



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:58 am BST

PDB ID : 4V7U  
Title : Crystal structure of the E. coli ribosome bound to erythromycin.  
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.  
Deposited on : 2010-08-15  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

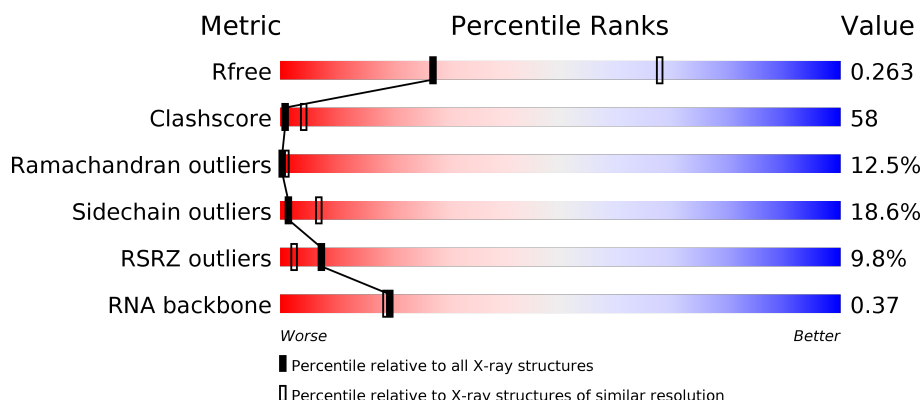
# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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>15%</div> <div>49%</div> <div>20%</div> <div>17%</div> </div>
1	CA	1533	<div> <div>3%</div> <div>12%</div> <div>48%</div> <div>25%</div> <div>14%</div> </div>
2	AB	218	<div> <div>33%</div> <div>21%</div> <div>54%</div> <div>23%</div> </div>
2	CB	218	<div> <div>31%</div> <div>22%</div> <div>63%</div> <div>14%</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2904	
22	DA	2904	
23	BB	118	
23	DB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	178	
27	DF	178	

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

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

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
53	MG	BA	3130	-	-	-	X
53	MG	CA	1614	-	-	-	X
53	MG	CA	1628	-	-	-	X
53	MG	DA	3003	-	-	-	X
53	MG	DA	3007	-	-	-	X
53	MG	DA	3010	-	-	-	X
53	MG	DA	3013	-	-	-	X
53	MG	DA	3015	-	-	-	X
53	MG	DA	3016	-	-	-	X
53	MG	DA	3020	-	-	-	X
53	MG	DA	3026	-	-	-	X
53	MG	DA	3028	-	-	-	X
53	MG	DA	3033	-	-	-	X
53	MG	DA	3043	-	-	-	X
53	MG	DA	3045	-	-	-	X
53	MG	DA	3057	-	-	-	X
53	MG	DA	3058	-	-	-	X
53	MG	DA	3062	-	-	-	X
53	MG	DA	3063	-	-	-	X
53	MG	DA	3064	-	-	-	X
53	MG	DA	3074	-	-	-	X
53	MG	DA	3078	-	-	-	X
53	MG	DA	3109	-	-	-	X
53	MG	DA	3111	-	-	-	X
53	MG	DA	3127	-	-	-	X
53	MG	DA	3130	-	-	-	X
53	MG	DA	3133	-	-	-	X
53	MG	DJ	201	-	-	-	X

## 2 Entry composition [i](#)

There are 56 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			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

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

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

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

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

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



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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	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			
16	CP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
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			
23	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	178	Total	C	N	O	S	0	0	1
			1411	899	250	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			
			596	367	120	108	1	0	0	0
44	DW	79	Total	C	N	O	S			
			596	367	120	108	1	0	0	0

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

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

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

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

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

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



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

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

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

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

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

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

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

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

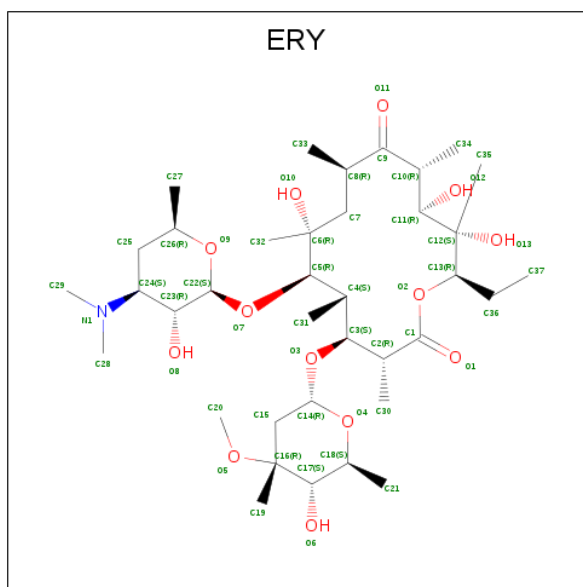
- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	BB	4	Total Mg 4 4	0	0
53	BA	135	Total Mg 135 135	0	0
53	CA	42	Total Mg 42 42	0	0
53	DJ	1	Total Mg 1 1	0	0
53	AA	41	Total Mg 41 41	0	0
53	AN	2	Total Mg 2 2	0	0
53	DA	133	Total Mg 133 133	0	0
53	DC	2	Total Mg 2 2	0	0
53	DB	1	Total Mg 1 1	0	0

- Molecule 54 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BA	1	Total C N O 51 37 1 13	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	197	Total O 197 197	0	0
56	AE	1	Total O 1 1	0	0
56	AL	1	Total O 1 1	0	0
56	AN	7	Total O 7 7	0	0
56	AT	1	Total O 1 1	0	0
56	AU	1	Total O 1 1	0	0
56	BA	605	Total O 605 605	0	0
56	BB	19	Total O 19 19	0	0
56	BC	7	Total O 7 7	0	0
56	BD	3	Total O 3 3	0	0
56	BE	1	Total O 1 1	0	0
56	BL	4	Total O 4 4	0	0
56	BN	2	Total O 2 2	0	0
56	BR	1	Total O 1 1	0	0
56	BT	2	Total O 2 2	0	0
56	BV	1	Total O 1 1	0	0
56	B3	3	Total O 3 3	0	0
56	B4	2	Total O 2 2	0	0

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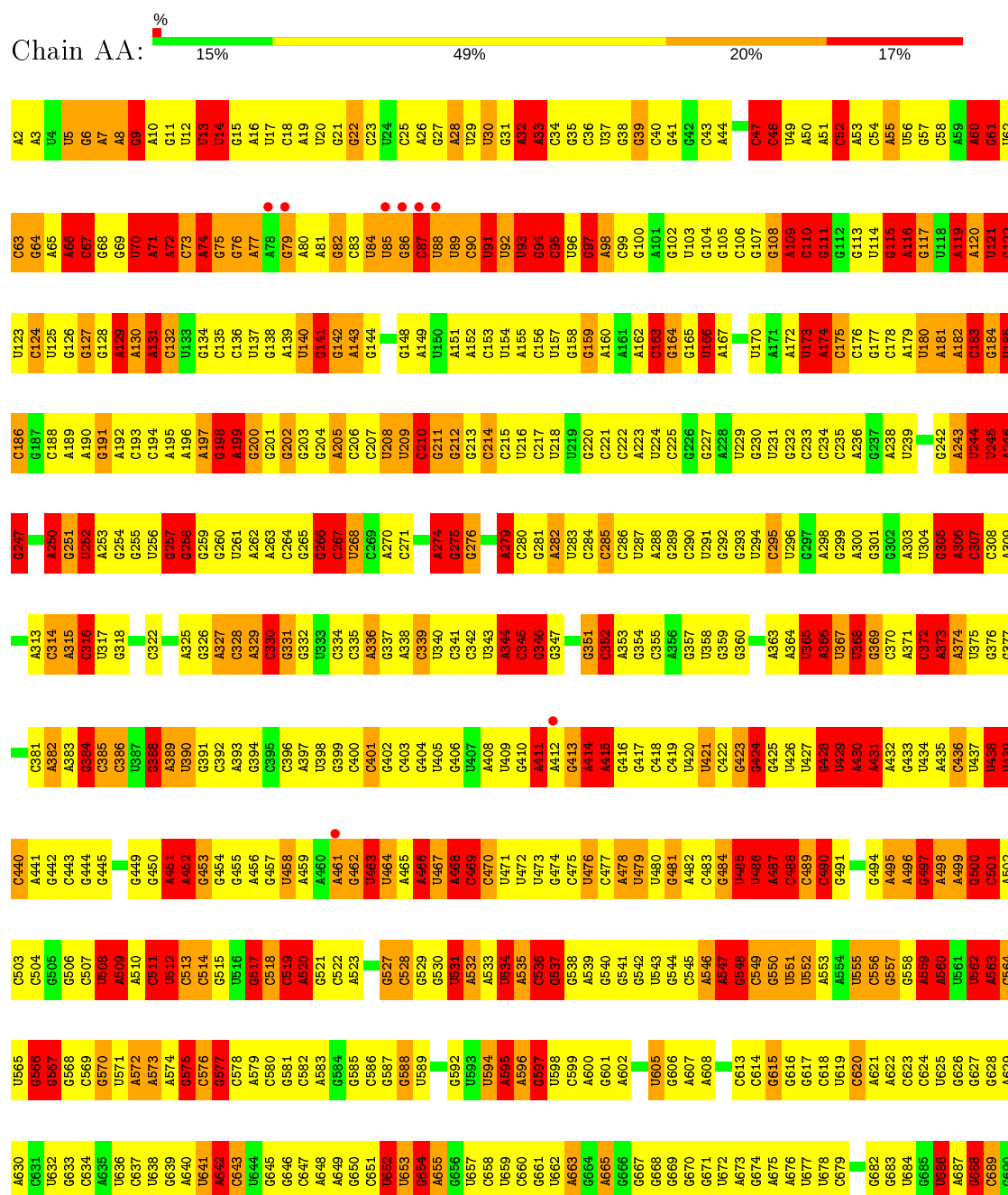
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	195	Total 195	O 195	0	0
56	CE	3	Total 3	O 3	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	3	Total 3	O 3	0	0
56	CT	4	Total 4	O 4	0	0
56	CU	1	Total 1	O 1	0	0
56	DA	600	Total 600	O 600	0	0
56	DB	3	Total 3	O 3	0	0
56	DC	13	Total 13	O 13	0	0
56	DD	2	Total 2	O 2	0	0
56	DE	4	Total 4	O 4	0	0
56	DJ	3	Total 3	O 3	0	0
56	DL	4	Total 4	O 4	0	0
56	DN	2	Total 2	O 2	0	0
56	DT	2	Total 2	O 2	0	0
56	DU	2	Total 2	O 2	0	0
56	DV	2	Total 2	O 2	0	0
56	D2	1	Total 1	O 1	0	0
56	D3	1	Total 1	O 1	0	0
56	D4	4	Total 4	O 4	0	0

### 3 Residue-property plots

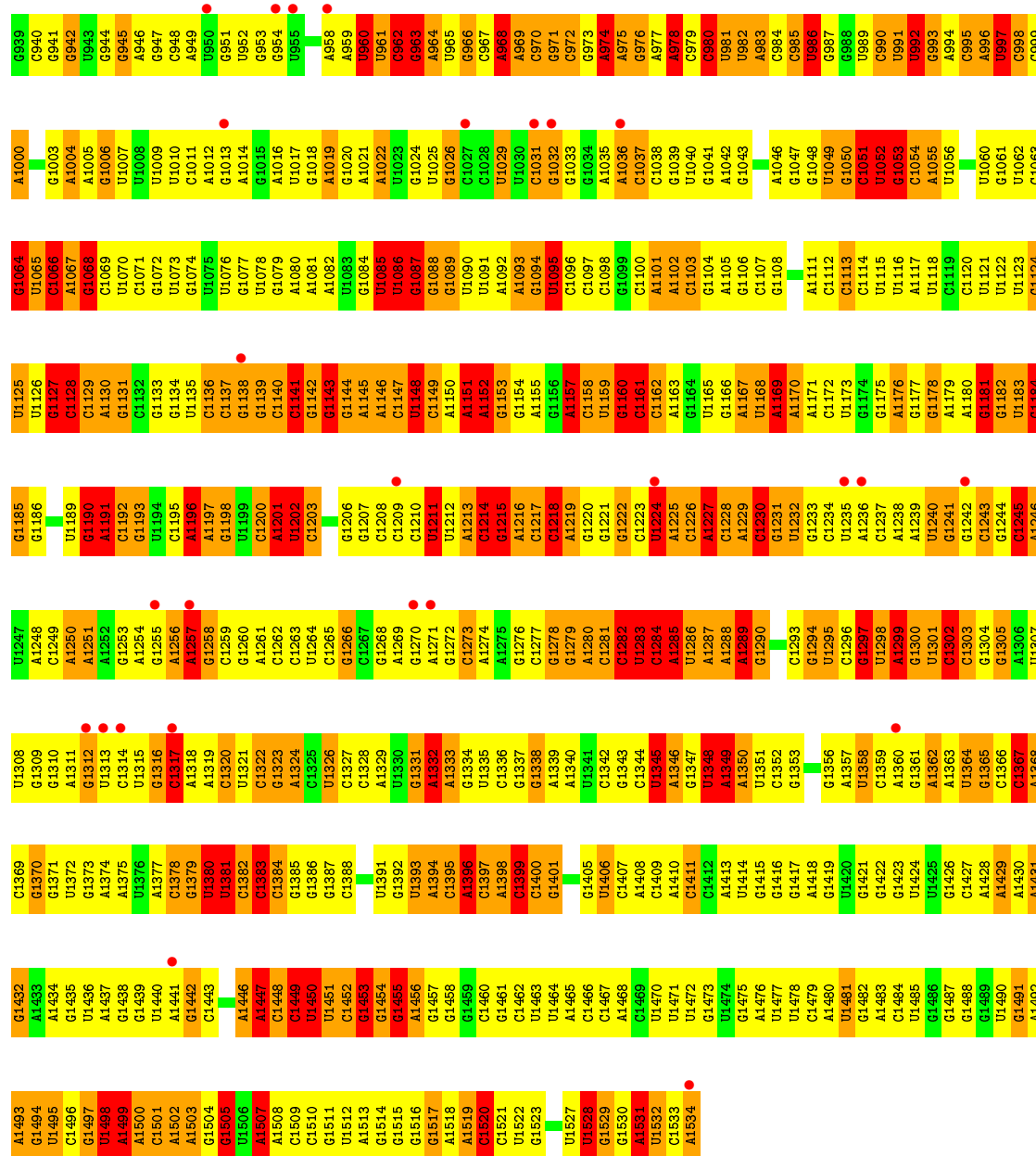
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA

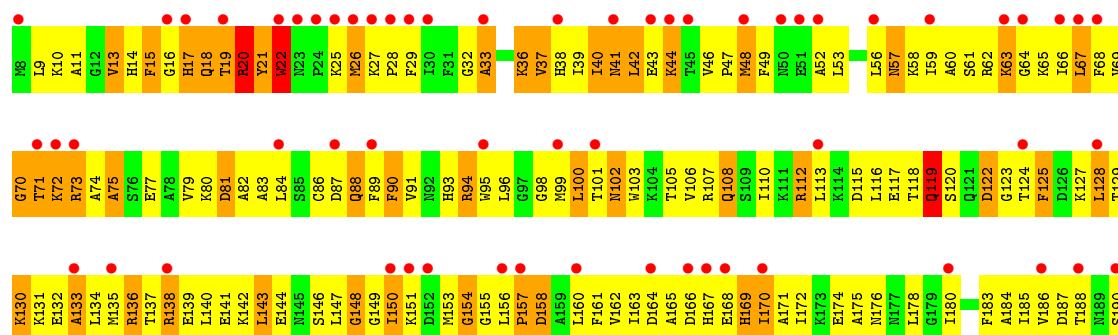


G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575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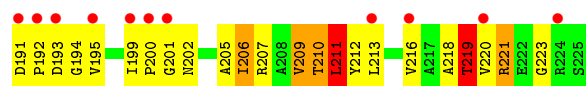




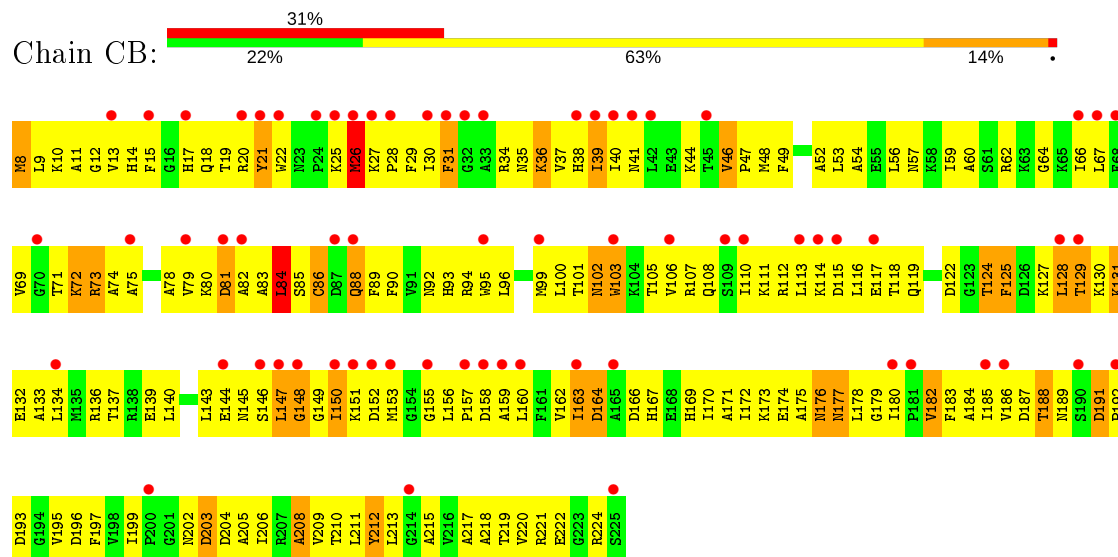
## • Molecule 2: 30S ribosomal protein S2



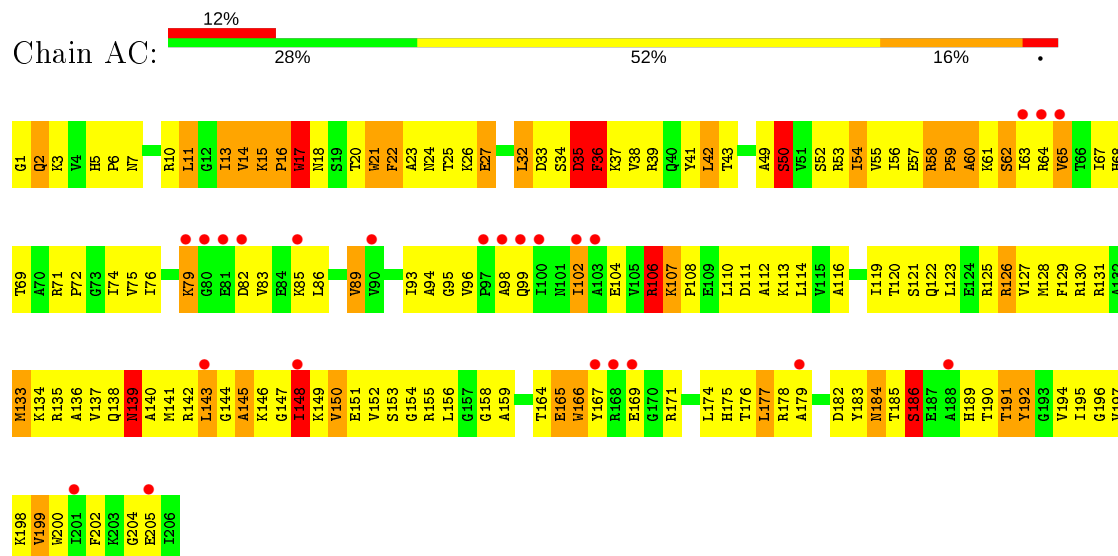




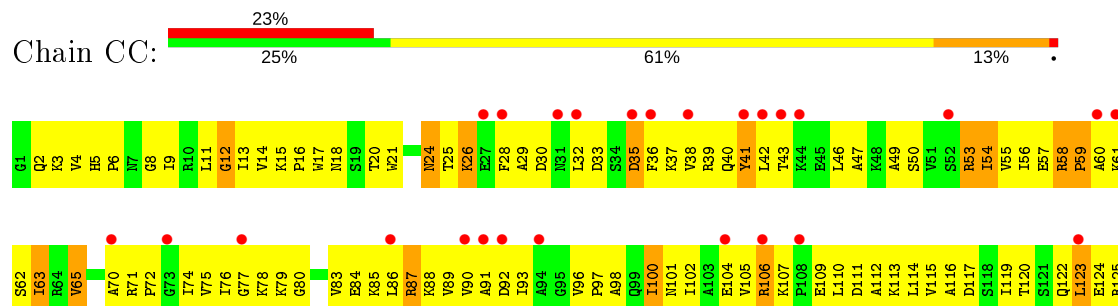
• Molecule 2: 30S ribosomal protein S2

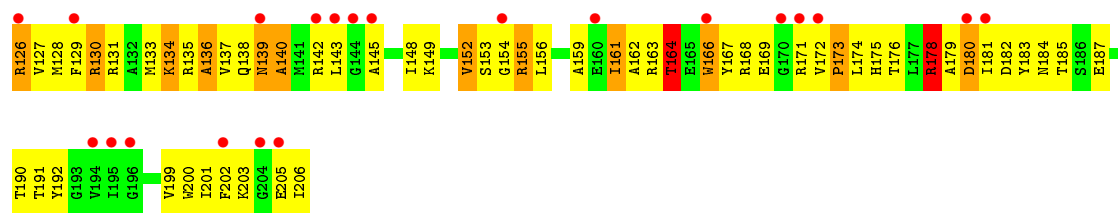


• Molecule 3: 30S ribosomal protein S3

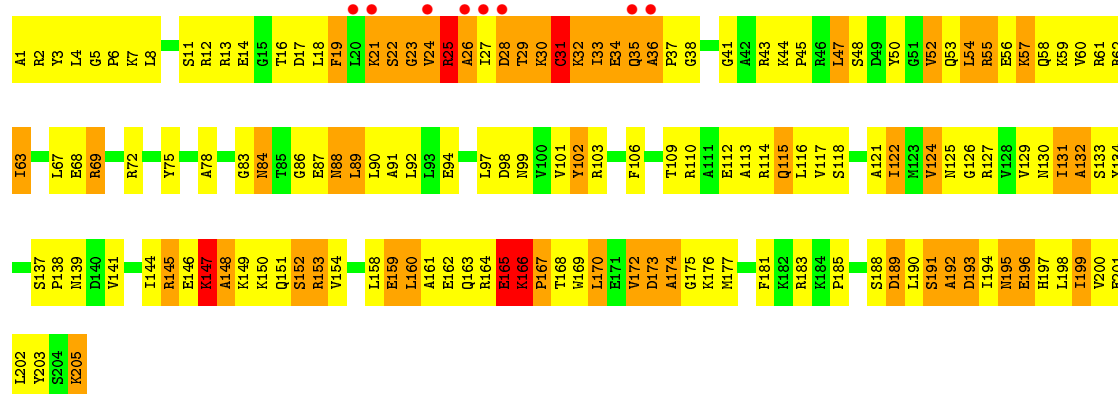


• Molecule 3: 30S ribosomal protein S3

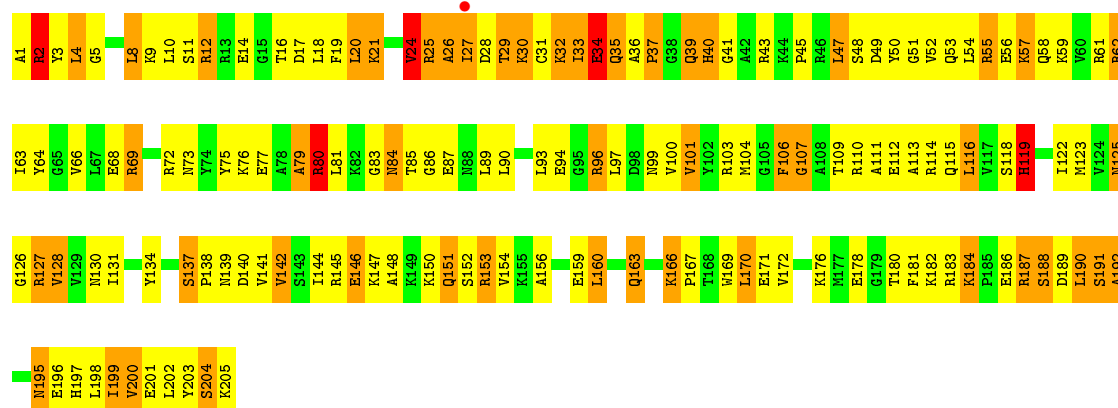




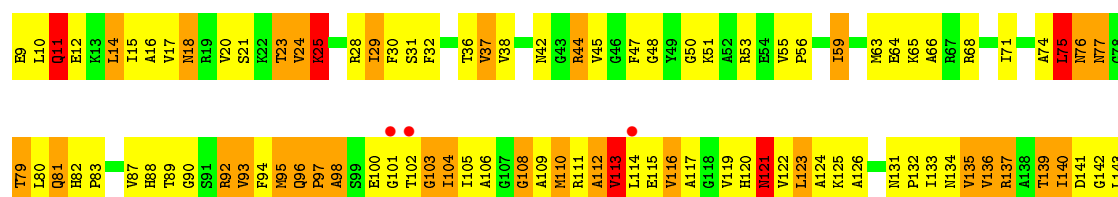
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

