3079	-	-	-	X
59	MG	DA	3097	-	-	-	X
59	MG	DA	3100	-	-	-	X
59	MG	DA	3106	-	-	-	X
59	MG	DA	3108	-	-	-	X
59	MG	DA	3129	-	-	-	X
60	TEL	BA	3135	X	-	-	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			892	552	178	162				
36	DO	116	Total	C	N	O	S	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	0	0	0
			780	492	146	142			
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called 16S rRNA.

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

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

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

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

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

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

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

- Molecule 57 is a RNA chain called 5S rRNA.

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

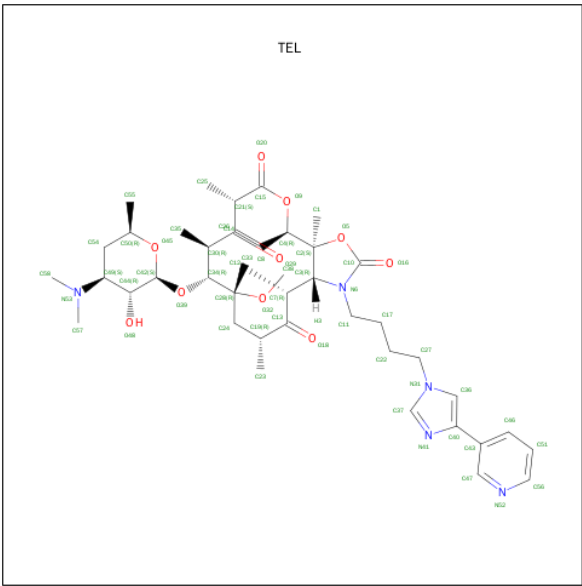
- Molecule 58 is a protein called 50S ribosomal protein L5.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BB	4	Total	Mg	0	0
			4	4		
59	BA	134	Total	Mg	0	0
			134	134		
59	CA	41	Total	Mg	0	0
			41	41		
59	DJ	1	Total	Mg	0	0
			1	1		
59	AA	43	Total	Mg	0	0
			43	43		
59	DA	133	Total	Mg	0	0
			133	133		
59	CE	1	Total	Mg	0	0
			1	1		
59	DC	2	Total	Mg	0	0
			2	2		
59	DB	1	Total	Mg	0	0
			1	1		

- Molecule 60 is TELITHROMYCIN (three-letter code: TEL) (formula: C₄₃H₆₅N₅O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	BA	1	Total	C	N	O	0	0
			58	43	5	10		

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AA	198	Total	O	0	0
			198	198		
62	AL	1	Total	O	0	0
			1	1		
62	AN	6	Total	O	0	0
			6	6		
62	AT	2	Total	O	0	0
			2	2		
62	AU	1	Total	O	0	0
			1	1		
62	BA	598	Total	O	0	0
			598	598		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	BB	20	Total 20	O 20	0	0
62	BC	10	Total 10	O 10	0	0
62	BD	2	Total 2	O 2	0	0
62	BE	1	Total 1	O 1	0	0
62	BL	2	Total 2	O 2	0	0
62	BN	3	Total 3	O 3	0	0
62	BQ	1	Total 1	O 1	0	0
62	BR	1	Total 1	O 1	0	0
62	BT	1	Total 1	O 1	0	0
62	B2	1	Total 1	O 1	0	0
62	B3	3	Total 3	O 3	0	0
62	B4	1	Total 1	O 1	0	0
62	CA	192	Total 192	O 192	0	0
62	CE	5	Total 5	O 5	0	0
62	CI	1	Total 1	O 1	0	0
62	CL	1	Total 1	O 1	0	0
62	CN	3	Total 3	O 3	0	0
62	CT	3	Total 3	O 3	0	0
62	CU	2	Total 2	O 2	0	0
62	DA	595	Total 595	O 595	0	0
62	DB	4	Total 4	O 4	0	0

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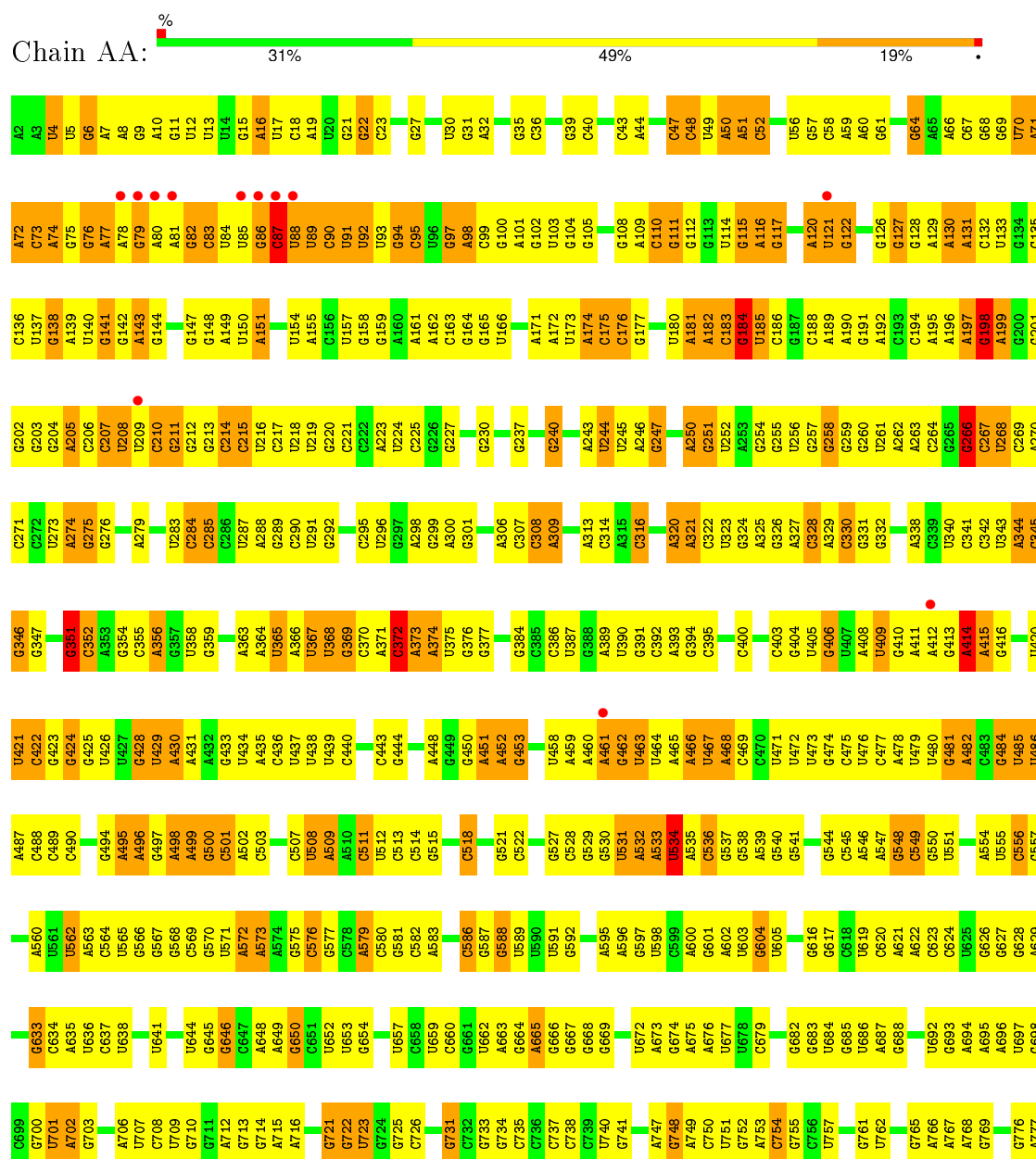
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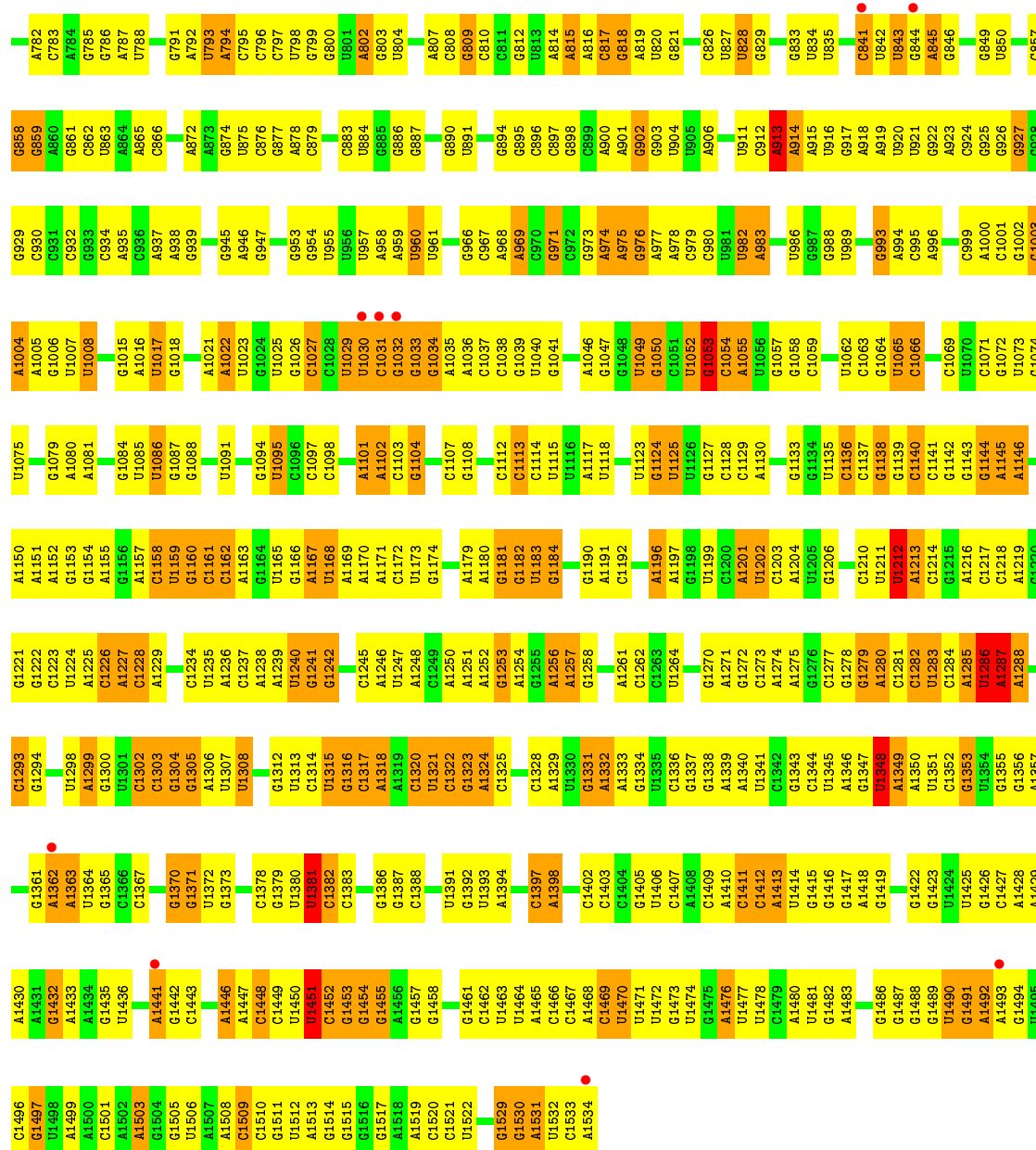
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62	DD	3	Total 3	O 3	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	6	Total 6	O 6	0	0
62	DL	6	Total 6	O 6	0	0
62	DN	2	Total 2	O 2	0	0
62	DT	3	Total 3	O 3	0	0
62	DU	2	Total 2	O 2	0	0
62	DV	1	Total 1	O 1	0	0
62	D2	1	Total 1	O 1	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	3	Total 3	O 3	0	0

