



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:33 PM BST

PDB ID : 4V9M
Title : 70S Ribosome translocation intermediate FA-4.2A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-25
Resolution : 4.00 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>

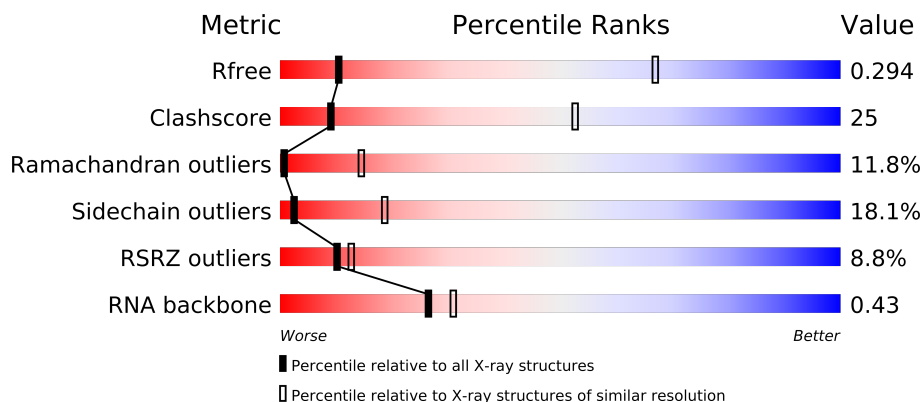
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)
RNA backbone	1838	1018 (5.00-2.80)

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

Mol	Chain	Length	Quality of chain
1	AB	235	
1	CB	235	
2	AC	207	
2	CC	207	
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	

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Mol	Chain	Length	Quality of chain
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	BC	228	
24	DC	228	
25	BD	275	
25	DD	275	
26	BE	205	
26	DE	205	
27	BF	208	
27	DF	208	

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Mol	Chain	Length	Quality of chain
28	BG	181	
28	DG	181	
29	BH	167	
29	DH	167	
30	BJ	170	
30	DJ	170	
31	BK	140	
31	DK	140	
32	BN	138	
32	DN	138	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	99	
38	BT	138	
38	DT	138	
39	BU	117	
39	DU	117	
40	BV	101	
40	DV	101	
41	BW	113	
41	DW	113	
42	BX	93	
42	DX	93	
43	BY	107	
43	DY	107	
44	BZ	185	
44	DZ	185	
45	B0	84	
45	D0	84	
46	B2	71	
46	D2	71	
47	B3	60	
47	D3	60	
48	B5	59	
48	D5	59	

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Mol	Chain	Length	Quality of chain
49	B6	50	
49	D6	50	
50	B7	49	
50	D7	49	
51	B8	64	
51	D8	64	
52	B9	37	
52	D9	37	
53	Be	102	
53	De	102	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	BA	2879	
58	DA	2879	
59	BB	119	
59	DB	119	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 308068 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			
2	CC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
4	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	HIS	ARG	CONFLICT	UNP P62669
CI	58	HIS	ARG	CONFLICT	UNP P62669

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			
9	CJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	96	GLU	GLN	CONFLICT	UNP P62658
CQ	96	GLU	GLN	CONFLICT	UNP P62658

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			
18	CS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	41	ILE	VAL	CONFLICT	UNP P62661
CT	41	ILE	VAL	CONFLICT	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
20	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			
21	CW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			
22	CV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			
23	CY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	CONFLICT	UNP Q72I01
AY	226	ASN	HIS	CONFLICT	UNP Q72I01
CY	129	LYS	HIS	CONFLICT	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
24	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	CONFLICT	UNP Q72GV9
BC	28	ARG	HIS	CONFLICT	UNP Q72GV9
DC	20	VAL	ILE	CONFLICT	UNP Q72GV9
DC	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
25	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
26	DE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
27	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05
BF	5	ALA	-	INSERTION	UNP Q72I05
BF	6	VAL	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05
DF	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	CONFLICT	UNP Q72I16
DG	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
29	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 30 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BJ	170	Total	C	N	O		0	0	0
			851	510	170	171				
30	DJ	170	Total	C	N	O		0	0	0
			851	510	170	171				

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			
31	DK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	CONFLICT	UNP Q72I14
DO	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	CONFLICT	UNP Q72I11
DQ	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BS	99	Total	C	N	O		0	0	0
			775	488	155	132				
37	DS	99	Total	C	N	O		0	0	0
			775	488	155	132				

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
38	DT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	CONFLICT	UNP Q72JU9
BT	135	ALA	VAL	CONFLICT	UNP Q72JU9
DT	123	GLN	LYS	CONFLICT	UNP Q72JU9
DT	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BX	93	Total	C	N	O	0	0	0
			734	477	132	125			
42	DX	93	Total	C	N	O	0	0	0
			734	477	132	125			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			
43	DY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	DZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	CONFLICT	UNP Q72HR3
D0	11	ARG	LYS	CONFLICT	UNP Q72HR3

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
47	D3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
48	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	CONFLICT	UNP P62652
D5	29	THR	ILE	CONFLICT	UNP P62652

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
50	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
51	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

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

- Molecule 53 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Be	102	Total	C	N	O		0	0	0
			686	430	119	137				
53	De	102	Total	C	N	O		0	0	0
			686	430	119	137				

- Molecule 54 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	Bf	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Bg	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Df	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Dg	31	Total	C	N	O	0	0	0
			156	93	31	32			

- Molecule 55 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	Bh	30	Total	C	N	O	0	0	0
			151	90	30	31			
55	Dh	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 56 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
56	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	CONFLICT	UNP Q72G84
D1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
57	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

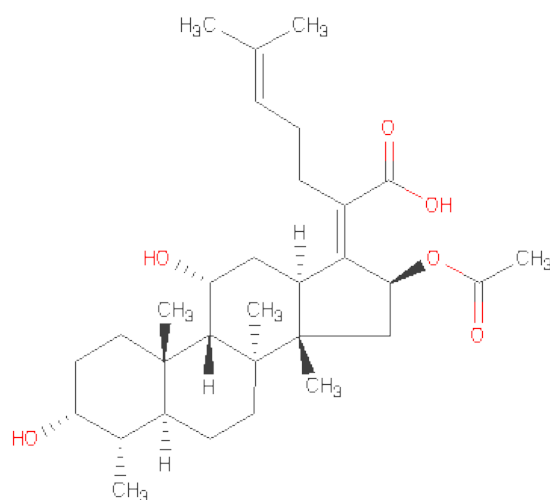
- Molecule 58 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
58	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 59 is a RNA chain called 5S ribosomal RNA.

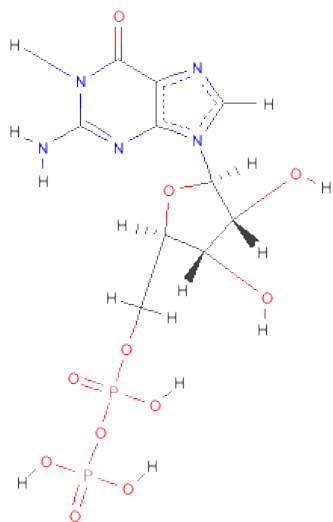
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
59	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 60 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	AY	1	Total	C	O	0	0
			37	31	6		
60	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

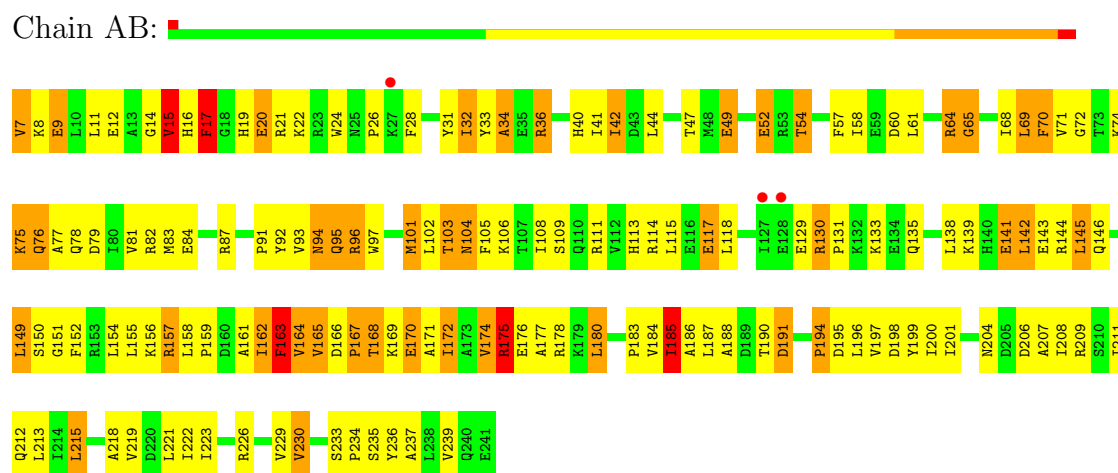


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
61	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

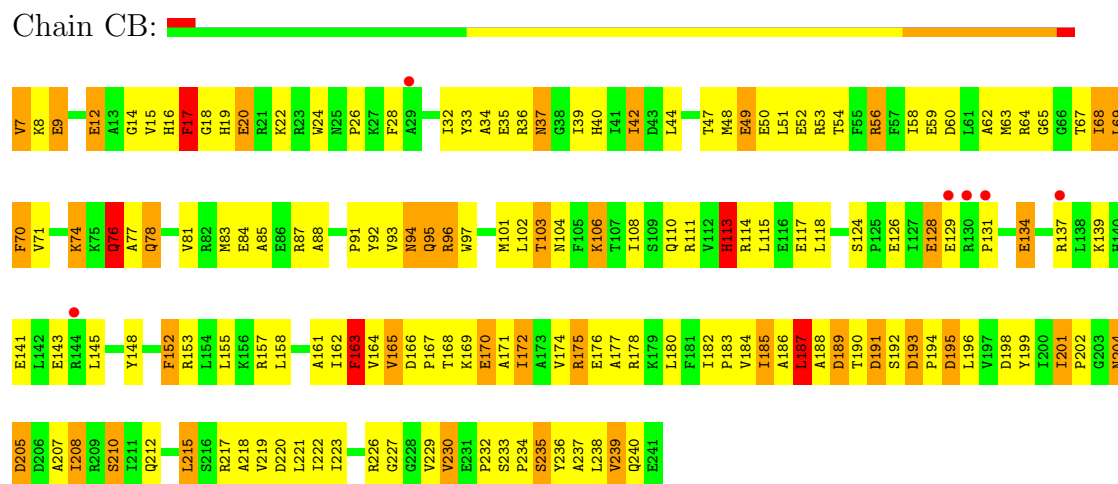
3 Residue-property plots

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.

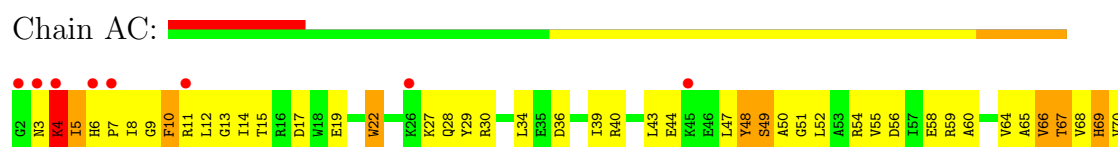
• Molecule 1: 30S ribosomal protein S2

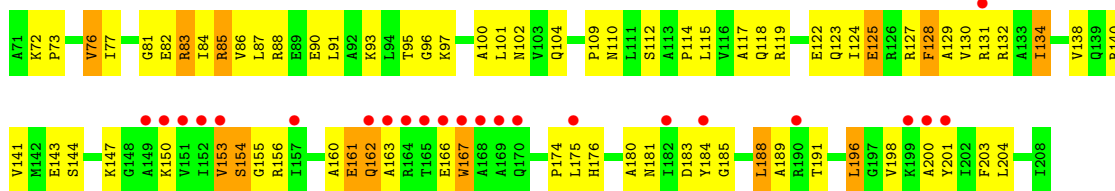


• Molecule 1: 30S ribosomal protein S2



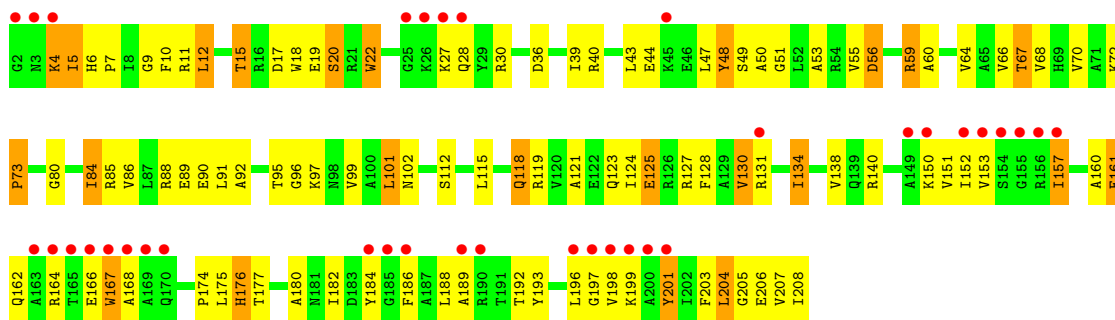
• Molecule 2: 30S ribosomal protein S3





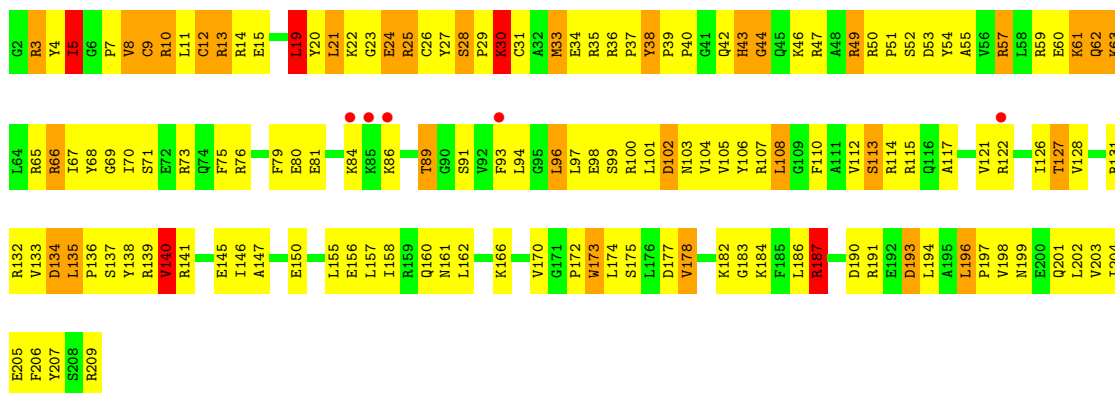
• Molecule 2: 30S ribosomal protein S3

Chain CC:



