



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:13 PM UTC

PDB ID : 4V9D / pdb_00004v9d
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.
Deposited on : 2012-07-31
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

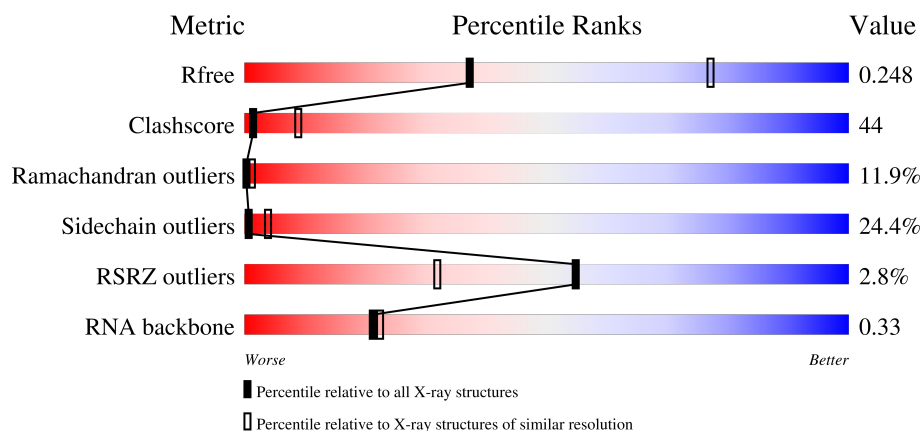
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1539	17% 58% 25%
1	BA	1539	15% 60% 25%
2	AB	218	7% 8% 43% 39% 10%
2	BB	218	5% 12% 52% 27% 8%

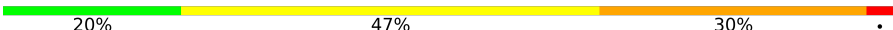
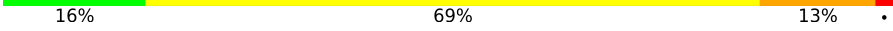
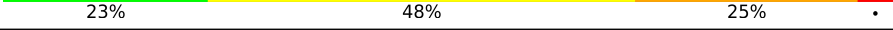
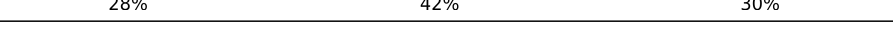
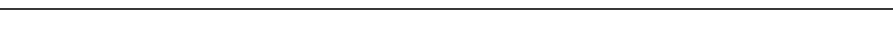
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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	150	
5	BE	150	
6	AF	100	
6	BF	100	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

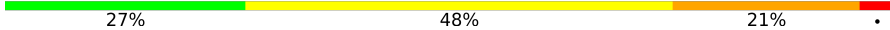
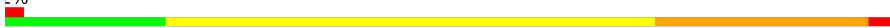
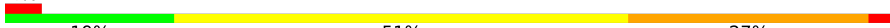
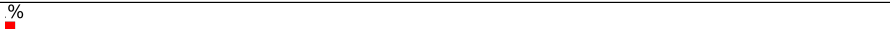
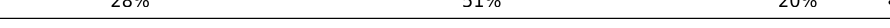
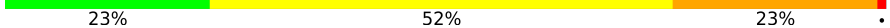
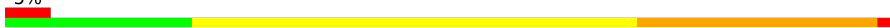
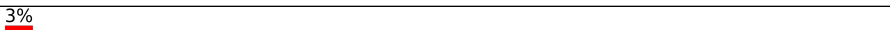
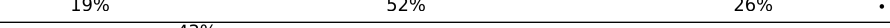
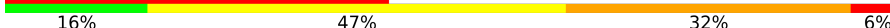
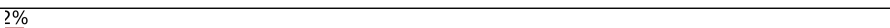
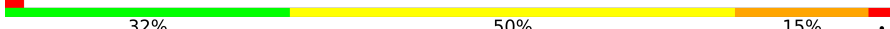
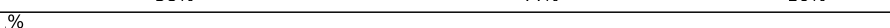
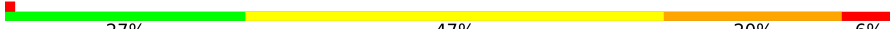
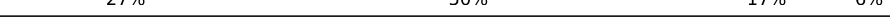
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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	85	
20	BT	85	
21	AU	51	
21	BU	51	
22	AV	76	
22	BV	76	
23	AX	16	
23	BX	16	
24	AY	183	
25	CA	2903	
25	DA	2903	
26	CB	119	
27	CC	271	
27	DC	271	
28	CD	209	
28	DD	209	

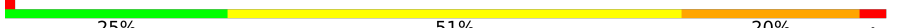
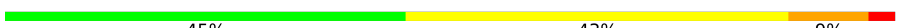
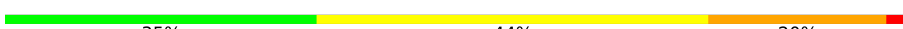
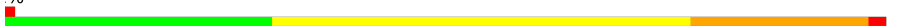
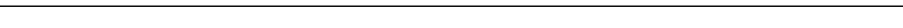
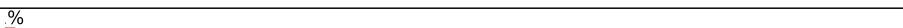
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Mol	Chain	Length	Quality of chain
29	CE	201	
29	DE	201	
30	CF	177	
30	DF	177	
31	CG	176	
31	DG	176	
32	CH	149	
32	DH	149	
33	CI	141	
33	DI	141	
34	CJ	142	
34	DJ	142	
35	CK	122	
35	DK	122	
36	CL	143	
36	DL	143	
37	CM	136	
37	DM	136	
38	CN	120	
38	DN	120	
39	CO	116	
39	DO	116	
40	CP	114	
40	DP	114	
41	CQ	117	

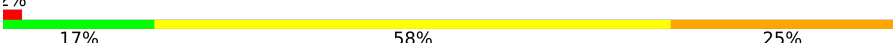
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Mol	Chain	Length	Quality of chain
41	DQ	117	
42	CR	103	
42	DR	103	
43	CS	110	
43	DS	110	
44	CT	93	
44	DT	93	
45	CU	102	
45	DU	102	
46	CV	94	
46	DV	94	
47	CW	76	
48	CX	77	
48	DX	77	
49	CY	63	
49	DY	63	
50	CZ	58	
50	DZ	58	
51	C0	56	
51	D0	56	
52	C1	50	
52	D1	50	
53	C2	46	
53	D2	46	
54	C3	64	

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Mol	Chain	Length	Quality of chain
54	D3	64	
55	C4	38	
55	D4	38	
56	DB	118	
57	DW	75	

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
58	MG	CA	3062	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	BB	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	BC	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	BD	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	BE	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	BF	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	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	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	BI	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	BJ	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	BK	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	BL	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	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	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	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	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	BR	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	BS	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	BT	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	BU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	BV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	BX	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	2	GLY	-	expression tag	UNP P0A805

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	DA	2896	Total	C	N	O	P	0	0	0
			62173	27735	11441	20101	2896			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CB	119	Total	C	N	O	P	0	0	0
			2548	1135	466	829	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
41	DQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CW	76	Total	C	N	O	S	0	0	0
			575	356	117	101	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	C1	50	Total	C	N	O	0	0	0
			410	263	75	72			
52	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a RNA chain called 5S rRNA.

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

- Molecule 57 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DW	75	Total	C	N	O	S	0	0	0
			564	350	113	100	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	72	Total	Mg	0	0
			72	72		
58	BA	56	Total	Mg	0	0
			56	56		
58	CA	194	Total	Mg	0	0
			194	194		
58	CB	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CQ	1	Total 1	Mg 1	0	0
58	DA	166	Total 166	Mg 166	0	0
58	DB	3	Total 3	Mg 3	0	0
58	DL	1	Total 1	Mg 1	0	0
58	DQ	1	Total 1	Mg 1	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C4	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	197	Total 197	O 197	0	0
60	AN	4	Total 4	O 4	0	0
60	AT	1	Total 1	O 1	0	0
60	AU	1	Total 1	O 1	0	0
60	BA	190	Total 190	O 190	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	5	Total 5	O 5	0	0
60	BT	1	Total 1	O 1	0	0
60	BU	1	Total 1	O 1	0	0
60	CA	625	Total 625	O 625	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CB	13	Total 13	O 13	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	2	Total 2	O 2	0	0
60	CE	2	Total 2	O 2	0	0
60	CF	1	Total 1	O 1	0	0
60	CJ	1	Total 1	O 1	0	0
60	CL	6	Total 6	O 6	0	0
60	CN	4	Total 4	O 4	0	0
60	CS	1	Total 1	O 1	0	0
60	CV	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	622	Total 622	O 622	0	0
60	DB	14	Total 14	O 14	0	0
60	DC	4	Total 4	O 4	0	0
60	DD	5	Total 5	O 5	0	0
60	DE	2	Total 2	O 2	0	0
60	DJ	1	Total 1	O 1	0	0
60	DL	4	Total 4	O 4	0	0
60	DN	1	Total 1	O 1	0	0

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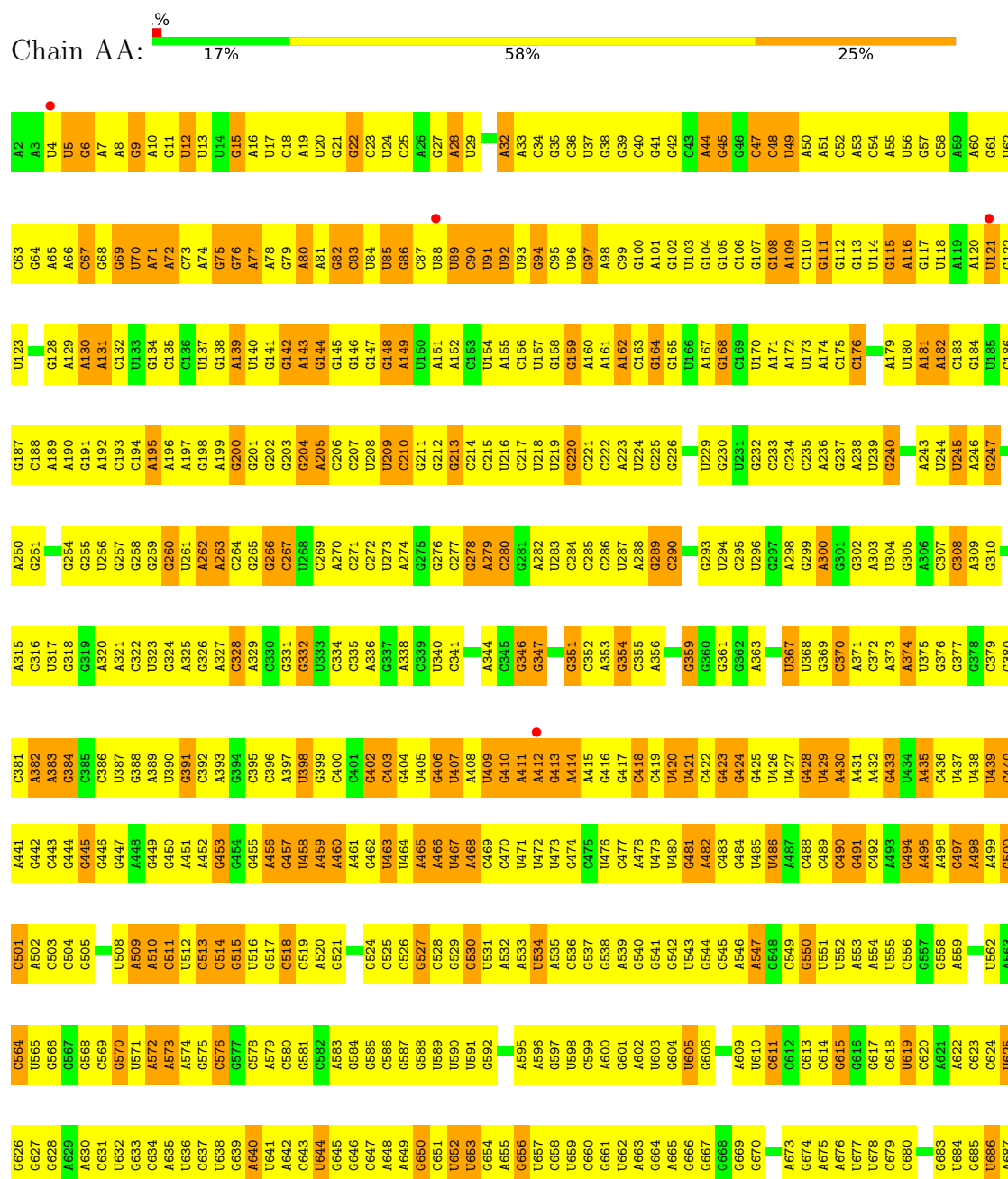
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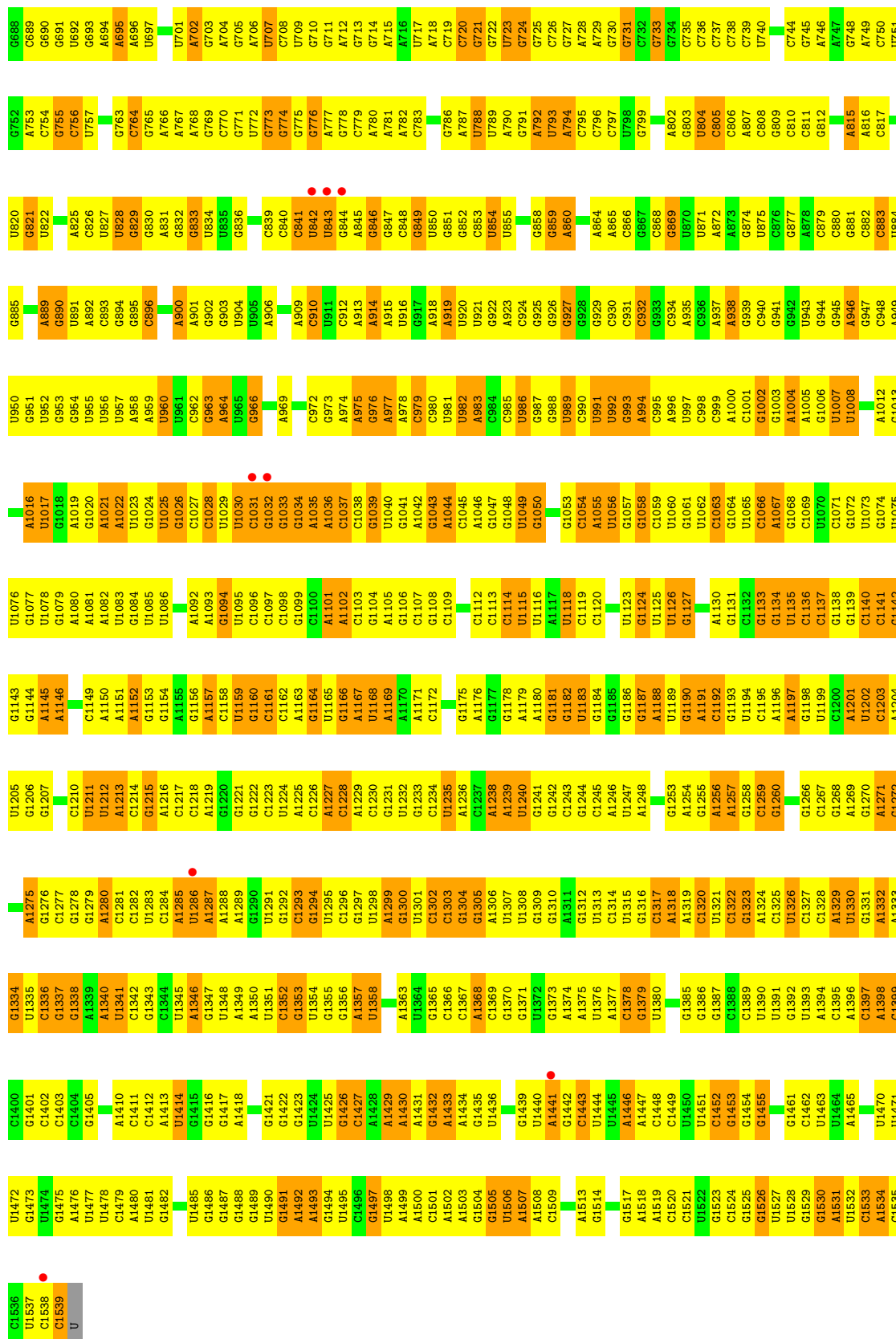
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			1	1		
60	D2	1	Total	O	0	0
			1	1		
60	D3	2	Total	O	0	0
			2	2		
60	D4	1	Total	O	0	0
			1	1		

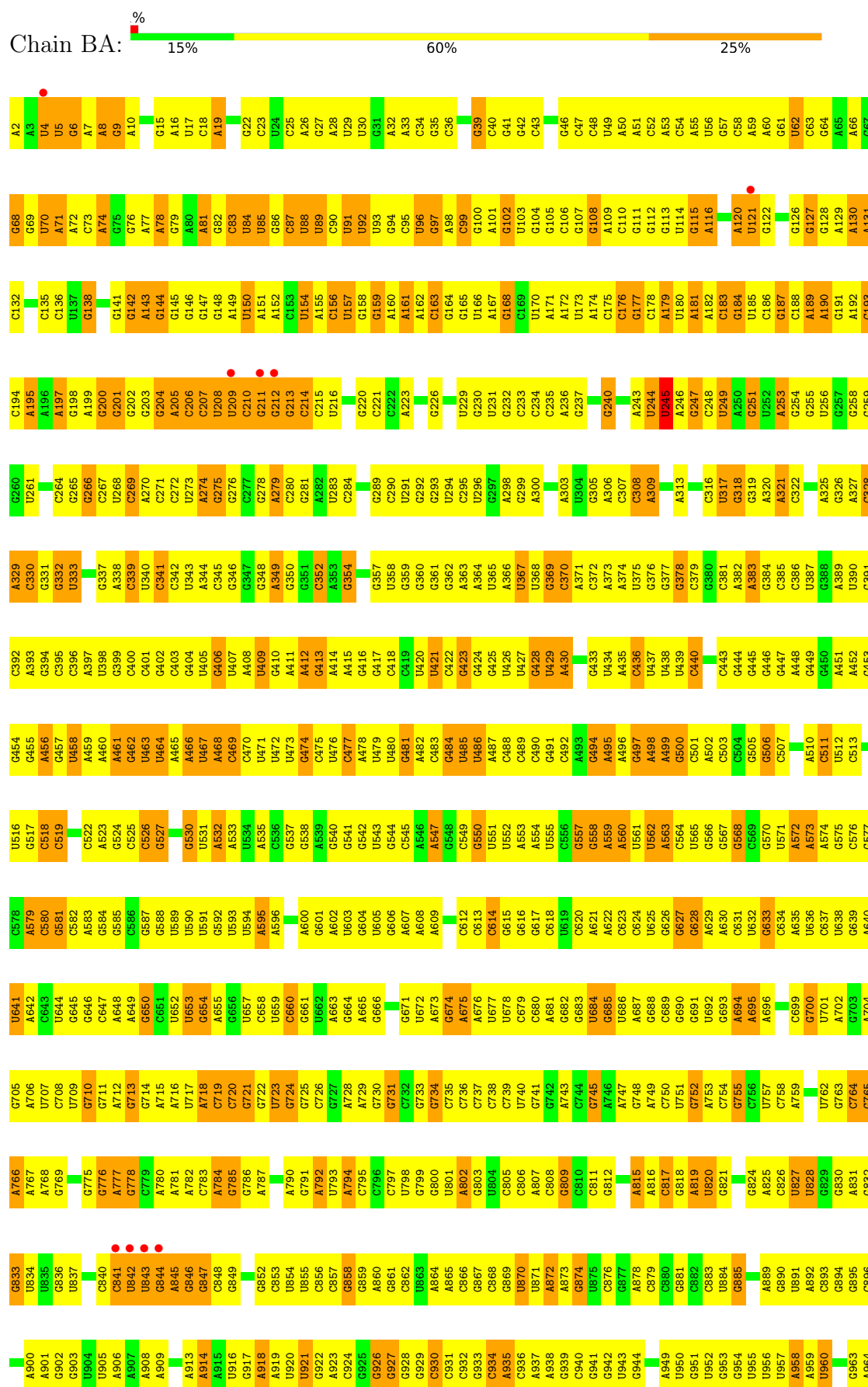
3 Residue-property plots

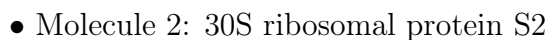
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA



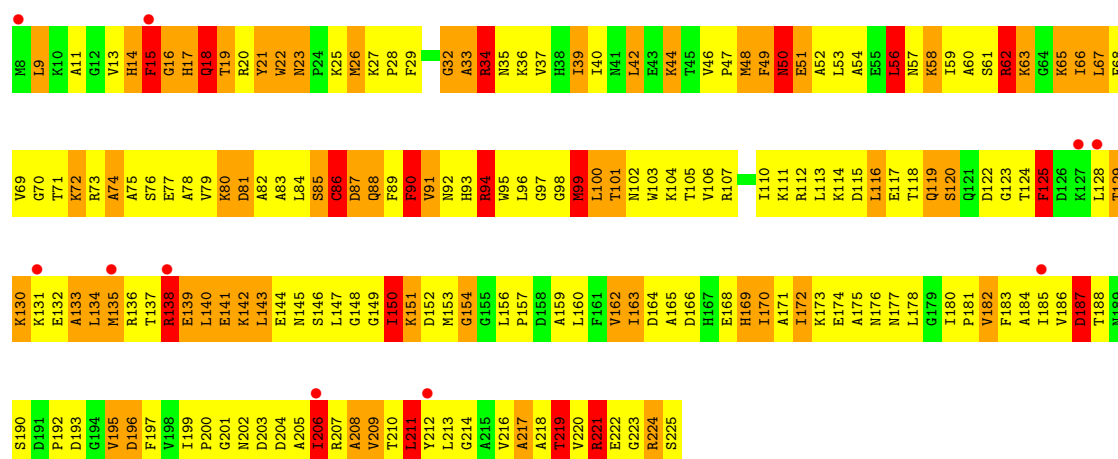
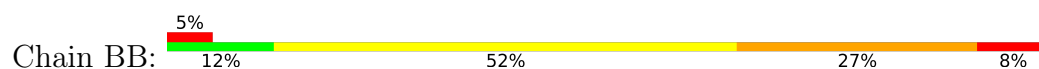




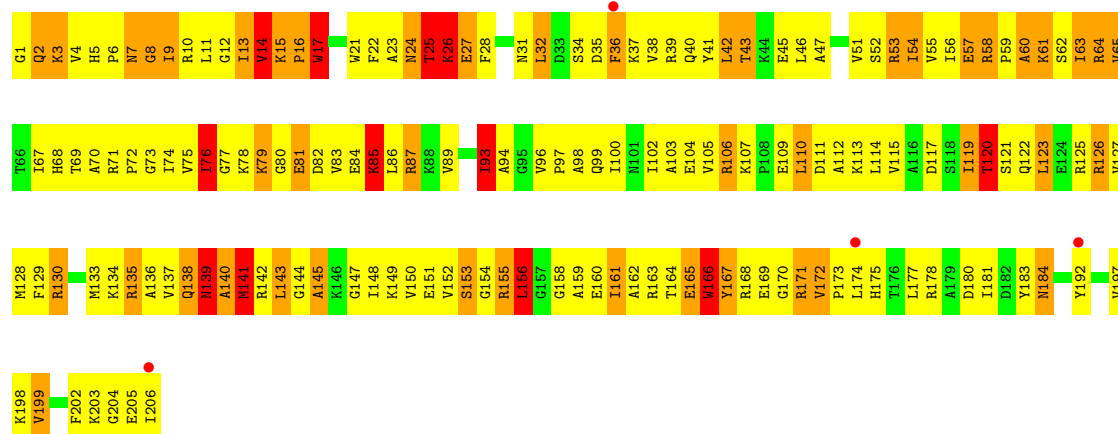




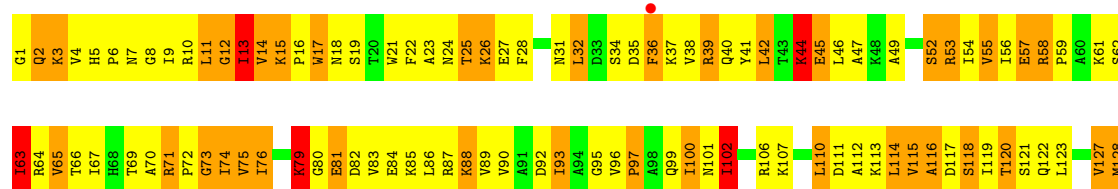
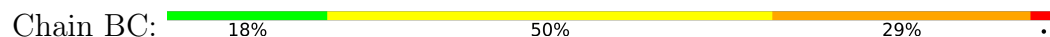
• Molecule 2: 30S ribosomal protein S2