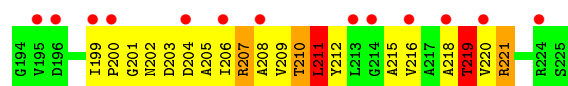
3 Residue-property plots

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

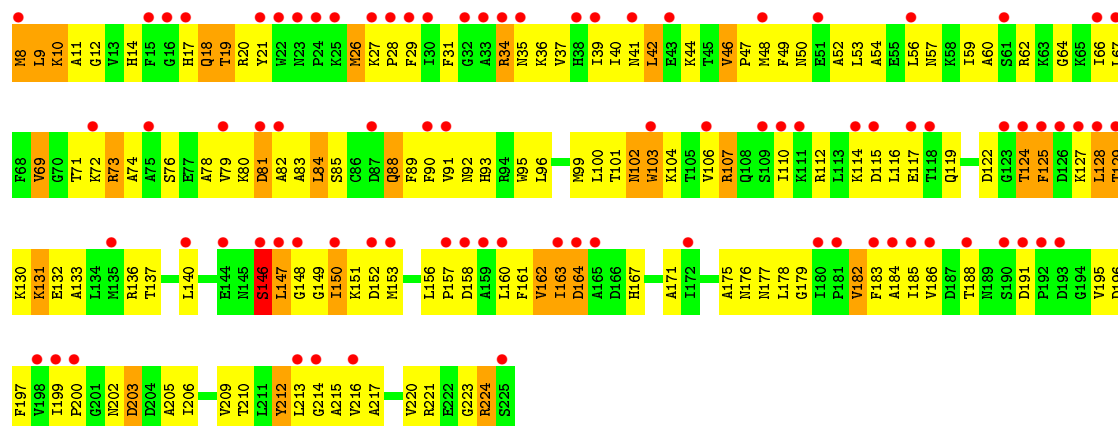
• Molecule 1: 16S rRNA



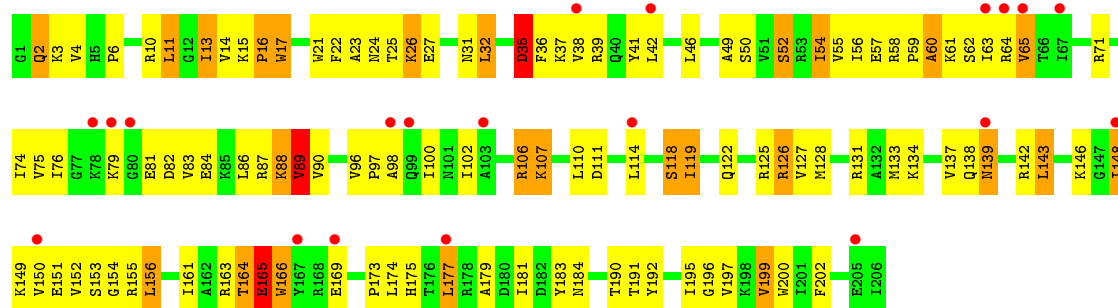




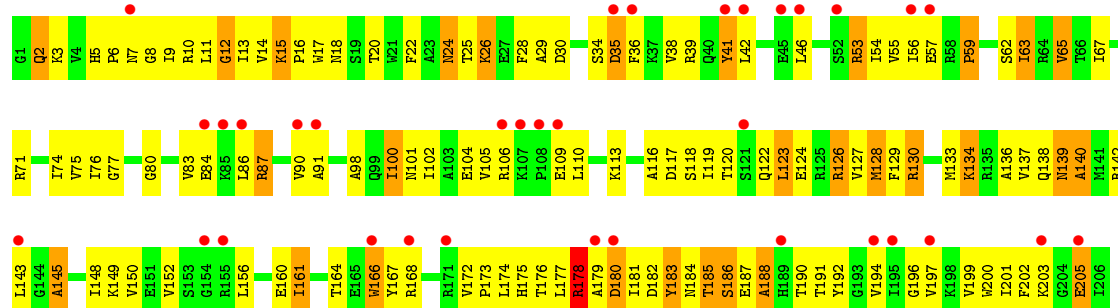
• Molecule 2: 30S ribosomal protein S2



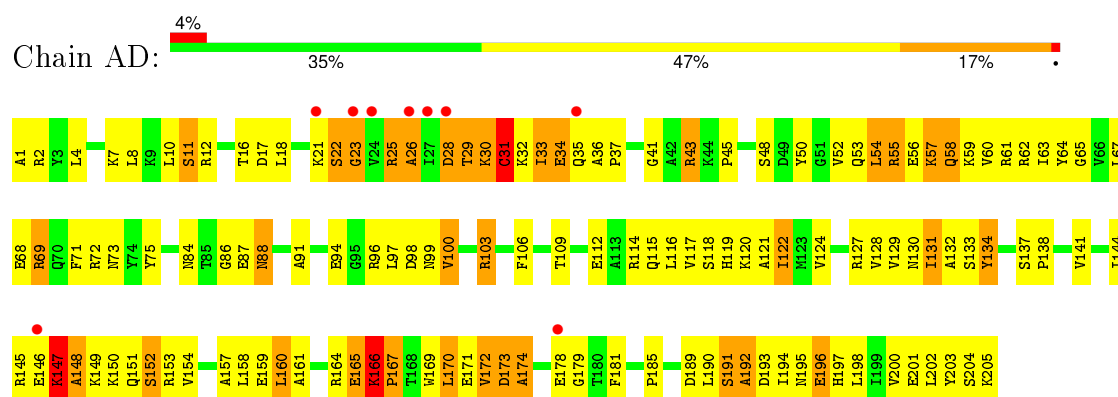
• Molecule 3: 30S ribosomal protein S3



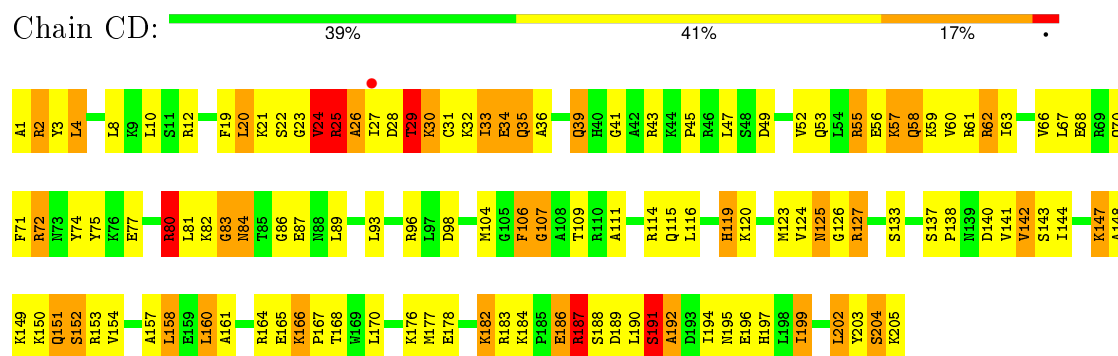
• Molecule 3: 30S ribosomal protein S3



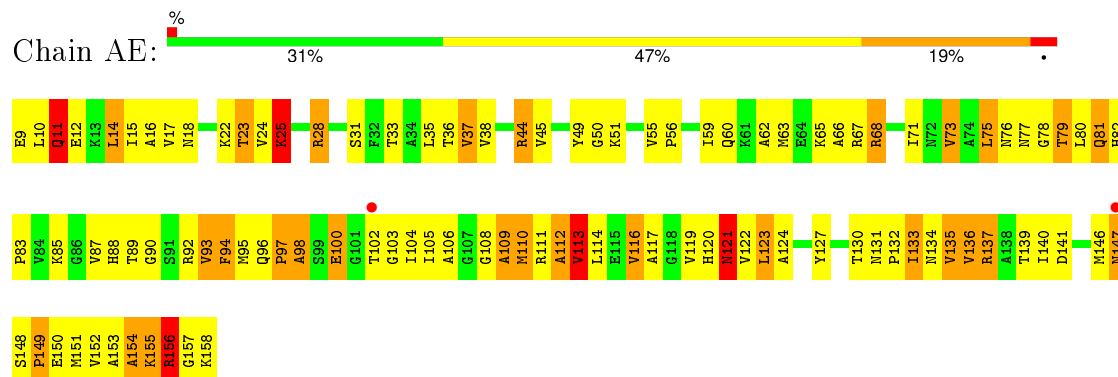
• Molecule 4: 30S ribosomal protein S4



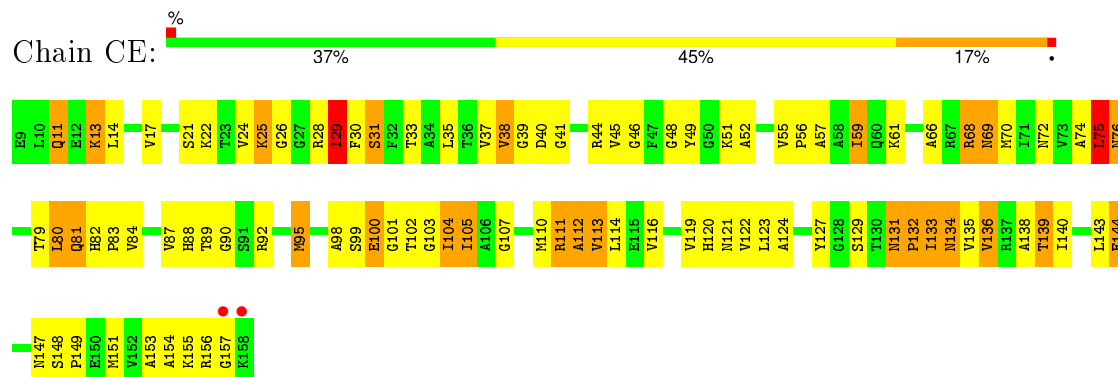
• Molecule 4: 30S ribosomal protein S4



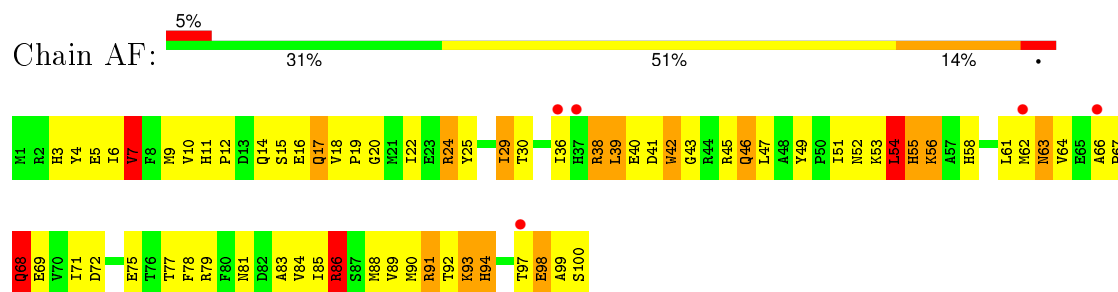
• Molecule 5: 30S ribosomal protein S5



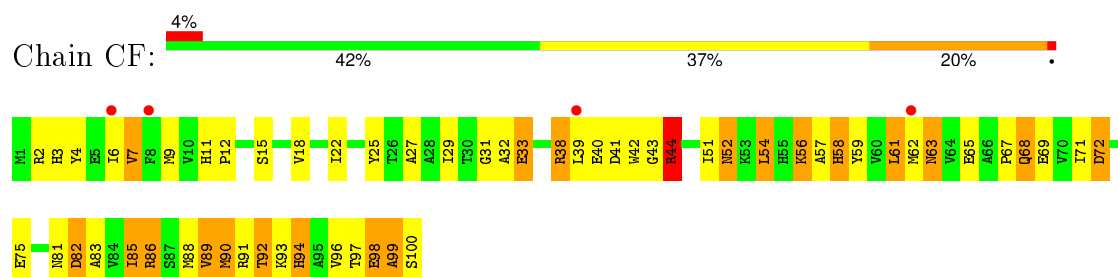
• Molecule 5: 30S ribosomal protein S5



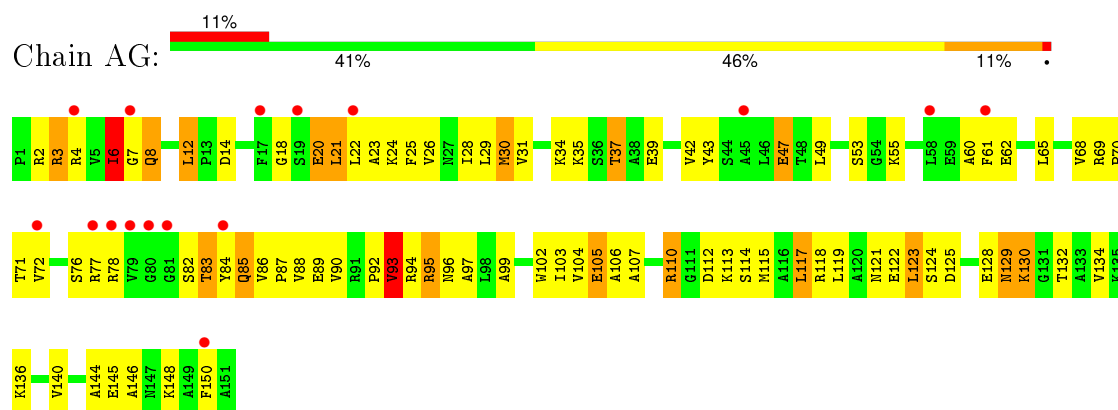
- Molecule 6: 30S ribosomal protein S6



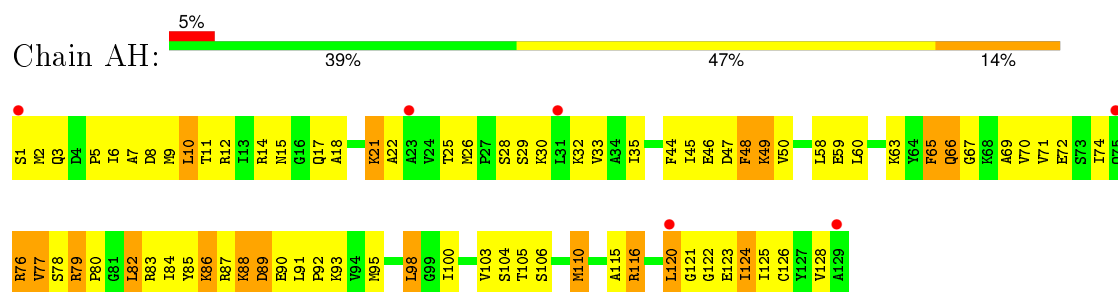
- Molecule 6: 30S ribosomal protein S6



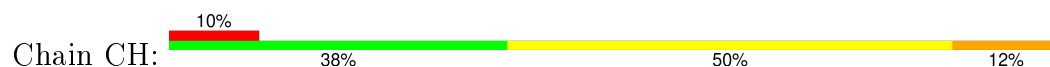
- Molecule 7: 30S ribosomal protein S7

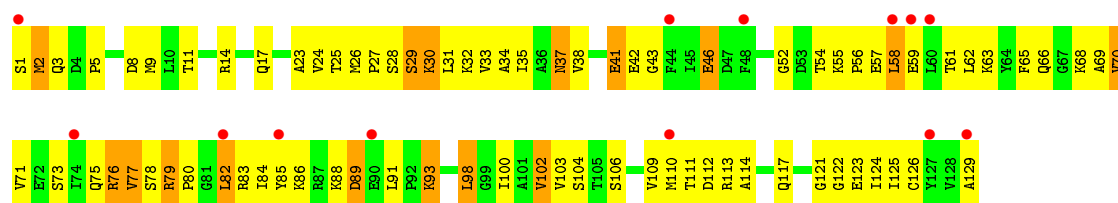


- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8





• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9



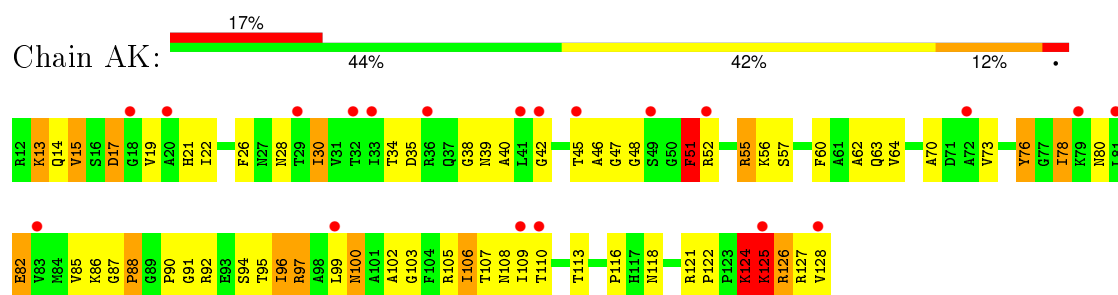
• Molecule 10: 30S ribosomal protein S10



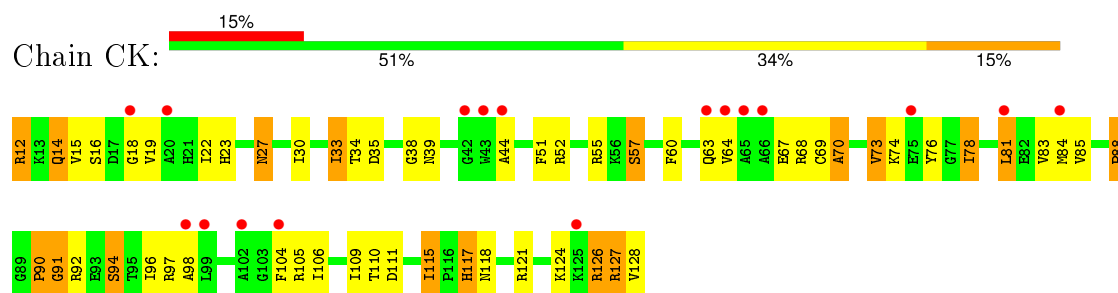
• Molecule 10: 30S ribosomal protein S10



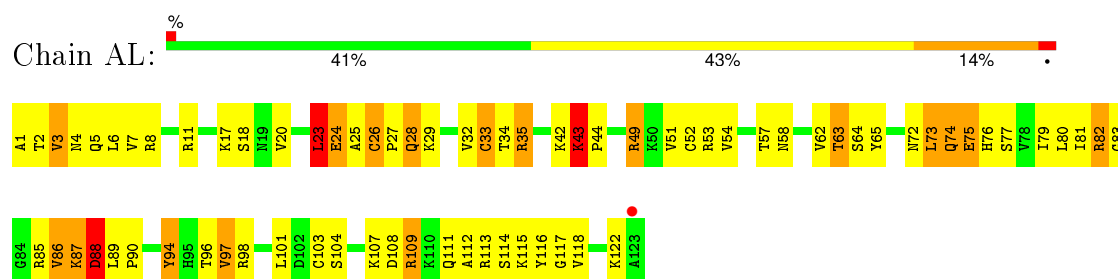
• Molecule 11: 30S ribosomal protein S11



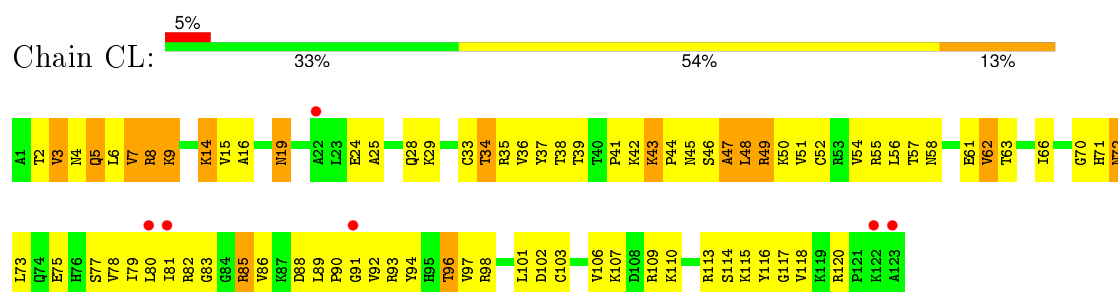
- Molecule 11: 30S ribosomal protein S11



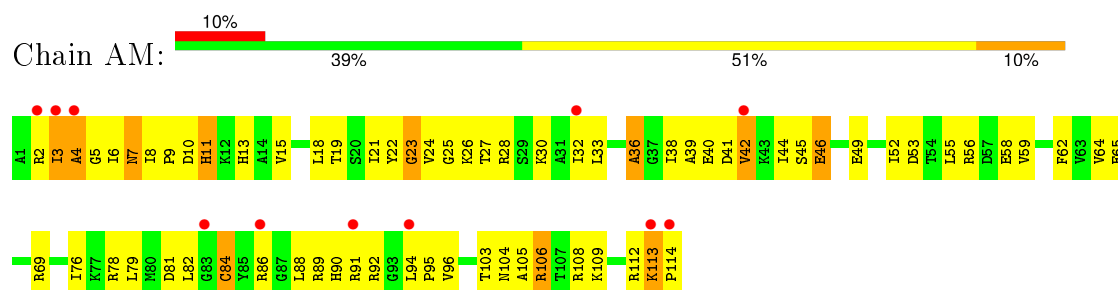
- Molecule 12: 30S ribosomal protein S12



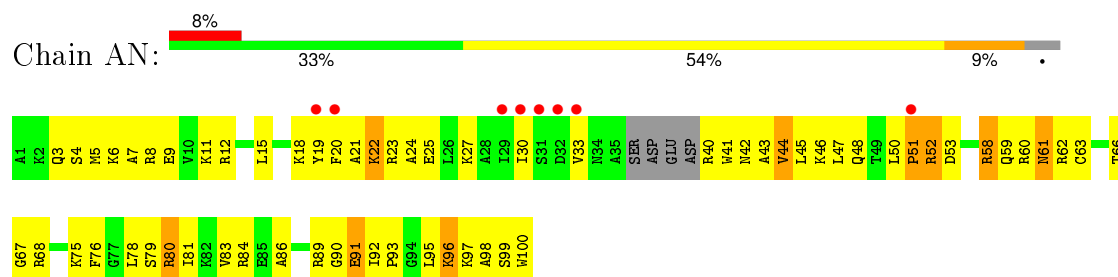
- Molecule 12: 30S ribosomal protein S12



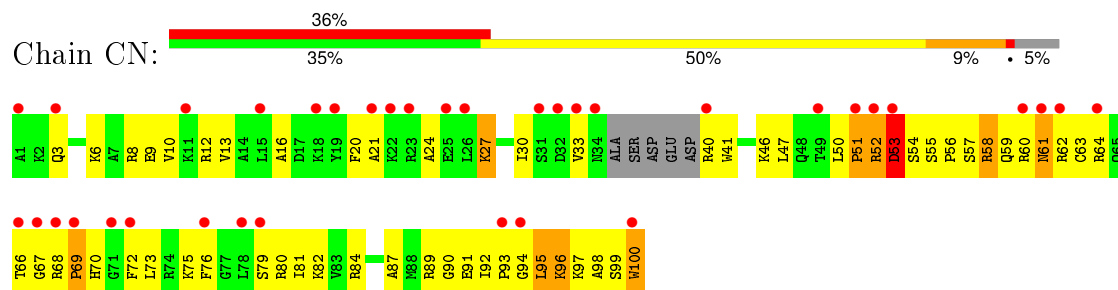
- Molecule 13: 30S ribosomal protein S13



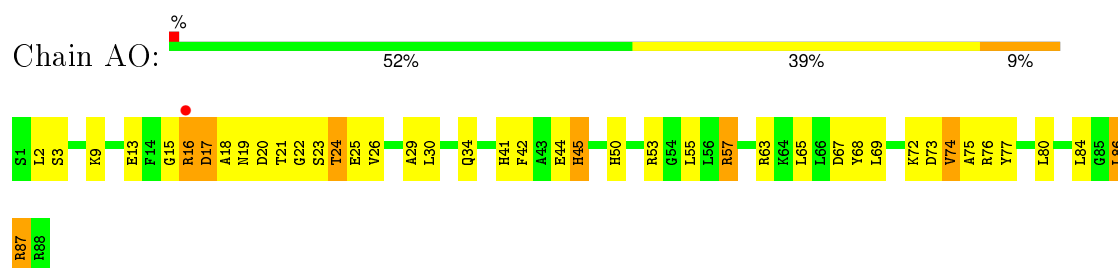
- Molecule 14: 30S ribosomal protein S14



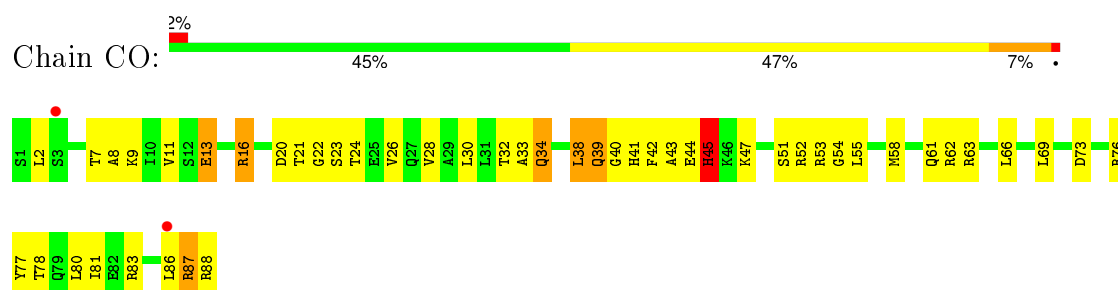
- Molecule 14: 30S ribosomal protein S14



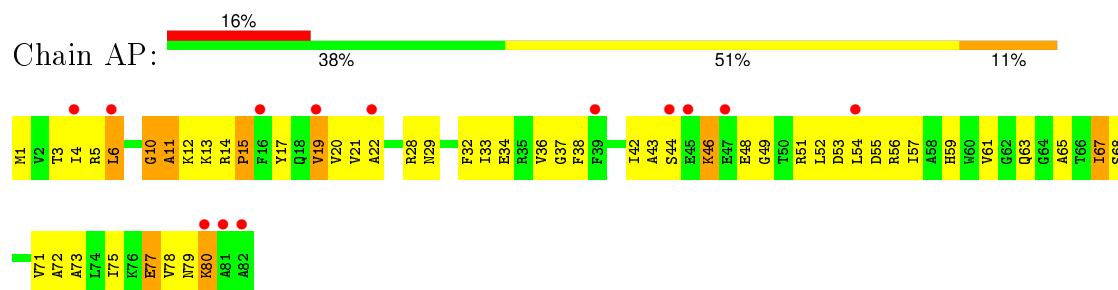
- Molecule 15: 30S ribosomal protein S15



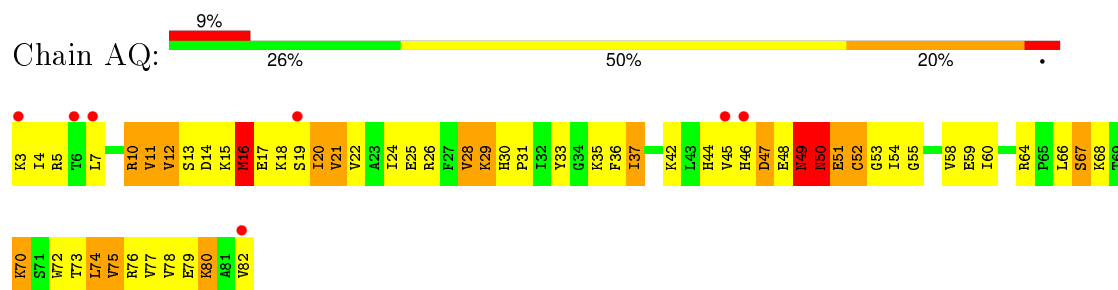
- Molecule 15: 30S ribosomal protein S15



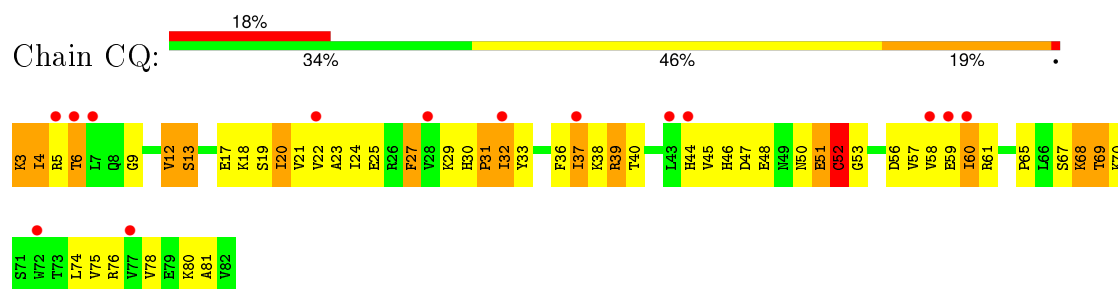
- Molecule 16: 30S ribosomal protein S16



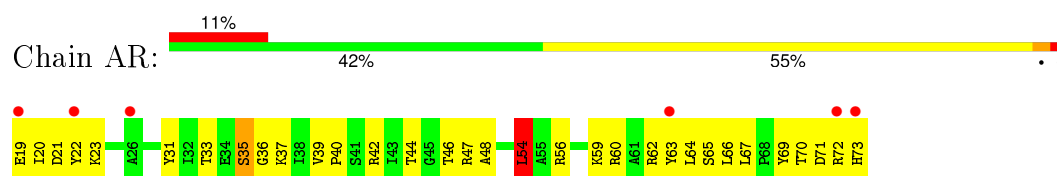
- Molecule 17: 30S ribosomal protein S17



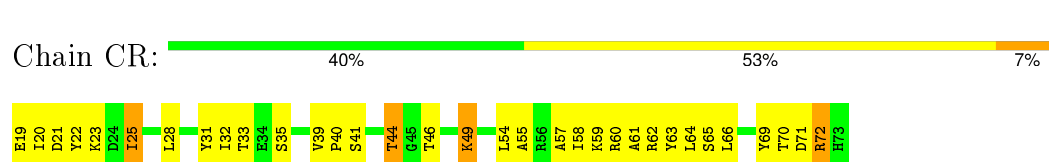
- Molecule 17: 30S ribosomal protein S17



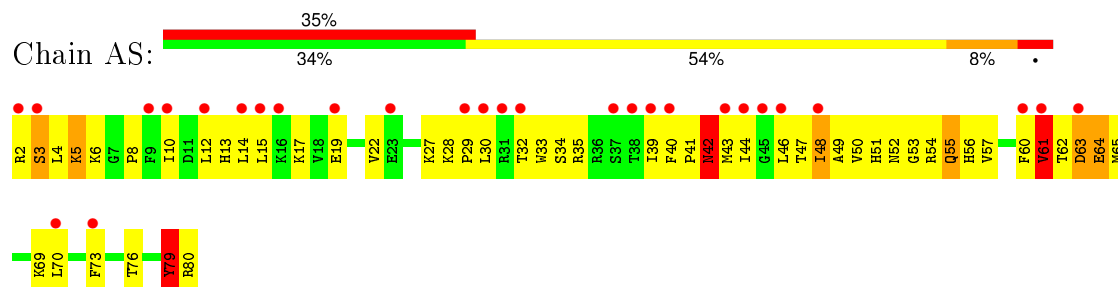
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

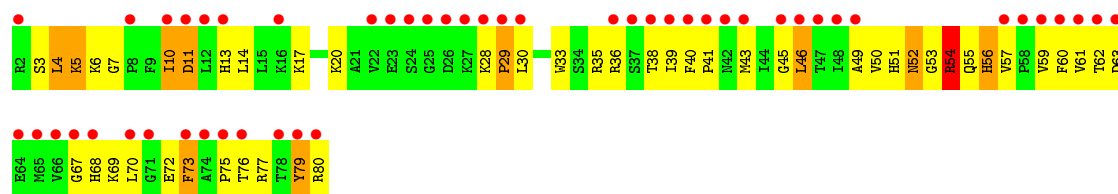


- Molecule 19: 30S ribosomal protein S19

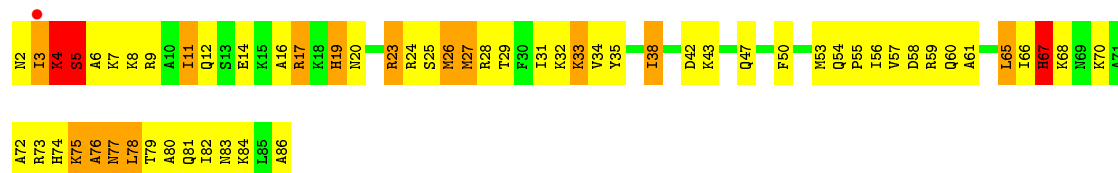


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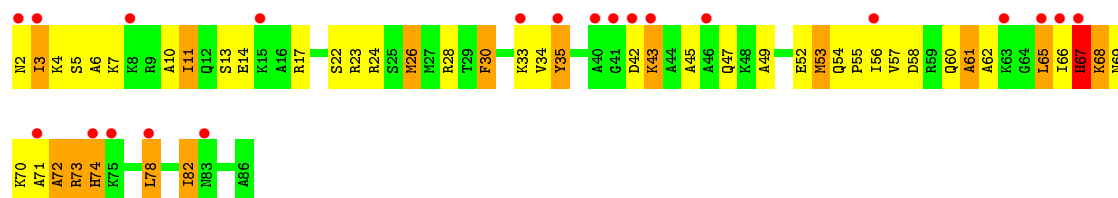




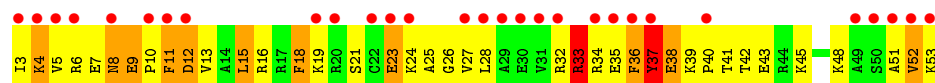
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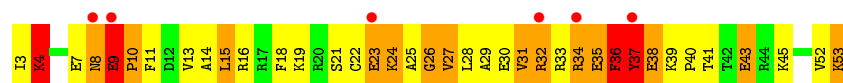
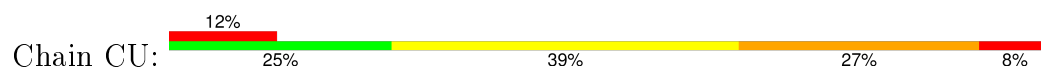
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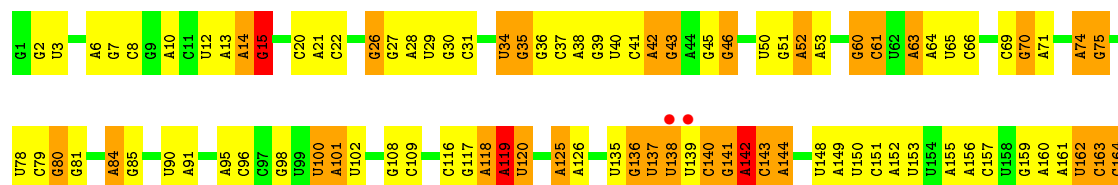
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