• Molecule 3: 30S ribosomal protein S4

Chain AD:



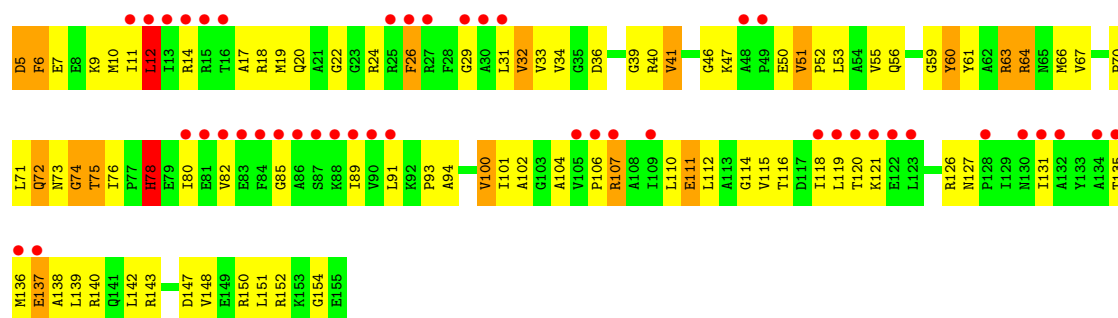
• Molecule 3: 30S ribosomal protein S4

Chain CD:



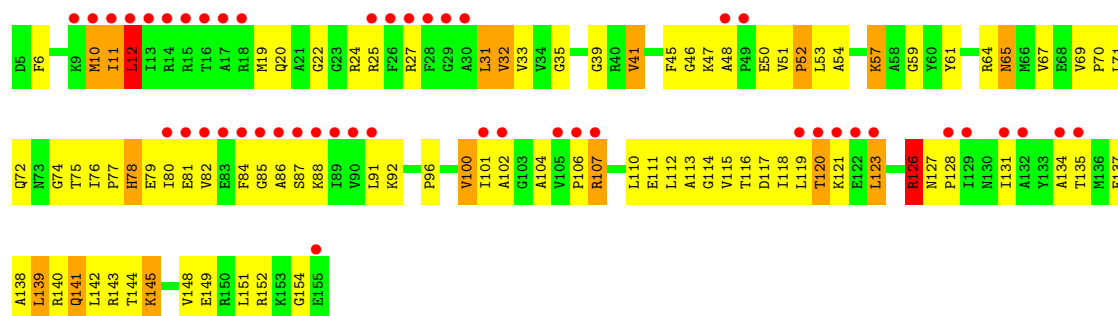
• Molecule 4: 30S ribosomal protein S5

Chain AE:



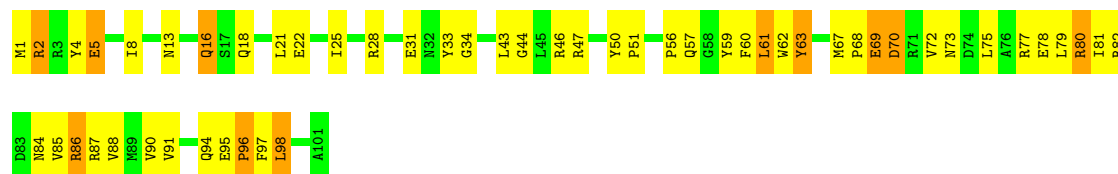
• Molecule 4: 30S ribosomal protein S5

Chain CE:



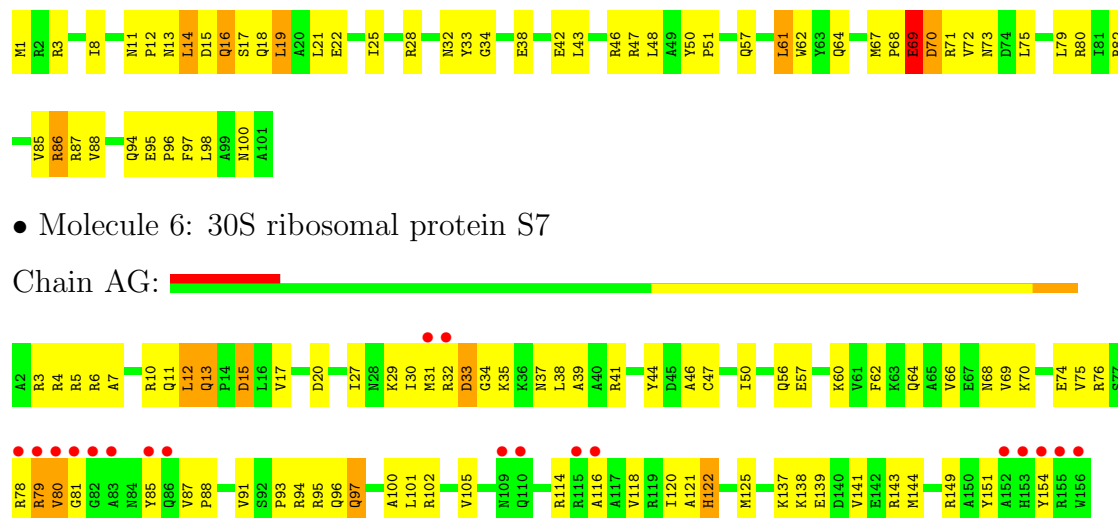
• Molecule 5: 30S ribosomal protein S6

Chain AF:



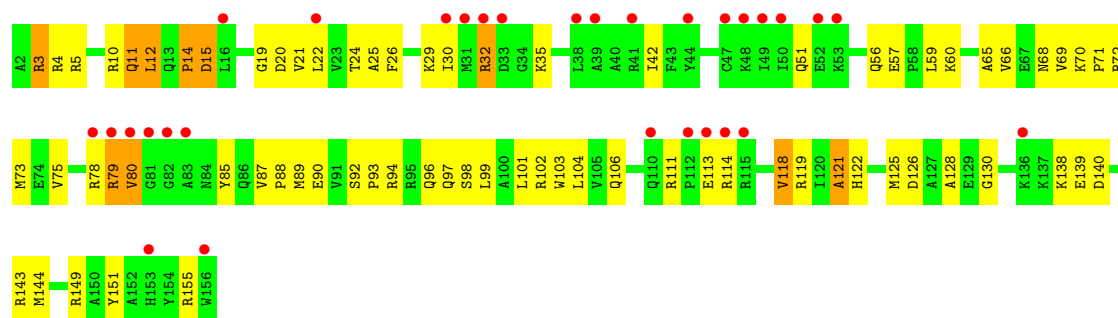
• Molecule 6: 30S ribosomal protein S7

Chain AG:



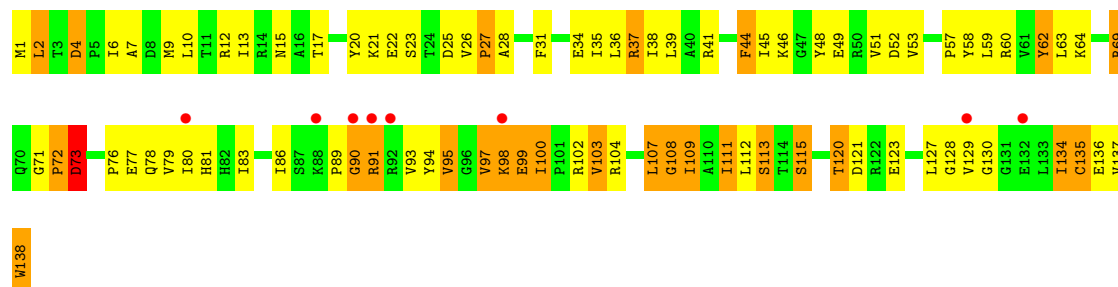
- Molecule 6: 30S ribosomal protein S7

Chain CG:



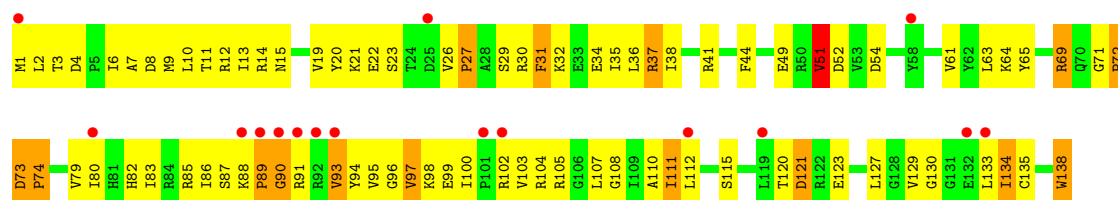
- Molecule 7: 30S ribosomal protein S8

Chain AH:



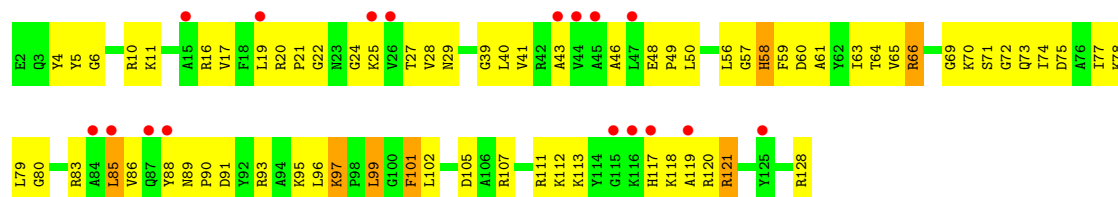
- Molecule 7: 30S ribosomal protein S8

Chain CH:



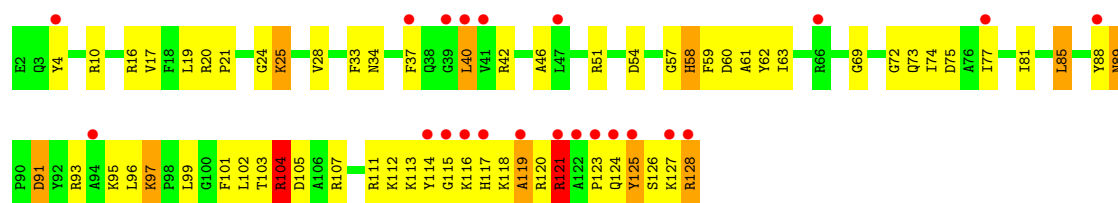
- Molecule 8: 30S ribosomal protein S9

Chain AI:



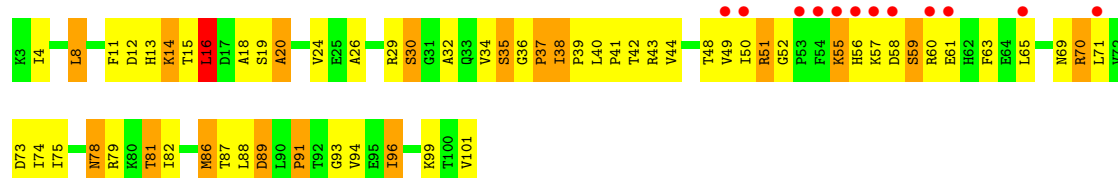
- Molecule 8: 30S ribosomal protein S9

Chain CI:



