



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:55 PM BST

PDB ID : 4V8N
Title : The crystal structure of agmatidine tRNA-Ile2 bound to the 70S ribosome in the A and P site.
Authors : Voorhees, R.M.; Mandal, D.; Neubauer, C.; Koehrer, C.; RajBhandary, U.L.; Ramakrishnan, V.
Deposited on : 2013-02-13
Resolution : 3.10 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>

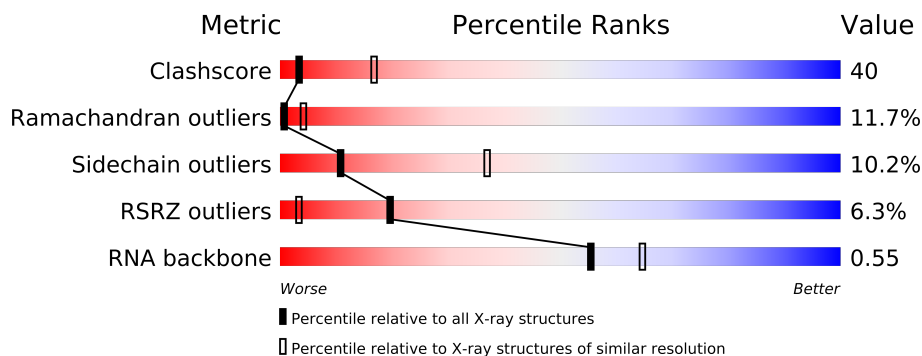
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	

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Mol	Chain	Length	Quality of chain
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	78	
22	AY	78	
22	CV	78	
22	CY	78	
23	AW	78	
23	CW	78	
24	AX	24	
24	CX	24	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	
27	D2	72	

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Mol	Chain	Length	Quality of chain
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	173	
44	DJ	173	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	

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Mol	Chain	Length	Quality of chain
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 298096 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 RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP Q5SHN3
AL	2	VAL	-	EXPRESSION TAG	UNP Q5SHN3
AL	3	ALA	-	EXPRESSION TAG	UNP Q5SHN3
AL	4	LEU	-	EXPRESSION TAG	UNP Q5SHN3
CL	1	MET	-	EXPRESSION TAG	UNP Q5SHN3
CL	2	VAL	-	EXPRESSION TAG	UNP Q5SHN3
CL	3	ALA	-	EXPRESSION TAG	UNP Q5SHN3
CL	4	LEU	-	EXPRESSION TAG	UNP Q5SHN3

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			
13	CM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	AY	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	CV	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	CY	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			

- Molecule 23 is a RNA chain called A-SITE TRNA ILE2 AGMATIDINE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	78	Total	C	N	O	P	0	0	0
			1659	741	295	546	77			
23	CW	78	Total	C	N	O	P	0	0	0
			1659	741	295	546	77			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			257	118	54	74	11			
24	CX	12	Total	C	N	O	P	0	0	0
			257	118	54	74	11			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
29	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			
30	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
31	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
32	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
35	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
43	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	131	Total	C	N	O	0	0	1
			651	390	131	130			
44	DJ	131	Total	C	N	O	0	0	1
			651	390	131	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
45	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
46	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
47	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			
48	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
49	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
50	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
51	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
52	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
53	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
54	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
56	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
57	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

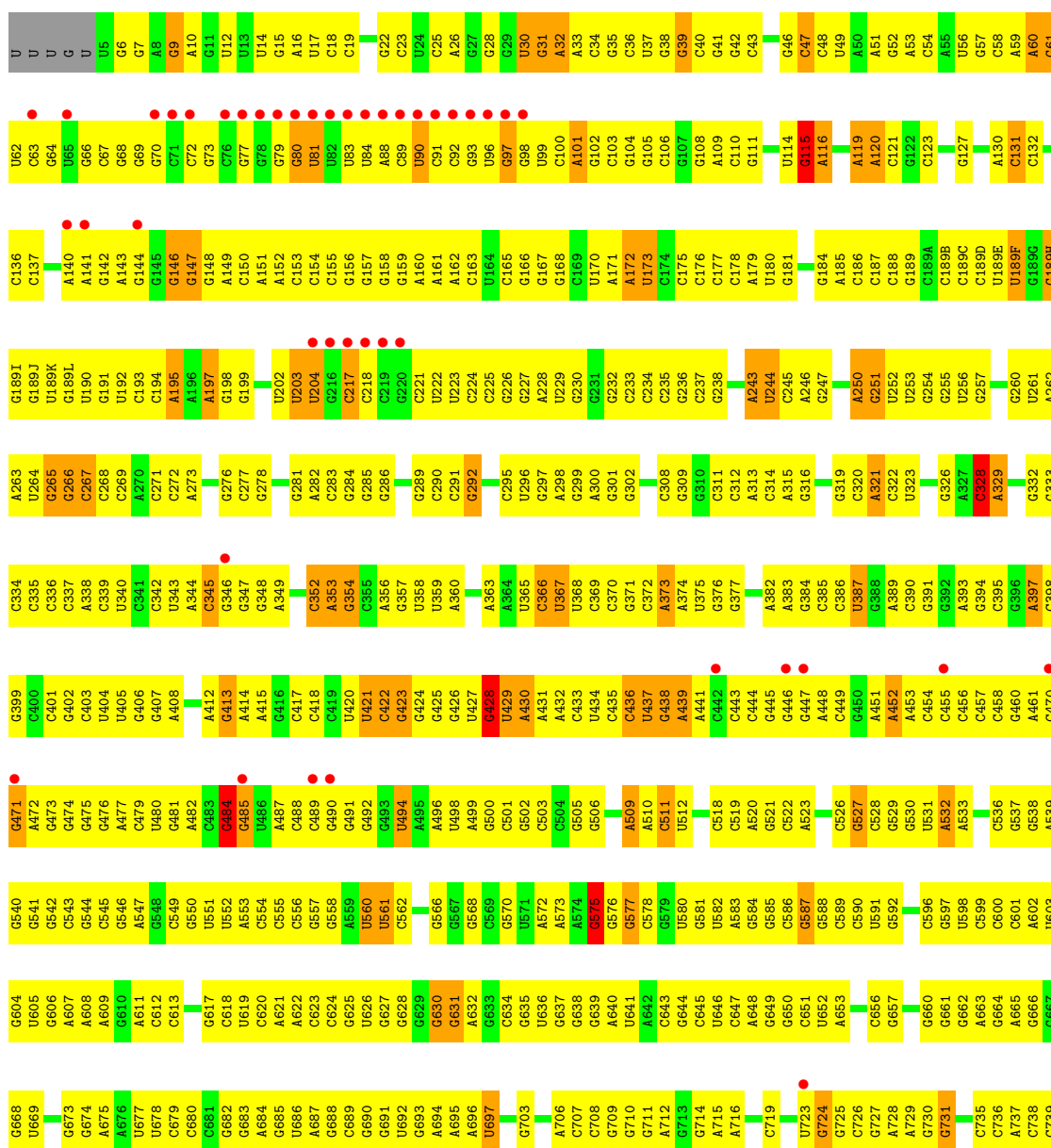
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CN	1	Total	Zn	0	0
			1	1		
58	AD	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	AN	1	Total	Zn	0	0
			1	1		

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: 16S rRNA

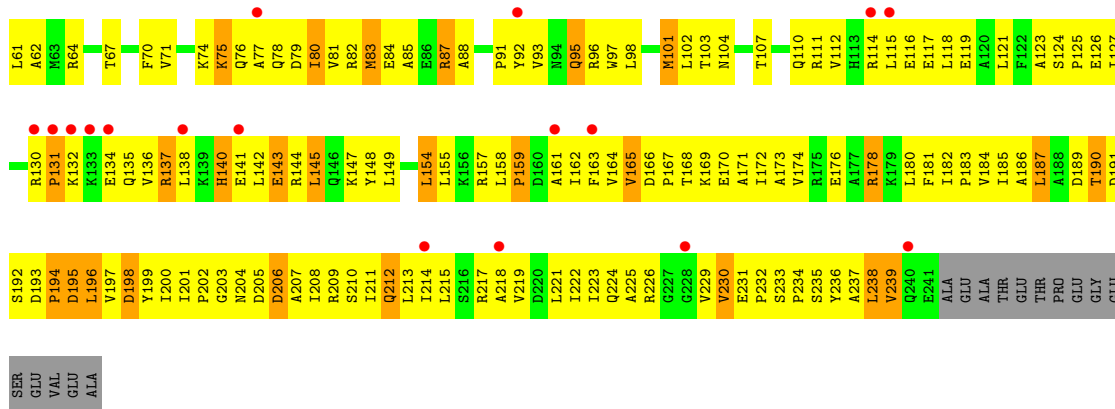
Chain AA: 





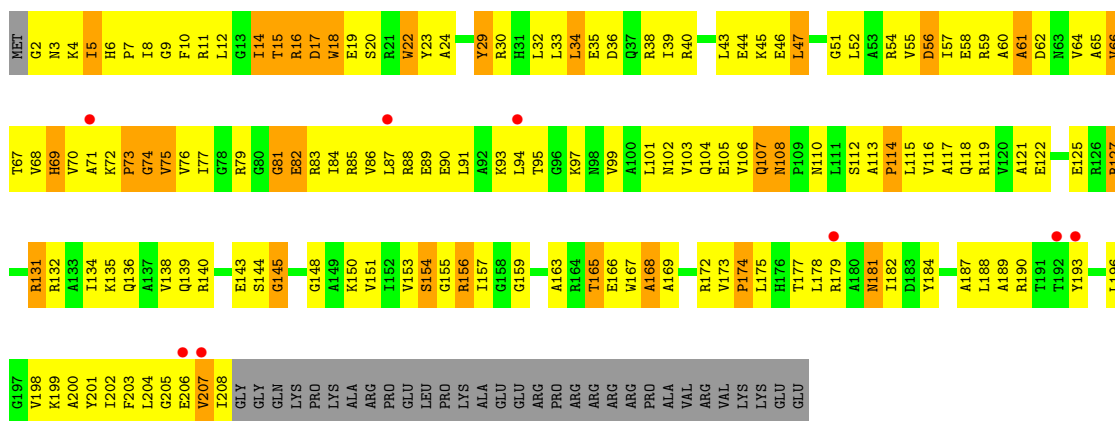






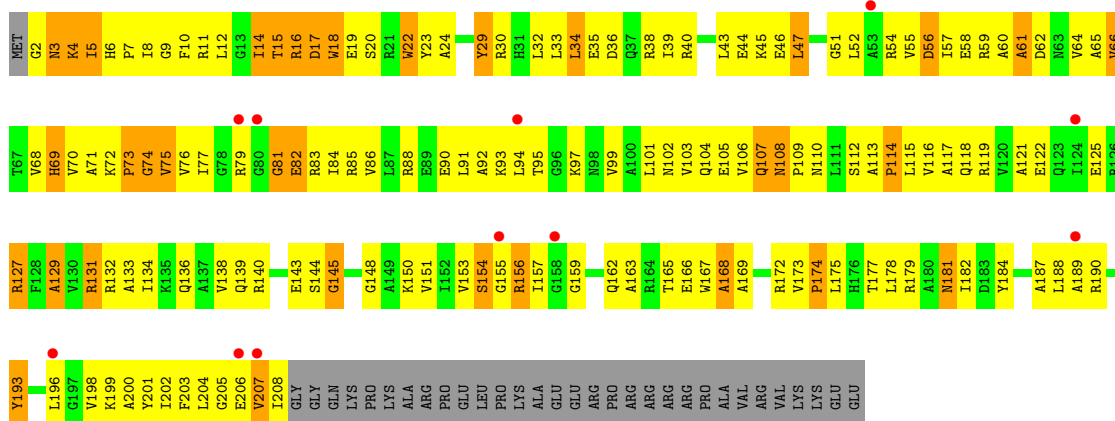
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:

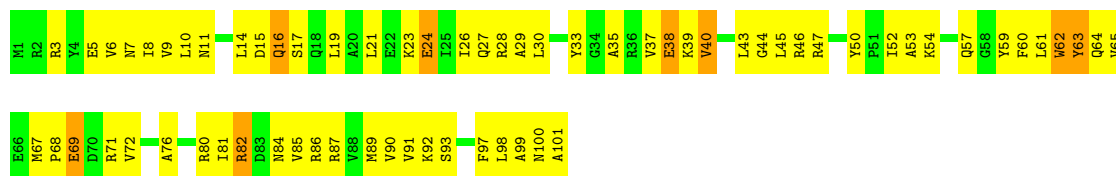


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



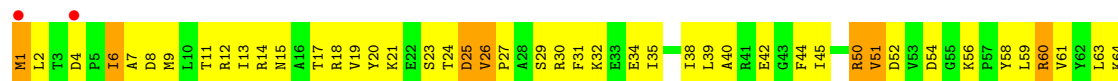
Chain AF:





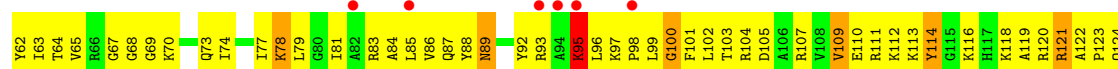
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



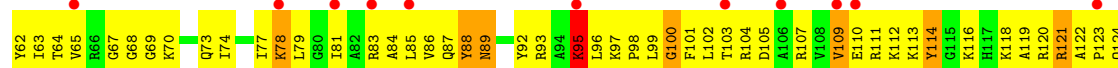
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



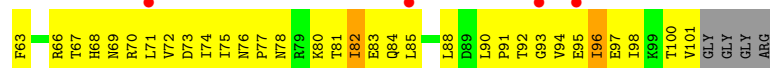
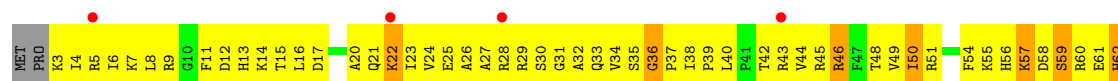
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



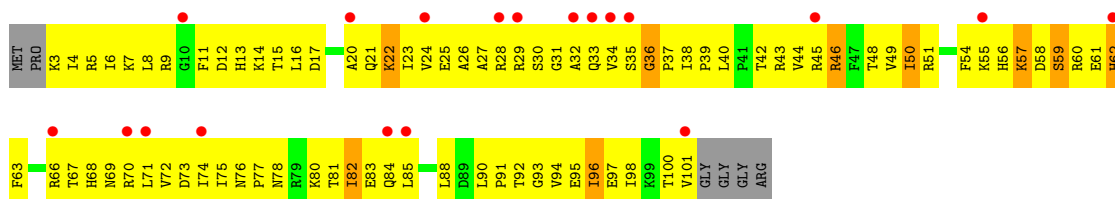
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



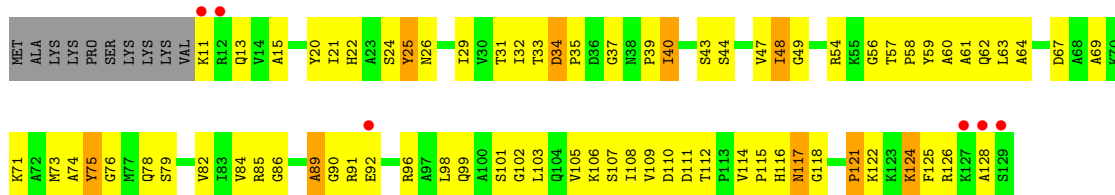
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ: 



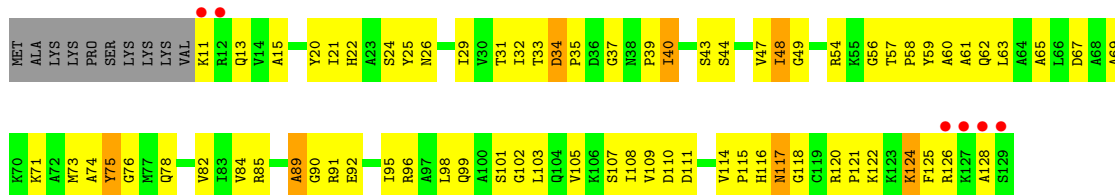
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK: 



