



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:06 PM BST

PDB ID : 4V5B
Title : Structure of PDF binding helix in complex with the ribosome
Authors : Bingel-Erlenmeyer, R.; Kohler, R.; Kramer, G.; Sandikci, A.; Antolic, S.;
Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.
Deposited on : 2007-11-22
Resolution : 3.74 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

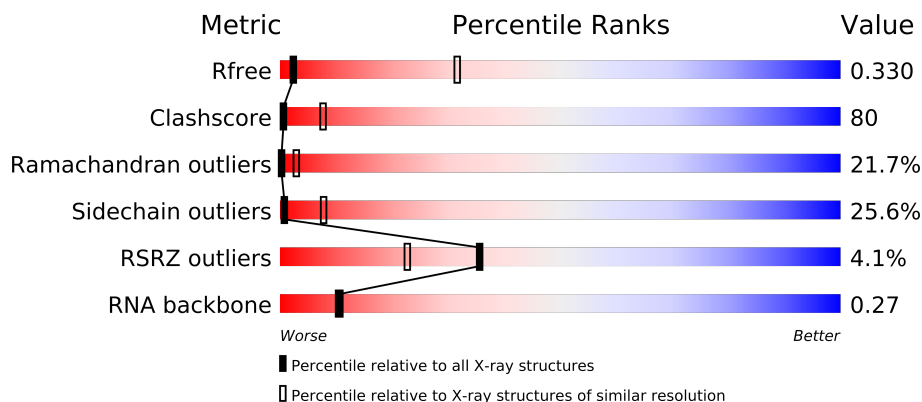
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.74 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}	66092	1103 (4.04-3.40)
Clashscore	79885	1072 (4.00-3.48)
Ramachandran outliers	78287	1023 (4.00-3.48)
Sidechain outliers	78261	1016 (4.00-3.48)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A0	56	
1	C0	56	
2	A1	54	
2	C1	54	
3	A2	46	
3	C2	46	
4	A3	64	
4	C3	64	
5	A4	38	
5	C4	38	
6	A5	16	
7	AA	120	

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Mol	Chain	Length	Quality of chain
7	CA	120	
8	AB	2904	
8	CB	2904	
9	AC	273	
9	CC	273	
10	AD	209	
10	CD	209	
11	AE	201	
11	CE	201	
12	AF	178	
12	CF	178	
13	AG	176	
13	CG	176	
14	AH	149	
14	CH	149	
15	AI	141	
15	CI	141	
16	AJ	142	
16	CJ	142	
17	AK	123	
17	CK	123	
18	AL	144	
18	CL	144	
19	AM	136	
19	CM	136	
20	AN	127	
20	CN	127	
21	AO	117	
21	CO	117	
22	AP	114	
22	CP	114	
23	AQ	117	
23	CQ	117	
24	AR	103	
24	CR	103	
25	AS	110	
25	CS	110	
26	AT	100	
26	CT	100	
27	AU	103	
27	CU	103	
28	AV	94	

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Mol	Chain	Length	Quality of chain
28	CV	94	
29	AW	84	
29	CW	84	
30	AX	63	
30	CX	63	
31	AY	58	
31	CY	58	
32	AZ	70	
32	CZ	70	
33	BA	1542	
33	DA	1542	
34	BB	240	
34	DB	240	
35	BC	232	
35	DC	232	
36	BD	205	
36	DD	205	
37	BE	166	
37	DE	166	
38	BF	135	
38	DF	135	
39	BG	178	
39	DG	178	
40	BH	129	
40	DH	129	
41	BI	129	
41	DI	129	
42	BJ	103	
42	DJ	103	
43	BK	128	
43	DK	128	
44	BL	123	
44	DL	123	
45	BM	117	
45	DM	117	
46	BN	100	
46	DN	100	
47	BO	89	
47	DO	89	
48	BP	82	
48	DP	82	
49	BQ	83	

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Mol	Chain	Length	Quality of chain
49	DQ	83	
50	BR	74	
50	DR	74	
51	BS	91	
51	DS	91	
52	BT	86	
52	DT	86	
53	BU	71	
53	DU	71	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
54	MG	AB	4014	-	X
54	MG	AB	4017	-	X
54	MG	AB	4020	-	X
54	MG	AB	4022	-	X
54	MG	AB	4027	-	X
54	MG	AB	4031	-	X
54	MG	AB	4032	-	X
54	MG	AB	4043	-	X
54	MG	AB	4048	-	X
54	MG	AB	4050	-	X
54	MG	AB	4056	-	X
54	MG	AB	4063	-	X
54	MG	AB	4069	-	X
54	MG	AB	4071	-	X
54	MG	AB	4075	-	X
54	MG	AB	4076	-	X
54	MG	AB	4077	-	X
54	MG	AB	4082	-	X
54	MG	AB	4085	-	X
54	MG	AB	4090	-	X
54	MG	AB	4091	-	X
54	MG	AB	4092	-	X
54	MG	AB	4096	-	X
54	MG	AB	4097	-	X
54	MG	AB	4098	-	X
54	MG	AB	4099	-	X
54	MG	AB	4108	-	X
54	MG	BA	4002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	BA	4007	-	X
54	MG	BA	4019	-	X
54	MG	BA	4020	-	X
54	MG	BA	4021	-	X
54	MG	BA	4022	-	X
54	MG	BA	4024	-	X
54	MG	BA	4027	-	X
54	MG	BA	4030	-	X
54	MG	BA	4035	-	X
54	MG	BA	4043	-	X
54	MG	BA	4053	-	X
54	MG	BA	4054	-	X
54	MG	CB	3005	-	X
54	MG	CB	3007	-	X
54	MG	CB	3014	-	X
54	MG	CB	3028	-	X
54	MG	CB	3029	-	X
54	MG	CB	3032	-	X
54	MG	CB	3036	-	X
54	MG	CB	3041	-	X
54	MG	CB	3044	-	X
54	MG	CB	3045	-	X
54	MG	CB	3051	-	X
54	MG	CB	3052	-	X
54	MG	CB	3054	-	X
54	MG	CB	3070	-	X
54	MG	CB	3071	-	X
54	MG	CB	3076	-	X
54	MG	CB	3077	-	X
54	MG	CB	3080	-	X
54	MG	CB	3085	-	X
54	MG	CB	3087	-	X
54	MG	CB	3093	-	X
54	MG	CB	3099	-	X
54	MG	CB	3101	-	X
54	MG	CB	3103	-	X
54	MG	CB	3104	-	X
54	MG	CB	3108	-	X
54	MG	DA	1607	-	X
54	MG	DA	1609	-	X
54	MG	DA	1612	-	X
54	MG	DA	1614	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	DA	1619	-	X
54	MG	DA	1622	-	X
54	MG	DA	1623	-	X
54	MG	DA	1624	-	X
54	MG	DA	1629	-	X
54	MG	DA	1632	-	X
54	MG	DA	1634	-	X
54	MG	DA	1644	-	X
54	MG	DA	1647	-	X
54	MG	DA	1651	-	X
54	MG	DA	1657	-	X
54	MG	DA	1658	-	X
54	MG	DA	1660	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284264 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
1	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A1	54	Total	C	N	O	0	0	0
			441	284	81	76			
2	C1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
3	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
4	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
5	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a protein called C-TERM HELIX PDF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A5	16	Total	C	N	O	0	0	0
			134	84	28	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	146	ALA	LEU	ENGINEERED MUTATION	UNP P0A6K3

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
7	CA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 8 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
8	CB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			
9	CC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
12	CF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
14	CH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			
16	CJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			
17	CK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
18	CL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
20	CN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
21	CO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			
26	CT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				
27	CU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			
29	CW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
30	CX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			
32	CZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			

- Molecule 33 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
33	DA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			
34	DB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			
35	DC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			
37	DE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			
38	DF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	1
			1175	730	227	214	4			
39	DG	153	Total	C	N	O	S	0	0	1
			1197	745	231	217	4			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			
42	DJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	115	Total	C	N	O	S	0	0	1
			884	546	179	156	3			
45	DM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	3			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	81	Total	C	N	O	S	0	0	1
			649	411	122	113	3			
49	DQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	56	Total	C	N	O	0	0	1
			456	288	87	81			
50	DR	56	Total	C	N	O	0	0	1
			456	288	87	81			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	80	Total	C	N	O	S	0	0	1
			638	408	121	107	2			
51	DS	81	Total	C	N	O	S	0	0	1
			645	413	122	108	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			
53	DU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BT	1	Total	Mg	0	0
			1	1		
54	BA	58	Total	Mg	0	0
			58	58		
54	BN	1	Total	Mg	0	0
			1	1		
54	AE	1	Total	Mg	0	0
			1	1		
54	CB	109	Total	Mg	0	0
			109	109		
54	AB	109	Total	Mg	0	0
			109	109		
54	CC	1	Total	Mg	0	0
			1	1		
54	DN	1	Total	Mg	0	0
			1	1		
54	DA	61	Total	Mg	0	0
			61	61		
54	CL	1	Total	Mg	0	0
			1	1		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	A2	2	Total	O	0	0
			2	2		
55	AB	489	Total	O	0	0
			489	489		
55	AC	3	Total	O	0	0
			3	3		
55	AD	1	Total	O	0	0
			1	1		
55	AE	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AJ	2	Total O 2 2	0	0
55	AL	3	Total O 3 3	0	0
55	BA	284	Total O 284 284	0	0
55	BE	3	Total O 3 3	0	0
55	BI	2	Total O 2 2	0	0
55	BK	1	Total O 1 1	0	0
55	BL	2	Total O 2 2	0	0
55	BN	3	Total O 3 3	0	0
55	BP	1	Total O 1 1	0	0
55	BT	2	Total O 2 2	0	0
55	C0	1	Total O 1 1	0	0
55	C2	2	Total O 2 2	0	0
55	CB	485	Total O 485 485	0	0
55	CC	3	Total O 3 3	0	0
55	CD	1	Total O 1 1	0	0
55	CE	1	Total O 1 1	0	0
55	CJ	2	Total O 2 2	0	0
55	CK	1	Total O 1 1	0	0
55	CL	5	Total O 5 5	0	0
55	CN	3	Total O 3 3	0	0
55	CP	1	Total O 1 1	0	0

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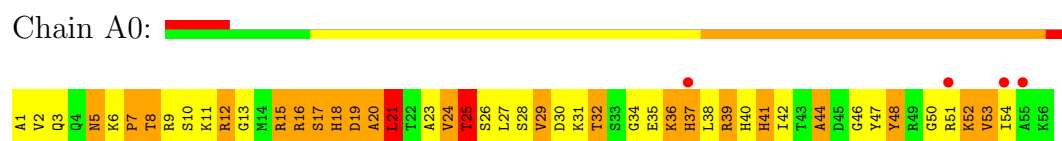
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	O 1	0	0
55	CT	2	Total 2	O 2	0	0
55	CU	1	Total 1	O 1	0	0
55	DA	293	Total 293	O 293	0	0
55	DD	1	Total 1	O 1	0	0
55	DE	2	Total 2	O 2	0	0
55	DG	1	Total 1	O 1	0	0
55	DL	4	Total 4	O 4	0	0
55	DN	2	Total 2	O 2	0	0
55	DP	1	Total 1	O 1	0	0
55	DT	3	Total 3	O 3	0	0

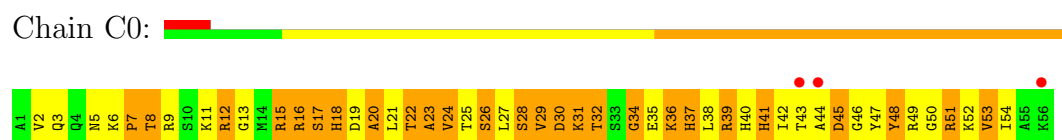
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

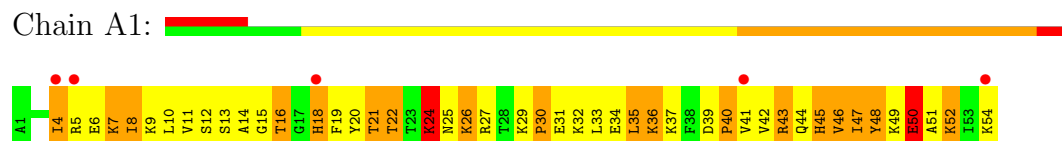
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



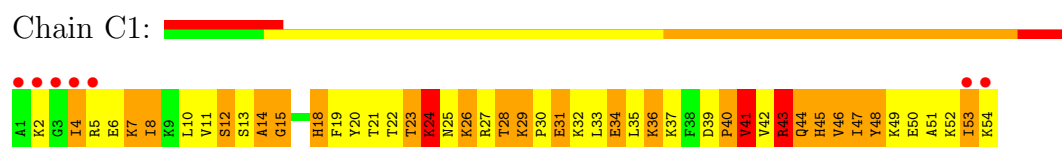
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



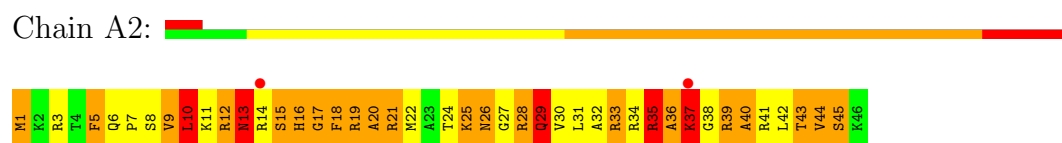
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



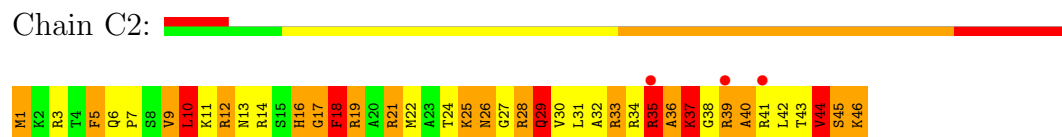
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 3: 50S RIBOSOMAL PROTEIN L34

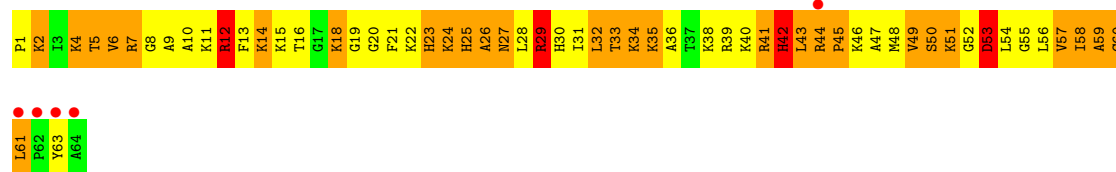


- Molecule 3: 50S RIBOSOMAL PROTEIN L34



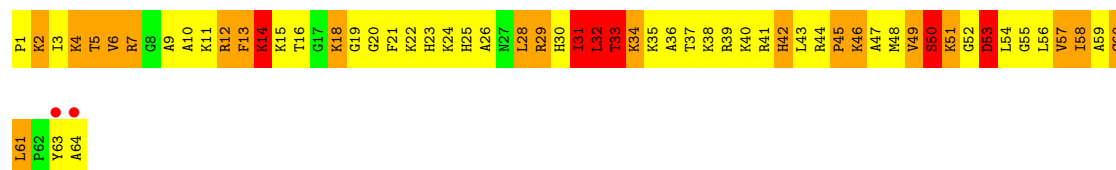
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain A3: 



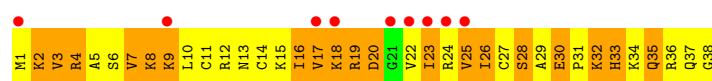
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain C3: 



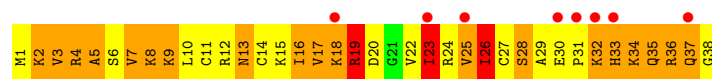
- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain A4: 



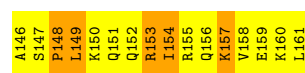
- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain C4: 



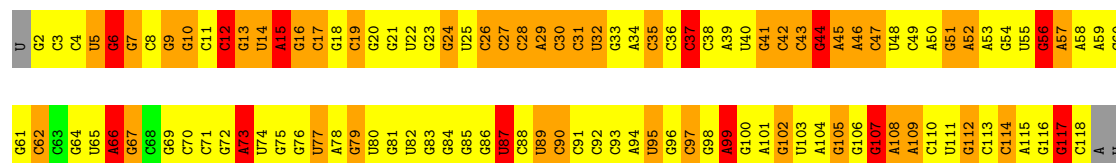
- Molecule 6: C-TERM HELIX PDF

Chain A5: 



- Molecule 7: 5S RIBOSOMAL RNA

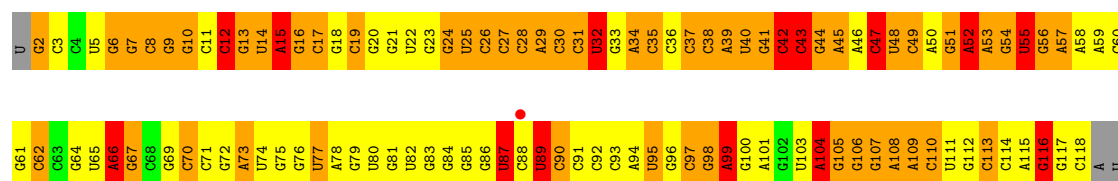
Chain AA: 



- Molecule 7: 5S RIBOSOMAL RNA

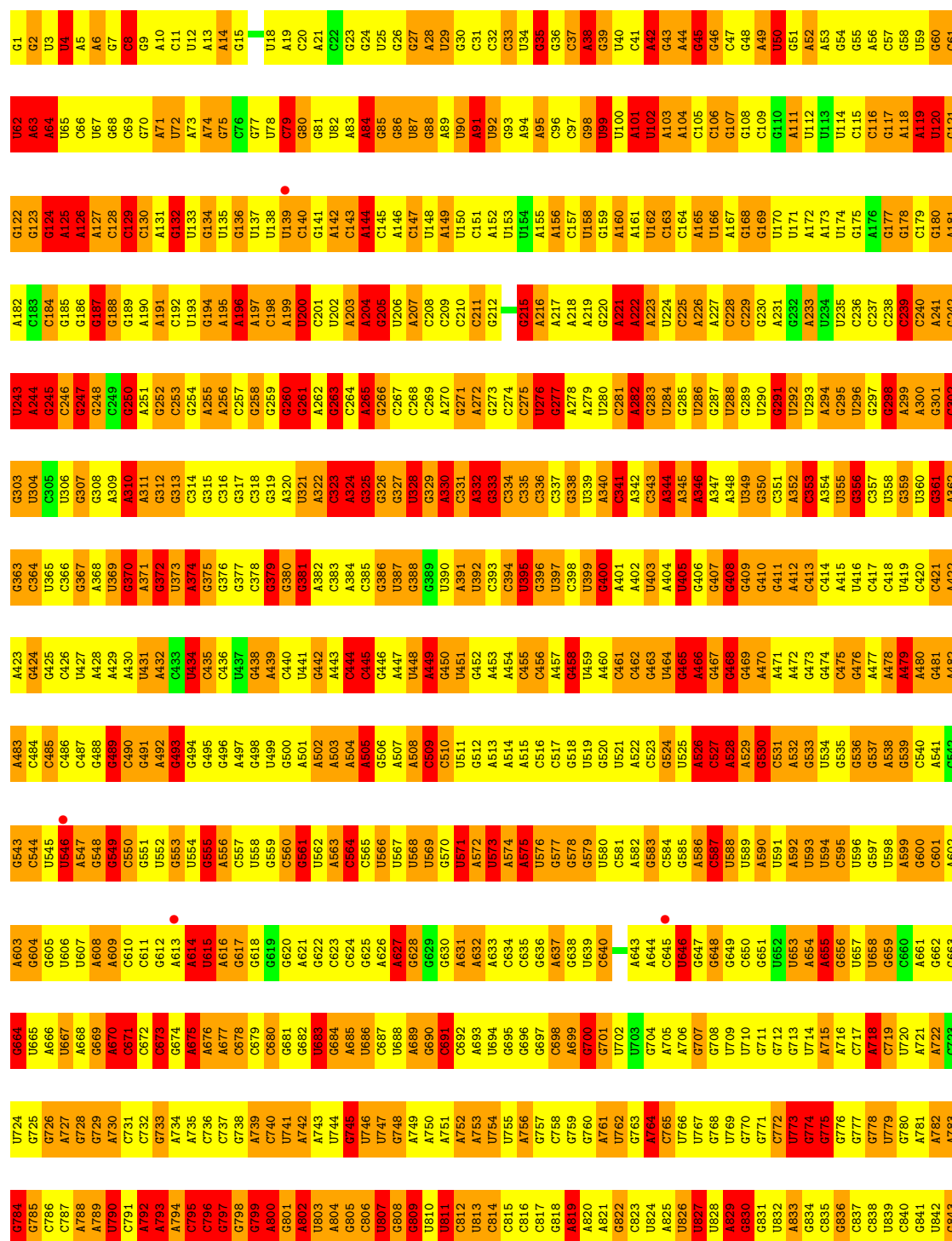
Chain CA: 