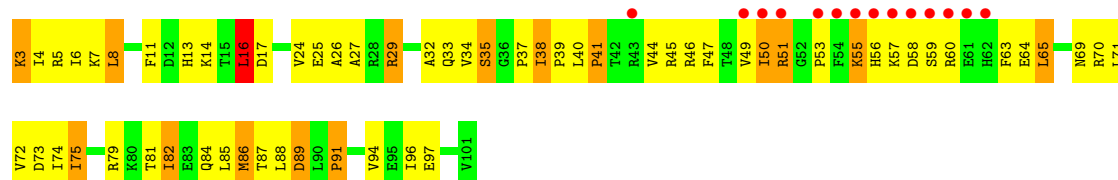
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



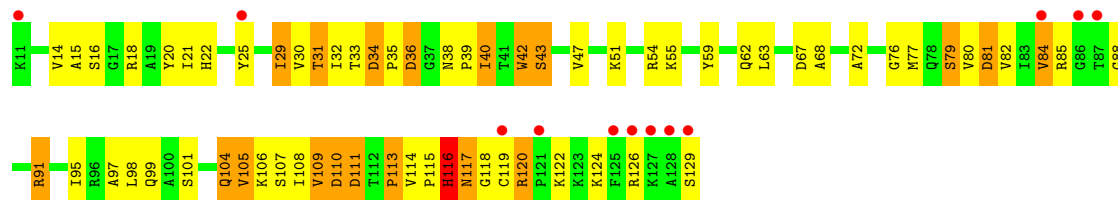
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



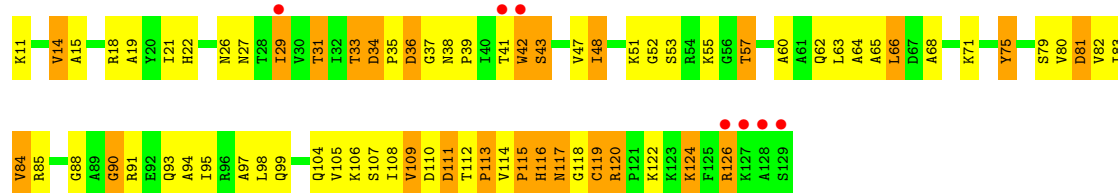
• Molecule 10: 30S ribosomal protein S11

Chain AK:



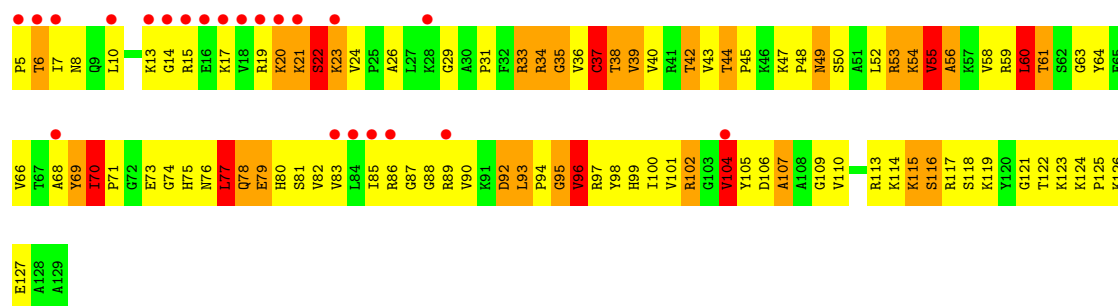
• Molecule 10: 30S ribosomal protein S11

Chain CK:



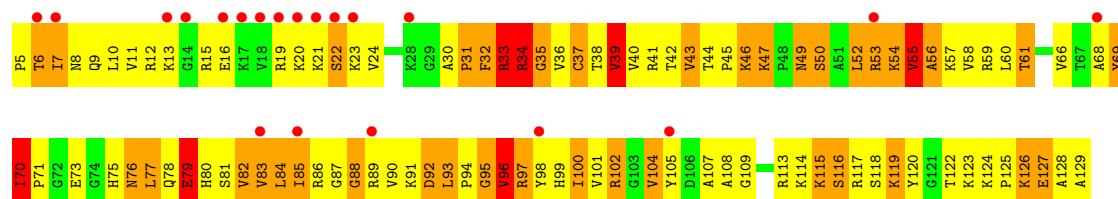
• Molecule 11: 30S ribosomal protein S12

Chain AL:



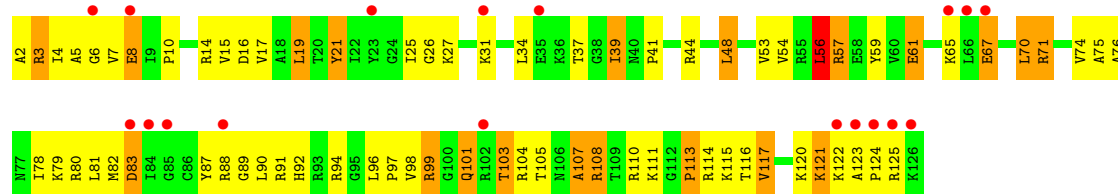
- Molecule 11: 30S ribosomal protein S12

Chain CL:



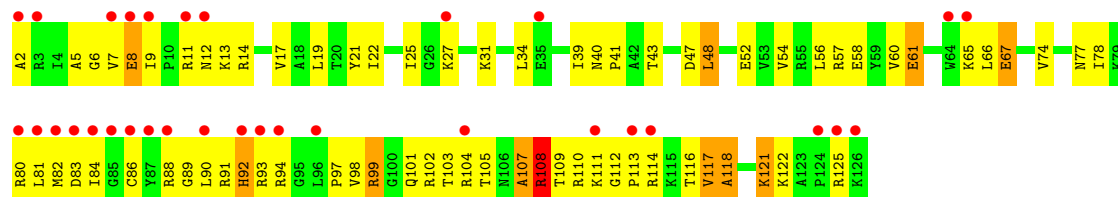
- Molecule 12: 30S ribosomal protein S13

Chain AM:



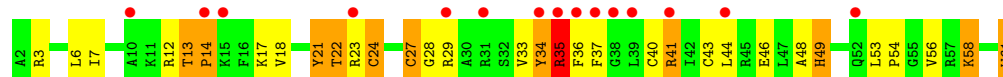
- Molecule 12: 30S ribosomal protein S13

Chain CM:



- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:



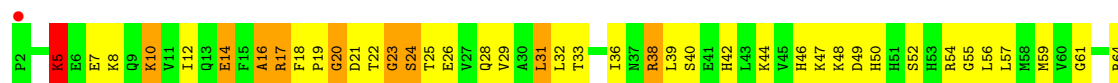
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN: 



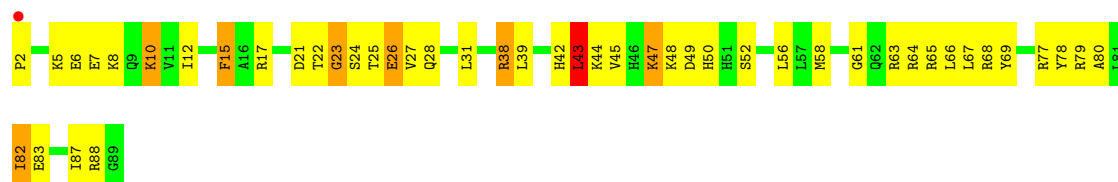
- Molecule 14: 30S ribosomal protein S15

Chain AO:



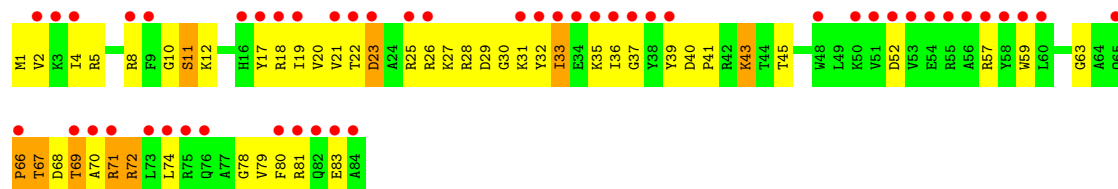
- Molecule 14: 30S ribosomal protein S15

Chain CO:



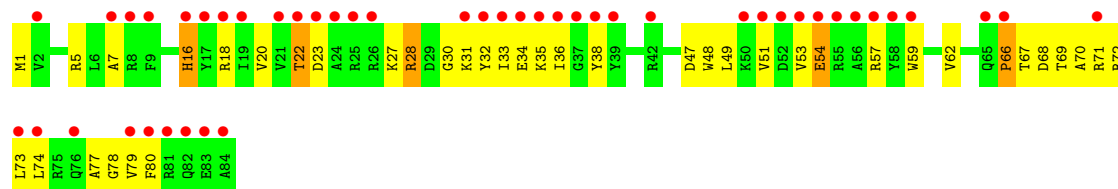
- Molecule 15: 30S ribosomal protein S16

Chain AP:



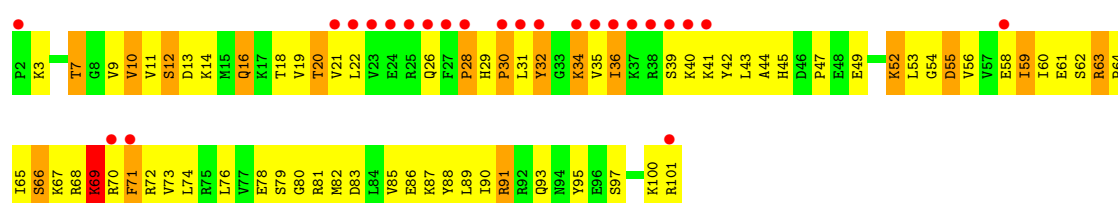
- Molecule 15: 30S ribosomal protein S16

Chain CP:

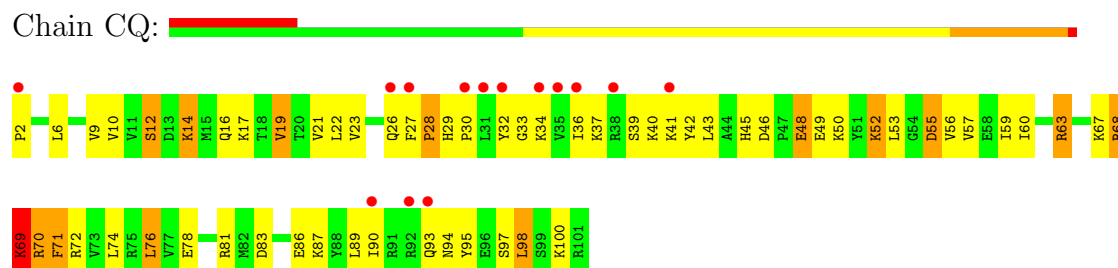


- Molecule 16: 30S ribosomal protein S17

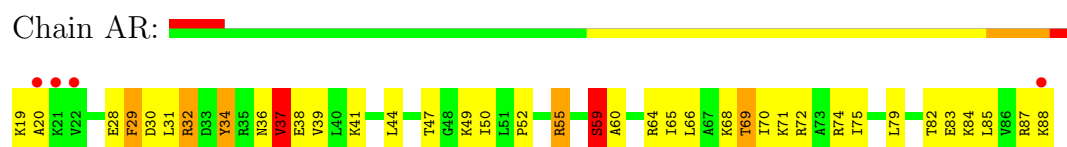
Chain AQ:



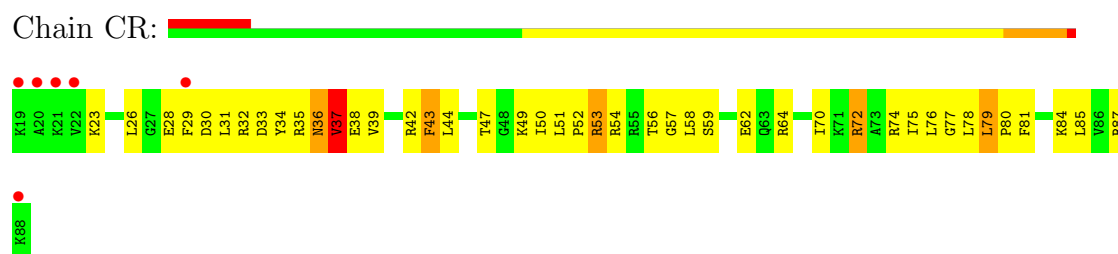
- Molecule 16: 30S ribosomal protein S17



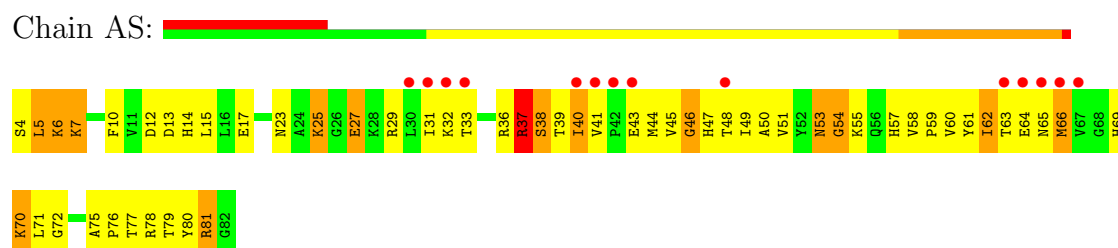
- Molecule 17: 30S ribosomal protein S18