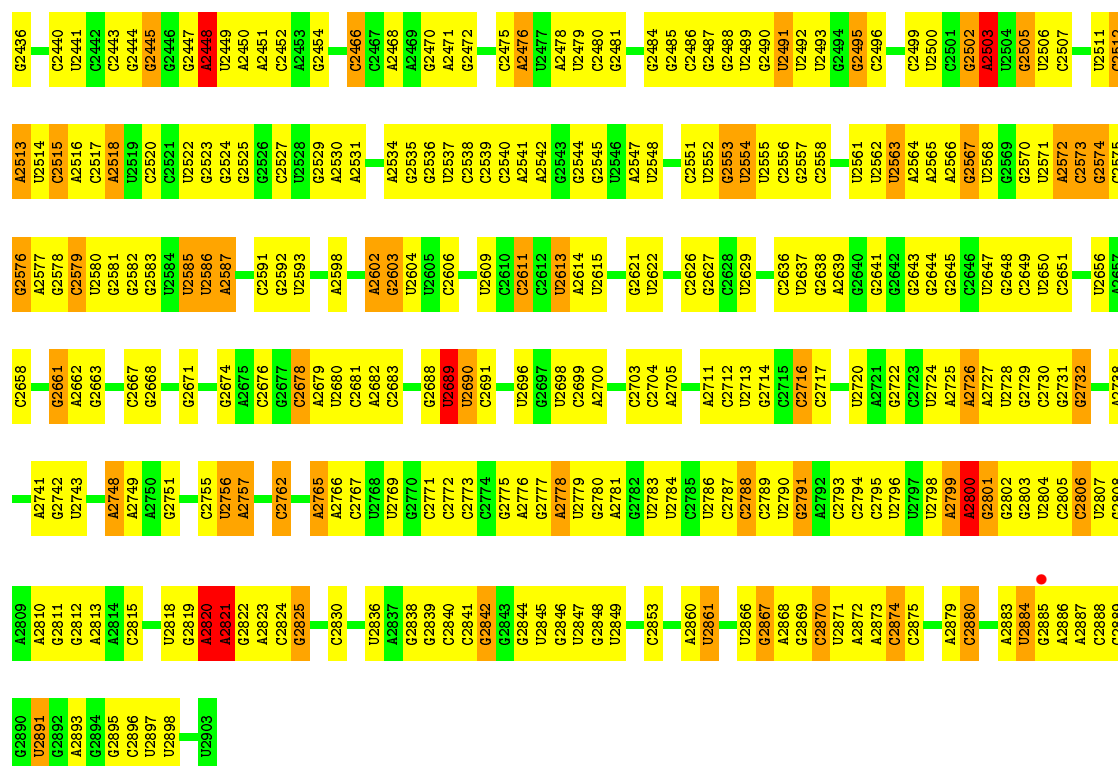


• Molecule 22: 23S rRNA

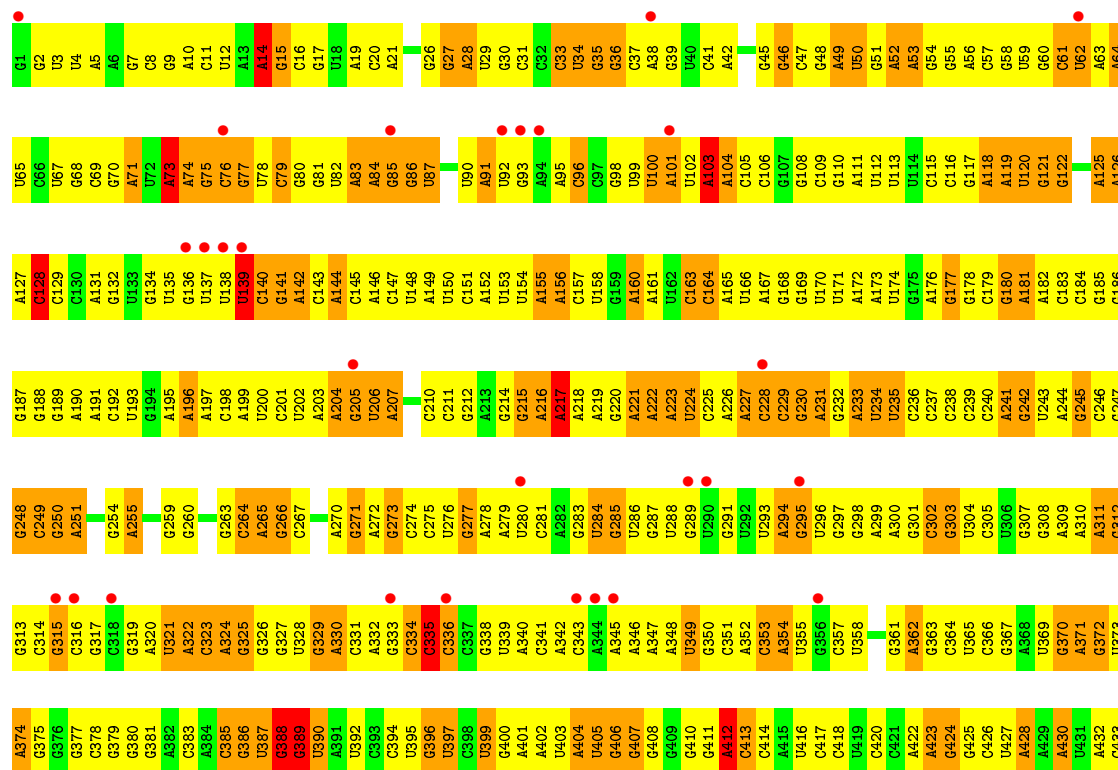
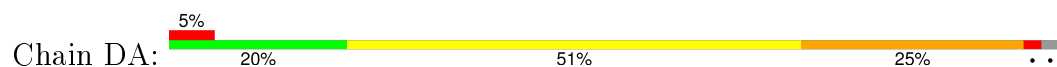


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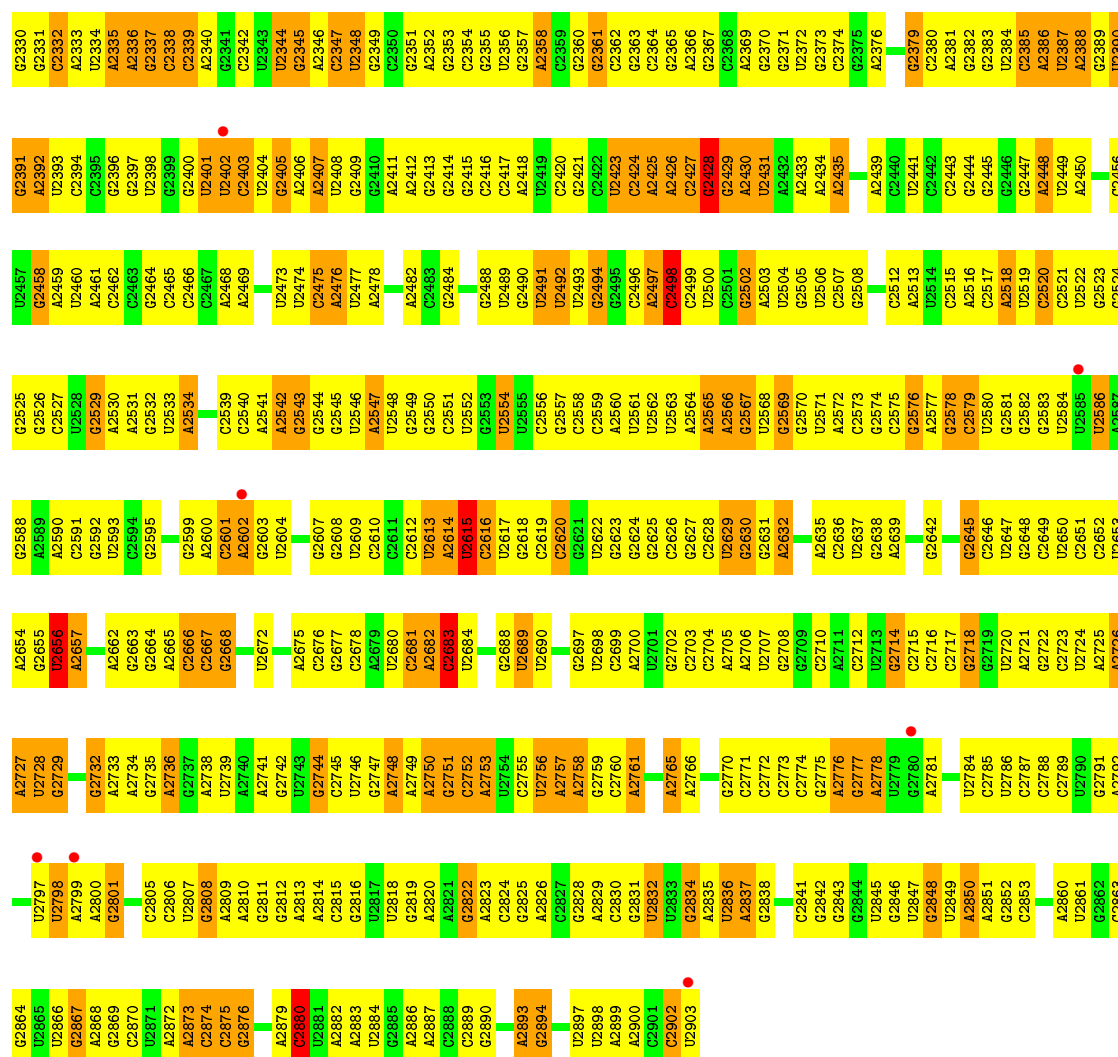


• Molecule 22: 23S rRNA



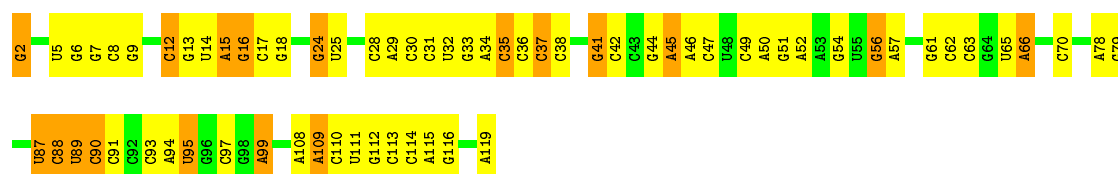
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A1378	C1314	G1252	U1184	C1117	G1055	A988	C922	G858	C795	C732	G662	A602	G537	A473
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G1380	G1316	G1254	G1186	U1119	A1057	A990	G924	U860	G797		G664	G604	C540	C475
G1381	G1317	U1255	G1187	G1120	U1058	A991	A925	A861	G798	C736	U665	G605	A541	A476
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A1383	A1383	C1257	U1189	U1122	U1060	C992	A927	A863	A800	G738	U667	U607	C544	A478
A1384	G1320	U1258	G1190	G1125	U1061	C993	A928	G864	G801	A739	G669	A608	U545	A479
C1386		G1259	C1191	G1126	G1062	C994	U929	C865	A802	G740	G670	A609	U546	A480
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G1389	U1327	U1263	G1197	U1129	U1065	C997	U932	U868	G805	A743	C673	C612	G549	A483
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A1391	G1324	U1265	U1198	G1132	G1068	A1000	C935	U870	U807	G745	G674	A614	C551	C485
A1392	U1329	G1266	C1200	U1133	A1069	A1001	A936	U871	G808	U746	A675	U615	G553	C486
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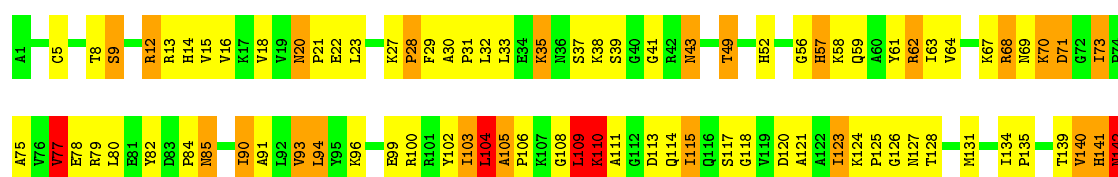
• Molecule 23: 5S rRNA