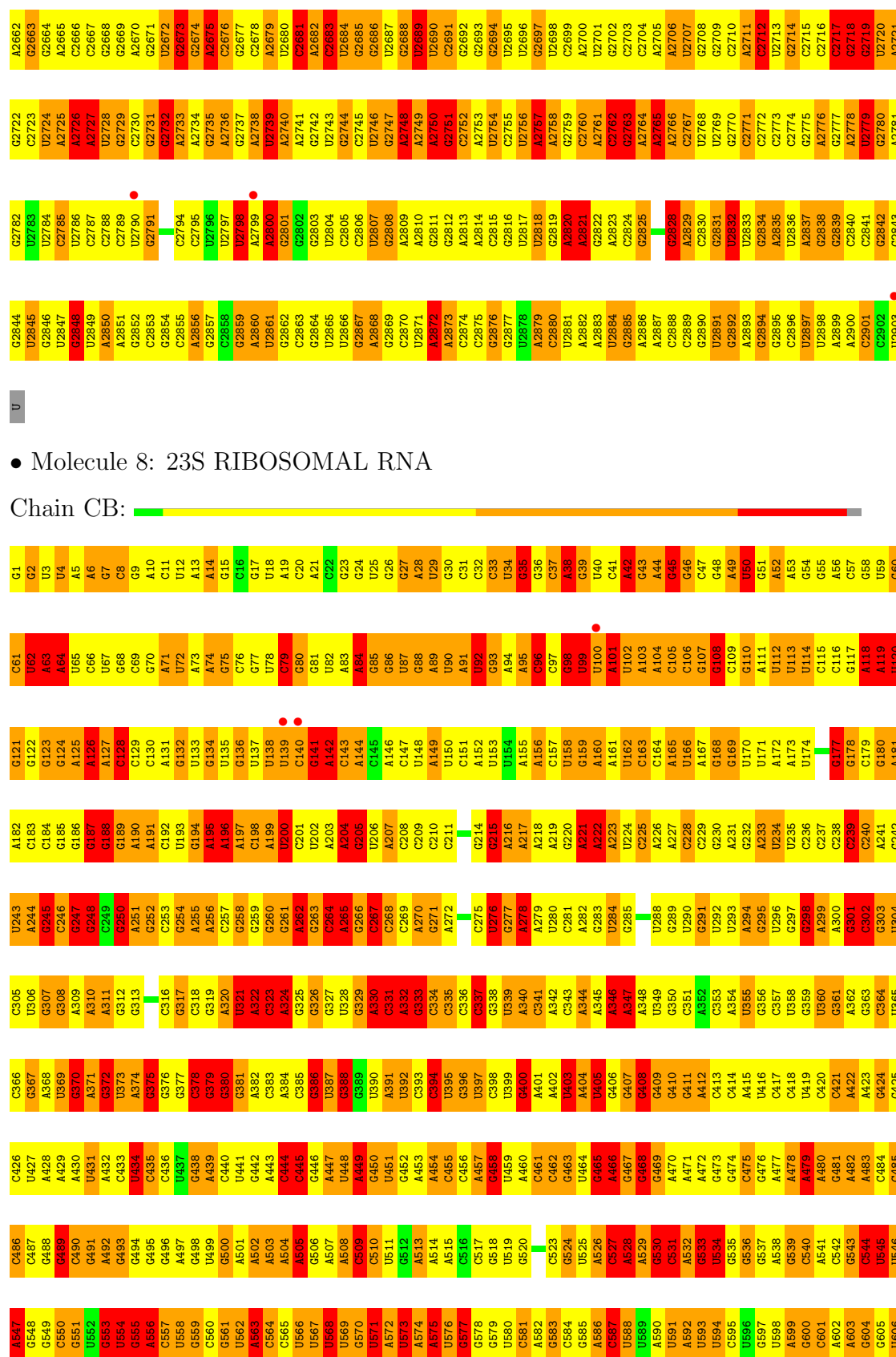
Molecule 8: 23S RIBOSOMAL RNA

Chain AB:





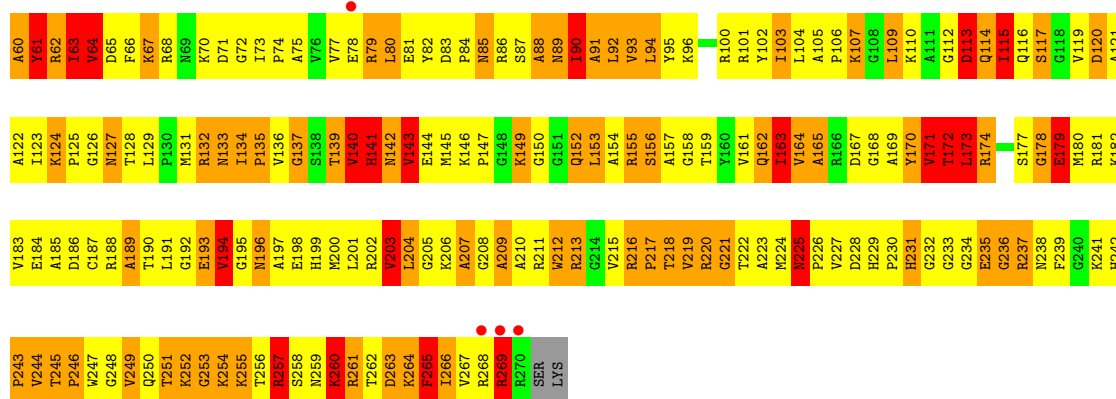
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G2603	A2542	A2482	C2422	G2302	G2242	U2182	U	A2062	G2002	C1942	C1881	C1760
G2604	G2543	G2483	U2423	G2303	U2243	A2183	G	C2063	A2003	U1943	C1882	C1761
G2605	G2544	G2484	C2424	G2304	U2244	A2184	G	C2064	G2004	U1944	U1883	A1762
G2606	G2545	G2485	A2425	U2305	U2245	U2185	G	C2065	A2005	G1945	G1884	G1763
G2607	U2546	G2486	A2426	U2306	G2246	G2186	A	C2066	G2006	U1946	C1885	C1764
G2608	G2547	G2487	C2427	G2307	A2247	U2187	G	G2067	U2007	C1947	U1886	U1765
G2609	U2548	G2488	G2428	G2308	C2248	U2188	G	U2068	C2008	G1948	G1887	G1766
G2610	G2549	G2489	G2429	A2309	U2249	U2189	C	G2069	A2009	G1949	G1888	G1767
G2611	G2550	G2490	A2430	G2310	G2250	A2190	U	A2070	G2010	G1950	A1889	C1768
G2612	G2551	U2491	U2431	A2311	G2251	A2191	U	A2071	G2011	U1951	A1890	U1769
U2613	U2552	U2492	A2432	U2312	G2252	U2192	U	C2072	G2012	A1952	G1891	G1770
A2614	G2553	U2493	A2433	G2313	G2253	G2193	G2133	C2073	A2013	A1953	C1892	C1771
U2615	U2554	G2494	A2434	A2314	C2254	U2194	A2134	U2074	A2014	G1954	C1893	A1772
G2616	U2555	A2495	A2435	G2315	G2255	U2195	A2135	U2075	A2015	U1955	C1894	A1773
G2617	G2556	G2496	G2436	G2316	G2256	U2196	A2136	U2076	U2016	U1956	G1896	C1774
G2618	G2557	A2497	G2437	G2317	U2257	U2197	U2137	A2077	G2017	C1957	G1897	U1775
G2619	G2558	G2498	U2438	G2318	U2258	A2198	U2138	C2078	G2018	G1958	U1898	G1776
G2620	G2559	C2499	A2439	G2319	U2259	A2199	U2139	U2079	A2019	G1959	A1899	U1777
G2621	U2560	U2500	C2440	U2320	C2260	G2200	G2140	A2080	A2020	A1960	A1900	U1778
G2622	U2561	C2501	U2441	U2321	C2261	G2201	G2141	U2081	C2021	C1961	A1901	U1779
G2623	U2562	G2502	C2442	A2322	U2262	U2202	A2142	A2082	U2022	C1962	C1902	U1780
G2624	G2563	A2503	C2443	G2323	G2263	U2203	G2143	G2083	C2023	U1963	G1903	U1781
G2625	U2564	U2504	G2444	U2324	C2264	G2204	G2144	C2084	G2024	G1964	G1904	U1782
G2626	G2565	G2505	G2445	G2325	U2265	A2205	C2145	U2085	C2025	C1965	C1905	A1783
G2627	U2566	U2506	G2446	C2326	A2266	C2206	C2146	U2086	U2026	A1966	G1906	A1784
G2628	G2567	G2507	G2447	A2327	A2267	G2207	A2147	G2087	G2027	C1967	C1907	A1785
G2629	U2568	C2508	A2448	A2328	A2268	C2208	A2148	A2088	U2028	G1968	C1908	A1786
G2630	G2569	G2509	U2449	U2329	G2269	G2209	U2149	C2089	G2029	A1969	C1909	A1787
G2631	G2570	C2510	A2450	U2330	A2270	U2210	C2150	A2090	A2030	A1970	G1910	C1788
A2632	U2571	U2511	A2451	G2331	G2271	A2211	U2151	C2091	A2031	U1971	U1911	A1789
G2633	U2572	A2512	C2452	C2332	U2272	A2212	C2152	U2092	G2032	G1972	A1912	C1790
A2634	C2573	A2513	A2453	A2333	A2273	U2213	C2153	G2093	A2033	G1973	A1913	A1791
A2635	G2574	C2514	G2454	U2334	A2274	C2214	A2154	A2094	U2034	C1974	G1914	G1792
G2636	G2575	C2515	G2455	A2335	G2275	C2215	U2155	A2095	G2035	G1975	U1915	C1793
G2637	G2576	A2516	C2456	A2336	G2276	G2216	G2156	C2096	C2036	U1976	A1916	A1794
U2638	G2577	C2517	U2457	G2337	G2277	G2217	G2157	A2097	A2037	A1977	U1917	G1795
A2639	G2578	A2518	G2458	C2338	A2278	G2218	A	U2098	G2038	A1978	A1918	U1796
G2640	G2579	U2519	A2459	G2339	G2279	U2219	G	U2099	U2039	U1979	G1919	U1797
G2641	U2580	C2520	U2460	A2340	G2280	U2220	C	G2100	G2040	G1980	C1920	G1798
G2642	G2581	C2521	A2461	G2341	A2281	G2221	C	A2101	U2041	A1981	G1921	G1799
G2643	G2582	U2522	C2462	C2342	G2282	C2222	G	G2102	A2042	U1982	G1922	C1800
G2644	U2583	G2523	C2463	U2343	G2283	G2223	C	C2103	C2043	G1983	U1923	A1801
G2645	G2584	G2524	G2464	U2344	A2284	G2224	C	C2104	C2044	G1984	U1924	A1802
G2646	U2585	G2525	C2465	G2345	G2285	A2225	C	U2105	C2045	C1985	C1925	A1803
U2647	U2586	G2526	A2466	A2346	G2286	C2226	U	G2106	G2046	G1986	U1926	C1804
G2648	A2587	C2527	C2467	C2347	A2287	A2227	U	G2107	C2047	A1987	U1927	A1805
G2649	G2588	U2528	A2468	U2348	A2288	G2228	G	A2108	G2048	G1988	A1928	C1806
U2650	A2589	G2529	A2469	G2349	G2289	U2229	A	U2109	G2049	G1989	G1929	G1807
G2651	U2590	A2530	G2470	C2350	G2290	G2230	A	G2110	C2050	C1990	G1930	A1808
G2652	C2591	A2531	A2471	G2351	U2291	G2231	U	U	A2051	U1991	U1931	A1809
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A2654	U2593	G2533	U2473	C2353	G2293	U2233	A	U	G2053	U1993	G1933	G1811
G2655	C2594	A2534	U2474	C2354	G2294	G2234	C	A	A2054	C1994	C1934	U1812
U2656	G2595	G2535	G2475	G2355	G2295	G2235	C	G	G2055	U1995	G1935	G1813
A2657	U2596	G2536	A2476	U2356	U2296	U2236	A	G	G2056	C1996	A1936	G1814
G2658	G2597	U2537	U2477	G2357	A2297	G2237	C	A	G2057	C1997	A1937	A1815
G2659	U2598	G2538	A2478	A2358	A2298	G2238	C	U	A2058	A1998	A1938	C1816
A2660	G2599	C2539	U2479	C2359	U2299	G2239	A	A	G2059	C1999	U1939	G1817
G2661	U2600	U2600	C2480	G2360	C2300	U2240	U2180	G	A2060	C2000	U1940	U1818



G1514	G1450	U1390	C1330	C1270	G1210	G1149	A1088	A1027	U967	G907	U847	C787	A727	U667	U607
A1515	C1451	U1391	G1331	G1271	G1211	C1150	A1089	A1028	C968	C908	C848	A788	G728	A668	A608
G1516	G1452	A1392	G1332	A1272	G1212	C1151	A1090	A1029	G969	A909	A849	A789	G729	G669	A609
G1517	A1453	A1393	G1333	U1273	A1213	C1152	G1091	C1030	U970	A910	U850	U790	A730	A670	C610
C1518	C1454	U1394	G1334	A1274	A1214	C1153	C1092	G1031	G971	C911	C851	C791	C731	C671	C611
G1519	G1455	A1395	C1335	A1275	G1215	C1154	C1093	A1032	A972	C912	U852	A792	C732	C672	G612
U1520	G1456	U1396	A1336	A1276	G1216	A1155	U1094	U1033	A973	U913	C853	A793	G733	G673	A613
G1521	A1457	U1397	G1337	G1277	G1217	A1156	A1095	G1034	G974	G914	C854	A794	A734	G674	A614
A1522	C1458	C1398	G1338	U1278	G1218	G1157	A1096	U1035	A975	C915	C855	A795	A735	A675	U615
G1523	G1459	C1399	G1339	G1279	U1219	C1158	U1097	G1036	G976	G916	G856	G796	C736	A676	A616
U1524	U1460	U1400	C1340	G1280	G1220	U1159	A1098	G1037	G977	A917	G857	G797	C737	A677	G617
A1525	C1461	G1401	G1341	G1281	C1221	U1160	G1099	G1038	G978	A918	G858	G798	G738	C678	G618
C1462	U1462	U1342	C1342	U1282	G1222	C1161	C1100	A1039	A979	U919	G859	G799	A739	C679	G619
G1527	G1463	A1403	G1343	G1283	G1223	G1162	U1101	A1040	A980	A920	U860	A800	C740	C680	G620
A1528	U1464	C1404	A1344	A1284	U1224	G1163	C1102	G1041	A981	C921	A861	G801	U741	G681	A621
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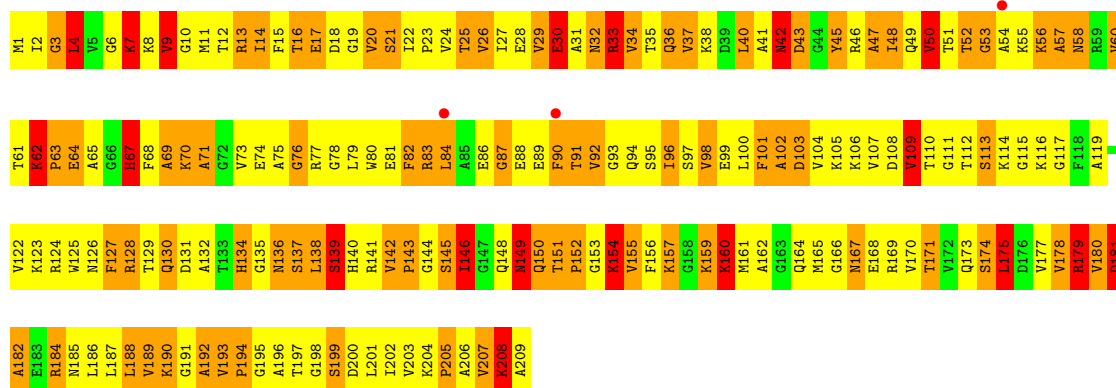
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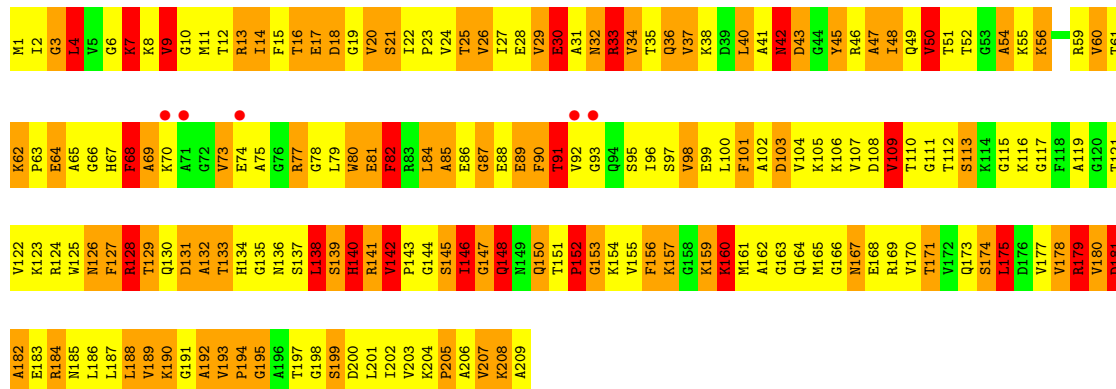
● Molecule 10: 50S RIBOSOMAL PROTEIN L3

Chain AD:



● Molecule 10: 50S RIBOSOMAL PROTEIN L3

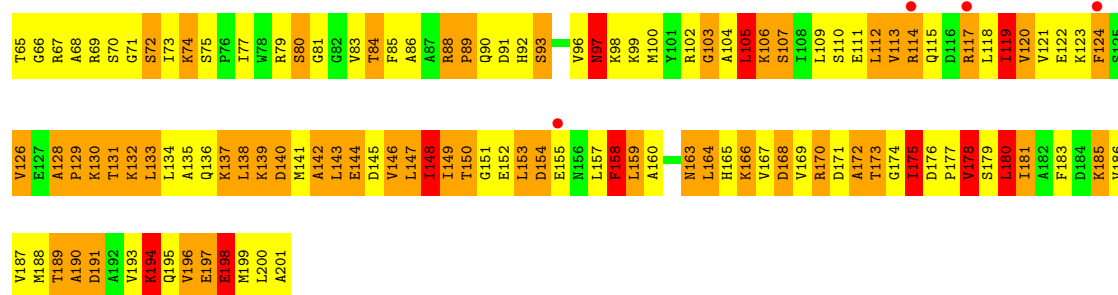
Chain CD:



● Molecule 11: 50S RIBOSOMAL PROTEIN L4

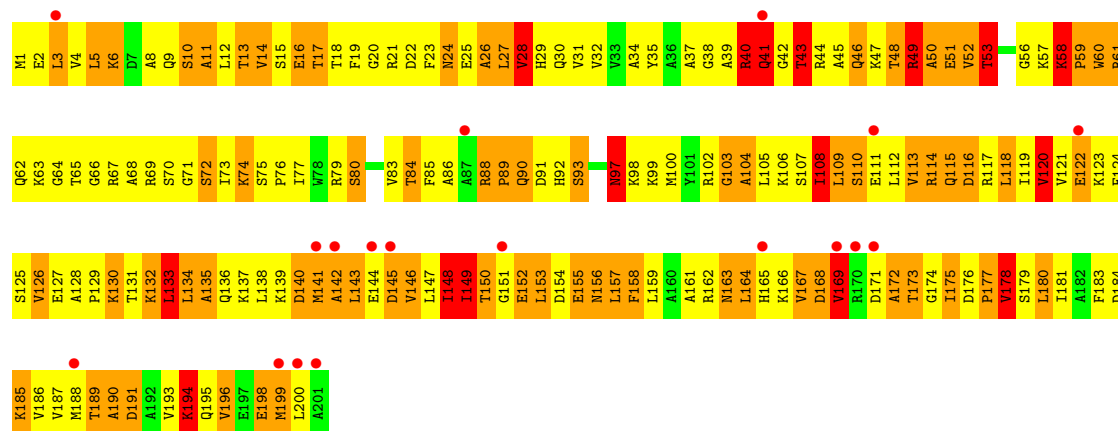
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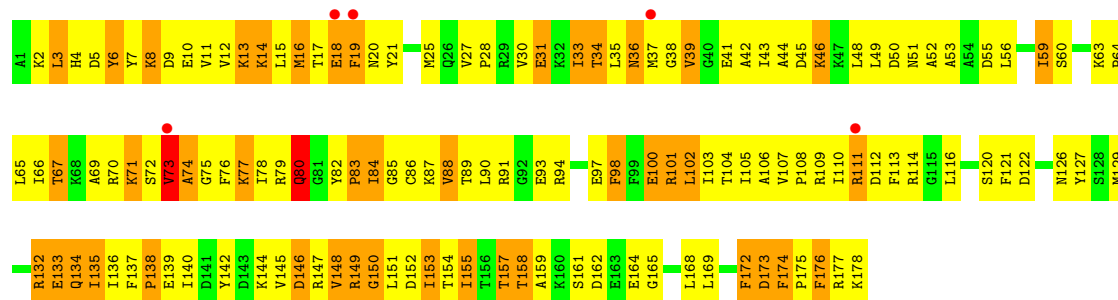
• Molecule 11: 50S RIBOSOMAL PROTEIN L4

Chain CE:



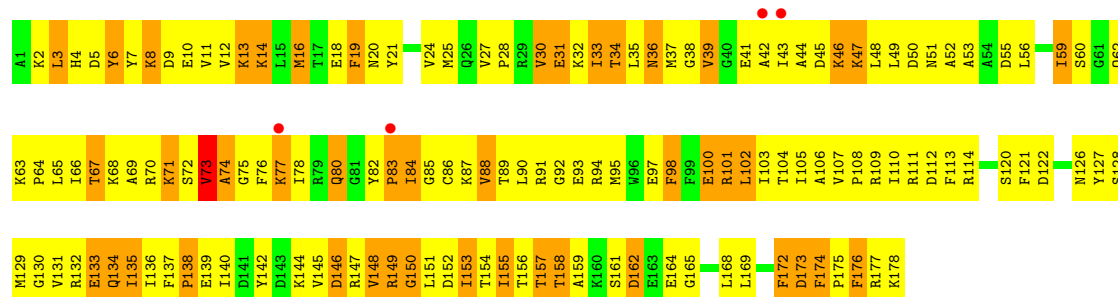
• Molecule 12: 50S RIBOSOMAL PROTEIN L5

Chain AF:



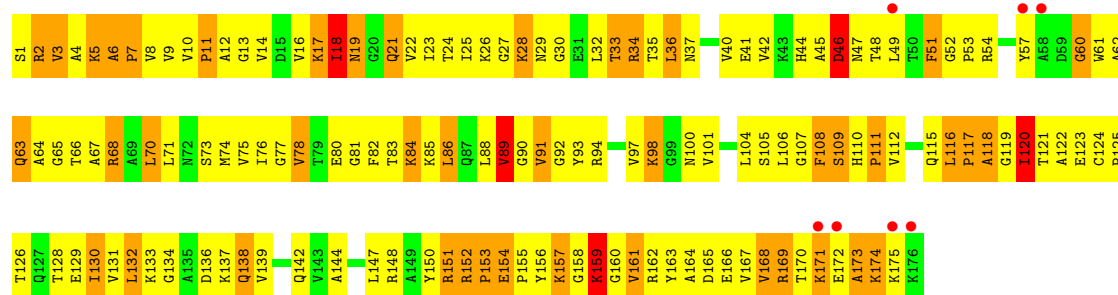
• Molecule 12: 50S RIBOSOMAL PROTEIN L5

Chain CF:



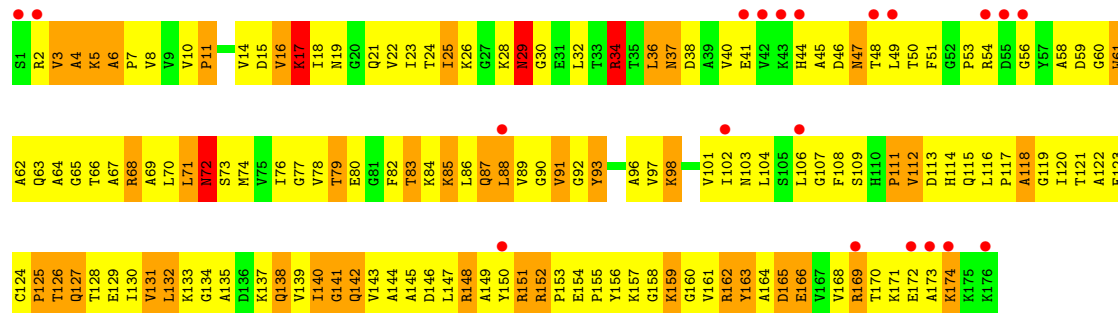
• Molecule 13: 50S RIBOSOMAL PROTEIN L6

Chain AG:



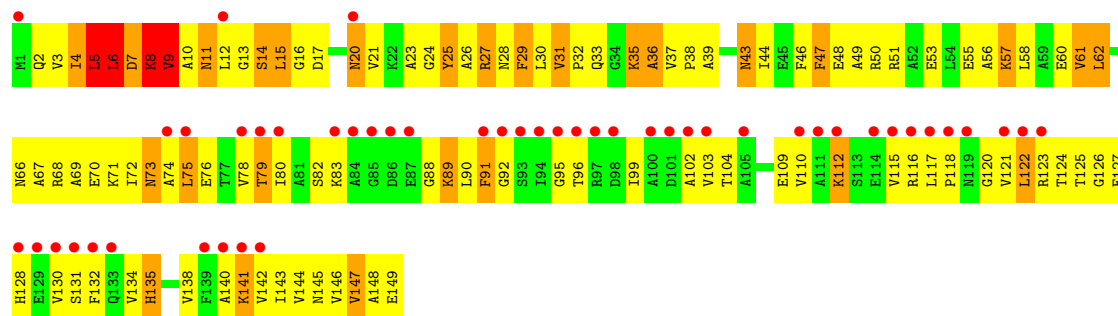
• Molecule 13: 50S RIBOSOMAL PROTEIN L6

Chain CG:



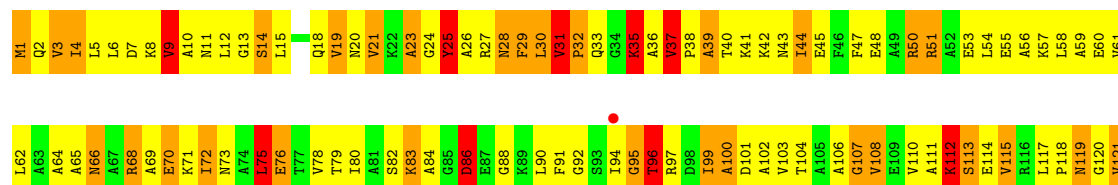
• Molecule 14: 50S RIBOSOMAL PROTEIN L9

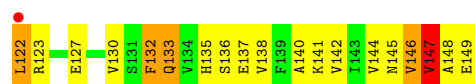
Chain AH:



• Molecule 14: 50S RIBOSOMAL PROTEIN L9

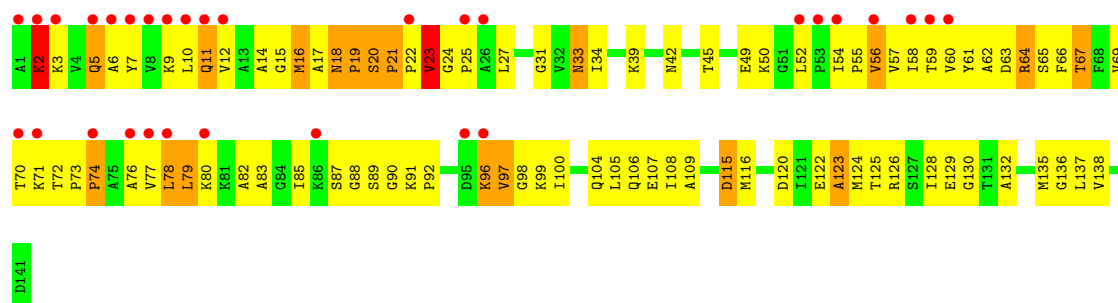
Chain CH:





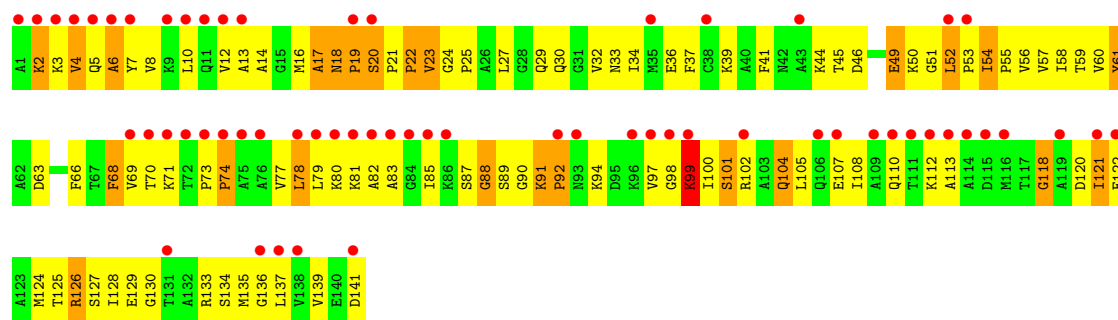
• Molecule 15: 50S RIBOSOMAL PROTEIN L11

Chain AI:



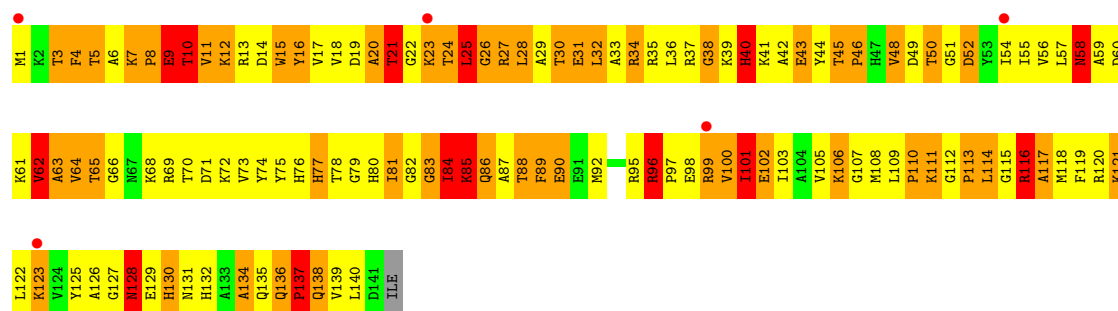
• Molecule 15: 50S RIBOSOMAL PROTEIN L11

Chain CI:



• Molecule 16: 50S RIBOSOMAL PROTEIN L13

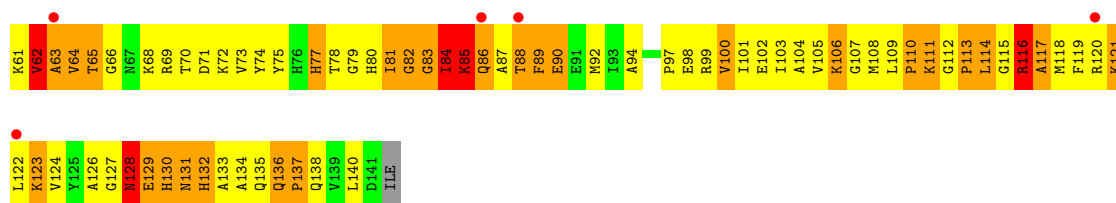
Chain AJ:



• Molecule 16: 50S RIBOSOMAL PROTEIN L13

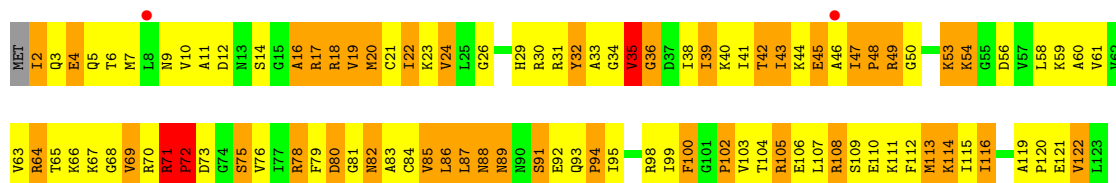
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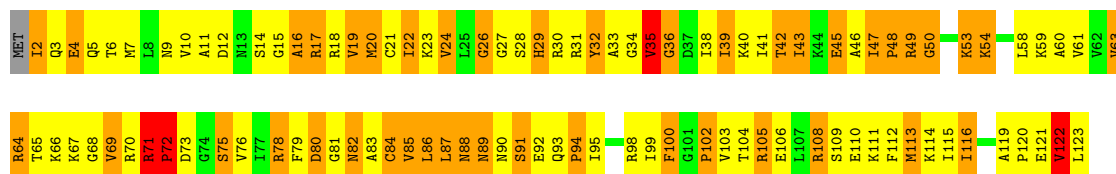
• Molecule 17: 50S RIBOSOMAL PROTEIN L14

Chain AK:



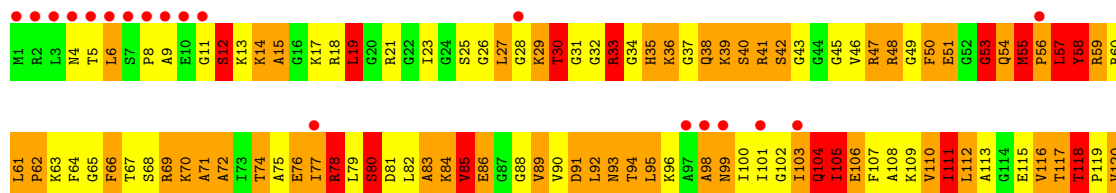
• Molecule 17: 50S RIBOSOMAL PROTEIN L14

Chain CK:



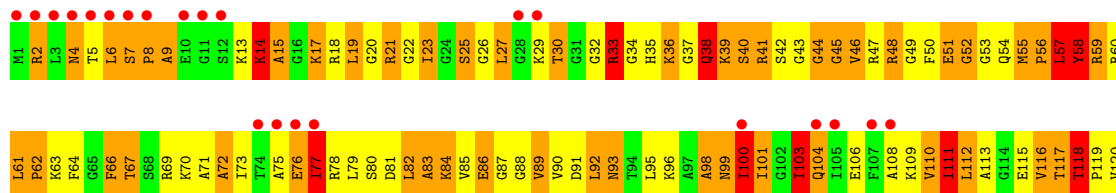
• Molecule 18: 50S RIBOSOMAL PROTEIN L15

Chain AL:



• Molecule 18: 50S RIBOSOMAL PROTEIN L15

Chain CL:



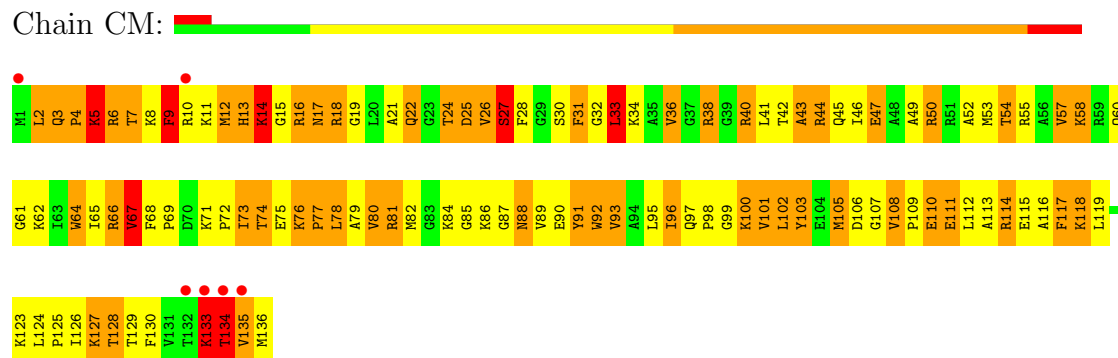
● Molecule 19: 50S RIBOSOMAL PROTEIN L16

Chain AM:



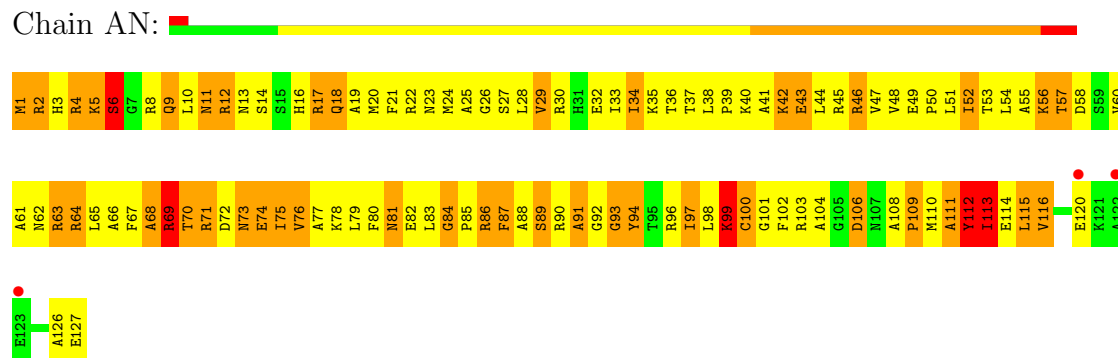
● Molecule 19: 50S RIBOSOMAL PROTEIN L16

Chain CM:



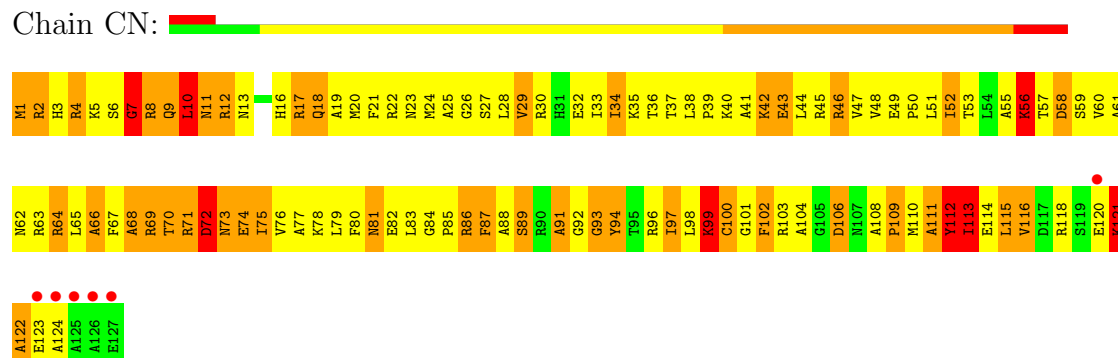
● Molecule 20: 50S RIBOSOMAL PROTEIN L17

Chain AN:



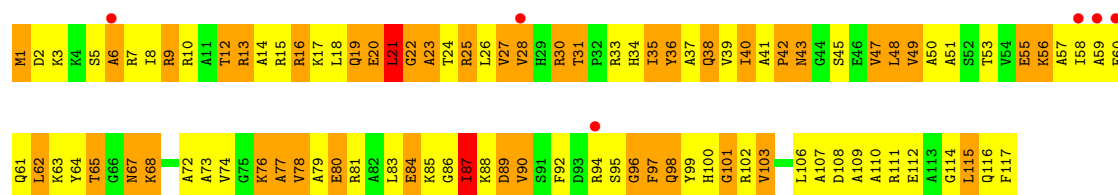
● Molecule 20: 50S RIBOSOMAL PROTEIN L17

Chain CN:



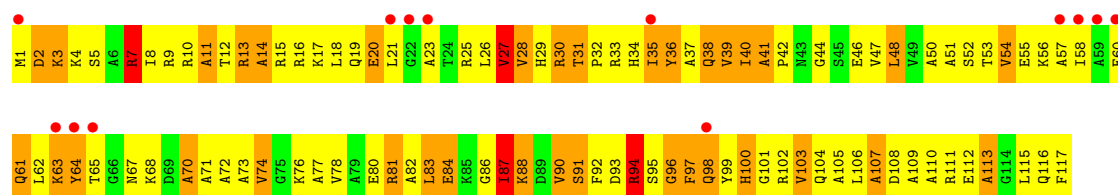
- Molecule 21: 50S RIBOSOMAL PROTEIN L18

Chain AO:



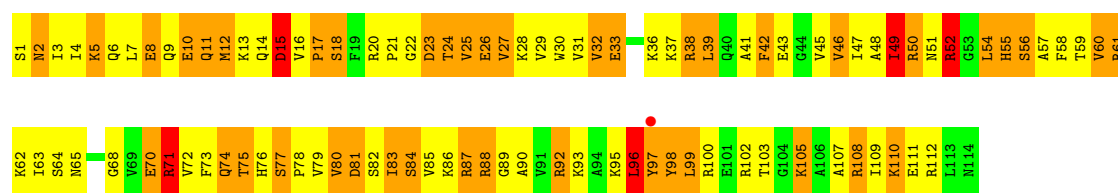
- Molecule 21: 50S RIBOSOMAL PROTEIN L18

Chain CO:



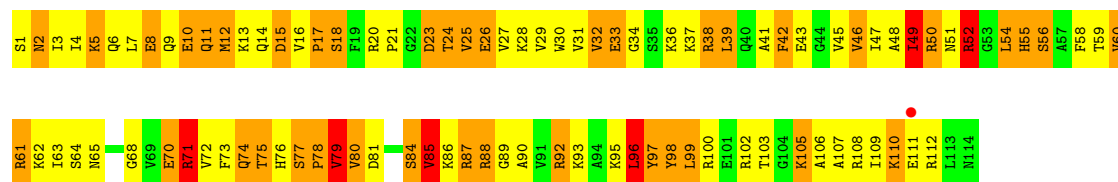
- Molecule 22: 50S RIBOSOMAL PROTEIN L19

Chain AP:



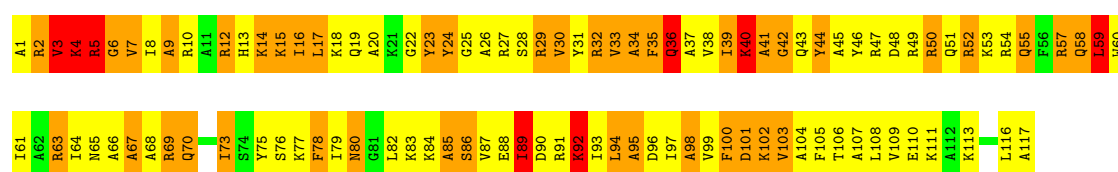
- Molecule 22: 50S RIBOSOMAL PROTEIN L19

Chain CP:



- Molecule 23: 50S RIBOSOMAL PROTEIN L20

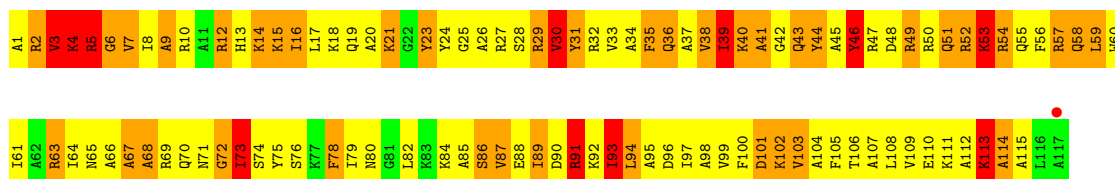
Chain AQ:



- Molecule 23: 50S RIBOSOMAL PROTEIN L20

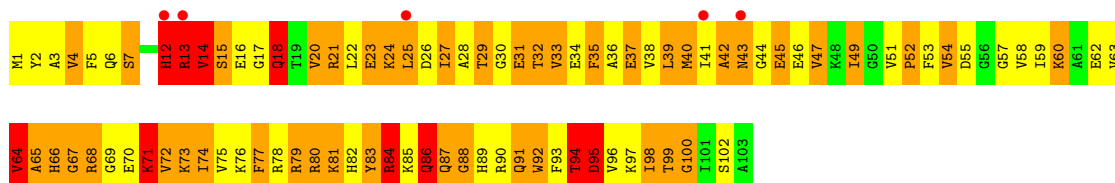
Chain CQ:





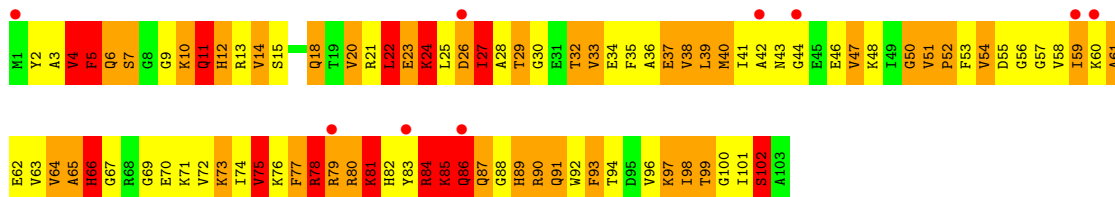
• Molecule 24: 50S RIBOSOMAL PROTEIN L21

Chain AR:



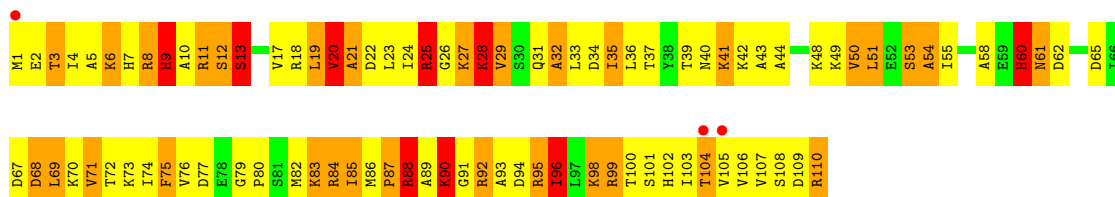
• Molecule 24: 50S RIBOSOMAL PROTEIN L21

Chain CR:



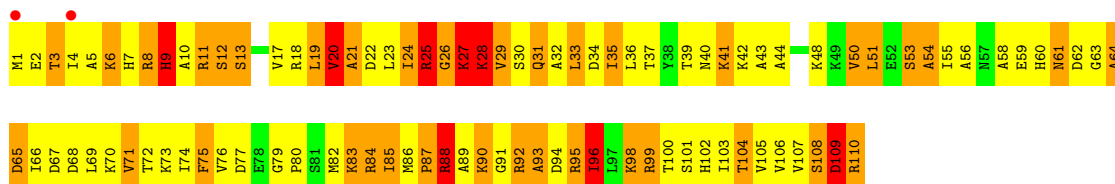
• Molecule 25: 50S RIBOSOMAL PROTEIN L22

Chain AS:



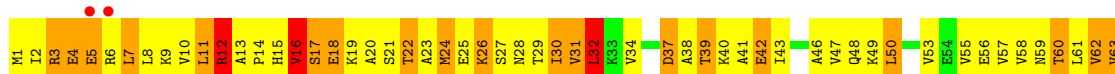
• Molecule 25: 50S RIBOSOMAL PROTEIN L22

Chain CS:



• Molecule 26: 50S RIBOSOMAL PROTEIN L23

Chain AT:



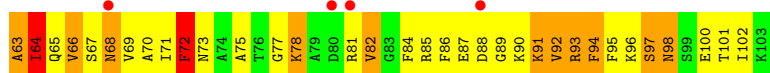
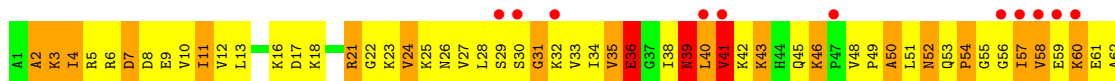
- Molecule 26: 50S RIBOSOMAL PROTEIN L23

Chain CT: 



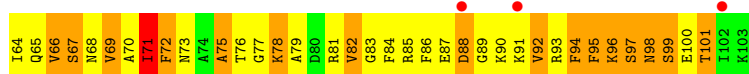
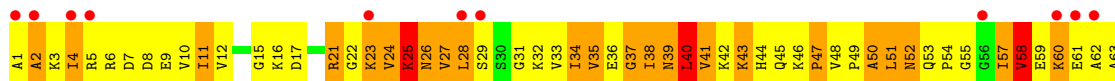
- Molecule 27: 50S RIBOSOMAL PROTEIN L24

Chain AU: 



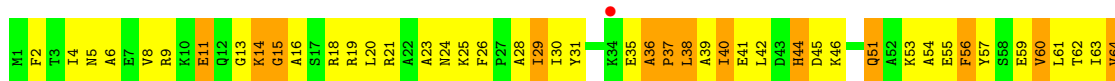
- Molecule 27: 50S RIBOSOMAL PROTEIN L24

Chain CU: 



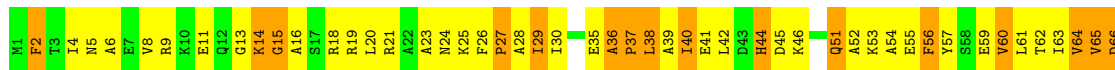
- Molecule 28: 50S RIBOSOMAL PROTEIN L25

Chain AV: 

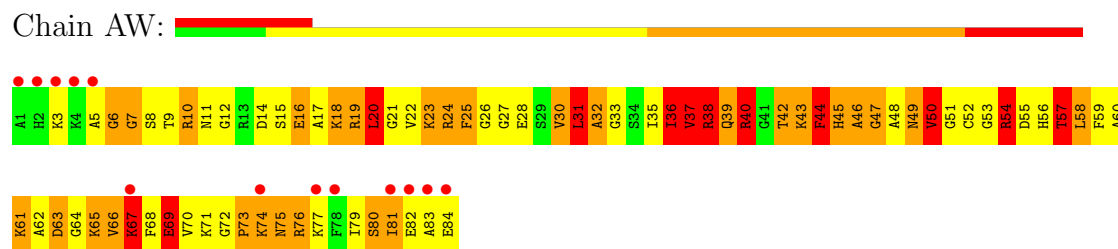


- Molecule 28: 50S RIBOSOMAL PROTEIN L25

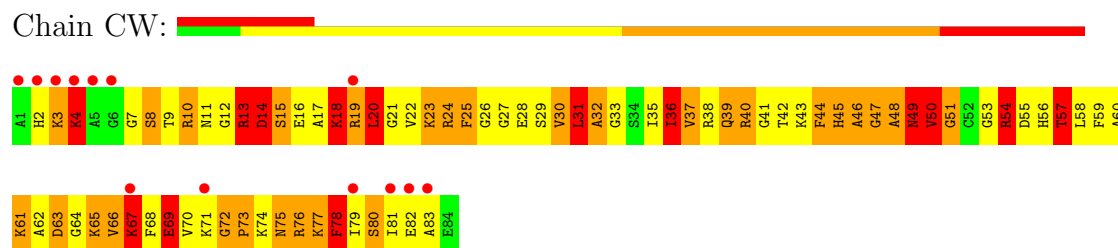
Chain CV: 



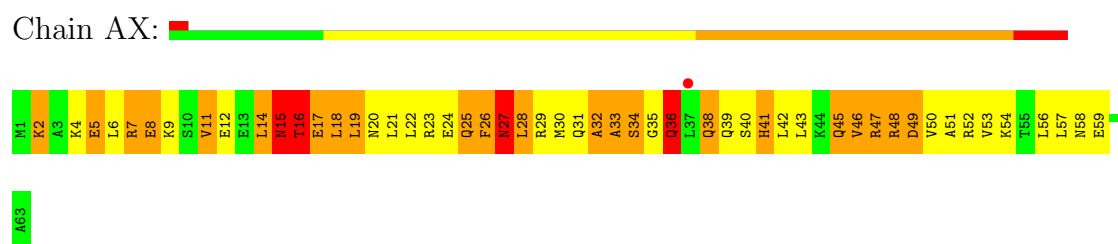
- Molecule 29: 50S RIBOSOMAL PROTEIN L27



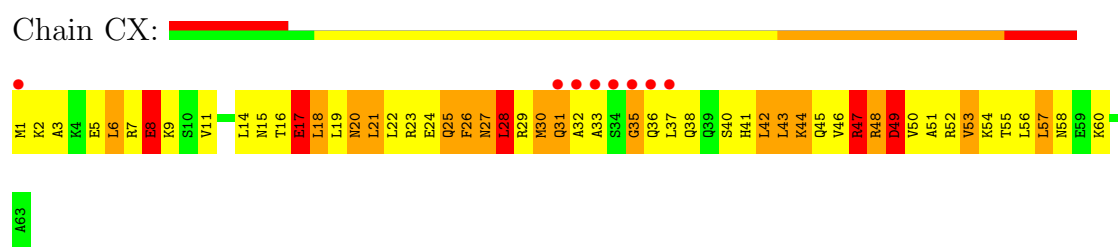
- Molecule 29: 50S RIBOSOMAL PROTEIN L27



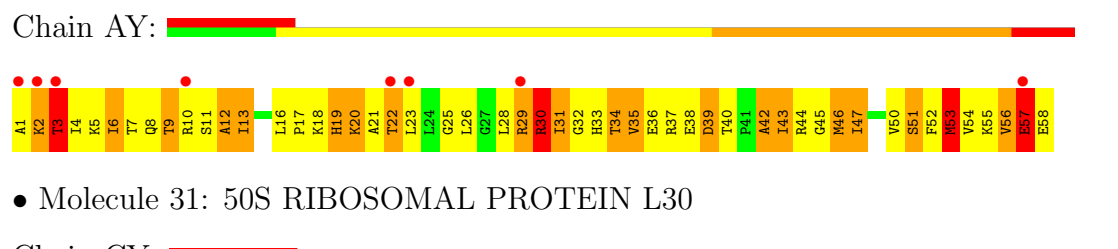
- Molecule 30: 50S RIBOSOMAL PROTEIN L29



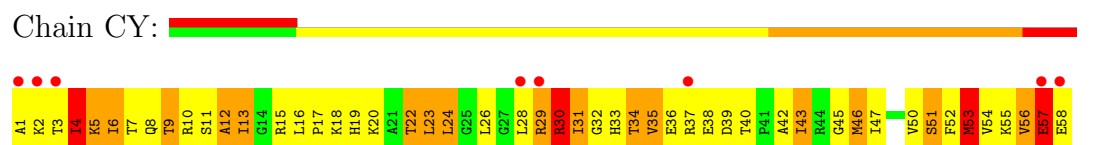
- Molecule 30: 50S RIBOSOMAL PROTEIN L29



- Molecule 31: 50S RIBOSOMAL PROTEIN L30

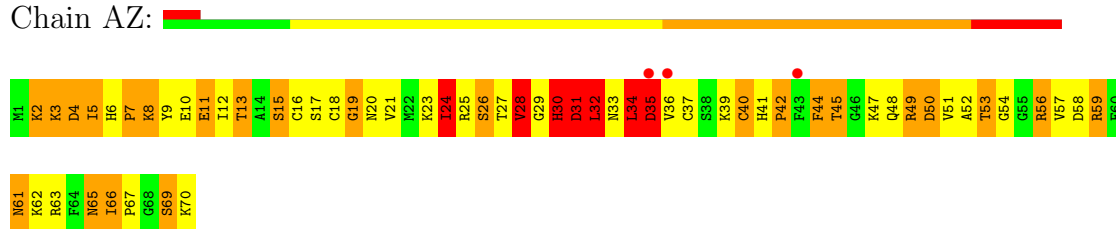


- Molecule 31: 50S RIBOSOMAL PROTEIN L30



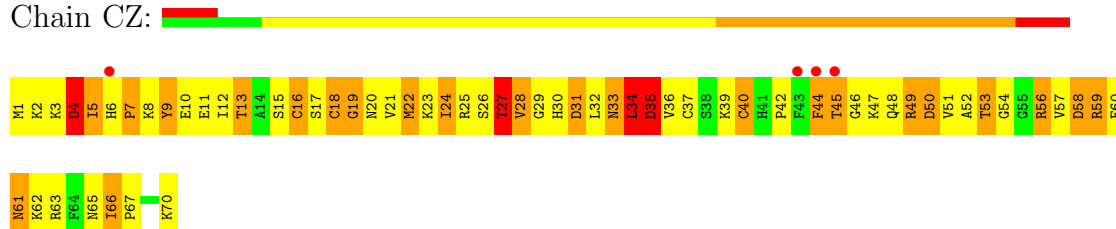
- Molecule 32: 50S RIBOSOMAL PROTEIN L31

Chain AZ:



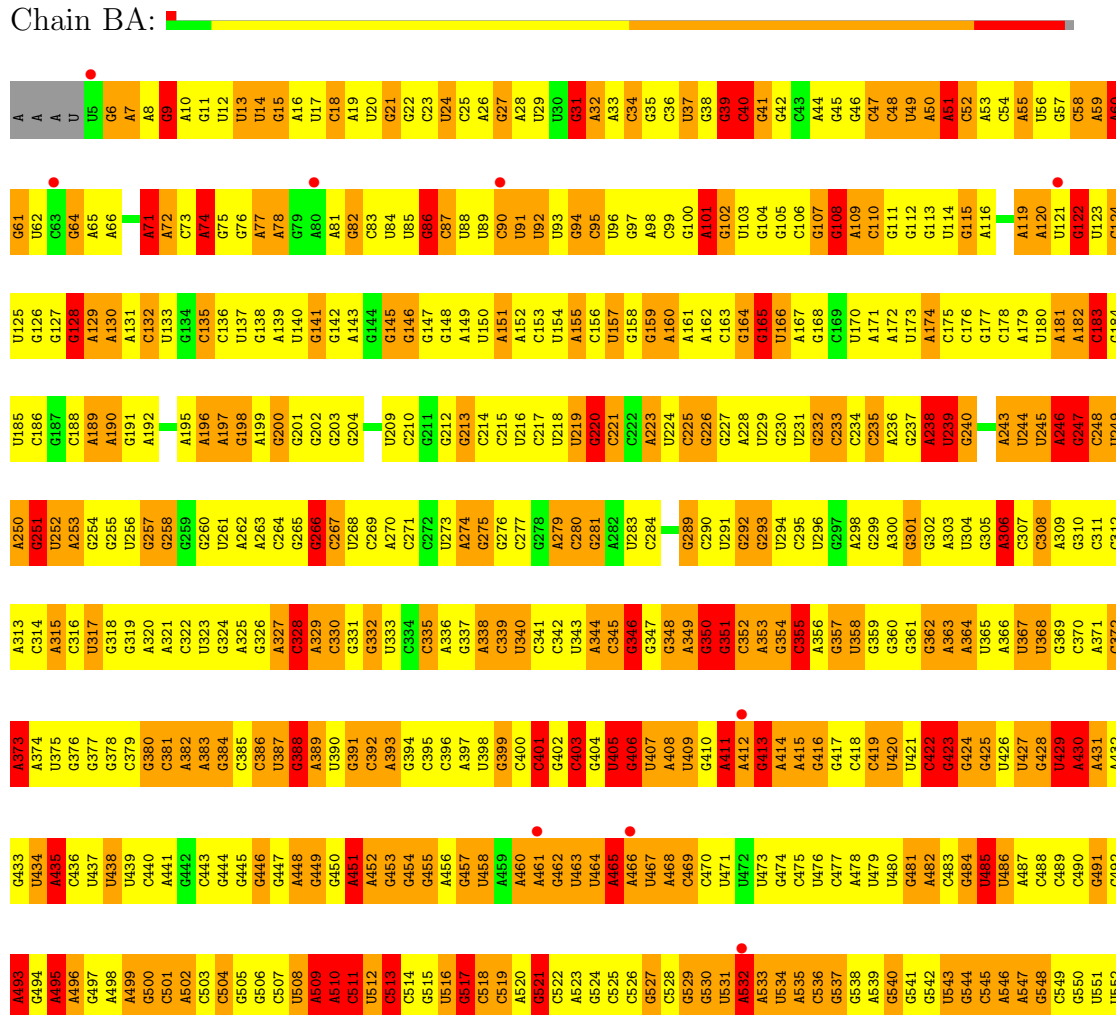
- Molecule 32: 50S RIBOSOMAL PROTEIN L31

Chain CZ:



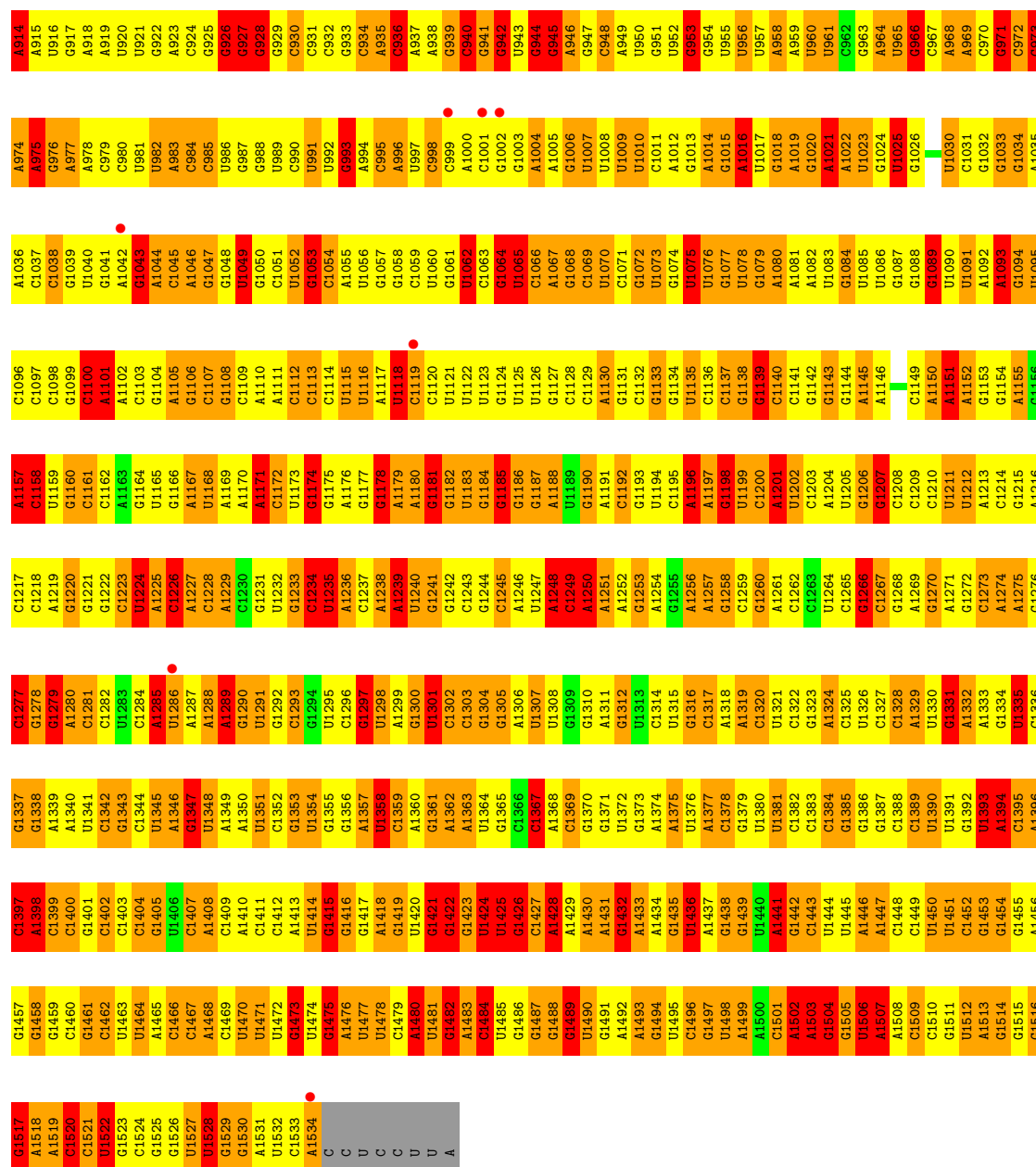
- Molecule 33: 16S RIBOSOMAL RNA

Chain BA:



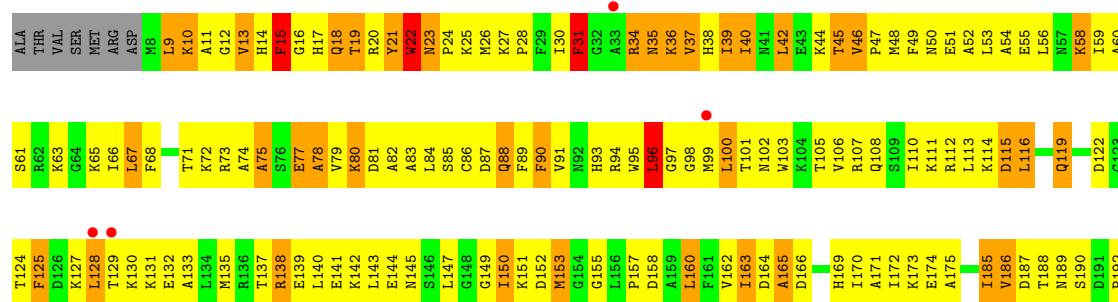
WORLDWIDE
PDB
PROTEIN DATA BANK

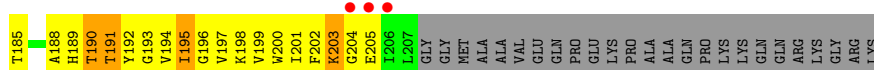




• Molecule 34: 30S RIBOSOMAL PROTEIN S2

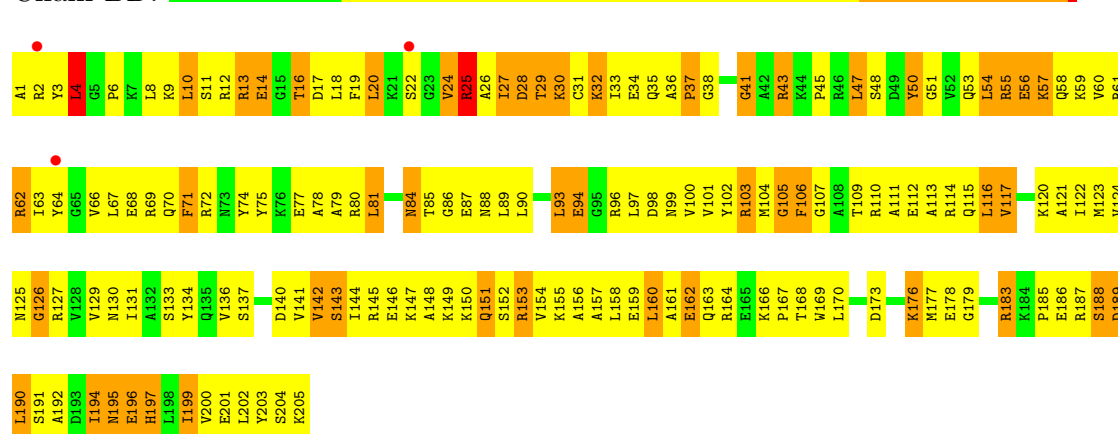
Chain BB:





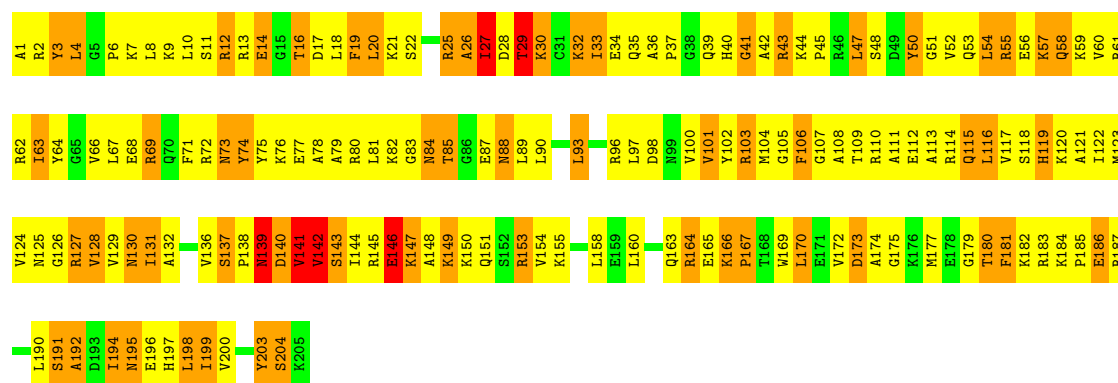
● Molecule 36: 30S RIBOSOMAL PROTEIN S4

Chain BD:



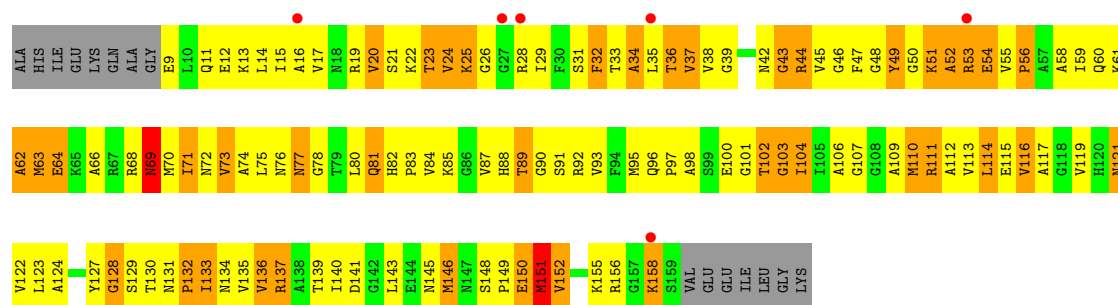
● Molecule 36: 30S RIBOSOMAL PROTEIN S4

Chain DD:



● Molecule 37: 30S RIBOSOMAL PROTEIN S5

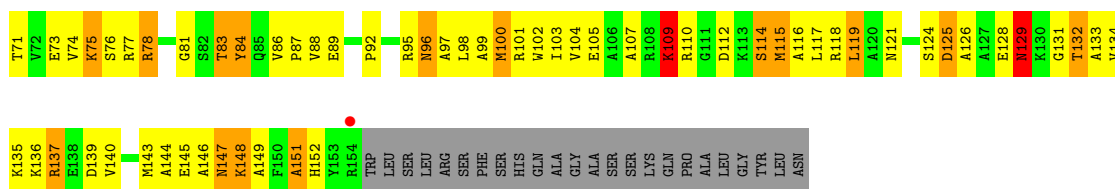
Chain BE:



● Molecule 37: 30S RIBOSOMAL PROTEIN S5

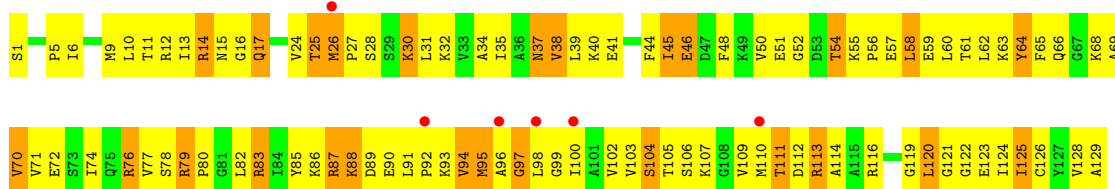
Chain DE:





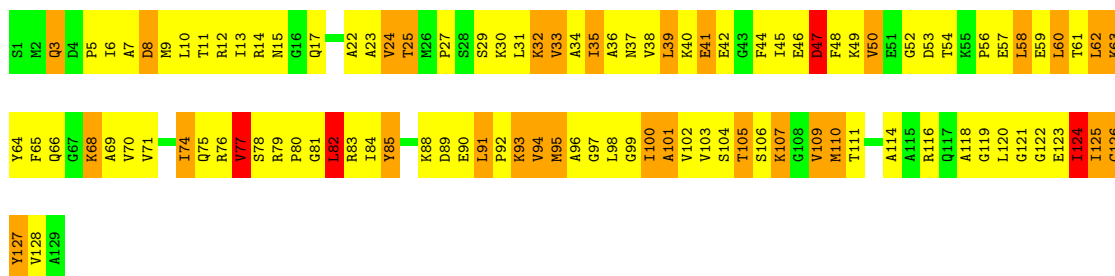
• Molecule 40: 30S RIBOSOMAL PROTEIN S8

Chain BH:



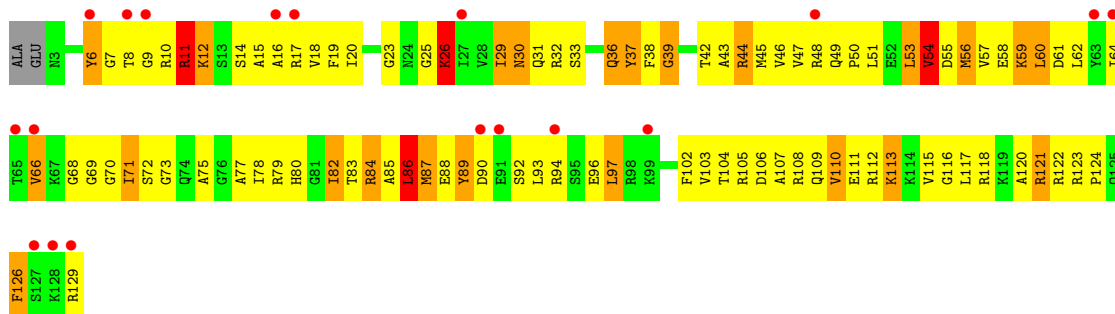
• Molecule 40: 30S RIBOSOMAL PROTEIN S8

Chain DH:



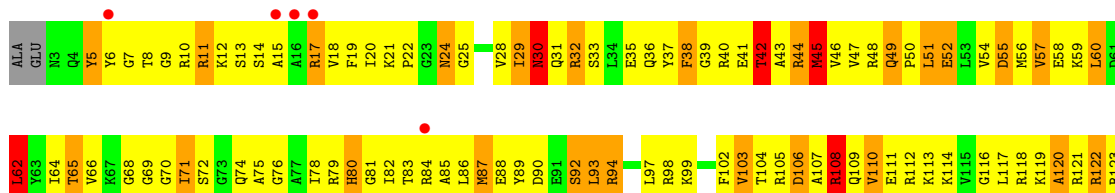
• Molecule 41: 30S RIBOSOMAL PROTEIN S9

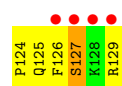
Chain BI:



• Molecule 41: 30S RIBOSOMAL PROTEIN S9

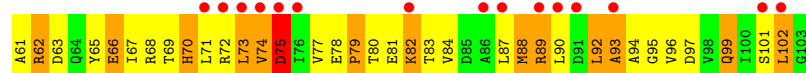
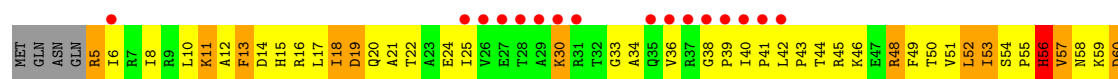
Chain DI:





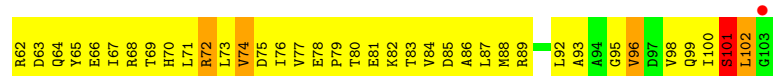
• Molecule 42: 30S RIBOSOMAL PROTEIN S10

Chain BJ:



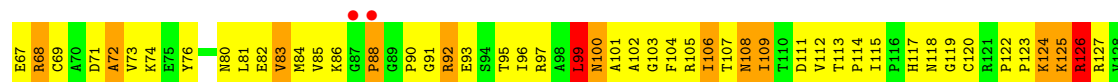
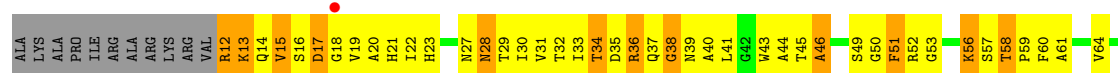
• Molecule 42: 30S RIBOSOMAL PROTEIN S10

Chain DJ:



• Molecule 43: 30S RIBOSOMAL PROTEIN S11

Chain BK:



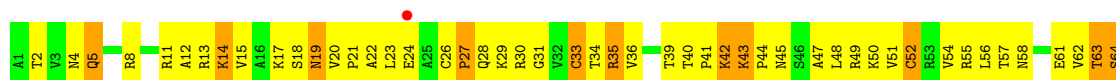
• Molecule 43: 30S RIBOSOMAL PROTEIN S11

Chain DK:



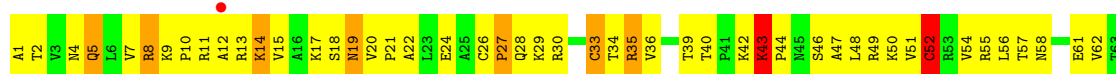
• Molecule 44: 30S RIBOSOMAL PROTEIN S12

Chain BL:



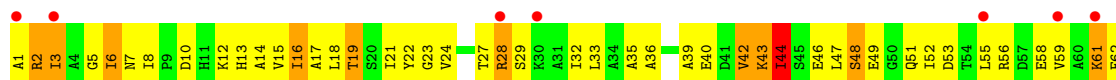
• Molecule 44: 30S RIBOSOMAL PROTEIN S12

Chain DL:



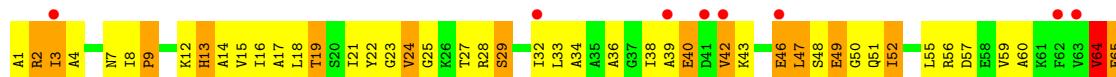
• Molecule 45: 30S RIBOSOMAL PROTEIN S13

Chain BM:



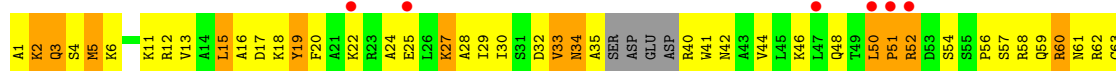
• Molecule 45: 30S RIBOSOMAL PROTEIN S13

Chain DM:



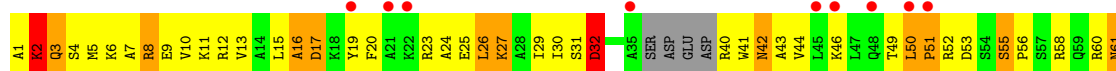
• Molecule 46: 30S RIBOSOMAL PROTEIN S14

Chain BN:



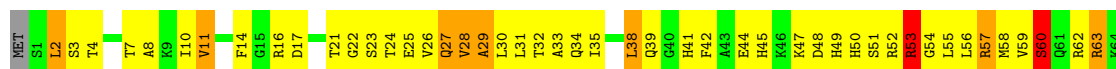
• Molecule 46: 30S RIBOSOMAL PROTEIN S14

Chain DN:



• Molecule 47: 30S RIBOSOMAL PROTEIN S15

Chain BO:



• Molecule 47: 30S RIBOSOMAL PROTEIN S15

Chain DO:



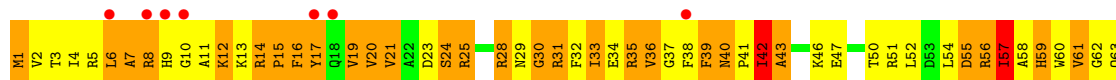
• Molecule 48: 30S RIBOSOMAL PROTEIN S16

Chain BP:



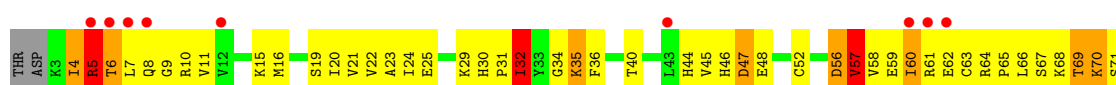
• Molecule 48: 30S RIBOSOMAL PROTEIN S16

Chain DP:



• Molecule 49: 30S RIBOSOMAL PROTEIN S17

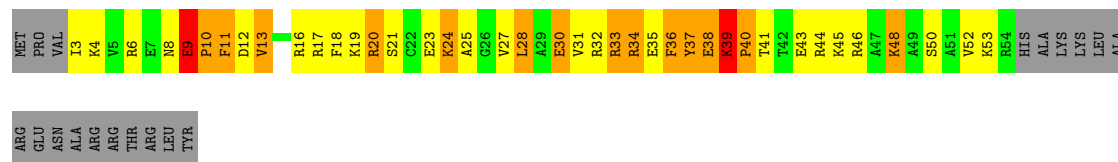
Chain BQ:



● Molecule 52: 30S RIBOSOMAL PROTEIN S20

• Molecule 53: 30S RIBOSOMAL PROTEIN S21

• Molecule 53: 30S RIBOSOMAL PROTEIN S21



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 49.74 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (49.74-3.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.323 0.276 , 0.330	Depositor DCC
R_{free} test set	5544 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 546832 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	284264	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A0	0.41	0/450	0.71	0/599
1	C0	0.48	0/450	0.78	0/599
2	A1	0.42	0/448	0.69	0/594
2	C1	0.46	0/448	0.73	0/594
3	A2	0.46	0/380	0.76	0/498
3	C2	0.46	0/380	0.83	1/498 (0.2%)
4	A3	0.52	0/513	0.79	0/676
4	C3	0.54	0/513	0.91	0/676
5	A4	0.43	0/303	0.69	0/397
5	C4	0.46	0/303	0.78	0/397
6	A5	0.64	0/134	0.72	0/176
7	AA	0.76	3/2803 (0.1%)	1.48	39/4371 (0.9%)
7	CA	0.79	2/2803 (0.1%)	1.52	47/4371 (1.1%)
8	AB	0.82	7/68314 (0.0%)	1.58	975/106569 (0.9%)
8	CB	0.90	15/68314 (0.0%)	1.64	1204/106569 (1.1%)
9	AC	0.51	0/2093	0.81	2/2815 (0.1%)
9	CC	0.55	0/2093	0.82	1/2815 (0.0%)
10	AD	0.45	0/1586	0.72	0/2134
10	CD	0.51	0/1586	0.77	0/2134
11	AE	0.47	0/1571	0.77	0/2113
11	CE	0.50	0/1571	0.75	0/2113
12	AF	0.30	0/1444	0.53	0/1937
12	CF	0.32	0/1444	0.54	0/1937
13	AG	0.38	0/1343	0.62	0/1816
13	CG	0.37	0/1343	0.62	0/1816
14	AH	0.34	0/1122	0.60	0/1515
14	CH	0.37	0/1122	0.64	0/1515
15	AI	0.29	0/1046	0.52	0/1410
15	CI	0.26	0/1045	0.52	0/1406
16	AJ	0.43	0/1136	0.71	0/1531
16	CJ	0.50	0/1136	0.75	0/1531
17	AK	0.50	0/940	0.71	0/1260

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CK	0.54	0/940	0.72	0/1260
18	AL	0.46	0/1062	0.84	1/1413 (0.1%)
18	CL	0.44	0/1062	0.81	0/1413
19	AM	0.46	0/1093	0.73	0/1460
19	CM	0.48	0/1093	0.77	0/1460
20	AN	0.41	0/1021	0.66	0/1364
20	CN	0.49	0/1021	0.73	0/1364
21	AO	0.38	0/910	0.69	0/1219
21	CO	0.45	0/910	0.77	0/1219
22	AP	0.44	0/929	0.77	1/1242 (0.1%)
22	CP	0.51	0/929	0.81	1/1242 (0.1%)
23	AQ	0.45	0/960	0.71	0/1278
23	CQ	0.53	0/960	0.81	1/1278 (0.1%)
24	AR	0.41	0/829	0.72	0/1107
24	CR	0.46	0/829	0.75	0/1107
25	AS	0.43	0/864	0.74	0/1156
25	CS	0.44	0/864	0.82	0/1156
26	AT	0.45	0/785	0.68	0/1050
26	CT	0.43	0/785	0.69	0/1050
27	AU	0.48	0/788	0.72	0/1053
27	CU	0.42	0/788	0.69	0/1053
28	AV	0.34	0/766	0.52	0/1025
28	CV	0.36	0/766	0.52	0/1025
29	AW	0.42	0/642	0.76	0/848
29	CW	0.45	0/642	0.78	0/848
30	AX	0.47	0/510	0.76	0/677
30	CX	0.40	0/510	0.69	0/677
31	AY	0.36	0/453	0.66	0/605
31	CY	0.34	0/453	0.67	0/605
32	AZ	0.56	0/559	0.94	2/745 (0.3%)
32	CZ	0.68	0/559	0.97	0/745
33	BA	0.70	4/36761 (0.0%)	1.42	407/57346 (0.7%)
33	DA	0.82	4/36762 (0.0%)	1.58	674/57350 (1.2%)
34	BB	0.32	0/1736	0.54	0/2340
34	DB	0.36	0/1736	0.61	0/2340
35	BC	0.33	0/1652	0.53	0/2227
35	DC	0.39	0/1652	0.61	0/2227
36	BD	0.36	0/1665	0.62	0/2227
36	DD	0.46	0/1665	0.68	0/2227
37	BE	0.37	0/1119	0.56	0/1506
37	DE	0.43	0/1119	0.67	0/1506
38	BF	0.40	1/836 (0.1%)	0.57	0/1130
38	DF	0.41	1/836 (0.1%)	0.63	1/1130 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BG	0.33	0/1188	0.52	0/1593
39	DG	0.38	0/1212	0.58	0/1626
40	BH	0.32	0/989	0.55	0/1326
40	DH	0.44	0/989	0.69	0/1326
41	BI	0.29	0/1034	0.51	0/1375
41	DI	0.33	0/1034	0.64	1/1375 (0.1%)
42	BJ	0.33	1/797 (0.1%)	0.53	0/1079
42	DJ	0.36	1/797 (0.1%)	0.57	0/1079
43	BK	0.35	0/893	0.61	0/1205
43	DK	0.43	0/893	0.70	0/1205
44	BL	0.33	0/969	0.58	0/1300
44	DL	0.42	0/969	0.67	0/1300
45	BM	0.29	0/893	0.50	0/1195
45	DM	0.37	1/885 (0.1%)	0.60	0/1183
46	BN	0.29	0/785	0.51	0/1043
46	DN	0.30	0/785	0.56	0/1043
47	BO	0.33	0/724	0.55	0/966
47	DO	0.38	0/724	0.63	0/966
48	BP	0.30	0/659	0.51	0/884
48	DP	0.49	0/649	0.69	0/872
49	BQ	0.37	0/658	0.59	0/883
49	DQ	0.39	0/666	0.65	0/892
50	BR	0.40	0/463	0.62	0/623
50	DR	0.49	0/463	0.70	0/623
51	BS	0.32	1/653 (0.2%)	0.50	0/879
51	DS	0.37	1/661 (0.2%)	0.62	0/890
52	BT	0.32	0/671	0.49	0/888
52	DT	0.39	0/671	0.58	0/888
53	BU	0.42	0/431	0.56	0/572
53	DU	0.55	0/431	0.73	0/572
All	All	0.73	42/306634 (0.0%)	1.39	3358/458333 (0.7%)