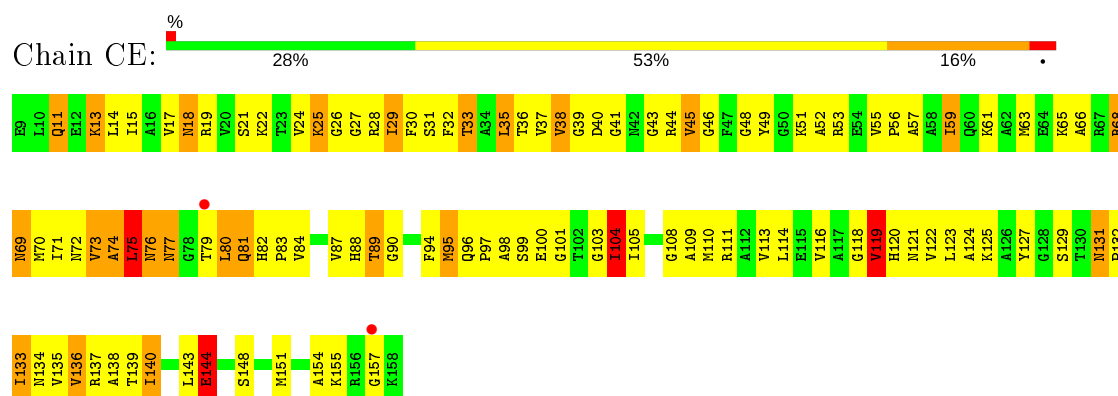


• Molecule 5: 30S ribosomal protein S5

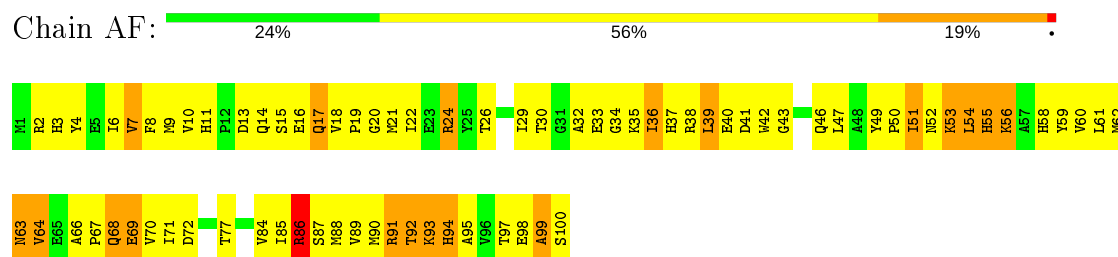


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M147  
S148  
P149  
E150  
M151  
V152  
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A154  
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G157  
K158

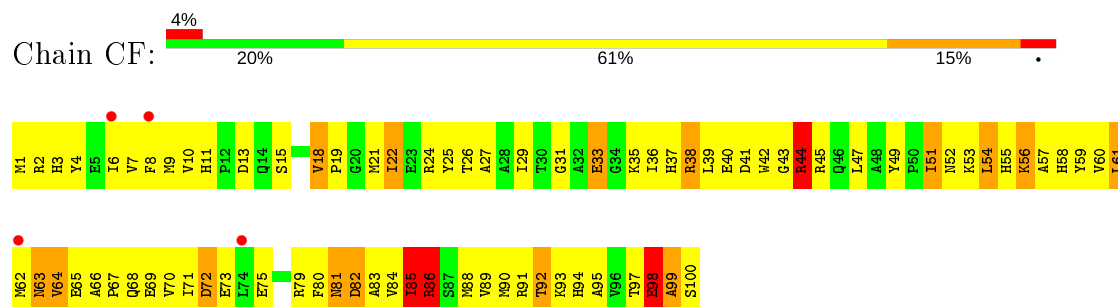
• Molecule 5: 30S ribosomal protein S5



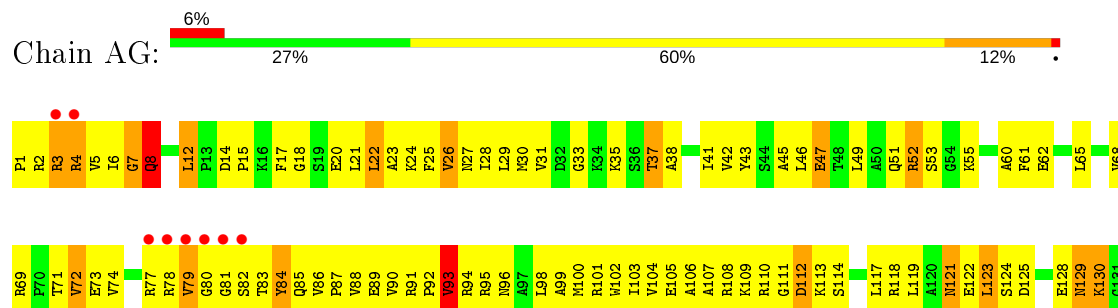
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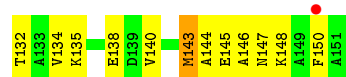


• Molecule 6: 30S ribosomal protein S6

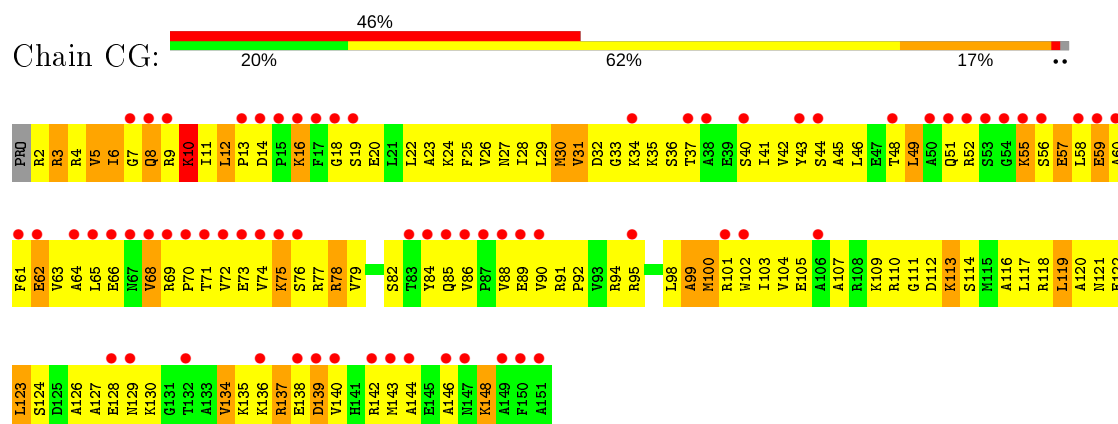


• Molecule 7: 30S ribosomal protein S7

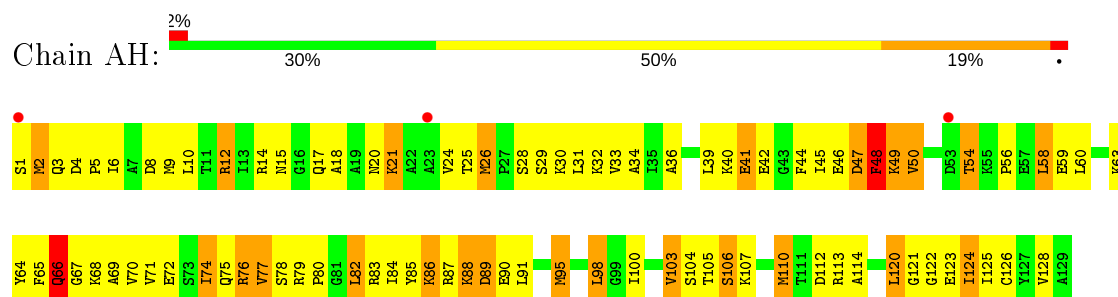




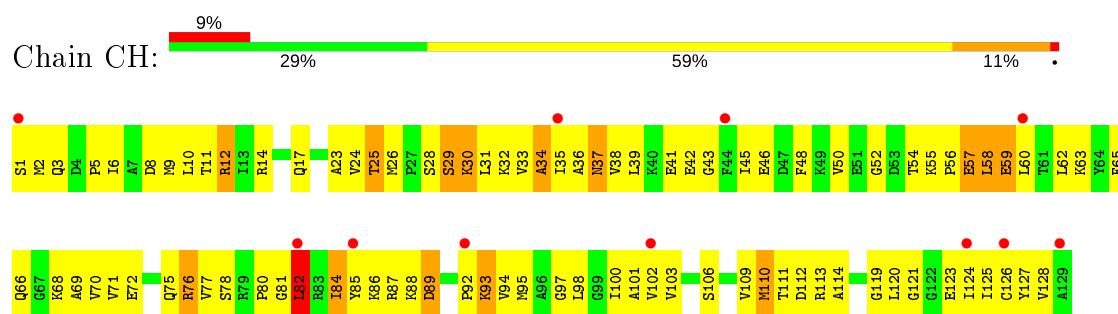
- Molecule 7: 30S ribosomal protein S7



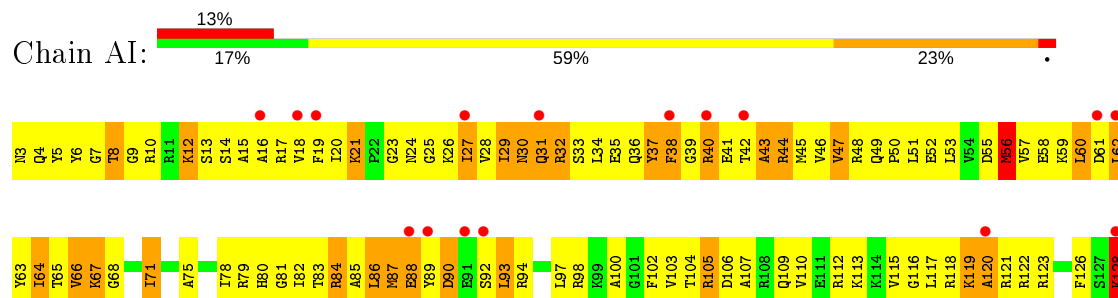
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

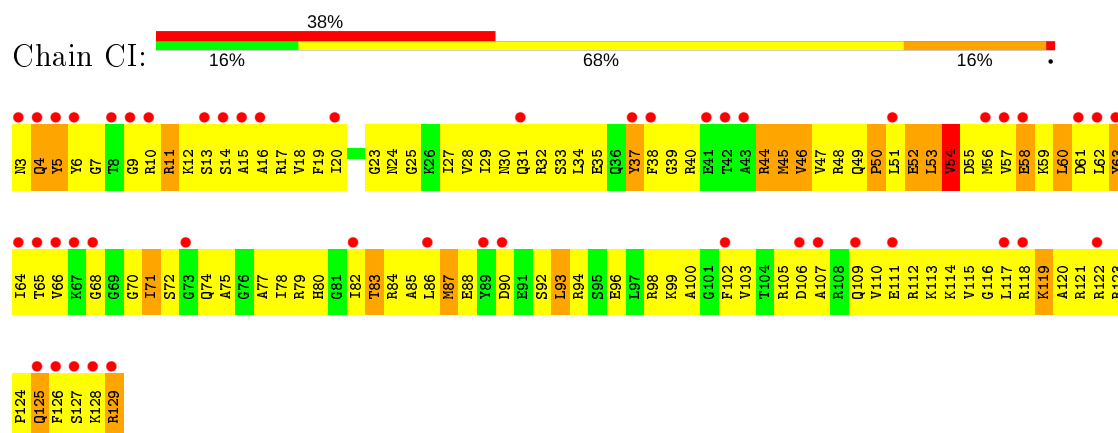


- Molecule 9: 30S ribosomal protein S9

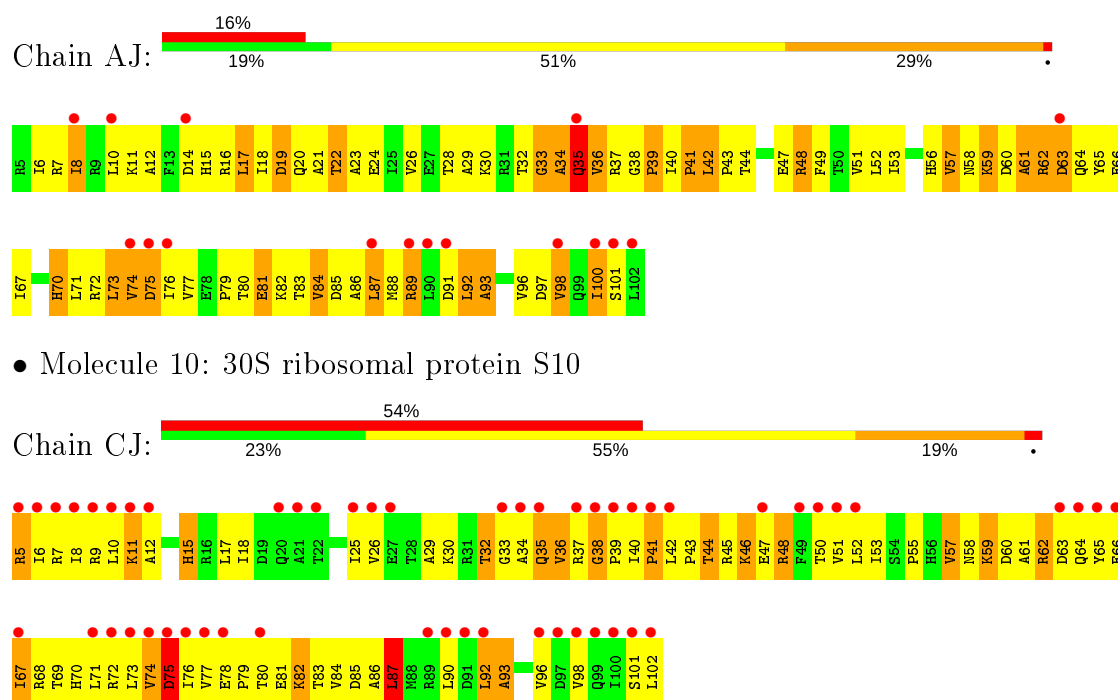


R129

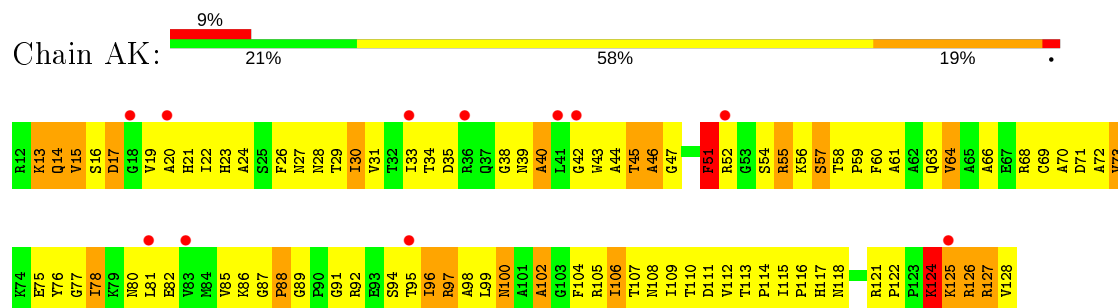
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10



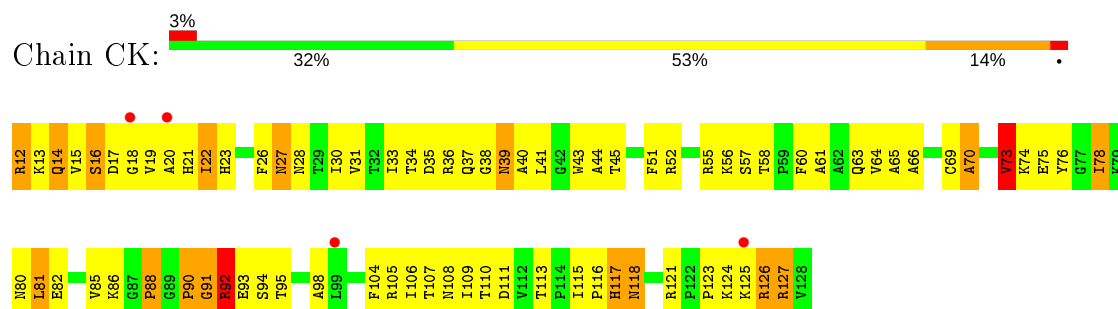
- Molecule 10: 30S ribosomal protein S10



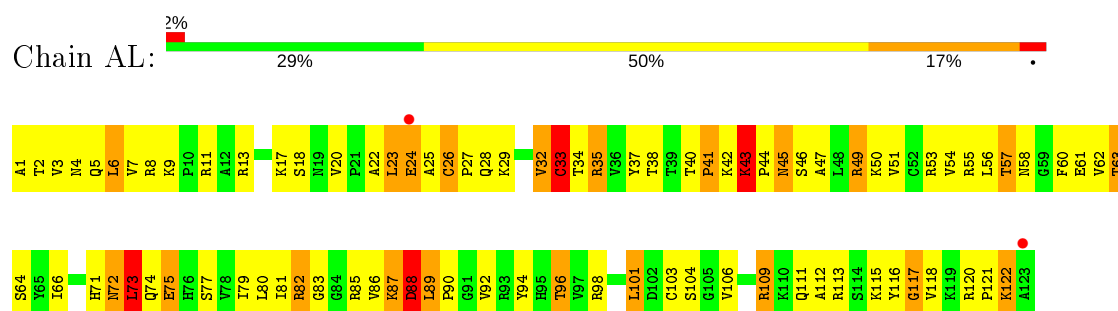
- Molecule 11: 30S ribosomal protein S11



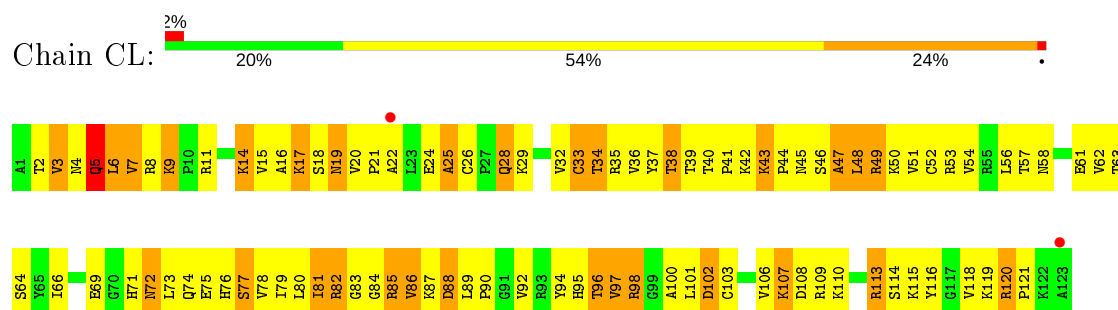
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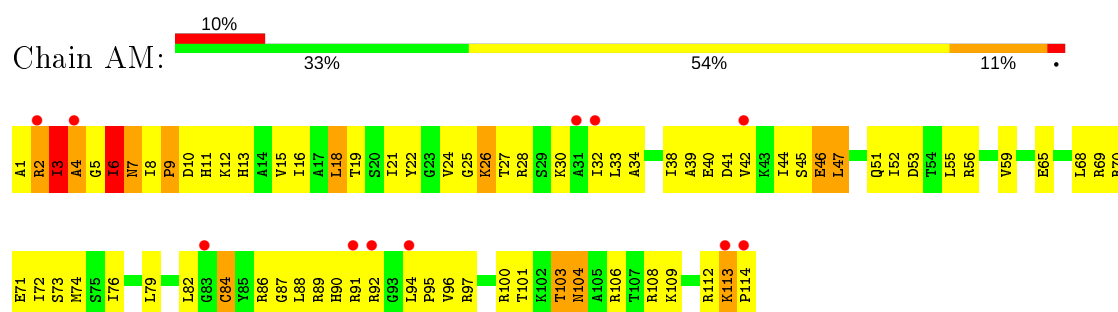
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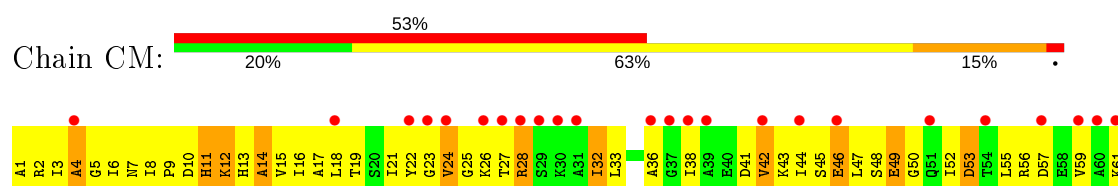
- Molecule 12: 30S ribosomal protein S12

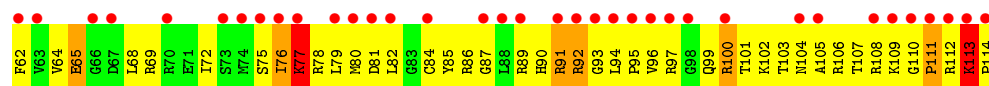


- Molecule 13: 30S ribosomal protein S13

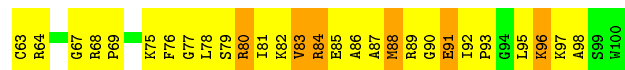


- Molecule 13: 30S ribosomal protein S13

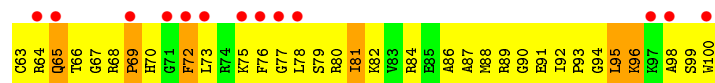
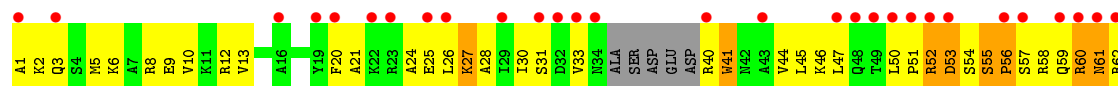




• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

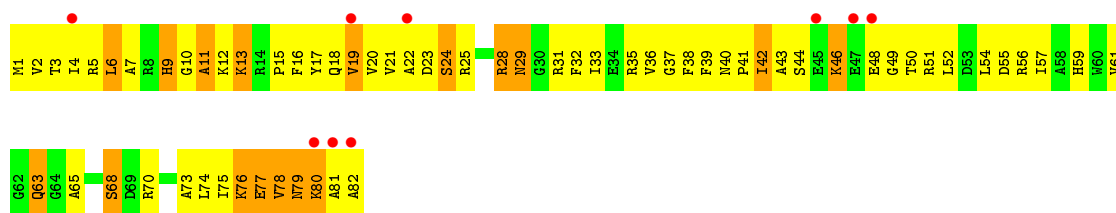


• Molecule 15: 30S ribosomal protein S15

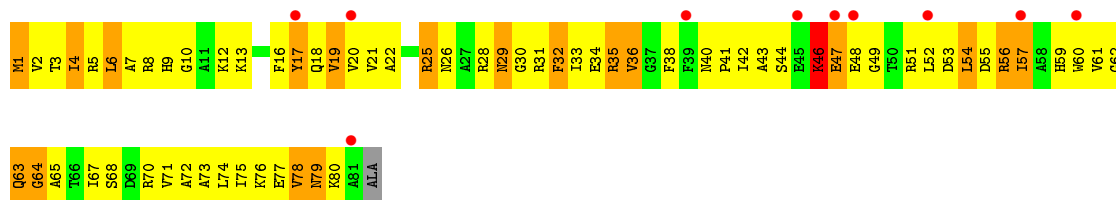


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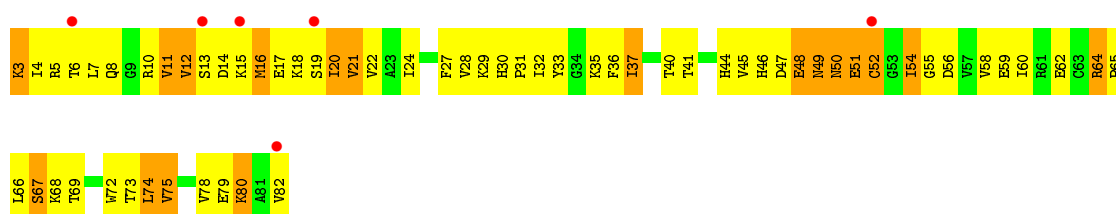