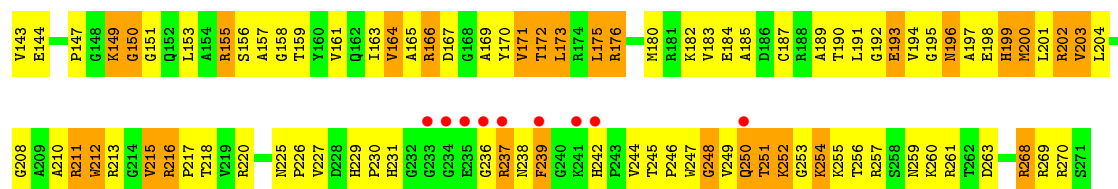
Chain BB: 43% 42% 15%



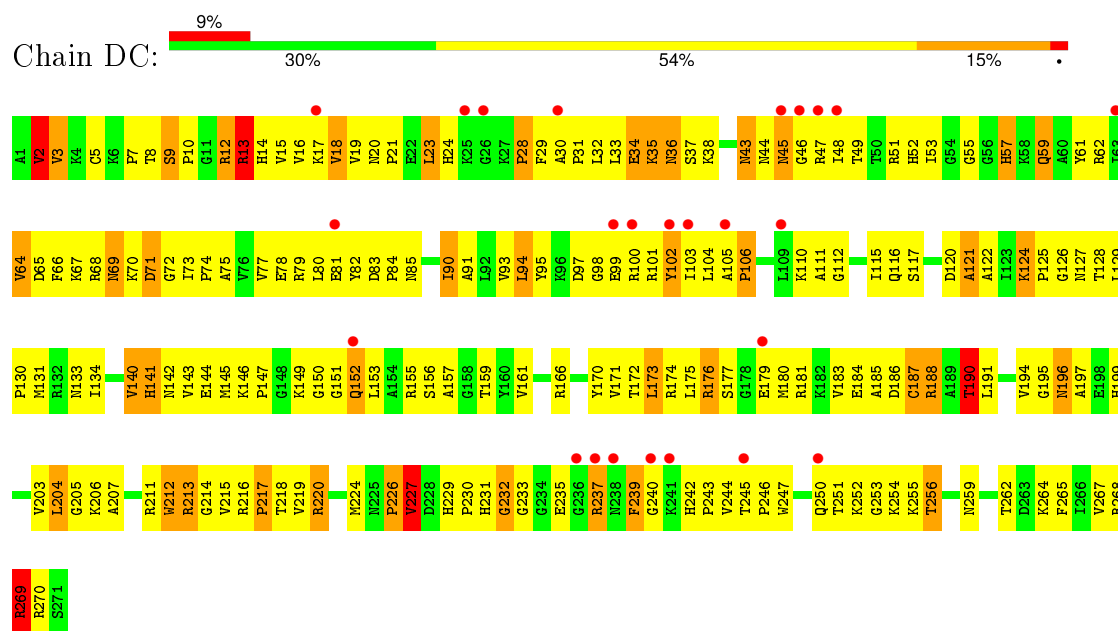
• Molecule 24: 50S ribosomal protein L2

Chain BC: 3% 35% 44% 19%

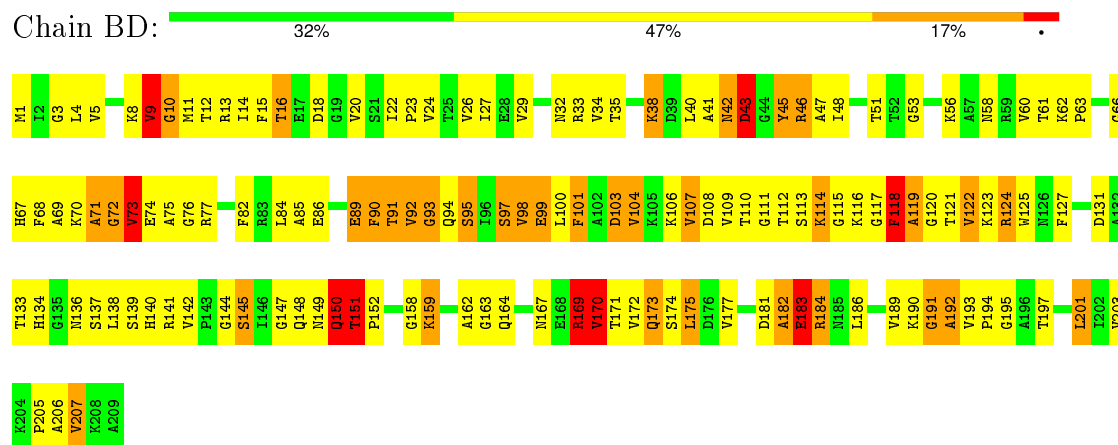




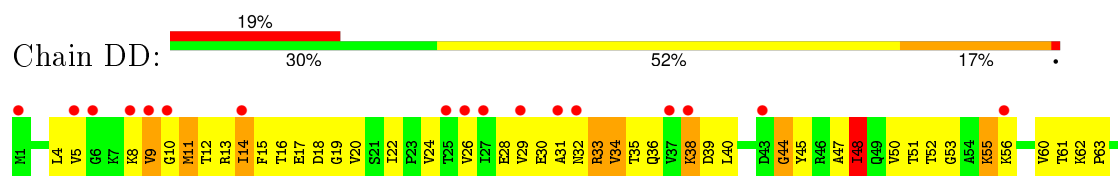
• Molecule 24: 50S ribosomal protein L2

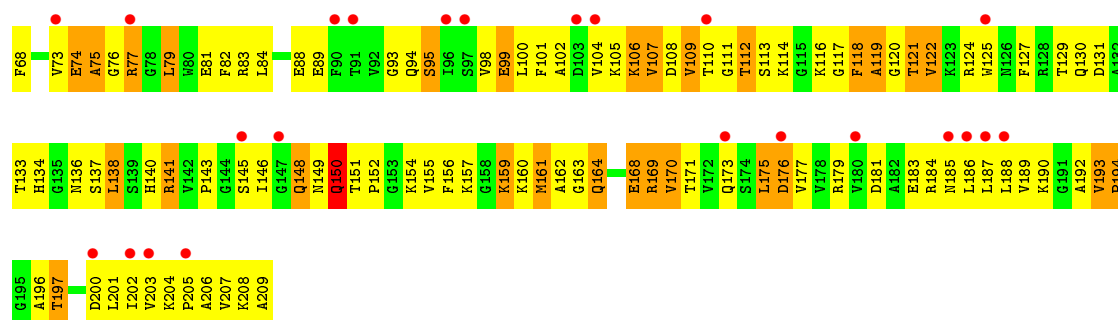


• Molecule 25: 50S ribosomal protein L3



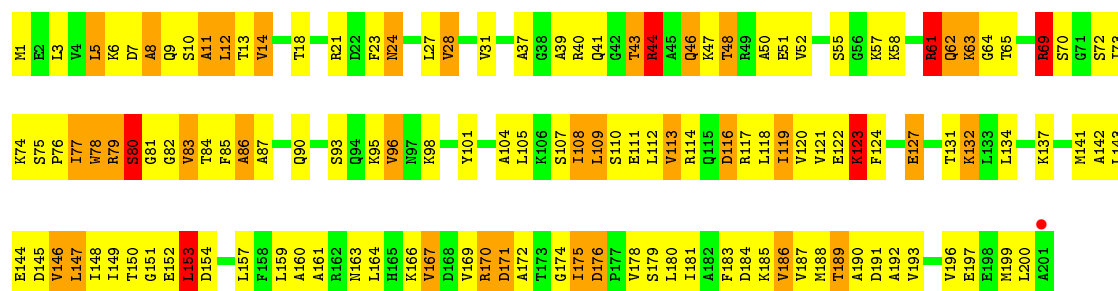
• Molecule 25: 50S ribosomal protein L3





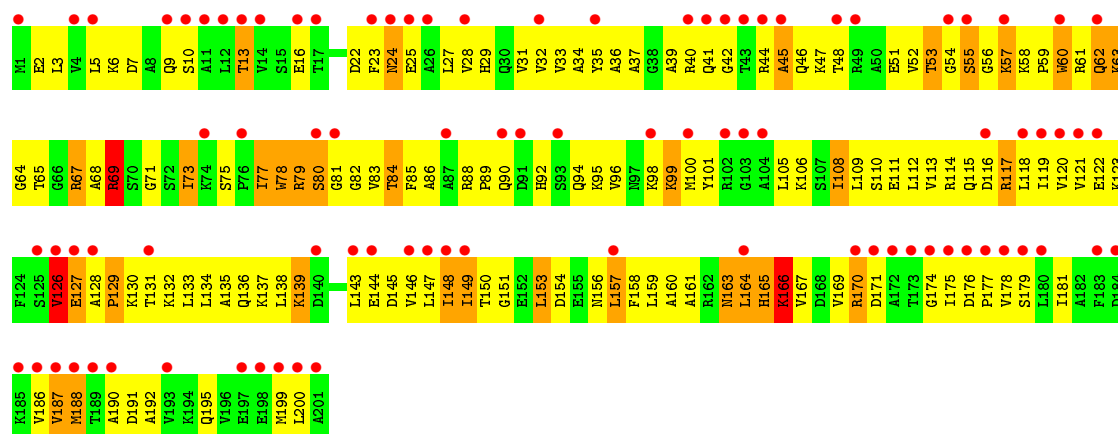
• Molecule 26: 50S ribosomal protein L4

Chain BE: 33% 47% 17%



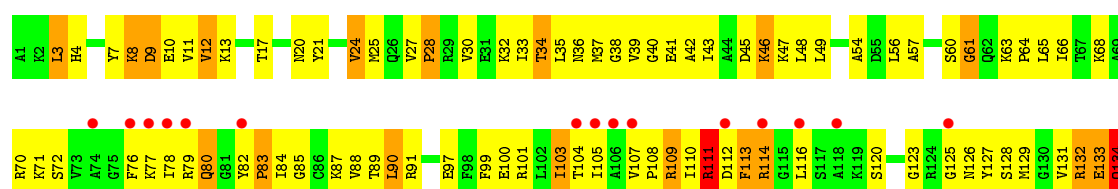
• Molecule 26: 50S ribosomal protein L4

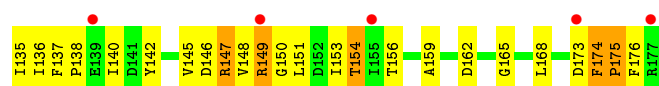
Chain DE: 27% 44% 56% 16%



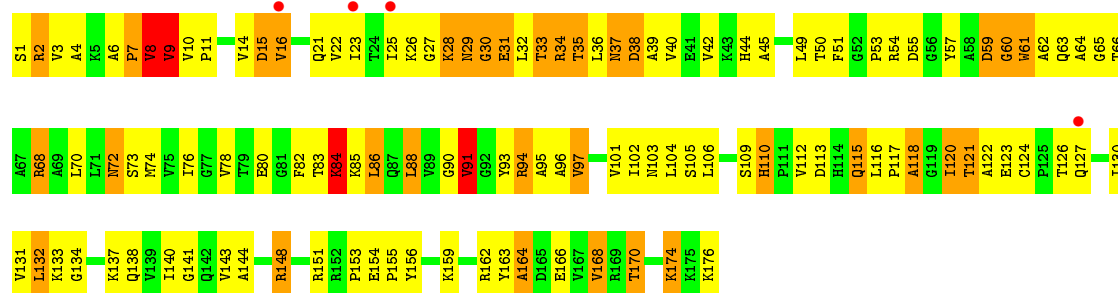
• Molecule 27: 50S ribosomal protein L5

Chain BF: 11% 37% 49% 13%

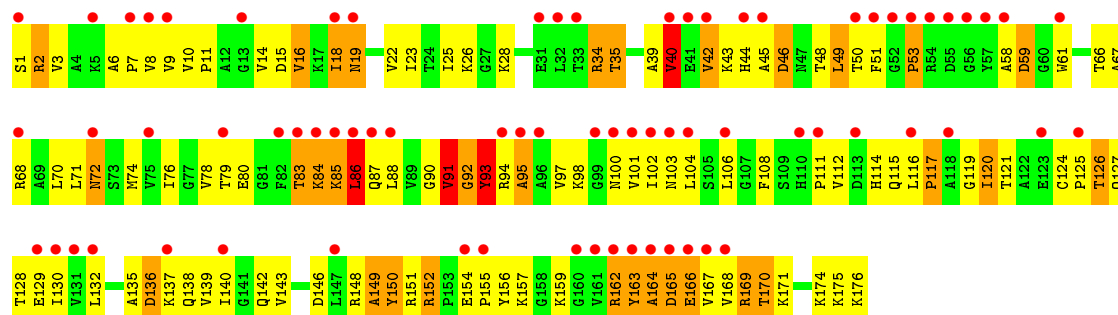




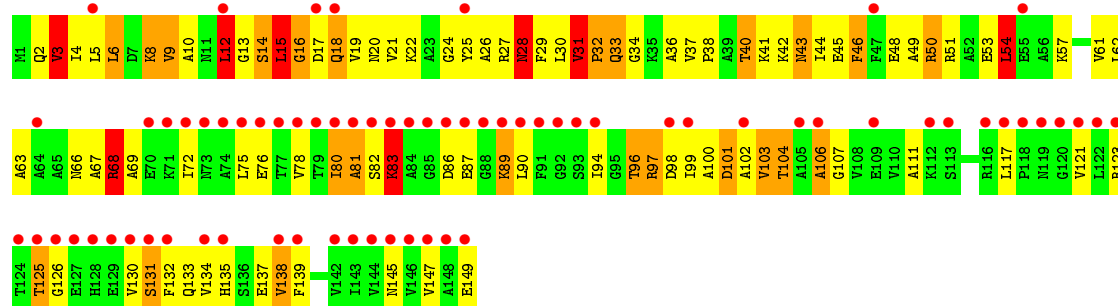
• Molecule 28: 50S ribosomal protein L6



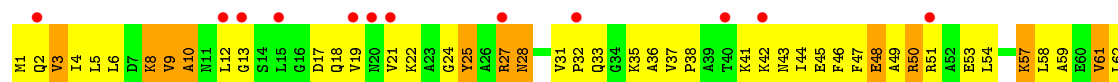
• Molecule 28: 50S ribosomal protein L6

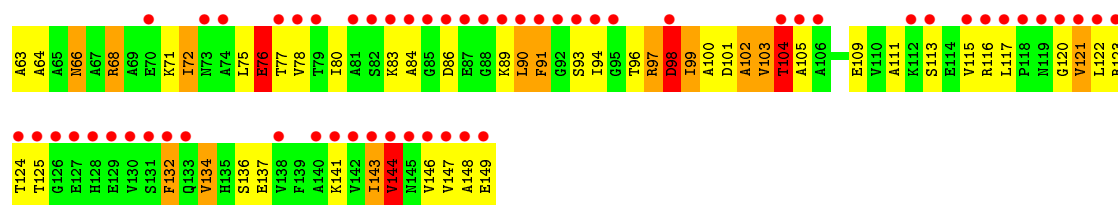


• Molecule 29: 50S ribosomal protein L9

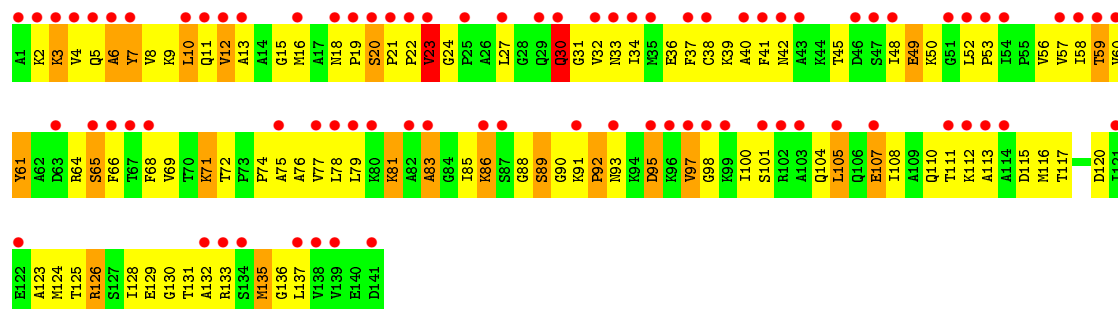


• Molecule 29: 50S ribosomal protein L9

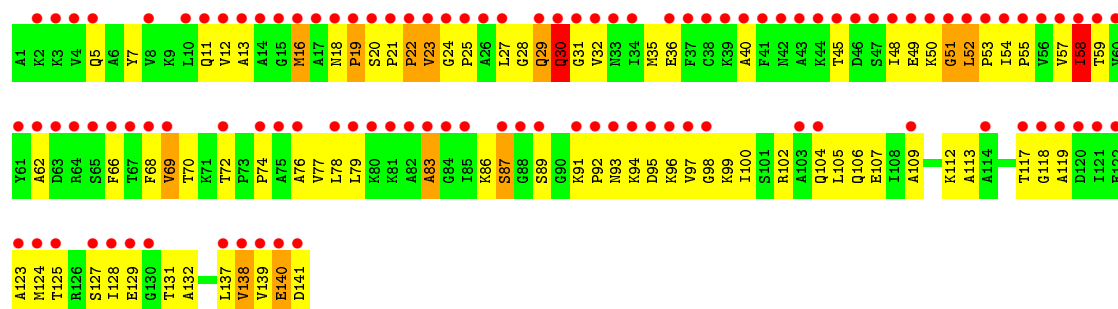
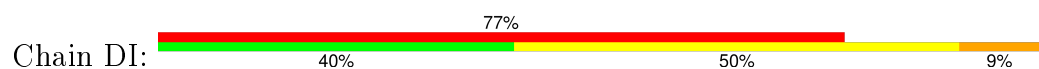




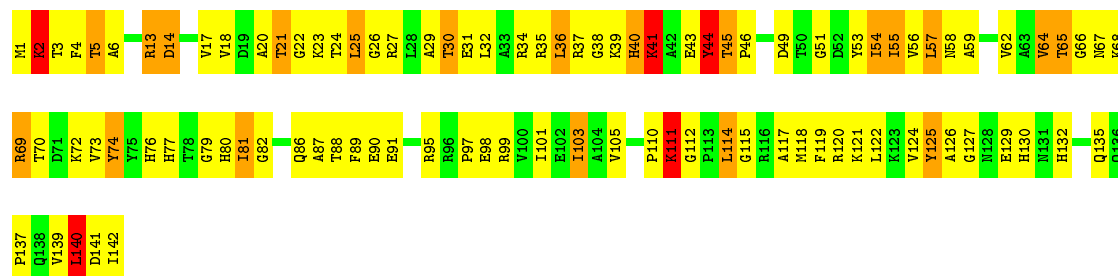
• Molecule 30: 50S ribosomal protein L11



• Molecule 30: 50S ribosomal protein L11

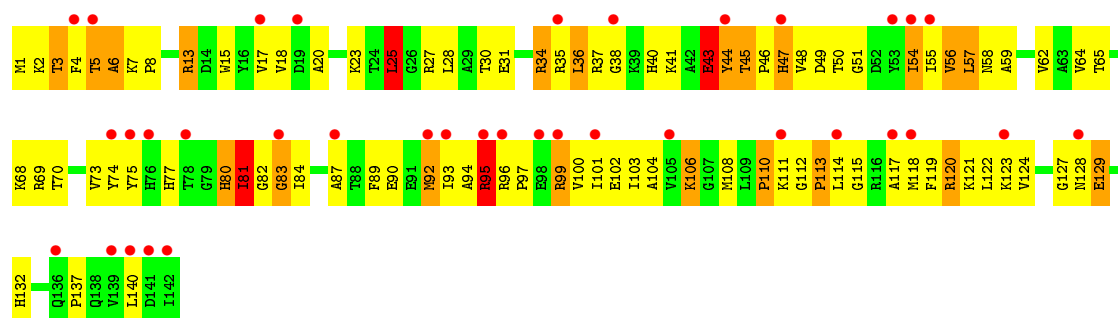


• Molecule 31: 50S ribosomal protein L13



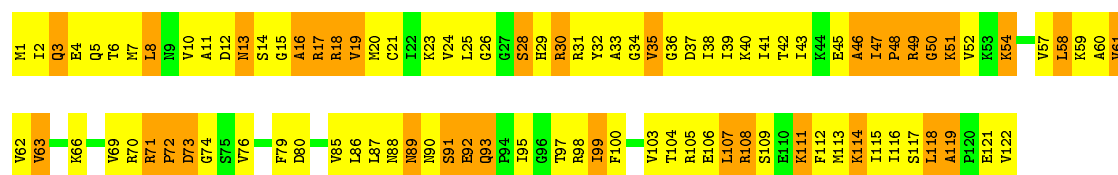
• Molecule 31: 50S ribosomal protein L13





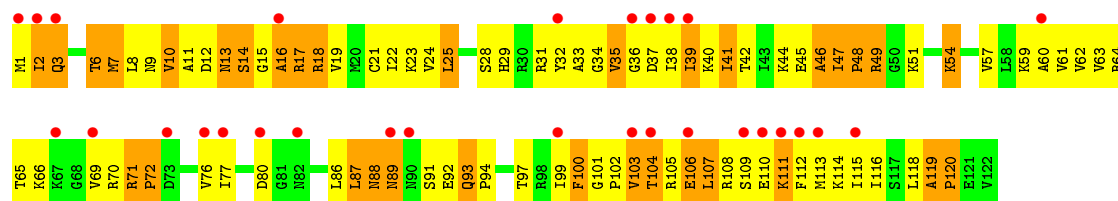
- Molecule 32: 50S ribosomal protein L14

Chain BK: 20% 52% 28%



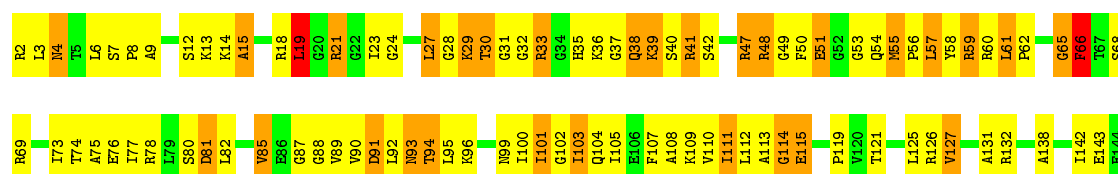
- Molecule 32: 50S ribosomal protein L14

Chain DK: 24% 26% 47% 27%



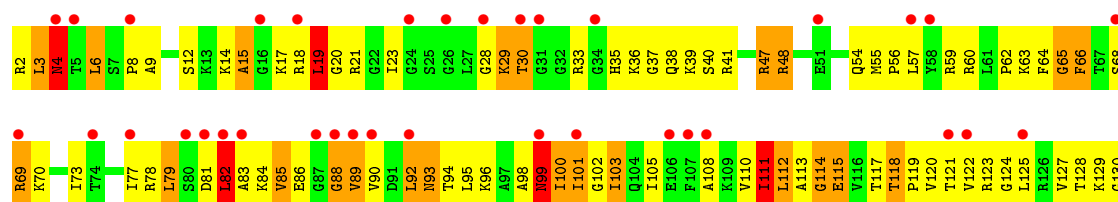
- Molecule 33: 50S ribosomal protein L15

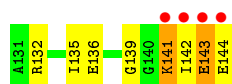
Chain BL: 33% 45% 20%



- Molecule 33: 50S ribosomal protein L15

Chain DL: 27% 34% 45% 17%





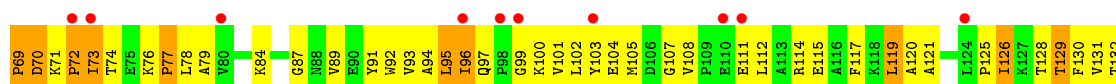
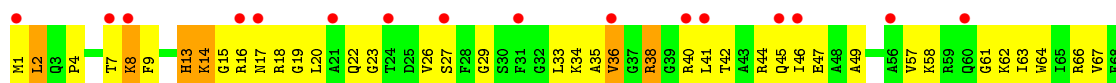
• Molecule 34: 50S ribosomal protein L16

Chain BM: 40% 42% 16%



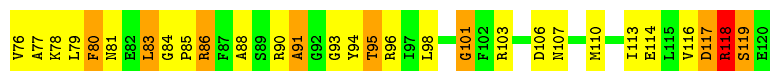
• Molecule 34: 50S ribosomal protein L16

Chain DM: 21% 35% 53% 12%



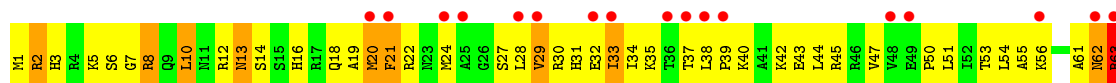
• Molecule 35: 50S ribosomal protein L17

Chain BN: 34% 48% 16%



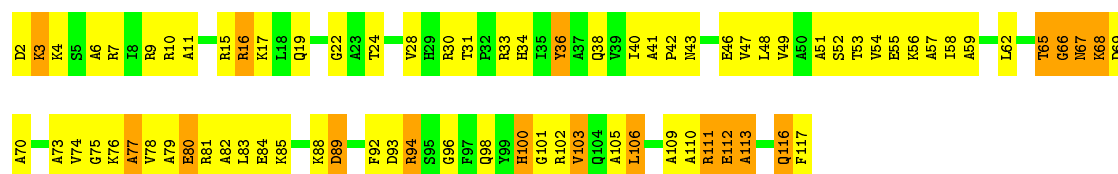
• Molecule 35: 50S ribosomal protein L17

Chain DN: 30% 32% 52% 16%

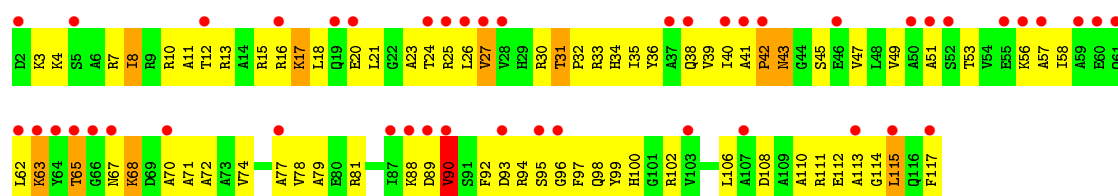
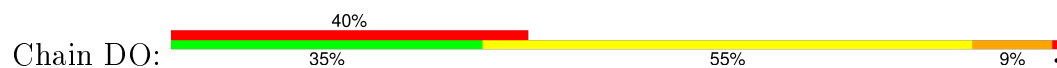


• Molecule 36: 50S ribosomal protein L18

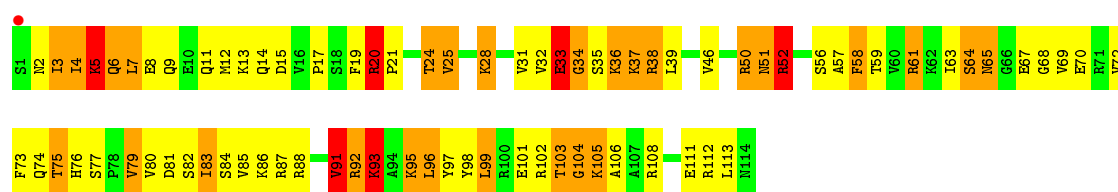
Chain BO: 33% 52% 16%



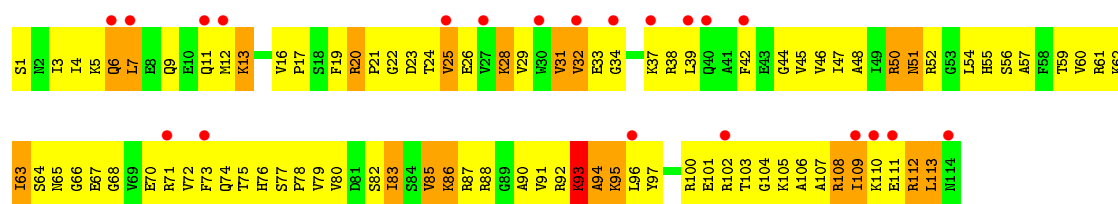
• Molecule 36: 50S ribosomal protein L18



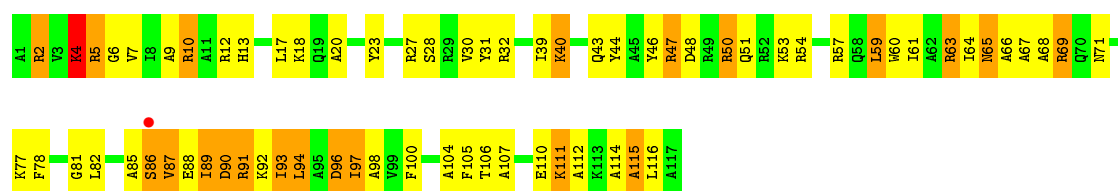
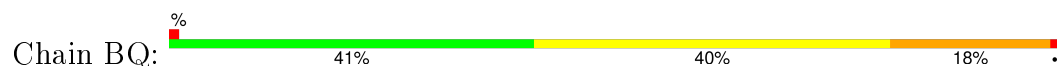
• Molecule 37: 50S ribosomal protein L19



• Molecule 37: 50S ribosomal protein L19

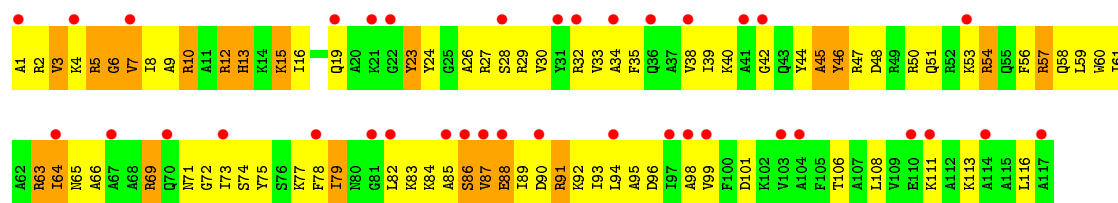


• Molecule 38: 50S ribosomal protein L20

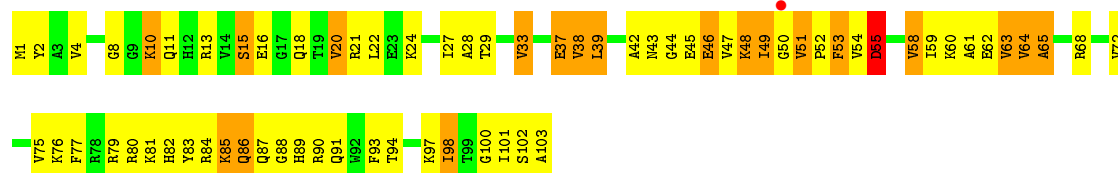


• Molecule 38: 50S ribosomal protein L20

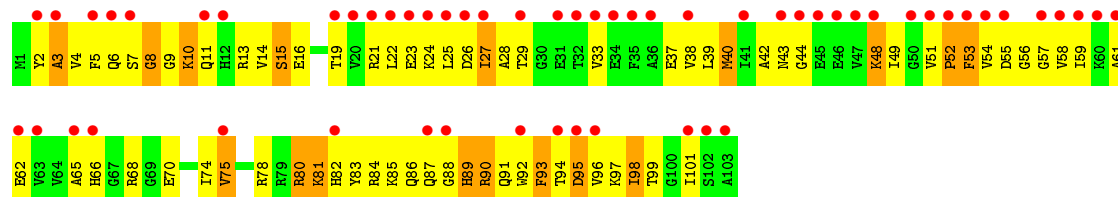




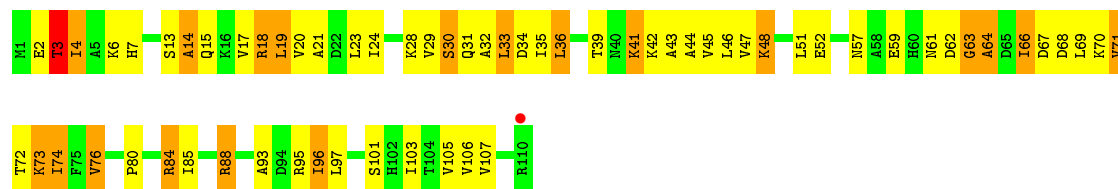
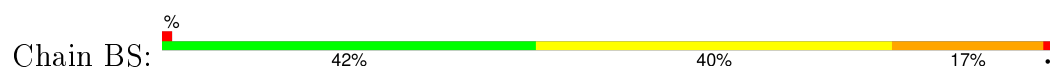
• Molecule 39: 50S ribosomal protein L21



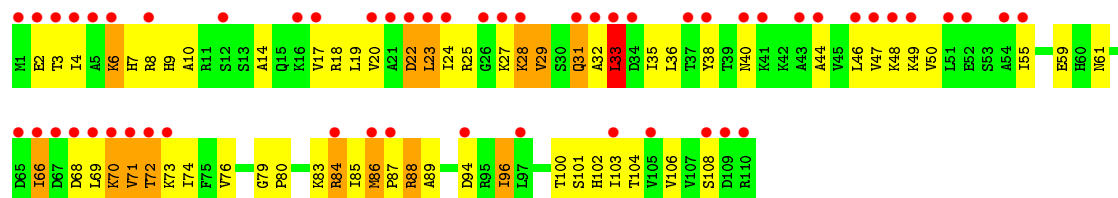
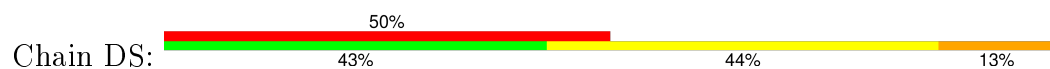
• Molecule 39: 50S ribosomal protein L21



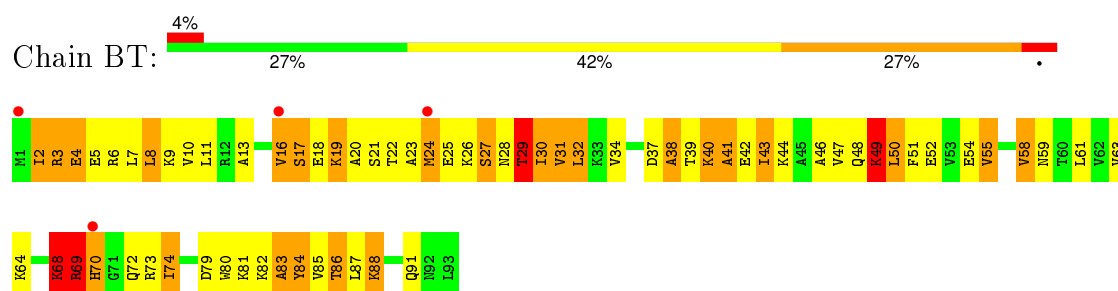
• Molecule 40: 50S ribosomal protein L22



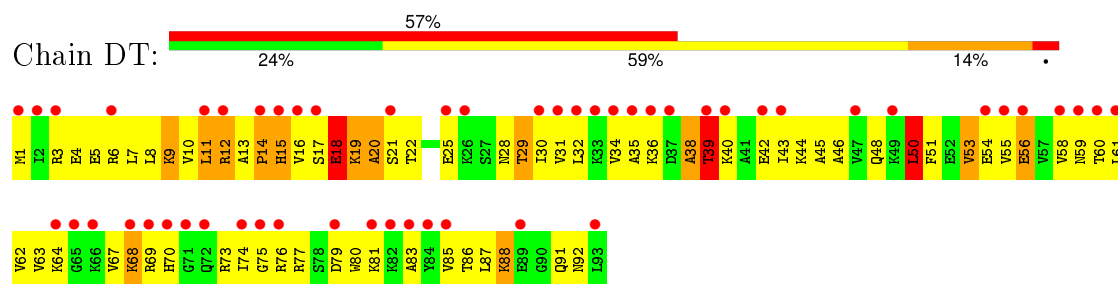
• Molecule 40: 50S ribosomal protein L22



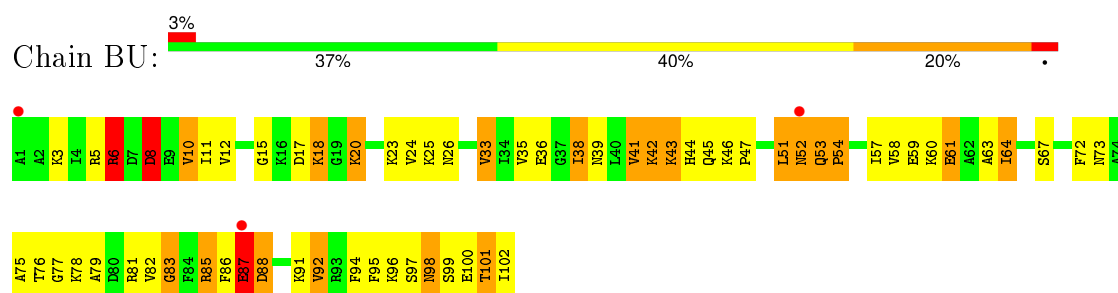
• Molecule 41: 50S ribosomal protein L23