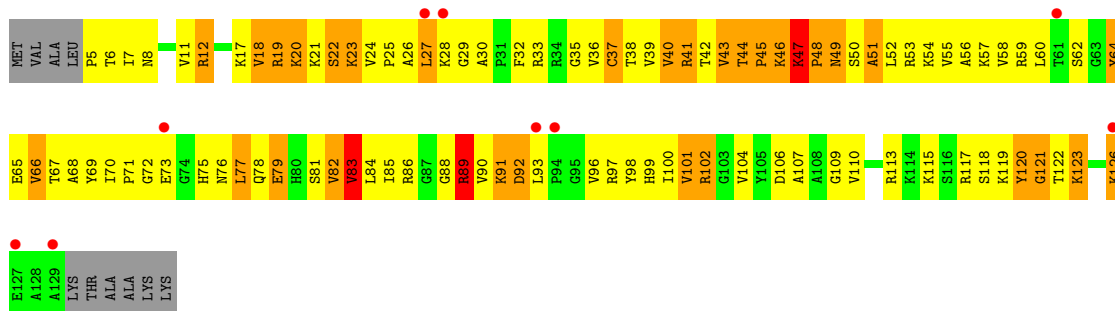
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK: 



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL: 



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

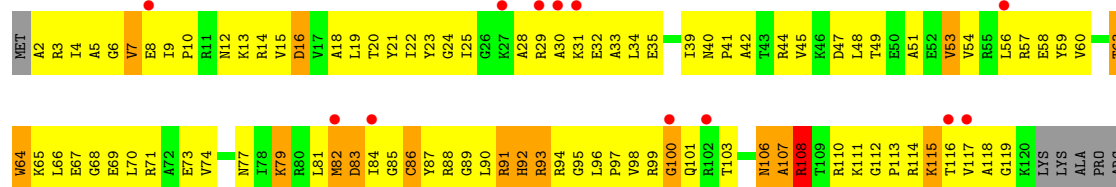
Chain CL: 



LYS
THR
ALA
ALA
LYS
LYS

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

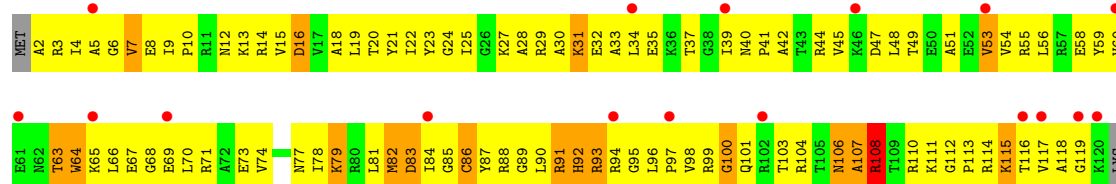
Chain AM:



LYS

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



LYS
ALA
PRO
ARG
LYS

• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



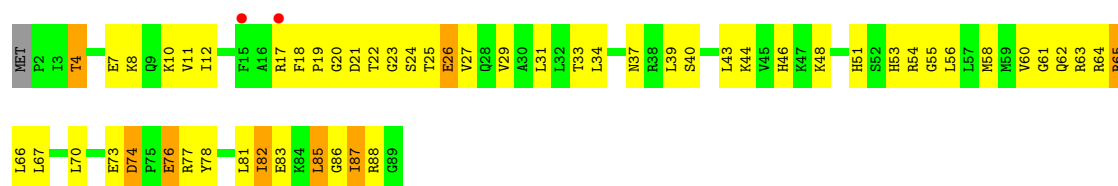
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



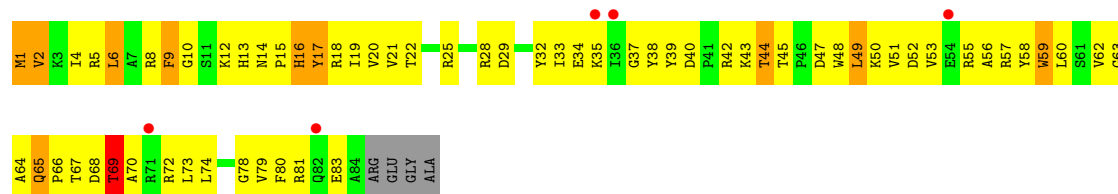
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



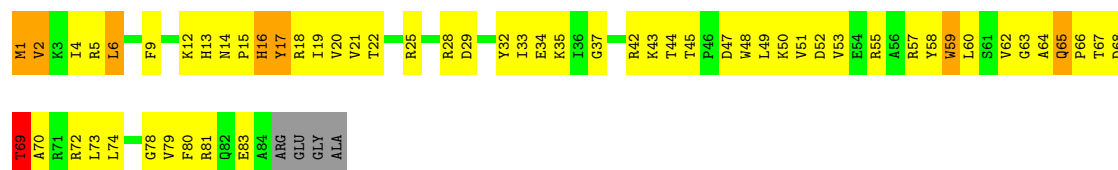
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



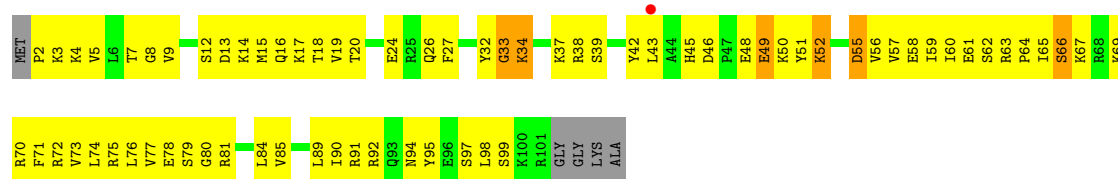
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



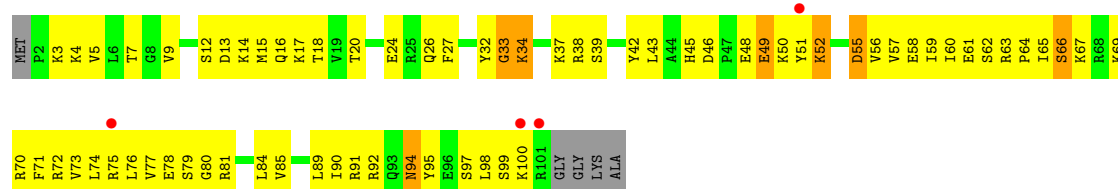
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



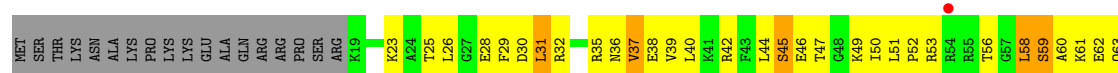
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



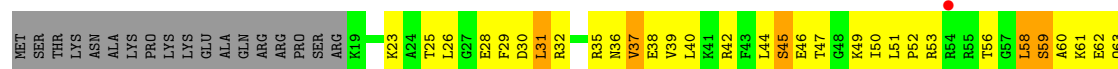
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



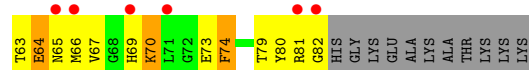
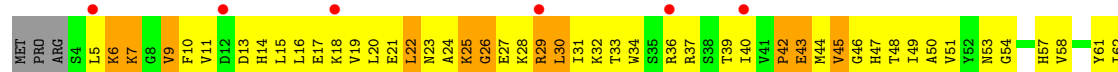
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



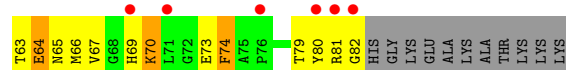
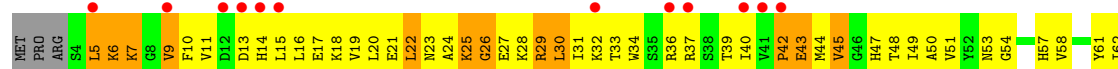
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



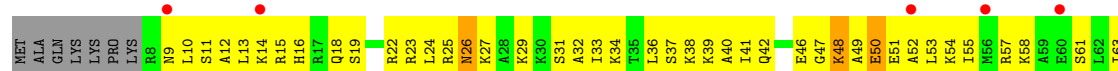
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

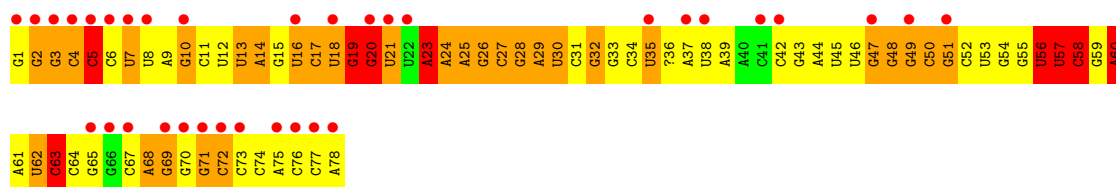
Chain AT:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

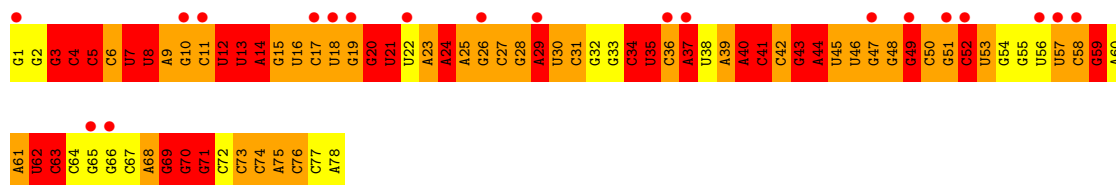
Chain CT:





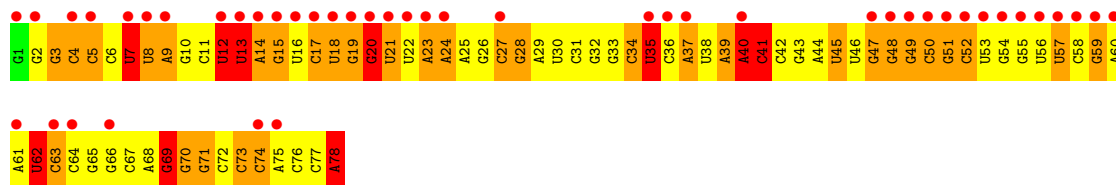
• Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

Chain AW:



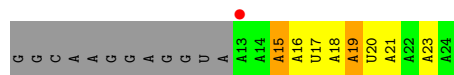
• Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

Chain CW:



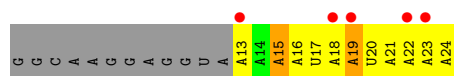
• Molecule 24: MRNA

Chain AX:



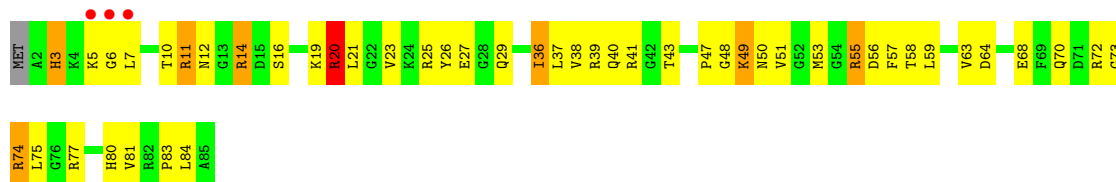
• Molecule 24: MRNA

Chain CX:



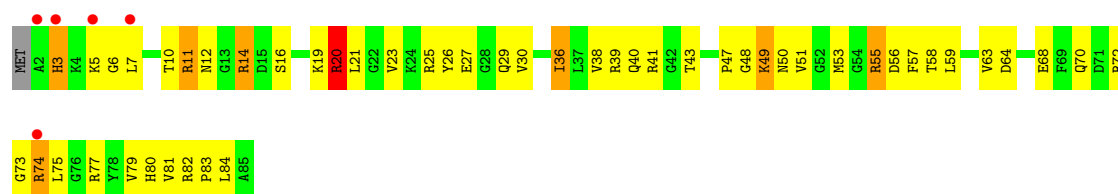
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



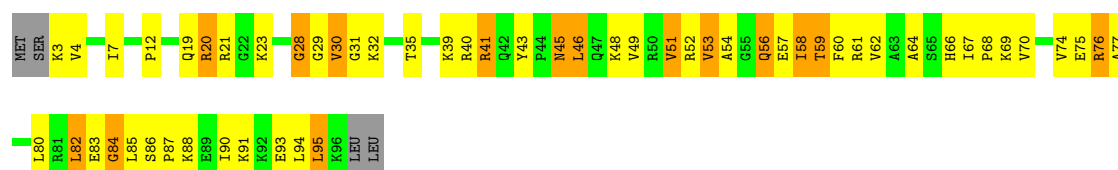
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



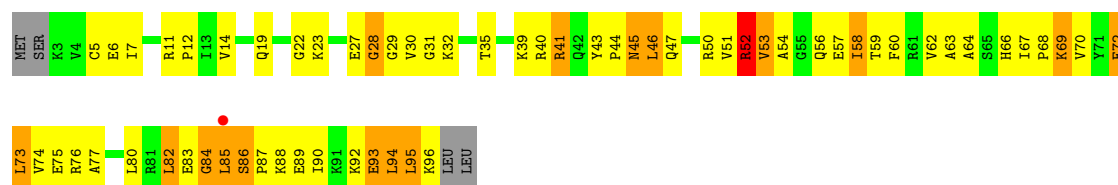
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



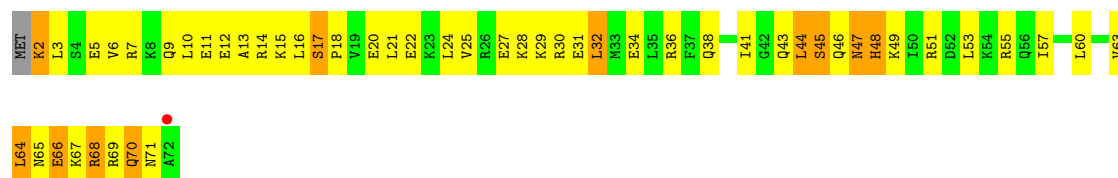
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



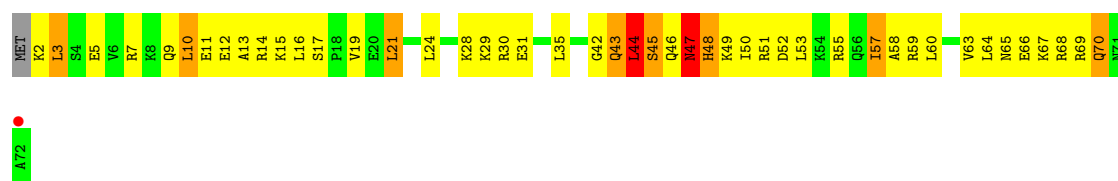
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



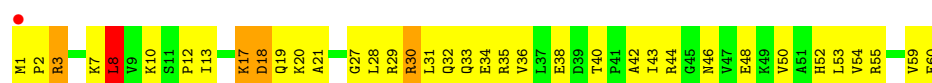
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



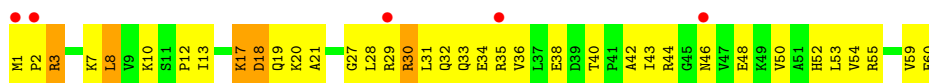
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



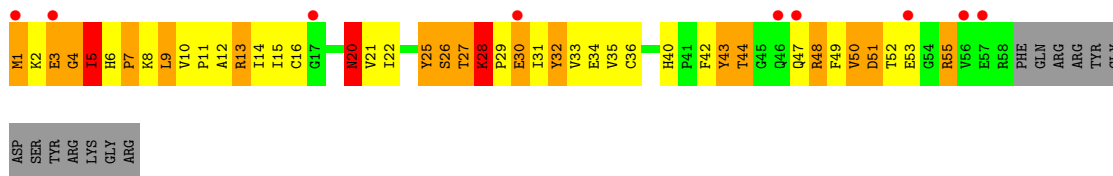
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



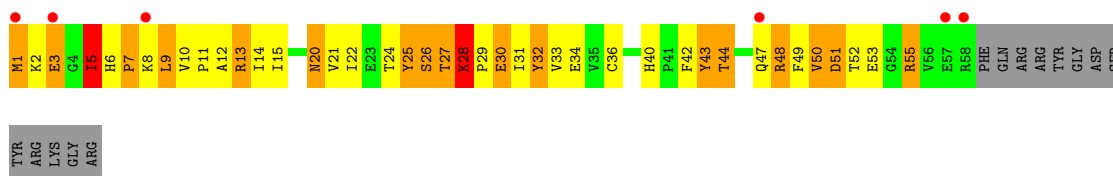
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