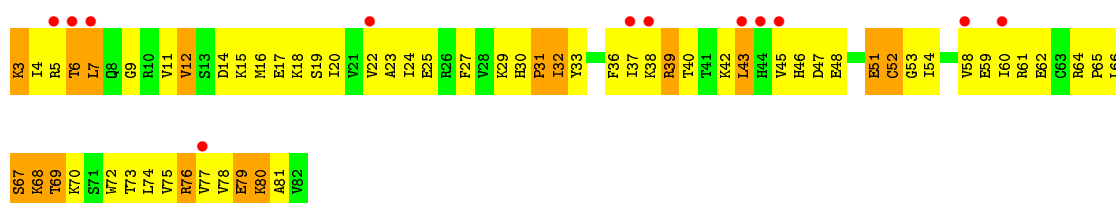
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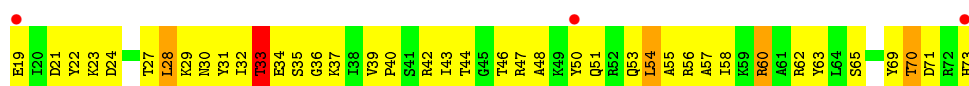
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18



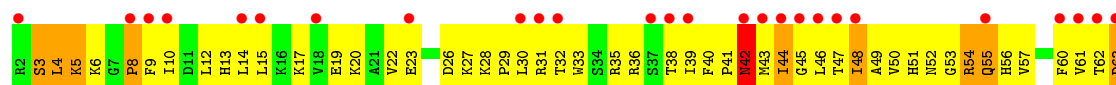
• Molecule 18: 30S ribosomal protein S18



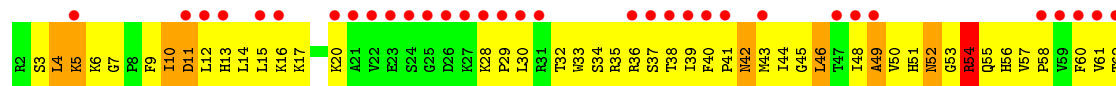




• Molecule 19: 30S ribosomal protein S19



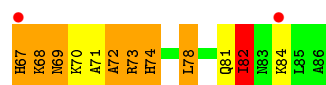
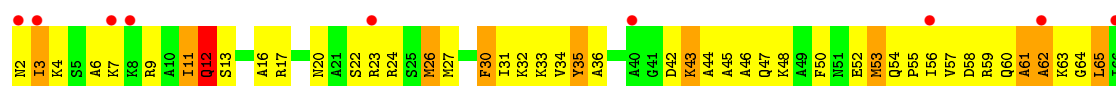
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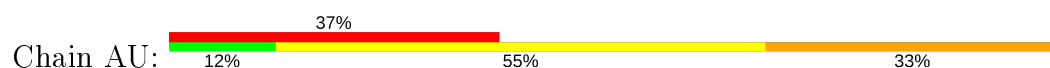
• Molecule 20: 30S ribosomal protein S20

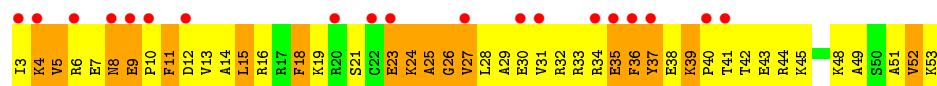


• Molecule 20: 30S ribosomal protein S20

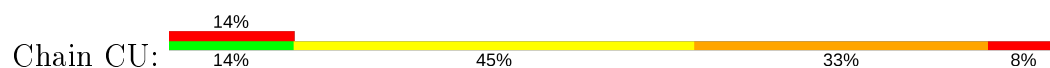


• Molecule 21: 30S ribosomal protein S21

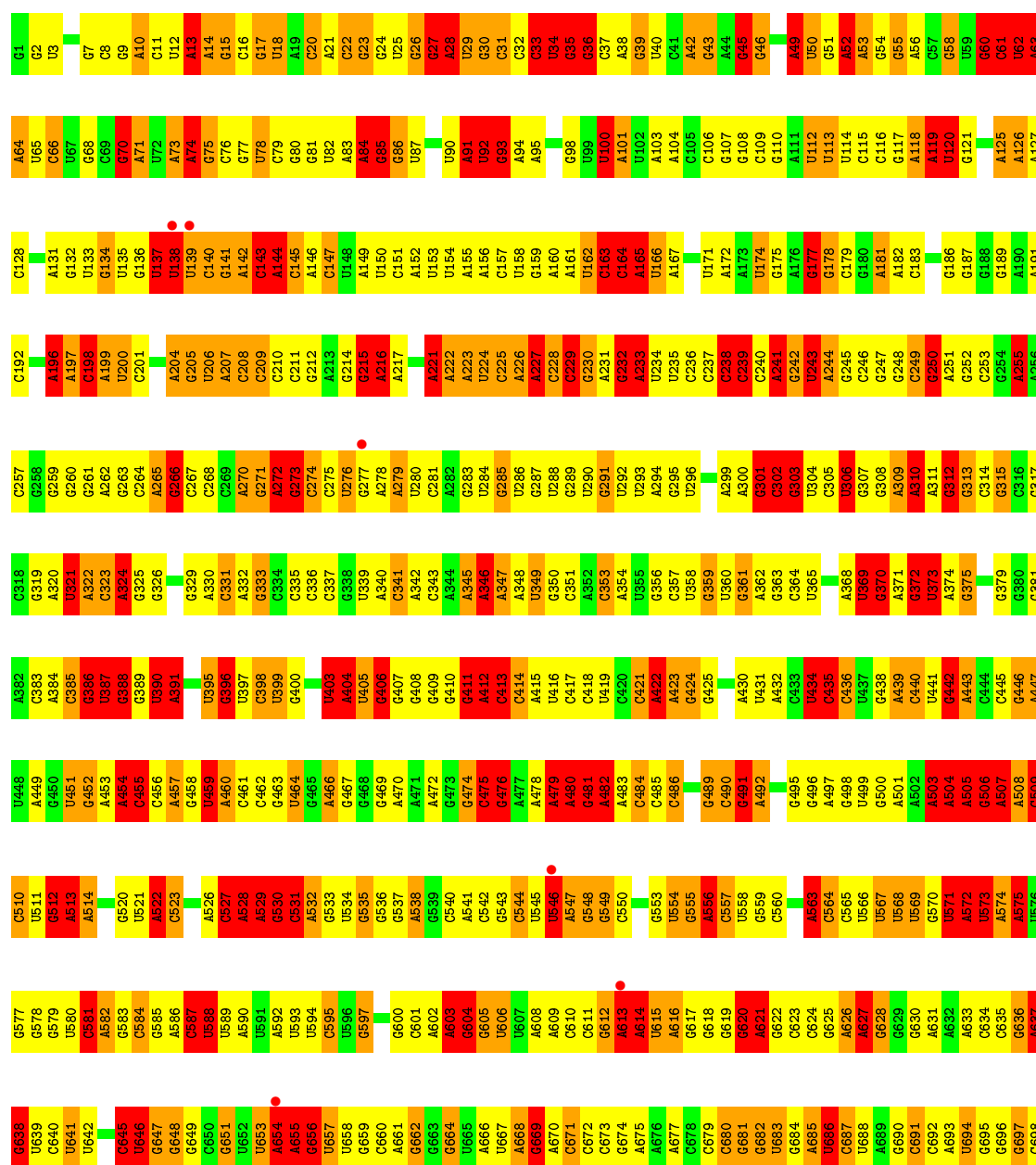
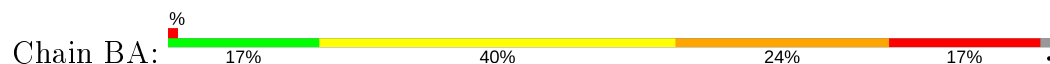




- Molecule 21: 30S ribosomal protein S21

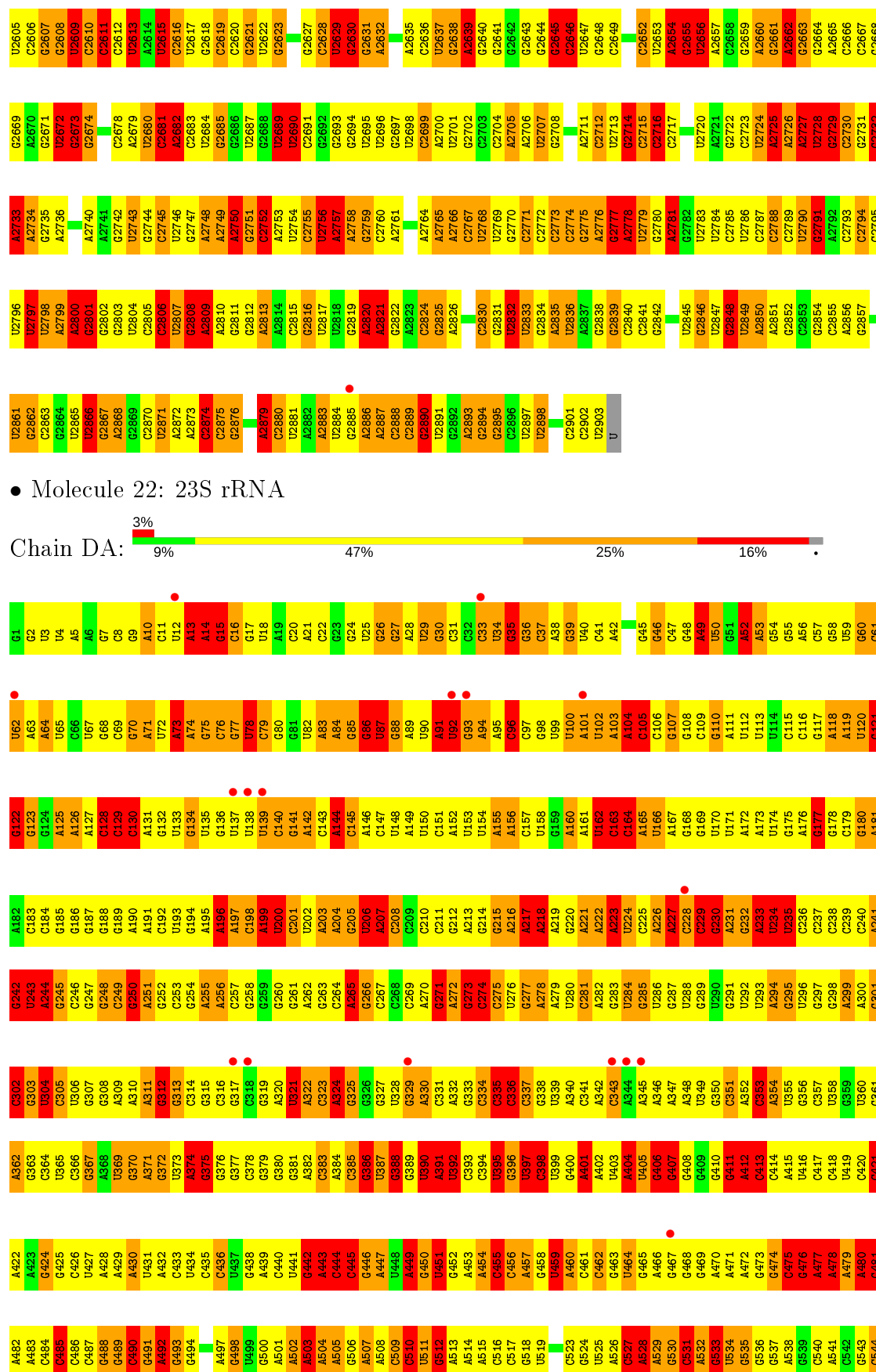


- Molecule 22: 23S rRNA



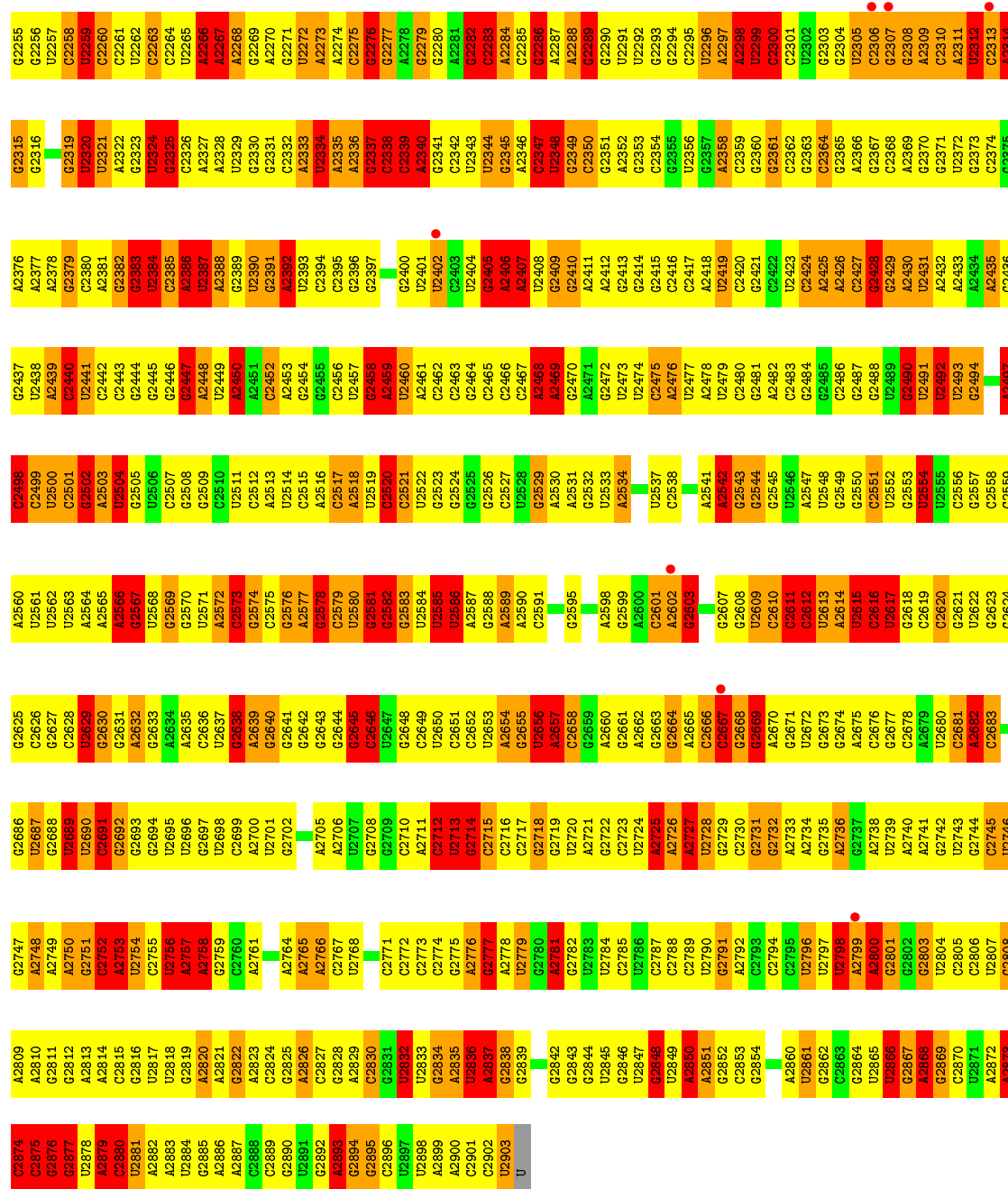
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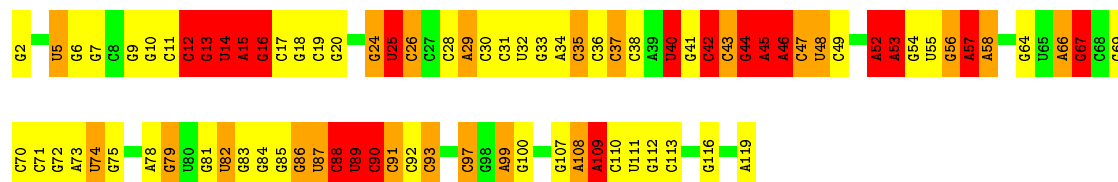
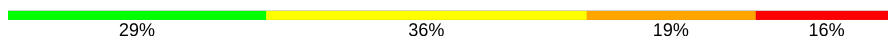
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U2243	A	G	C2063	C2001	G1941	A1877	A1815	A1755	G1695	A1635	C1574	G1452	G1452
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U2245	A	G	C2065	U1943	U1944	C1879	G1817	A1757	G1697	A1637	U1576	G1454	G1454
G2246	G	A	C2066	C2006	U1944	U1880	U1818	U1758	A1698	C1638	A1515	G1455	G1455
A2247	U	G	G2067	U2007	G1945	C1881	A1819	A1759	G1699	C1639	G1516	G1456	G1456
C2248	G	G	U2068	C2008	U1946	U1882	U1820	C1760	A1700	A1640	U1578	U1457	U1457
U2249	C	C	G2069	A2009	C1947	U1883	U1821	C1761	A1701	A1641	G1581	U1458	U1458
G2250	U	U	G2070	G1948	G1947	G1884	C1822	A1762	G1702	G1642	C1582	U1520	U1520
A2251	U	U	A2071	G1949	G1949	A1885	G1823	G1763	G1703	G1643	A1583	G1521	U1460
G2252	U	U	C2072	G2012	U1950	U1886	G1824	G1764	C1704	C1644	A1584	A1522	C1461
C2253	G	G	A2013	U1951	C1887	G1887	U1825	U1765	A1705	G1645	C1585	U1523	U1523
G2254	G	A2134	U2074	A2014	A1952	G1888	G1826	G1766	C1706	C1646	A1586	G1524	C1463

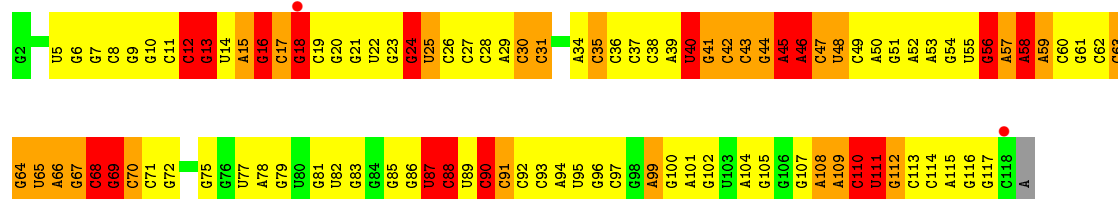
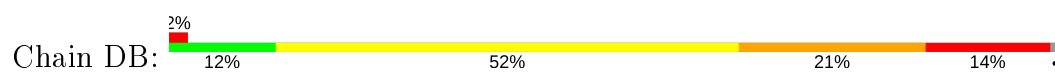


### • Molecule 23: 5S rRNA

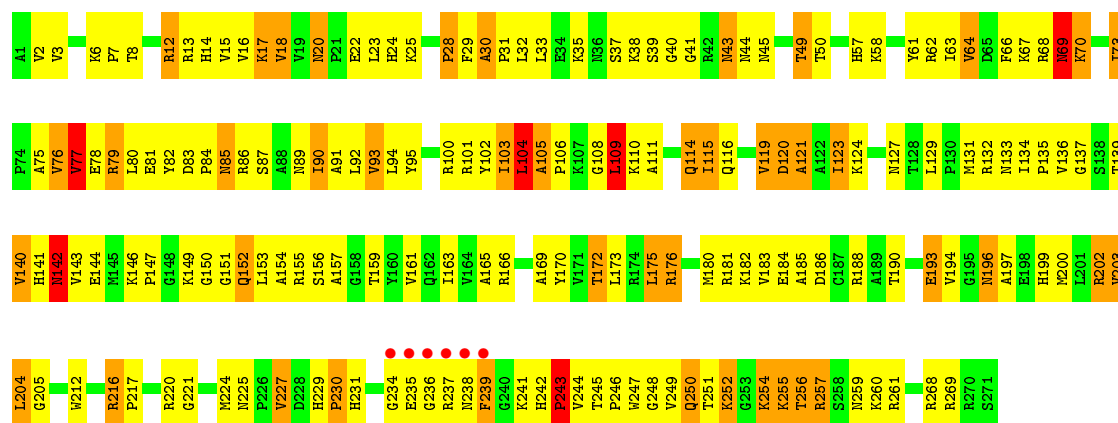
Chain BB:



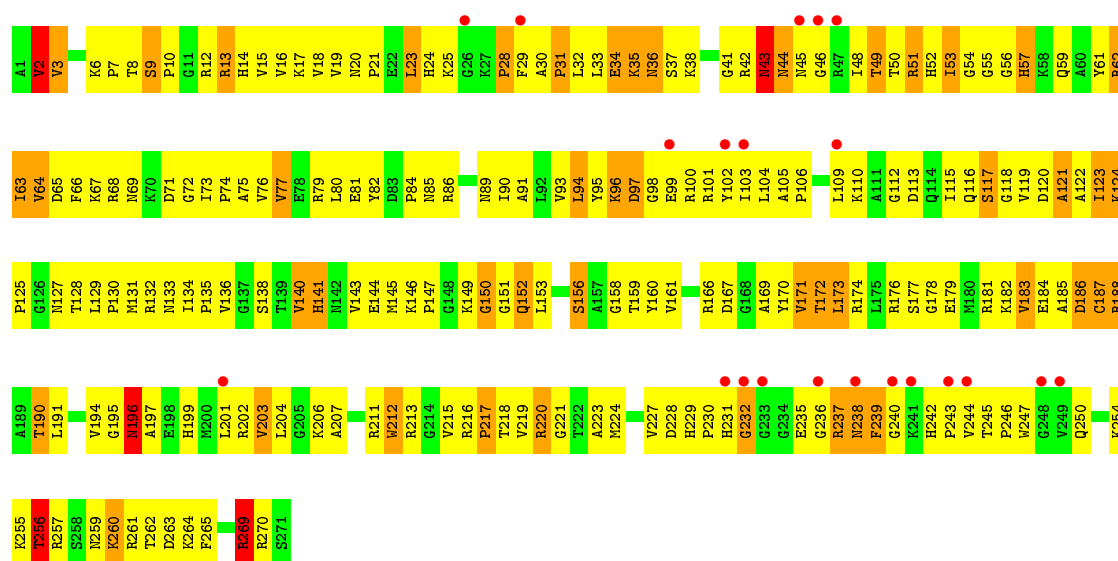




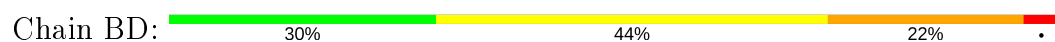
• Molecule 24: 50S ribosomal protein L2

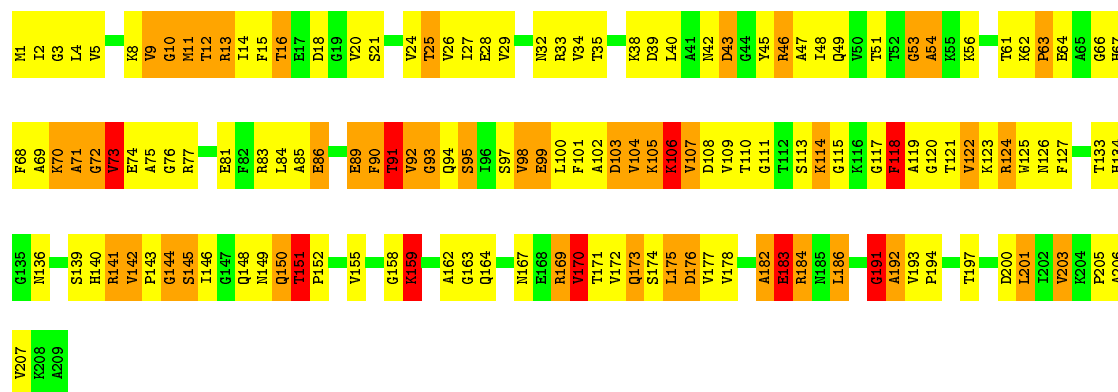


• Molecule 24: 50S ribosomal protein L2

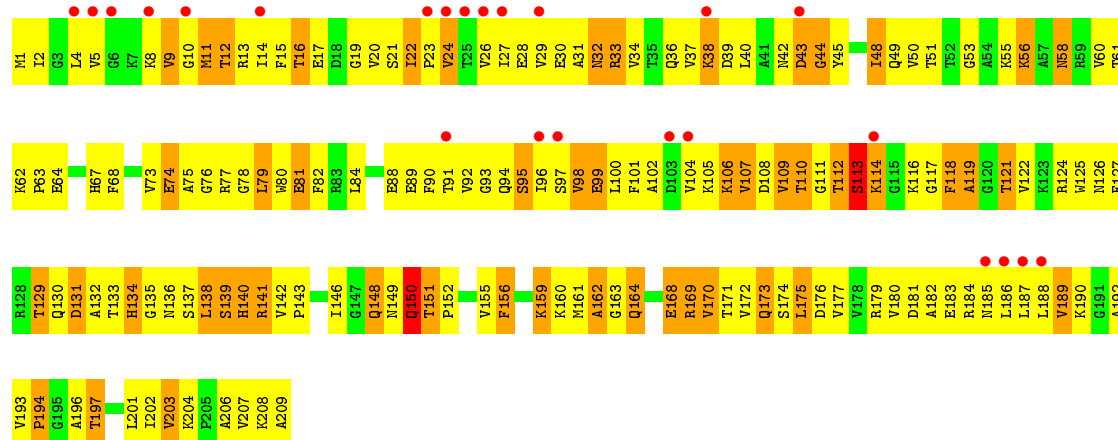


• Molecule 25: 50S ribosomal protein L3

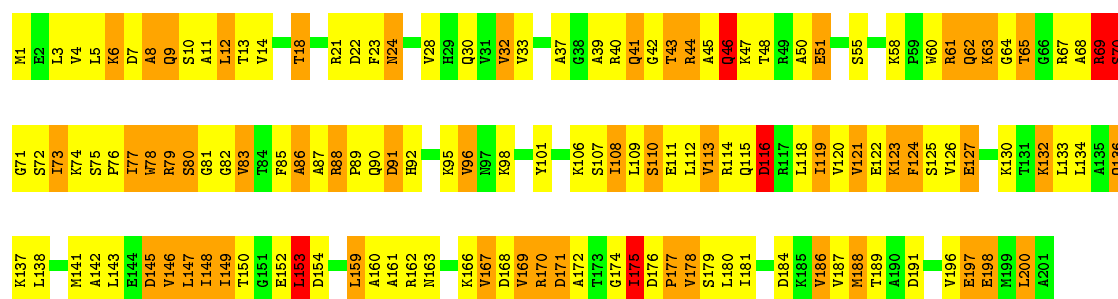




• Molecule 25: 50S ribosomal protein L3

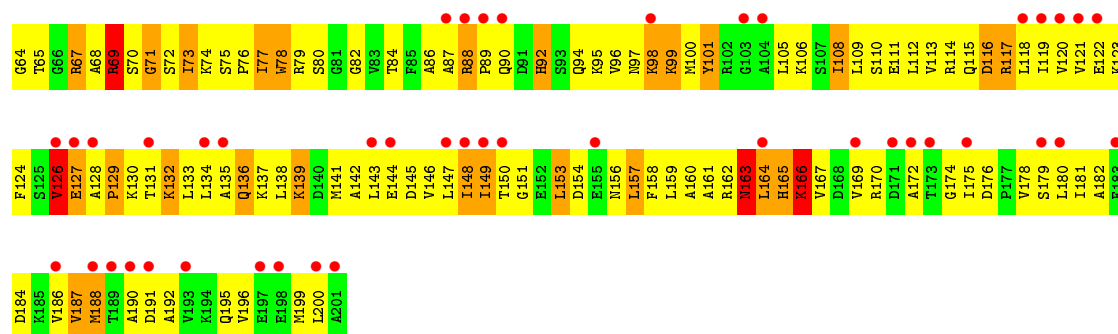


• Molecule 26: 50S ribosomal protein L4

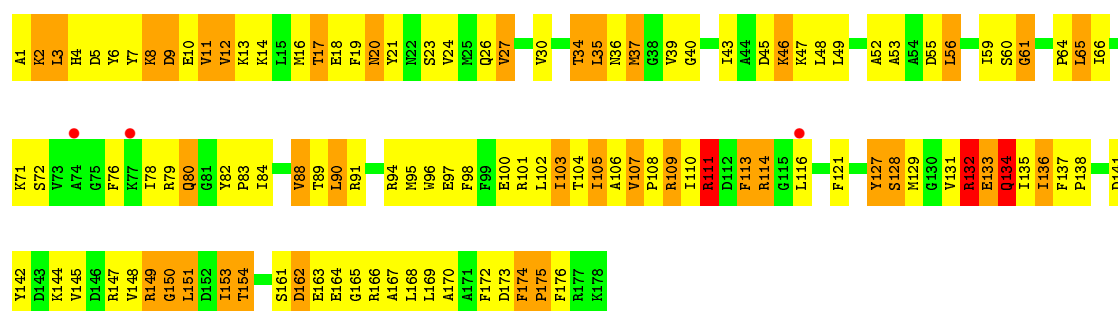


• Molecule 26: 50S ribosomal protein L4

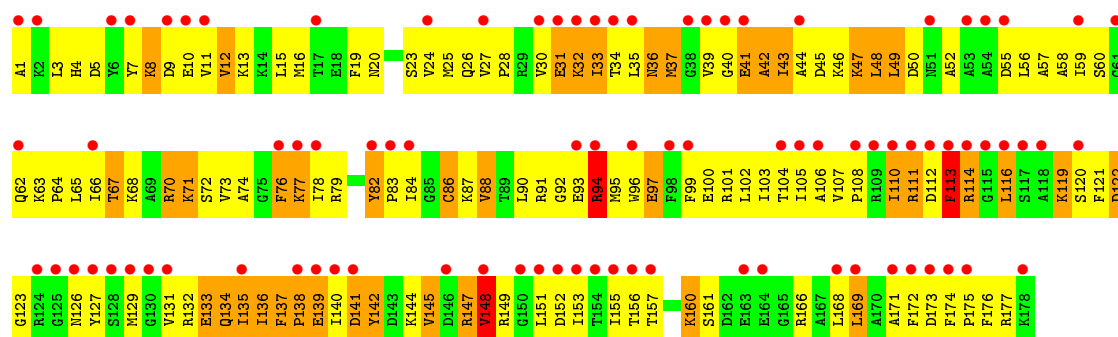




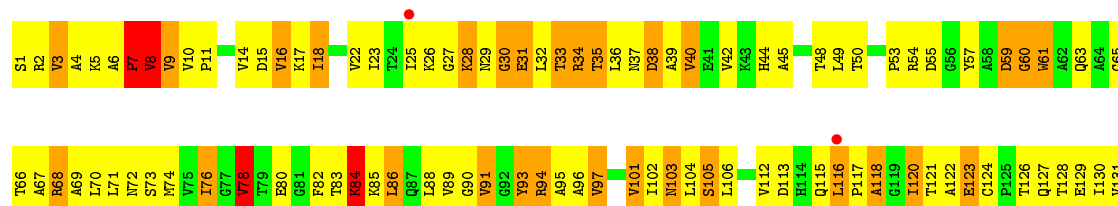
• Molecule 27: 50S ribosomal protein L5



• Molecule 27: 50S ribosomal protein L5

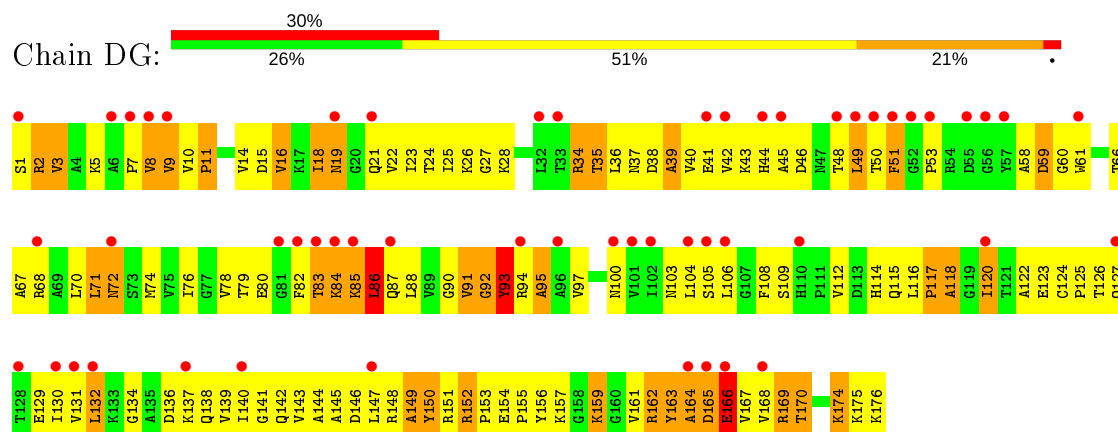


• Molecule 28: 50S ribosomal protein L6

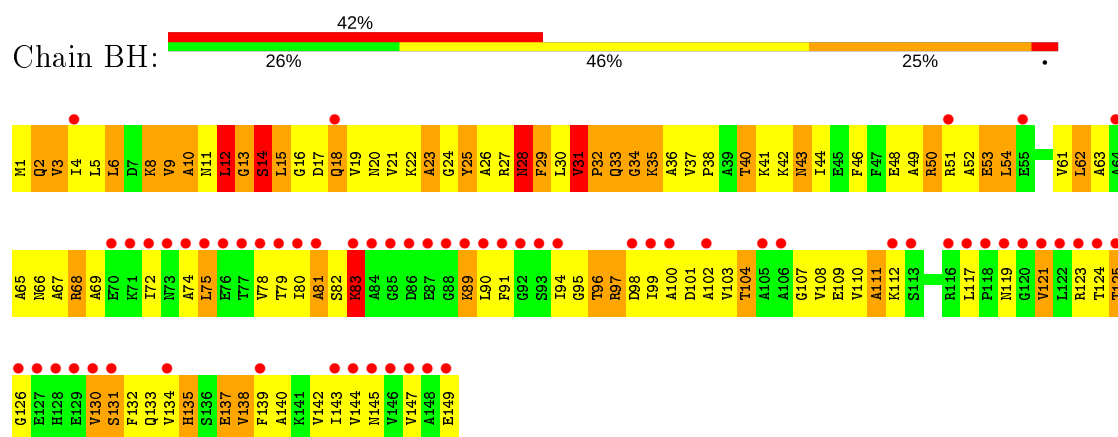




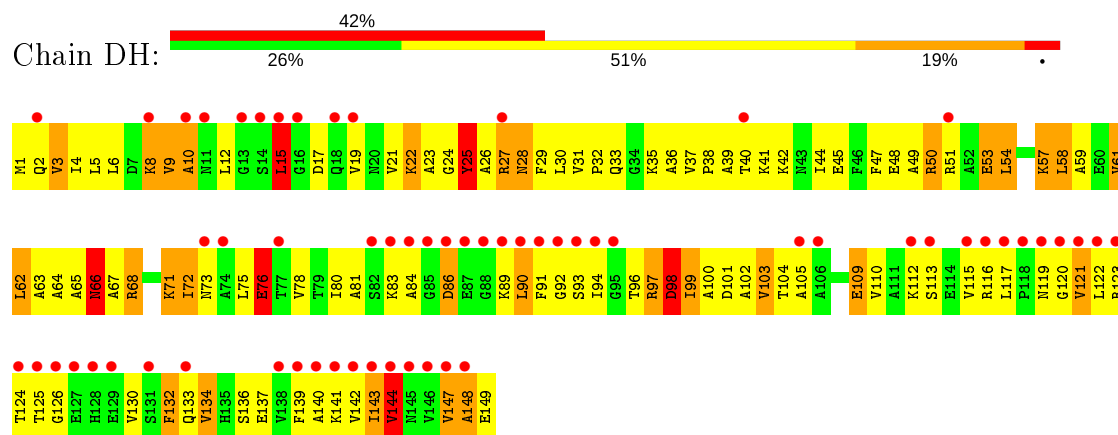
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9

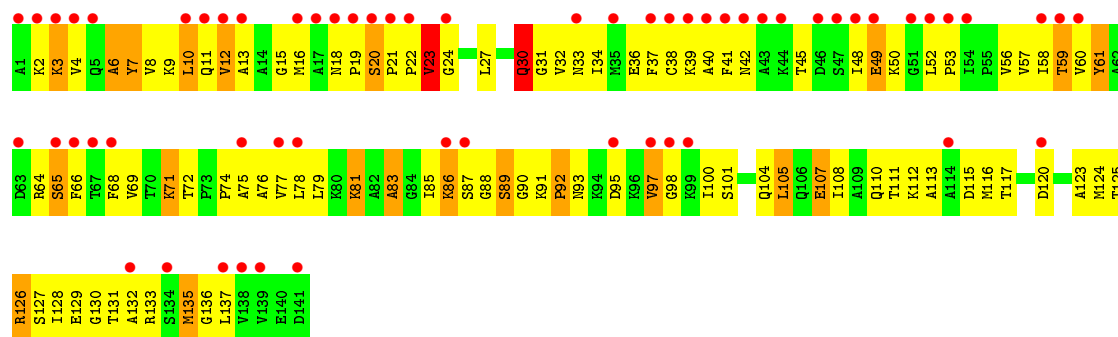


• Molecule 29: 50S ribosomal protein L9

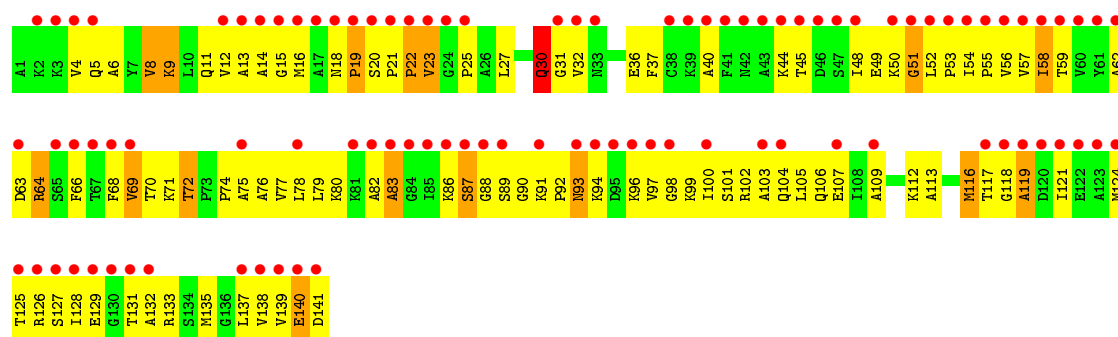


• Molecule 30: 50S ribosomal protein L11

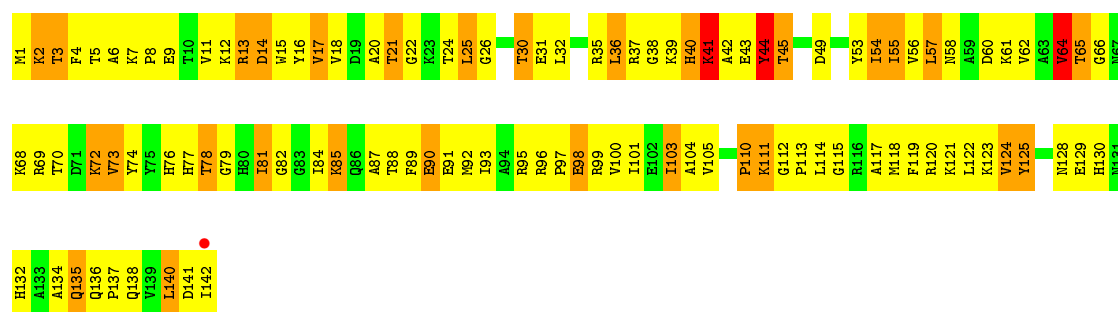
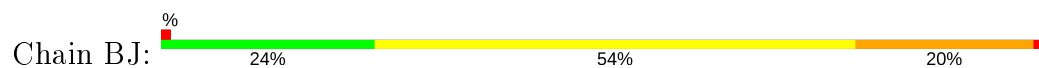




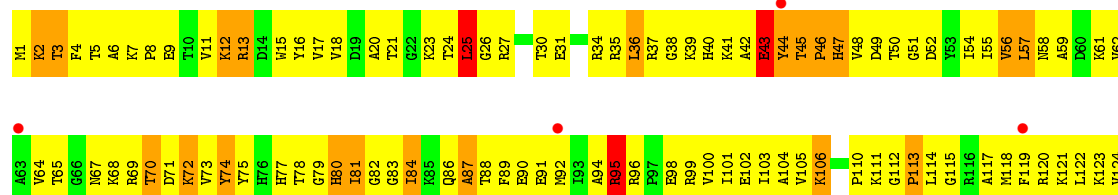
• Molecule 30: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L13



• Molecule 31: 50S ribosomal protein L13

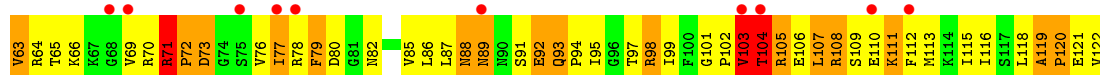
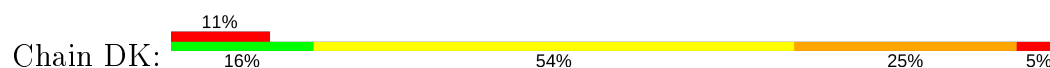




• Molecule 32: 50S ribosomal protein L14



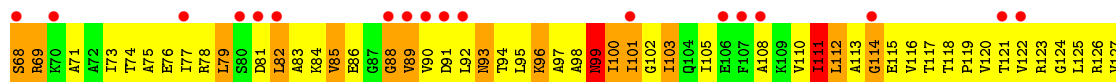
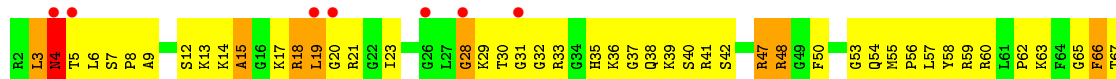
• Molecule 32: 50S ribosomal protein L14



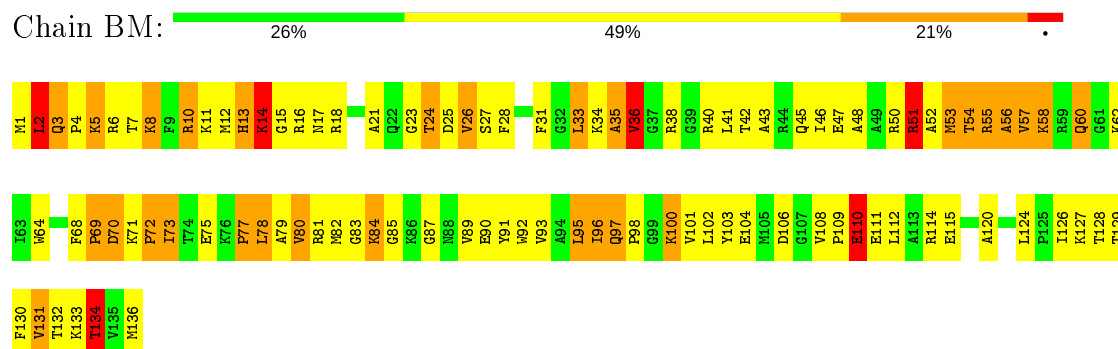
• Molecule 33: 50S ribosomal protein L15



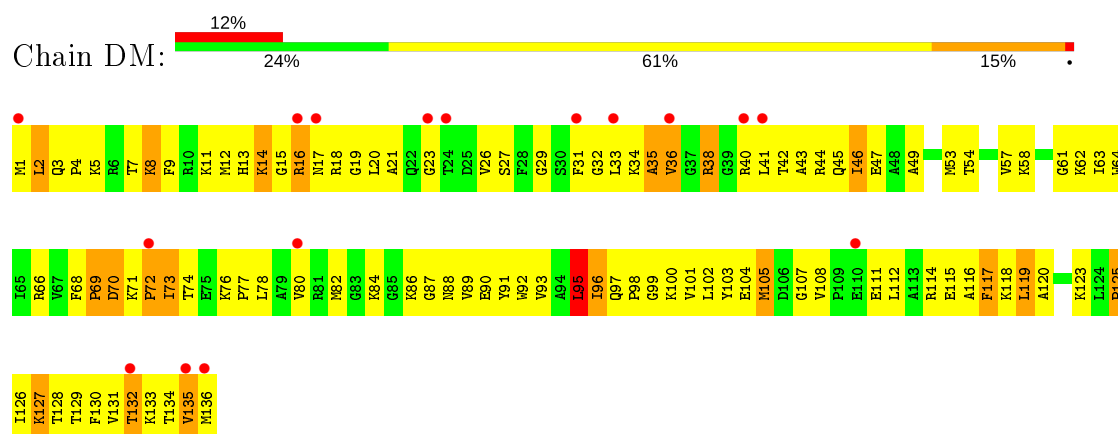
• Molecule 33: 50S ribosomal protein L15



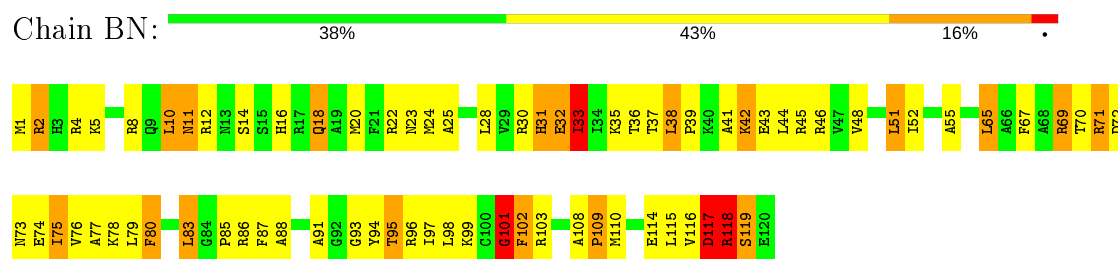
- Molecule 34: 50S ribosomal protein L16



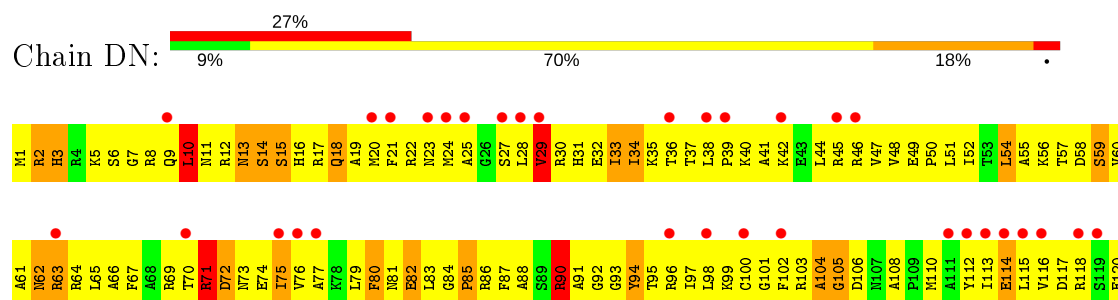
- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17

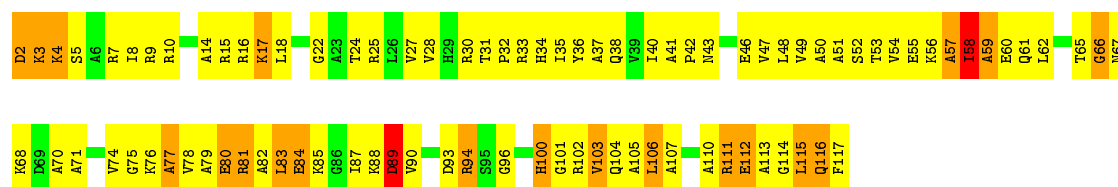


- Molecule 35: 50S ribosomal protein L17



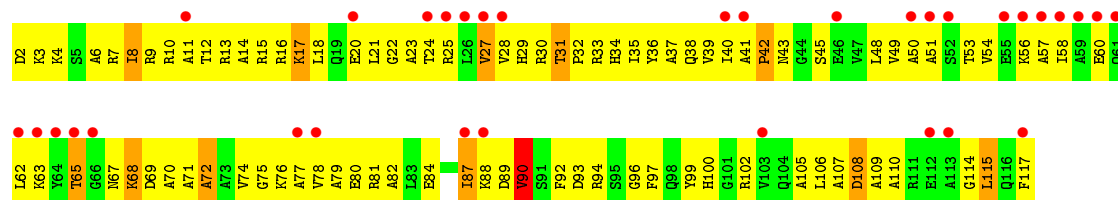
- Molecule 36: 50S ribosomal protein L18