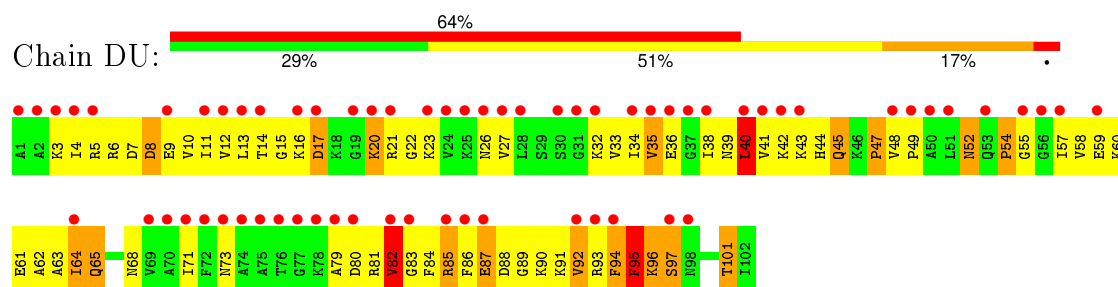
- Molecule 41: 50S ribosomal protein L23



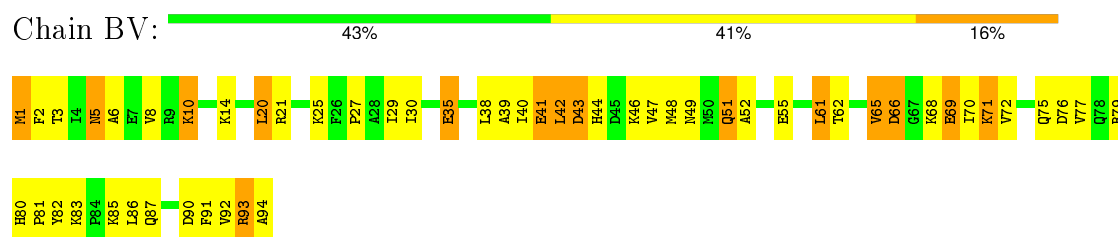
- Molecule 42: 50S ribosomal protein L24



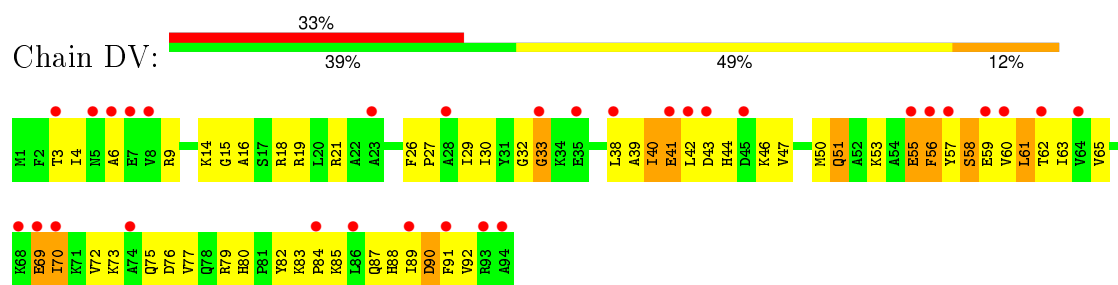
- Molecule 42: 50S ribosomal protein L24



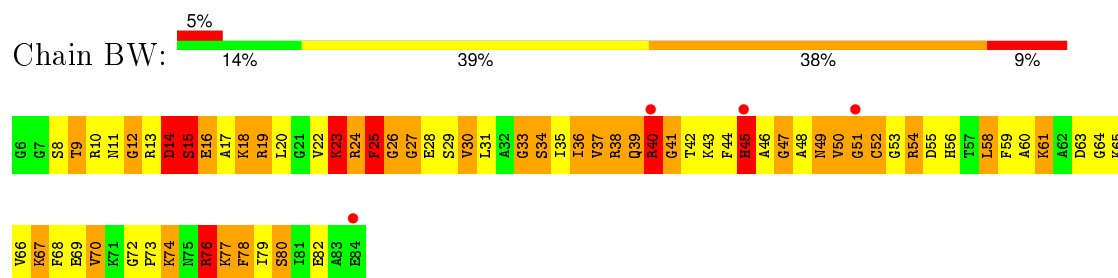
- Molecule 43: 50S ribosomal protein L25



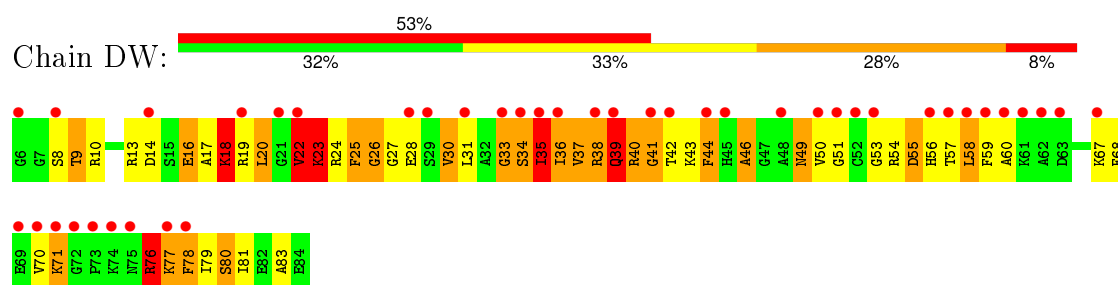
- Molecule 43: 50S ribosomal protein L25



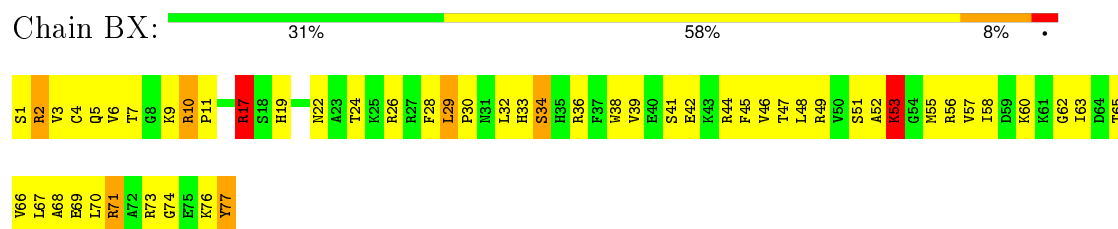
- Molecule 44: 50S ribosomal protein L27



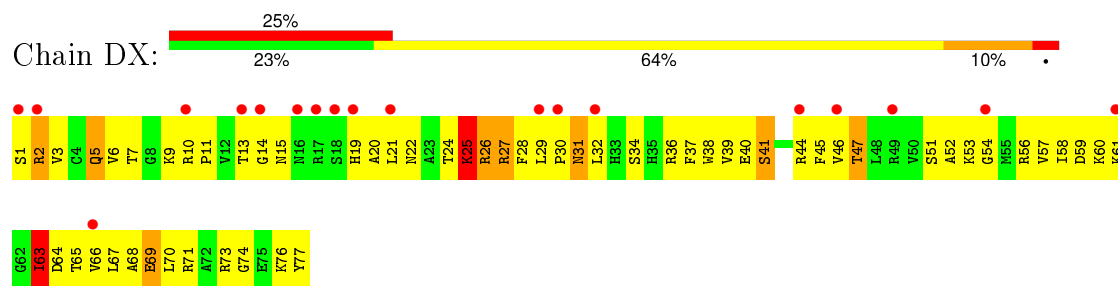
- Molecule 44: 50S ribosomal protein L27



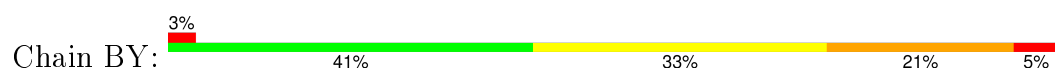
- Molecule 45: 50S ribosomal protein L28



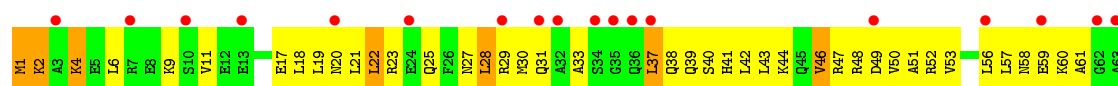
- Molecule 45: 50S ribosomal protein L28



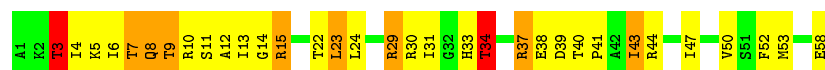
- Molecule 46: 50S ribosomal protein L29



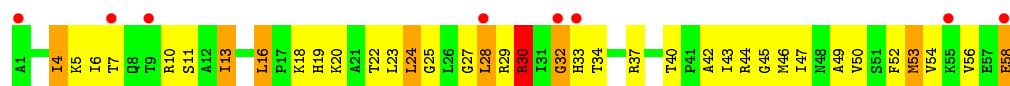
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



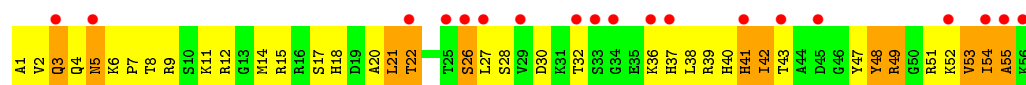
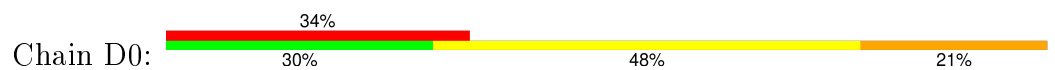
- Molecule 47: 50S ribosomal protein L30



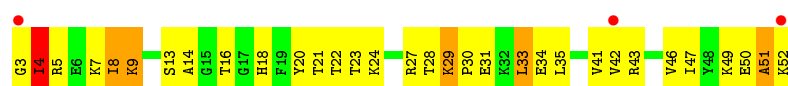
- Molecule 48: 50S ribosomal protein L32



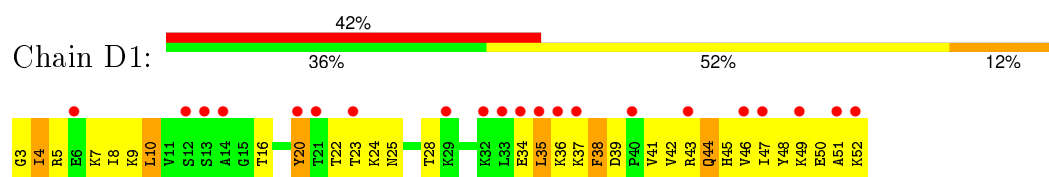
- Molecule 48: 50S ribosomal protein L32



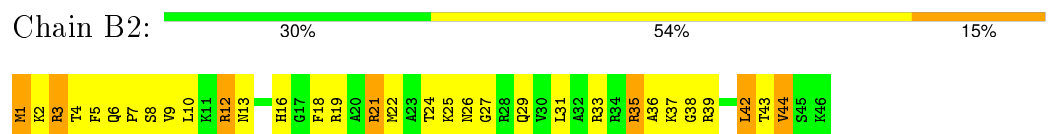
- Molecule 49: 50S ribosomal protein L33



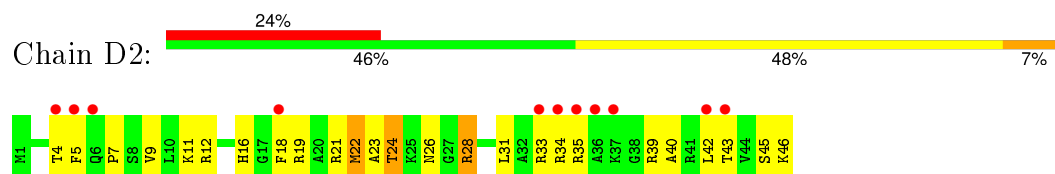
- Molecule 49: 50S ribosomal protein L33



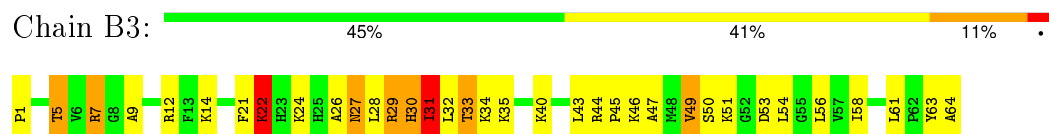
- Molecule 50: 50S ribosomal protein L34



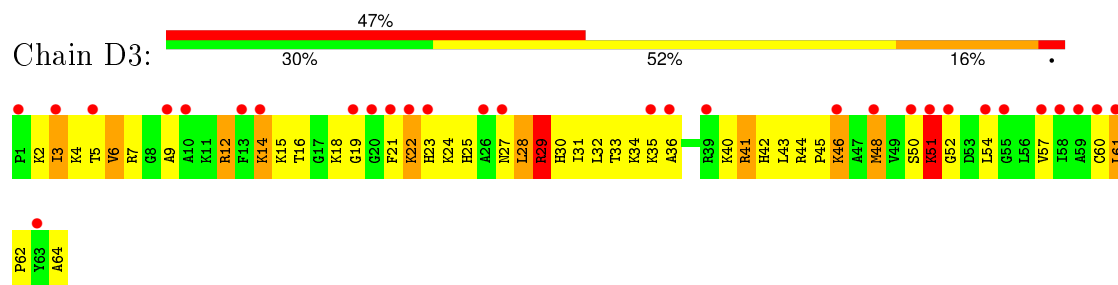
- Molecule 50: 50S ribosomal protein L34



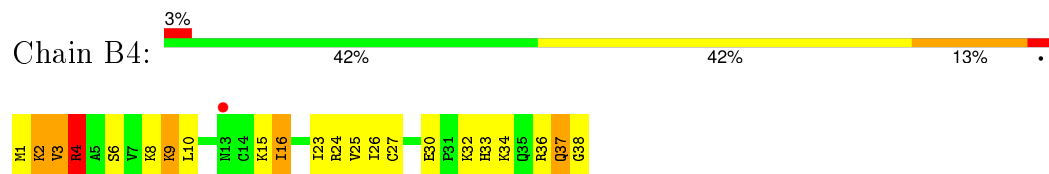
- Molecule 51: 50S ribosomal protein L35



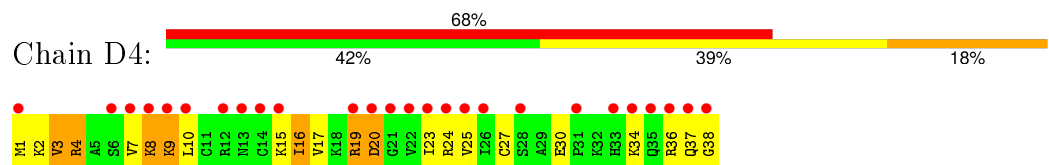
- Molecule 51: 50S ribosomal protein L35



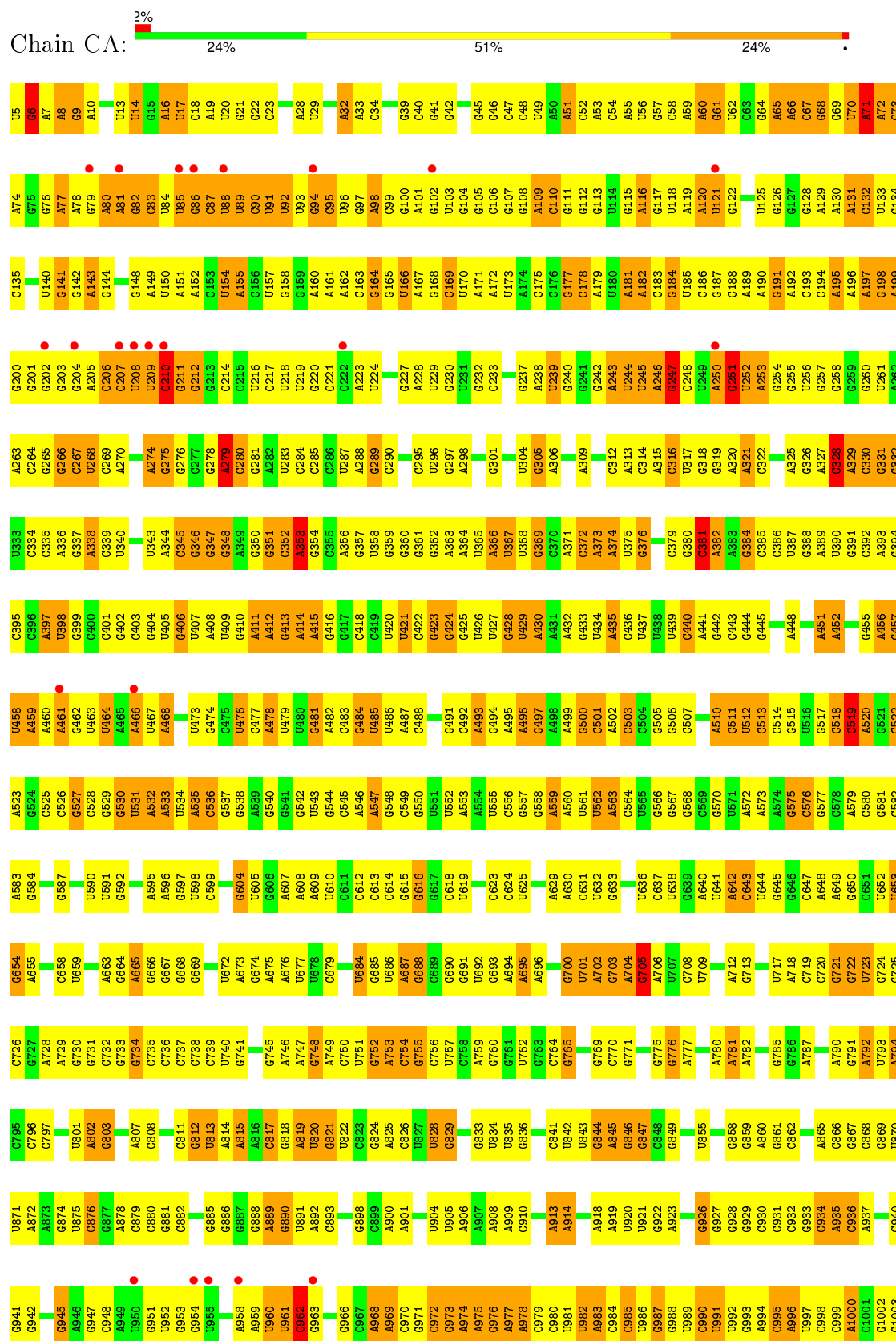
- Molecule 52: 50S ribosomal protein L36

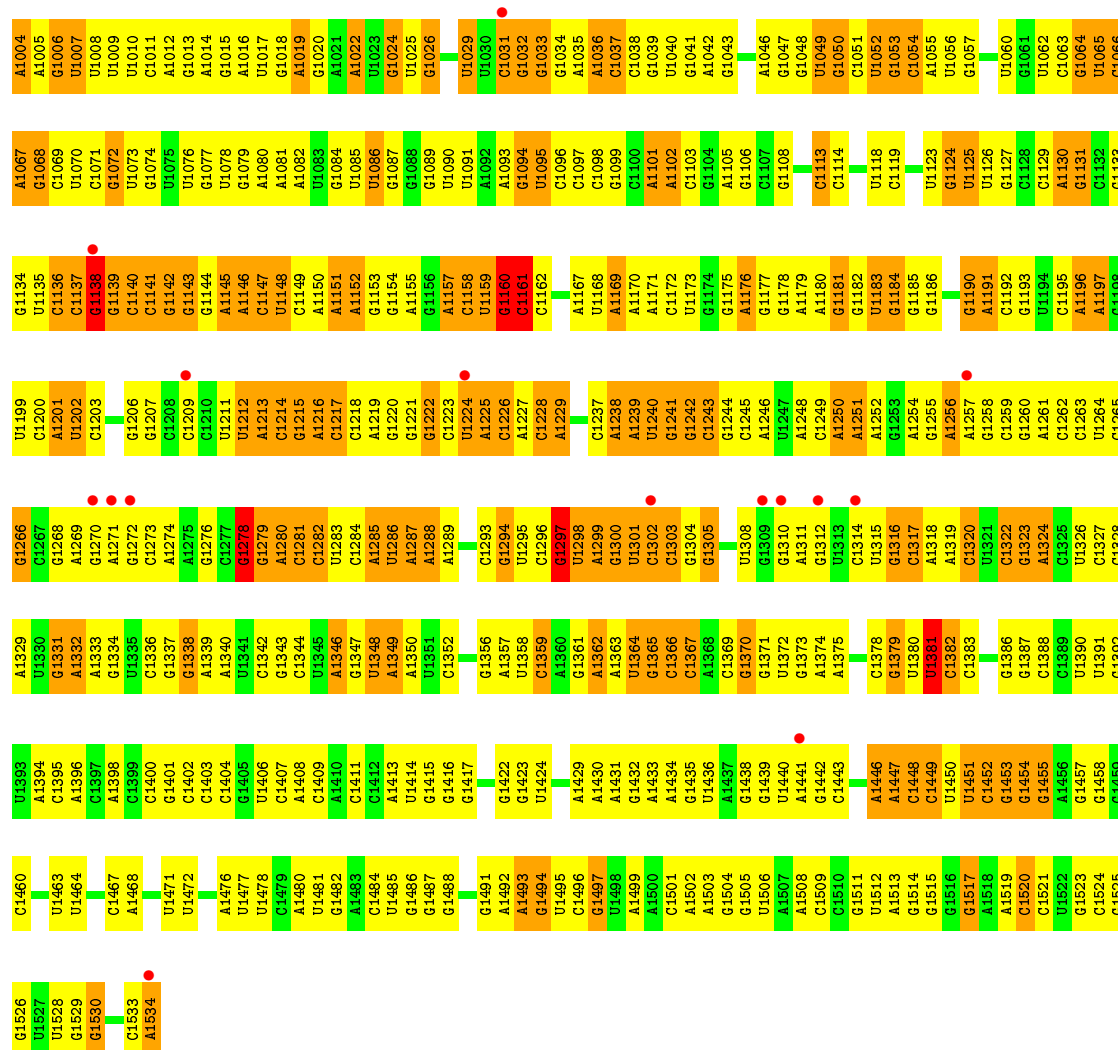


- Molecule 52: 50S ribosomal protein L36

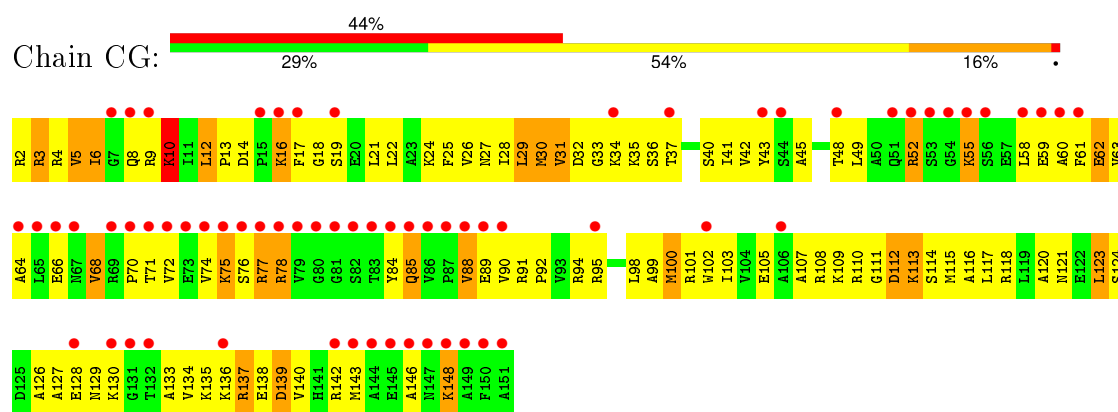


● Molecule 53: 16S rRNA



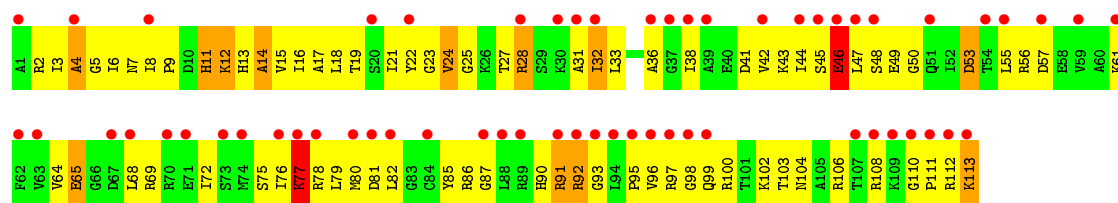


• Molecule 54: 30S ribosomal protein S7



• Molecule 55: 30S ribosomal protein S13

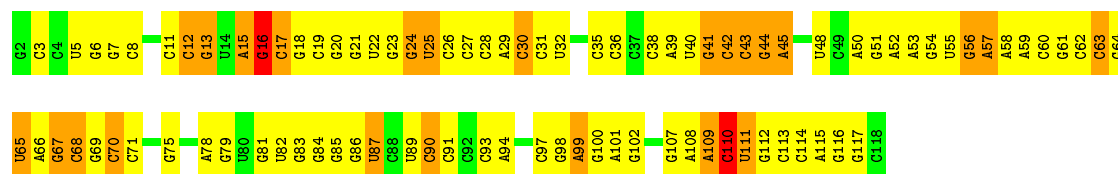




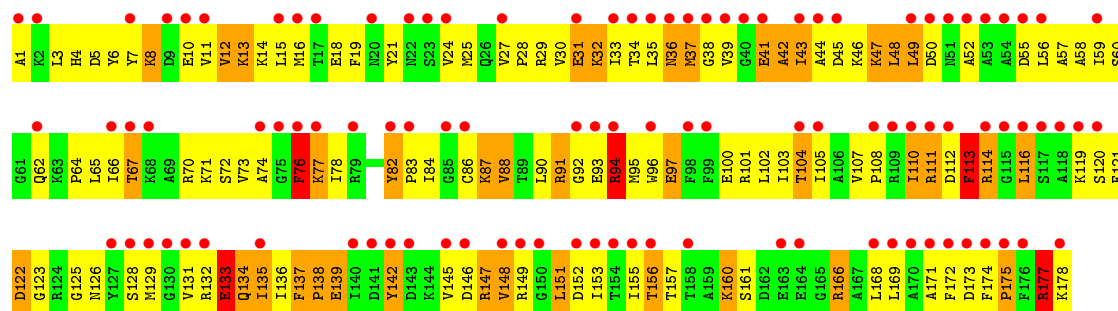
• Molecule 56: 30S ribosomal protein S16