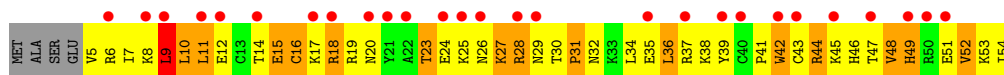
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



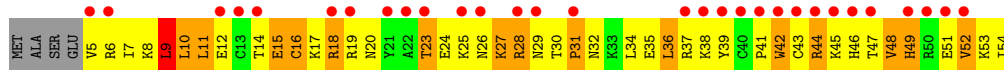
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:



• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7: 



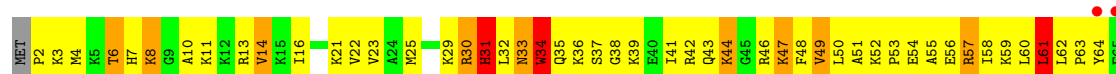
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7: 



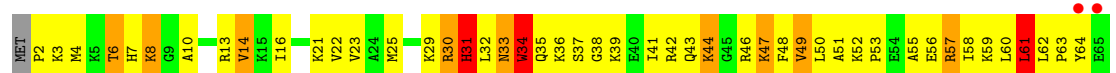
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



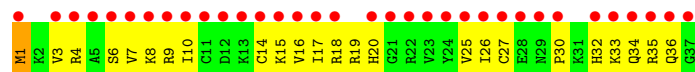
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



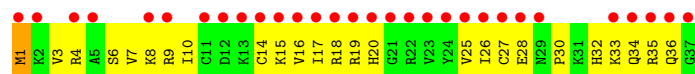
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



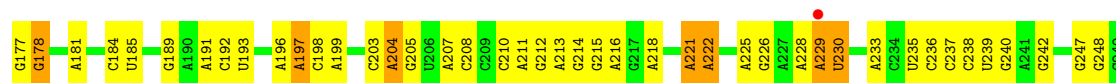
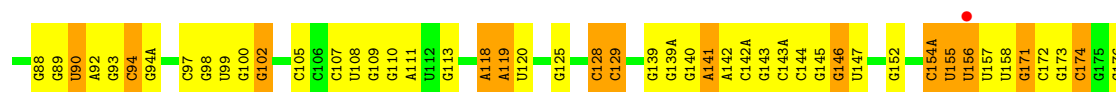
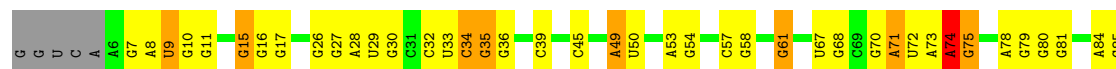
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

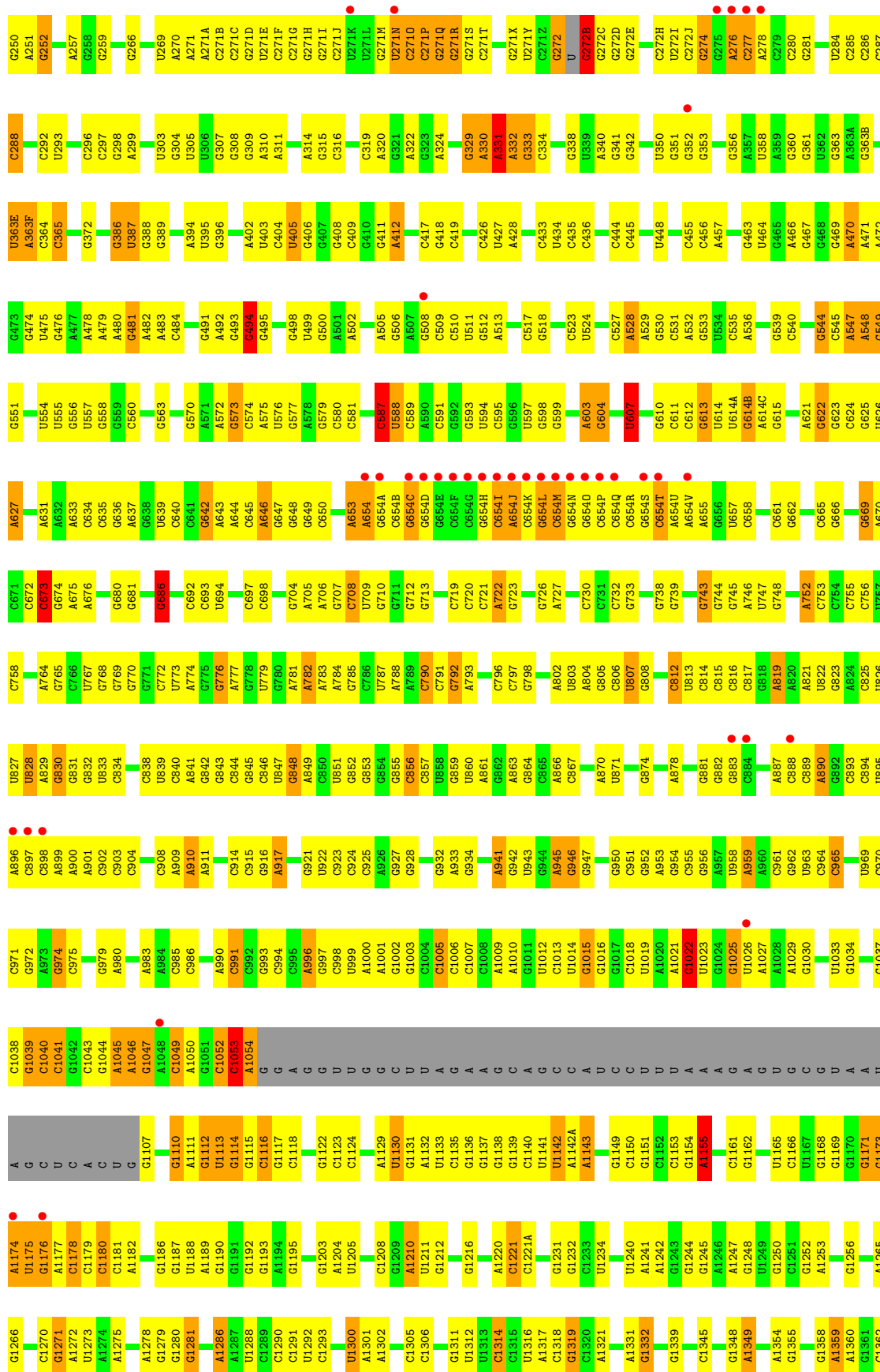
Chain D9: 



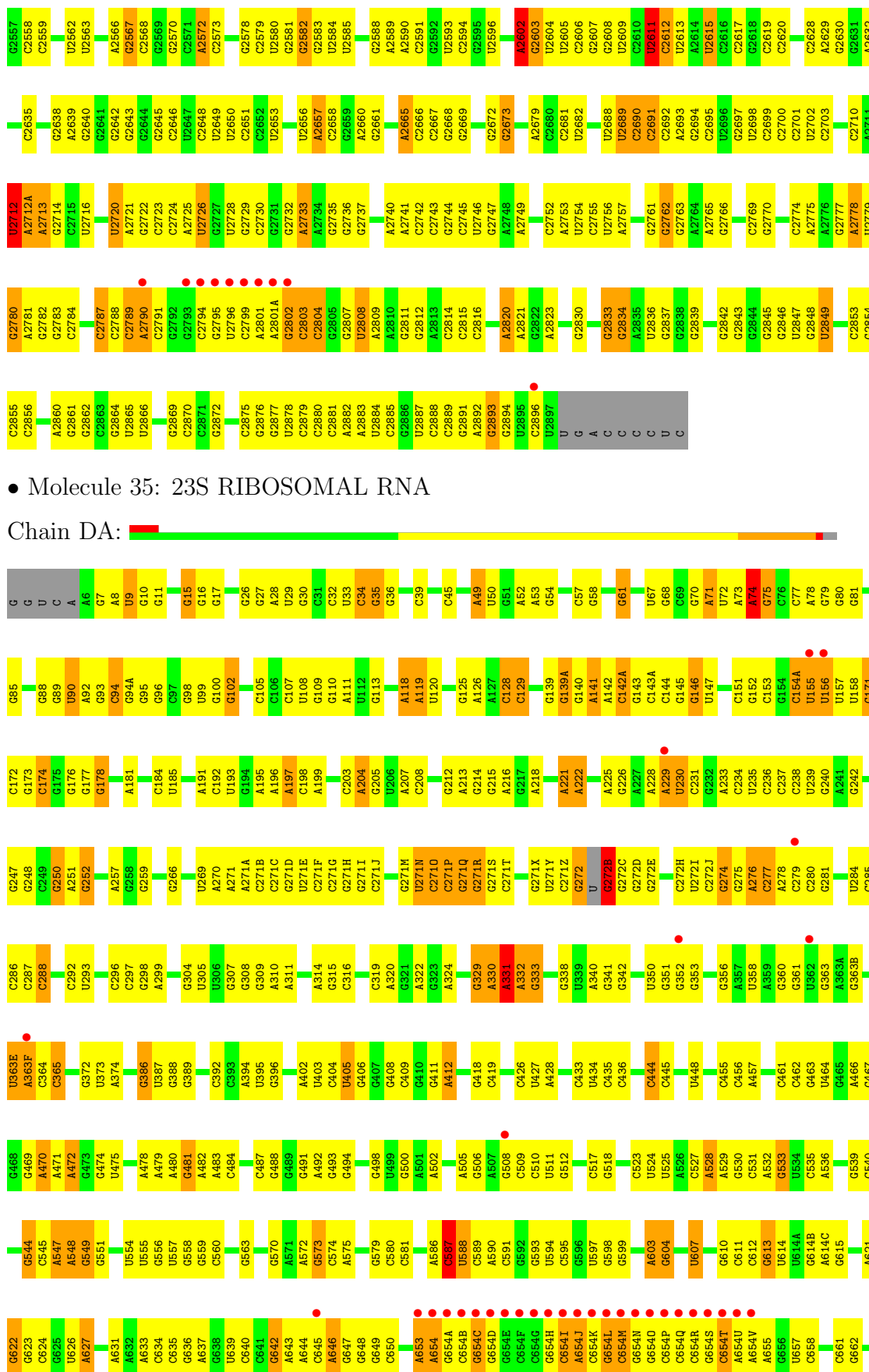
- Molecule 35: 23S RIBOSOMAL RNA

Chain BA: 





G2481	G2482	G2483	G2484	A2488	A2411	G2405	A2327	C2261	C2175	G2115	C2040	U1956	G1863	A1786	G1696	G1519	G1448	C1363
G2482	G2483	G2484	G2485	A2488	A2411	G2405	A2327	C2261	A2176	G2116	C2041	C1957	G1864	A1787	G1697	G1520	G1449	C1364
G2483	G2484	G2485	G2486	A2488	A2411	G2405	A2327	C2261	C2177	G2117	C2042	C1958	G1865	A1788	G1698	G1521	G1450	A1365
G2484	G2485	G2486	G2487	A2488	A2411	G2405	A2327	C2261	C2178	G2118	C2043	C1959	G1866	A1789	G1699	G1522	G1451	G1366
A2488	A2411	G2405	A2327	G2261	U2180	C2050	C2043	C1964	C1965	G1876	A1791	G1701	A1528	U1502	U1453	U1453	G1459	G1369
U2491	U2492	U2493	U2494	A2418	G2341	A2051	A2052	A1966	A1967	G1877	U1794	G1702	A1528A	A1603	G1459	A1460	U1372	A1373
U2492	U2493	U2494	U2495	A2419	G2342	A2052	A2053	A1968	A1969	G1878	C1795	G1703	A1529	C1607	A1461	U1373	G1374	G1375
U2493	U2494	U2495	U2496	A2420	G2343	A2053	A2054	A1970	A1971	G1881	U1796	G1704	A1530	A1608	G1462	U1374	G1375	G1376
C2498	C2499	U2500	U2501	U2418	G2344	A2054	A2055	A1972	A1973	G1882	U1797	G1705	A1531	A1609	C1464	U1375	G1376	G1377
C2499	U2500	U2501	U2502	U2419	G2345	A2055	A2056	A1973	A1974	G1883	U1798	G1706	A1532	A1610	U1376	U1377	A1378	A1379
U2500	U2501	U2502	U2503	U2420	G2346	A2056	A2057	A1974	A1975	G1884	U1799	G1707	A1533	A1611	C1467	A1468	A1380	A1381
U2501	U2502	U2503	U2504	A2425	C2347	A2057	A2058	A1975	A1976	G1885	U1800	G1710	A1534	A1612	C1468	A1469	A1382	A1383
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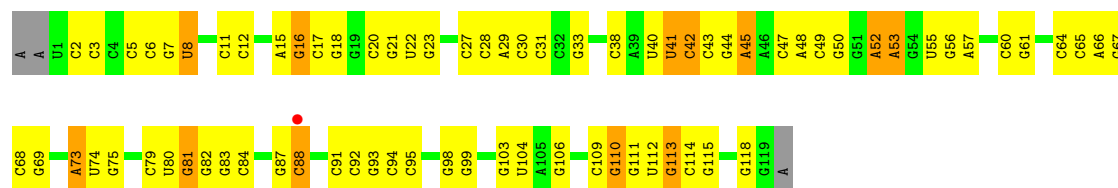


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G1740	C1642	C1546	U1481	C1402	C1318	G1243	A1155	A	U1023	C956	C989	C825	C756	A670
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G1742		C1548	G1484	C1404	C1320	G1245	C1161	G	U1025	U958	C992	U827	C758	G672
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G1746	G1653	A1554	G1487	C1407	C1331	A1248	U1165	U	A1028	C962	U895	G830	A764	A675
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G1748	G1656	G1559	G1491	G1410	G1337	C1251	G1168	U	U1033	C965	A899	U833		G680
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G1750	C1658	C1564	C1493	G1412	G1339	A1253	G1170	A	U1037	U969	A901	G835	G769	
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C1672	U1672	C1574	C1502	A1422	A1349	A1265	C1179	U	A1045	A980	A911	G844	G777	U694
U1673	U1673		U1503	G1423	U1349	G1266	G1180		A1046			G845	U779	G704
G1674	G1674	C1577	C1504	G1424	A1354	G1267	C1181	G	A1047	A983	C914	C846	A782	A705
C1675	C1675	U1578	C1505	C1430	G1355	C1270	A1182		U1048	A984	C915	U847	A783	A706
		U1579	U1580	U1431	G1358	G1271	G1186		G1049	C985	C916	C848	A784	G707
G1678	G1678	A1581	A1507	C1432	A1359	A1272	G1187		A1050	C986	A917	C849	G785	U709
G1681	G1681	C1582	C1508	U1433	G1360	G1273	U1188		G1051		A918		G786	G710
C1682	C1682	A1583	C1509	A1434	G1361	A1274	A1189		C1052	A990	C921	G852	C787	G711
G1683	C1683	A1584	A1509A	U1435	C1362	A1275	G1190		C1053	C991	U922	G853	A788	G712
		U1436	U1436	G1439	C1363	A1276	G1191		A1054	C992	C923	G854	A789	G713
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		G1515	G1516	G1442	A1368	G1280	A1194		G	A996	A926	U858	A793	A718
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A1698	A1698			U1453	C1375	A1287	G1209		C	G1002	G934	C865	A802	G726
				U1453	C1376	U1288	G1210		U	G1003	C935	A866	U803	A727
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U1701	U1701	A1528	A1528A	G1459	U1378	C1291	A1212		A	C1005	U937		G805	
G1702	G1702	U1529	G1530	A1460	A1379	U1292	G1212		G	C1006	G938	A870	C730	
G1703	G1703	C1530	C1531	G1461	G1380	C1293	G1215		A	C1007	U941	U871	U807	C736
G1704	G1704			U1464	A1384	U1300	G1216		G	C1008	G942	G874	G808	C737
U1706	U1706	C1532	C1533	C1464	G1385	A1301	G1216		A	A1009	U943			C738
		U1534	U1535	C1467	C1386	A1302	G1220		C	A1010	U944	C812	G739	
U1709	U1709	A1614	A1614	C1468	C1387	G1305	A1221		A	G1011	A945	U877	U813	G743
C1711	C1711	C1536	C1537	A1469	G1388	C1306	C1221A		G	U1012	C946	A978	C814	G744
G1712	G1712	U1537	G1538	A1470	G1389	C1306	U1142A		C	C1013	C947	G879	C815	G745
U1713	U1713			A1471	U1391	G1311	G1231		C	U1014	G948	G880	C816	G746
G1714	G1714			A1472	A1395	G1312	G1232		A	G1015	C949	G881	C817	A746
G1717	G1717	U1539	U1540	A1473	U1396	C1233	C1232		U	G1016	G950	G882	G818	A747
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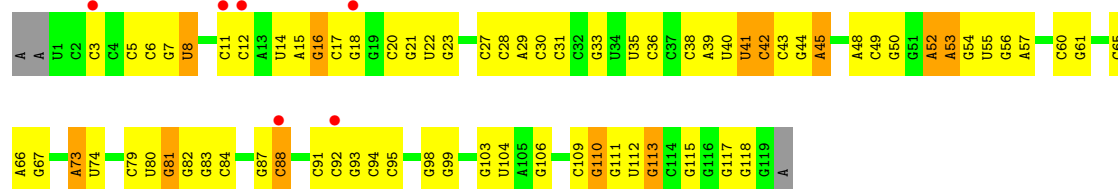
● Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