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
1	C0	0	2
4	C3	0	2
11	CE	0	3
13	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	CH	0	1
16	AJ	0	1
16	CJ	0	1
18	AL	0	1
18	CL	0	1
19	AM	0	1
20	CN	0	2
22	AP	0	3
22	CP	0	4
24	CR	0	1
25	CS	0	2
26	CT	0	1
30	CX	0	1
32	AZ	0	1
32	CZ	0	1
All	All	0	30

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	765	G	N9-C4	9.10	1.45	1.38
8	CB	301	G	C3'-O3'	7.66	1.52	1.42
7	CA	87	U	C1'-N1	7.10	1.59	1.48
7	AA	87	U	C1'-N1	6.70	1.58	1.48
33	DA	519	C	C1'-N1	6.38	1.58	1.48

The worst 5 of 3358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AB	2288	A	C2-N3-C4	-70.19	75.50	110.60
8	CB	2288	A	C2-N3-C4	-69.49	75.85	110.60
8	CB	2288	A	N1-C2-N3	59.84	159.22	129.30
8	AB	2288	A	C6-N1-C2	-58.83	83.30	118.60
8	AB	2288	A	N1-C2-N3	58.75	158.67	129.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	AG	109	SER	Peptide
16	AJ	9	GLU	Peptide

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Mol	Chain	Res	Type	Group
18	AL	53	GLY	Peptide
19	AM	88	ASN	Peptide
22	AP	46	VAL	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	444	0	461	86	0
1	C0	444	0	461	112	0
2	A1	441	0	485	104	0
2	C1	441	0	485	89	0
3	A2	377	0	418	106	0
3	C2	377	0	418	104	0
4	A3	504	0	574	171	0
4	C3	504	0	574	137	0
5	A4	302	0	340	104	0
5	C4	302	0	340	99	0
6	A5	134	0	153	17	0
7	AA	2507	0	1270	277	0
7	CA	2507	0	1270	303	0
8	AB	60995	0	30679	6970	0
8	CB	60995	0	30678	7146	0
9	AC	2054	0	2122	607	0
9	CC	2054	0	2122	625	0
10	AD	1565	0	1616	443	0
10	CD	1565	0	1616	508	0
11	AE	1552	0	1619	432	0
11	CE	1552	0	1619	401	0
12	AF	1420	0	1460	177	0
12	CF	1420	0	1460	216	0
13	AG	1323	0	1374	196	0
13	CG	1323	0	1374	226	0
14	AH	1111	0	1148	160	0
14	CH	1111	0	1148	191	0
15	AI	1032	0	1088	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CI	1032	0	1088	131	0
16	AJ	1113	0	1147	293	0
16	CJ	1113	0	1147	307	0
17	AK	931	0	1000	161	0
17	CK	931	0	1000	159	0
18	AL	1053	0	1129	403	0
18	CL	1053	0	1129	336	0
19	AM	1074	0	1157	276	0
19	CM	1074	0	1157	294	0
20	AN	1008	0	1045	219	0
20	CN	1008	0	1045	248	0
21	AO	900	0	935	206	0
21	CO	900	0	935	247	0
22	AP	917	0	965	248	0
22	CP	917	0	965	243	0
23	AQ	947	0	1022	269	0
23	CQ	947	0	1022	284	0
24	AR	816	0	839	236	0
24	CR	816	0	839	308	0
25	AS	857	0	922	172	0
25	CS	857	0	922	200	0
26	AT	778	0	840	178	0
26	CT	778	0	840	173	0
27	AU	780	0	834	183	0
27	CU	780	0	834	172	0
28	AV	753	0	780	100	0
28	CV	753	0	780	90	0
29	AW	634	0	656	205	0
29	CW	634	0	656	226	0
30	AX	509	0	543	111	0
30	CX	509	0	543	123	0
31	AY	449	0	491	66	0
31	CY	449	0	491	84	0
32	AZ	549	0	552	174	0
32	CZ	549	0	552	152	0
33	BA	32831	0	16522	3632	0
33	DA	32831	0	16521	4109	0
34	BB	1705	0	1732	245	0
34	DB	1705	0	1732	220	0
35	BC	1625	0	1699	214	0
35	DC	1625	0	1699	274	0
36	BD	1643	0	1710	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DD	1643	0	1710	280	0
37	BE	1106	0	1148	176	0
37	DE	1106	0	1148	200	0
38	BF	818	0	808	114	0
38	DF	818	0	808	143	0
39	BG	1175	0	1230	116	0
39	DG	1197	0	1246	145	0
40	BH	979	0	1034	141	0
40	DH	979	0	1034	156	0
41	BI	1022	0	1070	141	0
41	DI	1022	0	1070	158	0
42	BJ	787	0	828	99	0
42	DJ	787	0	828	129	0
43	BK	877	0	887	127	0
43	DK	877	0	887	134	0
44	BL	955	0	1019	145	0
44	DL	955	0	1019	149	0
45	BM	884	0	944	125	0
45	DM	877	0	937	107	0
46	BN	774	0	827	138	0
46	DN	774	0	827	127	0
47	BO	716	0	742	96	0
47	DO	716	0	742	106	0
48	BP	649	0	666	109	0
48	DP	639	0	656	121	0
49	BQ	649	0	691	70	0
49	DQ	657	0	702	91	0
50	BR	456	0	478	75	0
50	DR	456	0	478	100	0
51	BS	638	0	665	112	0
51	DS	645	0	675	97	0
52	BT	665	0	714	85	0
52	DT	665	0	714	91	0
53	BU	426	0	449	81	0
53	DU	426	0	449	67	0
54	AB	109	0	0	0	0
54	AE	1	0	0	0	0
54	BA	58	0	0	0	0
54	BN	1	0	0	0	0
54	BT	1	0	0	0	0
54	CB	109	0	0	0	0
54	CC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CL	1	0	0	0	0
54	DA	61	0	0	0	0
54	DN	1	0	0	0	0
55	A2	2	0	0	2	0
55	AB	489	0	0	65	0
55	AC	3	0	0	1	0
55	AD	1	0	0	0	0
55	AE	3	0	0	2	0
55	AJ	2	0	0	2	0
55	AL	3	0	0	1	0
55	BA	284	0	0	26	0
55	BE	3	0	0	0	0
55	BI	2	0	0	0	0
55	BK	1	0	0	0	0
55	BL	2	0	0	0	0
55	BN	3	0	0	0	0
55	BP	1	0	0	0	0
55	BT	2	0	0	0	0
55	C0	1	0	0	0	0
55	C2	2	0	0	0	0
55	CB	485	0	0	65	0
55	CC	3	0	0	0	0
55	CD	1	0	0	0	0
55	CE	1	0	0	0	0
55	CJ	2	0	0	0	0
55	CK	1	0	0	0	0
55	CL	5	0	0	1	0
55	CN	3	0	0	2	0
55	CP	1	0	0	0	0
55	CQ	1	0	0	0	0
55	CT	2	0	0	0	0
55	CU	1	0	0	2	0
55	DA	293	0	0	18	0
55	DD	1	0	0	0	0
55	DE	2	0	0	0	0
55	DG	1	0	0	0	0
55	DL	4	0	0	0	0
55	DN	2	0	0	1	0
55	DP	1	0	0	0	0
55	DT	3	0	0	2	0
All	All	284264	0	190919	37675	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 80.

The worst 5 of 37675 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:CB:2822:G:OP2	20:CN:2:ARG:HB3	1.29	1.26
33:DA:585:G:C8	33:DA:585:G:H5'	1.76	1.21
33:DA:235:C:H2'	33:DA:236:A:C8	1.77	1.19
1:C0:27:LEU:HG	8:CB:2886:A:C6	1.77	1.19
23:CQ:49:ARG:HG3	24:CR:77:PHE:CZ	1.79	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	54/56 (96%)	26 (48%)	13 (24%)	15 (28%)	0	1
1	C0	54/56 (96%)	24 (44%)	12 (22%)	18 (33%)	0	0
2	A1	52/54 (96%)	18 (35%)	15 (29%)	19 (36%)	0	0
2	C1	52/54 (96%)	18 (35%)	12 (23%)	22 (42%)	0	0
3	A2	44/46 (96%)	15 (34%)	16 (36%)	13 (30%)	0	1
3	C2	44/46 (96%)	16 (36%)	16 (36%)	12 (27%)	0	1
4	A3	62/64 (97%)	24 (39%)	17 (27%)	21 (34%)	0	0
4	C3	62/64 (97%)	29 (47%)	20 (32%)	13 (21%)	0	4
5	A4	36/38 (95%)	14 (39%)	13 (36%)	9 (25%)	0	2
5	C4	36/38 (95%)	9 (25%)	16 (44%)	11 (31%)	0	1
6	A5	14/16 (88%)	6 (43%)	5 (36%)	3 (21%)	0	3
9	AC	266/273 (97%)	101 (38%)	67 (25%)	98 (37%)	0	0
9	CC	266/273 (97%)	101 (38%)	70 (26%)	95 (36%)	0	0
10	AD	207/209 (99%)	80 (39%)	56 (27%)	71 (34%)	0	0
10	CD	207/209 (99%)	72 (35%)	65 (31%)	70 (34%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AE	199/201 (99%)	76 (38%)	58 (29%)	65 (33%)	0	0
11	CE	199/201 (99%)	71 (36%)	63 (32%)	65 (33%)	0	0
12	AF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	5
12	CF	176/178 (99%)	95 (54%)	45 (26%)	36 (20%)	0	4
13	AG	174/176 (99%)	98 (56%)	42 (24%)	34 (20%)	0	4
13	CG	174/176 (99%)	89 (51%)	52 (30%)	33 (19%)	0	5
14	AH	147/149 (99%)	94 (64%)	34 (23%)	19 (13%)	0	13
14	CH	147/149 (99%)	74 (50%)	39 (26%)	34 (23%)	0	2
15	AI	139/141 (99%)	92 (66%)	33 (24%)	14 (10%)	1	20
15	CI	137/141 (97%)	87 (64%)	32 (23%)	18 (13%)	0	13
16	AJ	139/142 (98%)	60 (43%)	34 (24%)	45 (32%)	0	0
16	CJ	139/142 (98%)	57 (41%)	37 (27%)	45 (32%)	0	0
17	AK	120/123 (98%)	67 (56%)	30 (25%)	23 (19%)	0	4
17	CK	120/123 (98%)	66 (55%)	29 (24%)	25 (21%)	0	4
18	AL	142/144 (99%)	53 (37%)	37 (26%)	52 (37%)	0	0
18	CL	142/144 (99%)	54 (38%)	39 (28%)	49 (34%)	0	0
19	AM	134/136 (98%)	51 (38%)	46 (34%)	37 (28%)	0	1
19	CM	134/136 (98%)	55 (41%)	45 (34%)	34 (25%)	0	2
20	AN	125/127 (98%)	55 (44%)	43 (34%)	27 (22%)	0	3
20	CN	125/127 (98%)	55 (44%)	44 (35%)	26 (21%)	0	4
21	AO	115/117 (98%)	49 (43%)	40 (35%)	26 (23%)	0	3
21	CO	115/117 (98%)	46 (40%)	41 (36%)	28 (24%)	0	2
22	AP	112/114 (98%)	48 (43%)	30 (27%)	34 (30%)	0	1
22	CP	112/114 (98%)	48 (43%)	31 (28%)	33 (30%)	0	1
23	AQ	115/117 (98%)	62 (54%)	26 (23%)	27 (24%)	0	2
23	CQ	115/117 (98%)	57 (50%)	30 (26%)	28 (24%)	0	2
24	AR	101/103 (98%)	31 (31%)	25 (25%)	45 (45%)	0	0
24	CR	101/103 (98%)	37 (37%)	23 (23%)	41 (41%)	0	0
25	AS	108/110 (98%)	58 (54%)	24 (22%)	26 (24%)	0	2
25	CS	108/110 (98%)	52 (48%)	29 (27%)	27 (25%)	0	2
26	AT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	CT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	2
27	AU	101/103 (98%)	40 (40%)	36 (36%)	25 (25%)	0	2
27	CU	101/103 (98%)	38 (38%)	31 (31%)	32 (32%)	0	0
28	AV	92/94 (98%)	58 (63%)	21 (23%)	13 (14%)	0	11
28	CV	92/94 (98%)	57 (62%)	21 (23%)	14 (15%)	0	8
29	AW	82/84 (98%)	20 (24%)	28 (34%)	34 (42%)	0	0
29	CW	82/84 (98%)	17 (21%)	29 (35%)	36 (44%)	0	0
30	AX	61/63 (97%)	17 (28%)	25 (41%)	19 (31%)	0	0
30	CX	61/63 (97%)	26 (43%)	22 (36%)	13 (21%)	0	3
31	AY	56/58 (97%)	25 (45%)	17 (30%)	14 (25%)	0	2
31	CY	56/58 (97%)	26 (46%)	19 (34%)	11 (20%)	0	4
32	AZ	68/70 (97%)	30 (44%)	19 (28%)	19 (28%)	0	1
32	CZ	68/70 (97%)	34 (50%)	21 (31%)	13 (19%)	0	5
34	BB	217/240 (90%)	128 (59%)	65 (30%)	24 (11%)	1	17
34	DB	217/240 (90%)	124 (57%)	59 (27%)	34 (16%)	0	8
35	BC	205/232 (88%)	116 (57%)	59 (29%)	30 (15%)	0	10
35	DC	205/232 (88%)	112 (55%)	67 (33%)	26 (13%)	0	14
36	BD	203/205 (99%)	120 (59%)	57 (28%)	26 (13%)	0	14
36	DD	203/205 (99%)	116 (57%)	50 (25%)	37 (18%)	0	5
37	BE	149/166 (90%)	94 (63%)	33 (22%)	22 (15%)	0	9
37	DE	149/166 (90%)	77 (52%)	49 (33%)	23 (15%)	0	8
38	BF	99/135 (73%)	62 (63%)	25 (25%)	12 (12%)	1	15
38	DF	99/135 (73%)	56 (57%)	22 (22%)	21 (21%)	0	4
39	BG	149/178 (84%)	100 (67%)	34 (23%)	15 (10%)	1	20
39	DG	151/178 (85%)	94 (62%)	43 (28%)	14 (9%)	1	24
40	BH	127/129 (98%)	73 (58%)	42 (33%)	12 (9%)	1	24
40	DH	127/129 (98%)	70 (55%)	34 (27%)	23 (18%)	0	5
41	BI	125/129 (97%)	78 (62%)	35 (28%)	12 (10%)	1	22
41	DI	125/129 (97%)	73 (58%)	32 (26%)	20 (16%)	0	8
42	BJ	97/103 (94%)	59 (61%)	23 (24%)	15 (16%)	0	8
42	DJ	97/103 (94%)	62 (64%)	24 (25%)	11 (11%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BK	115/128 (90%)	69 (60%)	31 (27%)	15 (13%)	0	13
43	DK	115/128 (90%)	73 (64%)	30 (26%)	12 (10%)	1	19
44	BL	121/123 (98%)	67 (55%)	37 (31%)	17 (14%)	0	11
44	DL	121/123 (98%)	73 (60%)	32 (26%)	16 (13%)	0	13
45	BM	113/117 (97%)	70 (62%)	32 (28%)	11 (10%)	1	22
45	DM	112/117 (96%)	78 (70%)	20 (18%)	14 (12%)	1	14
46	BN	92/100 (92%)	58 (63%)	18 (20%)	16 (17%)	0	6
46	DN	92/100 (92%)	55 (60%)	18 (20%)	19 (21%)	0	4
47	BO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	1	18
47	DO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	1	18
48	BP	80/82 (98%)	43 (54%)	22 (28%)	15 (19%)	0	5
48	DP	79/82 (96%)	38 (48%)	24 (30%)	17 (22%)	0	3
49	BQ	79/83 (95%)	53 (67%)	15 (19%)	11 (14%)	0	11
49	DQ	79/83 (95%)	53 (67%)	16 (20%)	10 (13%)	0	14
50	BR	54/74 (73%)	25 (46%)	19 (35%)	10 (18%)	0	5
50	DR	54/74 (73%)	24 (44%)	19 (35%)	11 (20%)	0	4
51	BS	78/91 (86%)	52 (67%)	20 (26%)	6 (8%)	1	30
51	DS	79/91 (87%)	50 (63%)	20 (25%)	9 (11%)	1	16
52	BT	83/86 (96%)	51 (61%)	20 (24%)	12 (14%)	0	10
52	DT	83/86 (96%)	52 (63%)	20 (24%)	11 (13%)	0	13
53	BU	50/71 (70%)	26 (52%)	14 (28%)	10 (20%)	0	4
53	DU	50/71 (70%)	13 (26%)	27 (54%)	10 (20%)	0	4
All	All	11307/11918 (95%)	5696 (50%)	3156 (28%)	2455 (22%)	0	3

5 of 2455 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	ASP
1	A0	21	LEU
1	A0	25	THR
1	A0	29	VAL
1	A0	36	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	47/47 (100%)	34 (72%)	13 (28%)	0	6
1	C0	47/47 (100%)	39 (83%)	8 (17%)	3	23
2	A1	48/48 (100%)	40 (83%)	8 (17%)	3	24
2	C1	48/48 (100%)	36 (75%)	12 (25%)	1	8
3	A2	38/38 (100%)	18 (47%)	20 (53%)	0	0
3	C2	38/38 (100%)	20 (53%)	18 (47%)	0	0
4	A3	51/51 (100%)	34 (67%)	17 (33%)	0	3
4	C3	51/51 (100%)	30 (59%)	21 (41%)	0	1
5	A4	34/34 (100%)	21 (62%)	13 (38%)	0	1
5	C4	34/34 (100%)	19 (56%)	15 (44%)	0	0
6	A5	15/15 (100%)	12 (80%)	3 (20%)	2	14
9	AC	213/218 (98%)	150 (70%)	63 (30%)	0	5
9	CC	213/218 (98%)	147 (69%)	66 (31%)	0	5
10	AD	164/164 (100%)	112 (68%)	52 (32%)	0	4
10	CD	164/164 (100%)	111 (68%)	53 (32%)	0	4
11	AE	165/165 (100%)	120 (73%)	45 (27%)	0	6
11	CE	165/165 (100%)	118 (72%)	47 (28%)	0	5
12	AF	149/149 (100%)	129 (87%)	20 (13%)	6	37
12	CF	149/149 (100%)	131 (88%)	18 (12%)	7	42
13	AG	137/137 (100%)	103 (75%)	34 (25%)	1	8
13	CG	137/137 (100%)	106 (77%)	31 (23%)	1	10
14	AH	114/114 (100%)	87 (76%)	27 (24%)	1	9
14	CH	114/114 (100%)	85 (75%)	29 (25%)	1	8
15	AI	109/109 (100%)	93 (85%)	16 (15%)	4	31
15	CI	109/109 (100%)	98 (90%)	11 (10%)	11	52
16	AJ	114/116 (98%)	74 (65%)	40 (35%)	0	2
16	CJ	114/116 (98%)	76 (67%)	38 (33%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AK	102/104 (98%)	68 (67%)	34 (33%)	0	3
17	CK	102/104 (98%)	65 (64%)	37 (36%)	0	2
18	AL	103/103 (100%)	61 (59%)	42 (41%)	0	1
18	CL	103/103 (100%)	63 (61%)	40 (39%)	0	1
19	AM	109/109 (100%)	59 (54%)	50 (46%)	0	0
19	CM	109/109 (100%)	66 (61%)	43 (39%)	0	1
20	AN	103/103 (100%)	74 (72%)	29 (28%)	0	5
20	CN	103/103 (100%)	69 (67%)	34 (33%)	0	4
21	AO	87/87 (100%)	64 (74%)	23 (26%)	1	7
21	CO	87/87 (100%)	69 (79%)	18 (21%)	2	13
22	AP	99/99 (100%)	79 (80%)	20 (20%)	2	14
22	CP	99/99 (100%)	81 (82%)	18 (18%)	2	19
23	AQ	89/89 (100%)	58 (65%)	31 (35%)	0	3
23	CQ	89/89 (100%)	55 (62%)	34 (38%)	0	1
24	AR	84/84 (100%)	59 (70%)	25 (30%)	0	5
24	CR	84/84 (100%)	52 (62%)	32 (38%)	0	1
25	AS	93/93 (100%)	66 (71%)	27 (29%)	0	5
25	CS	93/93 (100%)	66 (71%)	27 (29%)	0	5
26	AT	83/84 (99%)	60 (72%)	23 (28%)	0	6
26	CT	83/84 (99%)	59 (71%)	24 (29%)	0	5
27	AU	83/84 (99%)	63 (76%)	20 (24%)	1	8
27	CU	83/84 (99%)	63 (76%)	20 (24%)	1	8
28	AV	78/78 (100%)	63 (81%)	15 (19%)	2	16
28	CV	78/78 (100%)	62 (80%)	16 (20%)	2	14
29	AW	62/62 (100%)	42 (68%)	20 (32%)	0	4
29	CW	62/62 (100%)	39 (63%)	23 (37%)	0	2
30	AX	55/55 (100%)	40 (73%)	15 (27%)	0	6
30	CX	55/55 (100%)	38 (69%)	17 (31%)	0	5
31	AY	48/48 (100%)	33 (69%)	15 (31%)	0	5
31	CY	48/48 (100%)	32 (67%)	16 (33%)	0	3
32	AZ	62/62 (100%)	44 (71%)	18 (29%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	CZ	62/62 (100%)	43 (69%)	19 (31%)	0	5
34	BB	180/198 (91%)	143 (79%)	37 (21%)	2	13
34	DB	180/198 (91%)	140 (78%)	40 (22%)	1	11
35	BC	170/189 (90%)	142 (84%)	28 (16%)	3	25
35	DC	170/189 (90%)	130 (76%)	40 (24%)	1	9
36	BD	172/172 (100%)	137 (80%)	35 (20%)	2	14
36	DD	172/172 (100%)	126 (73%)	46 (27%)	1	7
37	BE	113/125 (90%)	86 (76%)	27 (24%)	1	8
37	DE	113/125 (90%)	82 (73%)	31 (27%)	0	6
38	BF	87/116 (75%)	71 (82%)	16 (18%)	2	18
38	DF	87/116 (75%)	67 (77%)	20 (23%)	1	9
39	BG	123/146 (84%)	105 (85%)	18 (15%)	5	32
39	DG	125/146 (86%)	95 (76%)	30 (24%)	1	8
40	BH	104/104 (100%)	78 (75%)	26 (25%)	1	8
40	DH	104/104 (100%)	78 (75%)	26 (25%)	1	8
41	BI	105/106 (99%)	81 (77%)	24 (23%)	1	10
41	DI	105/106 (99%)	82 (78%)	23 (22%)	1	11
42	BJ	86/90 (96%)	68 (79%)	18 (21%)	1	13
42	DJ	86/90 (96%)	71 (83%)	15 (17%)	3	21
43	BK	90/98 (92%)	68 (76%)	22 (24%)	1	8
43	DK	90/98 (92%)	61 (68%)	29 (32%)	0	4
44	BL	103/103 (100%)	82 (80%)	21 (20%)	2	14
44	DL	103/103 (100%)	79 (77%)	24 (23%)	1	9
45	BM	92/95 (97%)	76 (83%)	16 (17%)	3	21
45	DM	91/95 (96%)	74 (81%)	17 (19%)	2	17
46	BN	79/83 (95%)	66 (84%)	13 (16%)	3	25
46	DN	79/83 (95%)	64 (81%)	15 (19%)	2	17
47	BO	76/77 (99%)	63 (83%)	13 (17%)	3	23
47	DO	76/77 (99%)	60 (79%)	16 (21%)	1	12
48	BP	65/65 (100%)	54 (83%)	11 (17%)	3	24
48	DP	65/65 (100%)	42 (65%)	23 (35%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BQ	74/77 (96%)	65 (88%)	9 (12%)	7	42
49	DQ	75/77 (97%)	63 (84%)	12 (16%)	3	27
50	BR	48/64 (75%)	39 (81%)	9 (19%)	2	17
50	DR	48/64 (75%)	35 (73%)	13 (27%)	1	6
51	BS	70/78 (90%)	59 (84%)	11 (16%)	4	28
51	DS	71/78 (91%)	53 (75%)	18 (25%)	1	8
52	BT	65/65 (100%)	55 (85%)	10 (15%)	4	29
52	DT	65/65 (100%)	57 (88%)	8 (12%)	7	41
53	BU	44/61 (72%)	39 (89%)	5 (11%)	8	45
53	DU	44/61 (72%)	31 (70%)	13 (30%)	0	5
All	All	9356/9707 (96%)	6965 (74%)	2391 (26%)	1	8