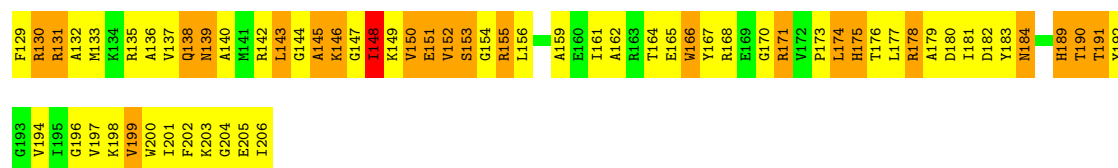


• Molecule 3: 30S ribosomal protein S3

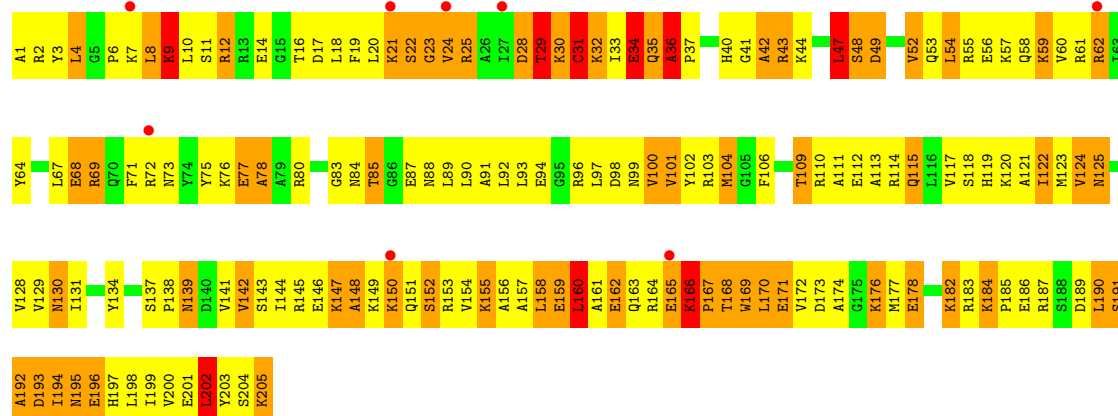
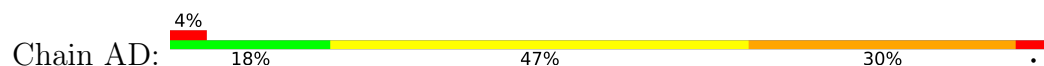


• Molecule 3: 30S ribosomal protein S3

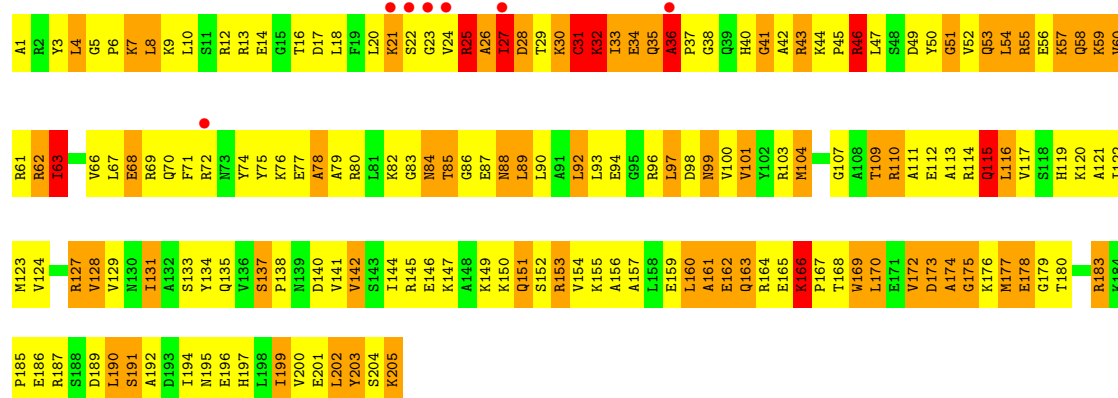
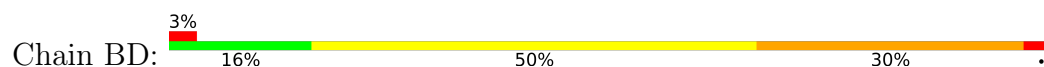




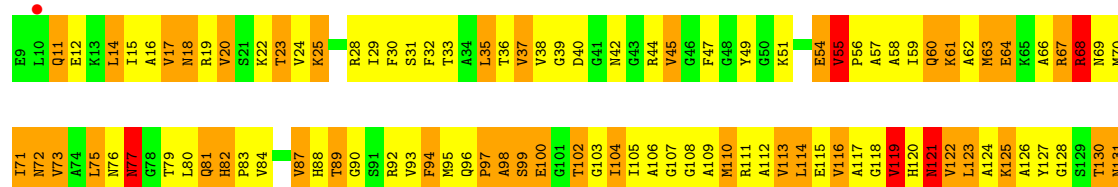
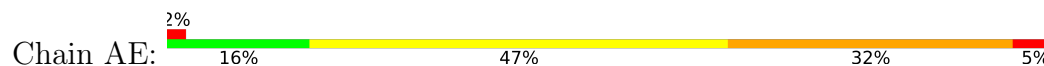
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

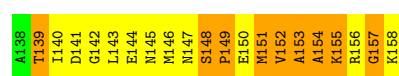
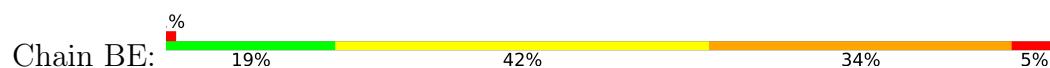


• Molecule 5: 30S ribosomal protein S5

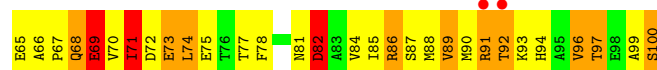
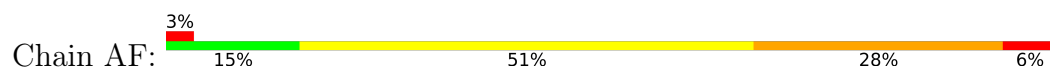




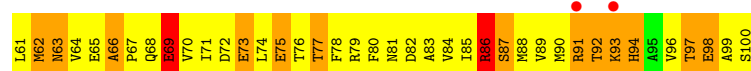
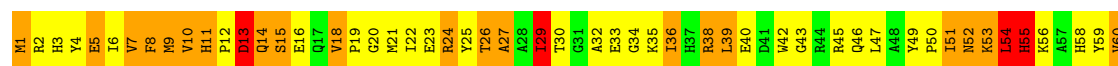
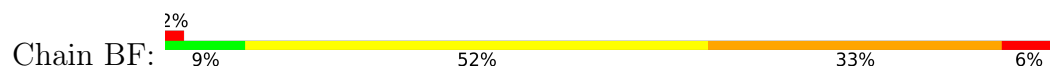
- Molecule 5: 30S ribosomal protein S5



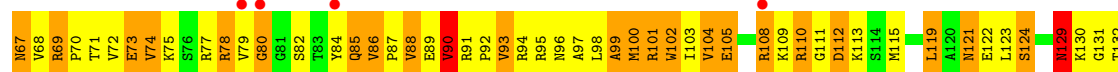
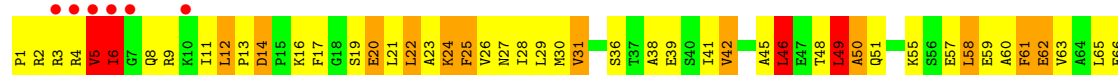
- Molecule 6: 30S ribosomal protein S6

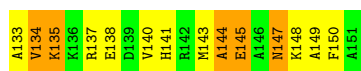


- Molecule 6: 30S ribosomal protein S6

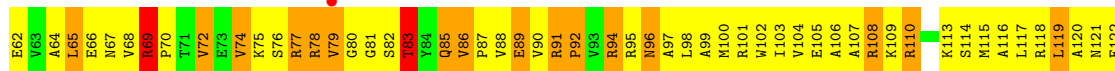
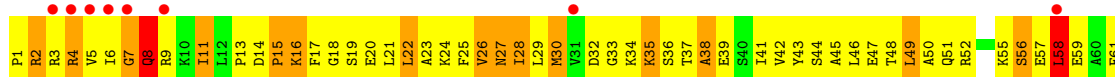
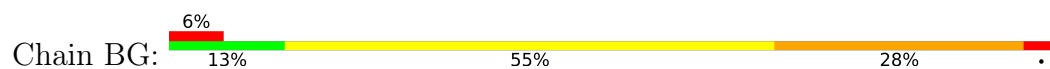


- Molecule 7: 30S ribosomal protein S7

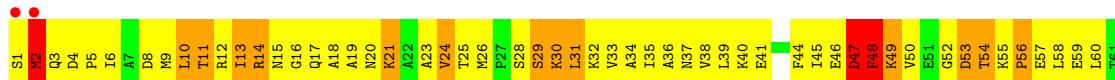




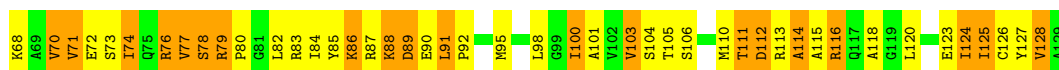
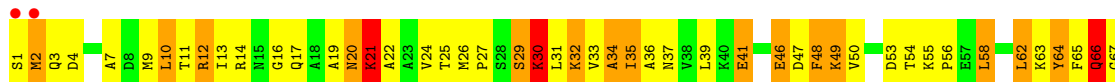
• Molecule 7: 30S ribosomal protein S7



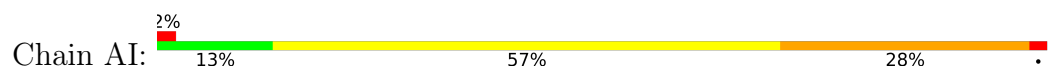
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

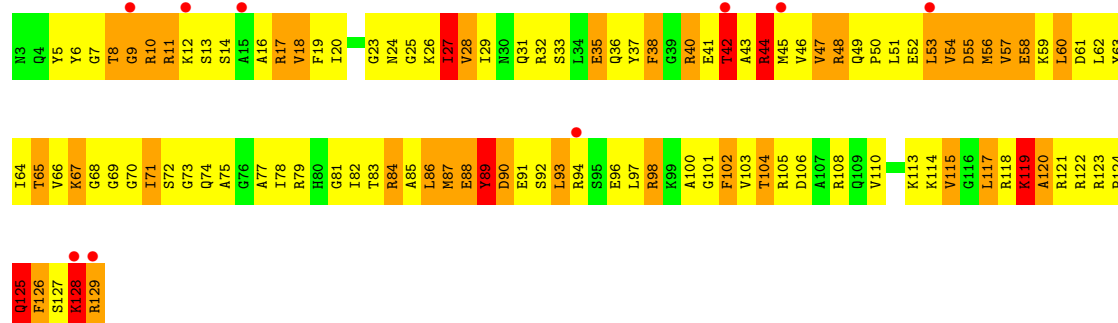
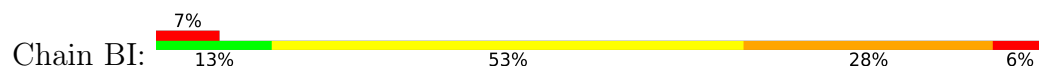


• Molecule 9: 30S ribosomal protein S9

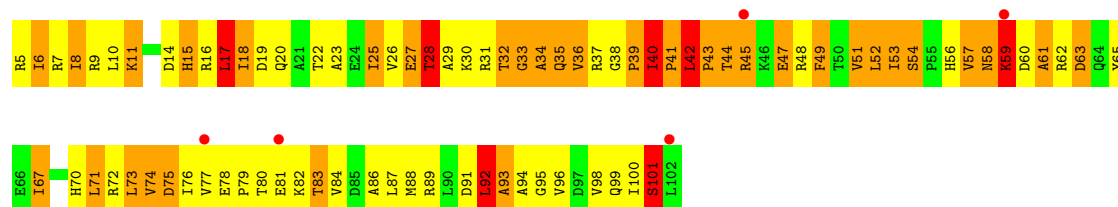
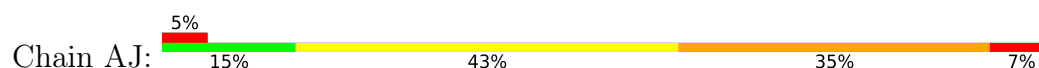




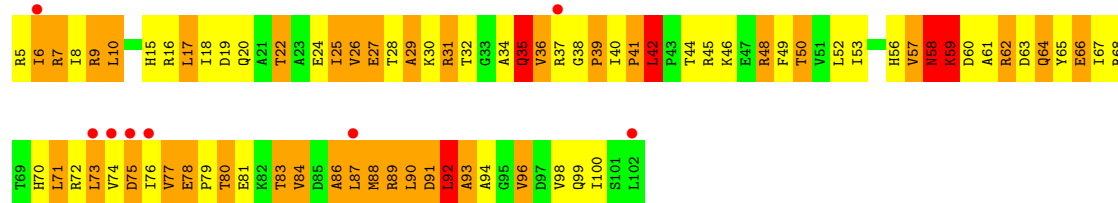
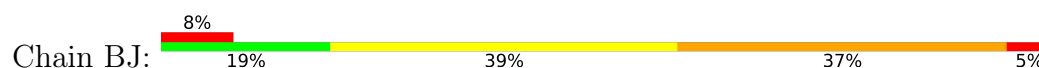
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

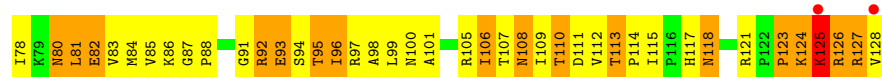


• Molecule 10: 30S ribosomal protein S10

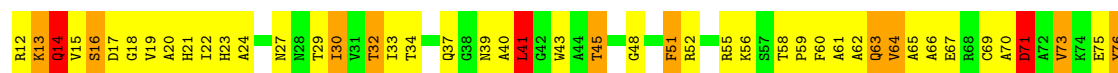


• Molecule 11: 30S ribosomal protein S11

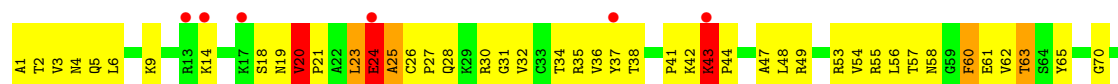




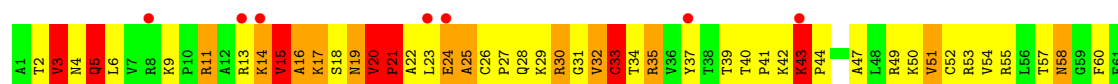
- Molecule 11: 30S ribosomal protein S11



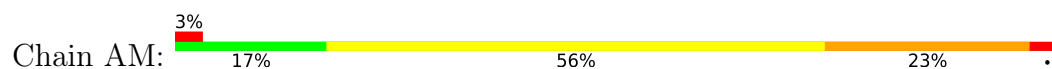
- Molecule 12: 30S ribosomal protein S12



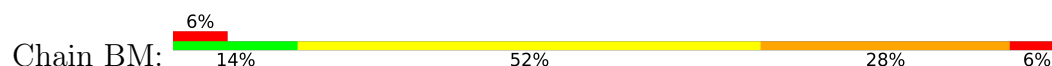
- Molecule 12: 30S ribosomal protein S12

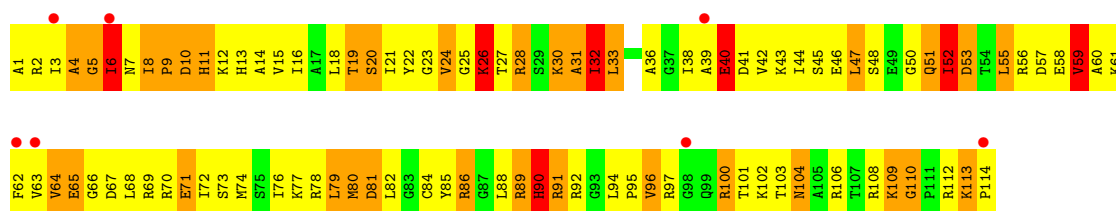


- Molecule 13: 30S ribosomal protein S13

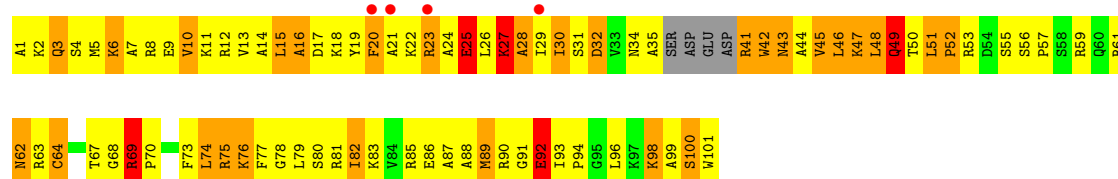
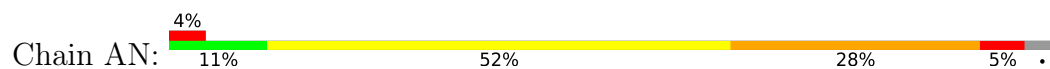


- Molecule 13: 30S ribosomal protein S13

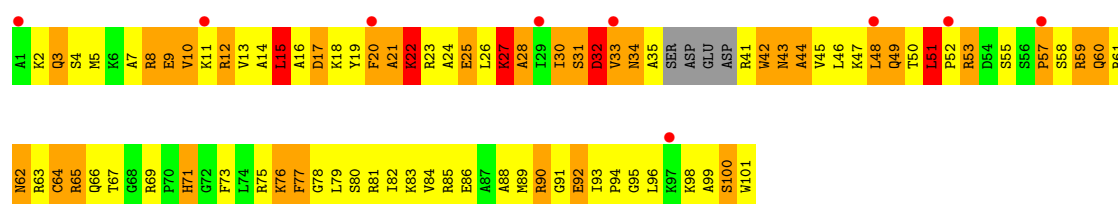
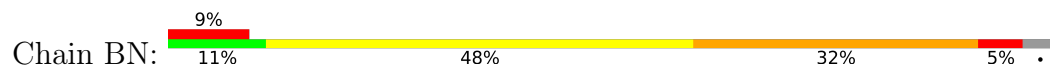




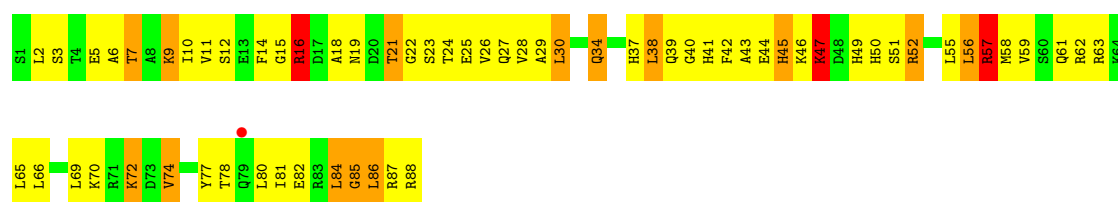
• Molecule 14: 30S ribosomal protein S14



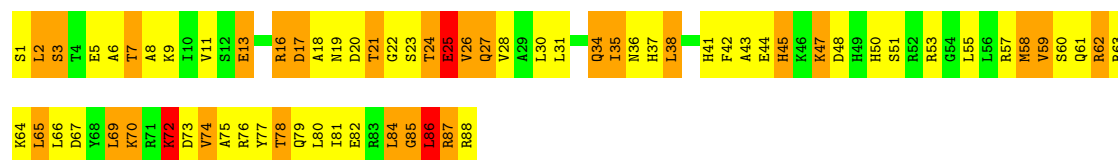
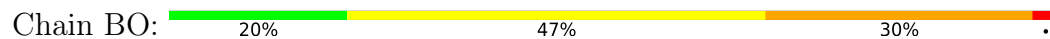
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

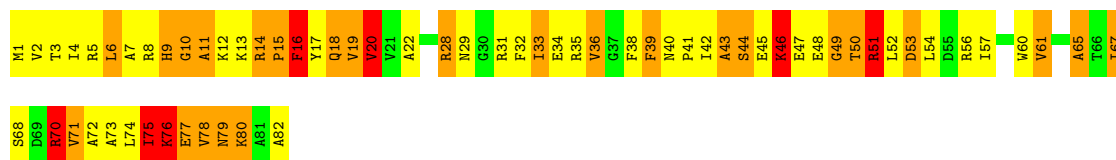


• Molecule 15: 30S ribosomal protein S15



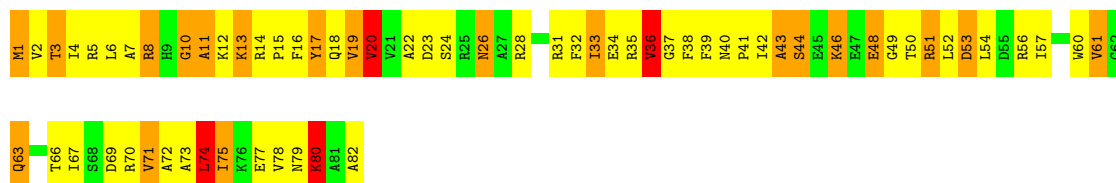
• Molecule 16: 30S ribosomal protein S16

Chain AP: 21% 40% 30% 9%



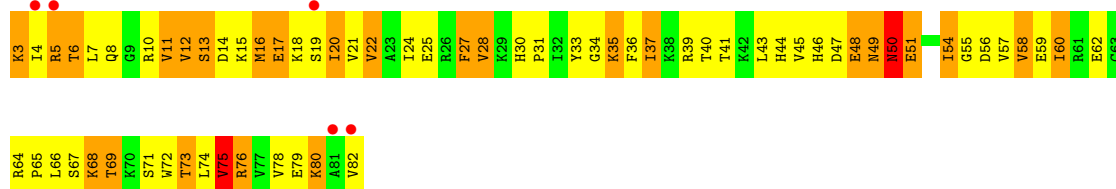
- Molecule 16: 30S ribosomal protein S16

Chain BP: 21% 50% 24% 5%



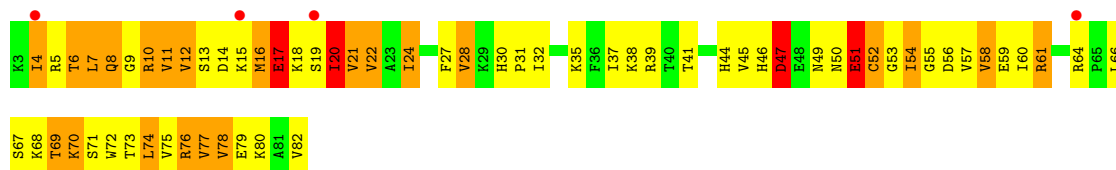
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 6% 18% 49% 31% .