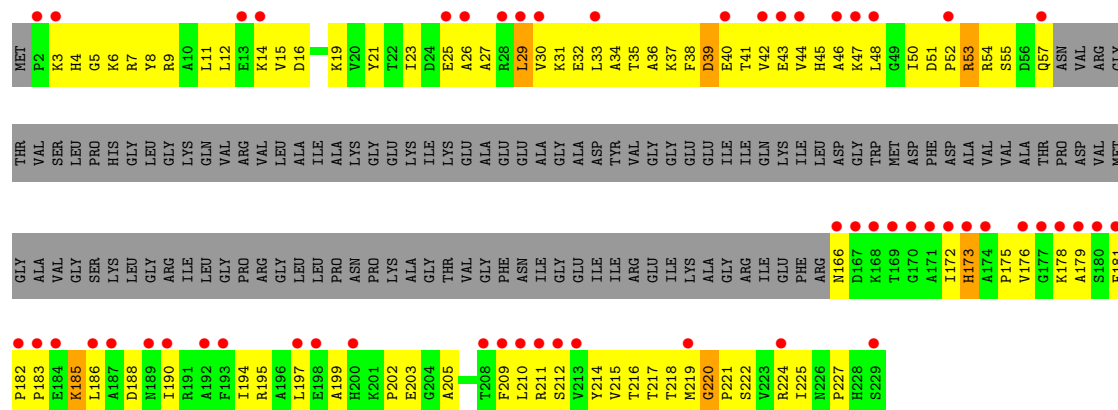
● Molecule 36: 5S RIBOSOMAL RNA

Chain DB:



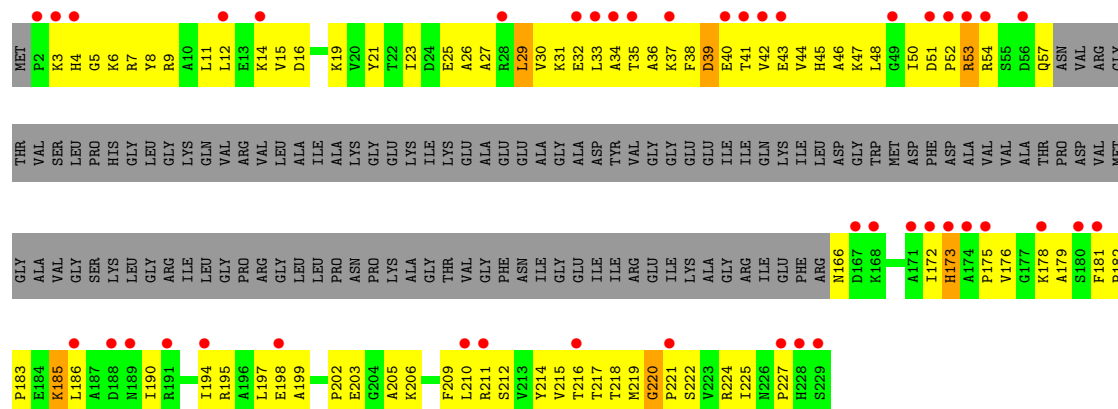
● Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC:



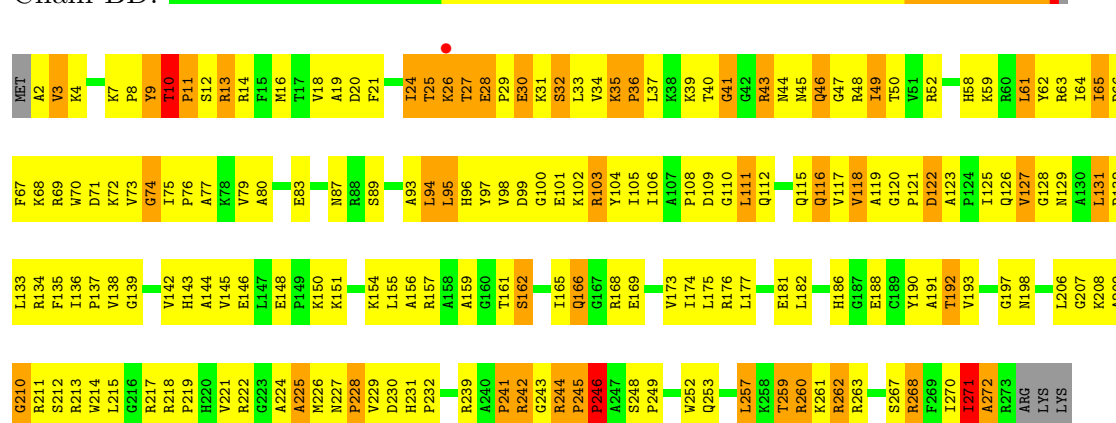
● Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain DC:



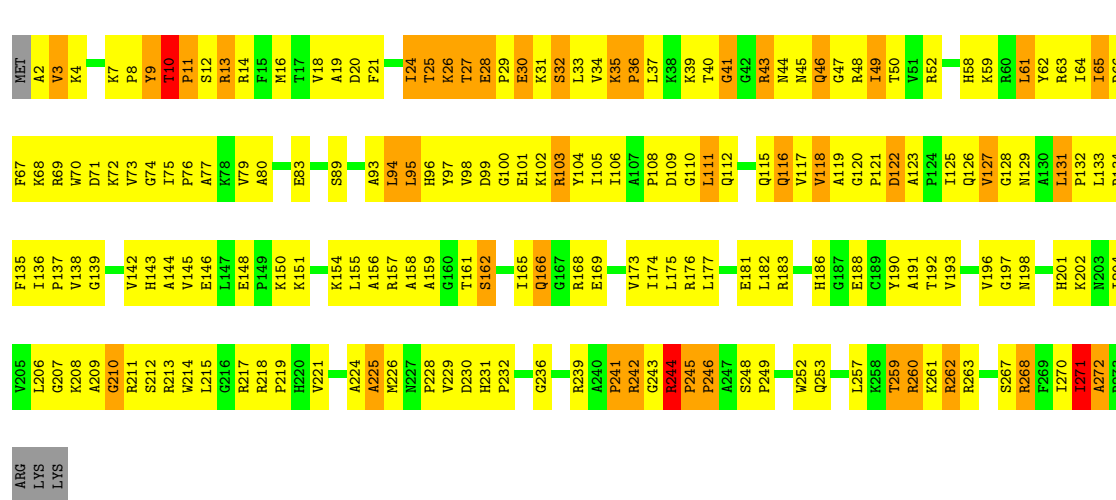
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:



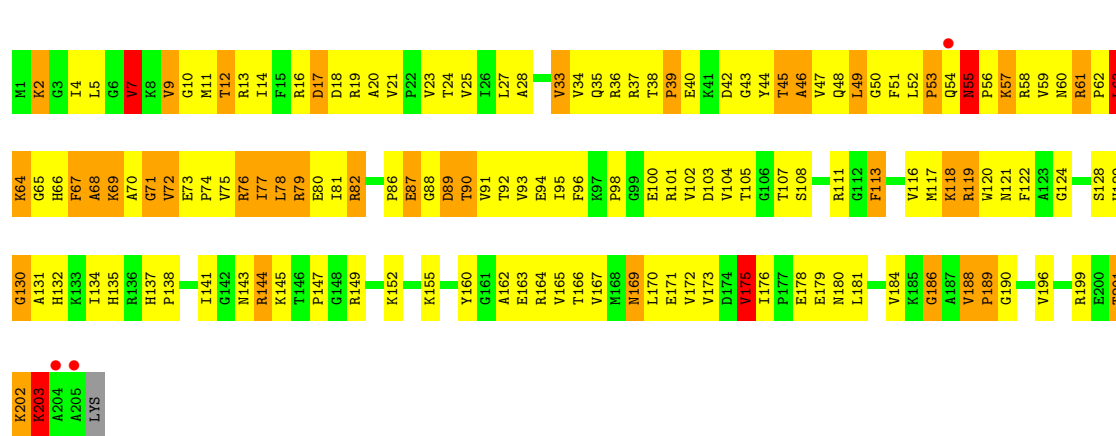
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:



- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



- Molecule 39: 50S RIBOSOMAL PROTEIN L3

K203	K64	H132	H1
A204	G65	K153	K2
A205	H66	I134	G3
LVS	F67	H135	I4
	R136	H137	L5
	K69	P138	G6
	A70		V7
	G71		K8
	V72	I141	V9
	E73	G142	G10
	P74	N143	M11
	V75	R144	T12
	R16	K145	R13
	I77	T146	F15
	L78	P147	I14
	R79	G148	R16
	E80	R149	D17
	T81	Y150	D18
	R82	Y151	R19
			A20
	P86	K154	V21
	E87	K155	P22
	G88		V23
	D89	Y160	T24
	T90	G161	V25
	V91	A162	I26
	E92	E163	L27
	R93	R164	
	E94	V165	
	T95	T166	
	P96	V167	
	K97	M168	
	P98	N169	K33
	G99	L170	V34
	E100	E171	Q35
	R101	V172	R36
	V102	V173	R37
	D103	D174	T38
	V104	V175	P39
	T105	I176	E40
	G106	P177	K41
	T107	E178	D42
	S108	E179	G43
		M180	Y44
	R111	L181	T45
			A46
	V116	V184	V47
	M117	K185	Q48
	K118	G186	L49
	R119	A187	G50
	W120	V188	F51
	N121	P189	L52
	F122	G190	P53
	A123		Q54
	G124		K55
			P56
			K57
			R58
			V59
			N60
			R61
			P62
			K63

T158	G159	M160	E161	L162	V163	R164	A165	I166	P167	R168	M169	W170	T171	V172	G173	L174	T175	L176	A177	P178	E179	G180	L181	M182	V183	Y184	D185	I186	V187	R188	G189	L190	T191	L192	V193	M194	D195	L196	D197	A198	V199	E200	V201	F202	G203	T204	G205	G206	GLU	ALA				
R74	H75	I82	F83	V84	G85	G86	G87	V88	V89	F90	R95	T100	L101	P102	K103	K104	V105	R106	K107	K108	G109	A110	A111	M112	A113	D116	R119	K122	L123	L124	L125	V126	E127	A128	F129	V132	M133	G134	K135	T136	W142	E145	L148	D149	G150	L155	L156	V157						
M1	K2	E3	V4	A5	V6	Y7	Q8	I9	P10	V11	L12	S13	P14	S15	G16	R17	R18	E19	L20	A21	A22	D23	L24	P25	A26	I28	H31	L32	L33	W34	E35	V36	V37	R38	W39	Q40	K43	R46	A58	Y59	S60	G61	R62	K63	I64	W65	P66	Q67	K68	H69	T70	G71	R72	A73

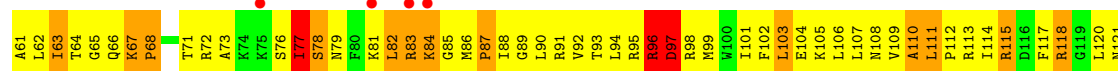
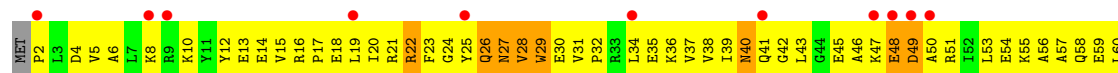
L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L69
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Gene	Chromosome	Position (kb)	Strand	Transcript	Feature
Q66	1	100	+	Q66	5'UTR
P67	1	100	+	P67	5'UTR
P68	1	100	+	P68	5'UTR
A69	1	100	+	A69	5'UTR
V70	1	100	+	V70	5'UTR
T71	1	100	+	T71	5'UTR
R72	1	100	+	R72	5'UTR
A73	1	100	+	A73	5'UTR
K74	1	100	+	K74	5'UTR
K75	1	100	+	K75	5'UTR
S76	1	100	+	S76	5'UTR
V77	1	100	+	V77	5'UTR
S78	1	100	+	S78	5'UTR
M79	1	100	+	M79	5'UTR
F80	1	100	+	F80	5'UTR
K81	1	100	+	K81	5'UTR
L82	1	100	+	L82	5'UTR
R83	1	100	+	R83	5'UTR
K84	1	100	+	K84	5'UTR
G85	1	100	+	G85	5'UTR
X86	1	100	+	X86	5'UTR
P87	1	100	+	P87	5'UTR
L88	1	100	+	L88	5'UTR
G89	1	100	+	G89	5'UTR
L90	1	100	+	L90	5'UTR
R91	1	100	+	R91	5'UTR
V92	1	100	+	V92	5'UTR
T93	1	100	+	T93	5'UTR
L94	1	100	+	L94	5'UTR
R95	1	100	+	R95	5'UTR
X96	1	100	+	X96	5'UTR
D97	1	100	+	D97	5'UTR
R98	1	100	+	R98	5'UTR
M99	1	100	+	M99	5'UTR
W100	1	100	+	W100	5'UTR
E104	1	100	+	E104	5'UTR
K105	1	100	+	K105	5'UTR
L106	1	100	+	L106	5'UTR
L107	1	100	+	L107	5'UTR
X108	1	100	+	X108	5'UTR
V109	1	100	+	V109	5'UTR
A110	1	100	+	A110	5'UTR
L111	1	100	+	L111	5'UTR
P112	1	100	+	P112	5'UTR
R113	1	100	+	R113	5'UTR
T114	1	100	+	T114	5'UTR
R115	1	100	+	R115	5'UTR
D116	1	100	+	D116	5'UTR
F117	1	100	+	F117	5'UTR
R118	1	100	+	R118	5'UTR
F122	1	100	+	F122	5'UTR
M123	1	100	+	M123	5'UTR
S124	1	100	+	S124	5'UTR
F125	1	100	+	F125	5'UTR
D126	1	100	+	D126	5'UTR
G127	1	100	+	G127	5'UTR
R128	1	100	+	R128	5'UTR
L129	1	100	+	L129	5'UTR
P2	2	100	+	P2	5'UTR
L3	2	100	+	L3	5'UTR
D4	2	100	+	D4	5'UTR
V5	2	100	+	V5	5'UTR
A6	2	100	+	A6	5'UTR
L7	2	100	+	L7	5'UTR
K8	2	100	+	K8	5'UTR
R9	2	100	+	R9	5'UTR
Y11	2	100	+	Y11	5'UTR
Y12	2	100	+	Y12	5'UTR
E13	2	100	+	E13	5'UTR
E14	2	100	+	E14	5'UTR
V15	2	100	+	V15	5'UTR
R16	2	100	+	R16	5'UTR
P17	2	100	+	P17	5'UTR
E18	2	100	+	E18	5'UTR
L19	2	100	+	L19	5'UTR
L20	2	100	+	L20	5'UTR
R21	2	100	+	R21	5'UTR
R22	2	100	+	R22	5'UTR
N27	2	100	+	N27	5'UTR
V28	2	100	+	V28	5'UTR
W29	2	100	+	W29	5'UTR
E30	2	100	+	E30	5'UTR
V31	2	100	+	V31	5'UTR
P32	2	100	+	P32	5'UTR
K36	2	100	+	K36	



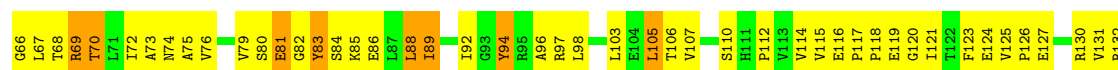
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