• Molecule 57: 5S rRNA



• Molecule 58: 50S ribosomal protein L5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.22 – 3.25 85.13 – 3.25	Depositor EDS
% Data completeness (in resolution range)	85.8 (85.22-3.25) 85.6 (85.13-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.193 , 0.245 0.227 , 0.270	Depositor DCC
R_{free} test set	16150 reflections (2.19%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 73.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 801754 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.45	2/36834 (0.0%)	0.87	33/57462 (0.1%)
2	AB	0.34	1/1736 (0.1%)	0.52	1/2338 (0.0%)
2	CB	0.30	1/1736 (0.1%)	0.58	4/2338 (0.2%)
3	AC	0.28	0/1652	0.50	0/2225
3	CC	0.25	0/1652	0.44	0/2225
4	AD	0.32	0/1665	0.53	0/2227
4	CD	0.39	0/1665	0.61	0/2227
5	AE	0.45	1/1119 (0.1%)	0.66	2/1504 (0.1%)
5	CE	0.36	0/1119	0.58	0/1504
6	AF	0.31	0/836	0.49	0/1128
6	CF	0.30	0/836	0.50	0/1128
7	AG	0.25	0/1196	0.45	0/1602
8	AH	0.33	0/989	0.55	0/1326
8	CH	0.30	0/989	0.52	0/1326
9	AI	0.26	0/1034	0.48	0/1375
9	CI	0.23	0/1034	0.43	0/1375
10	AJ	0.28	0/797	0.48	0/1077
10	CJ	0.24	0/797	0.47	0/1077
11	AK	0.30	0/893	0.53	0/1205
11	CK	0.28	0/893	0.52	0/1205
12	AL	0.38	0/969	0.69	1/1300 (0.1%)
12	CL	0.36	0/969	0.58	0/1300
13	AM	0.25	0/893	0.47	0/1193
14	AN	0.28	0/785	0.50	0/1043
14	CN	0.23	0/780	0.39	0/1036
15	AO	0.29	0/722	0.48	0/964
15	CO	0.39	1/722 (0.1%)	0.48	0/964
16	AP	0.31	0/659	0.51	0/884
17	AQ	0.40	0/658	0.62	0/881
17	CQ	0.34	0/658	0.52	0/881
18	AR	0.31	0/463	0.50	0/621
18	CR	0.31	0/463	0.47	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.25	0/653	0.45	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.37	0/671	0.56	0/888
20	CT	0.28	0/671	0.50	0/888
21	AU	0.29	0/431	0.46	0/570
21	CU	0.34	0/431	0.59	0/570
22	BA	0.77	9/68626 (0.0%)	1.12	282/107056 (0.3%)
22	DA	0.39	1/68314 (0.0%)	0.86	83/106569 (0.1%)
23	BB	0.68	0/2828	1.04	4/4410 (0.1%)
24	BC	0.48	0/2122	0.73	1/2852 (0.0%)
24	DC	0.31	0/2122	0.54	0/2852
25	BD	0.55	0/1586	0.78	1/2134 (0.0%)
25	DD	0.31	0/1586	0.58	0/2134
26	BE	0.45	0/1571	0.68	1/2113 (0.0%)
26	DE	0.26	0/1571	0.48	0/2113
27	BF	0.34	0/1435	0.53	0/1926
28	BG	0.39	0/1343	0.62	0/1816
28	DG	0.24	0/1343	0.47	0/1816
29	BH	0.33	0/1122	0.52	0/1515
29	DH	0.38	1/1122 (0.1%)	0.52	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.42	0/1410
31	BJ	0.58	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.29	0/1152	0.57	1/1551 (0.1%)
32	BK	0.55	0/948	0.80	0/1268
32	DK	0.35	0/948	0.57	0/1268
33	BL	0.46	0/1054	0.79	1/1403 (0.1%)
33	DL	0.27	0/1054	0.53	0/1403
34	BM	0.54	0/1093	0.73	0/1460
34	DM	0.30	0/1093	0.50	0/1460
35	BN	0.51	0/974	0.75	0/1301
35	DN	0.28	0/974	0.51	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.24	0/902	0.43	0/1209
37	BP	0.51	0/929	0.74	0/1242
37	DP	0.32	0/929	0.50	0/1242
38	BQ	0.61	0/960	0.78	0/1278
38	DQ	0.29	0/960	0.47	0/1278
39	BR	0.63	1/829 (0.1%)	0.79	0/1107
39	DR	0.29	0/829	0.51	0/1107
40	BS	0.57	0/864	0.78	0/1156
40	DS	0.28	0/864	0.52	0/1156
41	BT	0.45	0/745	0.70	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DT	0.24	0/745	0.48	0/994
42	BU	0.43	0/788	0.70	0/1051
42	DU	0.24	0/788	0.46	0/1051
43	BV	0.44	0/766	0.61	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.61	0/603	0.89	0/797
44	DW	0.29	0/603	0.51	0/797
45	BX	0.41	0/635	0.70	0/848
45	DX	0.29	0/635	0.56	0/848
46	BY	0.37	0/510	0.64	0/677
46	DY	0.23	0/510	0.44	0/677
47	BZ	0.52	0/453	0.83	0/605
47	DZ	0.28	0/453	0.51	0/605
48	B0	0.48	0/450	0.73	0/599
48	D0	0.29	0/450	0.50	0/599
49	B1	0.38	0/417	0.62	0/554
49	D1	0.27	0/417	0.46	0/554
50	B2	0.53	0/380	0.78	0/498
50	D2	0.27	0/380	0.49	0/498
51	B3	0.49	0/513	0.70	0/676
51	D3	0.29	0/513	0.53	0/676
52	B4	0.53	0/303	0.70	0/397
52	D4	0.45	0/303	0.50	0/397
53	CA	0.41	2/36762 (0.0%)	0.83	32/57350 (0.1%)
54	CG	0.23	0/1188	0.44	0/1591
55	CM	0.20	0/885	0.40	0/1181
56	CP	0.29	0/649	0.53	0/870
57	DB	0.36	1/2803 (0.0%)	0.81	2/4371 (0.0%)
58	DF	0.23	0/1444	0.53	3/1937 (0.2%)
All	All	0.51	21/306773 (0.0%)	0.86	453/458565 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
35	BN	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2092	U	O3'-P	-13.97	1.44	1.61
22	DA	2197	U	O3'-P	-13.44	1.45	1.61
53	CA	1396	A	O3'-P	-13.34	1.45	1.61
22	BA	1142	A	N9-C4	-9.96	1.31	1.37
57	DB	107	G	O3'-P	-9.89	1.49	1.61

The worst 5 of 453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	783	A	C5-N7-C8	-11.37	98.22	103.90
22	BA	974	G	C5-N7-C8	-11.01	98.79	104.30
22	BA	974	G	C4-C5-N7	10.99	115.20	110.80
2	CB	146	SER	O-C-N	-10.79	105.44	122.70
22	BA	2499	C	N1-C2-O2	-10.28	112.73	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
35	BN	101	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	32895	0	16553	1232	1
2	AB	1705	0	1732	183	0
2	CB	1705	0	1732	151	0
3	AC	1625	0	1699	109	0
3	CC	1625	0	1699	128	0
4	AD	1643	0	1710	145	0
4	CD	1643	0	1710	157	0
5	AE	1106	0	1148	148	0
5	CE	1106	0	1148	101	0
6	AF	818	0	808	87	0
6	CF	818	0	808	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	86	0
8	AH	979	0	1034	99	0
8	CH	979	0	1034	92	0
9	AI	1022	0	1070	84	0
9	CI	1022	0	1070	107	0
10	AJ	787	0	828	78	0
10	CJ	787	0	828	91	0
11	AK	877	0	887	91	0
11	CK	877	0	887	71	0
12	AL	955	0	1019	90	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	73	0
14	AN	774	0	827	69	0
14	CN	769	0	822	77	0
15	AO	714	0	737	46	0
15	CO	714	0	737	52	0
16	AP	649	0	666	50	0
17	AQ	649	0	691	71	0
17	CQ	649	0	691	66	0
18	AR	456	0	478	30	0
18	CR	456	0	478	39	0
19	AS	638	0	665	59	0
19	CS	638	0	665	65	0
20	AT	665	0	714	81	0
20	CT	665	0	714	45	0
21	AU	426	0	449	80	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	1937	6
22	DA	60995	0	30679	3516	8
23	BB	2529	0	1281	73	0
24	BC	2083	0	2157	217	0
24	DC	2083	0	2157	215	0
25	BD	1565	0	1616	196	1
25	DD	1565	0	1616	189	0
26	BE	1552	0	1619	151	0
26	DE	1552	0	1619	180	0
27	BF	1411	0	1447	135	0
28	BG	1323	0	1374	146	0
28	DG	1323	0	1374	126	0
29	BH	1111	0	1148	102	0
29	DH	1111	0	1148	96	0
30	BI	1032	0	1088	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DI	1032	0	1088	65	0
31	BJ	1129	0	1162	156	0
31	DJ	1129	0	1162	140	0
32	BK	939	0	1012	121	0
32	DK	939	0	1012	109	0
33	BL	1045	0	1117	130	1
33	DL	1045	0	1117	128	0
34	BM	1074	0	1157	90	0
34	DM	1074	0	1157	94	0
35	BN	961	0	1000	89	0
35	DN	961	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	79	0
37	BP	917	0	965	141	0
37	DP	917	0	965	121	0
38	BQ	947	0	1022	127	0
38	DQ	947	0	1022	121	0
39	BR	816	0	839	116	0
39	DR	816	0	839	93	0
40	BS	857	0	922	74	0
40	DS	857	0	922	60	0
41	BT	739	0	807	112	0
41	DT	739	0	807	99	0
42	BU	780	0	834	54	0
42	DU	780	0	834	92	0
43	BV	753	0	780	66	0
43	DV	753	0	780	60	0
44	BW	596	0	610	204	0
44	DW	596	0	610	115	0
45	BX	625	0	655	56	0
45	DX	625	0	655	75	0
46	BY	509	0	543	50	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	33	0
47	DZ	449	0	491	40	1
48	B0	444	0	461	30	0
48	D0	444	0	461	57	0
49	B1	410	0	440	33	0
49	D1	410	0	440	36	0
50	B2	377	0	418	35	0
50	D2	377	0	418	42	0
51	B3	504	0	574	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D3	504	0	574	57	0
52	B4	302	0	340	30	0
52	D4	302	0	342	27	0
53	CA	32831	0	16521	1619	0
54	CG	1175	0	1230	131	0
55	CM	877	0	937	91	0
56	CP	639	0	656	61	0
57	DB	2507	0	1270	159	0
58	DF	1420	0	1460	184	0
59	AA	43	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	CA	41	0	0	0	0
59	CE	1	0	0	0	0
59	DA	133	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	58	0	64	8	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	198	0	0	5	0
62	AL	1	0	0	0	0
62	AN	6	0	0	1	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	1	0	0	0	0
62	B3	3	0	0	0	0
62	B4	1	0	0	0	0
62	BA	598	0	0	29	0
62	BB	20	0	0	1	0
62	BC	10	0	0	0	0
62	BD	2	0	0	0	0
62	BE	1	0	0	0	0
62	BL	2	0	0	1	0
62	BN	3	0	0	1	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	0	0
62	BT	1	0	0	1	0
62	CA	192	0	0	6	0
62	CE	5	0	0	1	0
62	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	CL	1	0	0	0	0
62	CN	3	0	0	0	0
62	CT	3	0	0	0	0
62	CU	2	0	0	0	0
62	D2	1	0	0	1	0
62	D3	1	0	0	0	0
62	D4	3	0	0	0	0
62	DA	595	0	0	28	0
62	DB	4	0	0	0	0
62	DC	13	0	0	1	0
62	DD	3	0	0	1	0
62	DE	3	0	0	0	0
62	DJ	6	0	0	0	0
62	DL	6	0	0	1	0
62	DN	2	0	0	0	0
62	DT	3	0	0	0	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284525	0	190904	16341	9

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 35.

The worst 5 of 16341 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)
53:CA:1157:A:H4'	53:CA:1158:C:O5'	1.38	1.20
22:DA:1808:A:H3'	22:DA:1809:A:H8	1.05	1.20
53:CA:120:A:C3'	53:CA:121:U:H5''	1.73	1.19
22:DA:2091:C:OP2	22:DA:2092:U:H3'	1.39	1.18
22:BA:900:A:C2'	22:BA:901:C:H5'	1.74	1.17

The worst 5 of 9 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)
22:BA:138:U:O4	22:DA:305:C:OP1[3_545]	1.58	0.62
22:BA:138:U:O4	22:DA:305:C:P[3_545]	1.90	0.30
1:AA:416:G:OP1	22:DA:2139:U:O4'[4_455]	1.91	0.29
25:BD:181:ASP:OD1	22:DA:2903:U:O4[2_454]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:138:U:C4	22:DA:304:U:O3'[3_545]	1.98	0.22

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%)	132 (61%)	52 (24%)	32 (15%)	0	1
2	CB	216/218 (99%)	155 (72%)	46 (21%)	15 (7%)	1	11
3	AC	204/206 (99%)	156 (76%)	32 (16%)	16 (8%)	1	8
3	CC	204/206 (99%)	147 (72%)	37 (18%)	20 (10%)	1	5
4	AD	203/205 (99%)	138 (68%)	37 (18%)	28 (14%)	0	1
4	CD	203/205 (99%)	140 (69%)	43 (21%)	20 (10%)	1	4
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	2
5	CE	148/150 (99%)	112 (76%)	21 (14%)	15 (10%)	1	4
6	AF	98/100 (98%)	73 (74%)	13 (13%)	12 (12%)	0	2
6	CF	98/100 (98%)	65 (66%)	24 (24%)	9 (9%)	1	5
7	AG	149/151 (99%)	111 (74%)	32 (22%)	6 (4%)	4	26
8	AH	127/129 (98%)	92 (72%)	28 (22%)	7 (6%)	2	18
8	CH	127/129 (98%)	94 (74%)	22 (17%)	11 (9%)	1	6
9	AI	125/127 (98%)	89 (71%)	26 (21%)	10 (8%)	1	8
9	CI	125/127 (98%)	89 (71%)	25 (20%)	11 (9%)	1	6
10	AJ	96/98 (98%)	70 (73%)	13 (14%)	13 (14%)	0	2
10	CJ	96/98 (98%)	55 (57%)	28 (29%)	13 (14%)	0	2
11	AK	115/117 (98%)	85 (74%)	20 (17%)	10 (9%)	1	6
11	CK	115/117 (98%)	89 (77%)	19 (16%)	7 (6%)	2	15
12	AL	121/123 (98%)	88 (73%)	22 (18%)	11 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	121/123 (98%)	86 (71%)	27 (22%)	8 (7%)	1	12
13	AM	112/114 (98%)	88 (79%)	13 (12%)	11 (10%)	1	5
14	AN	92/100 (92%)	60 (65%)	20 (22%)	12 (13%)	0	2
14	CN	91/100 (91%)	59 (65%)	27 (30%)	5 (6%)	2	18
15	AO	86/88 (98%)	59 (69%)	23 (27%)	4 (5%)	3	22
15	CO	86/88 (98%)	67 (78%)	16 (19%)	3 (4%)	4	30
16	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	1	4
17	AQ	78/80 (98%)	51 (65%)	15 (19%)	12 (15%)	0	1
17	CQ	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	1	4
18	AR	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	4	28
18	CR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
19	AS	77/79 (98%)	58 (75%)	10 (13%)	9 (12%)	0	3
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	5
20	AT	83/85 (98%)	58 (70%)	19 (23%)	6 (7%)	1	10
20	CT	83/85 (98%)	63 (76%)	12 (14%)	8 (10%)	1	5
21	AU	49/51 (96%)	25 (51%)	15 (31%)	9 (18%)	0	1
21	CU	49/51 (96%)	22 (45%)	8 (16%)	19 (39%)	0	0
24	BC	269/271 (99%)	203 (76%)	40 (15%)	26 (10%)	1	5
24	DC	269/271 (99%)	183 (68%)	54 (20%)	32 (12%)	0	2
25	BD	207/209 (99%)	148 (72%)	31 (15%)	28 (14%)	0	2
25	DD	207/209 (99%)	136 (66%)	40 (19%)	31 (15%)	0	1
26	BE	199/201 (99%)	149 (75%)	32 (16%)	18 (9%)	1	6
26	DE	199/201 (99%)	125 (63%)	46 (23%)	28 (14%)	0	1
27	BF	175/177 (99%)	130 (74%)	30 (17%)	15 (9%)	1	6
28	BG	174/176 (99%)	118 (68%)	32 (18%)	24 (14%)	0	1
28	DG	174/176 (99%)	102 (59%)	41 (24%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	52 (35%)	28 (19%)	0	1
29	DH	147/149 (99%)	76 (52%)	53 (36%)	18 (12%)	0	2
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	4
30	DI	139/141 (99%)	84 (60%)	38 (27%)	17 (12%)	0	2
31	BJ	140/142 (99%)	103 (74%)	26 (19%)	11 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DJ	140/142 (99%)	96 (69%)	29 (21%)	15 (11%)	0	3
32	BK	120/122 (98%)	88 (73%)	12 (10%)	20 (17%)	0	1
32	DK	120/122 (98%)	82 (68%)	18 (15%)	20 (17%)	0	1
33	BL	141/143 (99%)	103 (73%)	28 (20%)	10 (7%)	1	10
33	DL	141/143 (99%)	80 (57%)	41 (29%)	20 (14%)	0	1
34	BM	134/136 (98%)	100 (75%)	21 (16%)	13 (10%)	1	5
34	DM	134/136 (98%)	95 (71%)	27 (20%)	12 (9%)	1	6
35	BN	118/120 (98%)	92 (78%)	14 (12%)	12 (10%)	1	4
35	DN	118/120 (98%)	70 (59%)	36 (30%)	12 (10%)	1	4
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	8
36	DO	114/116 (98%)	81 (71%)	26 (23%)	7 (6%)	2	15
37	BP	112/114 (98%)	74 (66%)	21 (19%)	17 (15%)	0	1
37	DP	112/114 (98%)	64 (57%)	29 (26%)	19 (17%)	0	1
38	BQ	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	10
38	DQ	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	1	4
39	BR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	1	11
39	DR	101/103 (98%)	71 (70%)	18 (18%)	12 (12%)	0	2
40	BS	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	1	13
40	DS	108/110 (98%)	74 (68%)	25 (23%)	9 (8%)	1	7
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	1
41	DT	91/93 (98%)	48 (53%)	28 (31%)	15 (16%)	0	1
42	BU	100/102 (98%)	67 (67%)	17 (17%)	16 (16%)	0	1
42	DU	100/102 (98%)	51 (51%)	28 (28%)	21 (21%)	0	0
43	BV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	17	60
43	DV	92/94 (98%)	64 (70%)	21 (23%)	7 (8%)	1	9
44	BW	77/79 (98%)	28 (36%)	22 (29%)	27 (35%)	0	0
44	DW	77/79 (98%)	33 (43%)	23 (30%)	21 (27%)	0	0
45	BX	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	18
45	DX	75/77 (97%)	50 (67%)	17 (23%)	8 (11%)	0	3
46	BY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	1	5
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BZ	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	4	29
47	DZ	56/58 (97%)	34 (61%)	17 (30%)	5 (9%)	1	6
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	10
48	D0	54/56 (96%)	40 (74%)	8 (15%)	6 (11%)	0	3
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	7
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	7
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	3	23
50	D2	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	5
51	B3	62/64 (97%)	50 (81%)	7 (11%)	5 (8%)	1	8
51	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	8
52	B4	36/38 (95%)	29 (81%)	3 (8%)	4 (11%)	0	3
52	D4	36/38 (95%)	23 (64%)	8 (22%)	5 (14%)	0	1
54	CG	148/150 (99%)	100 (68%)	36 (24%)	12 (8%)	1	8
55	CM	111/113 (98%)	64 (58%)	35 (32%)	12 (11%)	0	3
56	CP	78/80 (98%)	50 (64%)	18 (23%)	10 (13%)	0	2
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7713 (69%)	2283 (20%)	1242 (11%)	0	3