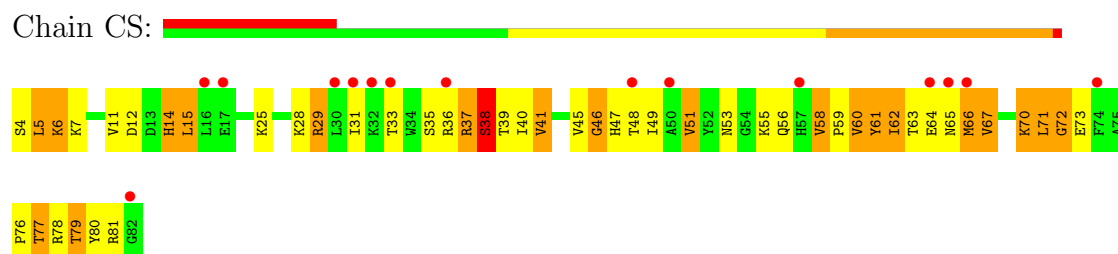
- Molecule 17: 30S ribosomal protein S18



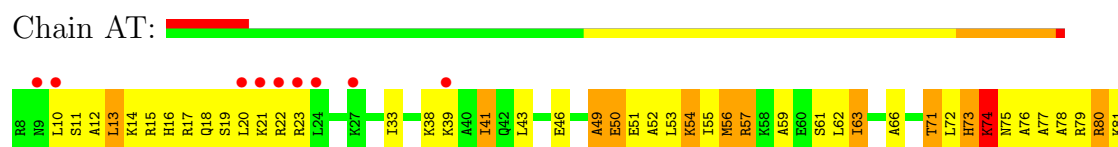
- Molecule 18: 30S ribosomal protein S19



- Molecule 18: 30S ribosomal protein S19



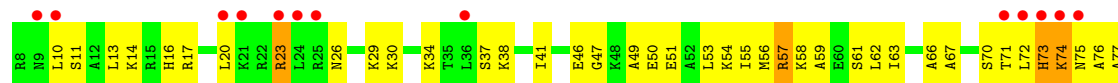
- Molecule 19: 30S ribosomal protein S20





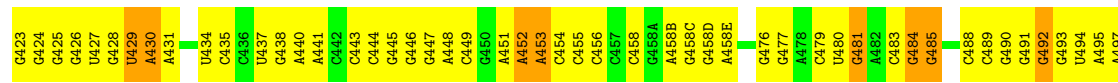
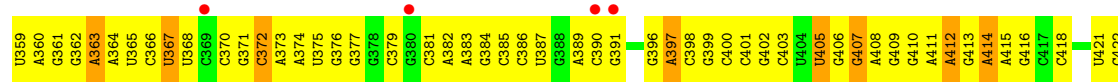
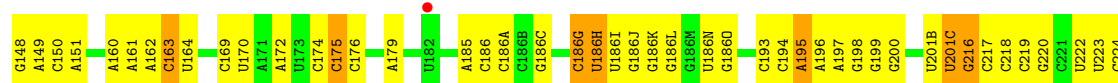
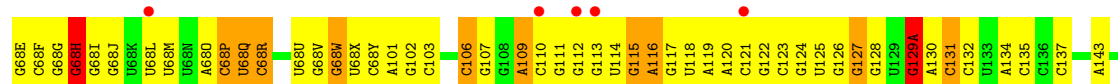
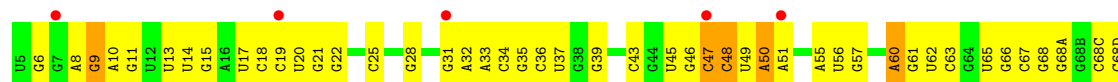
- Molecule 19: 30S ribosomal protein S20

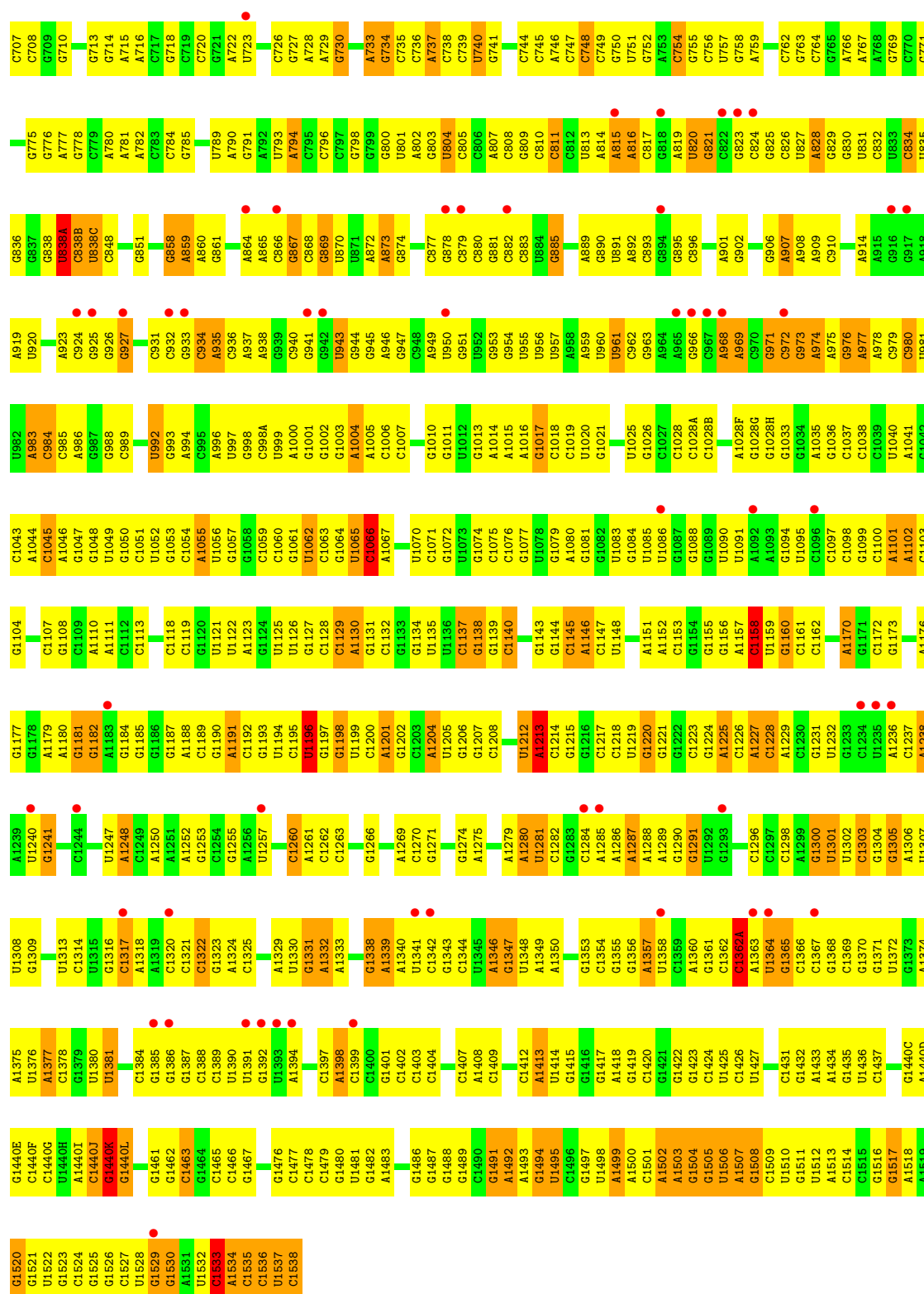
Chain CT:



- Molecule 20: ribosomal RNA 16S

Chain AA:

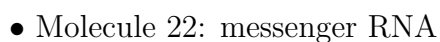




• Molecule 20: ribosomal RNA 16S

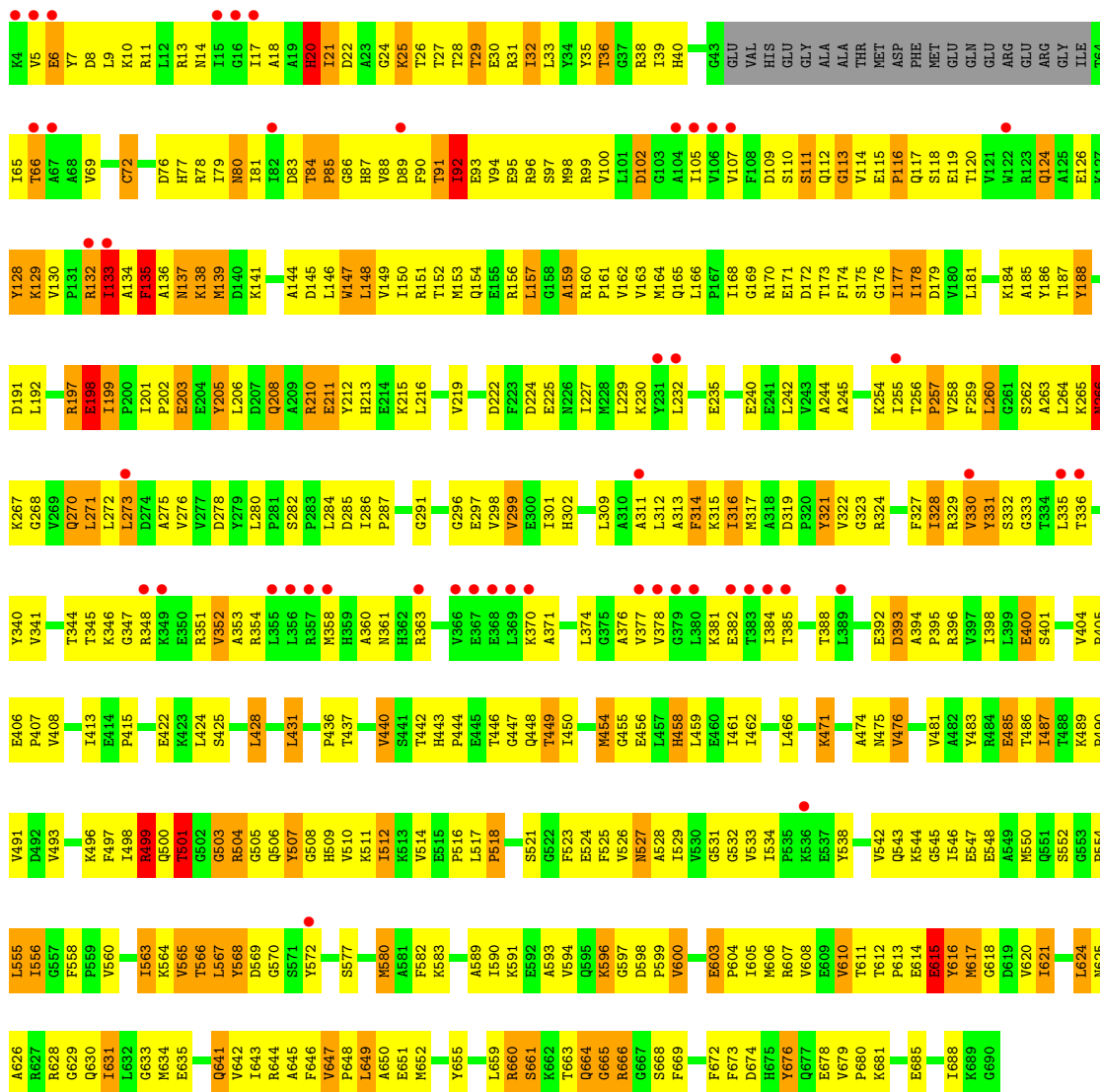
Chain CA:



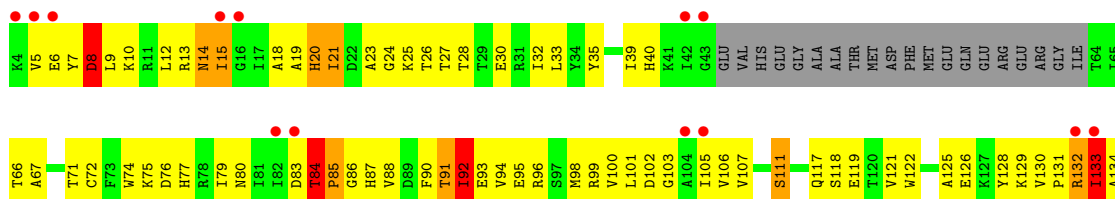


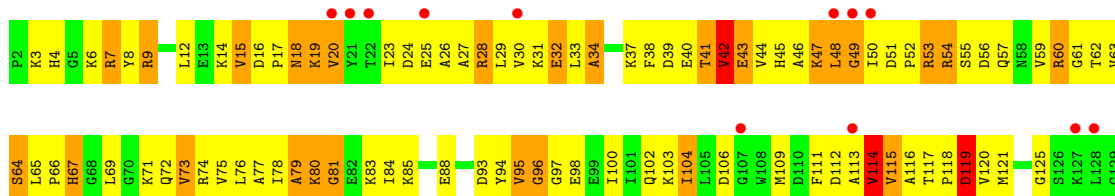
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G6	1
G7	1
A8	1
G9	1
G10	1
U11	1
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A15	1
A16	1
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G19	1
U20	1
A21	1
A22	1
A23	1
A24	1
A25	1
A26	1