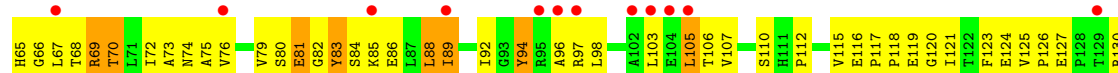
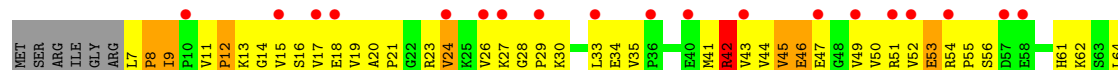
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



• Molecule 42: 50S RIBOSOMAL PROTEIN L6

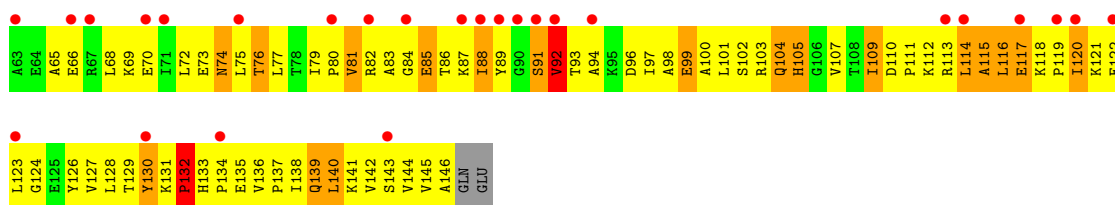
Chain DH:



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

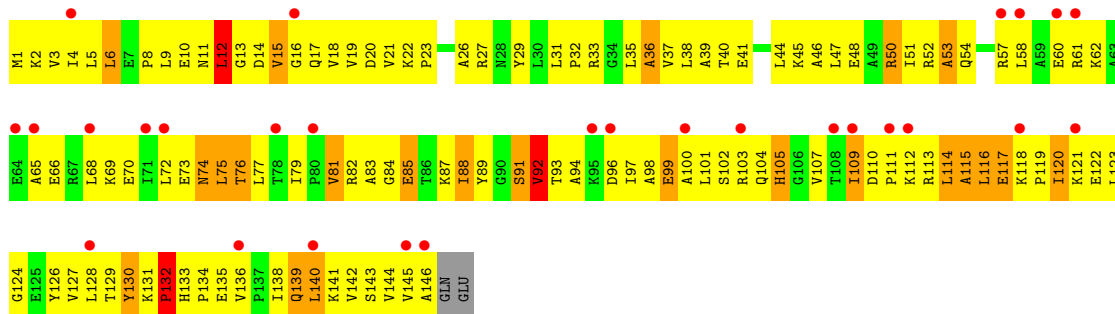
Chain BI:





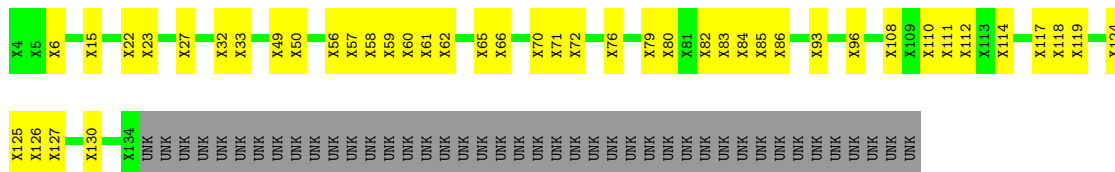
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain DI:



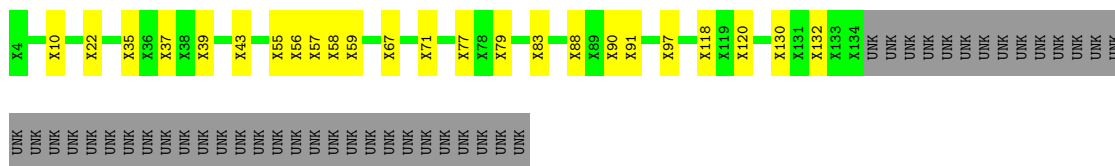
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



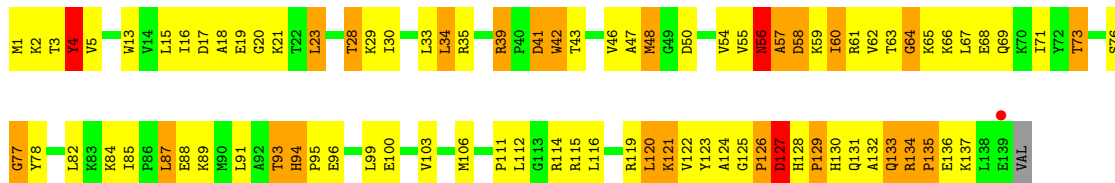
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



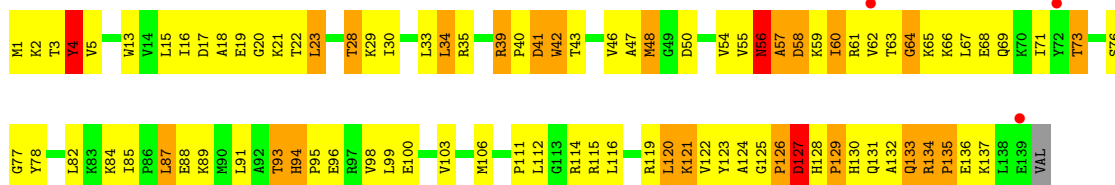
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:



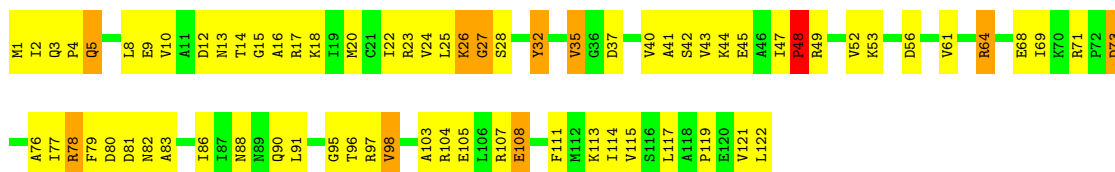
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain DN:



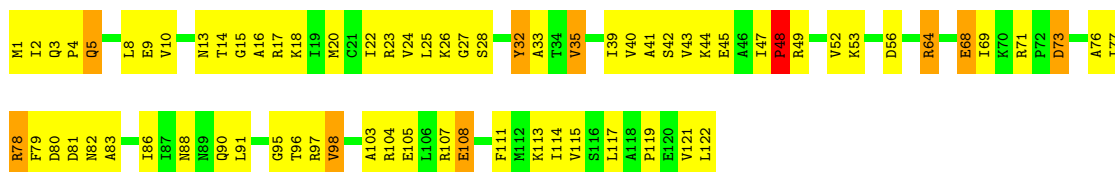
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



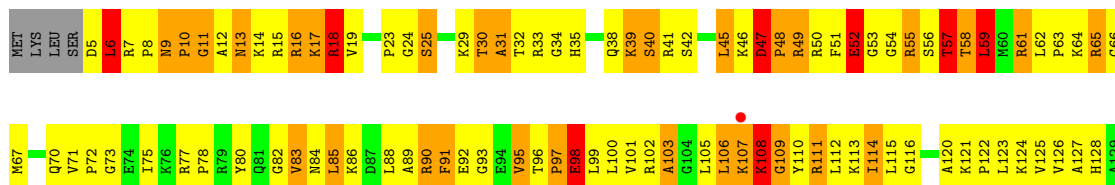
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain DO:



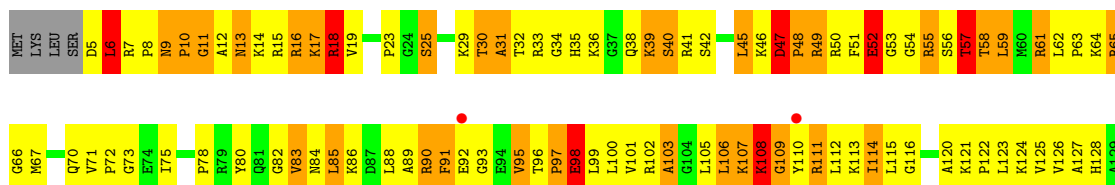
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain BP:



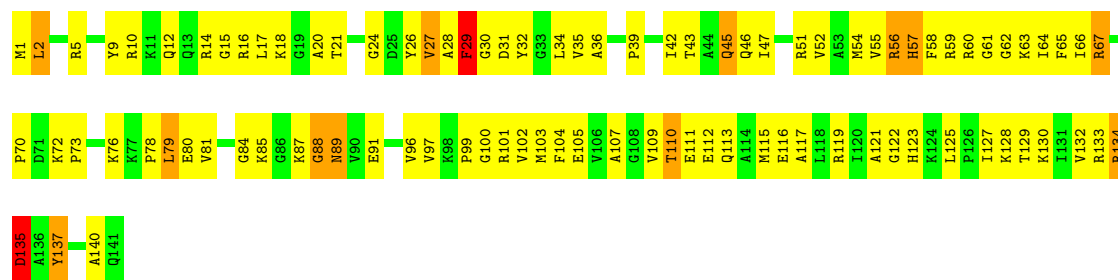
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain DP:



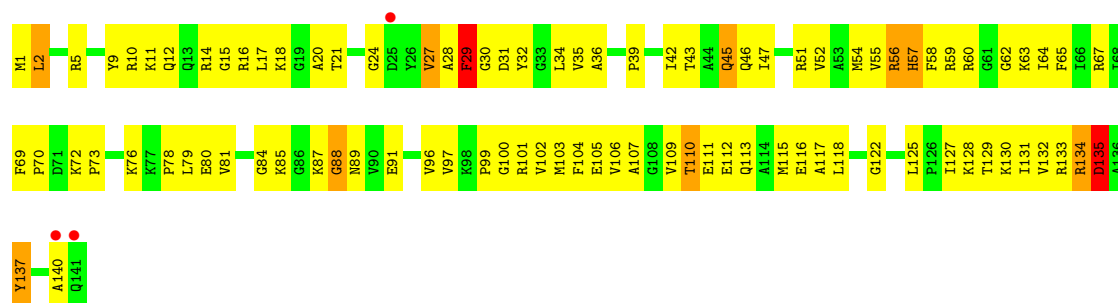
- Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



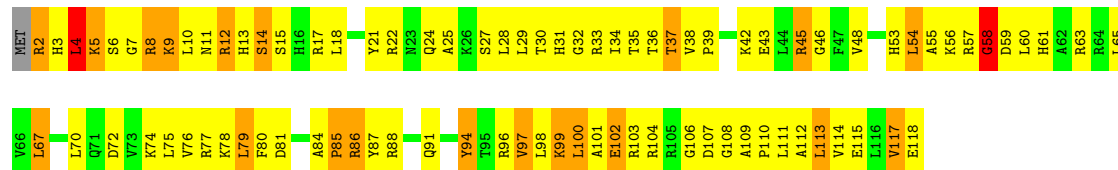
- Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



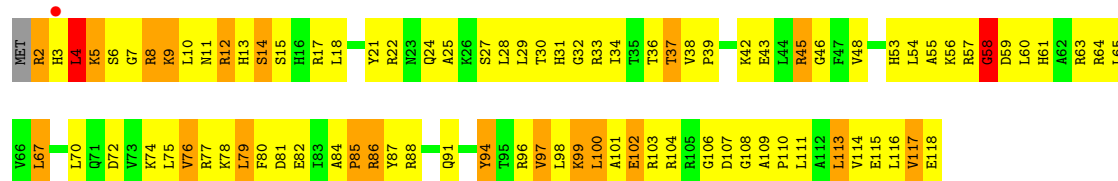
- Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:



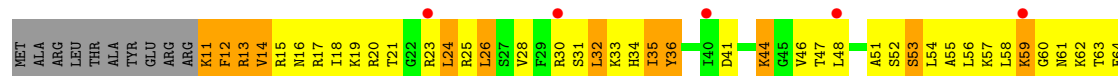
- Molecule 49: 50S RIBOSOMAL PROTEIN L17

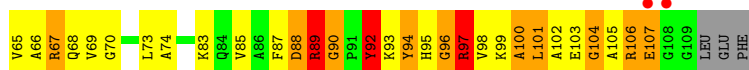
Chain DR:



- Molecule 50: 50S RIBOSOMAL PROTEIN L18

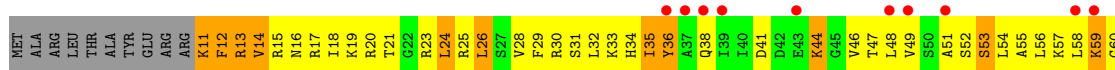
Chain BS:





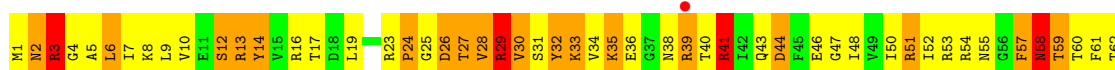
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain DS:



• Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain BT:



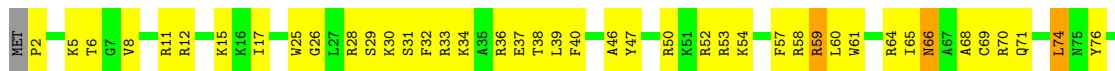
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain DT:



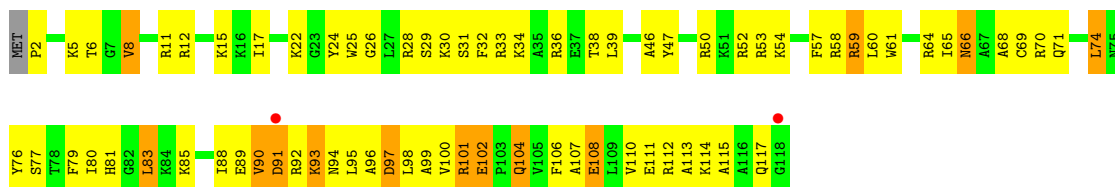
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



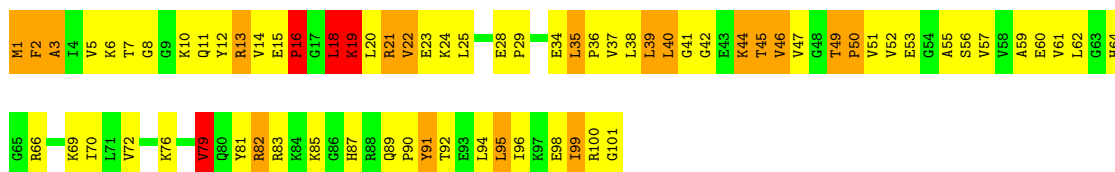
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain DU:



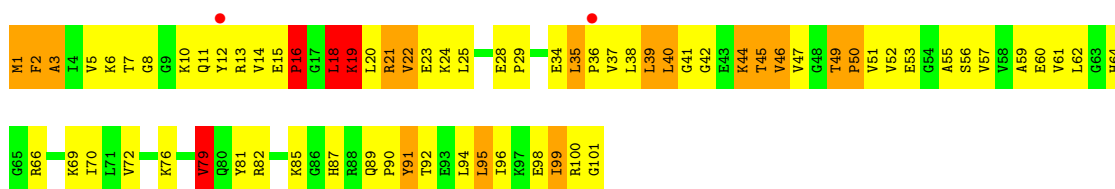
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain BV:



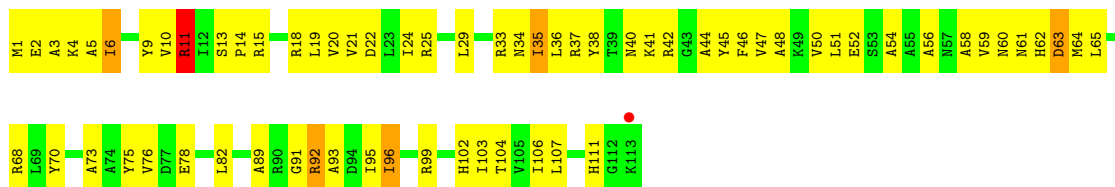
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain DV:



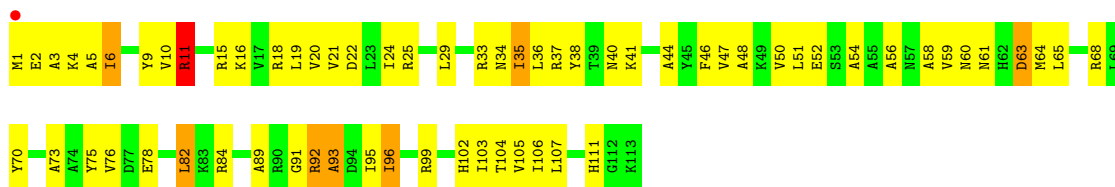
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain BW:



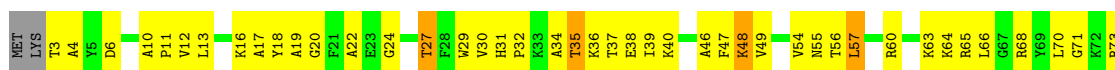
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

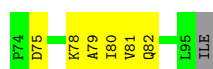
Chain DW:



• Molecule 55: 50S RIBOSOMAL PROTEIN L23

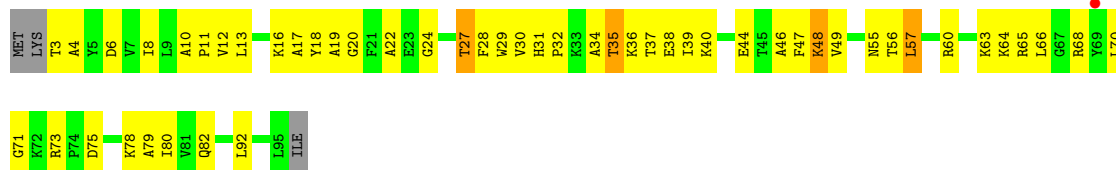
Chain BX:





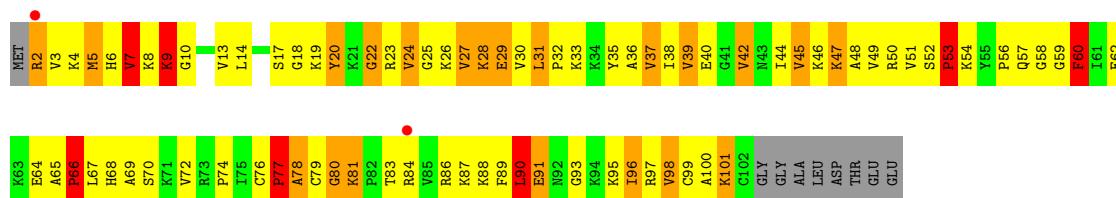
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain DX:



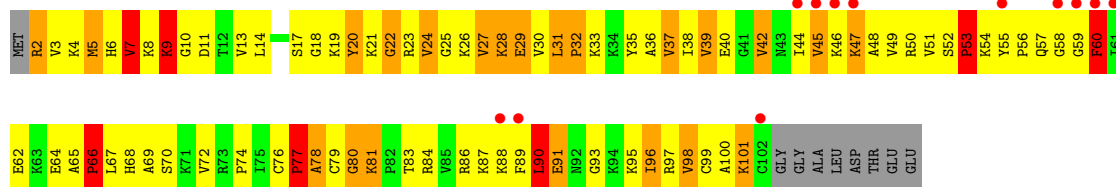
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:



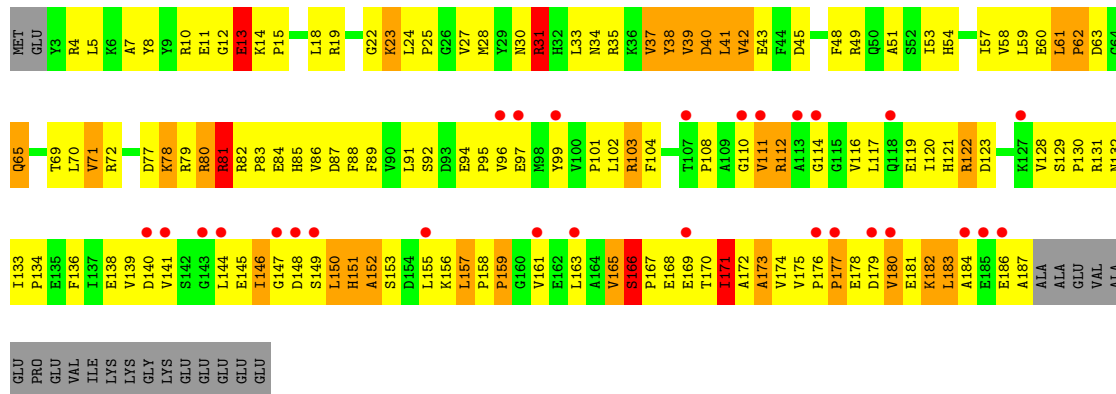
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain DY:



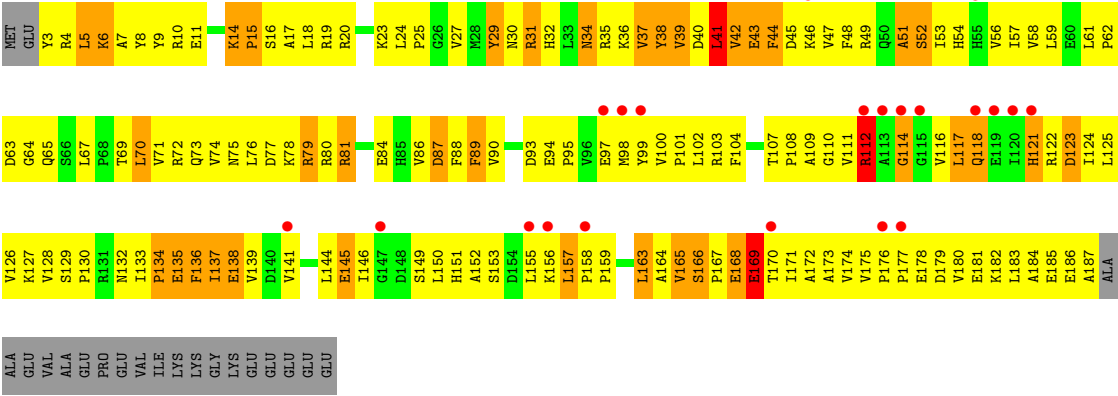
• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.90Å 450.79Å 625.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.10) 97.6 (49.95-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.280 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045150 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	298096	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: ZN, AG9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.44	0/36190	0.70	7/56486 (0.0%)
1	CA	0.42	0/36190	0.70	7/56486 (0.0%)
2	AB	0.30	0/1936	0.58	0/2611
2	CB	0.31	0/1936	0.58	0/2611
3	AC	0.31	0/1637	0.56	0/2207
3	CC	0.31	0/1637	0.56	0/2207
4	AD	0.37	0/1733	0.61	0/2318
4	CD	0.36	0/1733	0.60	0/2318
5	AE	0.36	0/1163	0.62	0/1566
5	CE	0.36	0/1163	0.63	0/1566
6	AF	0.34	0/856	0.59	0/1154
6	CF	0.34	0/856	0.59	0/1154
7	AG	0.29	0/1276	0.52	0/1709
7	CG	0.30	0/1276	0.52	0/1709
8	AH	0.32	0/1136	0.60	0/1527
8	CH	0.33	0/1136	0.60	0/1527
9	AI	0.31	0/1027	0.54	0/1373
9	CI	0.31	0/1027	0.55	0/1373
10	AJ	0.33	0/808	0.58	0/1087
10	CJ	0.33	0/808	0.57	0/1087
11	AK	0.33	0/900	0.60	0/1213
11	CK	0.33	0/900	0.60	0/1213
12	AL	0.46	0/987	0.79	0/1322
12	CL	0.43	0/987	0.78	0/1322
13	AM	0.32	0/943	0.61	0/1256
13	CM	0.33	0/943	0.61	0/1256
14	AN	0.31	0/501	0.51	0/664
14	CN	0.33	0/501	0.51	0/664
15	AO	0.33	0/745	0.58	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.38	0/717	0.61	0/965
16	CP	0.37	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/837	0.63	0/1119
17	CQ	0.37	0/837	0.62	0/1119
18	AR	0.33	0/579	0.64	0/768
18	CR	0.32	0/579	0.64	0/768
19	AS	0.36	0/643	0.58	0/867
19	CS	0.37	0/643	0.58	0/867
20	AT	0.32	0/765	0.54	0/1007
20	CT	0.31	0/765	0.54	0/1007
21	AU	0.42	0/213	0.53	0/279
21	CU	0.43	0/213	0.53	0/279
22	AV	1.84	39/1830 (2.1%)	0.95	3/2849 (0.1%)
22	AY	1.92	52/1830 (2.8%)	0.98	2/2849 (0.1%)
22	CV	0.88	0/1830	0.88	3/2849 (0.1%)
22	CY	1.56	22/1830 (1.2%)	1.25	27/2849 (0.9%)
23	AW	2.12	62/1853 (3.3%)	1.06	9/2887 (0.3%)
23	CW	0.83	0/1853	0.99	8/2887 (0.3%)
24	AX	0.55	0/290	0.83	0/450
24	CX	0.81	0/290	0.81	0/450
25	B0	0.42	0/671	0.62	0/892
25	D0	0.38	0/671	0.62	0/892
26	B1	0.48	0/741	0.78	2/986 (0.2%)
26	D1	0.44	0/741	0.76	0/986
27	B2	0.43	0/600	0.74	0/793
27	D2	0.34	0/600	0.59	0/793
28	B3	0.43	0/473	0.66	1/636 (0.2%)
28	D3	0.40	0/473	0.67	0/636
29	B4	0.38	0/461	0.64	0/623
29	D4	0.38	0/461	0.64	0/623
30	B5	0.56	0/442	0.73	0/598
30	D5	0.48	0/442	0.72	0/598
31	B6	0.37	0/440	0.72	1/586 (0.2%)
31	D6	0.37	0/440	0.72	1/586 (0.2%)
32	B7	0.54	0/418	0.65	0/552
32	D7	0.51	0/418	0.66	0/552
33	B8	0.59	0/516	0.84	0/681
33	D8	0.52	0/516	0.84	0/681
34	B9	0.31	0/310	0.59	0/407
34	D9	0.32	0/310	0.58	0/407
35	BA	0.60	1/68704 (0.0%)	0.73	42/107260 (0.0%)
35	DA	0.51	0/68704	0.73	35/107260 (0.0%)
36	BB	0.41	0/2853	0.69	0/4451
36	DB	0.38	0/2853	0.69	0/4451
37	BC	0.30	0/956	0.53	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.31	0/956	0.53	0/1288
38	BD	0.50	0/2155	0.78	2/2907 (0.1%)
38	DD	0.46	0/2155	0.78	3/2907 (0.1%)
39	BE	0.50	0/1597	0.74	0/2155
39	DE	0.45	0/1597	0.74	0/2155
40	BF	0.46	0/1659	0.69	0/2246
40	DF	0.42	0/1659	0.68	0/2246
41	BG	0.35	0/1498	0.67	0/2013
41	DG	0.34	0/1498	0.67	0/2013
42	BH	0.36	0/1285	0.70	1/1741 (0.1%)
42	DH	0.37	0/1285	0.69	1/1741 (0.1%)
43	BI	0.36	0/1147	0.86	3/1553 (0.2%)
43	DI	0.35	0/1147	0.85	3/1553 (0.2%)
45	BN	0.43	0/1132	0.70	0/1527
45	DN	0.41	0/1132	0.69	0/1527
46	BO	0.46	0/943	0.67	0/1269
46	DO	0.45	0/943	0.69	0/1269
47	BP	0.47	0/1131	0.93	5/1504 (0.3%)
47	DP	0.42	0/1131	0.92	4/1504 (0.3%)
48	BQ	0.43	0/1134	0.59	0/1517
48	DQ	0.42	0/1134	0.59	0/1517
49	BR	0.45	0/974	0.78	2/1302 (0.2%)
49	DR	0.42	0/974	0.78	2/1302 (0.2%)
50	BS	0.36	0/779	0.63	0/1038
50	DS	0.36	0/779	0.64	0/1038
51	BT	0.44	0/1138	0.76	1/1521 (0.1%)
51	DT	0.44	0/1138	0.76	1/1521 (0.1%)
52	BU	0.50	0/975	0.69	0/1297
52	DU	0.45	0/975	0.67	0/1297
53	BV	0.40	0/790	0.70	0/1057
53	DV	0.38	0/790	0.69	0/1057
54	BW	0.52	0/907	0.73	0/1216
54	DW	0.45	0/907	0.73	0/1216
55	BX	0.46	0/740	0.69	0/995
55	DX	0.45	0/740	0.69	0/995
56	BY	0.46	0/789	0.72	1/1053 (0.1%)
56	DY	0.42	0/789	0.71	1/1053 (0.1%)
57	BZ	0.44	0/1500	0.68	0/2037
57	DZ	0.38	0/1500	0.64	0/2037
All	All	0.56	176/322506 (0.1%)	0.72	178/482452 (0.0%)

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	AA	0	18
1	CA	0	19
22	AV	0	17
22	AY	0	19
22	CV	0	10
22	CY	0	17
23	AW	0	21
23	CW	0	11
35	BA	5	46
35	DA	4	41
All	All	9	219

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	56	U	C2-N3	28.94	1.58	1.37
22	CY	57	U	C3'-O3'	17.68	1.67	1.42
22	CY	56	U	N3-C4	14.74	1.51	1.38
22	CY	56	U	N1-C2	13.32	1.50	1.38
22	CY	58	C	P-O5'	12.55	1.72	1.59

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CY	56	U	C5-C6-N1	16.14	130.77	122.70
43	BI	50	ARG	NE-CZ-NH1	13.96	127.28	120.30
43	BI	50	ARG	NE-CZ-NH2	-13.50	113.55	120.30
43	DI	50	ARG	NE-CZ-NH2	-13.46	113.57	120.30
43	DI	50	ARG	NE-CZ-NH1	13.32	126.96	120.30

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	752	A	C3'
35	BA	790	C	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'
35	BA	1820	U	C3'

5 of 219 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	265	G	Sidechain
1	AA	292	G	Sidechain
1	AA	387	U	Sidechain
1	AA	436	C	Sidechain
1	AA	97	G	Sidechain

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	AA	32329	0	16318	1333	0
1	CA	32329	0	16318	1413	0
2	AB	1901	0	1951	265	0
2	CB	1901	0	1951	274	0
3	AC	1613	0	1677	225	0
3	CC	1613	0	1677	239	0
4	AD	1703	0	1765	227	1
4	CD	1703	0	1766	223	0
5	AE	1147	0	1207	149	0
5	CE	1147	0	1207	155	0
6	AF	843	0	857	81	0
6	CF	843	0	857	81	1
7	AG	1257	0	1296	124	0
7	CG	1257	0	1296	123	0
8	AH	1116	0	1177	123	0
8	CH	1116	0	1177	126	0
9	AI	1010	0	1035	154	0
9	CI	1010	0	1035	159	0
10	AJ	795	0	840	181	0
10	CJ	795	0	840	178	0
11	AK	885	0	904	85	0
11	CK	885	0	904	85	0
12	AL	971	0	1057	215	0
12	CL	971	0	1057	213	0
13	AM	938	0	991	131	0
13	CM	938	0	991	131	0
14	AN	492	0	531	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	532	52	0
15	AO	734	0	771	57	0
15	CO	734	0	771	62	0
16	AP	701	0	720	83	0
16	CP	701	0	720	82	0
17	AQ	824	0	891	83	0
17	CQ	824	0	891	79	0
18	AR	574	0	644	72	0
18	CR	574	0	644	73	0
19	AS	630	0	652	87	0
19	CS	630	0	652	79	0
20	AT	763	0	861	90	0
20	CT	763	0	861	85	0
21	AU	209	0	221	22	0
21	CU	209	0	221	24	0
22	AV	1667	0	857	264	0
22	AY	1667	0	857	327	0
22	CV	1667	0	857	235	0
22	CY	1667	0	854	330	0
23	AW	1659	0	843	396	0
23	CW	1659	0	843	323	0
24	AX	257	0	132	12	0
24	CX	257	0	132	35	0
25	B0	662	0	688	69	0
25	D0	662	0	688	72	0
26	B1	734	0	808	71	0
26	D1	734	0	808	87	0
27	B2	598	0	653	72	0
27	D2	598	0	653	70	0
28	B3	468	0	523	35	0
28	D3	468	0	523	37	0
29	B4	451	0	449	97	0
29	D4	451	0	449	82	0
30	B5	428	0	445	73	0
30	D5	428	0	445	72	0
31	B6	433	0	461	85	0
31	D6	433	0	461	86	0
32	B7	410	0	454	23	0
32	D7	410	0	454	24	0
33	B8	508	0	576	110	0
33	D8	508	0	576	110	0
34	B9	307	0	338	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	307	0	338	32	0
35	BA	61341	0	30928	1764	0
35	DA	61341	0	30928	1844	0
36	BB	2551	0	1295	93	0
36	DB	2551	0	1295	112	0
37	BC	937	0	957	113	0
37	DC	937	0	957	112	0
38	BD	2105	0	2182	267	0
38	DD	2105	0	2182	278	0
39	BE	1564	0	1629	236	0
39	DE	1564	0	1629	240	0
40	BF	1624	0	1677	169	0
40	DF	1624	0	1677	173	0
41	BG	1474	0	1534	248	0
41	DG	1474	0	1534	305	0
42	BH	1260	0	1326	154	0
42	DH	1260	0	1326	157	0
43	BI	1132	0	1218	204	0
43	DI	1132	0	1218	196	0
44	BJ	651	0	166	32	0
44	DJ	651	0	170	17	0
45	BN	1105	0	1180	145	0
45	DN	1105	0	1180	150	0
46	BO	933	0	996	116	0
46	DO	933	0	996	112	0
47	BP	1114	0	1187	284	0
47	DP	1114	0	1187	288	0
48	BQ	1113	0	1171	132	0
48	DQ	1113	0	1171	140	0
49	BR	960	0	1021	124	0
49	DR	960	0	1021	126	0
50	BS	771	0	832	153	0
50	DS	771	0	832	146	0
51	BT	1124	0	1181	251	0
51	DT	1124	0	1181	242	0
52	BU	958	0	1015	138	0
52	DU	958	0	1015	132	0
53	BV	779	0	852	151	0
53	DV	779	0	852	149	0
54	BW	896	0	953	70	0
54	DW	896	0	953	75	0
55	BX	726	0	778	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DX	726	0	778	60	0
56	BY	776	0	870	175	0
56	DY	776	0	870	175	0
57	BZ	1468	0	1492	265	0
57	DZ	1468	0	1491	341	0
58	AD	1	0	0	2	0
58	AN	1	0	0	1	0
58	CD	1	0	0	2	0
58	CN	1	0	0	1	0
All	All	298096	0	201782	19801	1

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 40.