5 of 2391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BO	11	VAL
10	CD	188	LEU
43	DK	52	ARG
50	BR	22	TYR
5	C4	23	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 328 such sidechains are listed below:

Mol	Chain	Res	Type
45	BM	90	HIS
9	CC	196	ASN
44	DL	71	HIS
47	BO	39	GLN
52	BT	69	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	BA	1528/1542 (99%)	618 (40%)	204 (13%)
33	DA	1529/1542 (99%)	663 (43%)	211 (13%)
7	AA	116/120 (96%)	40 (34%)	12 (10%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	CA	117/120 (97%)	48 (41%)	15 (12%)
8	AB	2839/2904 (97%)	1140 (40%)	396 (13%)
8	CB	2838/2904 (97%)	1137 (40%)	386 (13%)
All	All	8967/9132 (98%)	3646 (40%)	1224 (13%)

5 of 3646 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	AA	6	G
7	AA	7	G
7	AA	9	G
7	AA	12	C
7	AA	13	G

5 of 1224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	BA	1107	C
8	CB	396	G
33	DA	820	U
33	BA	1198	G
7	CA	44	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 343 ligands modelled in this entry, 343 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	BA	1
15	CI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1045:C	O3'	1046:A	P	4.69
1	CI	72:THR	C	73:PRO	N	4.33

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	A0	56/56 (100%)	0.43	4 (7%) 16 11	109, 149, 271, 317	0
1	C0	56/56 (100%)	0.33	3 (5%) 25 16	97, 120, 190, 244	0
2	A1	54/54 (100%)	0.64	5 (9%) 9 8	124, 143, 239, 296	0
2	C1	54/54 (100%)	0.85	7 (12%) 4 5	92, 113, 223, 254	0
3	A2	46/46 (100%)	0.48	2 (4%) 34 22	74, 92, 165, 271	0
3	C2	46/46 (100%)	0.30	3 (6%) 18 13	68, 103, 198, 264	0
4	A3	64/64 (100%)	0.36	5 (7%) 13 10	80, 106, 228, 309	0
4	C3	64/64 (100%)	0.25	2 (3%) 47 29	69, 99, 174, 229	0
5	A4	38/38 (100%)	1.09	9 (23%) 1 2	115, 135, 250, 284	0
5	C4	38/38 (100%)	1.08	8 (21%) 1 2	124, 144, 238, 298	0
6	A5	16/16 (100%)	-0.07	0 100 100	73, 108, 197, 216	0
7	AA	117/120 (97%)	-0.53	0 100 100	78, 127, 174, 316	0
7	CA	117/120 (97%)	-0.56	1 (0%) 81 61	71, 127, 170, 285	0
8	AB	2841/2904 (97%)	-0.50	25 (0%) 81 61	57, 105, 213, 373	0
8	CB	2841/2904 (97%)	-0.62	10 (0%) 90 78	41, 89, 202, 421	0
9	AC	268/273 (98%)	0.25	10 (3%) 39 25	71, 107, 196, 257	0
9	CC	268/273 (98%)	0.16	10 (3%) 39 25	63, 91, 165, 248	0
10	AD	209/209 (100%)	0.21	3 (1%) 72 48	12, 127, 226, 325	0
10	CD	209/209 (100%)	0.16	5 (2%) 56 35	11, 94, 186, 271	0
11	AE	201/201 (100%)	0.29	8 (3%) 36 23	92, 120, 206, 299	0
11	CE	201/201 (100%)	0.45	18 (8%) 10 9	88, 117, 224, 290	0
12	AF	178/178 (100%)	0.31	5 (2%) 50 31	121, 170, 253, 334	0
12	CF	178/178 (100%)	0.32	4 (2%) 59 37	92, 155, 224, 286	0
13	AG	176/176 (100%)	0.10	7 (3%) 36 23	100, 137, 207, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CG	176/176 (100%)	0.47	20 (11%) 6 6	88, 138, 222, 271	0
14	AH	149/149 (100%)	1.46	48 (32%) 1 2	71, 314, 427, 456	0
14	CH	149/149 (100%)	0.34	2 (1%) 74 50	107, 147, 233, 274	0
15	AI	141/141 (100%)	1.33	31 (21%) 1 2	155, 233, 307, 356	0
15	CI	141/141 (100%)	2.43	61 (43%) 1 1	219, 343, 422, 470	0
16	AJ	141/142 (99%)	0.33	5 (3%) 42 26	105, 130, 217, 267	0
16	CJ	141/142 (99%)	0.35	6 (4%) 34 22	104, 121, 207, 250	0
17	AK	122/123 (99%)	0.12	2 (1%) 68 45	81, 109, 162, 234	0
17	CK	122/123 (99%)	-0.08	0 100 100	80, 94, 127, 208	0
18	AL	144/144 (100%)	1.09	21 (14%) 3 4	94, 138, 281, 363	0
18	CL	144/144 (100%)	0.77	23 (15%) 3 3	83, 128, 275, 315	0
19	AM	136/136 (100%)	0.26	10 (7%) 14 11	105, 126, 222, 268	0
19	CM	136/136 (100%)	0.17	6 (4%) 33 21	77, 108, 223, 279	0
20	AN	127/127 (100%)	0.24	3 (2%) 56 35	96, 114, 200, 251	0
20	CN	127/127 (100%)	0.12	6 (4%) 30 20	58, 78, 155, 257	0
21	AO	117/117 (100%)	0.45	6 (5%) 27 17	107, 162, 236, 299	0
21	CO	117/117 (100%)	0.56	13 (11%) 6 6	52, 118, 211, 255	0
22	AP	114/114 (100%)	0.11	1 (0%) 81 61	85, 123, 219, 281	0
22	CP	114/114 (100%)	0.02	1 (0%) 81 61	77, 96, 196, 257	0
23	AQ	117/117 (100%)	-0.02	0 100 100	70, 106, 152, 203	0
23	CQ	117/117 (100%)	-0.09	1 (0%) 81 61	70, 93, 148, 225	0
24	AR	103/103 (100%)	0.62	5 (4%) 28 18	105, 145, 250, 346	0
24	CR	103/103 (100%)	0.41	9 (8%) 10 9	87, 132, 229, 286	0
25	AS	110/110 (100%)	0.25	3 (2%) 52 32	77, 106, 167, 279	0
25	CS	110/110 (100%)	0.14	2 (1%) 65 43	49, 85, 152, 211	0
26	AT	100/100 (100%)	0.26	4 (4%) 36 23	94, 130, 222, 250	0
26	CT	100/100 (100%)	0.50	7 (7%) 16 11	85, 120, 248, 278	0
27	AU	103/103 (100%)	0.80	15 (14%) 3 4	90, 140, 235, 264	0
27	CU	103/103 (100%)	0.89	14 (13%) 4 4	118, 162, 256, 281	0
28	AV	94/94 (100%)	-0.02	1 (1%) 77 54	86, 136, 209, 234	0
28	CV	94/94 (100%)	0.10	2 (2%) 60 38	87, 125, 194, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	AW	84/84 (100%)	1.02	13 (15%) 3 4	116, 147, 244, 330	0
29	CW	84/84 (100%)	0.82	13 (15%) 3 4	111, 136, 238, 275	0
30	AX	63/63 (100%)	0.08	1 (1%) 68 45	84, 130, 208, 247	0
30	CX	63/63 (100%)	0.58	8 (12%) 4 5	86, 150, 233, 320	0
31	AY	58/58 (100%)	1.10	8 (13%) 4 4	116, 143, 272, 279	0
31	CY	58/58 (100%)	1.07	8 (13%) 4 4	126, 138, 240, 249	0
32	AZ	70/70 (100%)	0.40	3 (4%) 34 22	66, 104, 170, 258	0
32	CZ	70/70 (100%)	0.40	4 (5%) 23 15	70, 91, 169, 255	0
33	BA	1530/1542 (99%)	-0.36	15 (0%) 79 57	70, 137, 279, 497	0
33	DA	1530/1542 (99%)	-0.54	8 (0%) 88 73	45, 111, 224, 368	0
34	BB	219/240 (91%)	0.15	4 (1%) 65 43	94, 175, 269, 316	0
34	DB	219/240 (91%)	0.25	6 (2%) 52 32	108, 159, 243, 292	0
35	BC	207/232 (89%)	0.33	13 (6%) 19 13	87, 169, 255, 315	0
35	DC	207/232 (89%)	0.16	9 (4%) 34 22	113, 140, 207, 226	0
36	BD	205/205 (100%)	0.06	3 (1%) 70 46	61, 139, 230, 325	0
36	DD	205/205 (100%)	0.02	0 100 100	71, 102, 169, 227	0
37	BE	151/166 (90%)	0.39	6 (3%) 36 23	75, 156, 254, 336	0
37	DE	151/166 (90%)	0.08	3 (1%) 62 39	56, 99, 174, 250	0
38	BF	101/135 (74%)	0.16	5 (4%) 28 18	57, 140, 224, 279	0
38	DF	101/135 (74%)	0.20	5 (4%) 28 18	110, 137, 200, 247	0
39	BG	151/178 (84%)	0.63	14 (9%) 9 8	94, 206, 288, 333	0
39	DG	153/178 (85%)	0.29	2 (1%) 74 50	44, 144, 206, 228	0
40	BH	129/129 (100%)	0.39	6 (4%) 30 20	76, 157, 231, 297	0
40	DH	129/129 (100%)	-0.06	0 100 100	70, 98, 166, 216	0
41	BI	127/129 (98%)	0.74	18 (14%) 3 4	90, 194, 271, 307	0
41	DI	127/129 (98%)	0.46	9 (7%) 16 11	103, 165, 231, 281	0
42	BJ	99/103 (96%)	1.53	31 (31%) 1 2	131, 254, 373, 423	0
42	DJ	99/103 (96%)	0.40	4 (4%) 36 23	130, 173, 223, 237	0
43	BK	117/128 (91%)	0.12	3 (2%) 53 33	54, 128, 245, 290	0
43	DK	117/128 (91%)	0.16	2 (1%) 67 44	69, 100, 165, 222	0
44	BL	123/123 (100%)	0.17	4 (3%) 44 28	50, 138, 215, 332	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DL	123/123 (100%)	0.04	3 (2%) 56 35	64, 95, 150, 211	0
45	BM	115/117 (98%)	1.18	28 (24%) 1 2	144, 252, 315, 344	0
45	DM	114/117 (97%)	0.57	10 (8%) 10 9	113, 171, 221, 288	0
46	BN	96/100 (96%)	0.64	6 (6%) 19 13	85, 188, 308, 367	0
46	DN	96/100 (96%)	0.59	10 (10%) 7 7	105, 153, 250, 295	0
47	BO	88/89 (98%)	-0.01	0 100 100	67, 133, 213, 255	0
47	DO	88/89 (98%)	-0.12	1 (1%) 77 54	73, 105, 170, 201	0
48	BP	82/82 (100%)	0.90	9 (10%) 6 7	90, 168, 269, 347	0
48	DP	81/82 (98%)	0.57	7 (8%) 11 9	69, 93, 145, 202	0
49	BQ	81/83 (97%)	0.93	12 (14%) 3 4	101, 180, 266, 301	0
49	DQ	81/83 (97%)	0.12	0 100 100	65, 109, 172, 212	0
50	BR	56/74 (75%)	0.08	1 (1%) 65 43	66, 117, 216, 283	0
50	DR	56/74 (75%)	0.62	4 (7%) 16 11	74, 103, 172, 253	0
51	BS	80/91 (87%)	1.57	23 (28%) 1 2	152, 267, 315, 366	0
51	DS	81/91 (89%)	0.81	12 (14%) 3 4	122, 182, 230, 249	0
52	BT	85/86 (98%)	0.27	0 100 100	76, 155, 224, 256	0
52	DT	85/86 (98%)	0.40	0 100 100	79, 97, 185, 219	0
53	BU	52/71 (73%)	0.47	5 (9%) 8 8	91, 171, 256, 300	0
53	DU	52/71 (73%)	-0.08	0 100 100	95, 140, 201, 249	0
All	All	20487/21050 (97%)	0.00	841 (4%) 35 23	11, 121, 254, 497	0