5 of 1242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLN
2	AB	20	ARG
2	AB	33	ALA
2	AB	40	ILE
2	AB	72	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	141 (78%)	39 (22%)	1	6
2	CB	180/180 (100%)	152 (84%)	28 (16%)	3	16
3	AC	170/170 (100%)	142 (84%)	28 (16%)	3	14
3	CC	170/170 (100%)	151 (89%)	19 (11%)	7	31
4	AD	172/172 (100%)	145 (84%)	27 (16%)	3	15
4	CD	172/172 (100%)	135 (78%)	37 (22%)	1	6
5	AE	113/113 (100%)	86 (76%)	27 (24%)	1	3
5	CE	113/113 (100%)	90 (80%)	23 (20%)	1	7
6	AF	87/87 (100%)	73 (84%)	14 (16%)	3	14
6	CF	87/87 (100%)	74 (85%)	13 (15%)	4	17
7	AG	124/124 (100%)	106 (86%)	18 (14%)	4	19
8	AH	104/104 (100%)	89 (86%)	15 (14%)	4	19
8	CH	104/104 (100%)	91 (88%)	13 (12%)	6	26
9	AI	105/105 (100%)	83 (79%)	22 (21%)	1	7
9	CI	105/105 (100%)	91 (87%)	14 (13%)	5	23
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	4	20
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	5	24
11	AK	90/90 (100%)	75 (83%)	15 (17%)	3	13
11	CK	90/90 (100%)	78 (87%)	12 (13%)	5	23
12	AL	103/103 (100%)	85 (82%)	18 (18%)	2	12
12	CL	103/103 (100%)	86 (84%)	17 (16%)	3	14
13	AM	92/92 (100%)	87 (95%)	5 (5%)	27	67
14	AN	79/83 (95%)	75 (95%)	4 (5%)	29	69
14	CN	79/83 (95%)	69 (87%)	10 (13%)	5	25
15	AO	76/76 (100%)	70 (92%)	6 (8%)	15	51
15	CO	76/76 (100%)	70 (92%)	6 (8%)	15	51
16	AP	65/65 (100%)	58 (89%)	7 (11%)	8	33
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	4
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	2	10
18	AR	48/48 (100%)	45 (94%)	3 (6%)	22	62
18	CR	48/48 (100%)	43 (90%)	5 (10%)	9	34
19	AS	70/70 (100%)	62 (89%)	8 (11%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/70 (100%)	63 (90%)	7 (10%)	9	36
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	51 (78%)	14 (22%)	1	6
21	AU	44/44 (100%)	34 (77%)	10 (23%)	1	5
21	CU	44/44 (100%)	36 (82%)	8 (18%)	2	10
24	BC	216/216 (100%)	167 (77%)	49 (23%)	1	5
24	DC	216/216 (100%)	189 (88%)	27 (12%)	6	26
25	BD	164/164 (100%)	134 (82%)	30 (18%)	2	10
25	DD	164/164 (100%)	144 (88%)	20 (12%)	6	27
26	BE	165/165 (100%)	122 (74%)	43 (26%)	0	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	8	32
27	BF	148/148 (100%)	130 (88%)	18 (12%)	6	27
28	BG	137/137 (100%)	105 (77%)	32 (23%)	1	4
28	DG	137/137 (100%)	119 (87%)	18 (13%)	5	24
29	BH	114/114 (100%)	96 (84%)	18 (16%)	3	15
29	DH	114/114 (100%)	96 (84%)	18 (16%)	3	15
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	14
30	DI	109/109 (100%)	102 (94%)	7 (6%)	22	61
31	BJ	116/116 (100%)	88 (76%)	28 (24%)	1	3
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	21
32	BK	103/103 (100%)	81 (79%)	22 (21%)	1	6
32	DK	103/103 (100%)	83 (81%)	20 (19%)	2	9
33	BL	102/102 (100%)	76 (74%)	26 (26%)	1	2
33	DL	102/102 (100%)	85 (83%)	17 (17%)	3	13
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	7
34	DM	109/109 (100%)	96 (88%)	13 (12%)	6	28
35	BN	100/100 (100%)	82 (82%)	18 (18%)	2	11
35	DN	100/100 (100%)	85 (85%)	15 (15%)	3	17
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	8
36	DO	86/86 (100%)	77 (90%)	9 (10%)	8	34
37	BP	99/99 (100%)	73 (74%)	26 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	89 (90%)	10 (10%)	9	36
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	7
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	13
39	BR	84/84 (100%)	70 (83%)	14 (17%)	3	13
39	DR	84/84 (100%)	71 (84%)	13 (16%)	3	16
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	7
40	DS	93/93 (100%)	79 (85%)	14 (15%)	3	17
41	BT	80/80 (100%)	61 (76%)	19 (24%)	1	3
41	DT	80/80 (100%)	73 (91%)	7 (9%)	12	44
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	7
42	DU	83/83 (100%)	74 (89%)	9 (11%)	8	33
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
43	DV	78/78 (100%)	68 (87%)	10 (13%)	5	24
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	42 (71%)	17 (29%)	0	1
45	BX	67/67 (100%)	54 (81%)	13 (19%)	2	9
45	DX	67/67 (100%)	58 (87%)	9 (13%)	5	22
46	BY	55/55 (100%)	41 (74%)	14 (26%)	1	2
46	DY	55/55 (100%)	52 (94%)	3 (6%)	27	67
47	BZ	48/48 (100%)	33 (69%)	15 (31%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	13
48	B0	47/47 (100%)	39 (83%)	8 (17%)	2	13
48	D0	47/47 (100%)	39 (83%)	8 (17%)	2	13
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	11
49	D1	45/45 (100%)	41 (91%)	4 (9%)	12	43
50	B2	38/38 (100%)	29 (76%)	9 (24%)	1	4
50	D2	38/38 (100%)	33 (87%)	5 (13%)	5	23
51	B3	51/51 (100%)	44 (86%)	7 (14%)	4	21
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	6
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	11
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	CG	123/123 (100%)	102 (83%)	21 (17%)	2	13
55	CM	91/91 (100%)	80 (88%)	11 (12%)	6	27
56	CP	65/65 (100%)	57 (88%)	8 (12%)	6	26
58	DF	149/149 (100%)	123 (83%)	26 (17%)	2	12
All	All	9331/9339 (100%)	7786 (83%)	1545 (17%)	3	13

5 of 1545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	20	VAL
50	B2	9	VAL
39	DR	58	VAL
40	BS	48	LYS
44	BW	14	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	91	GLN
3	CC	31	ASN
42	DU	44	HIS
43	BV	44	HIS
47	BZ	33	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	363 (23%)	63 (4%)
22	BA	2850/2903 (98%)	554 (19%)	87 (3%)
22	DA	2837/2903 (97%)	869 (30%)	183 (6%)
23	BB	117/118 (99%)	19 (16%)	0
53	CA	1529/1530 (99%)	445 (29%)	81 (5%)
57	DB	116/117 (99%)	33 (28%)	7 (6%)
All	All	8981/9104 (98%)	2283 (25%)	421 (4%)

5 of 2283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 421 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	CA	512	U
22	DA	52	A
22	DA	2492	U
53	CA	701	U
53	CA	1142	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 363 ligands modelled in this entry, 362 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	TEL	BA	3135	-	59,62,62	2.21	10 (16%)	72,92,92	3.13	25 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TEL	BA	3135	-	2/2/19/19	0/73/108/108	0/4/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	TEL	O9-C4	-3.95	1.39	1.46
60	BA	3135	TEL	O45-C50	-3.44	1.38	1.44
60	BA	3135	TEL	C37-N41	-2.93	1.29	1.35
60	BA	3135	TEL	C43-C40	-2.51	1.45	1.48
60	BA	3135	TEL	C7-C13	-2.39	1.48	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3135	TEL	C3-N6-C10	-15.48	93.00	111.94
60	BA	3135	TEL	O5-C10-O16	-11.28	110.75	122.53
60	BA	3135	TEL	O16-C10-N6	-7.05	117.54	127.98
60	BA	3135	TEL	O48-C44-C42	-4.86	99.36	110.02
60	BA	3135	TEL	C42-C44-C49	-4.86	100.69	109.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	BA	3135	TEL	C3
60	BA	3135	TEL	C21

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	3135	TEL	8	0

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	1533/1533 (100%)	-0.41	21 (1%) 78 69	31, 83, 185, 422	0
2	AB	218/218 (100%)	1.67	72 (33%) 0 1	67, 161, 222, 300	0
2	CB	218/218 (100%)	1.80	86 (39%) 0 1	76, 168, 231, 274	0
3	AC	206/206 (100%)	0.83	20 (9%) 10 7	53, 101, 156, 201	0
3	CC	206/206 (100%)	1.02	34 (16%) 2 2	76, 138, 202, 264	0
4	AD	205/205 (100%)	0.33	9 (4%) 38 29	48, 93, 168, 305	0
4	CD	205/205 (100%)	-0.14	1 (0%) 91 88	26, 60, 114, 257	0
5	AE	150/150 (100%)	0.16	2 (1%) 79 71	38, 76, 150, 231	0
5	CE	150/150 (100%)	0.27	2 (1%) 79 71	34, 85, 143, 282	0
6	AF	100/100 (100%)	0.23	5 (5%) 32 24	52, 100, 147, 188	0
6	CF	100/100 (100%)	0.28	4 (4%) 42 32	69, 109, 169, 214	0
7	AG	151/151 (100%)	0.72	16 (10%) 8 5	77, 131, 195, 217	0
8	AH	129/129 (100%)	0.40	6 (4%) 35 27	45, 82, 133, 191	0
8	CH	129/129 (100%)	0.70	13 (10%) 9 6	60, 101, 151, 212	0
9	AI	127/127 (100%)	1.11	27 (21%) 1 1	64, 137, 207, 266	0
9	CI	127/127 (100%)	1.58	40 (31%) 1 1	98, 168, 246, 283	0
10	AJ	98/98 (100%)	0.88	14 (14%) 4 3	65, 111, 196, 260	0
10	CJ	98/98 (100%)	2.78	51 (52%) 0 0	94, 178, 248, 272	0
11	AK	117/117 (100%)	0.96	20 (17%) 2 1	45, 108, 190, 238	0
11	CK	117/117 (100%)	0.83	17 (14%) 3 2	49, 112, 169, 192	0
12	AL	123/123 (100%)	-0.00	1 (0%) 87 82	24, 62, 106, 208	0
12	CL	123/123 (100%)	0.47	6 (4%) 33 25	37, 73, 124, 211	0
13	AM	114/114 (100%)	0.55	11 (9%) 10 7	86, 135, 206, 262	0
14	AN	96/100 (96%)	0.58	8 (8%) 14 9	58, 105, 187, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.90	36 (37%) 0 1	95, 187, 280, 335	0
15	AO	88/88 (100%)	-0.19	1 (1%) 82 75	43, 81, 124, 170	0
15	CO	88/88 (100%)	0.19	2 (2%) 64 54	57, 107, 153, 265	0
16	AP	82/82 (100%)	0.82	13 (15%) 3 2	56, 80, 166, 241	0
17	AQ	80/80 (100%)	0.71	7 (8%) 12 8	44, 78, 145, 219	0
17	CQ	80/80 (100%)	1.06	14 (17%) 2 1	57, 106, 146, 163	0
18	AR	55/55 (100%)	0.46	6 (10%) 7 5	60, 88, 151, 212	0
18	CR	55/55 (100%)	0.08	0 100 100	55, 88, 179, 249	0
19	AS	79/79 (100%)	1.68	28 (35%) 0 1	96, 137, 193, 233	0
19	CS	79/79 (100%)	3.19	50 (63%) 0 0	183, 316, 391, 403	0
20	AT	85/85 (100%)	0.01	1 (1%) 81 72	47, 84, 131, 157	0
20	CT	85/85 (100%)	1.35	21 (24%) 1 1	66, 115, 191, 210	0
21	AU	51/51 (100%)	2.28	29 (56%) 0 0	96, 152, 206, 217	0
21	CU	51/51 (100%)	0.83	6 (11%) 6 4	66, 117, 183, 253	0
22	BA	2854/2903 (98%)	-0.36	38 (1%) 79 71	5, 32, 160, 403	0
22	DA	2841/2903 (97%)	0.56	133 (4%) 35 27	53, 122, 250, 469	0
23	BB	118/118 (100%)	-0.40	0 100 100	13, 44, 74, 101	0
24	BC	271/271 (100%)	-0.13	9 (3%) 50 40	12, 42, 93, 209	0
24	DC	271/271 (100%)	0.76	25 (9%) 11 8	59, 93, 144, 185	0
25	BD	209/209 (100%)	-0.29	0 100 100	4, 26, 73, 178	0
25	DD	209/209 (100%)	1.22	40 (19%) 2 1	58, 109, 173, 246	0
26	BE	201/201 (100%)	-0.24	1 (0%) 91 88	5, 43, 103, 156	0
26	DE	201/201 (100%)	2.19	89 (44%) 0 0	65, 192, 378, 459	0
27	BF	177/177 (100%)	0.52	20 (11%) 7 5	27, 75, 156, 242	0
28	BG	176/176 (100%)	0.18	4 (2%) 64 54	22, 62, 121, 186	0
28	DG	176/176 (100%)	1.86	72 (40%) 0 1	100, 185, 264, 328	0
29	BH	149/149 (100%)	3.12	70 (46%) 0 0	49, 179, 279, 375	0
29	DH	149/149 (100%)	2.73	69 (46%) 0 0	93, 184, 287, 326	0
30	BI	141/141 (100%)	3.02	82 (58%) 0 0	136, 253, 308, 367	0
30	DI	141/141 (100%)	3.91	108 (76%) 0 0	167, 294, 351, 377	0
31	BJ	142/142 (100%)	-0.42	0 100 100	7, 23, 64, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	DJ	142/142 (100%)	1.19	36 (25%) 1 1	52, 106, 159, 195	0
32	BK	122/122 (100%)	-0.24	0 100 100	10, 31, 80, 254	0
32	DK	122/122 (100%)	1.29	29 (23%) 1 1	57, 91, 150, 229	0
33	BL	143/143 (100%)	-0.22	0 100 100	7, 38, 75, 111	0
33	DL	143/143 (100%)	1.40	39 (27%) 1 1	69, 149, 262, 337	0
34	BM	136/136 (100%)	-0.32	0 100 100	6, 29, 76, 120	0
34	DM	136/136 (100%)	1.03	28 (20%) 1 1	46, 107, 161, 204	0
35	BN	120/120 (100%)	-0.48	0 100 100	9, 25, 46, 155	0
35	DN	120/120 (100%)	1.45	36 (30%) 1 1	73, 124, 194, 293	0
36	BO	116/116 (100%)	0.00	0 100 100	24, 44, 83, 116	0
36	DO	116/116 (100%)	1.79	46 (39%) 0 1	113, 162, 224, 259	0
37	BP	114/114 (100%)	-0.10	1 (0%) 85 80	11, 41, 104, 161	0
37	DP	114/114 (100%)	1.03	21 (18%) 2 1	63, 105, 164, 195	0
38	BQ	117/117 (100%)	-0.51	1 (0%) 85 80	4, 20, 47, 206	0
38	DQ	117/117 (100%)	1.64	37 (31%) 1 1	67, 108, 191, 312	0
39	BR	103/103 (100%)	-0.33	1 (0%) 84 78	5, 30, 80, 109	0
39	DR	103/103 (100%)	2.53	57 (55%) 0 0	80, 138, 239, 291	0
40	BS	110/110 (100%)	-0.39	1 (0%) 85 80	6, 21, 61, 178	0
40	DS	110/110 (100%)	2.37	55 (50%) 0 0	70, 133, 241, 285	0
41	BT	93/93 (100%)	0.22	4 (4%) 39 29	23, 51, 121, 235	0
41	DT	93/93 (100%)	2.77	53 (56%) 0 0	110, 202, 299, 369	0
42	BU	102/102 (100%)	0.11	3 (2%) 55 46	19, 55, 136, 246	0
42	DU	102/102 (100%)	3.33	65 (63%) 0 0	122, 287, 418, 543	0
43	BV	94/94 (100%)	-0.02	0 100 100	13, 43, 85, 124	0
43	DV	94/94 (100%)	1.73	31 (32%) 0 1	100, 144, 196, 226	0
44	BW	79/79 (100%)	0.17	4 (5%) 32 23	10, 36, 110, 208	0
44	DW	79/79 (100%)	2.37	42 (53%) 0 0	87, 141, 230, 253	0
45	BX	77/77 (100%)	-0.23	0 100 100	15, 46, 88, 135	0
45	DX	77/77 (100%)	1.23	19 (24%) 1 1	67, 118, 172, 239	0
46	BY	63/63 (100%)	0.15	2 (3%) 51 42	34, 75, 134, 210	0
46	DY	63/63 (100%)	1.61	18 (28%) 1 1	130, 305, 419, 450	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BZ	58/58 (100%)	-0.29	0 100 100	6, 24, 74, 116	0
47	DZ	58/58 (100%)	1.00	8 (13%) 4 3	86, 123, 190, 236	0
48	B0	56/56 (100%)	-0.55	0 100 100	3, 22, 75, 168	0
48	D0	56/56 (100%)	1.64	19 (33%) 0 1	66, 132, 242, 278	0
49	B1	50/50 (100%)	0.38	3 (6%) 25 18	30, 50, 98, 178	0
49	D1	50/50 (100%)	1.83	21 (42%) 0 0	98, 155, 211, 275	0
50	B2	46/46 (100%)	-0.45	0 100 100	13, 27, 51, 183	0
50	D2	46/46 (100%)	1.46	11 (23%) 1 1	78, 118, 155, 203	0
51	B3	64/64 (100%)	-0.30	0 100 100	9, 27, 46, 71	0
51	D3	64/64 (100%)	1.99	30 (46%) 0 0	90, 125, 198, 250	0
52	B4	38/38 (100%)	0.37	1 (2%) 59 50	28, 49, 87, 112	0
52	D4	38/38 (100%)	2.97	26 (68%) 0 0	78, 141, 210, 225	0
53	CA	1530/1530 (100%)	0.07	38 (2%) 61 51	38, 100, 272, 376	0
54	CG	150/150 (100%)	2.37	66 (44%) 0 0	118, 209, 283, 333	0
55	CM	113/113 (100%)	2.38	59 (52%) 0 0	196, 344, 437, 471	0
56	CP	80/80 (100%)	0.95	12 (15%) 3 2	59, 91, 145, 249	0
57	DB	117/117 (100%)	0.15	0 100 100	95, 167, 229, 249	0
58	DF	178/178 (100%)	2.38	103 (57%) 0 0	135, 220, 279, 350	0
All	All	20431/20551 (99%)	0.54	2486 (12%) 5 4	3, 97, 258, 543	0