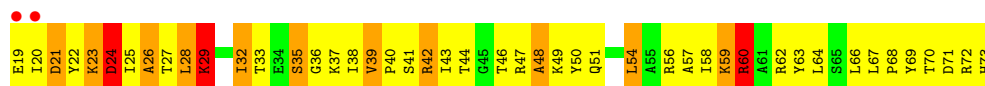
- Molecule 17: 30S ribosomal protein S17

Chain BQ: 5% 20% 48% 28% 5%



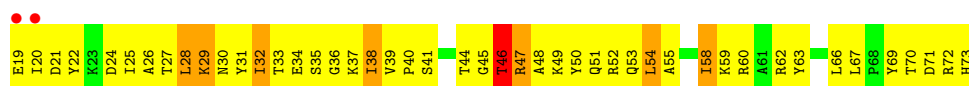
- Molecule 18: 30S ribosomal protein S18

Chain AR: 4% 16% 58% 20% 5%

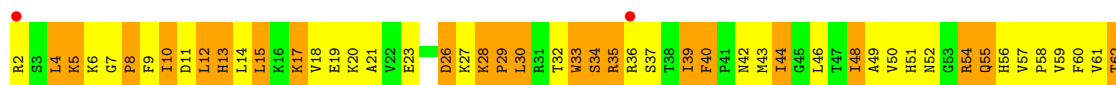
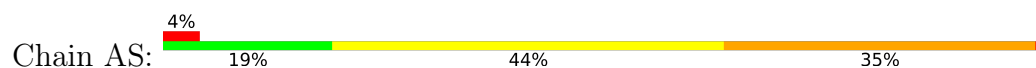


- Molecule 18: 30S ribosomal protein S18

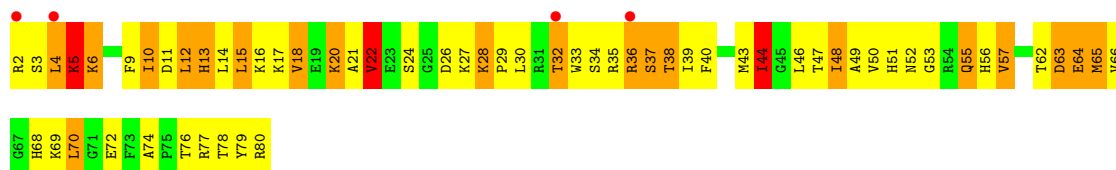
Chain BR: 4% 16% 69% 13% .



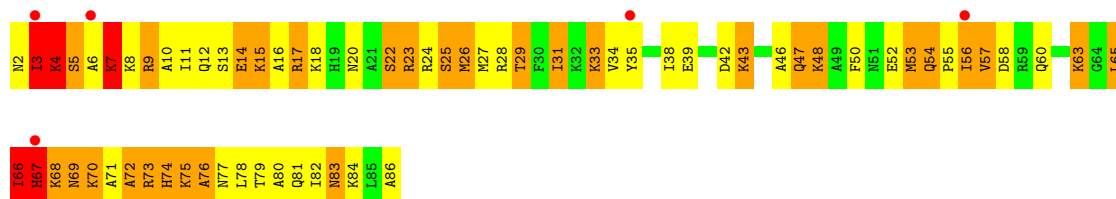
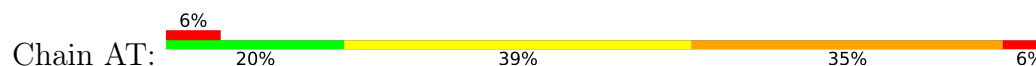
- Molecule 19: 30S ribosomal protein S19



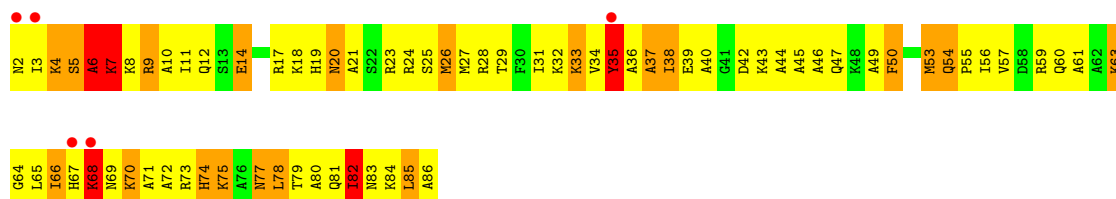
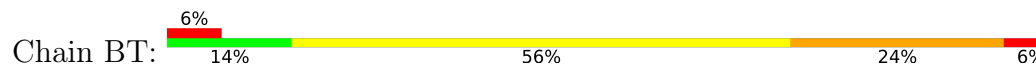
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

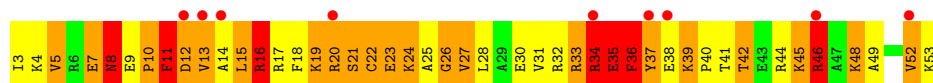


- Molecule 21: 30S ribosomal protein S21

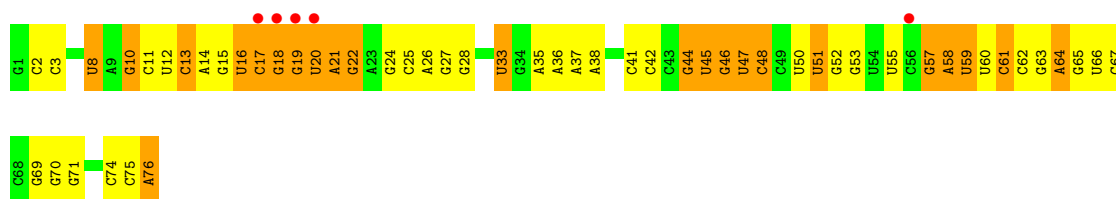




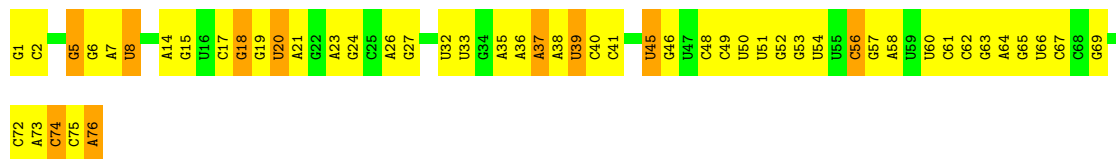
- Molecule 21: 30S ribosomal protein S21



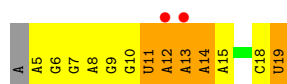
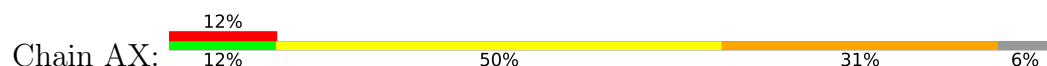
- Molecule 22: phenylalanine specific transfer RNA



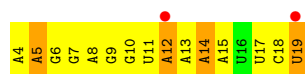
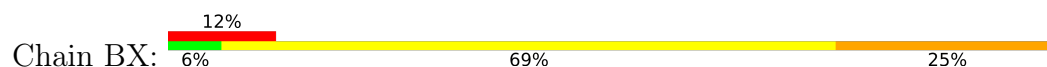
- Molecule 22: phenylalanine specific transfer RNA



- Molecule 23: messenger RNA

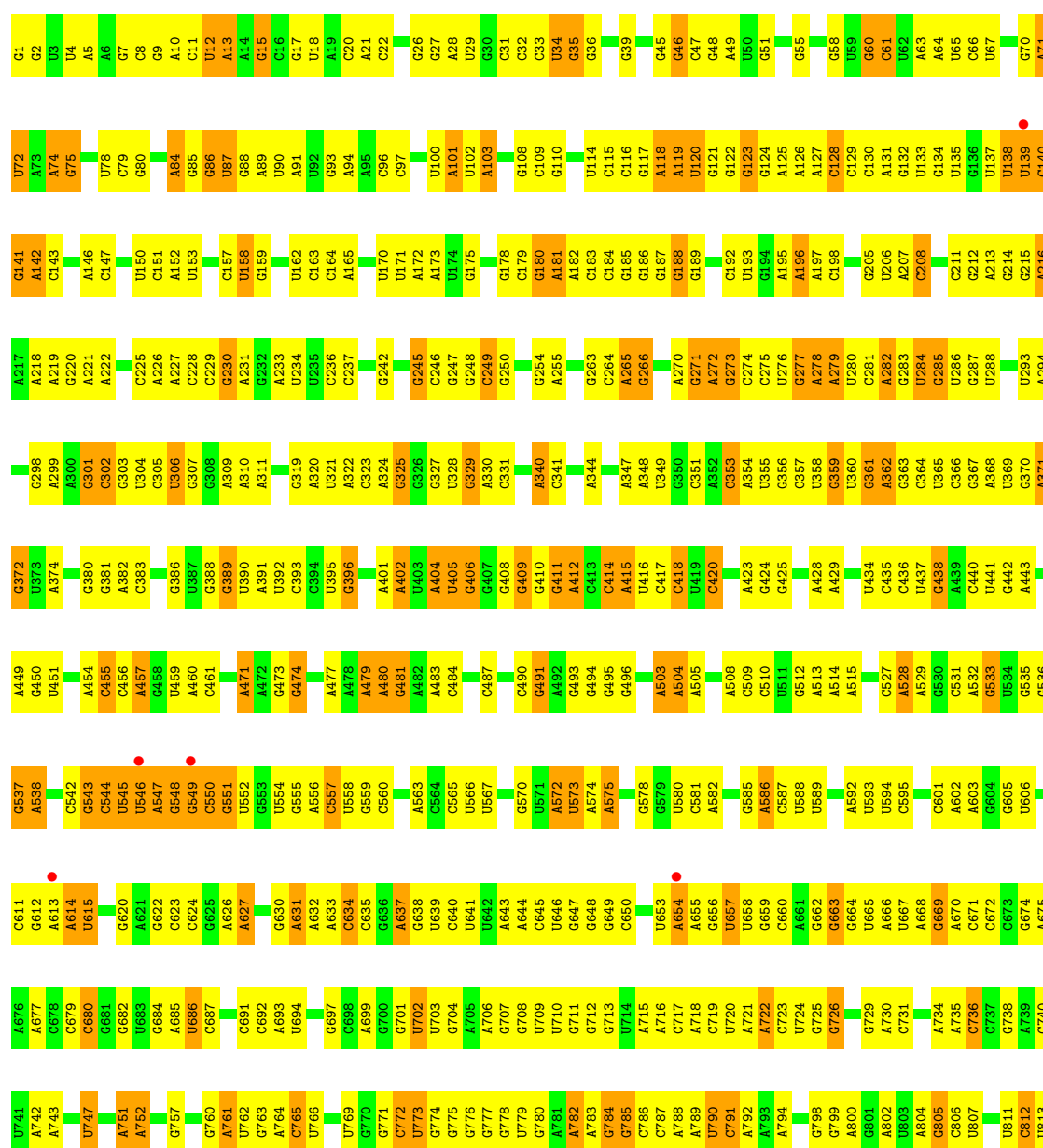


- Molecule 23: messenger RNA



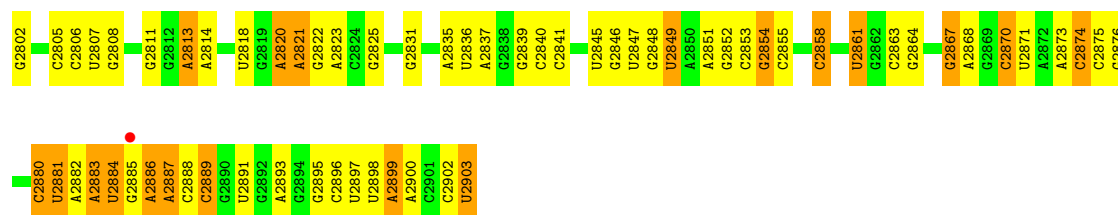
- Molecule 24: ribosome recycling factor



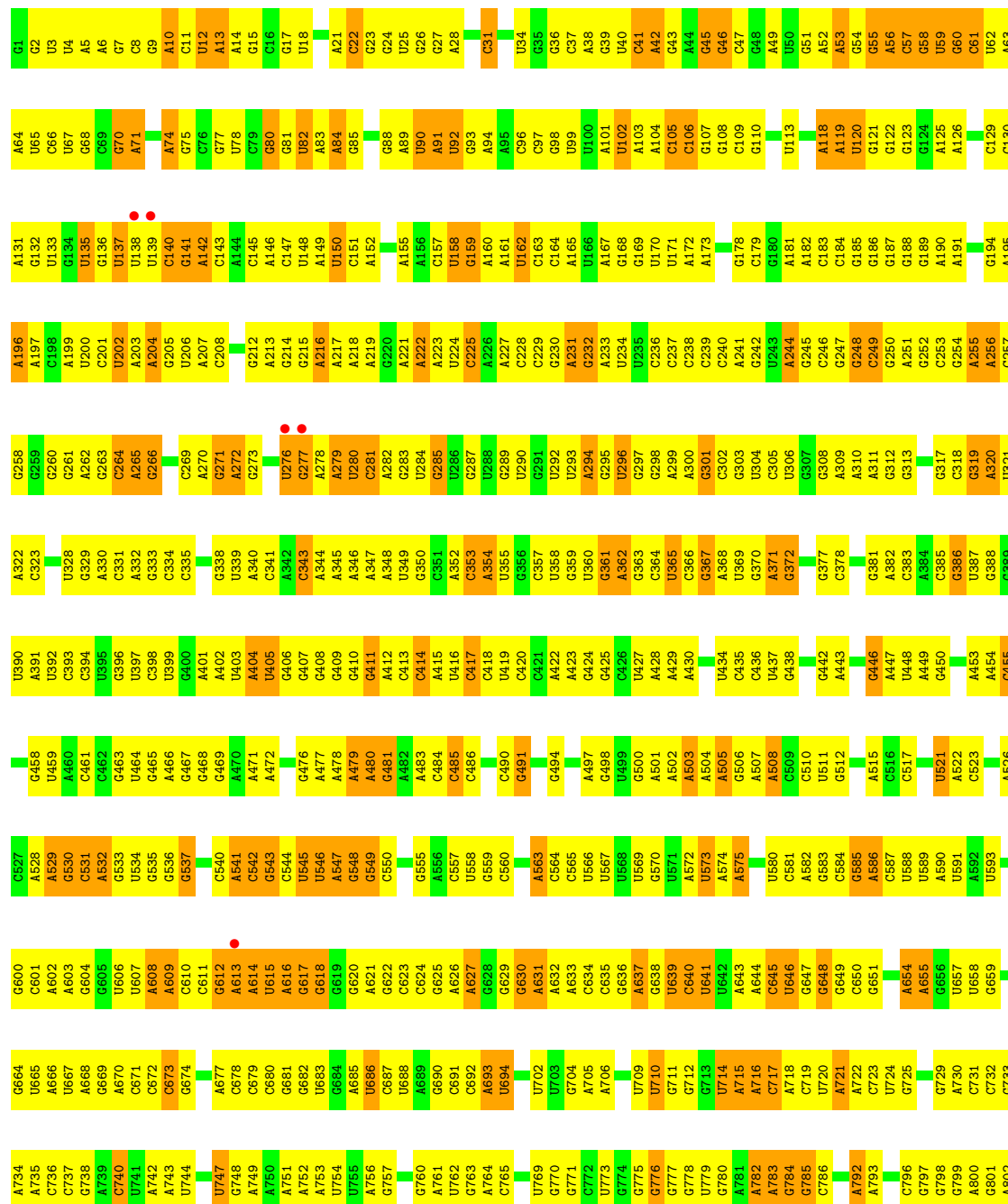


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G1743	A1676	C1606	C1541	U1476	A1413	C1345	U1267	G1181	U1181	C1045	U967	C	G819
A1744	A1677	C1607	C1541	A1477	C1414	C1348	A1268	G1182	G1106	A1046	C967	C	G823
A1745	A1678	A1608	G1546	G1478	U1415	C1349	A1269	U1183	G1107	G1047	C968	C	G824
A1746	A1679	A1609	C1547	G1479	U1416	C1350	C1270	U1184	U1108	A1048	G969	C	G825
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A1754	G1687	A1618	G1555	U1487	G1424	G1358	C1278	U1198	C1118	G1056	A899	C	G831
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C1774	G1714	U1642	U1578	G1510	G1449	G1380	G1302	U1240	C1140	U1078	C1007	C	C852
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G1799	G1733	C1665	C1595	G1530	U1466	C1404	U1326	G1256	G1171	A1095	U1033	C	A878
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A1801	A1735	U1669	C1599	A1532	U1468	U1406	A1328	U1258	U1173	U1097	A947	C	G880
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G1807	U1739	U1602	U1602	C1536	G1472	U1409	G1341	A1262	G1177	U1101	A960	C	U884
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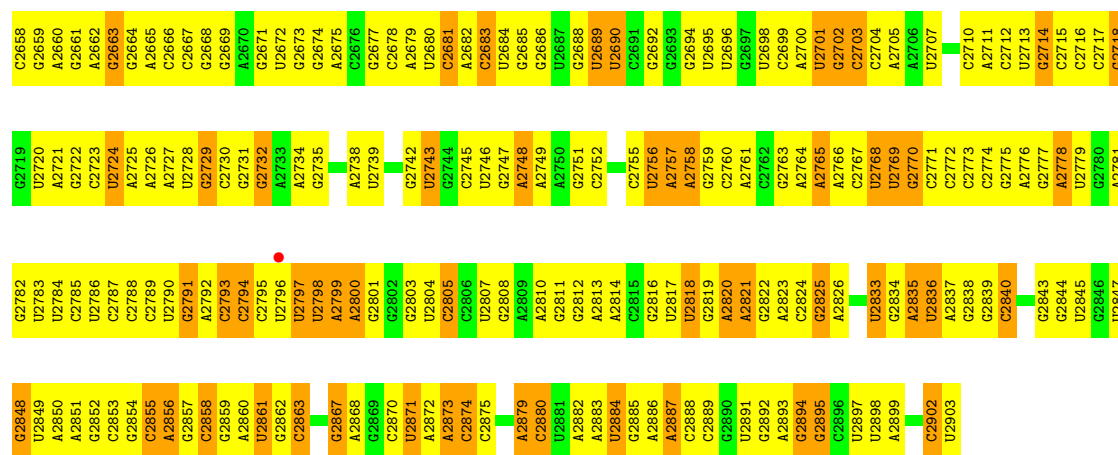


• Molecule 25: 23S rRNA

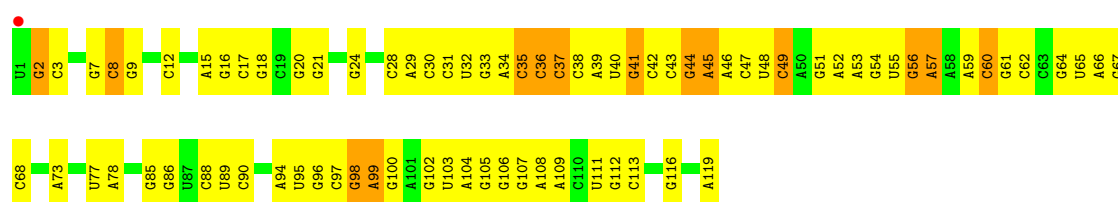


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C1639	C1577	U1513	A1453	A1393	G1259	G1194	G1132	A1070	U1004	A936	U872	C806
C1644	U1578	G1514	C1454	U1394	A1262	G1195	A1133	G1071	C1005	G839	C873	U807
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C1647	G1581	G1518	U1458	C1398	G1266	U1199	G1136	G1074	A1010	A941	C876	U810
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A1650	U1584	G1521	C1461	G1401	U1269	G1202	G1139	A1077	U1013	C944	C879	U813
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G1660	U1594	C1531	G1471	U1411	U1282	G1215	C1151	A1089	U1023	U958	C	U827
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G1667	A1596	C1533	G1473	A1413	A1284	U1219	C1153	G1091	G1025	C961	A892	A829
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C1677	G1606	G1543	G1483	G1423	C1295	G1229	A1165	C1102	G975	A975	C903	G841
A1678	A1608	A1544	U1484	G1424	G1299	U1230	A1166	U1106	C1043	A981	A910	U842
U1679	A1609	G1545	U1485	G1425	G1300	U1231	C1167	U1108	C1044	C982	A911	G843
A1680	U1610	C1546	U1486	G1426	A1301	G1232	G1168	C1109	C1049	A983	C912	U844
G1681	C1611	U1547	U1487	A1427	A1302	C1233	U1169	G1110	A1050	C984	G915	U845
G1682	C1612	A1548	C1488	G1428	G1302	G1234	A1170	G1112	C1052	C985	G916	A844
U1683	G1613	G1551	G1489	G1429	G1303	U1234	C1171	U1106	A1046	A980	U919	G854
A1614	A1614	A1552	A1490	G1430	G1310	G1235	G1172	G1107	A1047	A981	C992	G855
C1615	G1615	A1553	G1492	A1431	G1311	G1236	U1173	U1108	A1048	C982	A920	U856
A1616	C1616	U1554	C1493	G1432	U1312	A1237	C1174	C1109	A1049	A983	G917	G857
C1685	C1617	G1555	A1494	A1433	C1313	G1238	U1174	G1110	A1050	A984	U918	G858
U1688	A1618	C1556	U1495	A1434	C1314	G1239	U1175	A1111	C1051	C985	C921	U859
G1692	U1621	C1557	A1496	G1435	C1315	U1240	A1176	G1112	A1054	A988	U922	U860
U1693	G1622	U1558	U1497	G1436	U1316	U1241	G1177	U1113	G1055	G989	A917	A861
C1694	G1623	G1560	C1499	U1437	G1317	U1242	C1178	G1115	C1053	A990	U918	G862
G1695	A1626	C1561	G1500	U1438	U1318	A1244	G1179	C1116	A1056	C991	A927	A863
G1696	U1629	U1562	G1501	A1439	C1320	G1245	U1180	C1117	U1057	C992	U928	G864
G1697	A1630	A1563	A1502	U1440	A1321	G1246	U1181	C1118	U1058	A991	U929	C865
A1700	C1631	C1564	A1503	U1442	A1322	U1249	U1182	U1119	G1059	G993	U930	U866
A1701	U1632	U1565	A1504	G1444	G1323	G1251	U1183	G1120	U1060	C995	U931	A866
G1702	G1633	A1566	A1505	G1445	U1324	G1252	U1184	C1121	U1061	C996	U932	
A1703	A1634	C1567	U1506	C1446	U1325	G1253	U1185	G1122	G1062	A996		
C1704	A1635	U1568	C1507	C1447	U1326	G1254	G1186	C1123	G1063	C997		
		A1569	U1508	G1448	A1327	A1253	G1187	G1124	C1064	C998		
			A1509	G1449	A1328	U1254	U1188	G1125	U1065	U999		
					U1329	U1255	A1189	A1126	U1066	A1000		