The worst 5 of 841 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	CI	98	GLY	19.8
15	CI	83	ALA	16.9
15	CI	137	LEU	15.9
9	AC	5	CYS	14.0
15	AI	2	LYS	13.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	CB	3108	1/1	0.65	140.50	53,53,53,53	1
54	MG	DA	1622	1/1	0.23	129.00	27,27,27,27	0
54	MG	DA	1658	1/1	0.45	127.80	47,47,47,47	0
54	MG	BA	4054	1/1	0.81	55.07	90,90,90,90	0
54	MG	DA	1607	1/1	0.20	39.80	54,54,54,54	0
54	MG	DA	1632	1/1	0.45	39.43	90,90,90,90	0
54	MG	BA	4043	1/1	0.66	29.82	25,25,25,25	0
54	MG	CB	3036	1/1	0.34	29.40	19,19,19,19	0
54	MG	CB	3080	1/1	0.36	23.82	55,55,55,55	1
54	MG	AB	4092	1/1	0.42	22.77	27,27,27,27	1
54	MG	DA	1657	1/1	0.58	20.60	63,63,63,63	0
54	MG	BA	4002	1/1	0.34	20.53	86,86,86,86	0
54	MG	BA	4035	1/1	0.55	19.99	30,30,30,30	0
54	MG	DA	1647	1/1	0.24	19.58	30,30,30,30	0
54	MG	BA	4053	1/1	0.45	17.98	109,109,109,109	0
54	MG	AB	4099	1/1	0.25	15.20	12,12,12,12	1
54	MG	CB	3052	1/1	0.25	14.87	43,43,43,43	0
54	MG	CB	3007	1/1	0.19	14.09	25,25,25,25	0
54	MG	CB	3041	1/1	0.23	13.94	19,19,19,19	0
54	MG	AB	4014	1/1	0.21	13.28	18,18,18,18	0
54	MG	AB	4108	1/1	0.16	13.00	9,9,9,9	0
54	MG	BA	4021	1/1	0.20	12.75	28,28,28,28	1
54	MG	CB	3045	1/1	0.37	12.73	67,67,67,67	0
54	MG	AB	4017	1/1	0.39	12.62	10,10,10,10	0
54	MG	DA	1651	1/1	0.22	11.88	56,56,56,56	0
54	MG	DA	1619	1/1	0.44	11.67	64,64,64,64	0
54	MG	AB	4077	1/1	0.33	11.66	28,28,28,28	0
54	MG	AB	4096	1/1	0.32	11.16	46,46,46,46	0
54	MG	AB	4020	1/1	0.41	10.75	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AB	4098	1/1	0.26	10.67	37,37,37,37	0
54	MG	DA	1623	1/1	0.25	10.55	20,20,20,20	0
54	MG	AB	4056	1/1	0.29	10.22	9,9,9,9	0
54	MG	CB	3101	1/1	0.32	9.83	8,8,8,8	0
54	MG	DA	1660	1/1	0.25	9.52	14,14,14,14	0
54	MG	CB	3099	1/1	0.41	9.27	43,43,43,43	0
54	MG	CB	3087	1/1	0.26	9.11	25,25,25,25	0
54	MG	DA	1634	1/1	0.34	8.84	110,110,110,110	0
54	MG	BA	4007	1/1	0.36	8.73	81,81,81,81	0
54	MG	CB	3070	1/1	0.33	8.73	33,33,33,33	0
54	MG	CB	3076	1/1	0.22	8.67	15,15,15,15	0
54	MG	BA	4024	1/1	0.30	8.56	32,32,32,32	1
54	MG	DA	1612	1/1	0.36	8.22	81,81,81,81	0
54	MG	CB	3044	1/1	0.36	7.97	83,83,83,83	0
54	MG	CB	3103	1/1	0.31	7.93	10,10,10,10	0
54	MG	CB	3093	1/1	0.26	6.70	3,3,3,3	0
54	MG	CB	3005	1/1	0.16	6.69	26,26,26,26	0
54	MG	AB	4050	1/1	0.34	6.57	49,49,49,49	0
54	MG	CB	3104	1/1	0.38	6.38	6,6,6,6	0
54	MG	AB	4043	1/1	0.48	6.33	16,16,16,16	0
54	MG	AB	4076	1/1	0.24	6.33	23,23,23,23	0
54	MG	DA	1644	1/1	0.34	6.31	53,53,53,53	0
54	MG	CB	3051	1/1	0.24	6.24	12,12,12,12	0
54	MG	AB	4022	1/1	0.36	6.21	11,11,11,11	0
54	MG	CB	3054	1/1	0.27	6.20	13,13,13,13	0
54	MG	BA	4027	1/1	0.29	5.76	68,68,68,68	0
54	MG	AB	4048	1/1	0.21	5.48	22,22,22,22	0
54	MG	CB	3085	1/1	0.17	5.12	16,16,16,16	0
54	MG	CB	3032	1/1	0.24	5.07	52,52,52,52	0
54	MG	BA	4030	1/1	0.50	4.87	34,34,34,34	0
54	MG	DA	1624	1/1	0.33	4.33	57,57,57,57	0
54	MG	CB	3028	1/1	0.24	4.16	46,46,46,46	0
54	MG	AB	4091	1/1	0.20	4.13	34,34,34,34	0
54	MG	AB	4075	1/1	0.18	4.11	41,41,41,41	0
54	MG	AB	4032	1/1	0.19	4.06	35,35,35,35	0
54	MG	AB	4082	1/1	0.29	3.91	50,50,50,50	0
54	MG	AB	4063	1/1	0.21	3.81	16,16,16,16	0
54	MG	DA	1629	1/1	0.24	3.50	52,52,52,52	0
54	MG	AB	4071	1/1	0.18	3.28	29,29,29,29	0
54	MG	CB	3029	1/1	0.19	3.03	39,39,39,39	0
54	MG	AB	4027	1/1	0.20	2.97	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AB	4090	1/1	0.23	2.93	37,37,37,37	0
54	MG	BA	4022	1/1	0.25	2.90	14,14,14,14	0
54	MG	CB	3077	1/1	0.14	2.84	76,76,76,76	0
54	MG	CB	3014	1/1	0.20	2.72	33,33,33,33	0
54	MG	DA	1614	1/1	0.16	2.63	25,25,25,25	0
54	MG	BA	4019	1/1	0.31	2.53	11,11,11,11	0
54	MG	AB	4085	1/1	0.23	2.37	53,53,53,53	0
54	MG	AB	4097	1/1	0.23	2.32	17,17,17,17	0
54	MG	CB	3071	1/1	0.22	2.26	52,52,52,52	0
54	MG	AB	4031	1/1	0.17	2.18	56,56,56,56	0
54	MG	DA	1609	1/1	0.27	2.08	56,56,56,56	0
54	MG	AB	4069	1/1	0.19	2.07	51,51,51,51	0
54	MG	BA	4020	1/1	0.44	2.06	77,77,77,77	0
54	MG	CB	3040	1/1	0.26	1.91	46,46,46,46	0
54	MG	DA	1616	1/1	0.17	1.90	21,21,21,21	0
54	MG	CB	3096	1/1	0.21	1.90	38,38,38,38	0
54	MG	AB	4095	1/1	0.23	1.83	47,47,47,47	0
54	MG	CB	3063	1/1	0.17	1.70	11,11,11,11	0
54	MG	AB	4057	1/1	0.21	1.70	49,49,49,49	0
54	MG	BA	4013	1/1	0.19	1.56	73,73,73,73	0
54	MG	AB	4061	1/1	0.15	1.55	35,35,35,35	0
54	MG	AB	4065	1/1	0.17	1.55	20,20,20,20	0
54	MG	CB	3030	1/1	0.17	1.54	17,17,17,17	0
54	MG	AB	4101	1/1	0.17	1.37	25,25,25,25	0
54	MG	AB	4049	1/1	0.18	1.37	21,21,21,21	0
54	MG	BA	4005	1/1	0.24	1.29	59,59,59,59	0
54	MG	DA	1613	1/1	0.23	1.27	62,62,62,62	0
54	MG	AB	4002	1/1	0.20	1.23	27,27,27,27	0
54	MG	BA	4049	1/1	0.18	1.17	100,100,100,100	0
54	MG	CB	3094	1/1	0.16	1.14	16,16,16,16	0
54	MG	BA	4028	1/1	0.25	1.09	61,61,61,61	0
54	MG	CB	3010	1/1	0.17	1.09	30,30,30,30	0
54	MG	BA	4033	1/1	0.25	1.05	90,90,90,90	0
54	MG	DA	1611	1/1	0.18	1.05	51,51,51,51	0
54	MG	BA	4034	1/1	0.16	0.92	48,48,48,48	0
54	MG	DA	1659	1/1	0.23	0.89	85,85,85,85	0
54	MG	BA	4042	1/1	0.30	0.88	69,69,69,69	0
54	MG	CB	3027	1/1	0.16	0.83	40,40,40,40	0
54	MG	CB	3038	1/1	0.17	0.83	58,58,58,58	0
54	MG	CB	3020	1/1	0.21	0.73	8,8,8,8	0
54	MG	DA	1653	1/1	0.14	0.68	21,21,21,21	0
54	MG	BA	4046	1/1	0.28	0.64	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	4003	1/1	0.21	0.63	29,29,29,29	0
54	MG	CB	3049	1/1	0.16	0.63	30,30,30,30	1
54	MG	BA	4025	1/1	0.16	0.61	37,37,37,37	0
54	MG	CB	3026	1/1	0.13	0.60	10,10,10,10	0
54	MG	DA	1637	1/1	0.20	0.58	109,109,109,109	0
54	MG	CB	3060	1/1	0.16	0.55	78,78,78,78	0
54	MG	AB	4003	1/1	0.15	0.52	26,26,26,26	0
54	MG	AB	4011	1/1	0.18	0.43	45,45,45,45	0
54	MG	CB	3072	1/1	0.18	0.42	42,42,42,42	0
54	MG	BA	4032	1/1	0.16	0.41	27,27,27,27	0
54	MG	CB	3090	1/1	0.12	0.40	67,67,67,67	0
54	MG	AB	4066	1/1	0.15	0.35	33,33,33,33	0
54	MG	BA	4051	1/1	0.15	0.33	79,79,79,79	0
54	MG	DA	1610	1/1	0.19	0.30	48,48,48,48	0
54	MG	BA	4031	1/1	0.23	0.29	40,40,40,40	0
54	MG	DA	1617	1/1	0.14	0.29	10,10,10,10	0
54	MG	BA	4004	1/1	0.15	0.28	34,34,34,34	0
54	MG	AB	4103	1/1	0.21	0.28	13,13,13,13	0
54	MG	AB	4025	1/1	0.22	0.24	129,129,129,129	0
54	MG	AB	4016	1/1	0.17	0.21	68,68,68,68	0
54	MG	AB	4023	1/1	0.17	0.20	66,66,66,66	0
54	MG	AB	4088	1/1	0.18	0.20	24,24,24,24	0
54	MG	BA	4045	1/1	0.13	0.18	59,59,59,59	0
54	MG	AB	4079	1/1	0.23	0.17	43,43,43,43	0
54	MG	DA	1635	1/1	0.26	0.13	41,41,41,41	0
54	MG	AB	4029	1/1	0.15	0.10	55,55,55,55	0
54	MG	CB	3081	1/1	0.13	0.04	10,10,10,10	0
54	MG	AB	4080	1/1	0.16	-0.03	17,17,17,17	0
54	MG	CB	3075	1/1	0.14	-0.08	61,61,61,61	0
54	MG	DA	1615	1/1	0.13	-0.10	95,95,95,95	0
54	MG	CB	3004	1/1	0.13	-0.15	9,9,9,9	0
54	MG	BA	4039	1/1	0.18	-0.20	31,31,31,31	0
54	MG	AB	4060	1/1	0.17	-0.21	36,36,36,36	0
54	MG	AB	4004	1/1	0.17	-0.23	41,41,41,41	0
54	MG	AB	4109	1/1	0.16	-0.25	34,34,34,34	0
54	MG	AB	4013	1/1	0.15	-0.29	46,46,46,46	0
54	MG	CB	3037	1/1	0.14	-0.29	10,10,10,10	0
54	MG	CB	3066	1/1	0.16	-0.32	45,45,45,45	0
54	MG	BA	4037	1/1	0.12	-0.35	58,58,58,58	0
54	MG	BA	4012	1/1	0.18	-0.42	54,54,54,54	0
54	MG	CB	3109	1/1	0.13	-0.47	16,16,16,16	0
54	MG	CB	3048	1/1	0.16	-0.47	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	4057	1/1	0.11	-0.51	29,29,29,29	0
54	MG	CB	3067	1/1	0.14	-0.54	9,9,9,9	0
54	MG	CB	3095	1/1	0.14	-0.54	22,22,22,22	0
54	MG	CB	3073	1/1	0.13	-0.54	14,14,14,14	0
54	MG	CB	3008	1/1	0.13	-0.58	16,16,16,16	0
54	MG	AB	4053	1/1	0.11	-0.61	14,14,14,14	0
54	MG	DA	1638	1/1	0.11	-0.63	12,12,12,12	0
54	MG	CB	3105	1/1	0.12	-0.64	20,20,20,20	0
54	MG	BA	4026	1/1	0.16	-0.65	75,75,75,75	0
54	MG	DA	1646	1/1	0.15	-0.66	50,50,50,50	0
54	MG	AB	4100	1/1	0.13	-0.67	25,25,25,25	0
54	MG	CB	3078	1/1	0.12	-0.69	57,57,57,57	0
54	MG	CB	3089	1/1	0.15	-0.71	38,38,38,38	0
54	MG	AB	4026	1/1	0.14	-0.72	78,78,78,78	0
54	MG	AB	4042	1/1	0.11	-0.74	90,90,90,90	0
54	MG	CB	3031	1/1	0.12	-0.75	55,55,55,55	0
54	MG	AB	4062	1/1	0.12	-0.81	30,30,30,30	0
54	MG	CB	3009	1/1	0.12	-0.84	13,13,13,13	0
54	MG	CB	3082	1/1	0.14	-0.87	17,17,17,17	0
54	MG	CB	3022	1/1	0.08	-0.90	21,21,21,21	0
54	MG	BA	4008	1/1	0.12	-0.93	21,21,21,21	0
54	MG	CL	201	1/1	0.08	-0.94	43,43,43,43	0
54	MG	BA	4009	1/1	0.10	-0.94	34,34,34,34	0
54	MG	CB	3019	1/1	0.14	-0.97	11,11,11,11	0
54	MG	CB	3083	1/1	0.11	-0.99	9,9,9,9	0
54	MG	AB	4038	1/1	0.09	-0.99	30,30,30,30	0
54	MG	CB	3043	1/1	0.08	-1.00	69,69,69,69	0
54	MG	AB	4034	1/1	0.14	-1.00	51,51,51,51	0
54	MG	AB	4040	1/1	0.13	-1.16	77,77,77,77	0
54	MG	DA	1645	1/1	0.12	-1.16	56,56,56,56	0
54	MG	AB	4087	1/1	0.12	-1.18	38,38,38,38	0
54	MG	BA	4001	1/1	0.11	-1.18	69,69,69,69	0
54	MG	AB	4047	1/1	0.14	-1.20	48,48,48,48	0
54	MG	CB	3064	1/1	0.12	-1.21	63,63,63,63	0
54	MG	CB	3059	1/1	0.12	-1.22	12,12,12,12	0
54	MG	AB	4055	1/1	0.09	-1.27	68,68,68,68	0
54	MG	BA	4050	1/1	0.10	-1.27	51,51,51,51	0
54	MG	AB	4074	1/1	0.14	-1.28	50,50,50,50	0
54	MG	AB	4024	1/1	0.11	-1.29	54,54,54,54	0
54	MG	BA	4017	1/1	0.11	-1.29	42,42,42,42	0
54	MG	DA	1641	1/1	0.09	-1.29	63,63,63,63	0
54	MG	AB	4078	1/1	0.10	-1.30	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AB	4045	1/1	0.10	-1.30	51,51,51,51	0
54	MG	CB	3079	1/1	0.12	-1.31	54,54,54,54	0
54	MG	CB	3061	1/1	0.11	-1.33	31,31,31,31	0
54	MG	AB	4059	1/1	0.12	-1.36	55,55,55,55	0
54	MG	CB	3018	1/1	0.13	-1.37	25,25,25,25	0
54	MG	DA	1603	1/1	0.09	-1.37	22,22,22,22	0
54	MG	AB	4005	1/1	0.13	-1.40	11,11,11,11	0
54	MG	CB	3097	1/1	0.10	-1.42	9,9,9,9	0
54	MG	AB	4107	1/1	0.10	-1.43	6,6,6,6	0
54	MG	AB	4054	1/1	0.12	-1.43	10,10,10,10	0
54	MG	BA	4006	1/1	0.12	-1.44	42,42,42,42	0
54	MG	DA	1627	1/1	0.13	-1.44	51,51,51,51	0
54	MG	CB	3056	1/1	0.13	-1.45	8,8,8,8	0
54	MG	CC	301	1/1	0.08	-1.45	89,89,89,89	0
54	MG	CB	3034	1/1	0.10	-1.46	7,7,7,7	0
54	MG	DA	1648	1/1	0.14	-1.48	43,43,43,43	0
54	MG	CB	3006	1/1	0.10	-1.54	19,19,19,19	0
54	MG	DA	1605	1/1	0.11	-1.55	76,76,76,76	0
54	MG	CB	3091	1/1	0.09	-1.56	42,42,42,42	0
54	MG	BA	4038	1/1	0.09	-1.57	50,50,50,50	0
54	MG	BA	4055	1/1	0.13	-1.62	27,27,27,27	0
54	MG	DA	1601	1/1	0.06	-1.63	28,28,28,28	0
54	MG	CB	3107	1/1	0.14	-1.66	22,22,22,22	0
54	MG	CB	3033	1/1	0.11	-1.66	33,33,33,33	0
54	MG	CB	3086	1/1	0.10	-1.70	17,17,17,17	0
54	MG	DA	1649	1/1	0.09	-1.73	45,45,45,45	0
54	MG	CB	3015	1/1	0.15	-1.75	9,9,9,9	0
54	MG	DA	1618	1/1	0.09	-1.81	30,30,30,30	0
54	MG	CB	3023	1/1	0.12	-1.82	7,7,7,7	0
54	MG	DA	1636	1/1	0.07	-1.82	43,43,43,43	0
54	MG	CB	3092	1/1	0.11	-1.86	7,7,7,7	0
54	MG	AB	4001	1/1	0.05	-1.86	5,5,5,5	0
54	MG	BA	4041	1/1	0.11	-1.86	54,54,54,54	0
54	MG	CB	3017	1/1	0.10	-1.91	13,13,13,13	0
54	MG	AB	4067	1/1	0.09	-1.94	31,31,31,31	0
54	MG	CB	3025	1/1	0.10	-1.96	27,27,27,27	0
54	MG	AB	4104	1/1	0.09	-1.96	26,26,26,26	0
54	MG	CB	3084	1/1	0.09	-1.99	24,24,24,24	0
54	MG	AB	4070	1/1	0.07	-2.00	20,20,20,20	0
54	MG	AB	4021	1/1	0.13	-2.00	33,33,33,33	0
54	MG	AB	4081	1/1	0.10	-2.01	60,60,60,60	0
54	MG	AB	4009	1/1	0.10	-2.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	1604	1/1	0.12	-2.06	35,35,35,35	0
54	MG	AB	4028	1/1	0.11	-2.08	16,16,16,16	0
54	MG	CB	3050	1/1	0.08	-2.13	45,45,45,45	0
54	MG	CB	3065	1/1	0.08	-2.14	26,26,26,26	0
54	MG	AB	4093	1/1	0.08	-2.15	4,4,4,4	0
54	MG	AB	4102	1/1	0.09	-2.15	63,63,63,63	0
54	MG	CB	3098	1/1	0.07	-2.23	7,7,7,7	0
54	MG	BA	4011	1/1	0.09	-2.25	56,56,56,56	0
54	MG	CB	3024	1/1	0.08	-2.26	21,21,21,21	0
54	MG	AB	4073	1/1	0.11	-2.27	21,21,21,21	0
54	MG	DA	1620	1/1	0.09	-2.30	19,19,19,19	0
54	MG	AE	301	1/1	0.08	-2.34	10,10,10,10	0
54	MG	BA	4014	1/1	0.10	-2.37	44,44,44,44	0
54	MG	DA	1630	1/1	0.10	-2.39	29,29,29,29	0
54	MG	CB	3069	1/1	0.12	-2.39	10,10,10,10	0
54	MG	AB	4030	1/1	0.06	-2.40	34,34,34,34	0
54	MG	AB	4012	1/1	0.07	-2.42	44,44,44,44	0
54	MG	CB	3088	1/1	0.05	-2.43	52,52,52,52	0
54	MG	AB	4072	1/1	0.12	-2.46	44,44,44,44	0
54	MG	AB	4006	1/1	0.11	-2.46	12,12,12,12	0
54	MG	DN	201	1/1	0.09	-2.51	48,48,48,48	0
54	MG	DA	1602	1/1	0.10	-2.58	13,13,13,13	0
54	MG	AB	4084	1/1	0.08	-2.60	21,21,21,21	0
54	MG	BA	4015	1/1	0.08	-2.62	59,59,59,59	0
54	MG	CB	3055	1/1	0.06	-2.65	5,5,5,5	0
54	MG	CB	3001	1/1	0.06	-2.67	9,9,9,9	0
54	MG	AB	4036	1/1	0.08	-2.68	12,12,12,12	0
54	MG	AB	4051	1/1	0.09	-2.76	7,7,7,7	0
54	MG	DA	1631	1/1	0.06	-2.79	22,22,22,22	0
54	MG	CB	3074	1/1	0.10	-2.81	33,33,33,33	0
54	MG	AB	4007	1/1	0.10	-2.84	37,37,37,37	0
54	MG	AB	4086	1/1	0.09	-2.85	39,39,39,39	0
54	MG	BA	4016	1/1	0.07	-2.93	47,47,47,47	0
54	MG	BA	4036	1/1	0.08	-2.95	5,5,5,5	0
54	MG	DA	1661	1/1	0.09	-2.98	13,13,13,13	0
54	MG	DA	1621	1/1	0.10	-3.04	18,18,18,18	0
54	MG	BN	201	1/1	0.13	-3.05	61,61,61,61	0
54	MG	AB	4089	1/1	0.07	-3.07	31,31,31,31	0
54	MG	AB	4037	1/1	0.09	-3.08	25,25,25,25	0
54	MG	CB	3012	1/1	0.07	-3.09	10,10,10,10	0
54	MG	CB	3011	1/1	0.10	-3.14	33,33,33,33	0
54	MG	DA	1650	1/1	0.09	-3.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	1606	1/1	0.08	-3.14	18,18,18,18	0
54	MG	AB	4019	1/1	0.08	-3.15	29,29,29,29	0
54	MG	AB	4058	1/1	0.08	-3.17	20,20,20,20	0
54	MG	CB	3047	1/1	0.06	-3.26	10,10,10,10	0
54	MG	CB	3062	1/1	0.06	-3.30	7,7,7,7	0
54	MG	CB	3057	1/1	0.09	-3.31	7,7,7,7	0
54	MG	AB	4018	1/1	0.04	-3.33	32,32,32,32	0
54	MG	AB	4010	1/1	0.10	-3.36	32,32,32,32	0
54	MG	CB	3003	1/1	0.05	-3.44	8,8,8,8	0
54	MG	BA	4048	1/1	0.07	-3.45	73,73,73,73	0
54	MG	AB	4094	1/1	0.08	-3.45	15,15,15,15	0
54	MG	CB	3013	1/1	0.06	-3.54	14,14,14,14	0
54	MG	CB	3058	1/1	0.08	-3.55	31,31,31,31	0
54	MG	DA	1652	1/1	0.06	-3.55	21,21,21,21	0
54	MG	DA	1655	1/1	0.04	-3.56	12,12,12,12	0
54	MG	AB	4033	1/1	0.12	-3.67	52,52,52,52	0
54	MG	AB	4008	1/1	0.09	-3.69	38,38,38,38	0
54	MG	AB	4035	1/1	0.07	-3.71	39,39,39,39	0
54	MG	CB	3035	1/1	0.06	-3.72	20,20,20,20	0
54	MG	AB	4064	1/1	0.11	-3.73	43,43,43,43	0
54	MG	BA	4052	1/1	0.16	-3.75	33,33,33,33	0
54	MG	DA	1654	1/1	0.06	-3.76	13,13,13,13	0
54	MG	AB	4039	1/1	0.09	-3.85	25,25,25,25	0
54	MG	BA	4044	1/1	0.14	-3.86	86,86,86,86	0
54	MG	AB	4083	1/1	0.13	-3.92	29,29,29,29	0
54	MG	CB	3039	1/1	0.07	-3.94	27,27,27,27	0
54	MG	AB	4106	1/1	0.08	-3.99	9,9,9,9	0
54	MG	AB	4041	1/1	0.07	-4.03	11,11,11,11	0
54	MG	CB	3016	1/1	0.05	-4.04	18,18,18,18	0
54	MG	AB	4046	1/1	0.11	-4.13	26,26,26,26	0
54	MG	BA	4040	1/1	0.07	-4.16	49,49,49,49	0
54	MG	DA	1656	1/1	0.07	-4.41	15,15,15,15	0
54	MG	DA	1643	1/1	0.08	-4.41	70,70,70,70	0
54	MG	AB	4015	1/1	0.09	-4.44	3,3,3,3	0
54	MG	CB	3021	1/1	0.06	-4.45	22,22,22,22	0
54	MG	AB	4068	1/1	0.08	-4.50	21,21,21,21	0
54	MG	DA	1639	1/1	0.10	-4.53	79,79,79,79	0
54	MG	BT	101	1/1	0.25	-4.56	27,27,27,27	0
54	MG	DA	1642	1/1	0.05	-4.89	31,31,31,31	0
54	MG	DA	1633	1/1	0.06	-5.19	3,3,3,3	0
54	MG	AB	4052	1/1	0.09	-5.29	25,25,25,25	0
54	MG	CB	3068	1/1	0.10	-5.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CB	3002	1/1	0.07	-5.32	54,54,54,54	0
54	MG	DA	1640	1/1	0.13	-5.73	17,17,17,17	0
54	MG	BA	4010	1/1	0.07	-5.75	17,17,17,17	0
54	MG	CB	3042	1/1	0.07	-6.21	18,18,18,18	0
54	MG	CB	3046	1/1	0.07	-7.40	29,29,29,29	0
54	MG	AB	4044	1/1	0.05	-7.65	17,17,17,17	0
54	MG	BA	4029	1/1	0.09	-9.22	44,44,44,44	0
54	MG	BA	4018	1/1	0.12	-9.40	64,64,64,64	0
54	MG	CB	3053	1/1	0.10	-16.80	5,5,5,5	0
54	MG	AB	4105	1/1	0.09	-18.20	33,33,33,33	0
54	MG	BA	4058	1/1	0.07	-63.67	78,78,78,78	0
54	MG	BA	4047	1/1	0.10	-91.00	29,29,29,29	0
54	MG	BA	4023	1/1	0.19	-	63,63,63,63	1
54	MG	CB	3102	1/1	0.16	-	17,17,17,17	0
54	MG	DA	1626	1/1	0.20	-	11,11,11,11	1
54	MG	BA	4056	1/1	0.36	-	81,81,81,81	0
54	MG	DA	1628	1/1	0.47	-	33,33,33,33	1
54	MG	DA	1625	1/1	0.16	-	37,37,37,37	1
54	MG	CB	3106	1/1	0.25	-	20,20,20,20	0
54	MG	CB	3100	1/1	0.12	-	43,43,43,43	0
54	MG	DA	1608	1/1	0.36	-	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.