Chain BO:  23% 58% 17%




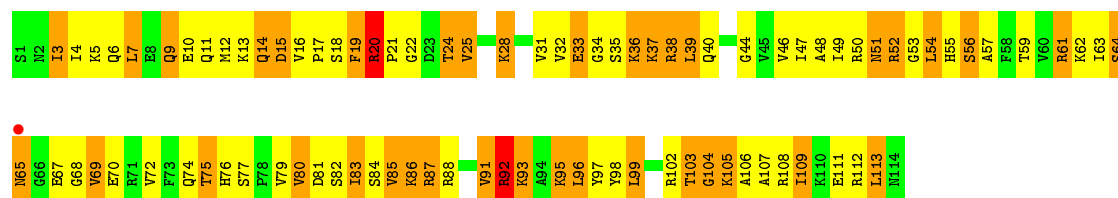
• Molecule 36: 50S ribosomal protein L18

Chain DO:  22% 67% 9%



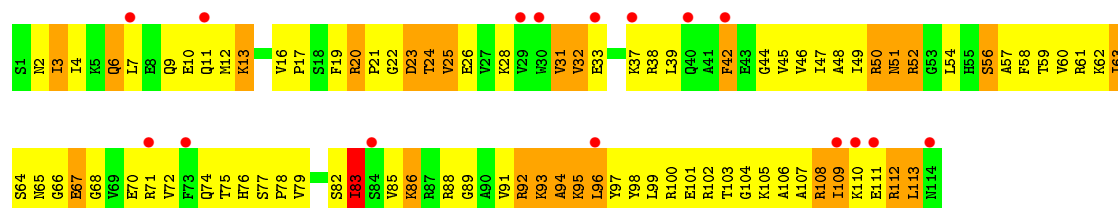
• Molecule 37: 50S ribosomal protein L19

Chain BP:  22% 43% 33%



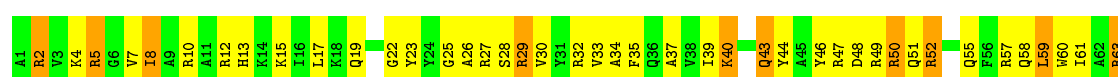
• Molecule 37: 50S ribosomal protein L19

Chain DP:  22% 54% 23%



• Molecule 38: 50S ribosomal protein L20

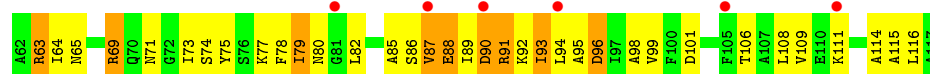
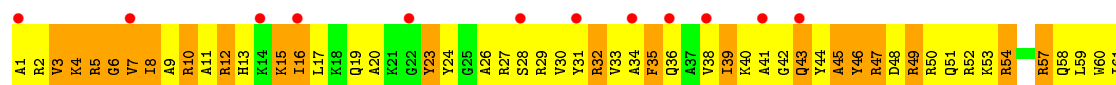
Chain BQ:  34% 47% 17%



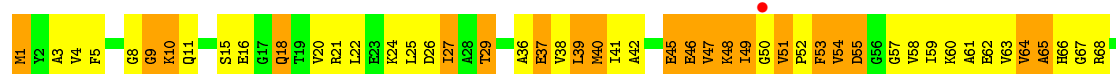




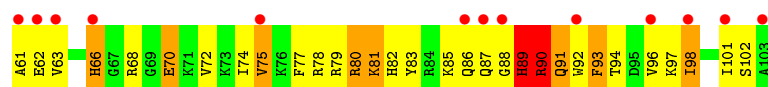
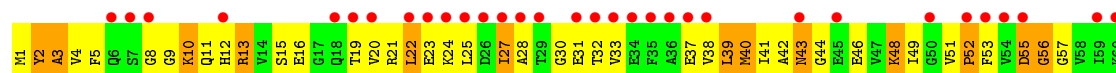
- Molecule 38: 50S ribosomal protein L20



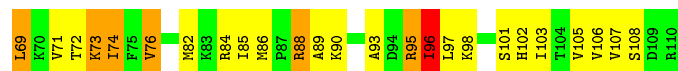
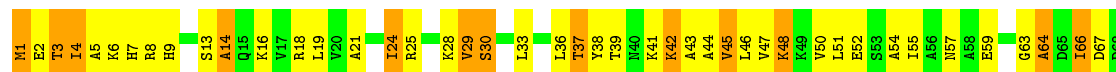
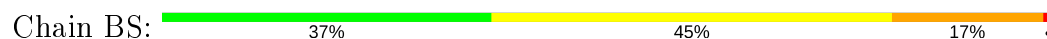
- Molecule 39: 50S ribosomal protein L21



- Molecule 39: 50S ribosomal protein L21

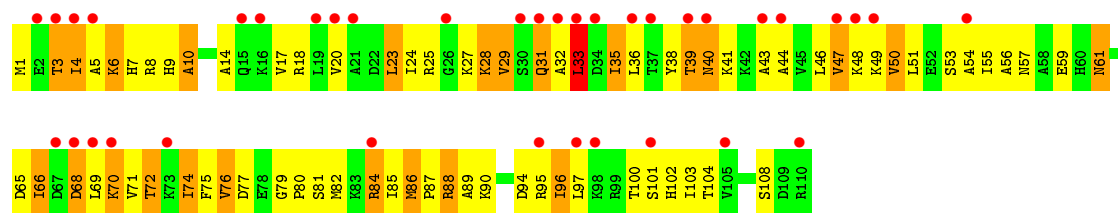


- Molecule 40: 50S ribosomal protein L22

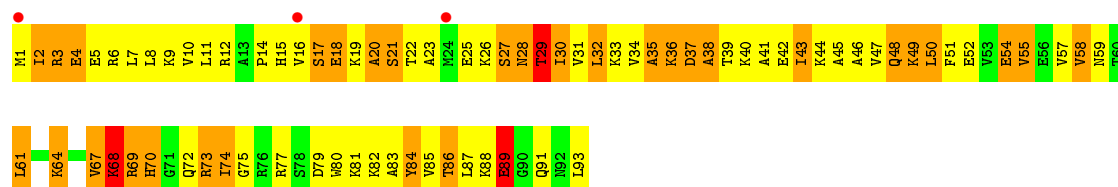
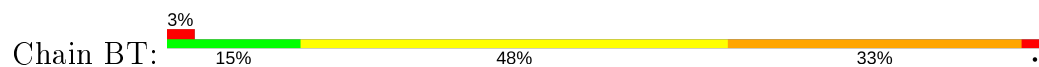


- Molecule 40: 50S ribosomal protein L22

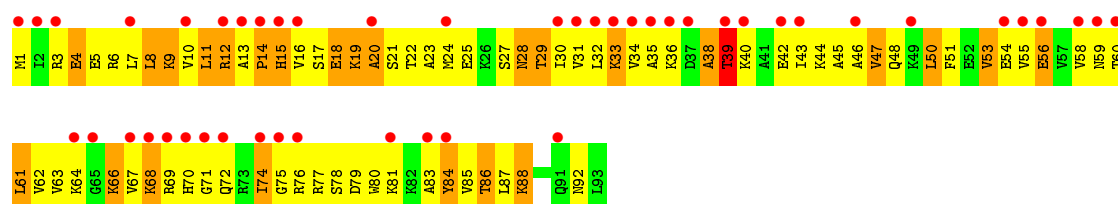
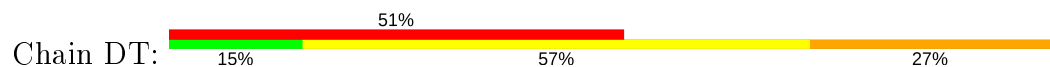




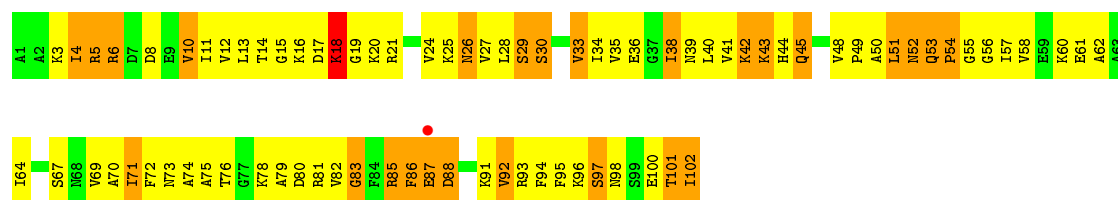
• Molecule 41: 50S ribosomal protein L23



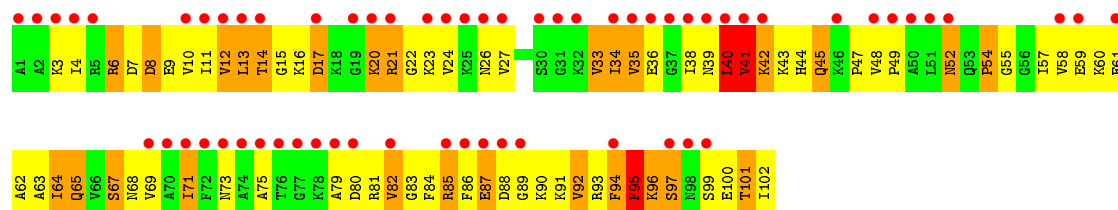
• Molecule 41: 50S ribosomal protein L23



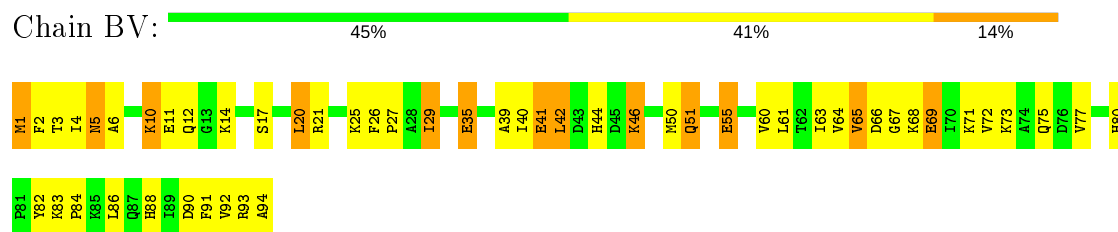
• Molecule 42: 50S ribosomal protein L24



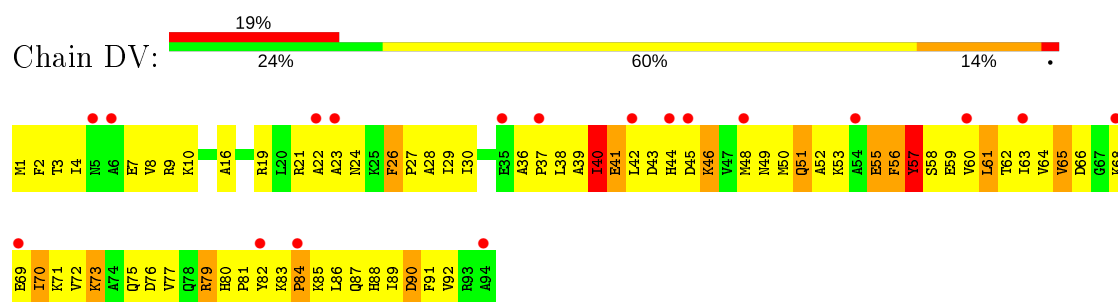
• Molecule 42: 50S ribosomal protein L24



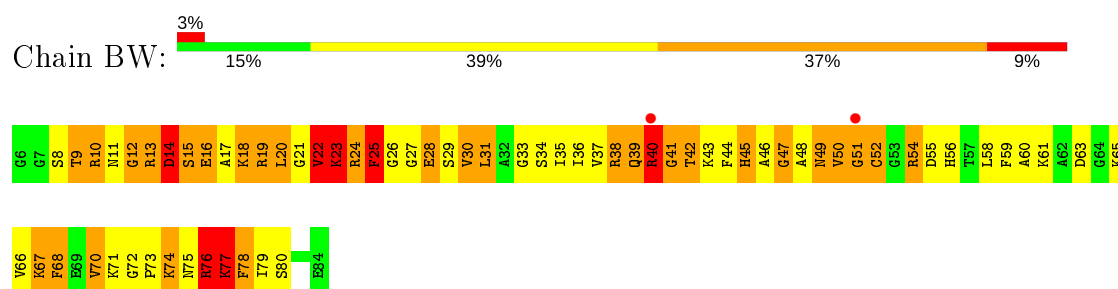
• Molecule 43: 50S ribosomal protein L25



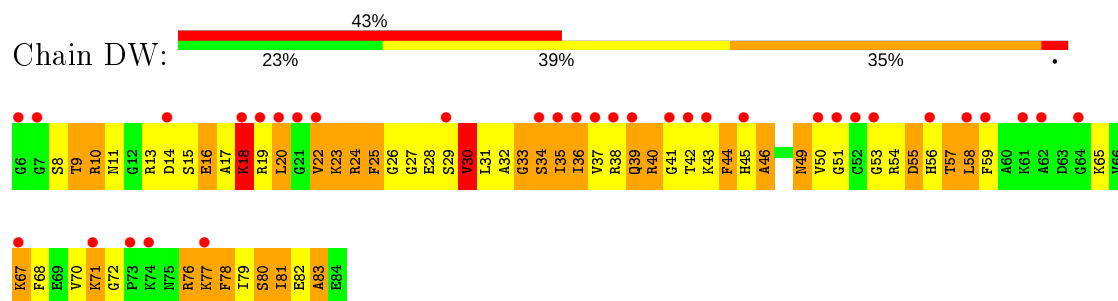
- Molecule 43: 50S ribosomal protein L25



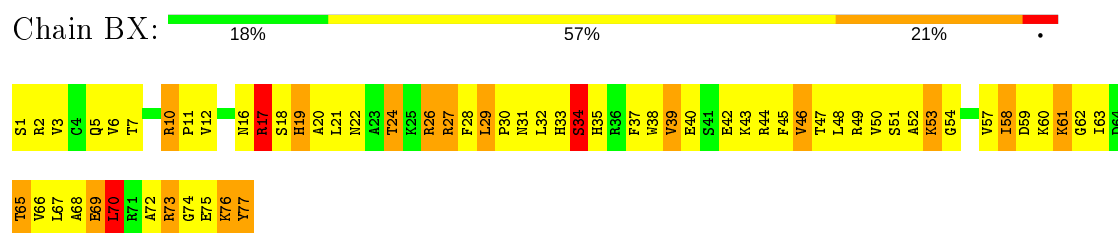
- Molecule 44: 50S ribosomal protein L27



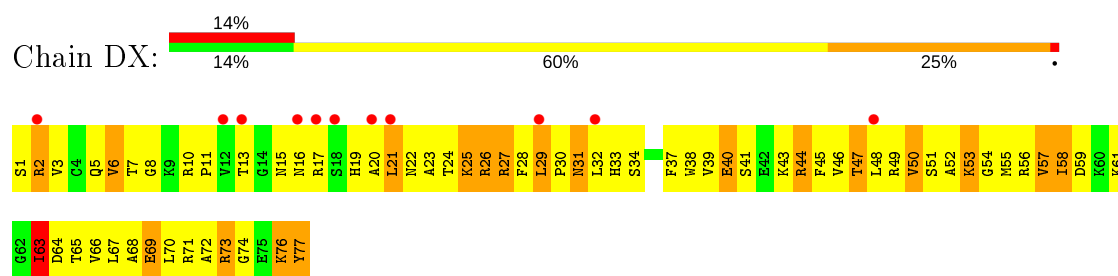
- Molecule 44: 50S ribosomal protein L27



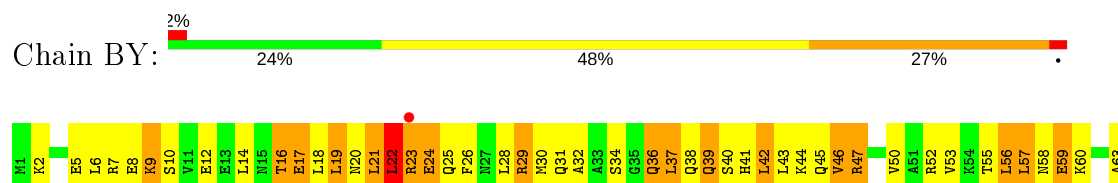
- Molecule 45: 50S ribosomal protein L28



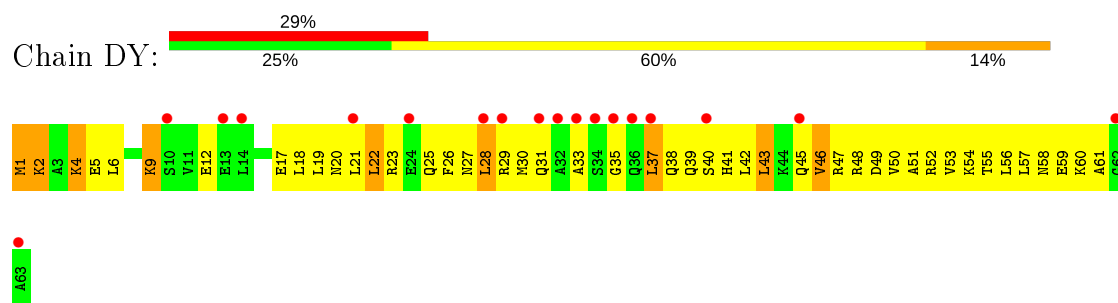
- Molecule 45: 50S ribosomal protein L28



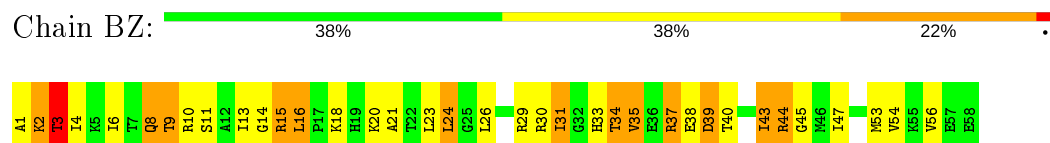
- Molecule 46: 50S ribosomal protein L29



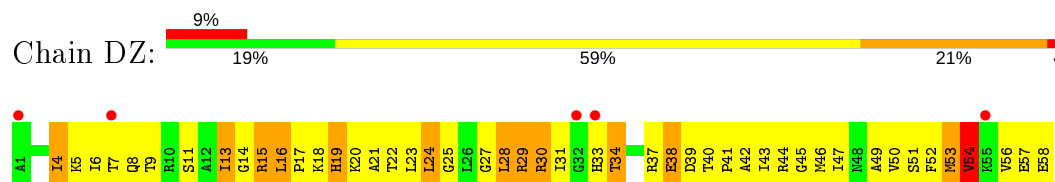
- Molecule 46: 50S ribosomal protein L29



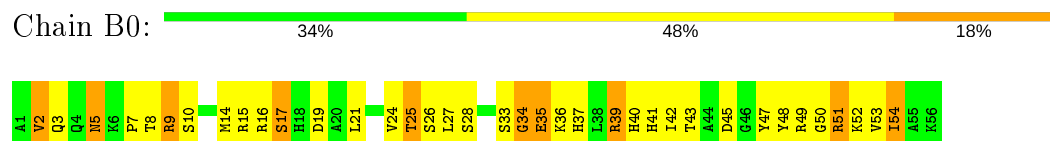
- Molecule 47: 50S ribosomal protein L30



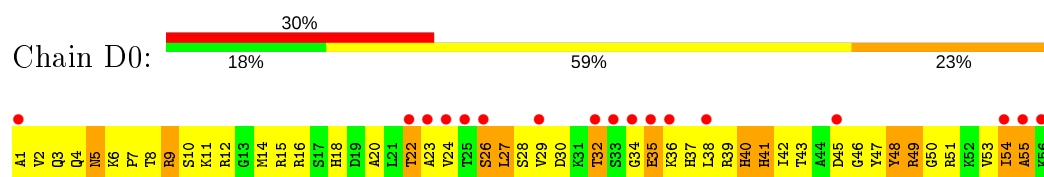
- Molecule 47: 50S ribosomal protein L30



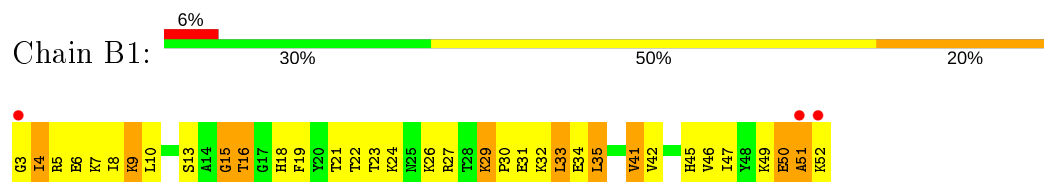
- Molecule 48: 50S ribosomal protein L32



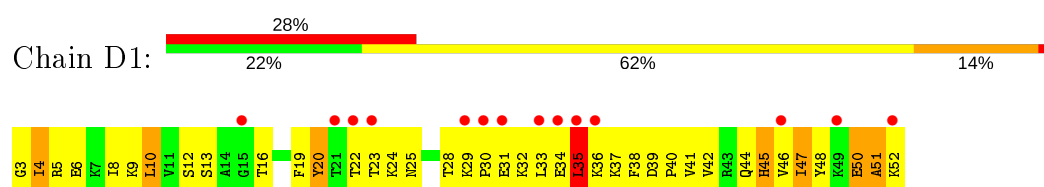
- Molecule 48: 50S ribosomal protein L32



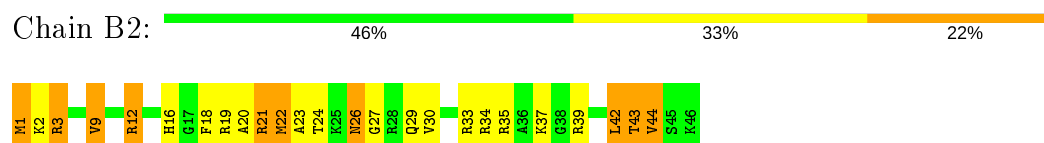
- Molecule 49: 50S ribosomal protein L33



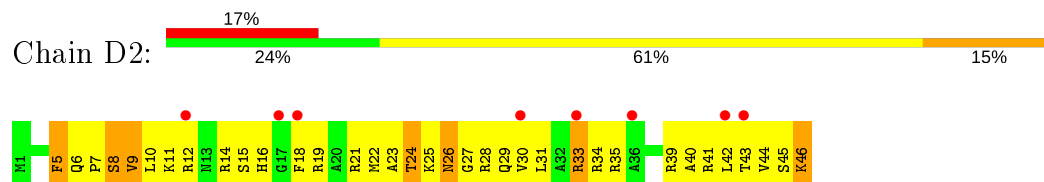
- Molecule 49: 50S ribosomal protein L33



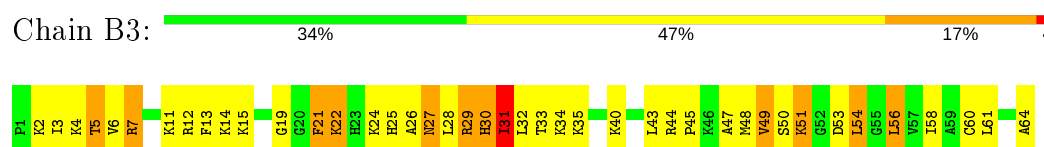
- Molecule 50: 50S ribosomal protein L34



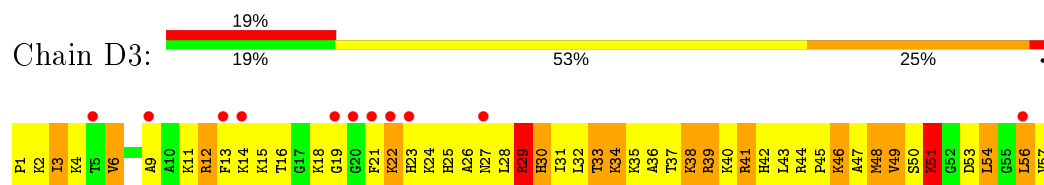
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35





• Molecule 52: 50S ribosomal protein L36



• Molecule 52: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.96Å 434.53Å 623.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.40 – 3.10 82.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (82.40-3.10) 83.9 (82.42-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.205 , 0.254 0.215 , 0.263	Depositor DCC
$R_{free}$ test set	18659 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 79.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.53	0/36834	1.32	524/57462 (0.9%)
1	CA	0.46	0/36762	1.21	433/57350 (0.8%)
2	AB	0.24	0/1736	0.47	0/2338
2	CB	0.22	0/1736	0.44	0/2338
3	AC	0.27	0/1652	0.50	0/2225
3	CC	0.24	0/1652	0.44	0/2225
4	AD	0.30	0/1665	0.52	0/2227
4	CD	0.37	0/1665	0.61	0/2227
5	AE	0.34	0/1119	0.61	0/1504
5	CE	0.31	0/1119	0.55	0/1504
6	AF	0.29	0/836	0.47	0/1128
6	CF	0.28	0/836	0.51	0/1128
7	AG	0.22	0/1196	0.44	0/1602
7	CG	0.22	0/1188	0.44	0/1591
8	AH	0.32	0/989	0.56	0/1326
8	CH	0.27	0/989	0.49	0/1326
9	AI	0.23	0/1034	0.45	0/1375
9	CI	0.22	0/1034	0.41	0/1375
10	AJ	0.24	0/797	0.47	0/1077
10	CJ	0.21	0/797	0.47	0/1077
11	AK	0.27	0/893	0.53	0/1205
11	CK	0.26	0/893	0.50	0/1205
12	AL	0.38	0/969	0.69	0/1300
12	CL	0.32	0/969	0.56	0/1300
13	AM	0.23	0/893	0.49	0/1193
13	CM	0.27	1/885 (0.1%)	0.39	0/1183
14	AN	0.25	0/785	0.48	0/1043
14	CN	0.21	0/780	0.38	0/1036
15	AO	0.30	0/722	0.49	0/964
15	CO	0.25	0/722	0.44	0/964
16	AP	0.31	0/659	0.51	0/884
16	CP	0.33	0/649	0.53	0/872