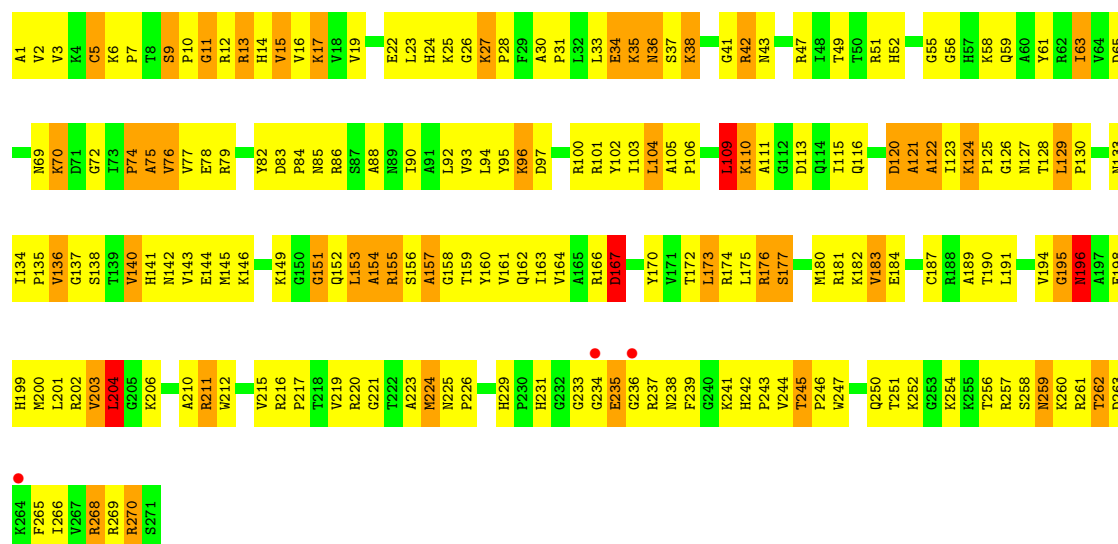




• Molecule 26: 5S rRNA

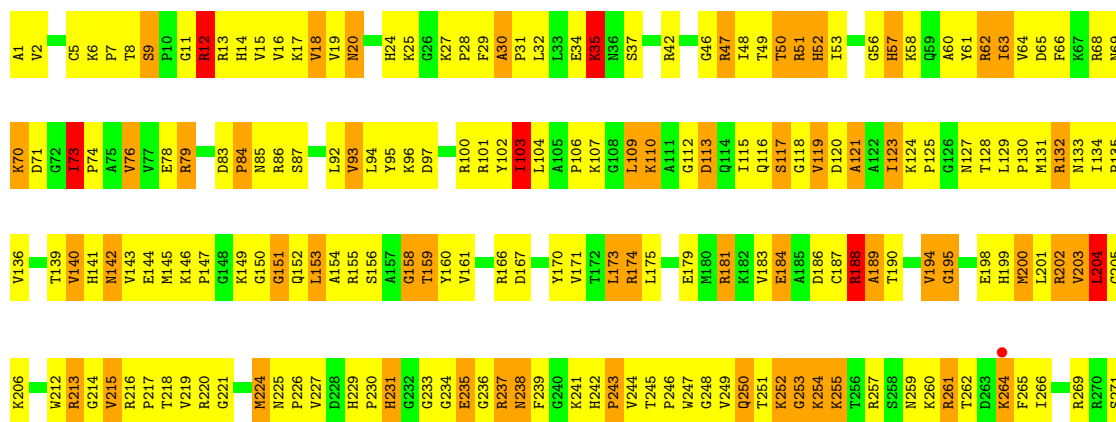


• Molecule 27: 50S ribosomal protein L2

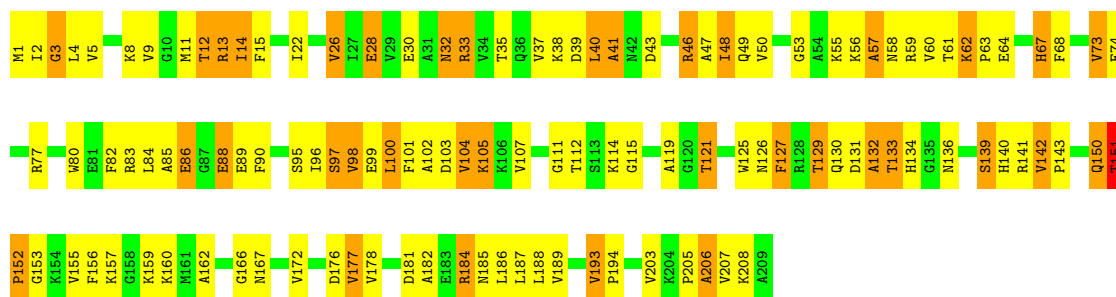


• Molecule 27: 50S ribosomal protein L2

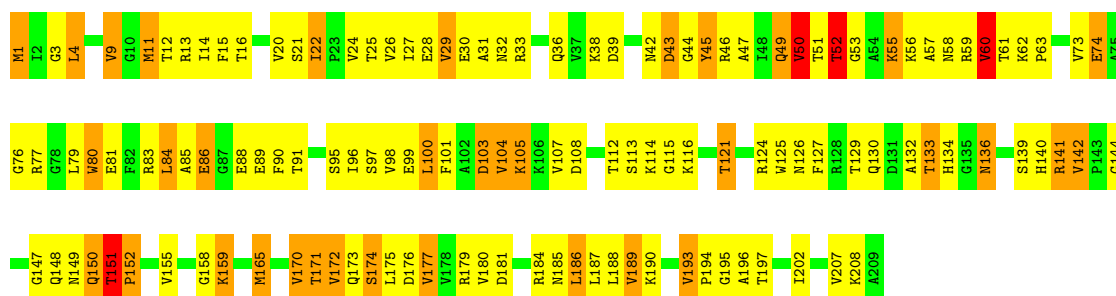




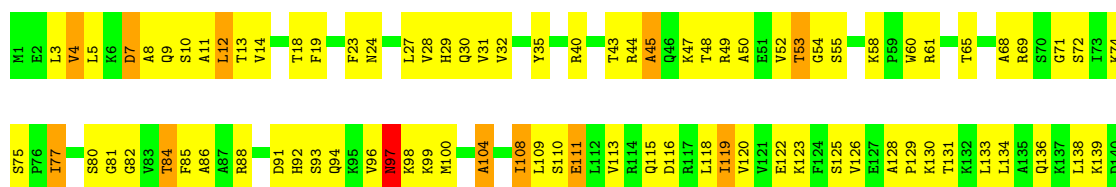
• Molecule 28: 50S ribosomal protein L3

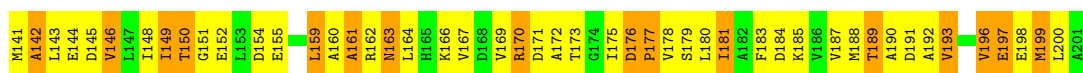


• Molecule 28: 50S ribosomal protein L3



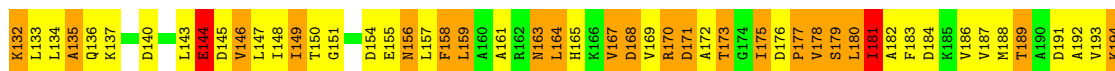
• Molecule 29: 50S ribosomal protein L4





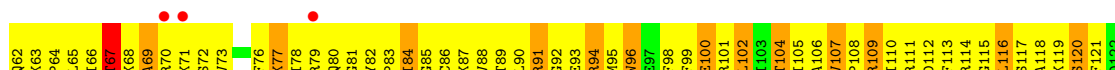
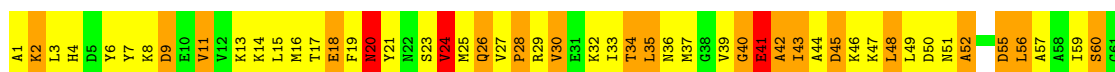
• Molecule 29: 50S ribosomal protein L4

Chain DE: 27% 48% 21% .



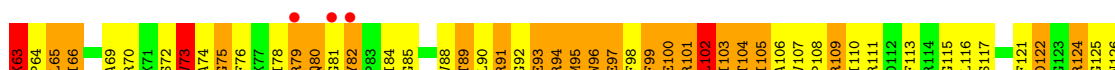
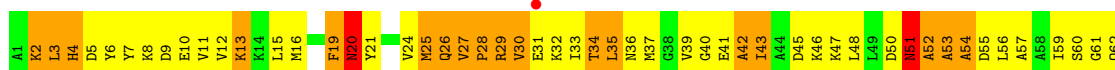
• Molecule 30: 50S ribosomal protein L5

Chain CF: 2% 18% 55% 24% .

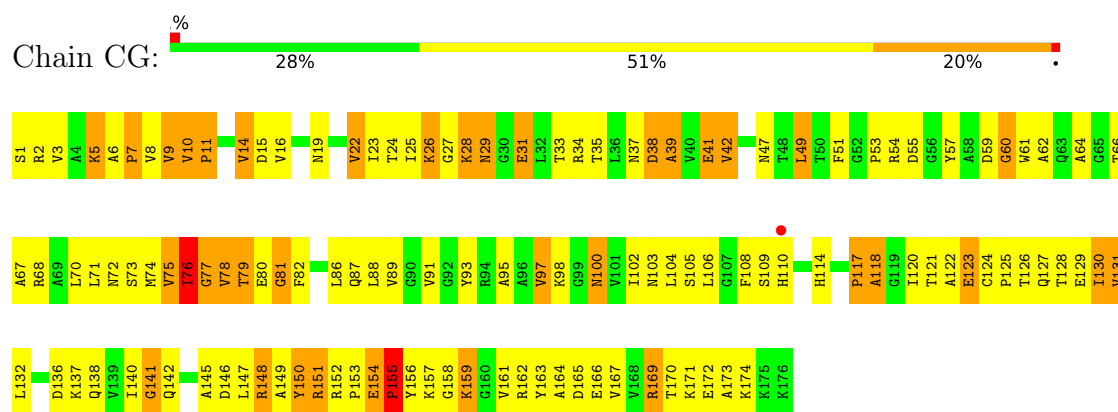


• Molecule 30: 50S ribosomal protein L5

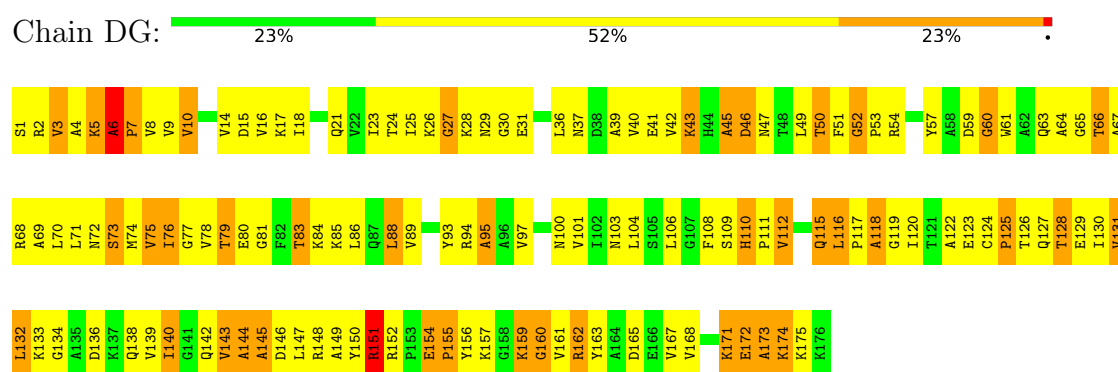
Chain DF: 4% 19% 51% 27% .



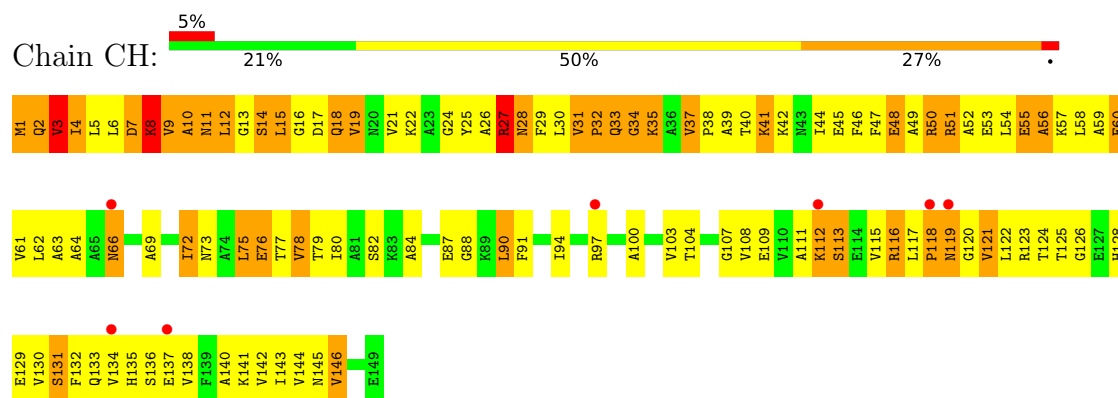
• Molecule 31: 50S ribosomal protein L6



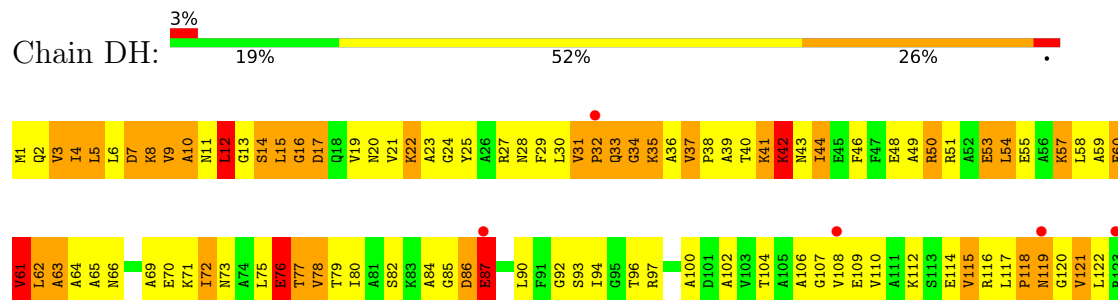
• Molecule 31: 50S ribosomal protein L6

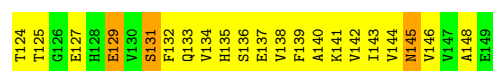


• Molecule 32: 50S ribosomal protein L9

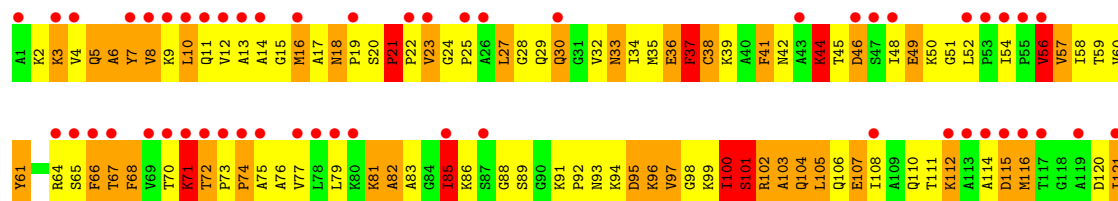
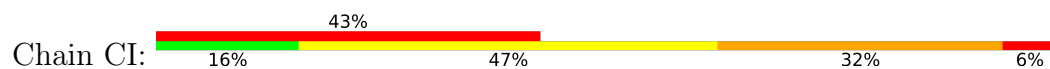


• Molecule 32: 50S ribosomal protein L9

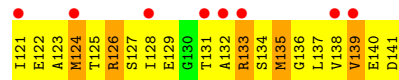
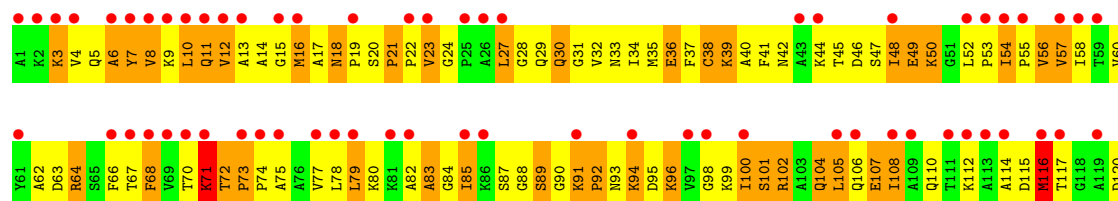
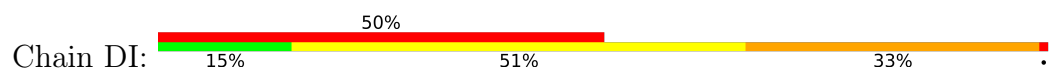




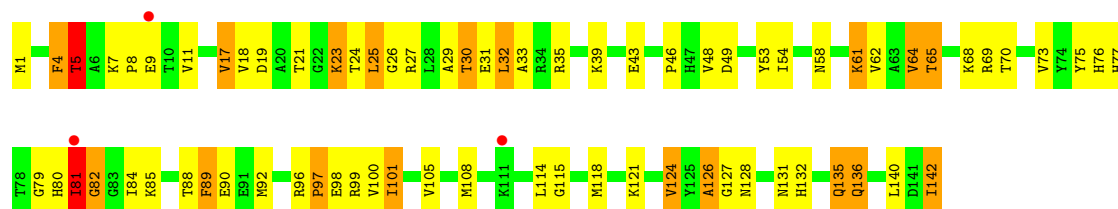
• Molecule 33: 50S ribosomal protein L11



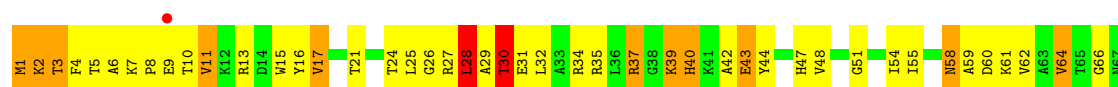
• Molecule 33: 50S ribosomal protein L11

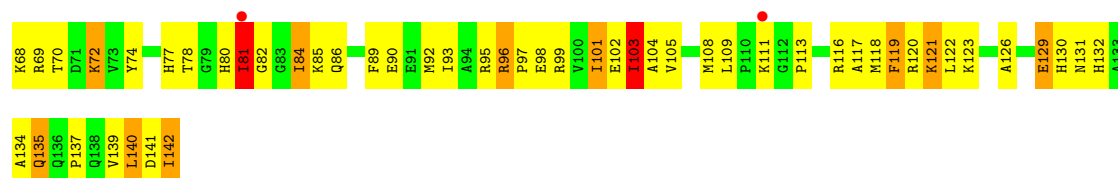


• Molecule 34: 50S ribosomal protein L13

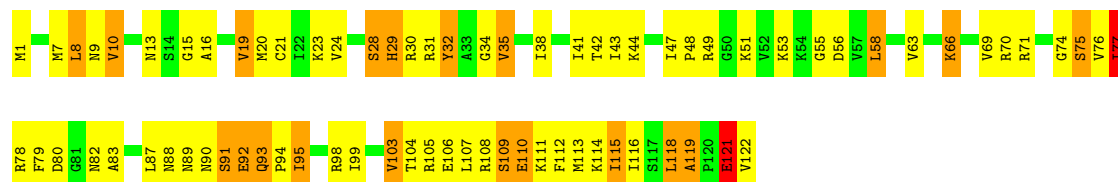


• Molecule 34: 50S ribosomal protein L13

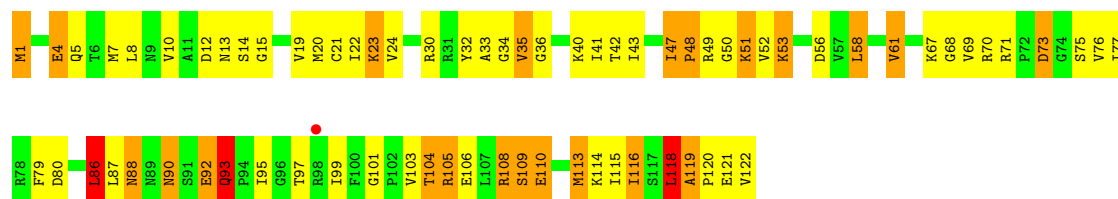
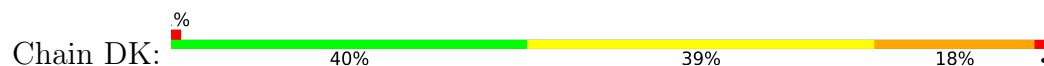




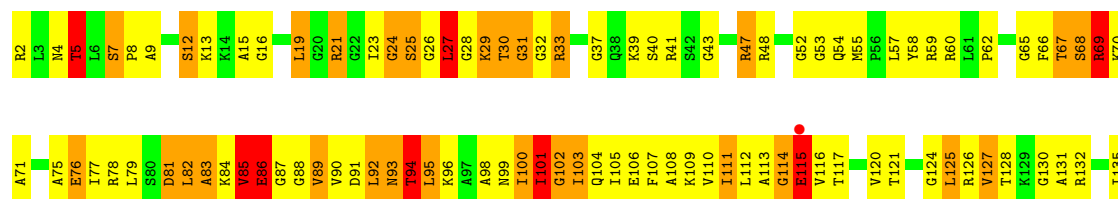
- Molecule 35: 50S ribosomal protein L14



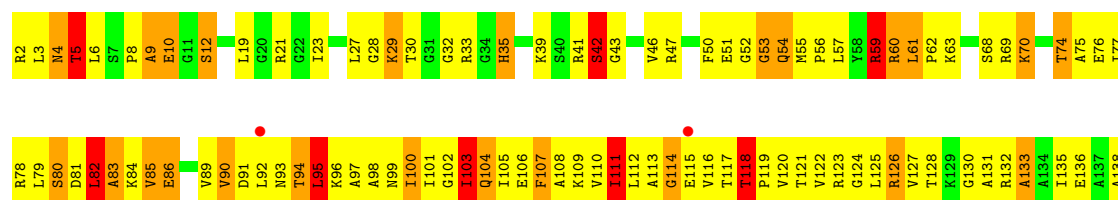
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



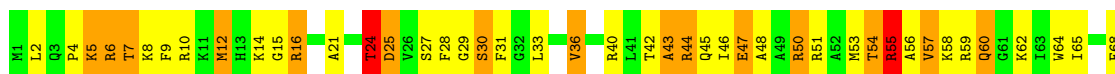
- Molecule 36: 50S ribosomal protein L15





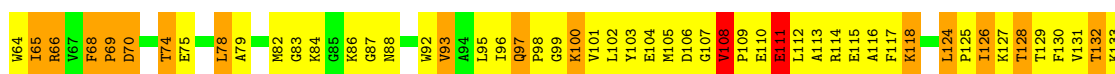
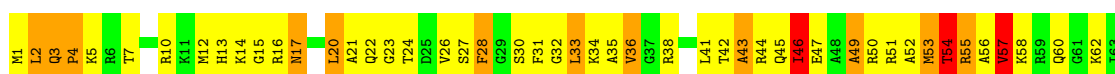
• Molecule 37: 50S ribosomal protein L16

Chain CM: 35% 42% 21% .



• Molecule 37: 50S ribosomal protein L16

Chain DM: 24% 51% 21% .



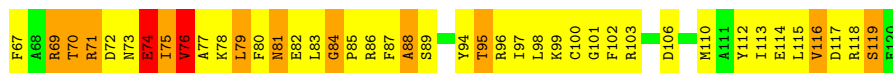
• Molecule 38: 50S ribosomal protein L17

Chain CN: 29% 52% 16% .



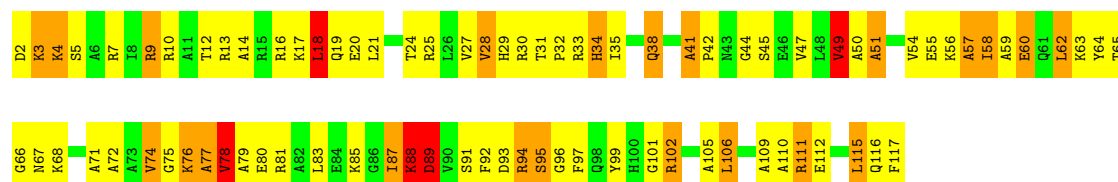
• Molecule 38: 50S ribosomal protein L17

Chain DN: 23% 55% 20% .

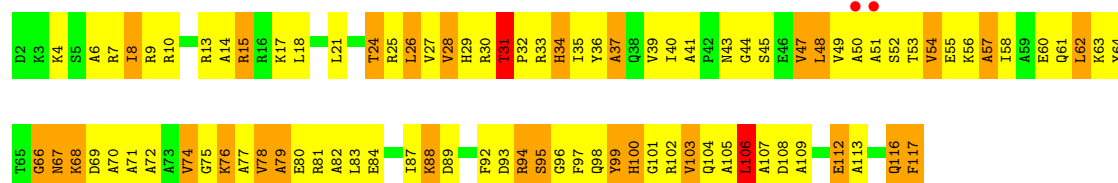


• Molecule 39: 50S ribosomal protein L18

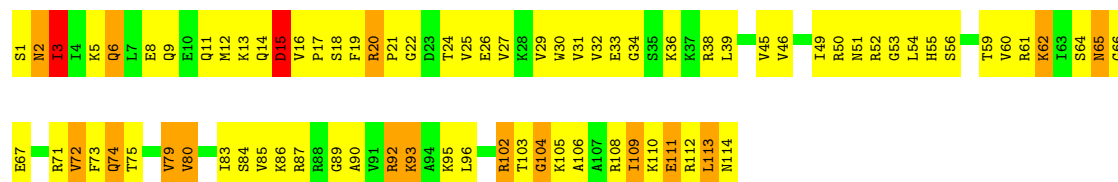
Chain CO: 28% 49% 19% .