The worst 5 of 19801 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:CY:57:U:C6	57:DZ:182:LYS:HA	1.08	1.58
1:CA:1196:U:C4	24:CX:23:A:C5	1.96	1.53
22:CY:57:U:H6	57:DZ:182:LYS:CA	1.20	1.50
1:CA:1196:U:O4	24:CX:23:A:C4	1.70	1.45
22:CY:62:U:O2'	57:DZ:186:GLU:CB	1.68	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:27:TYR:OH	6:CF:15:ASP:OD2[4_455]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	233/256 (91%)	153 (66%)	55 (24%)	25 (11%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	233/256 (91%)	152 (65%)	57 (24%)	24 (10%)	1	6
3	AC	205/239 (86%)	141 (69%)	43 (21%)	21 (10%)	1	6
3	CC	205/239 (86%)	142 (69%)	40 (20%)	23 (11%)	1	5
4	AD	206/209 (99%)	133 (65%)	46 (22%)	27 (13%)	0	3
4	CD	206/209 (99%)	135 (66%)	44 (21%)	27 (13%)	0	3
5	AE	149/162 (92%)	111 (74%)	24 (16%)	14 (9%)	1	7
5	CE	149/162 (92%)	110 (74%)	25 (17%)	14 (9%)	1	7
6	AF	99/101 (98%)	77 (78%)	15 (15%)	7 (7%)	2	12
6	CF	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	2	16
7	AG	153/156 (98%)	108 (71%)	41 (27%)	4 (3%)	8	41
7	CG	153/156 (98%)	110 (72%)	39 (26%)	4 (3%)	8	41
8	AH	136/138 (99%)	100 (74%)	29 (21%)	7 (5%)	3	22
8	CH	136/138 (99%)	99 (73%)	29 (21%)	8 (6%)	2	17
9	AI	121/128 (94%)	90 (74%)	22 (18%)	9 (7%)	2	11
9	CI	121/128 (94%)	91 (75%)	20 (16%)	10 (8%)	1	9
10	AJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	4	27
10	CJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	4	27
11	AK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	2	14
11	CK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	2	14
12	AL	123/135 (91%)	75 (61%)	28 (23%)	20 (16%)	0	0
12	CL	123/135 (91%)	75 (61%)	28 (23%)	20 (16%)	0	0
13	AM	107/126 (85%)	67 (63%)	25 (23%)	15 (14%)	0	2
13	CM	107/126 (85%)	66 (62%)	26 (24%)	15 (14%)	0	2
14	AN	58/61 (95%)	41 (71%)	9 (16%)	8 (14%)	0	2
14	CN	58/61 (95%)	40 (69%)	9 (16%)	9 (16%)	0	1
15	AO	86/89 (97%)	52 (60%)	25 (29%)	9 (10%)	1	5
15	CO	86/89 (97%)	50 (58%)	27 (31%)	9 (10%)	1	5
16	AP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	1	4
16	CP	82/88 (93%)	49 (60%)	24 (29%)	9 (11%)	1	5
17	AQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	2	16
17	CQ	98/105 (93%)	71 (72%)	20 (20%)	7 (7%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	8
18	CR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	8
19	AS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	0
19	CS	77/93 (83%)	48 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	17 (18%)	13 (13%)	0	2
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	1	3
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	3
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	3
25	B0	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	5	31
25	D0	82/85 (96%)	66 (80%)	13 (16%)	3 (4%)	5	31
26	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	1	4
26	D1	92/98 (94%)	71 (77%)	9 (10%)	12 (13%)	0	3
27	B2	69/72 (96%)	50 (72%)	14 (20%)	5 (7%)	2	12
27	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	1	4
28	B3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	9
28	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	9
29	B4	56/71 (79%)	26 (46%)	15 (27%)	15 (27%)	0	0
29	D4	56/71 (79%)	26 (46%)	16 (29%)	14 (25%)	0	0
30	B5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	2
30	D5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	2
31	B6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
32	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	3
33	D8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	3
34	B9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
34	D9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
37	BC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	8	41
37	DC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	8	41
38	BD	270/276 (98%)	209 (77%)	32 (12%)	29 (11%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	207 (77%)	34 (13%)	29 (11%)	1	5
39	BE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	0
39	DE	203/206 (98%)	134 (66%)	37 (18%)	32 (16%)	0	1
40	BF	206/210 (98%)	149 (72%)	31 (15%)	26 (13%)	0	3
40	DF	206/210 (98%)	148 (72%)	32 (16%)	26 (13%)	0	3
41	BG	177/182 (97%)	112 (63%)	39 (22%)	26 (15%)	0	2
41	DG	177/182 (97%)	93 (52%)	57 (32%)	27 (15%)	0	1
42	BH	163/180 (91%)	110 (68%)	29 (18%)	24 (15%)	0	2
42	DH	163/180 (91%)	110 (68%)	28 (17%)	25 (15%)	0	1
43	BI	144/148 (97%)	84 (58%)	37 (26%)	23 (16%)	0	1
43	DI	144/148 (97%)	85 (59%)	36 (25%)	23 (16%)	0	1
45	BN	137/140 (98%)	99 (72%)	22 (16%)	16 (12%)	1	4
45	DN	137/140 (98%)	101 (74%)	20 (15%)	16 (12%)	1	4
46	BO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	3	18
46	DO	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	2	14
47	BP	144/150 (96%)	69 (48%)	43 (30%)	32 (22%)	0	0
47	DP	144/150 (96%)	69 (48%)	43 (30%)	32 (22%)	0	0
48	BQ	139/141 (99%)	100 (72%)	27 (19%)	12 (9%)	1	9
48	DQ	139/141 (99%)	99 (71%)	28 (20%)	12 (9%)	1	9
49	BR	115/118 (98%)	88 (76%)	13 (11%)	14 (12%)	1	4
49	DR	115/118 (98%)	87 (76%)	14 (12%)	14 (12%)	1	4
50	BS	97/112 (87%)	54 (56%)	24 (25%)	19 (20%)	0	0
50	DS	97/112 (87%)	52 (54%)	26 (27%)	19 (20%)	0	0
51	BT	134/146 (92%)	85 (63%)	19 (14%)	30 (22%)	0	0
51	DT	134/146 (92%)	86 (64%)	18 (13%)	30 (22%)	0	0
52	BU	115/118 (98%)	90 (78%)	19 (16%)	6 (5%)	3	21
52	DU	115/118 (98%)	88 (76%)	20 (17%)	7 (6%)	2	16
53	BV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	3
53	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	3
54	BW	111/113 (98%)	91 (82%)	12 (11%)	8 (7%)	2	12
54	DW	111/113 (98%)	91 (82%)	13 (12%)	7 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BX	91/96 (95%)	71 (78%)	15 (16%)	5 (6%)	3	19
55	DX	91/96 (95%)	67 (74%)	19 (21%)	5 (6%)	3	19
56	BY	99/110 (90%)	48 (48%)	26 (26%)	25 (25%)	0	0
56	DY	99/110 (90%)	48 (48%)	26 (26%)	25 (25%)	0	0
57	BZ	183/206 (89%)	111 (61%)	45 (25%)	27 (15%)	0	2
57	DZ	183/206 (89%)	111 (61%)	42 (23%)	30 (16%)	0	0
All	All	11600/12592 (92%)	7946 (68%)	2292 (20%)	1362 (12%)	1	4

5 of 1362 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	75	LYS
2	AB	101	MET
2	AB	123	ALA
2	AB	165	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	186 (92%)	16 (8%)	18	55
2	CB	202/220 (92%)	187 (93%)	15 (7%)	20	59
3	AC	160/188 (85%)	145 (91%)	15 (9%)	13	43
3	CC	160/188 (85%)	146 (91%)	14 (9%)	14	49
4	AD	180/181 (99%)	162 (90%)	18 (10%)	11	38
4	CD	180/181 (99%)	162 (90%)	18 (10%)	11	38
5	AE	115/123 (94%)	107 (93%)	8 (7%)	21	61
5	CE	115/123 (94%)	107 (93%)	8 (7%)	21	61
6	AF	90/90 (100%)	87 (97%)	3 (3%)	50	86
6	CF	90/90 (100%)	87 (97%)	3 (3%)	50	86
7	AG	126/127 (99%)	121 (96%)	5 (4%)	42	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CG	126/127 (99%)	121 (96%)	5 (4%)	42	82
8	AH	119/119 (100%)	109 (92%)	10 (8%)	16	52
8	CH	119/119 (100%)	109 (92%)	10 (8%)	16	52
9	AI	98/99 (99%)	90 (92%)	8 (8%)	17	53
9	CI	98/99 (99%)	90 (92%)	8 (8%)	17	53
10	AJ	88/92 (96%)	83 (94%)	5 (6%)	29	70
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	29	70
11	AK	90/99 (91%)	85 (94%)	5 (6%)	30	70
11	CK	90/99 (91%)	85 (94%)	5 (6%)	30	70
12	AL	104/111 (94%)	85 (82%)	19 (18%)	2	10
12	CL	104/111 (94%)	84 (81%)	20 (19%)	2	9
13	AM	94/101 (93%)	84 (89%)	10 (11%)	10	35
13	CM	94/101 (93%)	84 (89%)	10 (11%)	10	35
14	AN	49/50 (98%)	47 (96%)	2 (4%)	41	82
14	CN	49/50 (98%)	47 (96%)	2 (4%)	41	82
15	AO	79/80 (99%)	75 (95%)	4 (5%)	33	74
15	CO	79/80 (99%)	75 (95%)	4 (5%)	33	74
16	AP	72/74 (97%)	66 (92%)	6 (8%)	16	53
16	CP	72/74 (97%)	66 (92%)	6 (8%)	16	53
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	40	80
17	CQ	94/97 (97%)	90 (96%)	4 (4%)	40	80
18	AR	61/77 (79%)	59 (97%)	2 (3%)	50	86
18	CR	61/77 (79%)	59 (97%)	2 (3%)	50	86
19	AS	69/80 (86%)	62 (90%)	7 (10%)	11	38
19	CS	69/80 (86%)	61 (88%)	8 (12%)	8	30
20	AT	76/82 (93%)	71 (93%)	5 (7%)	24	64
20	CT	76/82 (93%)	71 (93%)	5 (7%)	24	64
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	35
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	72
25	B0	66/67 (98%)	59 (89%)	7 (11%)	10	35
25	D0	66/67 (98%)	59 (89%)	7 (11%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	B1	78/83 (94%)	70 (90%)	8 (10%)	10	36
26	D1	78/83 (94%)	68 (87%)	10 (13%)	6	24
27	B2	66/67 (98%)	57 (86%)	9 (14%)	5	21
27	D2	66/67 (98%)	60 (91%)	6 (9%)	14	45
28	B3	51/52 (98%)	48 (94%)	3 (6%)	28	68
28	D3	51/52 (98%)	48 (94%)	3 (6%)	28	68
29	B4	51/63 (81%)	42 (82%)	9 (18%)	3	10
29	D4	51/63 (81%)	42 (82%)	9 (18%)	3	10
30	B5	47/52 (90%)	42 (89%)	5 (11%)	10	35
30	D5	47/52 (90%)	42 (89%)	5 (11%)	10	35
31	B6	49/52 (94%)	43 (88%)	6 (12%)	7	26
31	D6	49/52 (94%)	43 (88%)	6 (12%)	7	26
32	B7	40/42 (95%)	35 (88%)	5 (12%)	7	25
32	D7	40/42 (95%)	36 (90%)	4 (10%)	11	38
33	B8	53/55 (96%)	44 (83%)	9 (17%)	3	11
33	D8	53/55 (96%)	44 (83%)	9 (17%)	3	11
34	B9	34/34 (100%)	33 (97%)	1 (3%)	55	88
34	D9	34/34 (100%)	33 (97%)	1 (3%)	55	88
37	BC	99/181 (55%)	94 (95%)	5 (5%)	33	74
37	DC	99/181 (55%)	94 (95%)	5 (5%)	33	74
38	BD	213/218 (98%)	185 (87%)	28 (13%)	6	23
38	DD	213/218 (98%)	187 (88%)	26 (12%)	7	26
39	BE	165/166 (99%)	144 (87%)	21 (13%)	6	24
39	DE	165/166 (99%)	143 (87%)	22 (13%)	6	22
40	BF	165/166 (99%)	149 (90%)	16 (10%)	12	41
40	DF	165/166 (99%)	149 (90%)	16 (10%)	12	41
41	BG	155/156 (99%)	140 (90%)	15 (10%)	12	41
41	DG	155/156 (99%)	140 (90%)	15 (10%)	12	41
42	BH	137/148 (93%)	121 (88%)	16 (12%)	8	29
42	DH	137/148 (93%)	121 (88%)	16 (12%)	8	29
43	BI	122/124 (98%)	112 (92%)	10 (8%)	17	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DI	122/124 (98%)	112 (92%)	10 (8%)	17	53
45	BN	117/119 (98%)	101 (86%)	16 (14%)	5	21
45	DN	117/119 (98%)	101 (86%)	16 (14%)	5	21
46	BO	100/100 (100%)	94 (94%)	6 (6%)	27	67
46	DO	100/100 (100%)	94 (94%)	6 (6%)	27	67
47	BP	112/116 (97%)	93 (83%)	19 (17%)	3	11
47	DP	112/116 (97%)	93 (83%)	19 (17%)	3	11
48	BQ	110/111 (99%)	100 (91%)	10 (9%)	14	45
48	DQ	110/111 (99%)	101 (92%)	9 (8%)	17	53
49	BR	100/101 (99%)	87 (87%)	13 (13%)	6	23
49	DR	100/101 (99%)	86 (86%)	14 (14%)	5	21
50	BS	77/88 (88%)	64 (83%)	13 (17%)	3	11
50	DS	77/88 (88%)	64 (83%)	13 (17%)	3	11
51	BT	118/127 (93%)	96 (81%)	22 (19%)	2	9
51	DT	118/127 (93%)	95 (80%)	23 (20%)	2	8
52	BU	92/94 (98%)	83 (90%)	9 (10%)	12	40
52	DU	92/94 (98%)	81 (88%)	11 (12%)	7	27
53	BV	82/82 (100%)	67 (82%)	15 (18%)	2	10
53	DV	82/82 (100%)	68 (83%)	14 (17%)	3	11
54	BW	91/92 (99%)	81 (89%)	10 (11%)	9	34
54	DW	91/92 (99%)	81 (89%)	10 (11%)	9	34
55	BX	74/78 (95%)	69 (93%)	5 (7%)	22	62
55	DX	74/78 (95%)	69 (93%)	5 (7%)	22	62
56	BY	84/91 (92%)	70 (83%)	14 (17%)	3	11
56	DY	84/91 (92%)	69 (82%)	15 (18%)	2	10
57	BZ	162/179 (90%)	140 (86%)	22 (14%)	5	21
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	10	35
All	All	9790/10432 (94%)	8794 (90%)	996 (10%)	11	37