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.37	0/658	0.59	0/881
17	CQ	0.26	0/658	0.50	0/881
18	AR	0.29	0/463	0.49	0/621
18	CR	0.28	0/463	0.46	0/621
19	AS	0.23	0/653	0.46	0/877
19	CS	0.21	0/653	0.41	0/877
20	AT	0.34	0/671	0.57	0/888
20	CT	0.26	0/671	0.51	0/888
21	AU	0.25	0/431	0.46	0/570
21	CU	0.31	0/431	0.58	0/570
22	BA	0.85	15/68626 (0.0%)	1.69	1674/107056 (1.6%)
22	DA	0.46	0/68314	1.26	901/106569 (0.8%)
23	BB	0.74	0/2828	1.56	46/4410 (1.0%)
23	DB	0.40	0/2803	1.09	27/4371 (0.6%)
24	BC	0.48	0/2122	0.74	1/2852 (0.0%)
24	DC	0.29	0/2122	0.54	0/2852
25	BD	0.61	0/1586	0.80	2/2134 (0.1%)
25	DD	0.28	0/1586	0.55	0/2134
26	BE	0.51	0/1571	0.73	0/2113
26	DE	0.25	0/1571	0.48	0/2113
27	BF	0.35	0/1435	0.55	0/1928
27	DF	0.21	0/1444	0.44	0/1937
28	BG	0.38	0/1343	0.61	0/1816
28	DG	0.21	0/1343	0.44	0/1816
29	BH	0.28	0/1122	0.51	0/1515
29	DH	0.26	0/1122	0.48	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.20	0/1046	0.42	0/1410
31	BJ	0.60	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.27	0/1152	0.55	1/1551 (0.1%)
32	BK	0.61	1/948 (0.1%)	0.83	0/1268
32	DK	0.30	0/948	0.56	0/1268
33	BL	0.50	0/1054	0.80	2/1403 (0.1%)
33	DL	0.25	0/1054	0.51	0/1403
34	BM	0.55	0/1093	0.78	0/1460
34	DM	0.27	0/1093	0.49	0/1460
35	BN	0.55	0/974	0.82	2/1301 (0.2%)
35	DN	0.27	0/974	0.50	0/1301
36	BO	0.42	0/902	0.66	0/1209
36	DO	0.22	0/902	0.41	0/1209
37	BP	0.52	0/929	0.72	0/1242
37	DP	0.28	0/929	0.49	0/1242
38	BQ	0.72	0/960	0.89	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.27	0/960	0.46	0/1278
39	BR	0.67	2/829 (0.2%)	0.85	1/1107 (0.1%)
39	DR	0.27	0/829	0.48	0/1107
40	BS	0.63	0/864	0.84	0/1156
40	DS	0.26	0/864	0.51	0/1156
41	BT	0.51	0/745	0.80	0/994
41	DT	0.22	0/745	0.46	0/994
42	BU	0.44	0/788	0.75	0/1051
42	DU	0.23	0/788	0.45	0/1051
43	BV	0.47	0/766	0.65	0/1025
43	DV	0.23	0/766	0.43	0/1025
44	BW	0.67	0/603	0.93	1/797 (0.1%)
44	DW	0.24	0/603	0.48	0/797
45	BX	0.43	0/635	0.75	1/848 (0.1%)
45	DX	0.28	0/635	0.54	0/848
46	BY	0.39	0/510	0.63	0/677
46	DY	0.21	0/510	0.41	0/677
47	BZ	0.58	0/453	0.93	2/605 (0.3%)
47	DZ	0.25	0/453	0.49	0/605
48	B0	0.52	0/450	0.79	0/599
48	D0	0.27	0/450	0.49	0/599
49	B1	0.38	0/417	0.64	0/554
49	D1	0.23	0/417	0.46	0/554
50	B2	0.52	0/380	0.71	0/498
50	D2	0.27	0/380	0.52	0/498
51	B3	0.50	0/513	0.70	1/676 (0.1%)
51	D3	0.26	0/513	0.54	0/676
52	B4	0.41	0/303	0.64	0/397
52	D4	0.24	0/303	0.43	0/397
All	All	0.56	19/306773 (0.0%)	1.25	3621/458571 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	AL	0	1
20	AT	0	1
25	BD	0	1
31	BJ	0	1
35	BN	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-8.33	1.32	1.37
22	BA	984	A	C5-C6	-7.40	1.34	1.41
39	BR	86	GLN	CB-CG	7.19	1.72	1.52
22	BA	1783	A	N7-C5	-6.87	1.35	1.39
22	BA	984	A	N9-C4	-5.90	1.34	1.37

The worst 5 of 3621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	571	U	O4'-C1'-N1	17.46	122.17	108.20
22	BA	2848	G	P-O3'-C3'	17.00	140.09	119.70
22	BA	627	A	P-O3'-C3'	16.24	139.19	119.70
22	BA	984	A	N1-C6-N6	16.11	128.26	118.60
22	BA	1603	A	P-O3'-C3'	-15.84	100.69	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AL	22	ALA	Peptide
20	AT	6	ALA	Peptide
25	BD	191	GLY	Peptide
31	BJ	110	PRO	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	2319	0
1	CA	32831	0	16521	2706	0
2	AB	1705	0	1732	283	0
2	CB	1705	0	1732	260	0
3	AC	1625	0	1699	194	0
3	CC	1625	0	1699	238	0
4	AD	1643	0	1710	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CD	1643	0	1710	269	0
5	AE	1106	0	1148	203	0
5	CE	1106	0	1148	183	0
6	AF	818	0	808	113	0
6	CF	818	0	808	134	0
7	AG	1182	0	1240	150	0
7	CG	1175	0	1230	209	0
8	AH	979	0	1034	162	0
8	CH	979	0	1034	140	0
9	AI	1022	0	1070	165	0
9	CI	1022	0	1070	178	0
10	AJ	787	0	828	169	0
10	CJ	787	0	828	142	0
11	AK	877	0	887	165	0
11	CK	877	0	887	138	0
12	AL	955	0	1019	132	0
12	CL	955	0	1019	173	0
13	AM	884	0	944	120	0
13	CM	877	0	937	176	0
14	AN	774	0	827	131	0
14	CN	769	0	822	149	0
15	AO	714	0	737	93	0
15	CO	714	0	737	71	0
16	AP	649	0	666	105	0
16	CP	639	0	656	135	0
17	AQ	649	0	691	141	0
17	CQ	649	0	691	98	0
18	AR	456	0	478	51	0
18	CR	456	0	478	95	0
19	AS	638	0	665	97	0
19	CS	638	0	665	118	0
20	AT	665	0	714	117	0
20	CT	665	0	714	99	0
21	AU	426	0	449	131	0
21	CU	426	0	449	126	0
22	BA	61274	0	30819	3116	1
22	DA	60995	0	30679	5725	1
23	BB	2529	0	1281	109	0
23	DB	2507	0	1270	238	0
24	BC	2083	0	2157	313	0
24	DC	2083	0	2157	347	0
25	BD	1565	0	1616	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DD	1565	0	1616	319	0
26	BE	1552	0	1619	199	0
26	DE	1552	0	1619	321	0
27	BF	1411	0	1447	210	0
27	DF	1420	0	1460	289	0
28	BG	1323	0	1374	225	0
28	DG	1323	0	1374	229	0
29	BH	1111	0	1148	184	0
29	DH	1111	0	1148	208	0
30	BI	1032	0	1088	135	0
30	DI	1032	0	1088	149	0
31	BJ	1129	0	1162	214	0
31	DJ	1129	0	1162	205	0
32	BK	939	0	1012	150	0
32	DK	939	0	1012	188	0
33	BL	1045	0	1117	169	0
33	DL	1045	0	1117	224	0
34	BM	1074	0	1157	148	0
34	DM	1074	0	1157	156	0
35	BN	961	0	1000	131	0
35	DN	961	0	1000	228	0
36	BO	892	0	923	120	0
36	DO	892	0	923	118	0
37	BP	917	0	965	189	0
37	DP	917	0	965	184	0
38	BQ	947	0	1022	192	0
38	DQ	947	0	1022	203	0
39	BR	816	0	839	145	0
39	DR	816	0	839	147	0
40	BS	857	0	922	93	0
40	DS	857	0	922	125	0
41	BT	739	0	807	155	0
41	DT	739	0	807	174	0
42	BU	780	0	834	103	0
42	DU	780	0	834	147	0
43	BV	753	0	780	63	0
43	DV	753	0	780	118	0
44	BW	596	0	610	286	0
44	DW	596	0	610	180	0
45	BX	625	0	655	113	0
45	DX	625	0	655	128	0
46	BY	509	0	543	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DY	509	0	543	114	0
47	BZ	449	0	491	44	0
47	DZ	449	0	491	69	0
48	B0	444	0	461	52	0
48	D0	444	0	461	92	0
49	B1	410	0	440	66	0
49	D1	410	0	440	55	0
50	B2	377	0	418	29	0
50	D2	377	0	418	65	0
51	B3	504	0	574	71	0
51	D3	504	0	574	105	0
52	B4	302	0	340	48	0
52	D4	302	0	343	48	0
53	AA	41	0	0	0	0
53	AN	2	0	0	0	0
53	BA	135	0	0	0	0
53	BB	4	0	0	0	0
53	CA	42	0	0	0	0
53	DA	133	0	0	0	0
53	DB	1	0	0	0	0
53	DC	2	0	0	0	0
53	DJ	1	0	0	0	0
54	BA	51	0	67	4	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	197	0	0	12	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	7	0	0	0	0
56	AT	1	0	0	0	0
56	AU	1	0	0	0	0
56	B3	3	0	0	0	0
56	B4	2	0	0	0	0
56	BA	605	0	0	46	0
56	BB	19	0	0	0	0
56	BC	7	0	0	0	0
56	BD	3	0	0	2	0
56	BE	1	0	0	1	0
56	BL	4	0	0	1	0
56	BN	2	0	0	0	0
56	BR	1	0	0	0	0
56	BT	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BV	1	0	0	1	0
56	CA	195	0	0	3	0
56	CE	3	0	0	1	0
56	CL	1	0	0	0	0
56	CN	3	0	0	0	0
56	CT	4	0	0	0	0
56	CU	1	0	0	0	0
56	D2	1	0	0	1	0
56	D3	1	0	0	0	0
56	D4	4	0	0	0	0
56	DA	600	0	0	30	0
56	DB	3	0	0	0	0
56	DC	13	0	0	2	0
56	DD	2	0	0	0	0
56	DE	4	0	0	0	0
56	DJ	3	0	0	0	0
56	DL	4	0	0	1	0
56	DN	2	0	0	0	0
56	DT	2	0	0	0	0
56	DU	2	0	0	0	0
56	DV	2	0	0	0	0
All	All	284525	0	190908	27236	1

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 58.

The worst 5 of 27236 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)
37:BP:50:ARG:CG	37:BP:57:ALA:H	1.24	1.44
37:BP:50:ARG:HD2	37:BP:51:ASN:N	1.27	1.42
37:BP:50:ARG:HG2	37:BP:57:ALA:N	1.13	1.41
1:CA:238:A:C2'	1:CA:239:U:H5''	1.57	1.34
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.37	1.34

All (1) 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]	2.02	0.18

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	133 (62%)	51 (24%)	32 (15%)	0	0
2	CB	216/218 (99%)	158 (73%)	38 (18%)	20 (9%)	0	3
3	AC	204/206 (99%)	144 (71%)	36 (18%)	24 (12%)	0	1
3	CC	204/206 (99%)	138 (68%)	47 (23%)	19 (9%)	0	3
4	AD	203/205 (99%)	127 (63%)	43 (21%)	33 (16%)	0	0
4	CD	203/205 (99%)	138 (68%)	40 (20%)	25 (12%)	0	1
5	AE	148/150 (99%)	97 (66%)	28 (19%)	23 (16%)	0	0
5	CE	148/150 (99%)	111 (75%)	21 (14%)	16 (11%)	0	2
6	AF	98/100 (98%)	71 (72%)	15 (15%)	12 (12%)	0	1
6	CF	98/100 (98%)	66 (67%)	19 (19%)	13 (13%)	0	1
7	AG	149/151 (99%)	100 (67%)	37 (25%)	12 (8%)	1	5
7	CG	148/151 (98%)	96 (65%)	38 (26%)	14 (10%)	0	3
8	AH	127/129 (98%)	101 (80%)	15 (12%)	11 (9%)	1	4
8	CH	127/129 (98%)	96 (76%)	23 (18%)	8 (6%)	1	8
9	AI	125/127 (98%)	81 (65%)	28 (22%)	16 (13%)	0	1
9	CI	125/127 (98%)	84 (67%)	32 (26%)	9 (7%)	1	6
10	AJ	96/98 (98%)	69 (72%)	10 (10%)	17 (18%)	0	0
10	CJ	96/98 (98%)	61 (64%)	21 (22%)	14 (15%)	0	1
11	AK	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	1
11	CK	115/117 (98%)	87 (76%)	16 (14%)	12 (10%)	0	3
12	AL	121/123 (98%)	88 (73%)	21 (17%)	12 (10%)	0	3
12	CL	121/123 (98%)	84 (69%)	24 (20%)	13 (11%)	0	2
13	AM	112/114 (98%)	83 (74%)	19 (17%)	10 (9%)	1	4
13	CM	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	0	2
14	AN	92/100 (92%)	60 (65%)	18 (20%)	14 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	91/100 (91%)	57 (63%)	26 (29%)	8 (9%)	1	4
15	AO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	0	3
15	CO	86/88 (98%)	53 (62%)	30 (35%)	3 (4%)	3	20
16	AP	80/82 (98%)	59 (74%)	12 (15%)	9 (11%)	0	2
16	CP	79/82 (96%)	48 (61%)	23 (29%)	8 (10%)	0	3
17	AQ	78/80 (98%)	48 (62%)	24 (31%)	6 (8%)	1	5
17	CQ	78/80 (98%)	59 (76%)	11 (14%)	8 (10%)	0	3
18	AR	53/55 (96%)	40 (76%)	10 (19%)	3 (6%)	1	10
18	CR	53/55 (96%)	33 (62%)	17 (32%)	3 (6%)	1	10
19	AS	77/79 (98%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	4
20	AT	83/85 (98%)	57 (69%)	21 (25%)	5 (6%)	1	9
20	CT	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	1
21	AU	49/51 (96%)	25 (51%)	12 (24%)	12 (24%)	0	0
21	CU	49/51 (96%)	20 (41%)	13 (26%)	16 (33%)	0	0
24	BC	269/271 (99%)	197 (73%)	46 (17%)	26 (10%)	0	3
24	DC	269/271 (99%)	174 (65%)	64 (24%)	31 (12%)	0	2
25	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	0
25	DD	207/209 (99%)	131 (63%)	41 (20%)	35 (17%)	0	0
26	BE	199/201 (99%)	144 (72%)	35 (18%)	20 (10%)	0	3
26	DE	199/201 (99%)	115 (58%)	54 (27%)	30 (15%)	0	0
27	BF	176/178 (99%)	124 (70%)	36 (20%)	16 (9%)	1	4
27	DF	176/178 (99%)	87 (49%)	58 (33%)	31 (18%)	0	0
28	BG	174/176 (99%)	111 (64%)	38 (22%)	25 (14%)	0	1
28	DG	174/176 (99%)	99 (57%)	40 (23%)	35 (20%)	0	0
29	BH	147/149 (99%)	62 (42%)	50 (34%)	35 (24%)	0	0
29	DH	147/149 (99%)	70 (48%)	54 (37%)	23 (16%)	0	0
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	75 (54%)	48 (34%)	16 (12%)	0	2
31	BJ	140/142 (99%)	104 (74%)	24 (17%)	12 (9%)	1	4
31	DJ	140/142 (99%)	92 (66%)	28 (20%)	20 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	120/122 (98%)	89 (74%)	17 (14%)	14 (12%)	0	1
32	DK	120/122 (98%)	76 (63%)	17 (14%)	27 (22%)	0	0
33	BL	141/143 (99%)	100 (71%)	30 (21%)	11 (8%)	1	5
33	DL	141/143 (99%)	77 (55%)	44 (31%)	20 (14%)	0	1
34	BM	134/136 (98%)	96 (72%)	18 (13%)	20 (15%)	0	0
34	DM	134/136 (98%)	90 (67%)	26 (19%)	18 (13%)	0	1
35	BN	118/120 (98%)	91 (77%)	16 (14%)	11 (9%)	0	3
35	DN	118/120 (98%)	74 (63%)	25 (21%)	19 (16%)	0	0
36	BO	114/116 (98%)	85 (75%)	18 (16%)	11 (10%)	0	3
36	DO	114/116 (98%)	74 (65%)	30 (26%)	10 (9%)	1	4
37	BP	112/114 (98%)	78 (70%)	20 (18%)	14 (12%)	0	1
37	DP	112/114 (98%)	60 (54%)	31 (28%)	21 (19%)	0	0
38	BQ	115/117 (98%)	100 (87%)	7 (6%)	8 (7%)	1	7
38	DQ	115/117 (98%)	75 (65%)	27 (24%)	13 (11%)	0	2
39	BR	101/103 (98%)	76 (75%)	14 (14%)	11 (11%)	0	2
39	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
40	BS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	15
40	DS	108/110 (98%)	72 (67%)	25 (23%)	11 (10%)	0	3
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
41	DT	91/93 (98%)	41 (45%)	26 (29%)	24 (26%)	0	0
42	BU	100/102 (98%)	66 (66%)	16 (16%)	18 (18%)	0	0
42	DU	100/102 (98%)	52 (52%)	22 (22%)	26 (26%)	0	0
43	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	6	29
43	DV	92/94 (98%)	60 (65%)	24 (26%)	8 (9%)	1	4
44	BW	77/79 (98%)	31 (40%)	22 (29%)	24 (31%)	0	0
44	DW	77/79 (98%)	30 (39%)	25 (32%)	22 (29%)	0	0
45	BX	75/77 (97%)	58 (77%)	10 (13%)	7 (9%)	0	3
45	DX	75/77 (97%)	44 (59%)	20 (27%)	11 (15%)	0	0
46	BY	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	1
46	DY	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	1	5
47	BZ	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DZ	56/58 (97%)	31 (55%)	20 (36%)	5 (9%)	1	4
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	6
48	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	3
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	3
49	D1	48/50 (96%)	35 (73%)	8 (17%)	5 (10%)	0	3
50	B2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
50	D2	44/46 (96%)	29 (66%)	10 (23%)	5 (11%)	0	2
51	B3	62/64 (97%)	53 (86%)	5 (8%)	4 (6%)	1	8
51	D3	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	1
52	B4	36/38 (95%)	24 (67%)	9 (25%)	3 (8%)	1	5
52	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	0
All	All	11241/11452 (98%)	7412 (66%)	2420 (22%)	1409 (12%)	0	1

5 of 1409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	33	ALA
2	AB	37	VAL
2	AB	72	LYS
2	AB	75	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	142 (79%)	38 (21%)	1	5
2	CB	180/180 (100%)	154 (86%)	26 (14%)	3	14
3	AC	170/170 (100%)	136 (80%)	34 (20%)	1	5
3	CC	170/170 (100%)	153 (90%)	17 (10%)	7	28
4	AD	172/172 (100%)	138 (80%)	34 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	131 (76%)	41 (24%)	0	2
5	AE	113/113 (100%)	77 (68%)	36 (32%)	0	0
5	CE	113/113 (100%)	89 (79%)	24 (21%)	1	5
6	AF	87/87 (100%)	71 (82%)	16 (18%)	1	7
6	CF	87/87 (100%)	73 (84%)	14 (16%)	2	10
7	AG	124/124 (100%)	111 (90%)	13 (10%)	7	26
7	CG	123/124 (99%)	101 (82%)	22 (18%)	2	8
8	AH	104/104 (100%)	83 (80%)	21 (20%)	1	5
8	CH	104/104 (100%)	91 (88%)	13 (12%)	4	18
9	AI	105/105 (100%)	82 (78%)	23 (22%)	1	4
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	12
10	AJ	86/86 (100%)	70 (81%)	16 (19%)	1	7
10	CJ	86/86 (100%)	73 (85%)	13 (15%)	3	12
11	AK	90/90 (100%)	73 (81%)	17 (19%)	1	6
11	CK	90/90 (100%)	79 (88%)	11 (12%)	5	19
12	AL	103/103 (100%)	76 (74%)	27 (26%)	0	1
12	CL	103/103 (100%)	78 (76%)	25 (24%)	0	2
13	AM	92/92 (100%)	84 (91%)	8 (9%)	10	36
13	CM	91/92 (99%)	81 (89%)	10 (11%)	6	25
14	AN	79/83 (95%)	71 (90%)	8 (10%)	7	28
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	18
15	AO	76/76 (100%)	59 (78%)	17 (22%)	1	3
15	CO	76/76 (100%)	69 (91%)	7 (9%)	9	33
16	AP	65/65 (100%)	54 (83%)	11 (17%)	2	9
16	CP	65/65 (100%)	50 (77%)	15 (23%)	1	3
17	AQ	74/74 (100%)	60 (81%)	14 (19%)	1	6
17	CQ	74/74 (100%)	62 (84%)	12 (16%)	2	10
18	AR	48/48 (100%)	44 (92%)	4 (8%)	11	38
18	CR	48/48 (100%)	40 (83%)	8 (17%)	2	9
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	28
19	CS	70/70 (100%)	64 (91%)	6 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/65 (100%)	48 (74%)	17 (26%)	0	1
20	CT	65/65 (100%)	52 (80%)	13 (20%)	1	5
21	AU	44/44 (100%)	36 (82%)	8 (18%)	1	7
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	170 (79%)	46 (21%)	1	4
24	DC	216/216 (100%)	178 (82%)	38 (18%)	2	8
25	BD	164/164 (100%)	133 (81%)	31 (19%)	1	6
25	DD	164/164 (100%)	131 (80%)	33 (20%)	1	5
26	BE	165/165 (100%)	111 (67%)	54 (33%)	0	0
26	DE	165/165 (100%)	143 (87%)	22 (13%)	4	16
27	BF	148/149 (99%)	116 (78%)	32 (22%)	1	4
27	DF	149/149 (100%)	124 (83%)	25 (17%)	2	9
28	BG	137/137 (100%)	106 (77%)	31 (23%)	1	3
28	DG	137/137 (100%)	117 (85%)	20 (15%)	3	13
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	11
29	DH	114/114 (100%)	90 (79%)	24 (21%)	1	5
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	10
30	DI	109/109 (100%)	103 (94%)	6 (6%)	21	53
31	BJ	116/116 (100%)	92 (79%)	24 (21%)	1	5
31	DJ	116/116 (100%)	101 (87%)	15 (13%)	4	18
32	BK	103/103 (100%)	77 (75%)	26 (25%)	0	1
32	DK	103/103 (100%)	84 (82%)	19 (18%)	1	7
33	BL	102/102 (100%)	82 (80%)	20 (20%)	1	6
33	DL	102/102 (100%)	89 (87%)	13 (13%)	4	18
34	BM	109/109 (100%)	81 (74%)	28 (26%)	0	1
34	DM	109/109 (100%)	98 (90%)	11 (10%)	7	28
35	BN	100/100 (100%)	82 (82%)	18 (18%)	1	7
35	DN	100/100 (100%)	85 (85%)	15 (15%)	3	12
36	BO	86/86 (100%)	67 (78%)	19 (22%)	1	4
36	DO	86/86 (100%)	79 (92%)	7 (8%)	11	39
37	BP	99/99 (100%)	66 (67%)	33 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	88 (89%)	11 (11%)	6	24
38	BQ	89/89 (100%)	68 (76%)	21 (24%)	1	2
38	DQ	89/89 (100%)	69 (78%)	20 (22%)	1	3
39	BR	84/84 (100%)	66 (79%)	18 (21%)	1	4
39	DR	84/84 (100%)	69 (82%)	15 (18%)	2	8
40	BS	93/93 (100%)	72 (77%)	21 (23%)	1	3
40	DS	93/93 (100%)	72 (77%)	21 (23%)	1	3
41	BT	80/80 (100%)	53 (66%)	27 (34%)	0	0
41	DT	80/80 (100%)	75 (94%)	5 (6%)	18	48
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	5
42	DU	83/83 (100%)	72 (87%)	11 (13%)	4	16
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	5
43	DV	78/78 (100%)	66 (85%)	12 (15%)	2	11
44	BW	59/59 (100%)	38 (64%)	21 (36%)	0	0
44	DW	59/59 (100%)	45 (76%)	14 (24%)	1	2
45	BX	67/67 (100%)	51 (76%)	16 (24%)	0	2
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	8
46	BY	55/55 (100%)	42 (76%)	13 (24%)	1	2
46	DY	55/55 (100%)	51 (93%)	4 (7%)	14	43
47	BZ	48/48 (100%)	35 (73%)	13 (27%)	0	1
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	5
48	B0	47/47 (100%)	39 (83%)	8 (17%)	2	9
48	D0	47/47 (100%)	38 (81%)	9 (19%)	1	6
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	8
49	D1	45/45 (100%)	38 (84%)	7 (16%)	2	11
50	B2	38/38 (100%)	27 (71%)	11 (29%)	0	1
50	D2	38/38 (100%)	33 (87%)	5 (13%)	4	17
51	B3	51/51 (100%)	42 (82%)	9 (18%)	2	8
51	D3	51/51 (100%)	37 (72%)	14 (28%)	0	1
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	8
52	D4	34/34 (100%)	30 (88%)	4 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9342 (100%)	7599 (81%)	1732 (19%)	<b>1</b> <b>7</b>