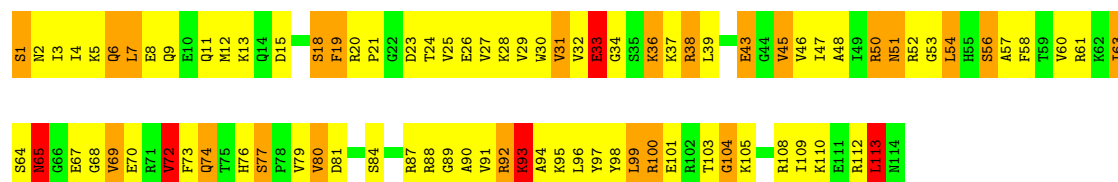
- Molecule 39: 50S ribosomal protein L18



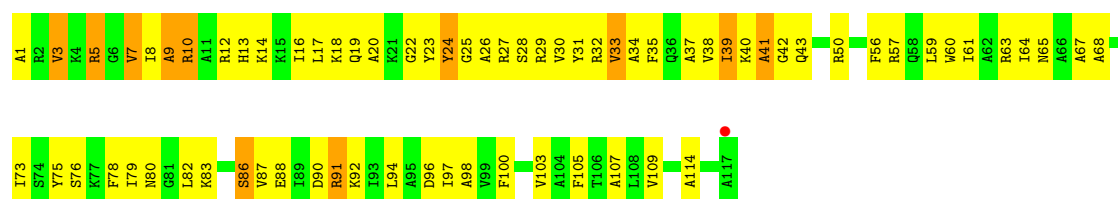
- Molecule 40: 50S ribosomal protein L19



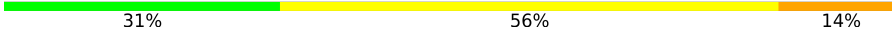
- Molecule 40: 50S ribosomal protein L19

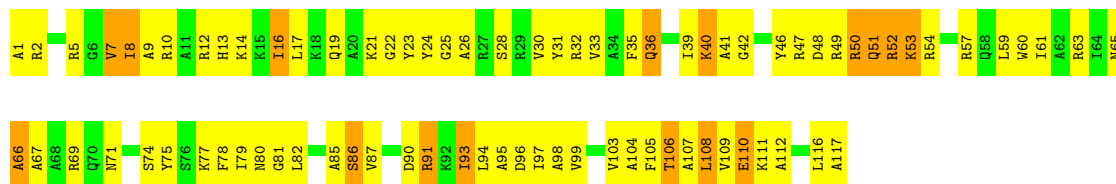


- Molecule 41: 50S ribosomal protein L20



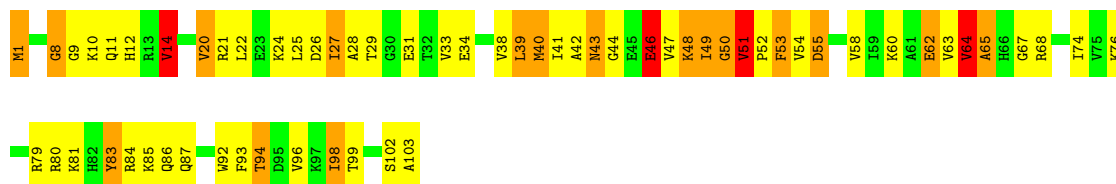
- Molecule 41: 50S ribosomal protein L20

Chain DQ:  31% 56% 14%

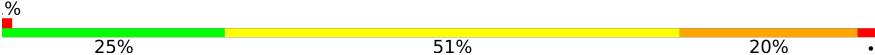


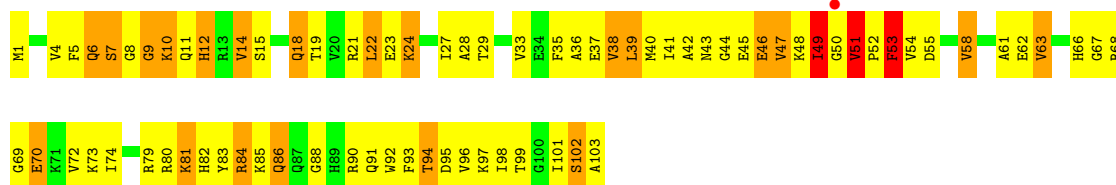
• Molecule 42: 50S ribosomal protein L21

Chain CR:  40% 40% 17% .



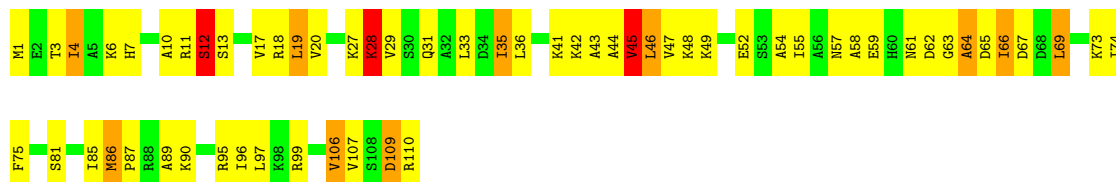
• Molecule 42: 50S ribosomal protein L21

Chain DR:  25% 51% 20% .

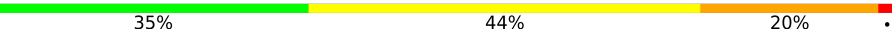


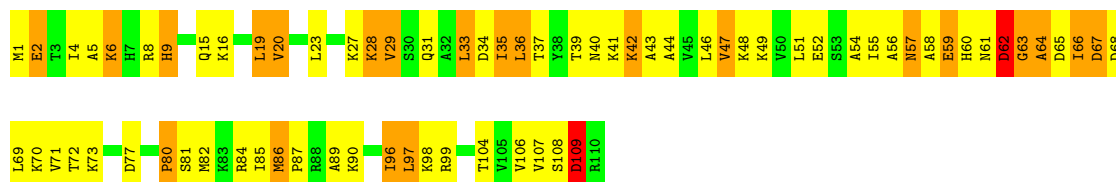
• Molecule 43: 50S ribosomal protein L22

Chain CS:  45% 43% 9% .

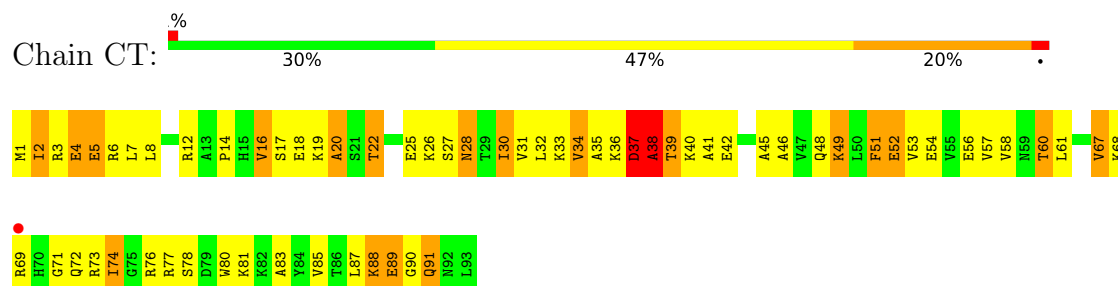


• Molecule 43: 50S ribosomal protein L22

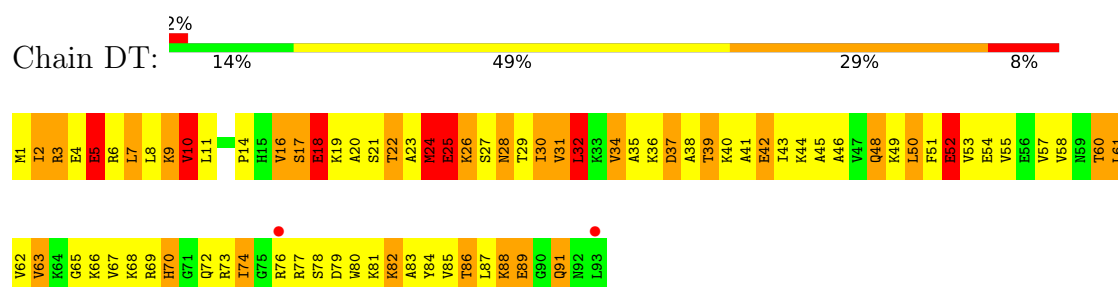
Chain DS:  35% 44% 20% .



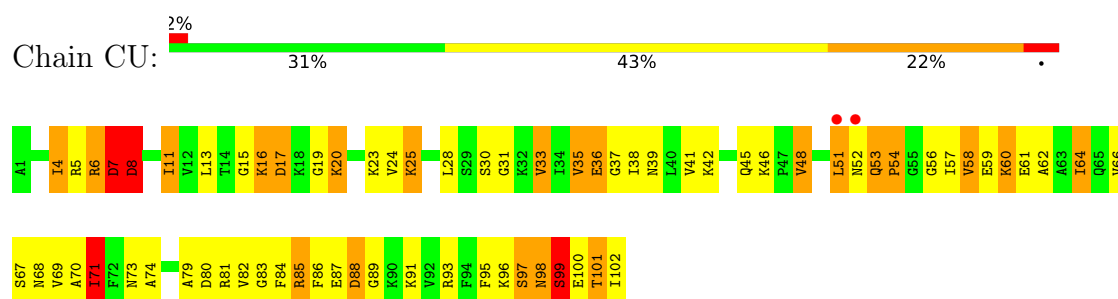
- Molecule 44: 50S ribosomal protein L23



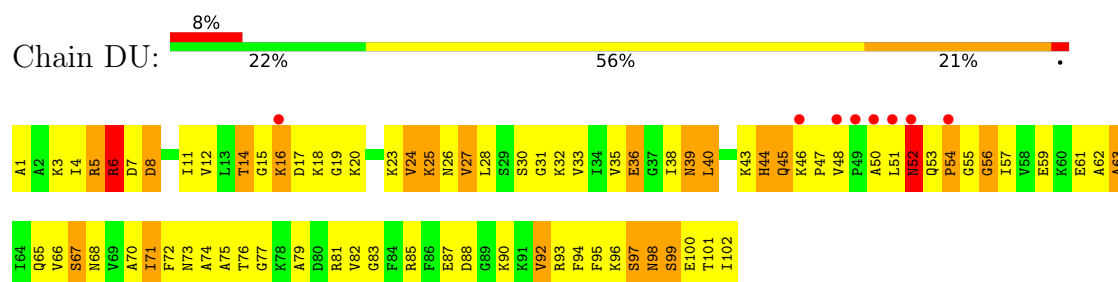
- Molecule 44: 50S ribosomal protein L23



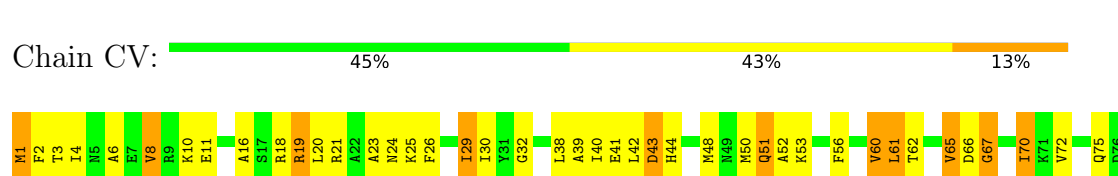
- Molecule 45: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L24



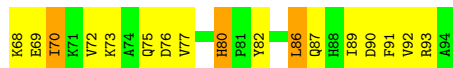
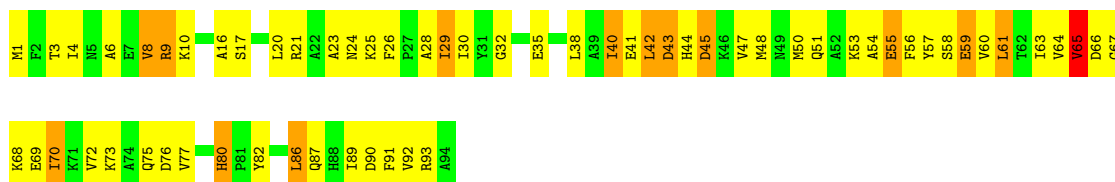
- Molecule 46: 50S ribosomal protein L25





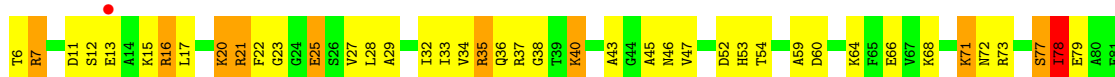
- Molecule 46: 50S ribosomal protein L25

Chain DV: 34% 51% 14% .



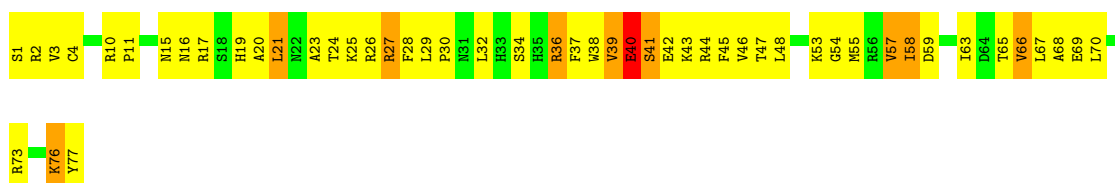
- Molecule 47: 50S ribosomal protein L27

Chain CW: % 45% 42% 12% .



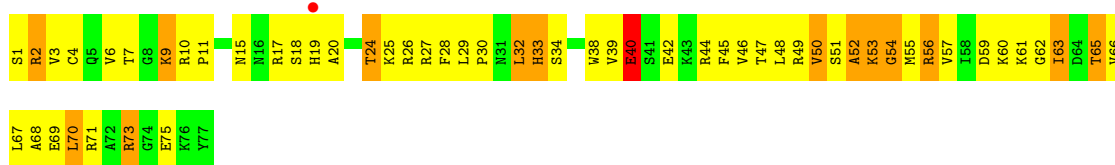
- Molecule 48: 50S ribosomal protein L28

Chain CX: 34% 53% 12% .



- Molecule 48: 50S ribosomal protein L28

Chain DX: % 27% 53% 18% .

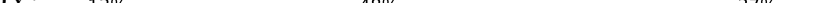


- Molecule 49: 50S ribosomal protein L29

Chain CY: 2% 22% 40% 30% 8% .

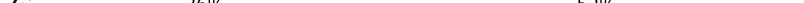


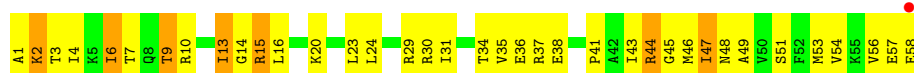
- Molecule 49: 50S ribosomal protein L29

Chain DY: 

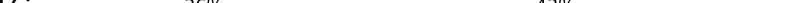


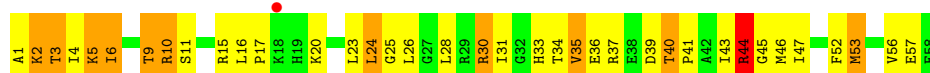
- Molecule 50: 50S ribosomal protein L30

Chain CZ: 

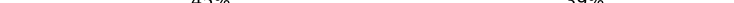


- Molecule 50: 50S ribosomal protein L30

Chain DZ: 

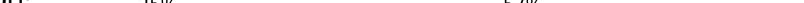


- Molecule 51: 50S ribosomal protein L32

Chain C0:  45% 39% 16%

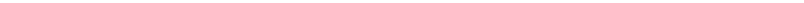


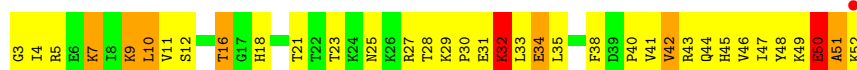
- Molecule 51: 50S ribosomal protein L32

Chain D0: 

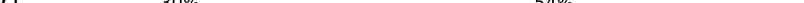


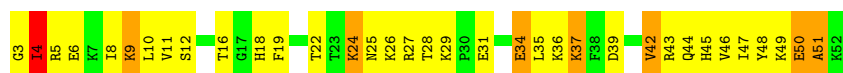
- Molecule 52: 50S ribosomal protein L33

Chain C1: 

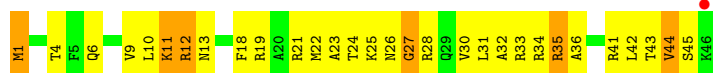


- Molecule 52: 50S ribosomal protein L33

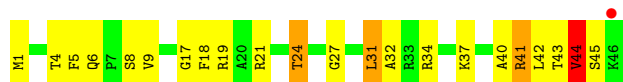
Chain D1:  30% 54% 14%



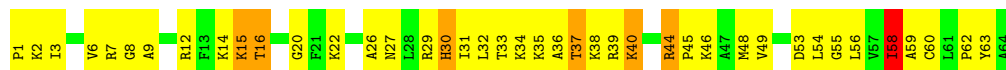
- Molecule 53: 50S ribosomal protein L34



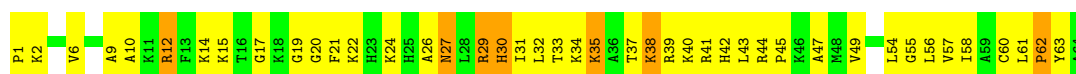
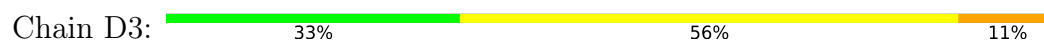
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



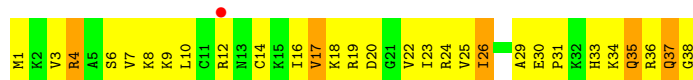
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36

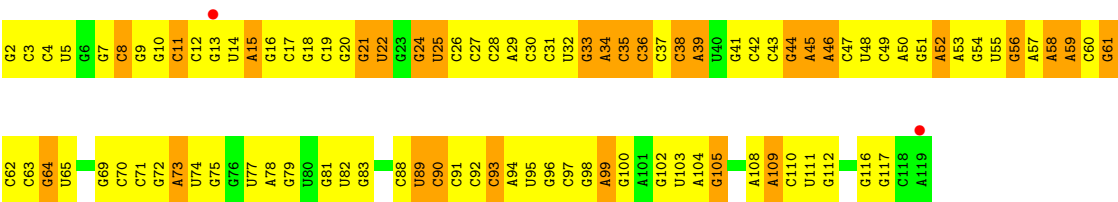


- Molecule 55: 50S ribosomal protein L36

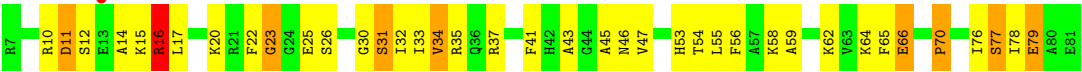


- Molecule 56: 5S rRNA





● Molecule 57: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.4 (40.00-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.260 0.194 , 0.248	Depositor DCC
R_{free} test set	19022 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 19.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292354	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.49	0/36944	0.50	0/57632
1	BA	0.49	0/36966	0.51	1/57666 (0.0%)
2	AB	0.76	0/1736	1.12	10/2338 (0.4%)
2	BB	0.67	0/1736	0.99	3/2338 (0.1%)
3	AC	0.71	0/1652	1.01	4/2225 (0.2%)
3	BC	0.62	0/1652	1.02	7/2225 (0.3%)
4	AD	0.70	0/1665	1.07	10/2227 (0.4%)
4	BD	0.80	0/1665	1.09	8/2227 (0.4%)
5	AE	0.80	1/1119 (0.1%)	1.20	8/1504 (0.5%)
5	BE	0.79	0/1119	1.25	11/1504 (0.7%)
6	AF	0.81	0/836	1.15	5/1128 (0.4%)
6	BF	0.68	0/836	1.05	3/1128 (0.3%)
7	AG	0.64	0/1196	1.04	7/1602 (0.4%)
7	BG	0.62	0/1196	0.97	2/1602 (0.1%)
8	AH	0.74	0/989	1.14	9/1326 (0.7%)
8	BH	0.72	0/989	1.11	5/1326 (0.4%)
9	AI	0.60	0/1034	1.01	5/1375 (0.4%)
9	BI	0.60	0/1034	1.05	5/1375 (0.4%)
10	AJ	0.75	0/797	1.05	4/1077 (0.4%)
10	BJ	0.70	0/797	1.02	1/1077 (0.1%)
11	AK	0.90	0/893	1.14	1/1205 (0.1%)
11	BK	0.78	0/893	1.14	6/1205 (0.5%)
12	AL	0.77	0/969	1.09	5/1300 (0.4%)
12	BL	0.91	0/969	1.35	13/1300 (1.0%)
13	AM	0.68	0/893	1.08	3/1193 (0.3%)
13	BM	0.64	0/893	1.01	2/1193 (0.2%)
14	AN	0.66	0/785	1.11	6/1043 (0.6%)
14	BN	0.61	0/785	0.91	3/1043 (0.3%)
15	AO	0.73	0/722	1.04	3/964 (0.3%)
15	BO	0.66	0/722	1.04	3/964 (0.3%)
16	AP	0.70	0/659	1.16	5/884 (0.6%)
16	BP	0.83	1/659 (0.2%)	1.09	3/884 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.65	0/658	1.03	3/881 (0.3%)
17	BQ	0.74	0/658	1.03	2/881 (0.2%)
18	AR	0.75	0/463	1.03	3/621 (0.5%)
18	BR	0.70	0/463	1.02	2/621 (0.3%)
19	AS	0.60	0/653	1.15	10/877 (1.1%)
19	BS	0.71	0/653	1.03	2/877 (0.2%)
20	AT	0.69	0/671	0.97	3/888 (0.3%)
20	BT	0.74	0/671	1.02	2/888 (0.2%)
21	AU	1.04	0/431	1.27	6/570 (1.1%)
21	BU	0.92	1/431 (0.2%)	1.15	1/570 (0.2%)
22	AV	0.43	0/1813	0.49	0/2823
22	BV	0.41	0/1813	0.51	0/2823
23	AX	0.49	0/363	0.52	0/564
23	BX	0.40	0/388	0.45	0/603
24	AY	0.86	0/1430	1.11	5/1924 (0.3%)
25	CA	0.88	1/69659 (0.0%)	0.60	1/108672 (0.0%)
25	DA	0.60	0/69633	0.55	0/108629
26	CB	0.73	0/2847	0.60	0/4440
27	CC	1.04	0/2122	1.20	6/2852 (0.2%)
27	DC	0.85	0/2122	1.20	17/2852 (0.6%)
28	CD	1.28	2/1586 (0.1%)	1.35	12/2134 (0.6%)
28	DD	0.92	1/1586 (0.1%)	1.20	12/2134 (0.6%)
29	CE	1.18	0/1571	1.19	5/2113 (0.2%)
29	DE	0.87	1/1571 (0.1%)	1.12	6/2113 (0.3%)
30	CF	0.81	0/1435	1.11	8/1926 (0.4%)
30	DF	0.59	0/1435	1.04	8/1926 (0.4%)
31	CG	0.94	0/1343	1.28	11/1816 (0.6%)
31	DG	0.64	0/1343	1.06	8/1816 (0.4%)
32	CH	0.86	0/1121	1.03	3/1515 (0.2%)
32	DH	0.84	1/1121 (0.1%)	1.08	2/1515 (0.1%)
33	CI	1.05	1/1046 (0.1%)	1.16	10/1410 (0.7%)
33	DI	0.97	1/1046 (0.1%)	1.15	9/1410 (0.6%)
34	CJ	1.36	4/1152 (0.3%)	1.15	4/1551 (0.3%)
34	DJ	0.97	0/1152	1.16	4/1551 (0.3%)
35	CK	1.17	1/948 (0.1%)	1.24	8/1268 (0.6%)
35	DK	0.89	0/948	1.19	6/1268 (0.5%)
36	CL	1.27	2/1054 (0.2%)	1.38	11/1403 (0.8%)
36	DL	0.81	0/1054	1.21	7/1403 (0.5%)
37	CM	1.27	4/1093 (0.4%)	1.31	8/1460 (0.5%)
37	DM	0.84	0/1093	1.18	11/1460 (0.8%)
38	CN	1.26	0/974	1.24	9/1301 (0.7%)
38	DN	0.90	0/974	1.15	7/1301 (0.5%)
39	CO	0.99	1/902 (0.1%)	1.19	6/1209 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DO	0.62	0/902	1.03	3/1209 (0.2%)
40	CP	1.10	1/929 (0.1%)	1.20	5/1242 (0.4%)
40	DP	0.85	0/929	1.18	10/1242 (0.8%)
41	CQ	1.46	3/960 (0.3%)	1.29	5/1278 (0.4%)
41	DQ	1.01	0/960	1.13	2/1278 (0.2%)
42	CR	1.26	1/829 (0.1%)	1.39	7/1107 (0.6%)
42	DR	0.96	0/829	1.24	5/1107 (0.5%)
43	CS	1.46	3/864 (0.3%)	1.29	6/1156 (0.5%)
43	DS	0.94	0/864	1.17	2/1156 (0.2%)
44	CT	1.02	2/745 (0.3%)	1.20	7/994 (0.7%)
44	DT	0.68	0/745	0.99	3/994 (0.3%)
45	CU	1.19	3/788 (0.4%)	1.22	3/1051 (0.3%)
45	DU	0.81	1/788 (0.1%)	1.10	1/1051 (0.1%)
46	CV	1.02	0/766	1.16	4/1025 (0.4%)
46	DV	0.62	0/766	1.02	0/1025
47	CW	1.37	3/582 (0.5%)	1.21	1/769 (0.1%)
48	CX	1.03	1/635 (0.2%)	1.13	4/848 (0.5%)
48	DX	0.74	0/635	1.05	2/848 (0.2%)
49	CY	0.98	0/510	1.39	8/677 (1.2%)
49	DY	0.66	0/510	1.00	2/677 (0.3%)
50	CZ	1.38	2/453 (0.4%)	1.34	3/605 (0.5%)
50	DZ	0.82	0/453	1.13	0/605
51	C0	1.23	0/450	1.32	4/599 (0.7%)
51	D0	0.94	0/450	1.24	3/599 (0.5%)
52	C1	0.90	0/417	1.02	0/554
52	D1	0.61	0/417	0.93	1/554 (0.2%)
53	C2	1.38	0/380	1.39	5/498 (1.0%)
53	D2	0.90	0/380	1.06	0/498
54	C3	1.20	1/513 (0.2%)	1.11	1/676 (0.1%)
54	D3	0.75	0/513	1.07	2/676 (0.3%)
55	C4	1.13	0/303	1.24	1/397 (0.3%)
55	D4	0.85	0/303	1.08	1/397 (0.3%)
56	DB	0.43	0/2828	0.49	0/4410
57	DW	0.76	0/571	1.00	2/755 (0.3%)
All	All	0.74	44/315257 (0.0%)	0.75	502/471496 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	BD	0	1
5	AE	0	1
5	BE	0	2
6	BF	0	1
9	AI	0	1
11	AK	0	1
11	BK	0	2
12	BL	0	2
13	AM	0	1
14	AN	0	1
20	BT	0	1
21	AU	0	2
21	BU	0	1
27	CC	0	1
27	DC	0	1
28	CD	0	2
28	DD	0	1
32	DH	0	2
33	CI	0	1
34	DJ	0	1
39	DO	0	1
42	CR	0	1
45	CU	0	1
50	CZ	0	1
All	All	0	31