5 of 996 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BW	11	ARG

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Mol	Chain	Res	Type
6	CF	63	TYR
51	DT	95	ARG
55	BX	68	ARG
2	CB	87	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 311 such sidechains are listed below:

Mol	Chain	Res	Type
51	BT	90	GLN
4	CD	62	GLN
48	DQ	123	HIS
52	BU	117	GLN
2	CB	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	215 (14%)	29 (1%)
1	CA	1503/1522 (98%)	218 (14%)	31 (2%)
22	AV	76/78 (97%)	25 (32%)	0
22	AY	76/78 (97%)	24 (31%)	2 (2%)
22	CV	76/78 (97%)	24 (31%)	0
22	CY	76/78 (97%)	23 (30%)	2 (2%)
23	AW	77/78 (98%)	41 (53%)	4 (5%)
23	CW	77/78 (98%)	39 (50%)	3 (3%)
24	AX	11/24 (45%)	2 (18%)	0
24	CX	11/24 (45%)	2 (18%)	0
35	BA	2847/2915 (97%)	498 (17%)	49 (1%)
35	DA	2847/2915 (97%)	498 (17%)	49 (1%)
36	BB	118/122 (96%)	18 (15%)	1 (0%)
36	DB	118/122 (96%)	17 (14%)	1 (0%)
All	All	9416/9634 (97%)	1644 (17%)	171 (1%)

5 of 1644 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	47	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2405	G
1	CA	429	U
35	DA	2126	A
35	BA	2439	A
1	CA	60	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	AG9	AV	36	22	27,29,30	1.10	3 (11%)	35,39,42	1.68	4 (11%)
22	AG9	AY	36	22	27,29,30	1.41	4 (14%)	35,39,42	1.77	5 (14%)
22	AG9	CV	36	22	27,29,30	1.68	3 (11%)	35,39,42	1.66	4 (11%)
22	AG9	CY	36	22	27,29,30	1.99	6 (22%)	35,39,42	1.76	5 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AG9	AV	36	22	-	0/17/47/48	0/2/2/2
22	AG9	AY	36	22	-	0/17/47/48	0/2/2/2
22	AG9	CV	36	22	-	0/17/47/48	0/2/2/2
22	AG9	CY	36	22	-	0/17/47/48	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	36	AG9	C2-N1	6.18	1.43	1.38
22	CV	36	AG9	C2-N1	5.68	1.43	1.38
22	CY	36	AG9	P-OP1	5.27	1.52	1.46
22	AY	36	AG9	C2-N1	5.18	1.42	1.38
22	CV	36	AG9	P-OP1	4.58	1.51	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CY	36	AG9	C4-N3-C2	7.27	120.84	112.23
22	AY	36	AG9	C4-N3-C2	6.73	120.20	112.23
22	AV	36	AG9	C4-N3-C2	6.62	120.07	112.23
22	CV	36	AG9	C4-N3-C2	6.48	119.90	112.23
22	AY	36	AG9	N1-C2-N3	-4.85	118.76	124.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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
13	CM	5
13	AM	5
9	AI	2
9	CI	2
41	DG	1
41	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AM	112:GLY	C	113:PRO	N	4.84
1	CM	112:GLY	C	113:PRO	N	4.84
1	AM	69:GLU	C	70:LEU	N	4.24
1	CM	69:GLU	C	70:LEU	N	4.23
1	DG	112:PRO	C	113:ARG	N	4.14

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.35	65 (4%) 34 5	44, 101, 184, 200	0
1	CA	1504/1522 (98%)	0.34	69 (4%) 31 5	55, 115, 186, 200	0
2	AB	235/256 (91%)	0.32	10 (4%) 34 5	75, 134, 176, 198	0
2	CB	235/256 (91%)	0.65	24 (10%) 7 2	94, 148, 183, 200	0
3	AC	207/239 (86%)	0.37	8 (3%) 37 5	82, 127, 157, 179	0
3	CC	207/239 (86%)	0.67	11 (5%) 25 4	92, 141, 170, 185	0
4	AD	208/209 (99%)	0.38	7 (3%) 43 6	64, 112, 142, 179	0
4	CD	208/209 (99%)	0.10	1 (0%) 88 39	56, 99, 135, 157	0
5	AE	151/162 (93%)	0.17	0 100 100	65, 95, 142, 167	0
5	CE	151/162 (93%)	0.49	4 (2%) 53 8	69, 119, 151, 160	0
6	AF	101/101 (100%)	-0.03	0 100 100	59, 98, 138, 173	0
6	CF	101/101 (100%)	0.01	0 100 100	64, 110, 133, 173	0
7	AG	155/156 (99%)	0.76	22 (14%) 3 1	76, 123, 155, 198	0
7	CG	155/156 (99%)	0.72	18 (11%) 5 1	94, 131, 160, 194	0
8	AH	138/138 (100%)	0.16	1 (0%) 84 32	61, 101, 128, 144	0
8	CH	138/138 (100%)	0.46	4 (2%) 49 7	83, 121, 148, 166	0
9	AI	127/128 (99%)	0.86	12 (9%) 9 2	81, 148, 176, 191	0
9	CI	127/128 (99%)	1.26	30 (23%) 1 0	99, 153, 181, 193	0
10	AJ	99/105 (94%)	0.94	8 (8%) 12 2	71, 149, 177, 185	0
10	CJ	99/105 (94%)	1.39	19 (19%) 2 0	97, 159, 182, 189	0
11	AK	119/129 (92%)	0.25	6 (5%) 28 4	63, 94, 136, 187	0
11	CK	119/129 (92%)	0.25	6 (5%) 28 4	78, 108, 141, 176	0
12	AL	125/135 (92%)	0.59	9 (7%) 15 2	53, 93, 146, 180	0
12	CL	125/135 (92%)	0.63	2 (1%) 68 15	63, 111, 149, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	119/126 (94%)	0.76	12 (10%) 7 2	75, 129, 161, 178	0
13	CM	119/126 (94%)	1.01	17 (14%) 3 1	96, 150, 169, 186	0
14	AN	60/61 (98%)	0.81	8 (13%) 4 1	71, 118, 145, 157	0
14	CN	60/61 (98%)	1.02	10 (16%) 2 0	108, 143, 166, 187	0
15	AO	88/89 (98%)	0.20	1 (1%) 77 22	60, 97, 130, 148	0
15	CO	88/89 (98%)	0.27	2 (2%) 57 9	67, 110, 138, 146	0
16	AP	84/88 (95%)	0.64	5 (5%) 21 3	67, 112, 156, 178	0
16	CP	84/88 (95%)	0.26	0 100 100	60, 87, 137, 157	0
17	AQ	100/105 (95%)	0.34	1 (1%) 79 23	74, 109, 138, 151	0
17	CQ	100/105 (95%)	0.43	4 (4%) 36 5	70, 109, 139, 165	0
18	AR	70/88 (79%)	0.34	2 (2%) 49 7	69, 98, 139, 157	0
18	CR	70/88 (79%)	0.53	2 (2%) 49 7	77, 111, 148, 156	0
19	AS	79/93 (84%)	1.15	12 (15%) 3 1	89, 137, 171, 185	0
19	CS	79/93 (84%)	1.34	18 (22%) 1 0	112, 154, 178, 200	0
20	AT	99/106 (93%)	0.68	10 (10%) 7 2	65, 117, 160, 167	0
20	CT	99/106 (93%)	0.55	5 (5%) 27 4	66, 107, 151, 163	0
21	AU	25/27 (92%)	1.47	7 (28%) 1 0	84, 120, 146, 156	0
21	CU	25/27 (92%)	2.49	16 (64%) 0 0	91, 135, 171, 188	0
22	AV	77/78 (98%)	0.96	8 (10%) 7 1	65, 141, 179, 199	0
22	AY	77/78 (98%)	1.11	12 (15%) 3 1	90, 140, 185, 189	0
22	CV	77/78 (98%)	1.61	23 (29%) 1 0	94, 175, 196, 200	0
22	CY	77/78 (98%)	2.46	34 (44%) 1 0	138, 176, 197, 200	0
23	AW	78/78 (100%)	1.58	20 (25%) 1 0	70, 173, 191, 199	0
23	CW	78/78 (100%)	2.60	45 (57%) 0 0	99, 188, 200, 200	0
24	AX	12/24 (50%)	0.98	1 (8%) 11 2	59, 88, 157, 160	0
24	CX	12/24 (50%)	1.87	5 (41%) 1 0	92, 163, 185, 185	0
25	B0	84/85 (98%)	0.41	3 (3%) 41 6	39, 66, 124, 167	0
25	D0	84/85 (98%)	0.81	5 (5%) 21 3	71, 105, 146, 165	0
26	B1	94/98 (95%)	-0.00	0 100 100	33, 61, 114, 141	0
26	D1	94/98 (95%)	0.09	1 (1%) 77 22	43, 74, 127, 149	0
27	B2	71/72 (98%)	-0.09	1 (1%) 72 17	41, 70, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.13	1 (1%)	72 17	57, 97, 139, 178	0
28	B3	60/60 (100%)	0.30	1 (1%)	67 15	42, 63, 108, 167	0
28	D3	60/60 (100%)	0.91	5 (8%)	11 2	65, 109, 149, 175	0
29	B4	58/71 (81%)	0.80	9 (15%)	3 1	96, 144, 171, 187	0
29	D4	58/71 (81%)	0.82	6 (10%)	7 2	86, 165, 194, 200	0
30	B5	56/60 (93%)	-0.10	0	100 100	25, 63, 126, 148	0
30	D5	56/60 (93%)	0.04	1 (1%)	65 14	48, 80, 128, 146	0
31	B6	50/54 (92%)	2.06	27 (54%)	0 0	99, 140, 171, 180	0
31	D6	50/54 (92%)	2.76	30 (60%)	0 0	113, 150, 174, 191	0
32	B7	48/49 (97%)	0.04	1 (2%)	60 11	23, 42, 83, 129	0
32	D7	48/49 (97%)	0.12	0	100 100	35, 54, 98, 131	0
33	B8	64/65 (98%)	0.23	2 (3%)	47 7	30, 61, 107, 123	0
33	D8	64/65 (98%)	0.46	2 (3%)	47 7	46, 89, 134, 177	0
34	B9	37/37 (100%)	3.35	34 (91%)	0 0	91, 136, 157, 159	0
34	D9	37/37 (100%)	4.19	30 (81%)	0 0	126, 149, 172, 183	0
35	BA	2848/2915 (97%)	0.13	97 (3%)	43 6	20, 56, 184, 200	0
35	DA	2848/2915 (97%)	0.17	123 (4%)	34 5	39, 82, 186, 200	0
36	BB	119/122 (97%)	0.43	1 (0%)	83 28	52, 81, 149, 178	0
36	DB	119/122 (97%)	0.66	6 (5%)	28 4	102, 151, 183, 195	0
37	BC	120/229 (52%)	2.10	55 (45%)	1 0	119, 168, 189, 200	0
37	DC	120/229 (52%)	1.83	44 (36%)	1 0	132, 170, 187, 199	0
38	BD	272/276 (98%)	-0.07	1 (0%)	90 45	24, 55, 93, 150	0
38	DD	272/276 (98%)	0.01	0	100 100	37, 73, 110, 144	0
39	BE	205/206 (99%)	0.06	3 (1%)	70 16	20, 62, 129, 165	0
39	DE	205/206 (99%)	0.12	1 (0%)	88 39	41, 82, 136, 159	0
40	BF	208/210 (99%)	0.09	6 (2%)	49 7	22, 63, 144, 195	0
40	DF	208/210 (99%)	0.05	2 (0%)	79 23	38, 90, 145, 184	0
41	BG	181/182 (99%)	0.53	7 (3%)	37 5	51, 103, 155, 182	0
41	DG	181/182 (99%)	0.70	15 (8%)	11 2	102, 141, 167, 183	0
42	BH	165/180 (91%)	0.38	5 (3%)	48 7	49, 86, 136, 174	0
42	DH	165/180 (91%)	1.15	36 (21%)	1 0	102, 139, 167, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.99	29 (19%) 2 0	55, 147, 187, 200	0
43	DI	146/148 (98%)	1.01	28 (19%) 2 0	59, 139, 183, 200	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	-0.00	1 (0%) 84 32	36, 64, 118, 147	0
45	DN	139/140 (99%)	0.29	3 (2%) 59 11	69, 104, 136, 155	0
46	BO	122/122 (100%)	-0.10	0 100 100	33, 60, 94, 116	0
46	DO	122/122 (100%)	0.06	0 100 100	54, 83, 110, 141	0
47	BP	146/150 (97%)	0.32	3 (2%) 60 11	29, 74, 128, 189	0
47	DP	146/150 (97%)	0.39	4 (2%) 52 8	41, 98, 144, 173	0
48	BQ	141/141 (100%)	0.17	0 100 100	38, 67, 109, 143	0
48	DQ	141/141 (100%)	0.48	3 (2%) 60 11	63, 113, 153, 178	0
49	BR	117/118 (99%)	0.05	0 100 100	36, 62, 103, 136	0
49	DR	117/118 (99%)	0.07	1 (0%) 81 25	42, 76, 118, 151	0
50	BS	99/112 (88%)	0.67	7 (7%) 16 3	52, 95, 141, 160	0
50	DS	99/112 (88%)	1.14	16 (16%) 2 1	101, 137, 163, 186	0
51	BT	136/146 (93%)	0.01	1 (0%) 84 32	47, 78, 140, 181	0
51	DT	136/146 (93%)	0.21	5 (3%) 39 6	58, 92, 151, 176	0
52	BU	117/118 (99%)	-0.09	1 (0%) 81 25	27, 53, 102, 144	0
52	DU	117/118 (99%)	0.16	2 (1%) 67 15	46, 97, 137, 163	0
53	BV	101/101 (100%)	-0.06	0 100 100	24, 72, 124, 168	0
53	DV	101/101 (100%)	0.45	2 (1%) 62 12	53, 116, 146, 171	0
54	BW	113/113 (100%)	-0.02	1 (0%) 81 25	28, 52, 105, 180	0
54	DW	113/113 (100%)	0.05	1 (0%) 81 25	49, 71, 119, 165	0
55	BX	93/96 (96%)	-0.15	0 100 100	29, 63, 100, 141	0
55	DX	93/96 (96%)	0.12	1 (1%) 77 22	55, 83, 115, 138	0
56	BY	101/110 (91%)	0.18	2 (1%) 62 12	47, 89, 131, 157	0
56	DY	101/110 (91%)	0.64	12 (11%) 5 1	60, 106, 149, 164	0
57	BZ	185/206 (89%)	0.86	28 (15%) 3 1	51, 113, 163, 188	0
57	DZ	185/206 (89%)	0.85	21 (11%) 6 1	99, 144, 171, 189	0
All	All	21266/22572 (94%)	0.40	1349 (6%) 19 3	20, 98, 177, 200	0

The worst 5 of 1349 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	277	C	16.2
43	BI	88	ILE	13.1
37	BC	171	ALA	13.0
22	CY	78	A	11.1
23	CW	36	C	10.7

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

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
22	AG9	AV	36	28/29	0.27	-	43,59,79,79	0
22	AG9	AY	36	28/29	0.32	-	43,59,79,79	0
22	AG9	CV	36	28/29	0.47	-	33,49,70,70	0
22	AG9	CY	36	28/29	0.54	-	33,49,70,70	0

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
58	ZN	CN	1000	1/1	0.07	-	178,178,178,178	0
58	ZN	AD	1000	1/1	0.25	-	165,165,165,165	0
58	ZN	CD	1000	1/1	0.28	-	200,200,200,200	0
58	ZN	AN	1000	1/1	0.08	-	88,88,88,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.