The worst 5 of 2486 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	CS	29	PRO	18.8
29	DH	124	THR	18.2
29	DH	91	PHE	18.0
29	BH	118	PRO	15.6
29	DH	105	ALA	15.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	BA	3129	1/1	0.93	1.06	90.68	243,243,243,243	0
59	MG	DA	3079	1/1	0.66	0.89	26.10	200,200,200,200	0
59	MG	CA	1627	1/1	0.88	1.25	23.02	237,237,237,237	0
59	MG	DA	3108	1/1	0.81	0.67	19.34	212,212,212,212	0
59	MG	DA	3106	1/1	0.45	0.74	14.68	316,316,316,316	0
59	MG	CA	1612	1/1	0.82	0.41	14.59	113,113,113,113	0
59	MG	DA	3002	1/1	-0.04	0.63	14.20	225,225,225,225	0
59	MG	BA	3021	1/1	0.84	0.34	13.93	158,158,158,158	0
59	MG	BA	3122	1/1	0.94	0.71	11.38	155,155,155,155	0
59	MG	DA	3069	1/1	0.84	0.58	8.79	233,233,233,233	0
59	MG	CA	1639	1/1	0.92	0.22	7.06	161,161,161,161	0
59	MG	AA	1641	1/1	0.91	0.23	6.13	148,148,148,148	0
59	MG	BA	3134	1/1	0.93	0.36	5.99	196,196,196,196	0
59	MG	DA	3075	1/1	0.88	0.41	4.83	172,172,172,172	0
59	MG	BA	3106	1/1	0.96	0.22	4.71	5,5,5,5	0
59	MG	BA	3102	1/1	0.96	0.21	4.66	9,9,9,9	0
59	MG	CA	1636	1/1	0.87	0.30	4.32	119,119,119,119	0
59	MG	DA	3097	1/1	0.57	0.39	3.97	137,137,137,137	0
59	MG	BA	3099	1/1	0.99	0.20	3.84	8,8,8,8	0
59	MG	BA	3070	1/1	0.91	0.21	3.71	135,135,135,135	0
59	MG	BA	3013	1/1	0.98	0.19	3.60	1,1,1,1	0
59	MG	CA	1618	1/1	0.45	0.30	3.36	146,146,146,146	0
59	MG	BA	3081	1/1	0.94	0.18	3.07	92,92,92,92	0
59	MG	BA	3040	1/1	0.98	0.18	2.96	13,13,13,13	0
59	MG	DA	3100	1/1	0.88	0.33	2.83	105,105,105,105	0
59	MG	BA	3105	1/1	0.98	0.17	2.32	27,27,27,27	0
59	MG	BA	3095	1/1	0.95	0.19	2.21	117,117,117,117	0
59	MG	DA	3129	1/1	0.52	0.53	2.10	210,210,210,210	0
59	MG	CA	1624	1/1	0.97	0.27	2.06	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3037	1/1	0.95	0.17	1.67	24,24,24,24	0
59	MG	DA	3133	1/1	0.43	0.38	1.66	198,198,198,198	0
59	MG	AA	1631	1/1	0.94	0.17	1.54	168,168,168,168	0
59	MG	DC	301	1/1	0.79	0.25	1.36	155,155,155,155	0
59	MG	CA	1607	1/1	0.81	0.23	1.35	134,134,134,134	0
59	MG	BA	3062	1/1	0.95	0.18	1.32	5,5,5,5	0
60	TEL	BA	3135	58/58	0.97	0.22	1.26	0,23,68,74	0
59	MG	AA	1622	1/1	0.99	0.18	1.25	40,40,40,40	0
59	MG	CA	1616	1/1	0.82	0.39	0.94	203,203,203,203	0
59	MG	BA	3028	1/1	0.92	0.20	0.91	49,49,49,49	0
59	MG	CA	1630	1/1	0.94	0.27	0.65	126,126,126,126	0
59	MG	CA	1606	1/1	0.90	0.16	0.44	54,54,54,54	0
59	MG	DA	3050	1/1	0.72	0.28	0.44	160,160,160,160	0
59	MG	BA	3008	1/1	0.96	0.16	0.35	12,12,12,12	0
59	MG	DA	3128	1/1	0.86	0.31	0.22	116,116,116,116	0
59	MG	DA	3027	1/1	0.51	0.27	0.14	157,157,157,157	0
59	MG	DA	3083	1/1	0.63	0.29	0.03	204,204,204,204	0
59	MG	BA	3110	1/1	0.95	0.16	-0.01	89,89,89,89	0
59	MG	BA	3103	1/1	0.91	0.17	-0.18	21,21,21,21	0
59	MG	CA	1621	1/1	0.91	0.18	-0.38	50,50,50,50	0
59	MG	BA	3022	1/1	0.96	0.16	-0.54	5,5,5,5	0
59	MG	BA	3116	1/1	0.96	0.14	-0.54	71,71,71,71	0
59	MG	AA	1635	1/1	0.94	0.14	-0.59	73,73,73,73	0
59	MG	BA	3114	1/1	0.92	0.15	-0.67	8,8,8,8	0
59	MG	BA	3130	1/1	0.97	0.14	-0.69	108,108,108,108	0
59	MG	AA	1633	1/1	0.94	0.10	-0.80	62,62,62,62	0
59	MG	CA	1611	1/1	0.91	0.19	-0.83	111,111,111,111	0
59	MG	AA	1617	1/1	0.79	0.16	-0.86	147,147,147,147	0
59	MG	DA	3115	1/1	0.80	0.21	-0.90	126,126,126,126	0
59	MG	BA	3053	1/1	0.98	0.15	-0.92	6,6,6,6	0
59	MG	BA	3057	1/1	0.86	0.14	-0.92	147,147,147,147	0
59	MG	CA	1628	1/1	0.56	0.17	-1.01	165,165,165,165	0
59	MG	BA	3119	1/1	0.97	0.07	-1.04	47,47,47,47	0
59	MG	CA	1617	1/1	0.61	0.12	-1.06	214,214,214,214	0
59	MG	DA	3105	1/1	0.93	0.20	-1.07	61,61,61,61	0
59	MG	DA	3084	1/1	0.55	0.17	-1.07	201,201,201,201	0
59	MG	BA	3064	1/1	0.97	0.13	-1.10	5,5,5,5	0
59	MG	BA	3077	1/1	0.93	0.13	-1.26	38,38,38,38	0
59	MG	CA	1640	1/1	0.96	0.16	-1.30	80,80,80,80	0
59	MG	DA	3012	1/1	0.90	0.21	-1.42	41,41,41,41	0
59	MG	BA	3027	1/1	0.97	0.17	-1.56	119,119,119,119	0
59	MG	AA	1616	1/1	0.69	0.14	-1.66	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3095	1/1	0.83	0.19	-1.72	122,122,122,122	0
61	ZN	D4	101	1/1	0.77	0.10	-1.74	157,157,157,157	0
59	MG	AA	1629	1/1	0.59	0.11	-1.81	84,84,84,84	0
59	MG	AA	1604	1/1	0.95	0.09	-1.83	121,121,121,121	0
59	MG	DA	3044	1/1	0.73	0.17	-1.95	92,92,92,92	0
59	MG	DA	3072	1/1	0.78	0.16	-1.96	131,131,131,131	0
59	MG	DA	3025	1/1	0.96	0.18	-1.98	104,104,104,104	0
59	MG	DA	3048	1/1	0.80	0.15	-2.02	95,95,95,95	0
59	MG	DA	3103	1/1	0.90	0.17	-2.04	76,76,76,76	0
59	MG	DA	3037	1/1	0.79	0.11	-2.12	97,97,97,97	0
59	MG	BA	3017	1/1	0.95	0.11	-2.14	33,33,33,33	0
59	MG	DA	3024	1/1	0.58	0.20	-2.15	100,100,100,100	0
59	MG	DA	3104	1/1	0.78	0.16	-2.16	33,33,33,33	0
59	MG	DA	3068	1/1	0.92	0.16	-2.16	67,67,67,67	0
59	MG	DA	3112	1/1	0.92	0.14	-2.25	80,80,80,80	0
59	MG	AA	1643	1/1	0.96	0.12	-2.27	43,43,43,43	0
59	MG	CA	1641	1/1	0.95	0.12	-2.40	82,82,82,82	0
59	MG	BA	3112	1/1	0.98	0.09	-2.43	41,41,41,41	0
59	MG	BA	3049	1/1	0.96	0.13	-2.47	6,6,6,6	0
59	MG	AA	1609	1/1	0.95	0.12	-2.53	54,54,54,54	0
59	MG	CA	1613	1/1	0.70	0.15	-2.56	107,107,107,107	0
59	MG	DA	3131	1/1	0.93	0.17	-2.61	91,91,91,91	0
59	MG	BA	3132	1/1	0.95	0.13	-2.62	1,1,1,1	0
61	ZN	B4	101	1/1	0.96	0.07	-2.75	118,118,118,118	0
59	MG	BA	3118	1/1	0.93	0.14	-2.78	23,23,23,23	0
59	MG	DA	3061	1/1	0.89	0.12	-2.84	131,131,131,131	0
59	MG	DA	3065	1/1	0.93	0.18	-2.86	77,77,77,77	0
59	MG	DA	3017	1/1	0.82	0.13	-3.01	51,51,51,51	0
59	MG	DA	3052	1/1	0.92	0.12	-3.06	56,56,56,56	0
59	MG	DA	3051	1/1	0.87	0.15	-3.19	91,91,91,91	0
59	MG	AA	1634	1/1	0.97	0.08	-3.26	62,62,62,62	0
59	MG	DA	3124	1/1	0.83	0.18	-3.46	70,70,70,70	0
59	MG	AA	1606	1/1	0.96	0.08	-3.54	72,72,72,72	0
59	MG	BA	3128	1/1	0.98	0.12	-3.62	15,15,15,15	0
59	MG	BA	3127	1/1	0.94	0.14	-3.63	2,2,2,2	0
59	MG	CA	1609	1/1	0.97	0.12	-3.82	97,97,97,97	0
59	MG	DB	201	1/1	0.82	0.10	-4.22	88,88,88,88	0
59	MG	AA	1625	1/1	0.88	0.08	-4.30	64,64,64,64	0
59	MG	DA	3039	1/1	0.45	0.17	-4.34	79,79,79,79	0
59	MG	BA	3002	1/1	0.96	0.10	-4.40	85,85,85,85	0
59	MG	BA	3024	1/1	0.94	0.12	-4.51	18,18,18,18	0
59	MG	BA	3050	1/1	0.98	0.09	-4.62	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BB	202	1/1	0.90	0.06	-4.74	64,64,64,64	0
59	MG	AA	1613	1/1	0.95	0.08	-4.76	50,50,50,50	0
59	MG	AA	1611	1/1	0.98	0.07	-5.04	60,60,60,60	0
59	MG	BA	3005	1/1	0.90	0.11	-5.07	75,75,75,75	0
59	MG	BA	3058	1/1	0.97	0.04	-5.48	47,47,47,47	0
59	MG	DA	3066	1/1	0.96	0.14	-5.50	61,61,61,61	0
59	MG	BA	3023	1/1	0.92	0.10	-5.51	16,16,16,16	0
59	MG	BA	3067	1/1	0.93	0.12	-5.83	17,17,17,17	0
59	MG	CA	1638	1/1	0.90	0.09	-5.99	141,141,141,141	0
59	MG	BA	3108	1/1	0.92	0.09	-6.07	83,83,83,83	0
59	MG	DA	3023	1/1	0.92	0.14	-6.17	111,111,111,111	0
59	MG	BA	3012	1/1	0.97	0.13	-6.67	1,1,1,1	0
59	MG	BA	3016	1/1	0.96	0.09	-6.99	4,4,4,4	0
59	MG	BA	3046	1/1	0.95	0.08	-7.01	12,12,12,12	0
59	MG	DA	3101	1/1	0.94	0.13	-7.20	75,75,75,75	0
59	MG	DA	3055	1/1	0.85	0.11	-7.68	72,72,72,72	0
59	MG	CA	1604	1/1	0.95	0.05	-8.16	57,57,57,57	0
59	MG	AA	1607	1/1	0.91	0.07	-8.24	105,105,105,105	0
59	MG	BA	3094	1/1	0.98	0.06	-24.73	22,22,22,22	0
59	MG	CA	1635	1/1	0.84	0.14	-	201,201,201,201	0
59	MG	DA	3126	1/1	0.67	0.25	-	112,112,112,112	0
59	MG	BA	3125	1/1	0.99	0.14	-	16,16,16,16	0
59	MG	BA	3097	1/1	0.95	0.10	-	33,33,33,33	0
59	MG	BA	3026	1/1	0.97	0.08	-	32,32,32,32	0
59	MG	DA	3028	1/1	0.54	0.63	-	222,222,222,222	0
59	MG	DA	3049	1/1	0.58	0.63	-	192,192,192,192	0
59	MG	DA	3040	1/1	0.77	0.15	-	65,65,65,65	0
59	MG	BB	203	1/1	0.94	0.11	-	34,34,34,34	0
59	MG	DA	3009	1/1	0.91	0.14	-	100,100,100,100	0
59	MG	DA	3007	1/1	0.56	0.62	-	248,248,248,248	0
59	MG	DA	3019	1/1	0.61	0.18	-	192,192,192,192	0
59	MG	AA	1626	1/1	0.79	0.10	-	52,52,52,52	0
59	MG	DA	3120	1/1	0.60	0.20	-	91,91,91,91	0
59	MG	BA	3107	1/1	0.97	0.16	-	12,12,12,12	0
59	MG	AA	1612	1/1	0.95	0.10	-	85,85,85,85	0
59	MG	DA	3086	1/1	0.73	0.39	-	84,84,84,84	0
59	MG	DA	3109	1/1	0.49	0.48	-	184,184,184,184	0
59	MG	DA	3026	1/1	0.63	0.91	-	258,258,258,258	0
59	MG	AA	1639	1/1	0.85	0.12	-	109,109,109,109	0
59	MG	AA	1620	1/1	0.92	0.10	-	126,126,126,126	0
59	MG	CA	1614	1/1	0.81	0.70	-	245,245,245,245	0
59	MG	DA	3029	1/1	0.91	0.94	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1631	1/1	0.89	0.10	-	160,160,160,160	0
59	MG	BA	3076	1/1	0.94	0.10	-	119,119,119,119	0
59	MG	BA	3123	1/1	0.98	0.14	-	11,11,11,11	0
59	MG	DA	3093	1/1	0.92	0.17	-	234,234,234,234	0
59	MG	DA	3114	1/1	0.92	0.10	-	147,147,147,147	0
59	MG	DA	3090	1/1	0.56	0.11	-	78,78,78,78	0
59	MG	BA	3104	1/1	0.98	0.16	-	13,13,13,13	0
59	MG	AA	1601	1/1	0.96	0.10	-	77,77,77,77	0
59	MG	CA	1610	1/1	0.72	0.06	-	151,151,151,151	0
59	MG	CA	1603	1/1	0.60	0.34	-	177,177,177,177	0
59	MG	DA	3013	1/1	0.83	0.38	-	189,189,189,189	0
59	MG	DA	3054	1/1	0.97	0.14	-	70,70,70,70	0
59	MG	BA	3101	1/1	0.95	0.09	-	18,18,18,18	0
59	MG	AA	1624	1/1	0.94	0.15	-	102,102,102,102	0
59	MG	AA	1608	1/1	0.98	0.22	-	47,47,47,47	0
59	MG	CA	1602	1/1	0.81	0.16	-	145,145,145,145	0
59	MG	BA	3087	1/1	0.98	0.12	-	36,36,36,36	0
59	MG	DA	3046	1/1	0.85	0.24	-	125,125,125,125	0
59	MG	BA	3115	1/1	0.92	0.10	-	7,7,7,7	0
59	MG	DA	3004	1/1	0.35	0.17	-	122,122,122,122	0
59	MG	DA	3021	1/1	0.78	0.15	-	83,83,83,83	0
59	MG	AA	1619	1/1	0.77	0.69	-	209,209,209,209	0
59	MG	AA	1632	1/1	0.96	0.07	-	90,90,90,90	0
59	MG	DA	3018	1/1	0.15	0.17	-	125,125,125,125	0
59	MG	BA	3031	1/1	0.90	0.11	-	26,26,26,26	0
59	MG	BA	3001	1/1	0.93	0.09	-	117,117,117,117	0
59	MG	BA	3124	1/1	0.95	0.14	-	33,33,33,33	0
59	MG	BA	3068	1/1	0.77	0.09	-	151,151,151,151	0
59	MG	DA	3058	1/1	0.71	0.32	-	202,202,202,202	0
59	MG	DA	3099	1/1	0.65	0.19	-	164,164,164,164	0
59	MG	AA	1621	1/1	0.91	0.17	-	143,143,143,143	0
59	MG	AA	1614	1/1	0.90	0.17	-	156,156,156,156	0
59	MG	DA	3102	1/1	0.71	0.21	-	87,87,87,87	0
59	MG	BA	3131	1/1	0.90	0.40	-	184,184,184,184	0
59	MG	DA	3001	1/1	0.66	0.09	-	149,149,149,149	0
59	MG	BA	3079	1/1	0.98	0.17	-	11,11,11,11	0
59	MG	BA	3093	1/1	0.98	0.07	-	35,35,35,35	0
59	MG	BA	3015	1/1	0.96	0.17	-	95,95,95,95	0
59	MG	DA	3094	1/1	0.84	0.26	-	134,134,134,134	0
59	MG	AA	1640	1/1	0.95	0.04	-	84,84,84,84	0
59	MG	BA	3113	1/1	0.96	0.09	-	138,138,138,138	0
59	MG	BA	3066	1/1	0.97	0.10	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3039	1/1	0.99	0.16	-	8,8,8,8	0
59	MG	AA	1623	1/1	0.82	0.12	-	89,89,89,89	0
59	MG	BA	3038	1/1	0.99	0.10	-	12,12,12,12	0
59	MG	DA	3056	1/1	0.77	0.18	-	72,72,72,72	0
59	MG	BA	3078	1/1	0.94	0.20	-	31,31,31,31	0
59	MG	BA	3109	1/1	0.96	0.16	-	112,112,112,112	0
59	MG	BA	3020	1/1	1.00	0.12	-	11,11,11,11	0
59	MG	BA	3084	1/1	0.98	0.16	-	3,3,3,3	0
59	MG	AA	1605	1/1	0.95	0.12	-	52,52,52,52	0
59	MG	DA	3063	1/1	0.37	2.20	-	213,213,213,213	0
59	MG	BA	3047	1/1	0.94	0.09	-	151,151,151,151	0
59	MG	BA	3100	1/1	0.98	0.13	-	85,85,85,85	0
59	MG	DA	3060	1/1	0.41	0.61	-	198,198,198,198	0
59	MG	AA	1602	1/1	0.85	0.12	-	152,152,152,152	0
59	MG	DA	3032	1/1	0.72	0.19	-	131,131,131,131	0
59	MG	BA	3063	1/1	0.95	0.13	-	12,12,12,12	0
59	MG	AA	1603	1/1	0.80	0.14	-	131,131,131,131	0
59	MG	AA	1638	1/1	0.84	0.17	-	47,47,47,47	0
59	MG	BA	3030	1/1	0.98	0.17	-	9,9,9,9	0
59	MG	CA	1622	1/1	0.93	0.13	-	190,190,190,190	0
59	MG	BA	3096	1/1	0.96	0.13	-	93,93,93,93	0
59	MG	AA	1628	1/1	0.90	0.35	-	136,136,136,136	0
59	MG	DA	3121	1/1	0.88	0.13	-	122,122,122,122	0
59	MG	DA	3057	1/1	0.89	0.55	-	185,185,185,185	0
59	MG	DA	3031	1/1	0.82	0.18	-	76,76,76,76	0
59	MG	BA	3121	1/1	0.94	0.13	-	35,35,35,35	0
59	MG	DA	3077	1/1	0.59	0.19	-	123,123,123,123	0
59	MG	DA	3003	1/1	0.65	0.81	-	229,229,229,229	0
59	MG	CA	1637	1/1	0.76	0.11	-	170,170,170,170	0
59	MG	DA	3092	1/1	0.25	0.25	-	119,119,119,119	0
59	MG	DA	3015	1/1	0.63	0.75	-	176,176,176,176	0
59	MG	BA	3059	1/1	0.88	0.33	-	129,129,129,129	0
59	MG	CA	1629	1/1	0.91	0.24	-	126,126,126,126	0
59	MG	BA	3011	1/1	0.96	0.21	-	126,126,126,126	0
59	MG	BA	3092	1/1	0.96	0.07	-	70,70,70,70	0
59	MG	DA	3005	1/1	-0.02	0.50	-	284,284,284,284	0
59	MG	DA	3033	1/1	0.77	0.32	-	132,132,132,132	0
59	MG	BA	3004	1/1	0.87	0.24	-	156,156,156,156	0
59	MG	DA	3082	1/1	0.67	0.19	-	132,132,132,132	0
59	MG	CA	1623	1/1	0.80	0.16	-	121,121,121,121	0
59	MG	DC	302	1/1	0.91	0.31	-	159,159,159,159	0
59	MG	DA	3118	1/1	0.85	0.10	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3064	1/1	0.66	0.66	-	280,280,280,280	0
59	MG	CA	1608	1/1	0.80	0.17	-	44,44,44,44	0
59	MG	BA	3010	1/1	0.92	0.07	-	17,17,17,17	0
59	MG	BA	3056	1/1	0.97	0.31	-	219,219,219,219	0
59	MG	DA	3070	1/1	0.85	0.13	-	60,60,60,60	0
59	MG	BA	3117	1/1	0.71	0.26	-	173,173,173,173	0
59	MG	DA	3080	1/1	0.91	0.11	-	152,152,152,152	0
59	MG	CA	1620	1/1	0.73	0.15	-	164,164,164,164	0
59	MG	DA	3010	1/1	0.63	0.57	-	195,195,195,195	0
59	MG	DA	3113	1/1	0.76	0.12	-	121,121,121,121	0
59	MG	DA	3132	1/1	0.62	0.88	-	185,185,185,185	0
59	MG	CA	1619	1/1	0.53	0.34	-	210,210,210,210	0
59	MG	CA	1605	1/1	0.98	0.14	-	32,32,32,32	0
59	MG	DA	3045	1/1	0.49	0.25	-	160,160,160,160	0
59	MG	BA	3042	1/1	0.99	0.11	-	16,16,16,16	0
59	MG	DA	3130	1/1	0.41	3.19	-	280,280,280,280	0
59	MG	BA	3044	1/1	0.99	0.06	-	43,43,43,43	0
59	MG	DA	3047	1/1	0.51	0.21	-	142,142,142,142	0
59	MG	BA	3075	1/1	0.97	0.06	-	26,26,26,26	0
59	MG	DA	3022	1/1	0.56	0.38	-	173,173,173,173	0
59	MG	BB	201	1/1	0.85	0.28	-	228,228,228,228	0
59	MG	AA	1636	1/1	0.94	0.32	-	199,199,199,199	0
59	MG	BA	3045	1/1	0.87	0.14	-	30,30,30,30	0
59	MG	BA	3098	1/1	0.97	0.13	-	26,26,26,26	0
59	MG	BA	3082	1/1	0.98	0.11	-	109,109,109,109	0
59	MG	BA	3036	1/1	0.95	0.34	-	187,187,187,187	0
59	MG	BA	3090	1/1	0.89	0.14	-	120,120,120,120	0
59	MG	DA	3034	1/1	0.95	0.17	-	78,78,78,78	0
59	MG	DA	3125	1/1	0.68	0.36	-	152,152,152,152	0
59	MG	DA	3008	1/1	0.74	0.17	-	112,112,112,112	0
59	MG	BA	3111	1/1	0.97	0.15	-	38,38,38,38	0
59	MG	DA	3071	1/1	0.75	0.18	-	74,74,74,74	0
59	MG	BA	3083	1/1	0.95	0.17	-	37,37,37,37	0
59	MG	BA	3065	1/1	0.97	0.11	-	20,20,20,20	0
59	MG	BA	3091	1/1	0.95	0.07	-	49,49,49,49	0
59	MG	CA	1634	1/1	0.95	0.09	-	74,74,74,74	0
59	MG	CA	1615	1/1	0.70	0.30	-	170,170,170,170	0
59	MG	DA	3085	1/1	0.89	0.44	-	132,132,132,132	0
59	MG	DA	3041	1/1	0.76	0.15	-	110,110,110,110	0
59	MG	DA	3016	1/1	0.07	1.15	-	214,214,214,214	0
59	MG	DA	3006	1/1	0.70	0.10	-	176,176,176,176	0
59	MG	DA	3111	1/1	0.35	0.19	-	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3048	1/1	0.95	0.17	-	101,101,101,101	0
59	MG	AA	1642	1/1	0.98	0.14	-	36,36,36,36	0
59	MG	BA	3080	1/1	0.98	0.04	-	26,26,26,26	0
59	MG	DA	3088	1/1	0.68	0.17	-	170,170,170,170	0
59	MG	DA	3042	1/1	0.87	0.19	-	99,99,99,99	0
59	MG	DA	3107	1/1	0.93	0.24	-	91,91,91,91	0
59	MG	BA	3025	1/1	0.89	0.56	-	165,165,165,165	0
59	MG	BA	3052	1/1	0.98	0.16	-	46,46,46,46	0
59	MG	BA	3089	1/1	0.84	0.13	-	95,95,95,95	0
59	MG	DA	3020	1/1	0.44	0.63	-	240,240,240,240	0
59	MG	DA	3059	1/1	0.76	0.39	-	197,197,197,197	0
59	MG	DA	3096	1/1	0.83	0.14	-	93,93,93,93	0
59	MG	BA	3086	1/1	0.95	0.12	-	134,134,134,134	0
59	MG	BA	3054	1/1	0.98	0.09	-	58,58,58,58	0
59	MG	DA	3116	1/1	0.76	0.12	-	54,54,54,54	0
59	MG	DA	3036	1/1	0.77	0.58	-	222,222,222,222	0
59	MG	DA	3089	1/1	0.71	0.18	-	100,100,100,100	0
59	MG	AA	1630	1/1	0.84	0.36	-	189,189,189,189	0
59	MG	DA	3110	1/1	0.47	0.38	-	146,146,146,146	0
59	MG	DA	3067	1/1	0.81	0.21	-	64,64,64,64	0
59	MG	CA	1626	1/1	0.80	0.39	-	196,196,196,196	0
59	MG	AA	1627	1/1	0.75	0.37	-	137,137,137,137	0
59	MG	AA	1618	1/1	0.94	0.18	-	87,87,87,87	0
59	MG	BA	3074	1/1	0.94	0.17	-	85,85,85,85	0
59	MG	BA	3073	1/1	0.94	0.17	-	17,17,17,17	0
59	MG	DA	3119	1/1	0.90	0.11	-	67,67,67,67	0
59	MG	BB	204	1/1	0.93	0.08	-	23,23,23,23	0
59	MG	BA	3034	1/1	0.91	0.28	-	197,197,197,197	0
59	MG	BA	3033	1/1	0.95	0.21	-	14,14,14,14	0
59	MG	BA	3014	1/1	0.98	0.21	-	44,44,44,44	0
59	MG	DJ	201	1/1	-0.24	1.06	-	312,312,312,312	0
59	MG	DA	3043	1/1	0.47	0.28	-	179,179,179,179	0
59	MG	BA	3043	1/1	0.96	0.06	-	18,18,18,18	0
59	MG	DA	3038	1/1	0.67	0.12	-	203,203,203,203	0
59	MG	BA	3006	1/1	0.98	0.07	-	31,31,31,31	0
59	MG	BA	3120	1/1	0.97	0.21	-	3,3,3,3	0
59	MG	DA	3073	1/1	0.87	0.07	-	148,148,148,148	0
59	MG	CA	1633	1/1	0.93	0.14	-	138,138,138,138	0
59	MG	BA	3088	1/1	0.94	0.10	-	62,62,62,62	0
59	MG	DA	3014	1/1	0.66	0.37	-	133,133,133,133	0
59	MG	DA	3081	1/1	0.90	0.28	-	78,78,78,78	0
59	MG	DA	3035	1/1	0.75	0.14	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3076	1/1	0.84	0.25	-	149,149,149,149	0
59	MG	DA	3127	1/1	0.58	0.85	-	228,228,228,228	0
59	MG	DA	3062	1/1	0.72	0.56	-	213,213,213,213	0
59	MG	BA	3055	1/1	0.89	0.35	-	215,215,215,215	0
59	MG	BA	3019	1/1	0.99	0.18	-	13,13,13,13	0
59	MG	DA	3117	1/1	0.90	0.20	-	73,73,73,73	0
59	MG	BA	3060	1/1	0.94	0.31	-	188,188,188,188	0
59	MG	BA	3009	1/1	0.96	0.17	-	38,38,38,38	0
59	MG	BA	3003	1/1	0.87	0.10	-	58,58,58,58	0
59	MG	BA	3061	1/1	0.97	0.17	-	11,11,11,11	0
59	MG	BA	3032	1/1	0.96	0.12	-	25,25,25,25	0
59	MG	AA	1610	1/1	0.94	0.11	-	201,201,201,201	0
59	MG	BA	3029	1/1	0.97	0.10	-	52,52,52,52	0
59	MG	BA	3069	1/1	0.93	0.25	-	136,136,136,136	0
59	MG	DA	3074	1/1	0.10	0.96	-	247,247,247,247	0
59	MG	DA	3091	1/1	0.30	0.37	-	154,154,154,154	0
59	MG	CA	1625	1/1	0.85	0.17	-	48,48,48,48	0
59	MG	CA	1632	1/1	0.97	0.09	-	65,65,65,65	0
59	MG	DA	3122	1/1	0.83	0.15	-	94,94,94,94	0
59	MG	DA	3087	1/1	0.76	0.28	-	152,152,152,152	0
59	MG	DA	3030	1/1	0.74	0.31	-	104,104,104,104	0
59	MG	CE	201	1/1	0.84	0.27	-	132,132,132,132	0
59	MG	BA	3072	1/1	0.97	0.21	-	97,97,97,97	0
59	MG	DA	3053	1/1	0.77	0.25	-	98,98,98,98	0
59	MG	BA	3133	1/1	0.94	0.26	-	146,146,146,146	0
59	MG	DA	3011	1/1	0.74	0.39	-	145,145,145,145	0
59	MG	DA	3078	1/1	0.69	0.24	-	182,182,182,182	0
59	MG	AA	1637	1/1	0.88	0.12	-	96,96,96,96	0
59	MG	AA	1615	1/1	0.96	0.10	-	128,128,128,128	0
59	MG	BA	3035	1/1	0.97	0.10	-	5,5,5,5	0
59	MG	DA	3098	1/1	0.72	0.33	-	151,151,151,151	0
59	MG	BA	3007	1/1	0.80	0.15	-	104,104,104,104	0
59	MG	DA	3123	1/1	0.71	0.30	-	183,183,183,183	0
59	MG	BA	3071	1/1	0.95	0.11	-	7,7,7,7	0
59	MG	BA	3085	1/1	0.85	0.20	-	124,124,124,124	0
59	MG	BA	3018	1/1	0.80	0.14	-	44,44,44,44	0
59	MG	BA	3041	1/1	0.98	0.17	-	21,21,21,21	0
59	MG	BA	3051	1/1	0.96	0.17	-	24,24,24,24	0
59	MG	CA	1601	1/1	0.79	0.10	-	120,120,120,120	0
59	MG	BA	3126	1/1	0.98	0.15	-	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.