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	BU	31	VAL	CA-CB	7.08	1.62	1.54
41	CQ	103	VAL	CA-CB	-7.04	1.46	1.54
35	CK	10	VAL	CA-CB	-6.56	1.46	1.54
44	CT	16	VAL	CA-CB	-6.50	1.46	1.54
28	DD	60	VAL	CA-CB	6.12	1.61	1.54

The worst 5 of 502 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CD	151	THR	CA-C-N	15.82	139.62	119.84
28	CD	151	THR	C-N-CA	15.82	139.62	119.84
42	CR	51	VAL	CA-C-N	-12.33	104.43	119.84
42	CR	51	VAL	C-N-CA	-12.33	104.43	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
49	CY	16	THR	N-CA-C	-12.13	98.06	111.28

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	2054	0
1	BA	33015	0	16617	2195	0
2	AB	1705	0	1732	393	0
2	BB	1705	0	1732	331	0
3	AC	1625	0	1699	247	0
3	BC	1625	0	1699	245	0
4	AD	1643	0	1710	317	0
4	BD	1643	0	1710	249	0
5	AE	1106	0	1148	222	0
5	BE	1106	0	1148	219	0
6	AF	818	0	808	124	0
6	BF	818	0	808	161	0
7	AG	1182	0	1240	130	0
7	BG	1182	0	1240	177	0
8	AH	979	0	1034	167	0
8	BH	979	0	1034	130	0
9	AI	1022	0	1070	198	0
9	BI	1022	0	1070	195	0
10	AJ	787	0	828	186	0
10	BJ	787	0	828	149	0
11	AK	877	0	887	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BK	877	0	887	140	0
12	AL	955	0	1019	96	0
12	BL	955	0	1019	122	0
13	AM	884	0	944	170	0
13	BM	884	0	944	156	0
14	AN	774	0	827	140	0
14	BN	774	0	827	144	0
15	AO	714	0	737	72	0
15	BO	714	0	737	97	0
16	AP	649	0	666	111	0
16	BP	649	0	666	91	0
17	AQ	649	0	691	122	0
17	BQ	649	0	691	106	0
18	AR	456	0	478	48	0
18	BR	456	0	478	60	0
19	AS	638	0	665	95	0
19	BS	638	0	665	102	0
20	AT	665	0	714	96	0
20	BT	665	0	714	134	0
21	AU	426	0	449	147	0
21	BU	426	0	449	128	0
22	AV	1623	0	821	88	0
22	BV	1623	0	821	47	0
23	AX	324	0	162	20	0
23	BX	346	0	173	24	0
24	AY	1419	0	1467	105	0
25	CA	62195	0	31271	2439	0
25	DA	62173	0	31270	3407	0
26	CB	2548	0	1292	100	0
27	CC	2083	0	2157	232	0
27	DC	2083	0	2157	220	0
28	CD	1565	0	1616	135	0
28	DD	1565	0	1616	121	0
29	CE	1552	0	1619	148	0
29	DE	1552	0	1619	173	0
30	CF	1411	0	1447	216	0
30	DF	1411	0	1447	209	0
31	CG	1323	0	1374	151	0
31	DG	1323	0	1374	184	0
32	CH	1110	0	1148	150	0
32	DH	1110	0	1148	215	0
33	CI	1032	0	1088	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DI	1032	0	1088	187	0
34	CJ	1129	0	1162	66	0
34	DJ	1129	0	1162	104	0
35	CK	939	0	1012	79	0
35	DK	939	0	1012	83	0
36	CL	1045	0	1117	138	0
36	DL	1045	0	1117	171	0
37	CM	1074	0	1157	105	0
37	DM	1074	0	1157	134	0
38	CN	961	0	1000	99	0
38	DN	961	0	1000	134	0
39	CO	892	0	923	90	0
39	DO	892	0	923	144	0
40	CP	917	0	965	97	0
40	DP	917	0	965	108	0
41	CQ	947	0	1022	68	0
41	DQ	947	0	1022	91	0
42	CR	816	0	839	90	0
42	DR	816	0	839	109	0
43	CS	857	0	922	47	0
43	DS	857	0	922	85	0
44	CT	739	0	807	76	0
44	DT	739	0	807	119	0
45	CU	780	0	834	68	0
45	DU	780	0	834	113	0
46	CV	753	0	780	64	0
46	DV	753	0	780	75	0
47	CW	575	0	589	30	0
48	CX	625	0	655	44	0
48	DX	625	0	655	62	0
49	CY	509	0	543	91	0
49	DY	509	0	543	113	0
50	CZ	449	0	491	28	0
50	DZ	449	0	491	50	0
51	C0	444	0	461	36	0
51	D0	444	0	461	48	0
52	C1	410	0	440	38	0
52	D1	410	0	440	48	0
53	C2	377	0	418	30	0
53	D2	377	0	418	20	0
54	C3	504	0	574	44	0
54	D3	504	0	574	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	C4	302	0	340	21	0
55	D4	302	0	340	34	0
56	DB	2529	0	1281	161	0
57	DW	564	0	576	36	0
58	AA	72	0	0	0	0
58	BA	56	0	0	0	0
58	CA	194	0	0	0	0
58	CB	4	0	0	0	0
58	CQ	1	0	0	0	0
58	DA	166	0	0	0	0
58	DB	3	0	0	0	0
58	DL	1	0	0	0	0
58	DQ	1	0	0	0	0
59	C4	1	0	0	0	0
59	D4	1	0	0	0	0
60	AA	197	0	0	10	0
60	AN	4	0	0	0	0
60	AT	1	0	0	0	0
60	AU	1	0	0	0	0
60	BA	190	0	0	12	0
60	BL	1	0	0	0	0
60	BN	5	0	0	1	0
60	BT	1	0	0	0	0
60	BU	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	625	0	0	62	0
60	CB	13	0	0	0	0
60	CC	8	0	0	0	0
60	CD	2	0	0	0	0
60	CE	2	0	0	0	0
60	CF	1	0	0	0	0
60	CJ	1	0	0	0	0
60	CL	6	0	0	2	0
60	CN	4	0	0	0	0
60	CS	1	0	0	0	0
60	CV	1	0	0	0	0
60	D2	1	0	0	0	0
60	D3	2	0	0	0	0
60	D4	1	0	0	0	0
60	DA	622	0	0	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DB	14	0	0	0	0
60	DC	4	0	0	0	0
60	DD	5	0	0	2	0
60	DE	2	0	0	0	0
60	DJ	1	0	0	0	0
60	DL	4	0	0	1	0
60	DN	1	0	0	0	0
60	DR	1	0	0	0	0
All	All	292354	0	195461	21524	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

The worst 5 of 21524 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)
32:DH:93:SER:OG	32:DH:121:VAL:HG12	1.46	1.15
1:BA:1053:G:H4'	1:BA:1054:C:H5'	1.29	1.11
32:DH:93:SER:OG	32:DH:121:VAL:CG1	2.03	1.06
25:DA:1153:C:OP2	60:DA:3363:HOH:O	1.78	1.01
12:BL:33:CYS:HA	12:BL:54:VAL:HA	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0	0
2	BB	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0	0
3	AC	204/206 (99%)	125 (61%)	49 (24%)	30 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BC	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	0
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	0
4	BD	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	0
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	0
5	BE	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	0
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	0
6	BF	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	AG	149/151 (99%)	86 (58%)	41 (28%)	22 (15%)	0	0
7	BG	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	0
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	0	3
8	BH	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	0	2
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	0	1
9	BI	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	0	1
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	0
10	BJ	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	0
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	0	1
11	BK	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	1
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	1	8
12	BL	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	0	1
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	0	2
13	BM	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	0
14	BN	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	3
15	BO	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	0
16	BP	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	1
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	0
17	BQ	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	0
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	1
18	BR	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	77/79 (98%)	36 (47%)	29 (38%)	12 (16%)	0	0
19	BS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	0	2
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	0
20	BT	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	0
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
21	BU	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0
24	AY	181/183 (99%)	135 (75%)	35 (19%)	11 (6%)	1	7
27	CC	269/271 (99%)	216 (80%)	32 (12%)	21 (8%)	1	4
27	DC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	0	2
28	CD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	1	9
28	DD	207/209 (99%)	162 (78%)	35 (17%)	10 (5%)	2	11
29	CE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	2	12
29	DE	199/201 (99%)	142 (71%)	38 (19%)	19 (10%)	0	2
30	CF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	0	1
30	DF	175/177 (99%)	113 (65%)	34 (19%)	28 (16%)	0	0
31	CG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	0	3
31	DG	174/176 (99%)	106 (61%)	43 (25%)	25 (14%)	0	0
32	CH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	0
32	DH	147/149 (99%)	95 (65%)	27 (18%)	25 (17%)	0	0
33	CI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	0
33	DI	139/141 (99%)	71 (51%)	46 (33%)	22 (16%)	0	0
34	CJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	12
34	DJ	140/142 (99%)	112 (80%)	24 (17%)	4 (3%)	3	20
35	CK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	5
35	DK	120/122 (98%)	87 (72%)	21 (18%)	12 (10%)	0	2
36	CL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	0
36	DL	141/143 (99%)	88 (62%)	36 (26%)	17 (12%)	0	1
37	CM	134/136 (98%)	110 (82%)	15 (11%)	9 (7%)	1	5
37	DM	134/136 (98%)	97 (72%)	23 (17%)	14 (10%)	0	2
38	CN	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	1	10
38	DN	118/120 (98%)	82 (70%)	28 (24%)	8 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	0	1
39	DO	114/116 (98%)	77 (68%)	25 (22%)	12 (10%)	0	2
40	CP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	2	16
40	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	6
41	CQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	7	32
41	DQ	115/117 (98%)	95 (83%)	18 (16%)	2 (2%)	7	32
42	CR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	3
42	DR	101/103 (98%)	78 (77%)	14 (14%)	9 (9%)	0	3
43	CS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	1	8
43	DS	108/110 (98%)	78 (72%)	19 (18%)	11 (10%)	0	2
44	CT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	0	1
44	DT	91/93 (98%)	59 (65%)	20 (22%)	12 (13%)	0	1
45	CU	100/102 (98%)	74 (74%)	14 (14%)	12 (12%)	0	1
45	DU	100/102 (98%)	73 (73%)	14 (14%)	13 (13%)	0	1
46	CV	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	5	26
46	DV	92/94 (98%)	71 (77%)	15 (16%)	6 (6%)	1	5
47	CW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	4	22
48	CX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	4	22
48	DX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	3
49	CY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	0
49	DY	61/63 (97%)	28 (46%)	16 (26%)	17 (28%)	0	0
50	CZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	DZ	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	2	16
51	C0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	2	15
51	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	2
52	C1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	0	3
52	D1	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	2	13
53	C2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	5	25
53	D2	44/46 (96%)	31 (70%)	8 (18%)	5 (11%)	0	1
54	C3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
54	D3	62/64 (97%)	49 (79%)	11 (18%)	2 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	C4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	21
55	D4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	21
57	DW	73/75 (97%)	57 (78%)	12 (16%)	4 (6%)	1	8
All	All	11416/11626 (98%)	7804 (68%)	2248 (20%)	1364 (12%)	0	1

5 of 1364 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

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%)	111 (62%)	69 (38%)	0	1
2	BB	180/180 (100%)	129 (72%)	51 (28%)	0	2
3	AC	170/170 (100%)	124 (73%)	46 (27%)	0	2
3	BC	170/170 (100%)	123 (72%)	47 (28%)	0	2
4	AD	172/172 (100%)	130 (76%)	42 (24%)	1	4
4	BD	172/172 (100%)	120 (70%)	52 (30%)	0	1
5	AE	113/113 (100%)	75 (66%)	38 (34%)	0	1
5	BE	113/113 (100%)	79 (70%)	34 (30%)	0	1
6	AF	87/87 (100%)	57 (66%)	30 (34%)	0	1
6	BF	87/87 (100%)	61 (70%)	26 (30%)	0	2
7	AG	124/124 (100%)	85 (68%)	39 (32%)	0	1
7	BG	124/124 (100%)	82 (66%)	42 (34%)	0	1
8	AH	104/104 (100%)	79 (76%)	25 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	104/104 (100%)	74 (71%)	30 (29%)	0	2
9	AI	105/105 (100%)	80 (76%)	25 (24%)	1	4
9	BI	105/105 (100%)	68 (65%)	37 (35%)	0	1
10	AJ	86/86 (100%)	60 (70%)	26 (30%)	0	1
10	BJ	86/86 (100%)	55 (64%)	31 (36%)	0	1
11	AK	90/90 (100%)	63 (70%)	27 (30%)	0	1
11	BK	90/90 (100%)	67 (74%)	23 (26%)	0	3
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	12
12	BL	103/103 (100%)	72 (70%)	31 (30%)	0	1
13	AM	92/92 (100%)	69 (75%)	23 (25%)	0	3
13	BM	92/92 (100%)	70 (76%)	22 (24%)	1	4
14	AN	79/83 (95%)	59 (75%)	20 (25%)	0	3
14	BN	79/83 (95%)	59 (75%)	20 (25%)	0	3
15	AO	76/76 (100%)	62 (82%)	14 (18%)	1	9
15	BO	76/76 (100%)	60 (79%)	16 (21%)	1	6
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0	2
16	BP	65/65 (100%)	46 (71%)	19 (29%)	0	2
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
17	BQ	74/74 (100%)	48 (65%)	26 (35%)	0	1
18	AR	48/48 (100%)	37 (77%)	11 (23%)	1	5
18	BR	48/48 (100%)	40 (83%)	8 (17%)	2	12
19	AS	70/70 (100%)	54 (77%)	16 (23%)	1	5
19	BS	70/70 (100%)	49 (70%)	21 (30%)	0	1
20	AT	65/65 (100%)	35 (54%)	30 (46%)	0	0
20	BT	65/65 (100%)	47 (72%)	18 (28%)	0	2
21	AU	44/44 (100%)	26 (59%)	18 (41%)	0	0
21	BU	44/44 (100%)	28 (64%)	16 (36%)	0	1
24	AY	157/157 (100%)	133 (85%)	24 (15%)	3	14
27	CC	216/216 (100%)	173 (80%)	43 (20%)	1	7
27	DC	216/216 (100%)	167 (77%)	49 (23%)	1	5
28	CD	164/164 (100%)	135 (82%)	29 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DD	164/164 (100%)	131 (80%)	33 (20%)	1	7
29	CE	165/165 (100%)	138 (84%)	27 (16%)	2	12
29	DE	165/165 (100%)	117 (71%)	48 (29%)	0	2
30	CF	148/148 (100%)	111 (75%)	37 (25%)	0	3
30	DF	148/148 (100%)	114 (77%)	34 (23%)	1	5
31	CG	137/137 (100%)	110 (80%)	27 (20%)	1	8
31	DG	137/137 (100%)	115 (84%)	22 (16%)	2	12
32	CH	114/114 (100%)	87 (76%)	27 (24%)	1	4
32	DH	114/114 (100%)	89 (78%)	25 (22%)	1	5
33	CI	109/109 (100%)	74 (68%)	35 (32%)	0	1
33	DI	109/109 (100%)	78 (72%)	31 (28%)	0	2
34	CJ	116/116 (100%)	95 (82%)	21 (18%)	2	9
34	DJ	116/116 (100%)	87 (75%)	29 (25%)	0	3
35	CK	103/103 (100%)	85 (82%)	18 (18%)	2	10
35	DK	103/103 (100%)	83 (81%)	20 (19%)	1	8
36	CL	102/102 (100%)	77 (76%)	25 (24%)	1	4
36	DL	102/102 (100%)	75 (74%)	27 (26%)	0	3
37	CM	109/109 (100%)	81 (74%)	28 (26%)	0	3
37	DM	109/109 (100%)	82 (75%)	27 (25%)	1	3
38	CN	100/100 (100%)	80 (80%)	20 (20%)	1	7
38	DN	100/100 (100%)	79 (79%)	21 (21%)	1	6
39	CO	86/86 (100%)	65 (76%)	21 (24%)	1	4
39	DO	86/86 (100%)	63 (73%)	23 (27%)	0	3
40	CP	99/99 (100%)	77 (78%)	22 (22%)	1	5
40	DP	99/99 (100%)	74 (75%)	25 (25%)	0	3
41	CQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
41	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	11
42	CR	84/84 (100%)	68 (81%)	16 (19%)	1	8
42	DR	84/84 (100%)	63 (75%)	21 (25%)	0	3
43	CS	93/93 (100%)	79 (85%)	14 (15%)	3	14
43	DS	93/93 (100%)	72 (77%)	21 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	CT	80/80 (100%)	67 (84%)	13 (16%)	2	12
44	DT	80/80 (100%)	53 (66%)	27 (34%)	0	1
45	CU	83/83 (100%)	64 (77%)	19 (23%)	1	5
45	DU	83/83 (100%)	62 (75%)	21 (25%)	0	3
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
46	DV	78/78 (100%)	60 (77%)	18 (23%)	1	5
47	CW	56/58 (97%)	44 (79%)	12 (21%)	1	6
48	CX	67/67 (100%)	55 (82%)	12 (18%)	2	10
48	DX	67/67 (100%)	54 (81%)	13 (19%)	1	8
49	CY	55/55 (100%)	44 (80%)	11 (20%)	1	7
49	DY	55/55 (100%)	44 (80%)	11 (20%)	1	7
50	CZ	48/48 (100%)	36 (75%)	12 (25%)	0	3
50	DZ	48/48 (100%)	34 (71%)	14 (29%)	0	2
51	C0	47/47 (100%)	41 (87%)	6 (13%)	4	19
51	D0	47/47 (100%)	40 (85%)	7 (15%)	3	15
52	C1	45/45 (100%)	35 (78%)	10 (22%)	1	5
52	D1	45/45 (100%)	36 (80%)	9 (20%)	1	7
53	C2	38/38 (100%)	32 (84%)	6 (16%)	2	13
53	D2	38/38 (100%)	33 (87%)	5 (13%)	4	18
54	C3	51/51 (100%)	42 (82%)	9 (18%)	2	10
54	D3	51/51 (100%)	46 (90%)	5 (10%)	7	30
55	C4	34/34 (100%)	27 (79%)	7 (21%)	1	7
55	D4	34/34 (100%)	29 (85%)	5 (15%)	3	15
57	DW	55/57 (96%)	48 (87%)	7 (13%)	4	20
All	All	9482/9494 (100%)	7166 (76%)	2316 (24%)	1	4

5 of 2316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	DF	91	ARG
52	D1	4	ILE
32	DH	79	THR
30	DF	82	TYR
39	DO	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 250 such sidechains are listed below:

Mol	Chain	Res	Type
20	BT	19	HIS
40	DP	65	ASN
34	CJ	58	ASN
39	DO	43	ASN
57	DW	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	442 (28%)	28 (1%)
1	BA	1538/1539 (99%)	446 (28%)	20 (1%)
22	AV	75/76 (98%)	29 (38%)	1 (1%)
22	BV	75/76 (98%)	15 (20%)	1 (1%)
23	AX	14/16 (87%)	5 (35%)	0
23	BX	15/16 (93%)	4 (26%)	0
25	CA	2895/2903 (99%)	754 (26%)	53 (1%)
25	DA	2893/2903 (99%)	765 (26%)	48 (1%)
26	CB	118/119 (99%)	24 (20%)	1 (0%)
56	DB	117/118 (99%)	34 (29%)	3 (2%)
All	All	9277/9305 (99%)	2518 (27%)	155 (1%)