5 of 1732 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BQ	89	ILE
50	B2	12	ARG
39	DR	86	GLN
40	BS	1	MET
43	BV	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 360 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	48	GLN
3	CC	139	ASN
42	DU	39	ASN
42	BU	73	ASN
48	B0	41	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	518 (33%)	236 (15%)
1	CA	1529/1533 (99%)	572 (37%)	242 (15%)
22	BA	2850/2904 (98%)	913 (32%)	429 (15%)
22	DA	2839/2904 (97%)	1105 (38%)	498 (17%)
23	BB	117/118 (99%)	34 (29%)	17 (14%)
23	DB	116/118 (98%)	44 (37%)	16 (13%)
All	All	8983/9110 (98%)	3186 (35%)	1438 (16%)

5 of 3186 RNA backbone outliers are listed below:

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

5 of 1438 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2781	A
1	CA	701	U
22	DA	2300	C
23	BB	25	U
1	CA	279	A

## 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 364 ligands modelled in this entry, 363 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
54	ERY	BA	3136	-	53,53,53	0.79	1 (1%)	82,82,82	1.66	19 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	ERY	BA	3136	-	-	7/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	3136	ERY	C6-C5	2.34	1.59	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	3136	ERY	C25-C24-C23	-5.00	102.77	109.97
54	BA	3136	ERY	O7-C5-C6	-4.81	100.45	106.39
54	BA	3136	ERY	O2-C1-O1	-3.57	117.27	123.94
54	BA	3136	ERY	C3-C2-C1	-3.44	102.98	110.01
54	BA	3136	ERY	C27-C26-C25	-3.10	108.53	113.40

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

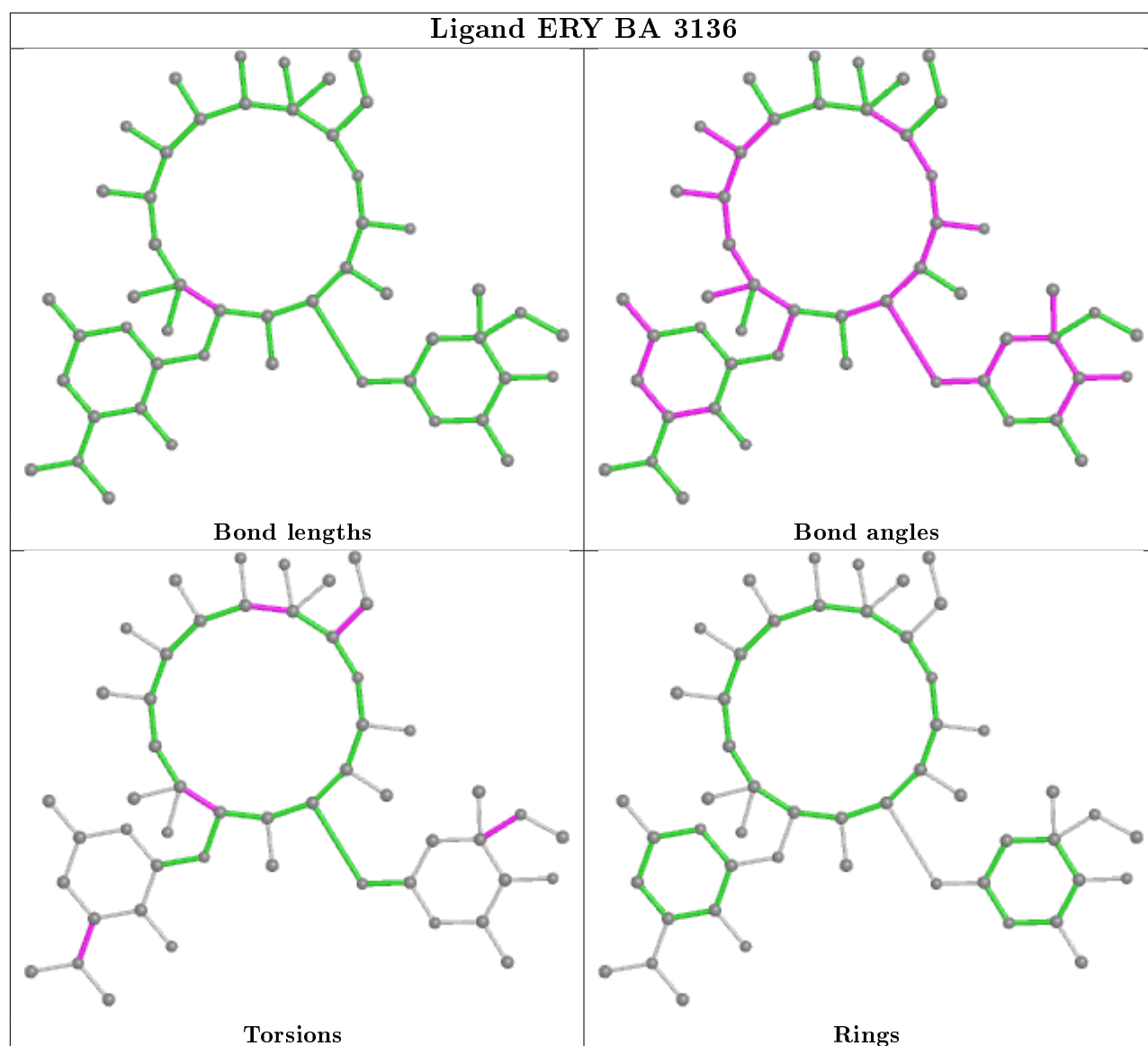
Mol	Chain	Res	Type	Atoms
54	BA	3136	ERY	C15-C16-O5-C20
54	BA	3136	ERY	C19-C16-O5-C20
54	BA	3136	ERY	C10-C11-C12-O13
54	BA	3136	ERY	C25-C24-N1-C28
54	BA	3136	ERY	C4-C5-C6-C32

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	BA	3136	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1533/1533 (100%)	-0.57	15 (0%) 82 67	21, 74, 188, 404	0
1	CA	1530/1533 (99%)	0.03	42 (2%) 54 31	38, 102, 287, 422	0
2	AB	218/218 (100%)	1.58	71 (32%) 0 0	72, 142, 202, 237	0
2	CB	218/218 (100%)	1.57	68 (31%) 0 0	98, 165, 222, 272	0
3	AC	206/206 (100%)	0.65	24 (11%) 4 2	54, 101, 149, 187	0
3	CC	206/206 (100%)	1.14	47 (22%) 0 0	80, 139, 210, 243	0
4	AD	205/205 (100%)	-0.07	8 (3%) 39 20	38, 80, 182, 310	0
4	CD	205/205 (100%)	-0.27	1 (0%) 91 81	29, 54, 103, 236	0
5	AE	150/150 (100%)	-0.10	3 (2%) 65 44	37, 70, 136, 207	0
5	CE	150/150 (100%)	0.33	2 (1%) 77 59	38, 87, 150, 253	0
6	AF	100/100 (100%)	-0.17	0 100 100	43, 85, 149, 174	0
6	CF	100/100 (100%)	0.03	4 (4%) 38 19	58, 109, 180, 202	0
7	AG	151/151 (100%)	0.24	9 (5%) 21 10	82, 155, 235, 286	0
7	CG	150/151 (99%)	2.32	69 (46%) 0 0	112, 196, 246, 272	0
8	AH	129/129 (100%)	-0.04	3 (2%) 60 39	41, 69, 120, 203	0
8	CH	129/129 (100%)	0.63	11 (8%) 10 4	52, 107, 161, 197	0
9	AI	127/127 (100%)	0.87	17 (13%) 3 1	68, 153, 256, 288	0
9	CI	127/127 (100%)	1.84	48 (37%) 0 0	102, 200, 285, 325	0
10	AJ	98/98 (100%)	0.61	16 (16%) 1 1	60, 119, 200, 251	0
10	CJ	98/98 (100%)	2.80	53 (54%) 0 0	102, 192, 267, 283	0
11	AK	117/117 (100%)	0.64	11 (9%) 8 3	38, 104, 176, 222	0
11	CK	117/117 (100%)	0.27	4 (3%) 45 24	53, 102, 161, 200	0
12	AL	123/123 (100%)	-0.34	2 (1%) 72 51	16, 49, 111, 187	0
12	CL	123/123 (100%)	0.19	2 (1%) 72 51	41, 81, 128, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.45	11 (9%) 8 2	69, 139, 213, 258	0
13	CM	114/114 (100%)	2.29	60 (52%) 0 0	190, 427, 522, 545	0
14	AN	96/100 (96%)	0.38	6 (6%) 20 8	68, 111, 199, 266	0
14	CN	95/100 (95%)	2.08	42 (44%) 0 0	112, 209, 319, 350	0
15	AO	88/88 (100%)	-0.41	0 100 100	34, 70, 111, 172	0
15	CO	88/88 (100%)	-0.14	1 (1%) 80 64	68, 112, 187, 286	0
16	AP	82/82 (100%)	0.70	9 (10%) 5 2	45, 68, 174, 288	0
16	CP	81/82 (98%)	0.71	10 (12%) 4 1	46, 97, 157, 229	0
17	AQ	80/80 (100%)	0.40	6 (7%) 14 5	35, 71, 134, 209	0
17	CQ	80/80 (100%)	0.81	12 (15%) 2 1	47, 103, 151, 188	0
18	AR	55/55 (100%)	0.10	3 (5%) 25 11	50, 80, 154, 211	0
18	CR	55/55 (100%)	-0.07	2 (3%) 42 22	51, 87, 157, 235	0
19	AS	79/79 (100%)	1.51	28 (35%) 0 0	81, 150, 212, 259	0
19	CS	79/79 (100%)	2.83	45 (56%) 0 0	217, 411, 508, 531	0
20	AT	85/85 (100%)	-0.32	0 100 100	35, 69, 129, 176	0
20	CT	85/85 (100%)	0.82	11 (12%) 3 1	66, 130, 204, 226	0
21	AU	51/51 (100%)	1.68	19 (37%) 0 0	90, 146, 226, 252	0
21	CU	51/51 (100%)	0.56	7 (13%) 3 1	54, 109, 189, 269	0
22	BA	2854/2904 (98%)	-0.49	36 (1%) 77 59	6, 25, 148, 390	0
22	DA	2841/2904 (97%)	0.23	91 (3%) 47 25	55, 116, 270, 526	0
23	BB	118/118 (100%)	-0.64	0 100 100	12, 40, 73, 109	0
23	DB	117/118 (99%)	-0.13	2 (1%) 70 49	88, 164, 221, 243	0
24	BC	271/271 (100%)	-0.36	6 (2%) 62 41	8, 35, 82, 192	0
24	DC	271/271 (100%)	0.52	21 (7%) 13 5	42, 95, 151, 215	0
25	BD	209/209 (100%)	-0.45	0 100 100	6, 21, 69, 179	0
25	DD	209/209 (100%)	0.73	24 (11%) 4 2	55, 115, 199, 284	0
26	BE	201/201 (100%)	-0.45	0 100 100	7, 36, 86, 151	0
26	DE	201/201 (100%)	1.57	63 (31%) 0 0	61, 235, 398, 470	0
27	BF	178/178 (100%)	-0.04	3 (1%) 70 49	21, 63, 136, 167	0
27	DF	178/178 (100%)	2.18	88 (49%) 0 0	142, 219, 259, 301	0
28	BG	176/176 (100%)	-0.03	2 (1%) 80 64	20, 61, 131, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	176/176 (100%)	1.49	53 (30%) 0 0	88, 239, 337, 389	0
29	BH	149/149 (100%)	3.01	62 (41%) 0 0	40, 171, 260, 304	0
29	DH	149/149 (100%)	2.59	62 (41%) 0 0	68, 188, 268, 298	0
30	BI	141/141 (100%)	2.38	60 (42%) 0 0	170, 245, 289, 301	0
30	DI	141/141 (100%)	3.15	95 (67%) 0 0	178, 312, 349, 370	0
31	BJ	142/142 (100%)	-0.56	1 (0%) 87 75	7, 16, 60, 137	0
31	DJ	142/142 (100%)	0.44	6 (4%) 36 18	50, 106, 169, 198	0
32	BK	122/122 (100%)	-0.41	1 (0%) 86 72	11, 24, 69, 242	0
32	DK	122/122 (100%)	0.58	13 (10%) 6 2	59, 97, 147, 210	0
33	BL	143/143 (100%)	-0.48	0 100 100	6, 30, 71, 123	0
33	DL	143/143 (100%)	1.31	28 (19%) 1 0	59, 164, 279, 354	0
34	BM	136/136 (100%)	-0.54	0 100 100	7, 22, 59, 147	0
34	DM	136/136 (100%)	0.78	16 (11%) 4 2	37, 112, 192, 250	0
35	BN	120/120 (100%)	-0.55	0 100 100	8, 17, 40, 149	0
35	DN	120/120 (100%)	1.36	32 (26%) 0 0	63, 131, 211, 305	0
36	BO	116/116 (100%)	-0.36	0 100 100	21, 41, 72, 113	0
36	DO	116/116 (100%)	1.44	33 (28%) 0 0	106, 172, 240, 273	0
37	BP	114/114 (100%)	-0.44	1 (0%) 84 69	12, 32, 87, 176	0
37	DP	114/114 (100%)	0.82	16 (14%) 2 1	50, 110, 175, 196	0
38	BQ	117/117 (100%)	-0.62	1 (0%) 84 69	6, 15, 39, 225	0
38	DQ	117/117 (100%)	0.90	18 (15%) 2 1	65, 113, 193, 331	0
39	BR	103/103 (100%)	-0.54	1 (0%) 82 67	6, 26, 67, 184	0
39	DR	103/103 (100%)	1.92	45 (43%) 0 0	73, 144, 238, 305	0
40	BS	110/110 (100%)	-0.57	0 100 100	7, 15, 48, 172	0
40	DS	110/110 (100%)	1.46	37 (33%) 0 0	71, 132, 214, 254	0
41	BT	93/93 (100%)	-0.02	3 (3%) 47 25	13, 43, 123, 233	0
41	DT	93/93 (100%)	2.36	47 (50%) 0 0	124, 265, 379, 423	0
42	BU	102/102 (100%)	-0.21	1 (0%) 82 67	21, 45, 131, 240	0
42	DU	102/102 (100%)	3.11	62 (60%) 0 0	148, 305, 420, 554	0
43	BV	94/94 (100%)	-0.31	0 100 100	14, 38, 78, 135	0
43	DV	94/94 (100%)	0.97	18 (19%) 1 0	88, 136, 193, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BW	79/79 (100%)	-0.15	2 (2%) 57 34	13, 29, 98, 213	0
44	DW	79/79 (100%)	2.08	34 (43%) 0 0	73, 169, 279, 323	0
45	BX	77/77 (100%)	-0.58	0 100 100	13, 37, 77, 108	0
45	DX	77/77 (100%)	0.76	11 (14%) 2 1	62, 118, 215, 280	0
46	BY	63/63 (100%)	-0.14	1 (1%) 72 51	27, 59, 126, 209	0
46	DY	63/63 (100%)	1.59	18 (28%) 0 0	152, 379, 492, 508	0
47	BZ	58/58 (100%)	-0.61	0 100 100	9, 16, 47, 61	0
47	DZ	58/58 (100%)	0.45	5 (8%) 10 4	68, 143, 251, 271	0
48	B0	56/56 (100%)	-0.69	0 100 100	6, 18, 71, 138	0
48	D0	56/56 (100%)	1.43	17 (30%) 0 0	63, 144, 246, 262	0
49	B1	50/50 (100%)	0.12	3 (6%) 21 10	27, 47, 93, 115	0
49	D1	50/50 (100%)	1.55	14 (28%) 0 0	97, 154, 208, 231	0
50	B2	46/46 (100%)	-0.55	0 100 100	10, 19, 43, 195	0
50	D2	46/46 (100%)	1.23	8 (17%) 1 0	59, 119, 184, 211	0
51	B3	64/64 (100%)	-0.54	0 100 100	8, 22, 38, 65	0
51	D3	64/64 (100%)	1.11	12 (18%) 1 0	64, 122, 197, 255	0
52	B4	38/38 (100%)	0.27	2 (5%) 26 12	25, 49, 94, 97	0
52	D4	38/38 (100%)	3.07	26 (68%) 0 0	87, 173, 235, 241	0
All	All	20434/20562 (99%)	0.30	2003 (9%) 7 2	6, 93, 274, 554	0

The worst 5 of 2003 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	21.2
29	DH	124	THR	18.3
29	DH	91	PHE	16.3
29	BH	118	PRO	15.6
16	AP	81	ALA	15.5