5 of 2518 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	614	A
25	DA	2311	A
25	DA	945	A
25	DA	1738	G
25	DA	2800	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.47	12 (0%) 82 64	0, 31, 105, 170	0
1	BA	1539/1539 (100%)	-0.38	19 (1%) 76 55	0, 33, 101, 147	0
2	AB	218/218 (100%)	0.44	16 (7%) 21 11	12, 52, 84, 115	0
2	BB	218/218 (100%)	0.42	10 (4%) 37 20	19, 59, 88, 113	0
3	AC	206/206 (100%)	-0.25	4 (1%) 66 43	0, 35, 69, 93	0
3	BC	206/206 (100%)	0.03	1 (0%) 87 72	9, 46, 75, 92	0
4	AD	205/205 (100%)	0.19	8 (3%) 43 24	14, 42, 73, 98	0
4	BD	205/205 (100%)	-0.13	7 (3%) 48 27	0, 24, 64, 82	0
5	AE	150/150 (100%)	-0.09	3 (2%) 65 41	0, 32, 68, 105	0
5	BE	150/150 (100%)	-0.06	2 (1%) 75 53	0, 31, 68, 98	0
6	AF	100/100 (100%)	-0.14	3 (3%) 52 30	0, 33, 68, 86	0
6	BF	100/100 (100%)	0.23	2 (2%) 65 41	17, 54, 80, 93	0
7	AG	151/151 (100%)	0.36	10 (6%) 24 12	12, 56, 86, 111	0
7	BG	151/151 (100%)	0.25	9 (5%) 27 14	20, 54, 81, 94	0
8	AH	129/129 (100%)	-0.30	2 (1%) 70 47	0, 32, 60, 71	0
8	BH	129/129 (100%)	-0.15	2 (1%) 70 47	4, 34, 58, 82	0
9	AI	127/127 (100%)	0.38	3 (2%) 59 36	6, 54, 79, 108	0
9	BI	127/127 (100%)	0.75	9 (7%) 22 11	20, 55, 85, 117	0
10	AJ	98/98 (100%)	0.59	5 (5%) 33 17	8, 55, 89, 104	0
10	BJ	98/98 (100%)	0.73	8 (8%) 17 9	25, 58, 82, 113	0
11	AK	117/117 (100%)	-0.24	3 (2%) 57 34	0, 19, 50, 87	0
11	BK	117/117 (100%)	-0.04	2 (1%) 69 45	0, 32, 66, 79	0
12	AL	123/123 (100%)	-0.03	7 (5%) 29 15	0, 22, 67, 93	0
12	BL	123/123 (100%)	-0.16	7 (5%) 29 15	0, 17, 58, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.21	3 (2%) 57 34	9, 53, 87, 100	0
13	BM	114/114 (100%)	0.50	7 (6%) 27 14	26, 63, 87, 97	0
14	AN	96/100 (96%)	0.41	4 (4%) 40 22	12, 45, 84, 106	0
14	BN	96/100 (96%)	0.75	9 (9%) 14 7	10, 56, 84, 98	0
15	AO	88/88 (100%)	-0.23	1 (1%) 78 57	0, 28, 55, 93	0
15	BO	88/88 (100%)	-0.14	0 100 100	1, 33, 66, 89	0
16	AP	82/82 (100%)	-0.05	0 100 100	5, 30, 73, 86	0
16	BP	82/82 (100%)	-0.12	0 100 100	0, 24, 67, 91	0
17	AQ	80/80 (100%)	0.13	5 (6%) 26 13	8, 42, 75, 96	0
17	BQ	80/80 (100%)	0.16	4 (5%) 34 18	7, 44, 79, 94	0
18	AR	55/55 (100%)	-0.24	2 (3%) 46 26	0, 25, 59, 93	0
18	BR	55/55 (100%)	0.08	2 (3%) 46 26	5, 38, 80, 101	0
19	AS	79/79 (100%)	0.31	3 (3%) 44 24	21, 52, 83, 98	0
19	BS	79/79 (100%)	0.69	4 (5%) 33 17	37, 65, 83, 95	0
20	AT	85/85 (100%)	0.35	5 (5%) 28 14	7, 37, 67, 80	0
20	BT	85/85 (100%)	0.30	5 (5%) 28 14	8, 38, 69, 96	0
21	AU	51/51 (100%)	1.16	10 (19%) 3 2	7, 39, 74, 77	0
21	BU	51/51 (100%)	0.97	9 (17%) 4 3	8, 47, 74, 80	0
22	AV	76/76 (100%)	0.11	5 (6%) 24 12	0, 70, 127, 154	0
22	BV	76/76 (100%)	-0.34	0 100 100	22, 43, 72, 119	0
23	AX	15/16 (93%)	0.89	2 (13%) 7 4	6, 76, 115, 133	0
23	BX	16/16 (100%)	0.35	2 (12%) 8 5	16, 77, 102, 124	0
24	AY	183/183 (100%)	0.19	6 (3%) 49 28	0, 50, 96, 117	0
25	CA	2897/2903 (99%)	-0.71	91 (3%) 51 30	0, 0, 103, 162	0
25	DA	2896/2903 (99%)	-0.62	51 (1%) 67 44	0, 15, 109, 162	0
26	CB	119/119 (100%)	-0.85	1 (0%) 82 64	0, 7, 32, 85	0
27	CC	271/271 (100%)	-0.56	3 (1%) 78 57	0, 1, 29, 56	0
27	DC	271/271 (100%)	-0.34	1 (0%) 88 76	0, 19, 46, 77	0
28	CD	209/209 (100%)	-0.59	0 100 100	0, 0, 19, 61	0
28	DD	209/209 (100%)	-0.48	0 100 100	0, 10, 52, 66	0
29	CE	201/201 (100%)	-0.50	0 100 100	0, 0, 39, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DE	201/201 (100%)	-0.35	0 100 100	0, 21, 60, 89	0
30	CF	177/177 (100%)	0.04	4 (2%) 61 38	0, 35, 82, 91	0
30	DF	177/177 (100%)	0.32	7 (3%) 42 23	12, 58, 84, 95	0
31	CG	176/176 (100%)	-0.55	1 (0%) 85 69	0, 15, 48, 88	0
31	DG	176/176 (100%)	0.04	0 100 100	15, 48, 73, 93	0
32	CH	149/149 (100%)	0.16	7 (4%) 36 19	0, 52, 87, 100	0
32	DH	149/149 (100%)	0.39	5 (3%) 48 27	8, 58, 92, 107	0
33	CI	141/141 (100%)	2.01	61 (43%) 0 1	44, 79, 102, 124	0
33	DI	141/141 (100%)	2.12	71 (50%) 0 0	54, 82, 104, 118	0
34	CJ	142/142 (100%)	-0.52	3 (2%) 63 40	0, 0, 21, 56	0
34	DJ	142/142 (100%)	-0.51	3 (2%) 63 40	0, 8, 37, 65	0
35	CK	122/122 (100%)	-0.61	0 100 100	0, 0, 27, 73	0
35	DK	122/122 (100%)	-0.46	1 (0%) 82 64	0, 15, 50, 71	0
36	CL	143/143 (100%)	-0.41	1 (0%) 84 66	0, 0, 27, 68	0
36	DL	143/143 (100%)	-0.29	2 (1%) 73 51	0, 18, 56, 82	0
37	CM	136/136 (100%)	-0.63	0 100 100	0, 0, 21, 83	0
37	DM	136/136 (100%)	-0.40	0 100 100	0, 21, 55, 88	0
38	CN	120/120 (100%)	-0.55	0 100 100	0, 0, 14, 68	0
38	DN	120/120 (100%)	-0.38	0 100 100	0, 12, 44, 78	0
39	CO	116/116 (100%)	-0.55	0 100 100	0, 11, 39, 49	0
39	DO	116/116 (100%)	0.32	2 (1%) 69 45	5, 49, 78, 98	0
40	CP	114/114 (100%)	-0.64	0 100 100	0, 0, 47, 70	0
40	DP	114/114 (100%)	-0.38	0 100 100	0, 21, 51, 81	0
41	CQ	117/117 (100%)	-0.39	1 (0%) 81 61	0, 0, 7, 63	0
41	DQ	117/117 (100%)	-0.68	0 100 100	0, 2, 27, 45	0
42	CR	103/103 (100%)	-0.60	0 100 100	0, 0, 35, 57	0
42	DR	103/103 (100%)	-0.37	1 (0%) 79 59	0, 10, 46, 78	0
43	CS	110/110 (100%)	-0.49	0 100 100	0, 0, 22, 98	0
43	DS	110/110 (100%)	-0.62	0 100 100	0, 8, 40, 77	0
44	CT	93/93 (100%)	-0.29	1 (1%) 78 57	0, 6, 68, 78	0
44	DT	93/93 (100%)	0.03	2 (2%) 62 39	0, 35, 71, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	CU	102/102 (100%)	-0.43	2 (1%) 65 41	0, 5, 42, 79	0
45	DU	102/102 (100%)	0.15	8 (7%) 19 10	0, 34, 74, 100	0
46	CV	94/94 (100%)	-0.55	0 100 100	0, 6, 42, 62	0
46	DV	94/94 (100%)	-0.07	0 100 100	11, 43, 68, 82	0
47	CW	76/76 (100%)	-0.51	1 (1%) 75 53	0, 1, 31, 69	0
48	CX	77/77 (100%)	-0.62	0 100 100	0, 1, 47, 74	0
48	DX	77/77 (100%)	-0.31	1 (1%) 75 53	0, 23, 55, 67	0
49	CY	63/63 (100%)	-0.18	1 (1%) 70 47	0, 14, 56, 97	0
49	DY	63/63 (100%)	0.20	3 (4%) 35 19	8, 43, 70, 111	0
50	CZ	58/58 (100%)	-0.54	1 (1%) 69 45	0, 0, 13, 50	0
50	DZ	58/58 (100%)	-0.43	1 (1%) 69 45	0, 20, 52, 72	0
51	C0	56/56 (100%)	-0.46	0 100 100	0, 0, 25, 69	0
51	D0	56/56 (100%)	-0.32	1 (1%) 67 44	0, 10, 53, 94	0
52	C1	50/50 (100%)	-0.42	1 (2%) 65 41	0, 8, 51, 93	0
52	D1	50/50 (100%)	0.11	0 100 100	21, 38, 70, 88	0
53	C2	46/46 (100%)	-0.24	1 (2%) 62 39	0, 0, 15, 101	0
53	D2	46/46 (100%)	-0.31	1 (2%) 62 39	0, 10, 26, 94	0
54	C3	64/64 (100%)	-0.50	0 100 100	0, 0, 11, 38	0
54	D3	64/64 (100%)	-0.32	0 100 100	0, 15, 35, 52	0
55	C4	38/38 (100%)	-0.26	1 (2%) 57 34	0, 1, 32, 72	0
55	D4	38/38 (100%)	0.17	1 (2%) 57 34	3, 26, 59, 65	0
56	DB	118/118 (100%)	-0.14	2 (1%) 69 45	6, 58, 86, 106	0
57	DW	75/75 (100%)	-0.18	1 (1%) 75 53	0, 27, 54, 94	0
All	All	20908/20931 (99%)	-0.29	589 (2%) 55 32	0, 23, 86, 170	0

The worst 5 of 589 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BT	3	ILE	9.7
53	C2	46	LYS	8.4
25	CA	2172	U	8.2
2	AB	156	LEU	7.9
25	DA	2172	U	7.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3062	1/1	0.37	0.43	46,46,46,46	0
58	MG	CA	3048	1/1	0.73	0.08	13,13,13,13	0
58	MG	DA	3150	1/1	0.75	0.17	0,0,0,0	0
58	MG	DA	3098	1/1	0.82	0.28	49,49,49,49	0
58	MG	CA	3106	1/1	0.84	0.15	0,0,0,0	0
58	MG	DA	3083	1/1	0.84	0.17	31,31,31,31	0
58	MG	AA	1670	1/1	0.85	0.12	11,11,11,11	0
58	MG	DA	3165	1/1	0.85	0.18	0,0,0,0	0
58	MG	CA	3108	1/1	0.86	0.04	0,0,0,0	0
58	MG	DA	3060	1/1	0.86	0.21	5,5,5,5	0
58	MG	CA	3173	1/1	0.87	0.18	0,0,0,0	0
58	MG	AA	1667	1/1	0.87	0.19	13,13,13,13	0
58	MG	CA	3158	1/1	0.87	0.28	0,0,0,0	0
58	MG	BA	1618	1/1	0.88	0.12	4,4,4,4	0
58	MG	DA	3147	1/1	0.88	0.19	0,0,0,0	0
58	MG	AA	1658	1/1	0.89	0.13	16,16,16,16	0
58	MG	BA	1653	1/1	0.89	0.08	7,7,7,7	0
58	MG	DA	3161	1/1	0.89	0.16	15,15,15,15	0
58	MG	BA	1654	1/1	0.89	0.13	22,22,22,22	0
58	MG	DA	3131	1/1	0.90	0.26	55,55,55,55	0
58	MG	AA	1653	1/1	0.90	0.15	1,1,1,1	0
58	MG	BA	1635	1/1	0.90	0.12	21,21,21,21	0
58	MG	BA	1655	1/1	0.90	0.14	9,9,9,9	0
58	MG	DA	3163	1/1	0.90	0.10	0,0,0,0	0
58	MG	DA	3115	1/1	0.90	0.15	27,27,27,27	0
58	MG	CA	3177	1/1	0.91	0.17	0,0,0,0	0
58	MG	CB	204	1/1	0.91	0.35	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	1644	1/1	0.91	0.17	5,5,5,5	0
58	MG	CA	3099	1/1	0.91	0.33	53,53,53,53	0
58	MG	AA	1663	1/1	0.91	0.09	6,6,6,6	0
58	MG	AA	1640	1/1	0.91	0.15	34,34,34,34	0
58	MG	DA	3116	1/1	0.91	0.12	13,13,13,13	0
58	MG	CA	3134	1/1	0.91	0.20	14,14,14,14	0
58	MG	DA	3138	1/1	0.91	0.34	0,0,0,0	0
58	MG	CA	3152	1/1	0.91	0.17	0,0,0,0	0
58	MG	CA	3153	1/1	0.91	0.18	0,0,0,0	0
58	MG	CA	3028	1/1	0.91	0.12	21,21,21,21	0
58	MG	CA	3160	1/1	0.91	0.21	0,0,0,0	0
58	MG	BA	1642	1/1	0.91	0.18	6,6,6,6	0
58	MG	AA	1664	1/1	0.92	0.09	4,4,4,4	0
58	MG	CA	3164	1/1	0.92	0.24	0,0,0,0	0
58	MG	AA	1655	1/1	0.92	0.19	0,0,0,0	0
58	MG	AA	1645	1/1	0.92	0.19	8,8,8,8	0
58	MG	CA	3178	1/1	0.92	0.07	0,0,0,0	0
58	MG	CA	3194	1/1	0.92	0.18	0,0,0,0	0
58	MG	AA	1625	1/1	0.92	0.04	6,6,6,6	0
58	MG	DA	3149	1/1	0.92	0.18	0,0,0,0	0
58	MG	CQ	201	1/1	0.92	0.27	0,0,0,0	0
58	MG	DA	3160	1/1	0.92	0.07	0,0,0,0	0
58	MG	DA	3055	1/1	0.92	0.11	28,28,28,28	0
58	MG	DA	3057	1/1	0.92	0.11	14,14,14,14	0
58	MG	BA	1631	1/1	0.92	0.09	35,35,35,35	0
58	MG	DA	3061	1/1	0.93	0.18	24,24,24,24	0
58	MG	AA	1666	1/1	0.93	0.09	13,13,13,13	0
58	MG	DA	3091	1/1	0.93	0.18	50,50,50,50	0
58	MG	AA	1660	1/1	0.93	0.16	15,15,15,15	0
58	MG	AA	1656	1/1	0.93	0.16	14,14,14,14	0
58	MG	BA	1649	1/1	0.93	0.18	11,11,11,11	0
58	MG	CA	3176	1/1	0.93	0.16	10,10,10,10	0
58	MG	BA	1615	1/1	0.93	0.17	9,9,9,9	0
58	MG	CA	3117	1/1	0.93	0.09	5,5,5,5	0
58	MG	AA	1654	1/1	0.93	0.15	5,5,5,5	0
58	MG	CA	3145	1/1	0.93	0.14	0,0,0,0	0
58	MG	CA	3147	1/1	0.93	0.29	0,0,0,0	0
58	MG	BA	1627	1/1	0.93	0.07	35,35,35,35	0
58	MG	BA	1630	1/1	0.93	0.07	41,41,41,41	0
58	MG	DA	3164	1/1	0.93	0.11	0,0,0,0	0
58	MG	CA	3154	1/1	0.93	0.21	0,0,0,0	0
58	MG	CA	3188	1/1	0.94	0.16	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3192	1/1	0.94	0.05	0,0,0,0	0
58	MG	CA	3026	1/1	0.94	0.20	30,30,30,30	0
58	MG	BA	1645	1/1	0.94	0.07	8,8,8,8	0
58	MG	BA	1647	1/1	0.94	0.07	0,0,0,0	0
58	MG	CA	3149	1/1	0.94	0.35	0,0,0,0	0
58	MG	CA	3151	1/1	0.94	0.28	0,0,0,0	0
58	MG	AA	1648	1/1	0.94	0.05	4,4,4,4	0
58	MG	CA	3081	1/1	0.94	0.03	0,0,0,0	0
58	MG	DA	3078	1/1	0.94	0.09	15,15,15,15	0
58	MG	CA	3085	1/1	0.94	0.09	12,12,12,12	0
58	MG	CA	3155	1/1	0.94	0.26	0,0,0,0	0
58	MG	CA	3156	1/1	0.94	0.28	0,0,0,0	0
58	MG	AA	1661	1/1	0.94	0.11	15,15,15,15	0
58	MG	CA	3159	1/1	0.94	0.18	0,0,0,0	0
58	MG	CA	3105	1/1	0.94	0.12	0,0,0,0	0
58	MG	CA	3161	1/1	0.94	0.12	0,0,0,0	0
58	MG	DA	3139	1/1	0.94	0.23	0,0,0,0	0
58	MG	CA	3163	1/1	0.94	0.16	0,0,0,0	0
58	MG	BA	1636	1/1	0.94	0.07	42,42,42,42	0
58	MG	CA	3167	1/1	0.94	0.23	0,0,0,0	0
58	MG	DA	3151	1/1	0.94	0.18	11,11,11,11	0
58	MG	DA	3152	1/1	0.94	0.20	6,6,6,6	0
58	MG	DA	3156	1/1	0.94	0.18	3,3,3,3	0
58	MG	AA	1662	1/1	0.94	0.13	8,8,8,8	0
58	MG	CA	3175	1/1	0.94	0.16	0,0,0,0	0
58	MG	CA	3116	1/1	0.94	0.17	10,10,10,10	0
58	MG	CA	3014	1/1	0.94	0.07	12,12,12,12	0
58	MG	CA	3132	1/1	0.94	0.26	24,24,24,24	0
58	MG	BA	1612	1/1	0.95	0.05	18,18,18,18	0
58	MG	DA	3119	1/1	0.95	0.09	44,44,44,44	0
58	MG	AA	1623	1/1	0.95	0.07	24,24,24,24	0
58	MG	DA	3025	1/1	0.95	0.17	16,16,16,16	0
58	MG	DA	3036	1/1	0.95	0.09	21,21,21,21	0
58	MG	DA	3143	1/1	0.95	0.18	0,0,0,0	0
58	MG	DA	3146	1/1	0.95	0.18	0,0,0,0	0
58	MG	DA	3047	1/1	0.95	0.05	28,28,28,28	0
58	MG	DA	3148	1/1	0.95	0.19	0,0,0,0	0
58	MG	CA	3140	1/1	0.95	0.35	0,0,0,0	0
58	MG	AA	1659	1/1	0.95	0.08	12,12,12,12	0
58	MG	BA	1643	1/1	0.95	0.15	3,3,3,3	0
58	MG	BA	1644	1/1	0.95	0.08	0,0,0,0	0
58	MG	CA	3180	1/1	0.95	0.10	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	1601	1/1	0.95	0.07	44,44,44,44	0
58	MG	DA	3090	1/1	0.95	0.06	15,15,15,15	0
58	MG	CA	3191	1/1	0.95	0.17	0,0,0,0	0
58	MG	AA	1616	1/1	0.95	0.07	11,11,11,11	0
58	MG	AA	1650	1/1	0.95	0.07	0,0,0,0	0
58	MG	BA	1633	1/1	0.96	0.11	11,11,11,11	0
58	MG	CA	3138	1/1	0.96	0.40	0,0,0,0	0
58	MG	CA	3165	1/1	0.96	0.13	0,0,0,0	0
58	MG	BA	1648	1/1	0.96	0.22	0,0,0,0	0
58	MG	DA	3079	1/1	0.96	0.06	27,27,27,27	0
58	MG	CA	3169	1/1	0.96	0.23	7,7,7,7	0
58	MG	DA	3084	1/1	0.96	0.12	32,32,32,32	0
58	MG	DA	3088	1/1	0.96	0.11	12,12,12,12	0
58	MG	CA	3170	1/1	0.96	0.11	0,0,0,0	0
58	MG	CA	3172	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3092	1/1	0.96	0.17	34,34,34,34	0
58	MG	DA	3095	1/1	0.96	0.07	10,10,10,10	0
58	MG	CA	3143	1/1	0.96	0.24	0,0,0,0	0
58	MG	DA	3102	1/1	0.96	0.07	12,12,12,12	0
58	MG	CA	3058	1/1	0.96	0.05	10,10,10,10	0
58	MG	AA	1639	1/1	0.96	0.08	22,22,22,22	0
58	MG	BA	1651	1/1	0.96	0.06	7,7,7,7	0
58	MG	CA	3150	1/1	0.96	0.13	0,0,0,0	0
58	MG	DA	3136	1/1	0.96	0.12	28,28,28,28	0
58	MG	CA	3082	1/1	0.96	0.06	0,0,0,0	0
58	MG	CA	3181	1/1	0.96	0.16	0,0,0,0	0
58	MG	DA	3140	1/1	0.96	0.21	0,0,0,0	0
58	MG	CA	3185	1/1	0.96	0.21	0,0,0,0	0
58	MG	CA	3084	1/1	0.96	0.05	22,22,22,22	0
58	MG	CA	3190	1/1	0.96	0.21	0,0,0,0	0
58	MG	AA	1668	1/1	0.96	0.08	0,0,0,0	0
58	MG	AA	1669	1/1	0.96	0.12	10,10,10,10	0
58	MG	AA	1620	1/1	0.96	0.07	10,10,10,10	0
58	MG	BA	1656	1/1	0.96	0.19	9,9,9,9	0
58	MG	CA	3013	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3155	1/1	0.96	0.11	1,1,1,1	0
58	MG	DA	3004	1/1	0.96	0.06	30,30,30,30	0
58	MG	DA	3157	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3015	1/1	0.96	0.16	23,23,23,23	0
58	MG	AA	1671	1/1	0.96	0.11	6,6,6,6	0
58	MG	CA	3015	1/1	0.96	0.12	36,36,36,36	0
58	MG	BA	1608	1/1	0.96	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3162	1/1	0.96	0.26	0,0,0,0	0
58	MG	DB	203	1/1	0.96	0.08	16,16,16,16	0
58	MG	DQ	801	1/1	0.96	0.24	0,0,0,0	0
58	MG	DA	3080	1/1	0.97	0.12	1,1,1,1	0
58	MG	CA	3070	1/1	0.97	0.12	25,25,25,25	0
58	MG	BA	1652	1/1	0.97	0.11	1,1,1,1	0
58	MG	BA	1637	1/1	0.97	0.09	19,19,19,19	0
58	MG	CA	3179	1/1	0.97	0.12	0,0,0,0	0
58	MG	BA	1641	1/1	0.97	0.07	20,20,20,20	0
58	MG	AA	1646	1/1	0.97	0.04	0,0,0,0	0
58	MG	CA	3182	1/1	0.97	0.28	0,0,0,0	0
58	MG	CA	3091	1/1	0.97	0.05	3,3,3,3	0
58	MG	CA	3186	1/1	0.97	0.27	0,0,0,0	0
58	MG	DA	3110	1/1	0.97	0.07	18,18,18,18	0
58	MG	BA	1620	1/1	0.97	0.06	19,19,19,19	0
58	MG	CA	3189	1/1	0.97	0.11	0,0,0,0	0
58	MG	CA	3001	1/1	0.97	0.05	0,0,0,0	0
58	MG	CA	3157	1/1	0.97	0.19	0,0,0,0	0
58	MG	DA	3133	1/1	0.97	0.19	16,16,16,16	0
58	MG	AA	1619	1/1	0.97	0.11	32,32,32,32	0
58	MG	AA	1665	1/1	0.97	0.04	0,0,0,0	0
58	MG	BA	1646	1/1	0.97	0.07	10,10,10,10	0
58	MG	CA	3024	1/1	0.97	0.06	0,0,0,0	0
58	MG	DA	3141	1/1	0.97	0.22	0,0,0,0	0
58	MG	AA	1627	1/1	0.97	0.08	19,19,19,19	0
58	MG	DA	3145	1/1	0.97	0.12	0,0,0,0	0
58	MG	DA	3011	1/1	0.97	0.04	0,0,0,0	0
58	MG	DA	3013	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3014	1/1	0.97	0.06	12,12,12,12	0
58	MG	BA	1609	1/1	0.97	0.06	26,26,26,26	0
58	MG	CA	3035	1/1	0.97	0.09	1,1,1,1	0
58	MG	CA	3139	1/1	0.97	0.37	0,0,0,0	0
58	MG	DA	3040	1/1	0.97	0.06	5,5,5,5	0
58	MG	DA	3153	1/1	0.97	0.12	11,11,11,11	0
58	MG	DA	3154	1/1	0.97	0.15	0,0,0,0	0
58	MG	CA	3166	1/1	0.97	0.14	0,0,0,0	0
58	MG	CA	3045	1/1	0.97	0.04	0,0,0,0	0
58	MG	CA	3141	1/1	0.97	0.26	0,0,0,0	0
58	MG	DA	3158	1/1	0.97	0.10	0,0,0,0	0
58	MG	DA	3159	1/1	0.97	0.17	3,3,3,3	0
58	MG	DA	3059	1/1	0.97	0.07	6,6,6,6	0
58	MG	AA	1652	1/1	0.97	0.16	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	3162	1/1	0.97	0.20	4,4,4,4	0
58	MG	CA	3144	1/1	0.97	0.26	0,0,0,0	0
58	MG	DA	3063	1/1	0.97	0.10	0,0,0,0	0
58	MG	DA	3069	1/1	0.97	0.06	41,41,41,41	0
58	MG	DA	3166	1/1	0.97	0.25	9,9,9,9	0
58	MG	BA	1650	1/1	0.97	0.21	5,5,5,5	0
58	MG	AA	1657	1/1	0.97	0.13	2,2,2,2	0
58	MG	DA	3043	1/1	0.98	0.05	6,6,6,6	0
58	MG	AA	1604	1/1	0.98	0.14	22,22,22,22	0
58	MG	DA	3050	1/1	0.98	0.04	0,0,0,0	0
58	MG	CA	3086	1/1	0.98	0.09	0,0,0,0	0
58	MG	CA	3089	1/1	0.98	0.12	19,19,19,19	0
58	MG	AA	1622	1/1	0.98	0.14	0,0,0,0	0
58	MG	CA	3092	1/1	0.98	0.06	16,16,16,16	0
58	MG	CA	3095	1/1	0.98	0.08	17,17,17,17	0
58	MG	AA	1610	1/1	0.98	0.05	32,32,32,32	0
58	MG	CA	3103	1/1	0.98	0.08	0,0,0,0	0
58	MG	DA	3070	1/1	0.98	0.04	0,0,0,0	0
58	MG	DA	3073	1/1	0.98	0.04	6,6,6,6	0
58	MG	AA	1614	1/1	0.98	0.03	12,12,12,12	0
58	MG	CA	3002	1/1	0.98	0.06	0,0,0,0	0
58	MG	CA	3168	1/1	0.98	0.16	0,0,0,0	0
58	MG	AA	1647	1/1	0.98	0.21	1,1,1,1	0
58	MG	CA	3109	1/1	0.98	0.10	0,0,0,0	0
58	MG	CA	3171	1/1	0.98	0.13	0,0,0,0	0
58	MG	CA	3112	1/1	0.98	0.05	4,4,4,4	0
58	MG	CA	3114	1/1	0.98	0.05	0,0,0,0	0
58	MG	CA	3174	1/1	0.98	0.18	0,0,0,0	0
58	MG	DA	3094	1/1	0.98	0.04	43,43,43,43	0
58	MG	BA	1603	1/1	0.98	0.04	13,13,13,13	0
58	MG	DA	3096	1/1	0.98	0.04	13,13,13,13	0
58	MG	BA	1606	1/1	0.98	0.06	24,24,24,24	0
58	MG	CA	3120	1/1	0.98	0.13	2,2,2,2	0
58	MG	DA	3103	1/1	0.98	0.05	0,0,0,0	0
58	MG	DA	3104	1/1	0.98	0.06	0,0,0,0	0
58	MG	DA	3105	1/1	0.98	0.04	0,0,0,0	0
58	MG	CA	3124	1/1	0.98	0.03	0,0,0,0	0
58	MG	DA	3111	1/1	0.98	0.05	1,1,1,1	0
58	MG	DA	3114	1/1	0.98	0.04	14,14,14,14	0
58	MG	CA	3021	1/1	0.98	0.04	0,0,0,0	0
58	MG	AA	1602	1/1	0.98	0.11	17,17,17,17	0
58	MG	AA	1649	1/1	0.98	0.20	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1611	1/1	0.98	0.08	13,13,13,13	0
58	MG	CA	3183	1/1	0.98	0.20	0,0,0,0	0
58	MG	DA	3135	1/1	0.98	0.08	11,11,11,11	0
58	MG	CA	3184	1/1	0.98	0.18	0,0,0,0	0
58	MG	DA	3137	1/1	0.98	0.36	0,0,0,0	0
58	MG	CA	3030	1/1	0.98	0.06	0,0,0,0	0
58	MG	CA	3031	1/1	0.98	0.15	0,0,0,0	0
58	MG	CA	3187	1/1	0.98	0.13	0,0,0,0	0
58	MG	CA	3142	1/1	0.98	0.37	0,0,0,0	0
58	MG	DA	3142	1/1	0.98	0.12	0,0,0,0	0
58	MG	AA	1630	1/1	0.98	0.10	16,16,16,16	0
58	MG	BA	1614	1/1	0.98	0.05	19,19,19,19	0
58	MG	AA	1651	1/1	0.98	0.18	0,0,0,0	0
58	MG	CA	3146	1/1	0.98	0.26	0,0,0,0	0
58	MG	CA	3193	1/1	0.98	0.17	0,0,0,0	0
58	MG	CA	3056	1/1	0.98	0.08	10,10,10,10	0
58	MG	CA	3148	1/1	0.98	0.28	0,0,0,0	0
58	MG	BA	1616	1/1	0.98	0.04	0,0,0,0	0
58	MG	CA	3061	1/1	0.98	0.05	9,9,9,9	0
58	MG	DA	3005	1/1	0.98	0.07	25,25,25,25	0
58	MG	DA	3006	1/1	0.98	0.05	10,10,10,10	0
58	MG	DA	3009	1/1	0.98	0.04	4,4,4,4	0
58	MG	DA	3010	1/1	0.98	0.04	7,7,7,7	0
58	MG	AA	1631	1/1	0.98	0.11	35,35,35,35	0
58	MG	AA	1635	1/1	0.98	0.09	18,18,18,18	0
58	MG	CA	3076	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3080	1/1	0.98	0.07	1,1,1,1	0
58	MG	DA	3016	1/1	0.98	0.04	1,1,1,1	0
58	MG	DA	3018	1/1	0.98	0.02	6,6,6,6	0
58	MG	DA	3023	1/1	0.98	0.04	0,0,0,0	0
58	MG	BA	1623	1/1	0.98	0.04	3,3,3,3	0
58	MG	DA	3034	1/1	0.98	0.04	11,11,11,11	0
58	MG	AA	1603	1/1	0.98	0.05	28,28,28,28	0
58	MG	DA	3039	1/1	0.98	0.03	3,3,3,3	0
58	MG	BA	1629	1/1	0.98	0.05	17,17,17,17	0
58	MG	DA	3028	1/1	0.99	0.05	0,0,0,0	0
58	MG	DA	3030	1/1	0.99	0.05	0,0,0,0	0
58	MG	DA	3033	1/1	0.99	0.06	0,0,0,0	0
58	MG	CA	3047	1/1	0.99	0.05	0,0,0,0	0
58	MG	AA	1642	1/1	0.99	0.03	1,1,1,1	0
58	MG	DA	3037	1/1	0.99	0.10	0,0,0,0	0
58	MG	DA	3038	1/1	0.99	0.03	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3053	1/1	0.99	0.03	0,0,0,0	0
58	MG	AA	1643	1/1	0.99	0.33	0,0,0,0	0
58	MG	AA	1612	1/1	0.99	0.09	0,0,0,0	0
58	MG	DA	3044	1/1	0.99	0.06	11,11,11,11	0
58	MG	DA	3045	1/1	0.99	0.04	0,0,0,0	0
58	MG	DA	3046	1/1	0.99	0.03	1,1,1,1	0
58	MG	CA	3059	1/1	0.99	0.03	4,4,4,4	0
58	MG	CA	3060	1/1	0.99	0.05	4,4,4,4	0
58	MG	DA	3053	1/1	0.99	0.01	0,0,0,0	0
58	MG	DA	3054	1/1	0.99	0.04	0,0,0,0	0
58	MG	AA	1607	1/1	0.99	0.03	10,10,10,10	0
58	MG	DA	3056	1/1	0.99	0.08	5,5,5,5	0
58	MG	AA	1615	1/1	0.99	0.08	9,9,9,9	0
58	MG	CA	3063	1/1	0.99	0.08	0,0,0,0	0
58	MG	AA	1626	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3074	1/1	0.99	0.10	0,0,0,0	0
58	MG	DA	3062	1/1	0.99	0.06	0,0,0,0	0
58	MG	CA	3075	1/1	0.99	0.02	0,0,0,0	0
58	MG	DA	3064	1/1	0.99	0.04	0,0,0,0	0
58	MG	DA	3066	1/1	0.99	0.04	0,0,0,0	0
58	MG	AA	1608	1/1	0.99	0.13	0,0,0,0	0
58	MG	CA	3077	1/1	0.99	0.05	0,0,0,0	0
58	MG	DA	3071	1/1	0.99	0.06	0,0,0,0	0
58	MG	AA	1617	1/1	0.99	0.06	21,21,21,21	0
58	MG	DA	3075	1/1	0.99	0.03	8,8,8,8	0
58	MG	DA	3076	1/1	0.99	0.06	5,5,5,5	0
58	MG	AA	1618	1/1	0.99	0.04	21,21,21,21	0
58	MG	BA	1622	1/1	0.99	0.07	4,4,4,4	0
58	MG	CA	3083	1/1	0.99	0.04	10,10,10,10	0
58	MG	DA	3081	1/1	0.99	0.03	0,0,0,0	0
58	MG	DA	3082	1/1	0.99	0.04	7,7,7,7	0
58	MG	AA	1632	1/1	0.99	0.03	15,15,15,15	0
58	MG	BA	1626	1/1	0.99	0.03	14,14,14,14	0
58	MG	DA	3085	1/1	0.99	0.10	0,0,0,0	0
58	MG	DA	3087	1/1	0.99	0.03	20,20,20,20	0
58	MG	AA	1606	1/1	0.99	0.04	6,6,6,6	0
58	MG	DA	3089	1/1	0.99	0.04	24,24,24,24	0
58	MG	AA	1636	1/1	0.99	0.04	0,0,0,0	0
58	MG	AA	1637	1/1	0.99	0.04	1,1,1,1	0
58	MG	CA	3004	1/1	0.99	0.03	11,11,11,11	0
58	MG	DA	3093	1/1	0.99	0.04	2,2,2,2	0
58	MG	CA	3093	1/1	0.99	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3094	1/1	0.99	0.03	3,3,3,3	0
58	MG	CA	3006	1/1	0.99	0.04	1,1,1,1	0
58	MG	DA	3097	1/1	0.99	0.03	13,13,13,13	0
58	MG	CA	3096	1/1	0.99	0.03	0,0,0,0	0
58	MG	DA	3099	1/1	0.99	0.03	0,0,0,0	0
58	MG	DA	3100	1/1	0.99	0.04	4,4,4,4	0
58	MG	CA	3098	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3007	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3100	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3009	1/1	0.99	0.03	0,0,0,0	0
58	MG	DA	3107	1/1	0.99	0.04	9,9,9,9	0
58	MG	DA	3108	1/1	0.99	0.10	0,0,0,0	0
58	MG	DA	3109	1/1	0.99	0.07	2,2,2,2	0
58	MG	AA	1611	1/1	0.99	0.05	0,0,0,0	0
58	MG	AA	1672	1/1	0.99	0.09	3,3,3,3	0
58	MG	DA	3112	1/1	0.99	0.04	5,5,5,5	0
58	MG	BA	1634	1/1	0.99	0.07	10,10,10,10	0
58	MG	CA	3017	1/1	0.99	0.09	0,0,0,0	0
58	MG	CA	3111	1/1	0.99	0.04	6,6,6,6	0
58	MG	CA	3019	1/1	0.99	0.04	0,0,0,0	0
58	MG	DA	3120	1/1	0.99	0.05	8,8,8,8	0
58	MG	DA	3121	1/1	0.99	0.04	7,7,7,7	0
58	MG	DA	3122	1/1	0.99	0.06	0,0,0,0	0
58	MG	DA	3123	1/1	0.99	0.04	6,6,6,6	0
58	MG	DA	3126	1/1	0.99	0.06	0,0,0,0	0
58	MG	DA	3128	1/1	0.99	0.07	0,0,0,0	0
58	MG	CA	3113	1/1	0.99	0.06	0,0,0,0	0
58	MG	DA	3132	1/1	0.99	0.04	6,6,6,6	0
58	MG	BA	1601	1/1	0.99	0.03	2,2,2,2	0
58	MG	CA	3115	1/1	0.99	0.03	0,0,0,0	0
58	MG	BA	1602	1/1	0.99	0.03	21,21,21,21	0
58	MG	CA	3025	1/1	0.99	0.09	0,0,0,0	0
58	MG	CA	3118	1/1	0.99	0.04	0,0,0,0	0
58	MG	AA	1621	1/1	0.99	0.06	10,10,10,10	0
58	MG	CA	3121	1/1	0.99	0.13	0,0,0,0	0
58	MG	BA	1638	1/1	0.99	0.05	27,27,27,27	0
58	MG	CA	3126	1/1	0.99	0.06	0,0,0,0	0
58	MG	CB	201	1/1	0.99	0.03	0,0,0,0	0
58	MG	DA	3144	1/1	0.99	0.11	0,0,0,0	0
58	MG	CB	202	1/1	0.99	0.08	0,0,0,0	0
58	MG	CA	3127	1/1	0.99	0.07	0,0,0,0	0
58	MG	CA	3129	1/1	0.99	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	3001	1/1	0.99	0.07	0,0,0,0	0
58	MG	DA	3002	1/1	0.99	0.04	1,1,1,1	0
58	MG	DA	3003	1/1	0.99	0.02	8,8,8,8	0
58	MG	BA	1640	1/1	0.99	0.10	0,0,0,0	0
58	MG	BA	1605	1/1	0.99	0.03	21,21,21,21	0
58	MG	CA	3135	1/1	0.99	0.07	0,0,0,0	0
58	MG	DA	3007	1/1	0.99	0.13	26,26,26,26	0
58	MG	CA	3136	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3137	1/1	0.99	0.07	4,4,4,4	0
58	MG	AA	1641	1/1	0.99	0.04	0,0,0,0	0
58	MG	DA	3012	1/1	0.99	0.04	0,0,0,0	0
58	MG	CA	3036	1/1	0.99	0.08	0,0,0,0	0
58	MG	CA	3037	1/1	0.99	0.09	11,11,11,11	0
58	MG	CA	3039	1/1	0.99	0.05	0,0,0,0	0
58	MG	CA	3040	1/1	0.99	0.06	0,0,0,0	0
58	MG	CA	3041	1/1	0.99	0.10	0,0,0,0	0
58	MG	DA	3020	1/1	0.99	0.03	0,0,0,0	0
58	MG	BA	1607	1/1	0.99	0.09	1,1,1,1	0
58	MG	CA	3046	1/1	0.99	0.06	0,0,0,0	0
58	MG	DB	201	1/1	0.99	0.02	24,24,24,24	0
58	MG	DB	202	1/1	0.99	0.04	9,9,9,9	0
58	MG	DA	3026	1/1	0.99	0.03	0,0,0,0	0
58	MG	DL	201	1/1	0.99	0.03	10,10,10,10	0
58	MG	DA	3027	1/1	0.99	0.08	14,14,14,14	0
58	MG	AA	1624	1/1	1.00	0.02	10,10,10,10	0
58	MG	CA	3032	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3033	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3034	1/1	1.00	0.12	0,0,0,0	0
58	MG	DA	3065	1/1	1.00	0.03	0,0,0,0	0
58	MG	BA	1604	1/1	1.00	0.06	13,13,13,13	0
58	MG	DA	3067	1/1	1.00	0.02	0,0,0,0	0
58	MG	DA	3068	1/1	1.00	0.02	6,6,6,6	0
58	MG	CA	3097	1/1	1.00	0.05	0,0,0,0	0
58	MG	BA	1617	1/1	1.00	0.06	13,13,13,13	0
58	MG	AA	1605	1/1	1.00	0.01	0,0,0,0	0
58	MG	DA	3072	1/1	1.00	0.02	0,0,0,0	0
58	MG	CA	3038	1/1	1.00	0.15	0,0,0,0	0
58	MG	DA	3074	1/1	1.00	0.08	0,0,0,0	0
58	MG	CA	3101	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3102	1/1	1.00	0.10	0,0,0,0	0
58	MG	DA	3077	1/1	1.00	0.04	12,12,12,12	0
58	MG	BA	1619	1/1	1.00	0.02	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3104	1/1	1.00	0.02	0,0,0,0	0
58	MG	CA	3003	1/1	1.00	0.02	0,0,0,0	0
58	MG	BA	1639	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3107	1/1	1.00	0.10	0,0,0,0	0
58	MG	CA	3042	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3043	1/1	1.00	0.02	0,0,0,0	0
58	MG	CA	3110	1/1	1.00	0.10	0,0,0,0	0
58	MG	DA	3086	1/1	1.00	0.09	0,0,0,0	0
58	MG	CA	3044	1/1	1.00	0.02	0,0,0,0	0
58	MG	CA	3005	1/1	1.00	0.01	14,14,14,14	0
58	MG	AA	1613	1/1	1.00	0.04	2,2,2,2	0
58	MG	BA	1621	1/1	1.00	0.03	12,12,12,12	0
58	MG	CA	3008	1/1	1.00	0.04	0,0,0,0	0
58	MG	CA	3049	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3050	1/1	1.00	0.05	0,0,0,0	0
58	MG	CA	3051	1/1	1.00	0.03	3,3,3,3	0
58	MG	CA	3119	1/1	1.00	0.04	8,8,8,8	0
58	MG	CA	3052	1/1	1.00	0.04	0,0,0,0	0
58	MG	AA	1633	1/1	1.00	0.06	3,3,3,3	0
58	MG	CB	203	1/1	1.00	0.04	5,5,5,5	0
58	MG	CA	3122	1/1	1.00	0.05	0,0,0,0	0
58	MG	CA	3123	1/1	1.00	0.09	0,0,0,0	0
58	MG	DA	3101	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3054	1/1	1.00	0.09	0,0,0,0	0
58	MG	CA	3125	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3055	1/1	1.00	0.06	6,6,6,6	0
58	MG	CA	3010	1/1	1.00	0.04	0,0,0,0	0
58	MG	DA	3106	1/1	1.00	0.11	0,0,0,0	0
58	MG	CA	3128	1/1	1.00	0.10	0,0,0,0	0
58	MG	CA	3057	1/1	1.00	0.05	0,0,0,0	0
58	MG	CA	3130	1/1	1.00	0.12	0,0,0,0	0
58	MG	DA	3008	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3131	1/1	1.00	0.08	0,0,0,0	0
58	MG	CA	3011	1/1	1.00	0.12	0,0,0,0	0
58	MG	DA	3113	1/1	1.00	0.06	0,0,0,0	0
58	MG	CA	3133	1/1	1.00	0.01	0,0,0,0	0
58	MG	CA	3012	1/1	1.00	0.11	0,0,0,0	0
58	MG	AA	1634	1/1	1.00	0.05	2,2,2,2	0
58	MG	DA	3117	1/1	1.00	0.02	5,5,5,5	0
58	MG	DA	3118	1/1	1.00	0.03	7,7,7,7	0
58	MG	BA	1624	1/1	1.00	0.02	1,1,1,1	0
58	MG	BA	1625	1/1	1.00	0.02	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3016	1/1	1.00	0.06	0,0,0,0	0
58	MG	DA	3017	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3064	1/1	1.00	0.13	0,0,0,0	0
58	MG	DA	3124	1/1	1.00	0.02	0,0,0,0	0
58	MG	DA	3125	1/1	1.00	0.03	0,0,0,0	0
58	MG	DA	3019	1/1	1.00	0.03	0,0,0,0	0
58	MG	DA	3127	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3065	1/1	1.00	0.03	0,0,0,0	0
58	MG	DA	3129	1/1	1.00	0.04	0,0,0,0	0
58	MG	DA	3130	1/1	1.00	0.03	0,0,0,0	0
58	MG	DA	3021	1/1	1.00	0.03	3,3,3,3	0
58	MG	DA	3022	1/1	1.00	0.01	0,0,0,0	0
58	MG	CA	3066	1/1	1.00	0.13	0,0,0,0	0
58	MG	DA	3134	1/1	1.00	0.01	0,0,0,0	0
58	MG	DA	3024	1/1	1.00	0.01	0,0,0,0	0
58	MG	CA	3067	1/1	1.00	0.09	0,0,0,0	0
58	MG	CA	3068	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3069	1/1	1.00	0.07	0,0,0,0	0
58	MG	AA	1609	1/1	1.00	0.05	0,0,0,0	0
58	MG	DA	3029	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3071	1/1	1.00	0.02	0,0,0,0	0
58	MG	DA	3031	1/1	1.00	0.04	0,0,0,0	0
58	MG	DA	3032	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3072	1/1	1.00	0.02	0,0,0,0	0
58	MG	CA	3073	1/1	1.00	0.06	0,0,0,0	0
58	MG	DA	3035	1/1	1.00	0.03	0,0,0,0	0
58	MG	CA	3018	1/1	1.00	0.12	0,0,0,0	0
58	MG	BA	1610	1/1	1.00	0.06	0,0,0,0	0
58	MG	CA	3020	1/1	1.00	0.04	0,0,0,0	0
58	MG	BA	1628	1/1	1.00	0.07	25,25,25,25	0
58	MG	CA	3078	1/1	1.00	0.05	0,0,0,0	0
58	MG	DA	3041	1/1	1.00	0.04	6,6,6,6	0
58	MG	DA	3042	1/1	1.00	0.02	5,5,5,5	0
58	MG	CA	3079	1/1	1.00	0.03	3,3,3,3	0
58	MG	CA	3022	1/1	1.00	0.07	0,0,0,0	0
58	MG	CA	3023	1/1	1.00	0.06	0,0,0,0	0
58	MG	AA	1628	1/1	1.00	0.04	1,1,1,1	0
58	MG	AA	1629	1/1	1.00	0.02	0,0,0,0	0
58	MG	DA	3048	1/1	1.00	0.03	0,0,0,0	0
58	MG	DA	3049	1/1	1.00	0.03	0,0,0,0	0
58	MG	BA	1613	1/1	1.00	0.07	0,0,0,0	0
58	MG	DA	3051	1/1	1.00	0.02	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	3052	1/1	1.00	0.01	0,0,0,0	0
58	MG	CA	3027	1/1	1.00	0.05	0,0,0,0	0
58	MG	BA	1632	1/1	1.00	0.05	18,18,18,18	0
58	MG	CA	3087	1/1	1.00	0.09	0,0,0,0	0
58	MG	CA	3088	1/1	1.00	0.05	0,0,0,0	0
58	MG	CA	3029	1/1	1.00	0.08	0,0,0,0	0
58	MG	DA	3058	1/1	1.00	0.02	6,6,6,6	0
58	MG	CA	3090	1/1	1.00	0.02	1,1,1,1	0
58	MG	AA	1638	1/1	1.00	0.07	12,12,12,12	0
59	ZN	C4	101	1/1	1.00	0.01	0,0,0,0	0
59	ZN	D4	101	1/1	1.00	0.02	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.