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
53	MG	DJ	201	1/1	-0.33	3.04	284,284,284,284	0
53	MG	DA	3016	1/1	-0.03	0.67	231,231,231,231	0
53	MG	DA	3099	1/1	0.00	0.23	180,180,180,180	0
53	MG	DA	3028	1/1	0.04	1.00	262,262,262,262	0
53	MG	DA	3003	1/1	0.08	1.79	268,268,268,268	0
53	MG	DA	3109	1/1	0.10	0.71	176,176,176,176	0
53	MG	DA	3130	1/1	0.12	2.63	279,279,279,279	0
53	MG	DA	3133	1/1	0.18	0.46	239,239,239,239	0
53	MG	DA	3111	1/1	0.22	0.40	127,127,127,127	0
53	MG	CA	1622	1/1	0.22	0.08	208,208,208,208	0
53	MG	CA	1636	1/1	0.28	0.18	155,155,155,155	0
53	MG	DA	3062	1/1	0.30	1.10	193,193,193,193	0
53	MG	DA	3064	1/1	0.31	1.24	230,230,230,230	0
53	MG	DA	3110	1/1	0.32	0.17	183,183,183,183	0
53	MG	DA	3078	1/1	0.38	1.03	210,210,210,210	0
53	MG	DA	3043	1/1	0.43	0.44	213,213,213,213	0
53	MG	DA	3082	1/1	0.51	0.36	189,189,189,189	0
53	MG	CA	1614	1/1	0.51	1.04	231,231,231,231	0
53	MG	DA	3087	1/1	0.54	0.17	164,164,164,164	0
53	MG	DA	3083	1/1	0.55	0.20	224,224,224,224	0
53	MG	DA	3014	1/1	0.56	0.29	128,128,128,128	0
53	MG	BA	3047	1/1	0.57	0.16	152,152,152,152	0
53	MG	DA	3127	1/1	0.57	0.59	199,199,199,199	0
53	MG	DA	3058	1/1	0.57	0.49	235,235,235,235	0
53	MG	CA	1628	1/1	0.57	1.56	236,236,236,236	0
53	MG	CA	1602	1/1	0.58	0.20	175,175,175,175	0
53	MG	DA	3033	1/1	0.59	0.53	149,149,149,149	0
53	MG	DA	3059	1/1	0.59	0.22	183,183,183,183	0
53	MG	DA	3010	1/1	0.60	0.50	171,171,171,171	0
53	MG	DA	3013	1/1	0.60	0.88	185,185,185,185	0
53	MG	DA	3074	1/1	0.60	1.20	240,240,240,240	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	DA	3045	1/1	0.61	0.49	233,233,233,233	0
53	MG	DA	3047	1/1	0.62	0.19	136,136,136,136	0
53	MG	DA	3015	1/1	0.62	0.40	145,145,145,145	0
53	MG	DA	3039	1/1	0.62	0.13	99,99,99,99	0
53	MG	DA	3084	1/1	0.62	0.18	182,182,182,182	0
53	MG	DA	3018	1/1	0.63	0.25	232,232,232,232	0
53	MG	DA	3038	1/1	0.63	0.12	204,204,204,204	0
53	MG	DA	3106	1/1	0.64	0.15	205,205,205,205	0
53	MG	DA	3097	1/1	0.65	0.25	116,116,116,116	0
53	MG	CA	1640	1/1	0.67	0.21	149,149,149,149	0
53	MG	DA	3020	1/1	0.67	0.51	218,218,218,218	0
53	MG	CA	1627	1/1	0.67	0.21	198,198,198,198	0
53	MG	DA	3006	1/1	0.67	0.21	267,267,267,267	0
53	MG	DA	3002	1/1	0.67	0.32	160,160,160,160	0
53	MG	CA	1620	1/1	0.67	0.10	170,170,170,170	0
53	MG	DA	3132	1/1	0.68	0.10	175,175,175,175	0
53	MG	BA	3130	1/1	0.70	0.47	205,205,205,205	0
53	MG	DA	3092	1/1	0.70	0.12	121,121,121,121	0
53	MG	DA	3026	1/1	0.71	0.98	244,244,244,244	0
53	MG	CA	1607	1/1	0.71	0.26	154,154,154,154	0
53	MG	CA	1601	1/1	0.71	0.12	179,179,179,179	0
53	MG	BB	201	1/1	0.71	0.32	236,236,236,236	0
53	MG	AA	1634	1/1	0.72	0.15	199,199,199,199	0
53	MG	DA	3125	1/1	0.72	0.31	163,163,163,163	0
53	MG	CA	1637	1/1	0.72	0.13	63,63,63,63	0
53	MG	DA	3007	1/1	0.72	0.45	253,253,253,253	0
53	MG	DA	3027	1/1	0.73	0.10	144,144,144,144	0
53	MG	DA	3063	1/1	0.73	2.07	192,192,192,192	0
53	MG	AA	1618	1/1	0.74	0.09	164,164,164,164	0
53	MG	DA	3050	1/1	0.74	0.13	125,125,125,125	0
53	MG	CA	1629	1/1	0.74	0.20	217,217,217,217	0
53	MG	DA	3032	1/1	0.74	0.14	100,100,100,100	0
53	MG	CA	1610	1/1	0.74	0.09	175,175,175,175	0
53	MG	DA	3095	1/1	0.74	0.21	116,116,116,116	0
53	MG	CA	1617	1/1	0.75	0.17	280,280,280,280	0
53	MG	DA	3009	1/1	0.76	0.17	101,101,101,101	0
53	MG	DA	3001	1/1	0.76	0.12	130,130,130,130	0
53	MG	BA	3057	1/1	0.76	0.23	161,161,161,161	0
53	MG	BA	3048	1/1	0.76	0.18	104,104,104,104	0
53	MG	BA	3132	1/1	0.76	0.23	165,165,165,165	0
53	MG	DA	3122	1/1	0.77	0.11	72,72,72,72	0
53	MG	DA	3073	1/1	0.78	0.11	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	DA	3049	1/1	0.78	0.32	235,235,235,235	0
53	MG	DA	3051	1/1	0.78	0.21	124,124,124,124	0
53	MG	DA	3036	1/1	0.79	0.16	211,211,211,211	0
53	MG	DA	3116	1/1	0.79	0.18	66,66,66,66	0
53	MG	AA	1638	1/1	0.79	0.12	102,102,102,102	0
53	MG	DA	3008	1/1	0.80	0.14	142,142,142,142	0
53	MG	BA	3083	1/1	0.80	0.20	113,113,113,113	0
53	MG	AA	1619	1/1	0.80	0.15	125,125,125,125	0
53	MG	DB	201	1/1	0.80	0.09	114,114,114,114	0
53	MG	DA	3057	1/1	0.80	0.50	212,212,212,212	0
53	MG	CA	1603	1/1	0.80	0.32	165,165,165,165	0
53	MG	CA	1618	1/1	0.80	0.31	139,139,139,139	0
53	MG	DA	3114	1/1	0.81	0.16	123,123,123,123	0
53	MG	DA	3070	1/1	0.81	0.11	56,56,56,56	0
53	MG	DA	3108	1/1	0.81	0.41	172,172,172,172	0
53	MG	AA	1607	1/1	0.81	0.15	119,119,119,119	0
53	MG	DA	3079	1/1	0.81	0.63	150,150,150,150	0
53	MG	AA	1604	1/1	0.82	0.14	120,120,120,120	0
53	MG	DA	3098	1/1	0.82	0.15	118,118,118,118	0
53	MG	DA	3022	1/1	0.82	0.27	162,162,162,162	0
53	MG	CA	1632	1/1	0.82	0.16	163,163,163,163	0
53	MG	AA	1617	1/1	0.82	0.68	203,203,203,203	0
53	MG	DA	3023	1/1	0.82	0.12	78,78,78,78	0
53	MG	BA	3091	1/1	0.82	0.26	113,113,113,113	0
53	MG	DA	3042	1/1	0.83	0.17	94,94,94,94	0
53	MG	DA	3120	1/1	0.83	0.23	76,76,76,76	0
53	MG	DA	3075	1/1	0.83	0.39	140,140,140,140	0
53	MG	CA	1633	1/1	0.83	0.10	77,77,77,77	0
53	MG	CA	1613	1/1	0.83	0.11	114,114,114,114	0
53	MG	DA	3115	1/1	0.83	0.25	139,139,139,139	0
53	MG	DA	3094	1/1	0.83	0.09	96,96,96,96	0
53	MG	DA	3101	1/1	0.84	0.21	104,104,104,104	0
53	MG	AA	1628	1/1	0.84	0.18	183,183,183,183	0
53	MG	CA	1639	1/1	0.84	0.10	226,226,226,226	0
53	MG	DA	3061	1/1	0.84	0.11	134,134,134,134	0
53	MG	CA	1630	1/1	0.84	0.09	123,123,123,123	0
53	MG	BA	3011	1/1	0.84	0.30	131,131,131,131	0
53	MG	DA	3017	1/1	0.84	0.13	68,68,68,68	0
53	MG	BA	3112	1/1	0.84	0.28	89,89,89,89	0
53	MG	BA	3090	1/1	0.85	0.07	73,73,73,73	0
53	MG	BA	3061	1/1	0.85	0.28	223,223,223,223	0
53	MG	DA	3035	1/1	0.86	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BA	3002	1/1	0.86	0.11	77,77,77,77	0
53	MG	BA	3084	1/1	0.86	0.20	50,50,50,50	0
53	MG	BA	3004	1/1	0.86	0.24	147,147,147,147	0
53	MG	DA	3131	1/1	0.86	0.16	70,70,70,70	0
53	MG	CA	1612	1/1	0.86	0.39	120,120,120,120	0
53	MG	DA	3126	1/1	0.86	0.10	76,76,76,76	0
53	MG	DA	3053	1/1	0.86	0.12	80,80,80,80	0
53	MG	DA	3088	1/1	0.86	0.14	141,141,141,141	0
53	MG	DA	3123	1/1	0.86	0.20	165,165,165,165	0
53	MG	DA	3089	1/1	0.86	0.24	69,69,69,69	0
53	MG	DA	3029	1/1	0.86	0.47	151,151,151,151	0
53	MG	CA	1631	1/1	0.86	0.22	88,88,88,88	0
53	MG	BA	3082	1/1	0.86	0.19	85,85,85,85	0
53	MG	DA	3104	1/1	0.86	0.17	34,34,34,34	0
53	MG	DA	3011	1/1	0.87	0.17	152,152,152,152	0
53	MG	AA	1610	1/1	0.87	0.12	210,210,210,210	0
53	MG	CA	1616	1/1	0.87	0.35	232,232,232,232	0
53	MG	DA	3072	1/1	0.87	0.14	132,132,132,132	0
53	MG	DA	3069	1/1	0.87	0.19	202,202,202,202	0
53	MG	BA	3059	1/1	0.87	0.22	109,109,109,109	0
53	MG	BA	3098	1/1	0.87	0.16	51,51,51,51	0
53	MG	BA	3007	1/1	0.87	0.10	69,69,69,69	0
53	MG	BA	3119	1/1	0.88	0.11	12,12,12,12	0
53	MG	DA	3005	1/1	0.88	1.07	309,309,309,309	0
53	MG	DA	3024	1/1	0.88	0.15	106,106,106,106	0
53	MG	DA	3086	1/1	0.88	0.16	94,94,94,94	0
53	MG	DA	3004	1/1	0.88	0.12	80,80,80,80	0
53	MG	DC	301	1/1	0.88	0.12	124,124,124,124	0
53	MG	CA	1638	1/1	0.88	0.15	139,139,139,139	0
53	MG	BA	3075	1/1	0.88	0.19	69,69,69,69	0
53	MG	CA	1611	1/1	0.88	0.20	122,122,122,122	0
53	MG	CA	1623	1/1	0.88	0.13	120,120,120,120	0
53	MG	DA	3054	1/1	0.88	0.08	71,71,71,71	0
53	MG	BA	3086	1/1	0.88	0.18	88,88,88,88	0
53	MG	AA	1616	1/1	0.88	0.16	78,78,78,78	0
53	MG	BA	3033	1/1	0.88	0.16	10,10,10,10	0
53	MG	DA	3025	1/1	0.88	0.12	110,110,110,110	0
53	MG	DC	302	1/1	0.88	0.27	121,121,121,121	0
53	MG	BA	3125	1/1	0.89	0.18	41,41,41,41	0
53	MG	AA	1626	1/1	0.89	0.18	106,106,106,106	0
53	MG	DA	3071	1/1	0.89	0.19	52,52,52,52	0
53	MG	BA	3073	1/1	0.89	0.18	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BA	3089	1/1	0.89	0.09	30,30,30,30	0
53	MG	DA	3096	1/1	0.89	0.09	92,92,92,92	0
53	MG	BA	3055	1/1	0.89	0.32	191,191,191,191	0
53	MG	CA	1608	1/1	0.89	0.15	51,51,51,51	0
53	MG	DA	3118	1/1	0.89	0.12	70,70,70,70	0
53	MG	CA	1619	1/1	0.89	0.15	201,201,201,201	0
53	MG	DA	3076	1/1	0.89	0.28	158,158,158,158	0
53	MG	CA	1625	1/1	0.89	0.30	91,91,91,91	0
53	MG	BA	3092	1/1	0.89	0.07	38,38,38,38	0
53	MG	BA	3087	1/1	0.89	0.17	125,125,125,125	0
53	MG	AA	1630	1/1	0.89	0.14	87,87,87,87	0
53	MG	DA	3068	1/1	0.89	0.11	78,78,78,78	0
53	MG	DA	3031	1/1	0.90	0.10	79,79,79,79	0
53	MG	DA	3046	1/1	0.90	0.10	76,76,76,76	0
53	MG	AA	1622	1/1	0.90	0.13	97,97,97,97	0
53	MG	BA	3060	1/1	0.90	0.48	174,174,174,174	0
53	MG	DA	3129	1/1	0.90	0.73	203,203,203,203	0
53	MG	AA	1635	1/1	0.90	0.10	88,88,88,88	0
53	MG	AA	1633	1/1	0.90	0.08	75,75,75,75	0
53	MG	AA	1602	1/1	0.90	0.12	119,119,119,119	0
53	MG	DA	3060	1/1	0.90	0.50	161,161,161,161	0
53	MG	AA	1639	1/1	0.90	0.15	126,126,126,126	0
53	MG	DA	3090	1/1	0.90	0.10	91,91,91,91	0
53	MG	DA	3085	1/1	0.90	0.29	148,148,148,148	0
53	MG	DA	3091	1/1	0.91	0.38	200,200,200,200	0
53	MG	DA	3103	1/1	0.91	0.16	98,98,98,98	0
53	MG	BA	3028	1/1	0.91	0.11	32,32,32,32	0
53	MG	DA	3080	1/1	0.91	0.15	137,137,137,137	0
53	MG	DA	3065	1/1	0.91	0.22	83,83,83,83	0
53	MG	AA	1603	1/1	0.91	0.17	121,121,121,121	0
53	MG	DA	3040	1/1	0.91	0.17	52,52,52,52	0
53	MG	DA	3093	1/1	0.91	0.16	228,228,228,228	0
53	MG	DA	3112	1/1	0.91	0.14	66,66,66,66	0
53	MG	BA	3078	1/1	0.91	0.08	41,41,41,41	0
53	MG	CA	1624	1/1	0.91	0.69	179,179,179,179	0
53	MG	CA	1615	1/1	0.91	0.09	124,124,124,124	0
53	MG	AA	1612	1/1	0.91	0.20	104,104,104,104	0
53	MG	AA	1614	1/1	0.91	0.14	197,197,197,197	0
53	MG	DA	3034	1/1	0.91	0.09	89,89,89,89	0
53	MG	BA	3069	1/1	0.91	0.10	176,176,176,176	0
53	MG	DA	3119	1/1	0.91	0.14	88,88,88,88	0
53	MG	DA	3037	1/1	0.91	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BA	3115	1/1	0.91	0.15	10,10,10,10	0
53	MG	AA	1606	1/1	0.91	0.11	58,58,58,58	0
53	MG	CA	1641	1/1	0.92	0.14	80,80,80,80	0
53	MG	BA	3114	1/1	0.92	0.16	144,144,144,144	0
53	MG	CA	1626	1/1	0.92	0.26	29,29,29,29	0
53	MG	DA	3030	1/1	0.92	0.17	111,111,111,111	0
53	MG	BA	3062	1/1	0.92	0.15	15,15,15,15	0
53	MG	DA	3044	1/1	0.92	0.17	83,83,83,83	0
53	MG	BA	3131	1/1	0.92	0.11	140,140,140,140	0
53	MG	DA	3048	1/1	0.92	0.18	132,132,132,132	0
53	MG	BA	3025	1/1	0.92	0.46	119,119,119,119	0
53	MG	CA	1609	1/1	0.92	0.20	80,80,80,80	0
53	MG	BA	3123	1/1	0.92	0.45	118,118,118,118	0
53	MG	AA	1636	1/1	0.92	0.08	25,25,25,25	0
53	MG	AA	1623	1/1	0.92	0.09	72,72,72,72	0
53	MG	BA	3001	1/1	0.92	0.14	110,110,110,110	0
53	MG	DA	3100	1/1	0.92	0.19	93,93,93,93	0
53	MG	BB	202	1/1	0.93	0.07	43,43,43,43	0
53	MG	DA	3107	1/1	0.93	0.18	121,121,121,121	0
53	MG	BA	3034	1/1	0.93	0.30	154,154,154,154	0
53	MG	BA	3079	1/1	0.93	0.18	30,30,30,30	0
53	MG	AN	202	1/1	0.93	0.15	169,169,169,169	0
53	MG	BB	203	1/1	0.93	0.12	17,17,17,17	0
53	MG	DA	3052	1/1	0.93	0.10	49,49,49,49	0
55	ZN	D4	101	1/1	0.93	0.09	151,151,151,151	0
53	MG	CA	1634	1/1	0.93	0.12	153,153,153,153	0
53	MG	DA	3128	1/1	0.93	0.24	123,123,123,123	0
53	MG	DA	3121	1/1	0.93	0.23	119,119,119,119	0
53	MG	BA	3122	1/1	0.93	0.11	21,21,21,21	0
53	MG	DA	3012	1/1	0.93	0.09	51,51,51,51	0
53	MG	CA	1606	1/1	0.93	0.14	63,63,63,63	0
53	MG	AA	1629	1/1	0.93	0.07	183,183,183,183	0
53	MG	BA	3134	1/1	0.93	0.22	143,143,143,143	0
53	MG	BA	3042	1/1	0.93	0.14	18,18,18,18	0
53	MG	BA	3099	1/1	0.93	0.10	18,18,18,18	0
53	MG	DA	3041	1/1	0.94	0.13	122,122,122,122	0
53	MG	DA	3113	1/1	0.94	0.07	96,96,96,96	0
53	MG	BA	3117	1/1	0.94	0.08	83,83,83,83	0
53	MG	DA	3056	1/1	0.94	0.13	112,112,112,112	0
53	MG	DA	3105	1/1	0.94	0.14	51,51,51,51	0
53	MG	BA	3052	1/1	0.94	0.12	25,25,25,25	0
53	MG	BA	3014	1/1	0.94	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	AA	1615	1/1	0.94	0.05	128,128,128,128	0
53	MG	BA	3103	1/1	0.94	0.20	7,7,7,7	0
53	MG	BA	3015	1/1	0.94	0.13	38,38,38,38	0
53	MG	AA	1609	1/1	0.94	0.06	28,28,28,28	0
53	MG	BA	3003	1/1	0.94	0.12	42,42,42,42	0
53	MG	BA	3036	1/1	0.94	0.39	169,169,169,169	0
53	MG	BA	3110	1/1	0.94	0.20	102,102,102,102	0
53	MG	DA	3117	1/1	0.94	0.17	71,71,71,71	0
53	MG	CA	1621	1/1	0.94	0.21	55,55,55,55	0
53	MG	DA	3019	1/1	0.94	0.20	224,224,224,224	0
53	MG	DA	3077	1/1	0.95	0.26	114,114,114,114	0
53	MG	BA	3076	1/1	0.95	0.06	32,32,32,32	0
53	MG	AA	1637	1/1	0.95	0.09	104,104,104,104	0
53	MG	BA	3100	1/1	0.95	0.21	24,24,24,24	0
53	MG	BA	3070	1/1	0.95	0.24	134,134,134,134	0
53	MG	AA	1605	1/1	0.95	0.16	35,35,35,35	0
53	MG	BA	3108	1/1	0.95	0.18	8,8,8,8	0
53	MG	BA	3018	1/1	0.95	0.16	40,40,40,40	0
53	MG	DA	3102	1/1	0.95	0.06	62,62,62,62	0
53	MG	AA	1625	1/1	0.95	0.31	121,121,121,121	0
53	MG	BA	3097	1/1	0.95	0.14	80,80,80,80	0
53	MG	AA	1613	1/1	0.95	0.08	57,57,57,57	0
53	MG	DA	3055	1/1	0.95	0.10	84,84,84,84	0
53	MG	BA	3101	1/1	0.95	0.13	64,64,64,64	0
53	MG	BA	3005	1/1	0.95	0.10	93,93,93,93	0
53	MG	CA	1605	1/1	0.95	0.21	40,40,40,40	0
53	MG	BA	3104	1/1	0.95	0.19	12,12,12,12	0
53	MG	BA	3009	1/1	0.95	0.13	13,13,13,13	0
53	MG	BA	3120	1/1	0.95	0.10	53,53,53,53	0
53	MG	BA	3010	1/1	0.95	0.08	19,19,19,19	0
53	MG	BA	3102	1/1	0.95	0.13	23,23,23,23	0
53	MG	BA	3118	1/1	0.95	0.37	168,168,168,168	0
53	MG	AA	1627	1/1	0.95	0.06	78,78,78,78	0
53	MG	BA	3050	1/1	0.95	0.12	37,37,37,37	0
53	MG	BA	3031	1/1	0.95	0.09	34,34,34,34	0
53	MG	AA	1621	1/1	0.95	0.14	91,91,91,91	0
53	MG	AA	1611	1/1	0.96	0.06	54,54,54,54	0
53	MG	BA	3046	1/1	0.96	0.15	16,16,16,16	0
53	MG	DA	3021	1/1	0.96	0.19	41,41,41,41	0
53	MG	BA	3135	1/1	0.96	0.44	196,196,196,196	0
53	MG	BA	3040	1/1	0.96	0.21	8,8,8,8	0
53	MG	BA	3021	1/1	0.96	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BA	3066	1/1	0.96	0.15	11,11,11,11	0
53	MG	BA	3016	1/1	0.96	0.13	7,7,7,7	0
53	MG	BA	3019	1/1	0.96	0.31	10,10,10,10	0
53	MG	BA	3067	1/1	0.96	0.12	10,10,10,10	0
53	MG	BA	3071	1/1	0.96	0.15	112,112,112,112	0
53	MG	AA	1601	1/1	0.96	0.13	78,78,78,78	0
53	MG	BA	3093	1/1	0.96	0.07	45,45,45,45	0
53	MG	BA	3096	1/1	0.96	0.11	45,45,45,45	0
53	MG	BA	3023	1/1	0.96	0.10	7,7,7,7	0
53	MG	AA	1608	1/1	0.96	0.15	32,32,32,32	0
53	MG	BA	3080	1/1	0.96	0.13	11,11,11,11	0
53	MG	BA	3106	1/1	0.96	0.15	25,25,25,25	0
53	MG	AN	201	1/1	0.96	0.07	105,105,105,105	0
53	MG	BA	3133	1/1	0.96	0.18	10,10,10,10	0
53	MG	BA	3113	1/1	0.96	0.09	21,21,21,21	0
53	MG	DA	3124	1/1	0.96	0.12	48,48,48,48	0
54	ERY	BA	3136	51/51	0.96	0.23	5,11,15,16	0
53	MG	BA	3128	1/1	0.96	0.17	7,7,7,7	0
53	MG	BA	3121	1/1	0.96	0.18	10,10,10,10	0
53	MG	BA	3049	1/1	0.96	0.16	11,11,11,11	0
53	MG	CA	1604	1/1	0.96	0.07	60,60,60,60	0
53	MG	BA	3111	1/1	0.96	0.16	74,74,74,74	0
53	MG	BA	3058	1/1	0.97	0.07	35,35,35,35	0
53	MG	BA	3038	1/1	0.97	0.13	7,7,7,7	0
53	MG	CA	1642	1/1	0.97	0.05	58,58,58,58	0
53	MG	AA	1631	1/1	0.97	0.13	69,69,69,69	0
53	MG	BA	3077	1/1	0.97	0.15	121,121,121,121	0
53	MG	BA	3027	1/1	0.97	0.19	109,109,109,109	0
53	MG	BA	3022	1/1	0.97	0.14	9,9,9,9	0
53	MG	BA	3043	1/1	0.97	0.12	29,29,29,29	0
53	MG	BA	3116	1/1	0.97	0.07	17,17,17,17	0
53	MG	BA	3008	1/1	0.97	0.14	13,13,13,13	0
53	MG	BA	3127	1/1	0.97	0.15	15,15,15,15	0
53	MG	BA	3064	1/1	0.97	0.10	6,6,6,6	0
53	MG	AA	1641	1/1	0.97	0.12	39,39,39,39	0
53	MG	BA	3072	1/1	0.97	0.12	10,10,10,10	0
53	MG	BA	3012	1/1	0.97	0.15	6,6,6,6	0
53	MG	DA	3066	1/1	0.97	0.08	48,48,48,48	0
53	MG	DA	3081	1/1	0.97	0.10	92,92,92,92	0
53	MG	BA	3065	1/1	0.97	0.09	7,7,7,7	0
53	MG	BA	3056	1/1	0.97	0.24	233,233,233,233	0
53	MG	BA	3035	1/1	0.97	0.12	11,11,11,11	0

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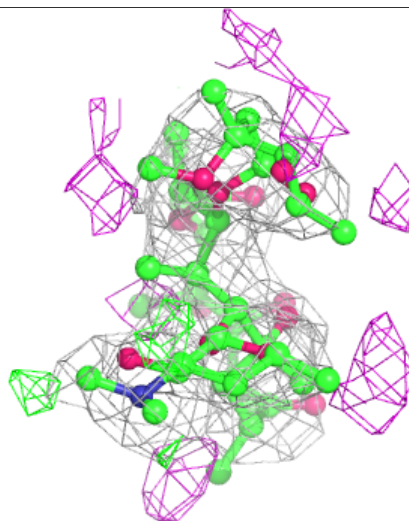
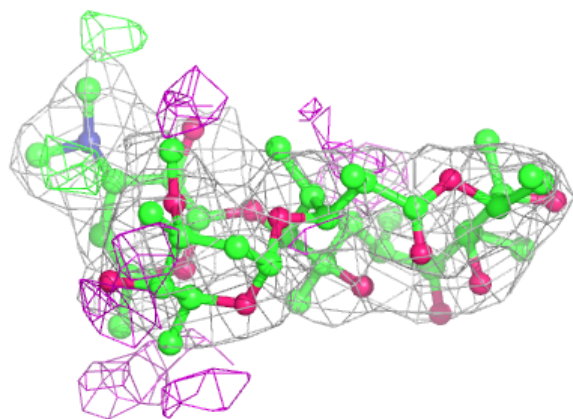
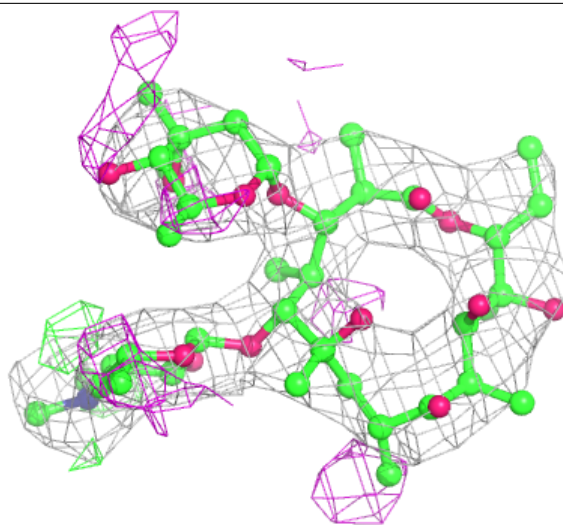
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BA	3017	1/1	0.97	0.09	30,30,30,30	0
53	MG	AA	1620	1/1	0.97	0.19	28,28,28,28	0
53	MG	BA	3129	1/1	0.97	0.12	14,14,14,14	0
53	MG	AA	1624	1/1	0.97	0.24	31,31,31,31	0
53	MG	CA	1635	1/1	0.97	0.08	85,85,85,85	0
53	MG	DA	3067	1/1	0.97	0.10	38,38,38,38	0
53	MG	BB	204	1/1	0.97	0.09	20,20,20,20	0
53	MG	BA	3041	1/1	0.98	0.19	13,13,13,13	0
53	MG	BA	3095	1/1	0.98	0.10	22,22,22,22	0
53	MG	BA	3054	1/1	0.98	0.10	25,25,25,25	0
53	MG	BA	3074	1/1	0.98	0.15	18,18,18,18	0
53	MG	BA	3024	1/1	0.98	0.11	17,17,17,17	0
53	MG	BA	3006	1/1	0.98	0.06	31,31,31,31	0
53	MG	AA	1640	1/1	0.98	0.18	17,17,17,17	0
53	MG	BA	3030	1/1	0.98	0.22	15,15,15,15	0
53	MG	BA	3088	1/1	0.98	0.05	11,11,11,11	0
53	MG	BA	3124	1/1	0.98	0.15	16,16,16,16	0
53	MG	BA	3020	1/1	0.98	0.15	35,35,35,35	0
53	MG	BA	3029	1/1	0.98	0.09	66,66,66,66	0
53	MG	BA	3107	1/1	0.98	0.17	8,8,8,8	0
53	MG	BA	3105	1/1	0.98	0.14	9,9,9,9	0
53	MG	BA	3026	1/1	0.98	0.07	19,19,19,19	0
53	MG	BA	3037	1/1	0.98	0.13	17,17,17,17	0
53	MG	BA	3109	1/1	0.98	0.06	57,57,57,57	0
53	MG	BA	3081	1/1	0.98	0.08	39,39,39,39	0
53	MG	BA	3032	1/1	0.98	0.13	16,16,16,16	0
53	MG	BA	3094	1/1	0.98	0.09	24,24,24,24	0
53	MG	BA	3085	1/1	0.98	0.13	6,6,6,6	0
53	MG	BA	3068	1/1	0.99	0.10	20,20,20,20	0
53	MG	BA	3044	1/1	0.99	0.22	14,14,14,14	0
55	ZN	B4	101	1/1	0.99	0.10	84,84,84,84	0
53	MG	AA	1632	1/1	0.99	0.11	31,31,31,31	0
53	MG	BA	3126	1/1	0.99	0.11	18,18,18,18	0
53	MG	BA	3039	1/1	0.99	0.17	20,20,20,20	0
53	MG	BA	3051	1/1	0.99	0.12	10,10,10,10	0
53	MG	BA	3053	1/1	0.99	0.09	9,9,9,9	0
53	MG	BA	3063	1/1	0.99	0.18	13,13,13,13	0
53	MG	BA	3045	1/1	0.99	0.13	17,17,17,17	0
53	MG	BA	3013	1/1	0.99	0.17	9,9,9,9	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

**Electron density around ERY BA 3136:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.