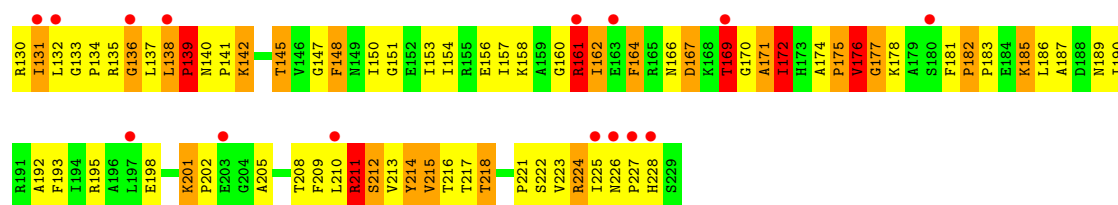
Chain AY:



Chain CY:

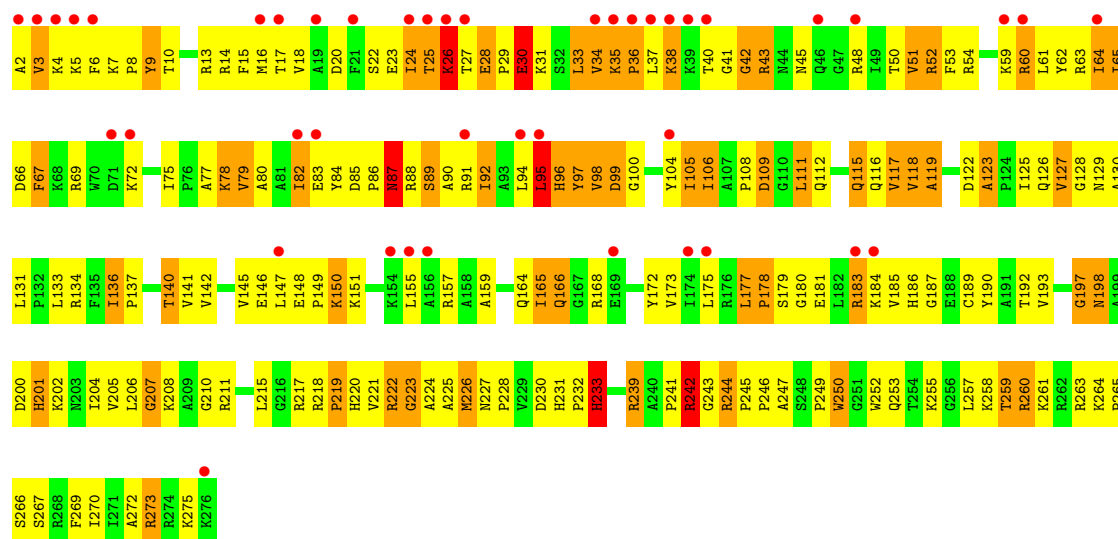






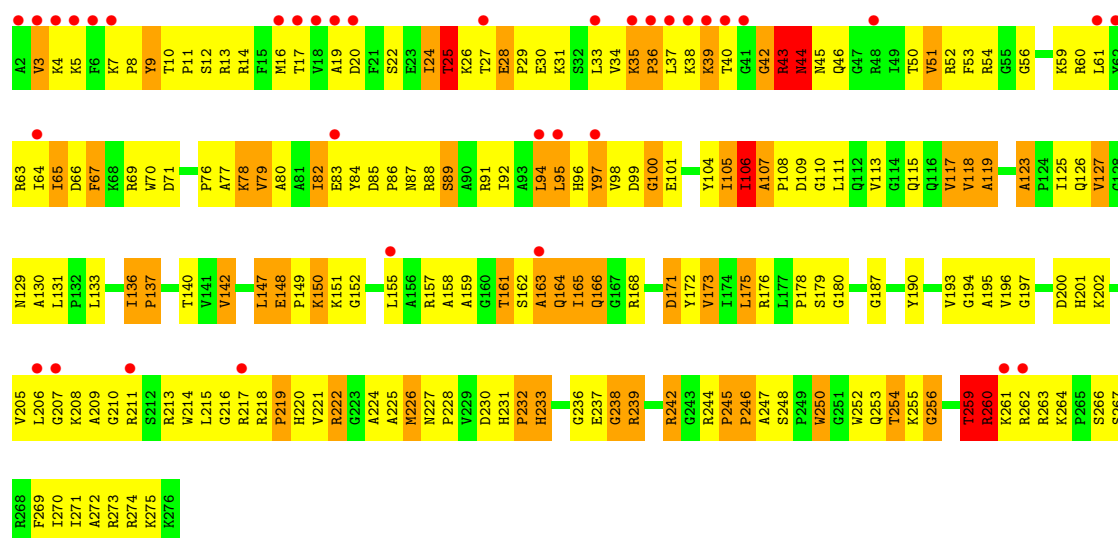
• Molecule 25: 50S ribosomal protein L2

Chain BD:



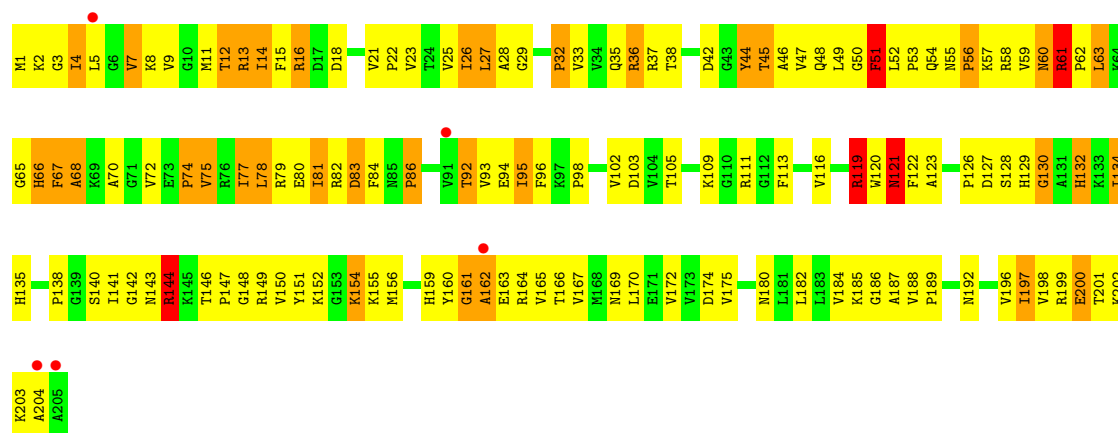
• Molecule 25: 50S ribosomal protein L2

Chain DD:



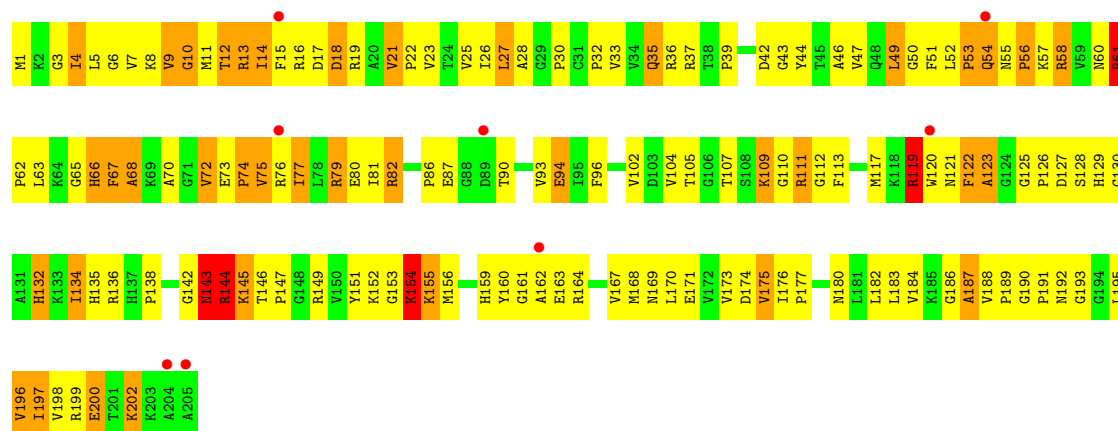
• Molecule 26: 50S ribosomal protein L3

Chain BE:



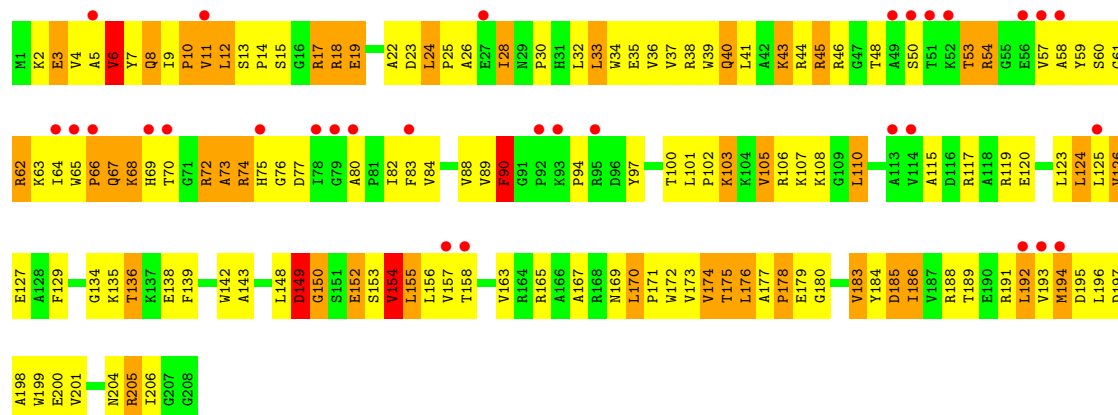
• Molecule 26: 50S ribosomal protein L3

Chain DE:



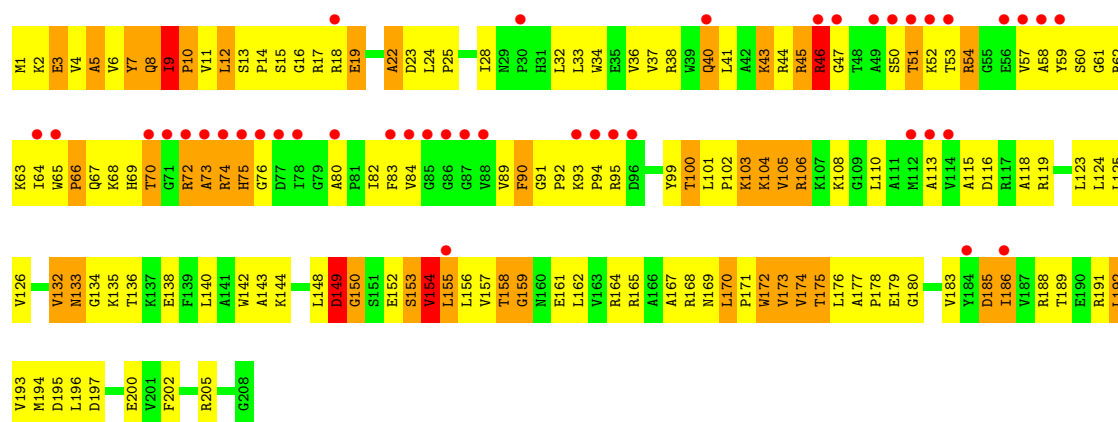
• Molecule 27: 50S ribosomal protein L4

Chain BF:



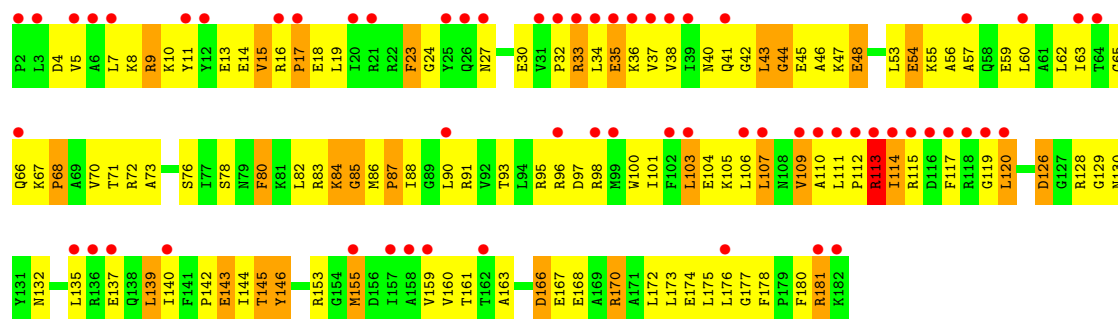
• Molecule 27: 50S ribosomal protein L4

Chain DF:



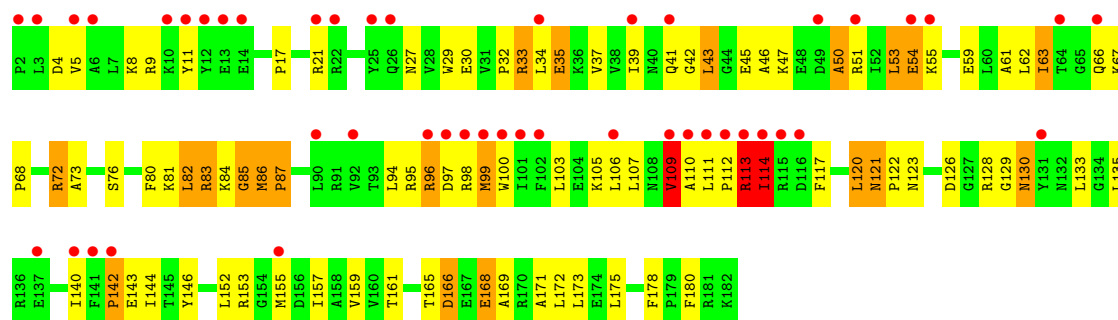
• Molecule 28: 50S ribosomal protein L5

Chain BG:



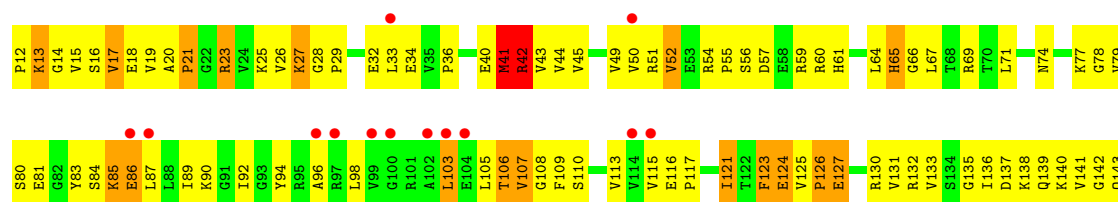
• Molecule 28: 50S ribosomal protein L5

Chain DG:



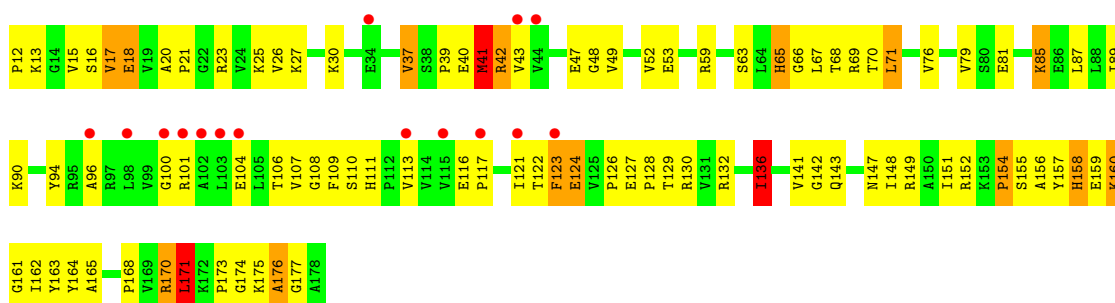
• Molecule 29: 50S ribosomal protein L6

Chain BH:



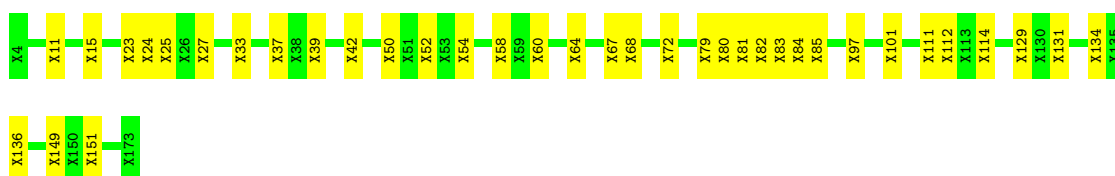
- Molecule 29: 50S ribosomal protein L6

Chain DH:



- Molecule 30: 50S ribosomal protein L10

Chain BJ:



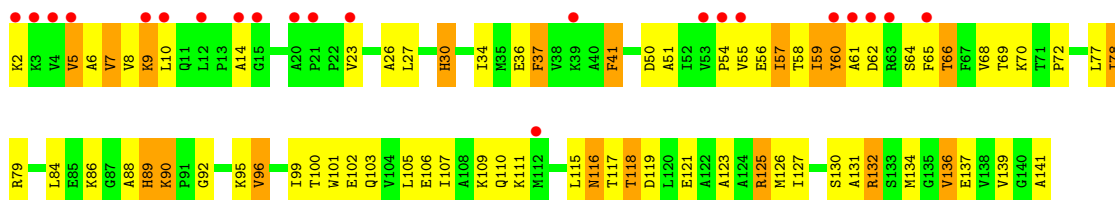
- Molecule 30: 50S ribosomal protein L10

Chain DJ:



- Molecule 31: 50S ribosomal protein L11

Chain BK:



- Molecule 31: 50S ribosomal protein L11

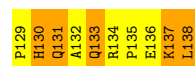
Chain DK:





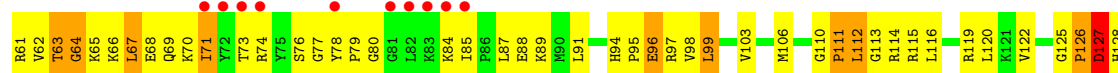
• Molecule 32: 50S ribosomal protein L13

Chain BN:



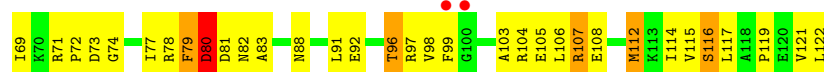
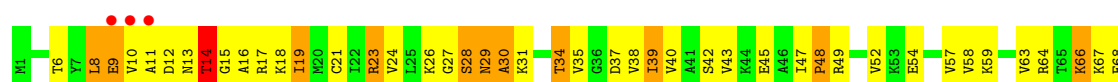
• Molecule 32: 50S ribosomal protein L13

Chain DN:



• Molecule 33: 50S ribosomal protein L14

Chain BO:



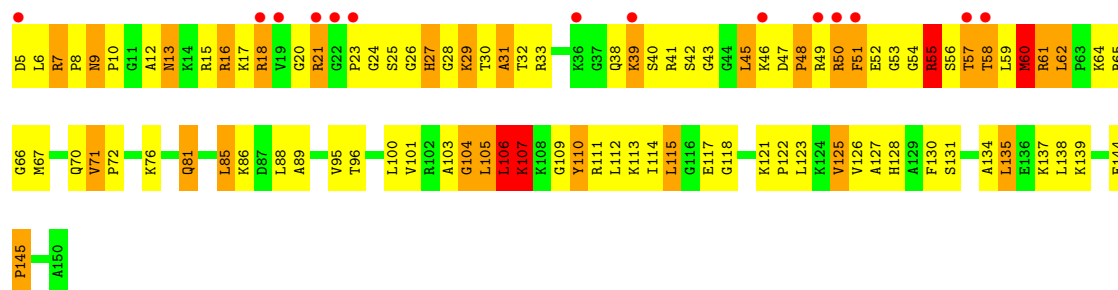
• Molecule 33: 50S ribosomal protein L14

Chain DO:



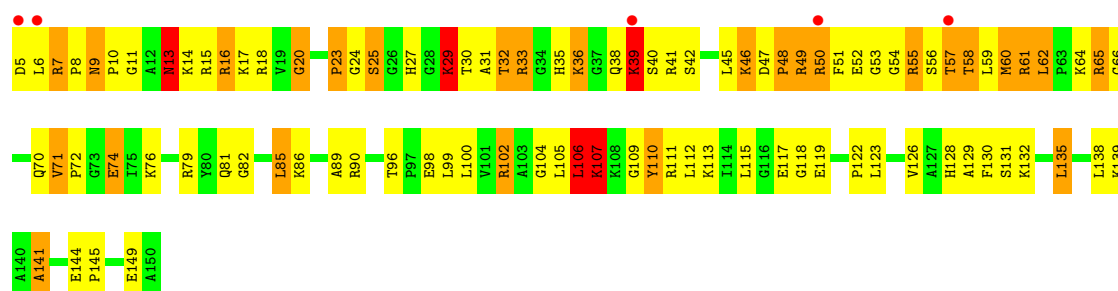
• Molecule 34: 50S ribosomal protein L15

Chain BP: 



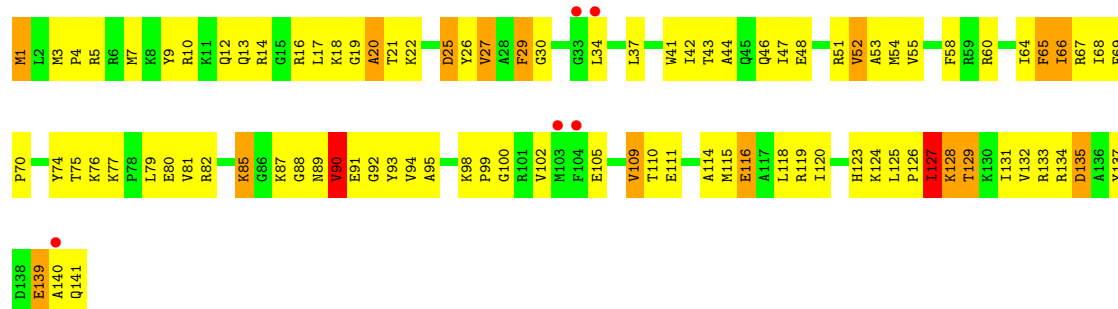
- Molecule 34: 50S ribosomal protein L15

Chain DP: 



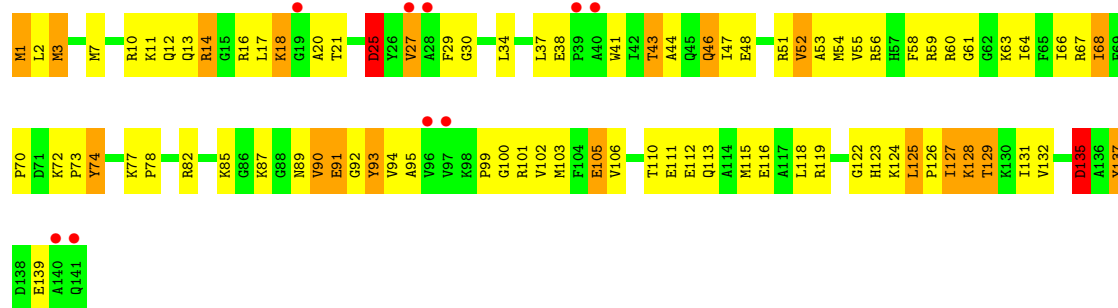
- Molecule 35: 50S ribosomal protein L16

Chain BQ: 



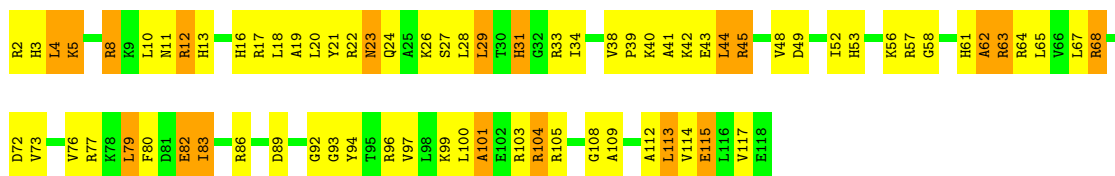
- Molecule 35: 50S ribosomal protein L16

Chain DQ: 



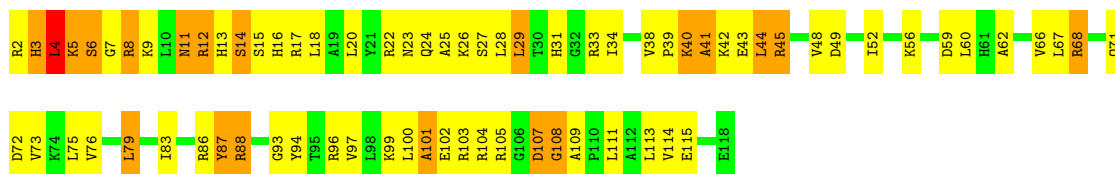
- Molecule 36: 50S ribosomal protein L17

Chain BR:



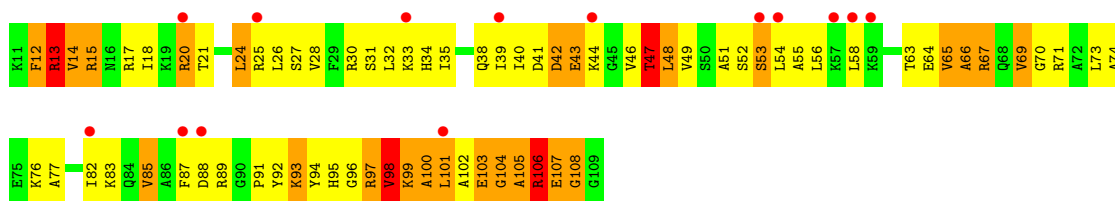
- Molecule 36: 50S ribosomal protein L17

Chain DR:



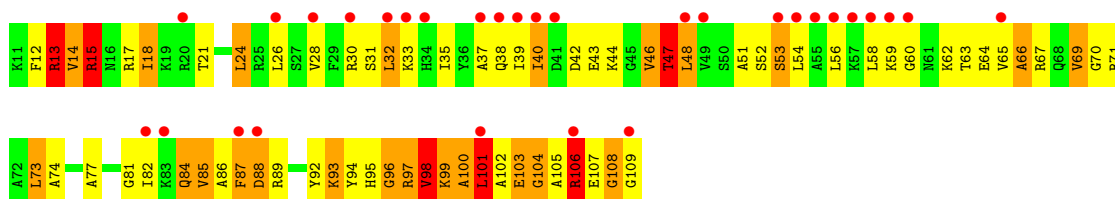
- Molecule 37: 50S ribosomal protein L18

Chain BS:



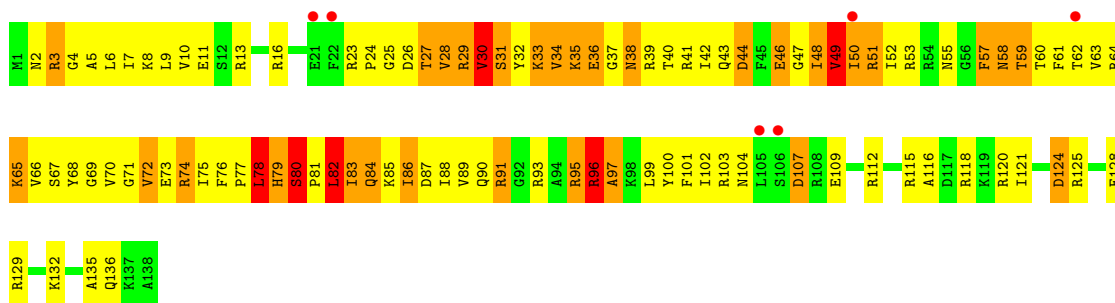
- Molecule 37: 50S ribosomal protein L18

Chain DS:



- Molecule 38: 50S ribosomal protein L19

Chain BT:



- Molecule 38: 50S ribosomal protein L19

Category	Item	Value	Color
A	A135	G69	Yellow
	Q136	V70	Red
	K137	G71	Yellow
	A138	V72	Green
		E73	Yellow
		R74	Yellow
		L75	Yellow
		F76	Yellow
		P77	Yellow
		L78	Yellow
B		H79	Orange
		S80	Red
		P81	Green
		L82	Yellow
		I83	Yellow
		O84	Yellow
		G85	Red
		T86	Yellow
		D87	Yellow
		L88	Yellow
C		V89	Yellow
		Q90	Yellow
		R91	Yellow
		G92	Yellow
		R93	Yellow
		A94	Yellow
		R95	Yellow
		K98	Yellow
		L99	Yellow
		Y100	Yellow
D		F101	Yellow
		I102	Yellow
		R103	Yellow
		N104	Yellow
		L105	Yellow
		S106	Green
		D107	Yellow
		R108	Yellow
		E109	Yellow
		I110	Yellow
E		R111	Yellow
		L114	Yellow
		R115	Orange
		K119	Yellow
		R120	Green
		I121	Yellow
		D124	Yellow
		R125	Yellow
		E128	Orange
		R129	Yellow
F		A130	Yellow
		A131	Yellow
		K132	Yellow
		E133	Yellow
		E134	Yellow
		M1	Yellow
		N2	Yellow
		R3	Yellow
		L6	Yellow
		I7	Green
G		K8	Yellow
		E11	Yellow
		S12	Yellow
		R13	Orange
		Y14	Yellow
		V15	Yellow
		R16	Yellow
		L19	Yellow
		P20	Yellow
		E21	Green
H		F22	Yellow
		R23	Yellow
		P24	Yellow
		G25	Yellow
		D26	Green
		T27	Yellow
		V28	Yellow
		R29	Yellow
		V30	Red
		S31	Yellow
I		Y32	Yellow
		K33	Yellow
		V34	Yellow
		K35	Yellow
		E36	Orange
		R41	Yellow
		D44	Yellow
		F45	Yellow
		E46	Yellow
		G47	Yellow
J		I48	Yellow
		V49	Yellow
		L50	Red
		R51	Yellow
		I52	Yellow
		R53	Yellow
		R54	Green
		N55	Yellow
		G56	Green
		F57	Yellow
K		N58	Yellow
		T59	Yellow
		T60	Yellow
		F61	Yellow
		T62	Yellow
		V63	Yellow
		R64	Yellow
		K65	Yellow
		V66	Yellow

- | Category | Item | Value | Color |
|-----------------------|------|-------|-------|
| Top Row | L74 | 100 | Blue |
| | N75 | 100 | Blue |
| | Y76 | 100 | Blue |
| | S77 | 100 | Blue |
| | T78 | 100 | Blue |
| | F79 | 100 | Red |
| | L80 | 100 | Blue |
| | K81 | 100 | Blue |
| | L83 | 100 | Blue |
| | K84 | 100 | Blue |
| Bottom Row | L88 | 100 | Blue |
| | E89 | 100 | Blue |
| | V90 | 100 | Blue |
| | D91 | 100 | Blue |
| | K92 | 100 | Blue |
| | R93 | 100 | Blue |
| | N94 | 100 | Blue |
| | L95 | 100 | Blue |
| | A96 | 100 | Blue |
| | D97 | 100 | Blue |
| Middle Row | L98 | 100 | Blue |
| | A99 | 100 | Blue |
| | V100 | 100 | Blue |
| | E101 | 100 | Blue |
| | E102 | 100 | Blue |
| | P103 | 100 | Blue |
| | Q104 | 100 | Blue |
| | V105 | 100 | Blue |
| | F106 | 100 | Blue |
| | A107 | 100 | Blue |
| Right Row | E108 | 100 | Blue |
| | L109 | 100 | Blue |
| | G118 | 100 | Blue |
| | P2 | 100 | Blue |
| | R3 | 100 | Blue |
| | A4 | 100 | Blue |
| | V8 | 100 | Blue |
| | V9 | 100 | Blue |
| | R10 | 100 | Blue |
| | R11 | 100 | Blue |
| Far Right | K12 | 100 | Blue |
| | K13 | 100 | Blue |
| | H14 | 100 | Blue |
| | K15 | 100 | Blue |
| | K16 | 100 | Blue |
| | I17 | 100 | Blue |
| | L18 | 100 | Blue |
| | K19 | 100 | Blue |
| | L20 | 100 | Blue |
| | A21 | 100 | Blue |
| Far Right (Continued) | K22 | 100 | Blue |
| | W25 | 100 | Blue |
| | G26 | 100 | Blue |
| | S29 | 100 | Blue |
| | F32 | 100 | Blue |
| | R33 | 100 | Blue |
| | K34 | 100 | Blue |
| | A35 | 100 | Blue |
| | R36 | 100 | Blue |
| | E37 | 100 | Blue |
| Far Right (Continued) | T38 | 100 | Blue |
| | L39 | 100 | Blue |
| | F40 | 100 | Blue |
| | A41 | 100 | Blue |
| | A42 | 100 | Blue |
| | Y45 | 100 | Blue |
| | H49 | 100 | Blue |
| | R50 | 100 | Blue |
| | K51 | 100 | Blue |
| | R52 | 100 | Blue |
| R53 | 100 | Blue | |
| Far Right (Continued) | K54 | 100 | Blue |
| | R55 | 100 | Blue |
| | D56 | 100 | Blue |
| | F57 | 100 | Blue |
| | R58 | 100 | Blue |
| | R59 | 100 | Blue |
| | L60 | 100 | Blue |
| | W61 | 100 | Blue |
| | I62 | 100 | Blue |
| | V63 | 100 | Blue |
| R64 | 100 | Blue | |
| Far Right (Continued) | I65 | 100 | Blue |
| | N66 | 100 | Blue |
| | A67 | 100 | Blue |
| | A68 | 100 | Blue |

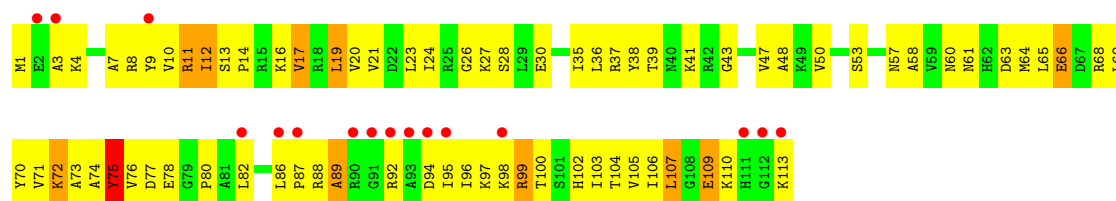
-
- The chart displays the frequency of 100 categories, each represented by a colored bar. The categories are labeled with IDs, and the bars are color-coded from green (low frequency) to red (high frequency). The chart is organized into two rows of 50 categories each.
- | Category ID | Frequency (approx.) |
|-------------|---------------------|
| F2 | 10 |
| R3 | 10 |
| A4 | 10 |
| X5 | 10 |
| T6 | 10 |
| R10 | 10 |
| R11 | 10 |
| R12 | 10 |
| K13 | 10 |
| H14 | 10 |
| K15 | 10 |
| L18 | 10 |
| K19 | 10 |
| L20 | 10 |
| T24 | 10 |
| G25 | 10 |
| G26 | 10 |
| L27 | 10 |
| R28 | 10 |
| S29 | 10 |
| F32 | 10 |
| R33 | 10 |
| K34 | 10 |
| A35 | 10 |
| R36 | 10 |
| S37 | 10 |
| T38 | 10 |
| L39 | 10 |
| F40 | 10 |
| A47 | 10 |
| A48 | 10 |
| H49 | 10 |
| R50 | 10 |
| K51 | 10 |
| R52 | 10 |
| R53 | 10 |
| K54 | 10 |
| R55 | 10 |
| D56 | 10 |
| F57 | 10 |
| R58 | 10 |
| S59 | 10 |
| L60 | 10 |
| A61 | 10 |
| L62 | 10 |
| V63 | 10 |
| R64 | 10 |
| L65 | 10 |
| G69 | 10 |
| R70 | 10 |
| L74 | 10 |
| R75 | 10 |
| T76 | 10 |
| F79 | 10 |
| I80 | 10 |
| L83 | 10 |
| R84 | 10 |
| R85 | 10 |
| A86 | 10 |
| G87 | 10 |
| I88 | 10 |
| E89 | 10 |
| V90 | 10 |
| D91 | 10 |
| R92 | 10 |
| K93 | 10 |
| N94 | 10 |
| L95 | 10 |
| A96 | 10 |
| D97 | 10 |
| L98 | 10 |
| A99 | 10 |
| V100 | 10 |
| R101 | 10 |
| E102 | 10 |
| P103 | 10 |
| Q104 | 10 |
| V105 | 10 |
| E108 | 10 |
| L109 | 10 |
| V110 | 10 |
| E111 | 10 |
| R112 | 10 |
| A113 | 10 |
| K114 | 10 |
| A115 | 10 |
| A116 | 10 |
| Q117 | 10 |
| G118 | 10 |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| K69 | L70 | L71 | L72 | V73 | V74 | K75 | F76 | A77 | K78 | V79 | Q80 | Y81 | R82 | R83 | K84 | K85 | G86 | H87 | R88 | Q89 | P90 | Y91 | T92 | E93 | L94 | I95 | I96 | K97 | E98 | R99 | R100 | G101 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| M1 | F2 | A3 | I4 | V5 | K6 | T7 | | Q10 | K11 | Q12 | R13 | V14 | E15 | P16 | G17 | I18 | K19 | L20 | R21 | | K24 | | E28 | P29 | | V33 | E34 | I35 | P36 | V37 | L38 | L39 | L40 | G41 | | T45 | V46 | V47 | G48 | T49 | P50 | V51 | V52 | E53 | G54 | A55 | S56 | V57 | V58 | A59 | E60 | V61 | L62 | G63 | H64 | G65 | R66 | G67 | V69 |

-

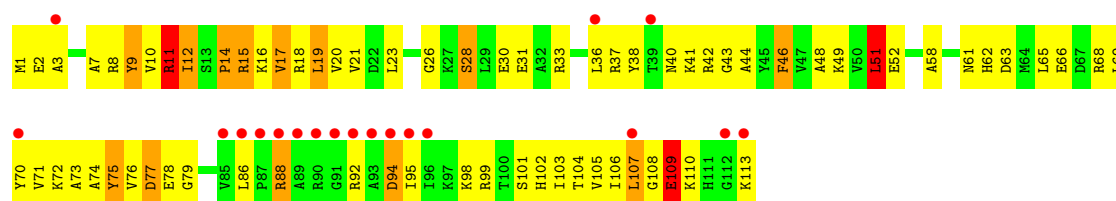
- Molecule 41: 50S ribosomal protein L22

Chain BW:



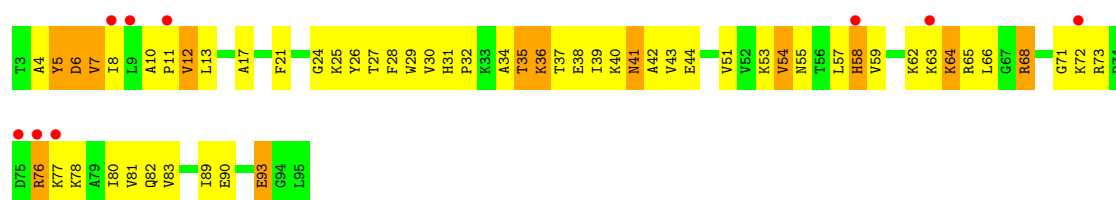
- Molecule 41: 50S ribosomal protein L22

Chain DW:



- Molecule 42: 50S ribosomal protein L23

Chain BX:



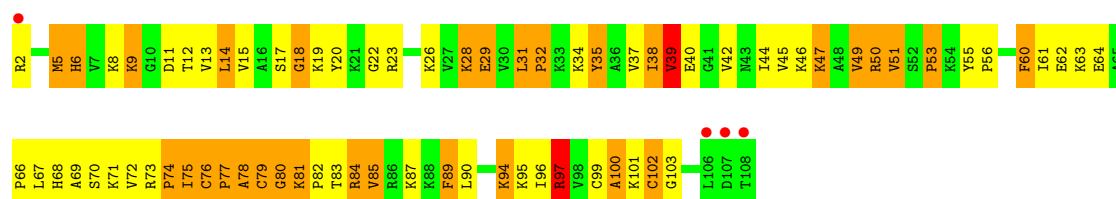
- Molecule 42: 50S ribosomal protein L23

Chain DX:



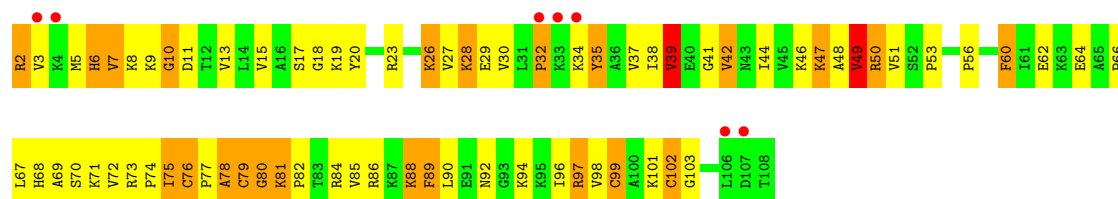
- Molecule 43: 50S ribosomal protein L24

Chain BY:



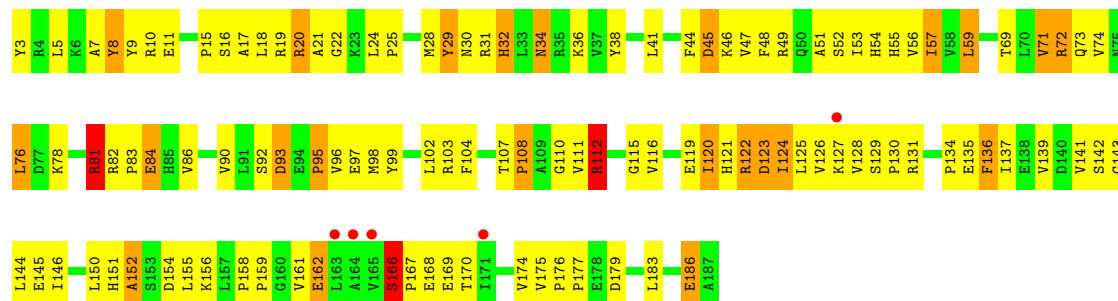
- Molecule 43: 50S ribosomal protein L24

Chain DY:



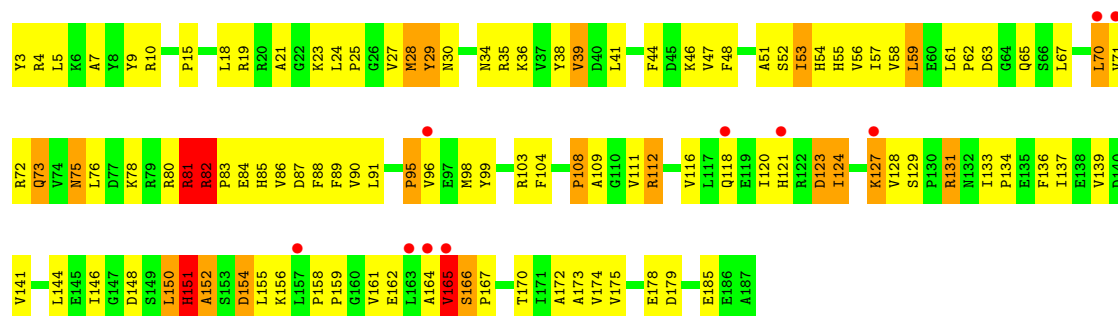
- Molecule 44: 50S ribosomal protein L25

Chain BZ:



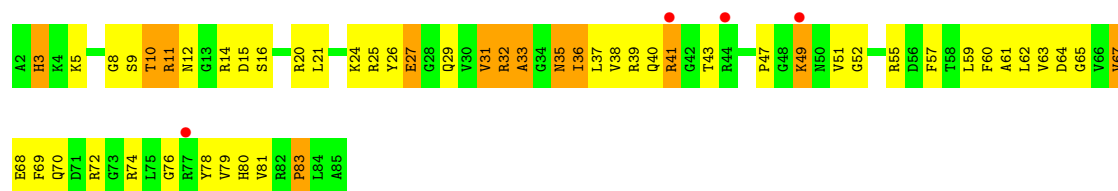
- Molecule 44: 50S ribosomal protein L25

Chain DZ:



- Molecule 45: 50S ribosomal protein L27

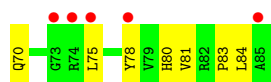
Chain B0:



- Molecule 45: 50S ribosomal protein L27

Chain D0:





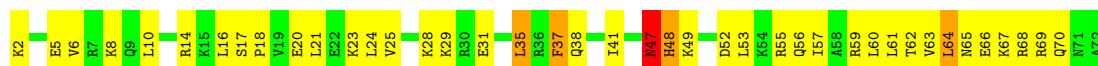
- Molecule 46: 50S ribosomal protein L29

Chain B2:



- Molecule 46: 50S ribosomal protein L29

Chain D2:



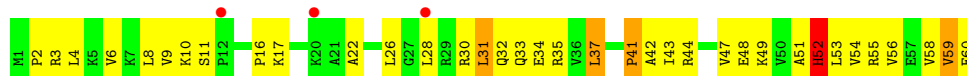
- Molecule 47: 50S ribosomal protein L30

Chain B3:



- Molecule 47: 50S ribosomal protein L30

Chain D3:



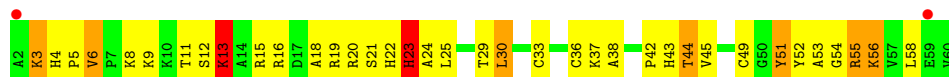
- Molecule 48: 50S ribosomal protein L32

Chain B5:



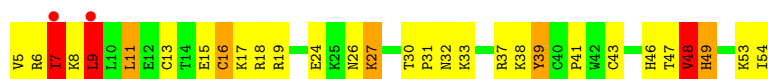
- Molecule 48: 50S ribosomal protein L32

Chain D5:



- Molecule 49: 50S ribosomal protein L33

Chain B6:



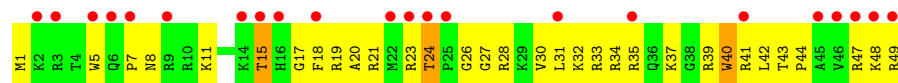
- Molecule 49: 50S ribosomal protein L33

Chain D6:



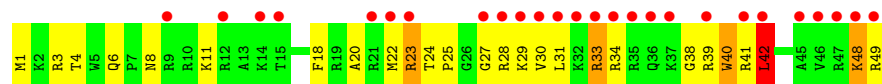
- Molecule 50: 50S ribosomal protein L34

Chain B7:



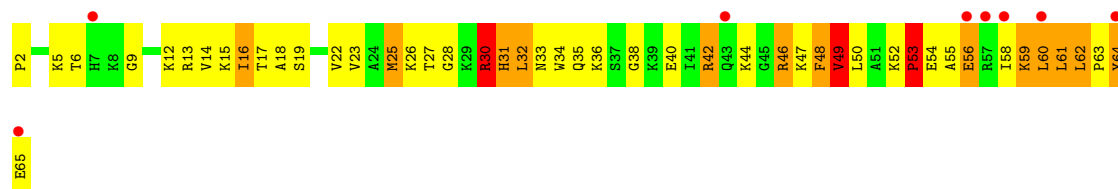
- Molecule 50: 50S ribosomal protein L34

Chain D7:



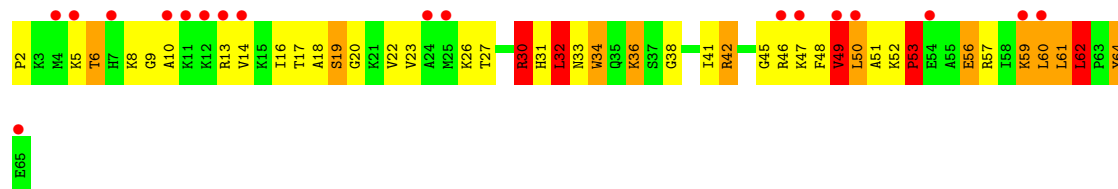
- Molecule 51: 50S ribosomal protein L35

Chain B8:



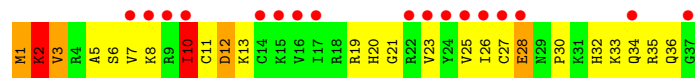
- Molecule 51: 50S ribosomal protein L35

Chain D8:



- Molecule 52: 50S ribosomal protein L36

Chain B9:



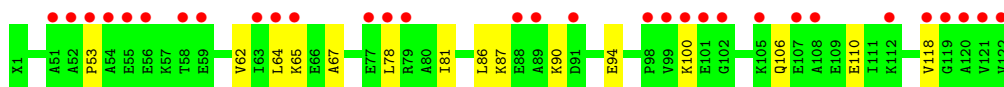
- Molecule 52: 50S ribosomal protein L36

Chain D9:



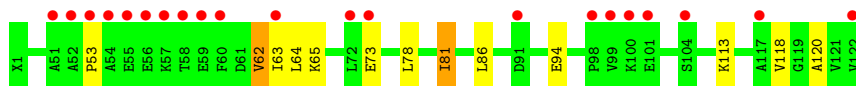
- Molecule 53: 50S ribosomal protein L7/L12

Chain Be: 



- Molecule 53: 50S ribosomal protein L7/L12

Chain De: 



- Molecule 54: 50S ribosomal protein L7/L12

Chain Bf: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

Chain Bg: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

Chain Df: 

There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

Chain Dg: 

There are no outlier residues recorded for this chain.

- Molecule 55: 50S ribosomal protein L7/L12

Chain Bh: 

There are no outlier residues recorded for this chain.

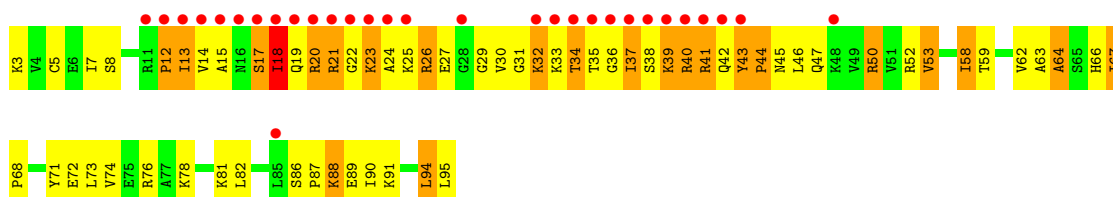
- Molecule 55: 50S ribosomal protein L7/L12

Chain Dh: 

There are no outlier residues recorded for this chain.

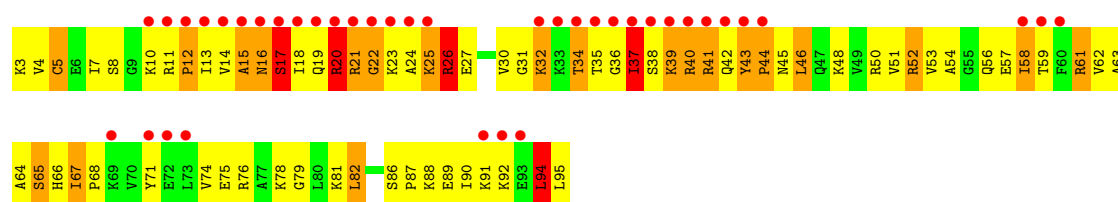
- Molecule 56: 50S ribosomal protein L28

Chain B1: 



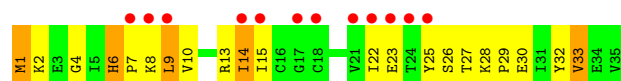
- Molecule 56: 50S ribosomal protein L28

Chain D1:



- Molecule 57: 50S ribosomal protein L31

Chain B4:



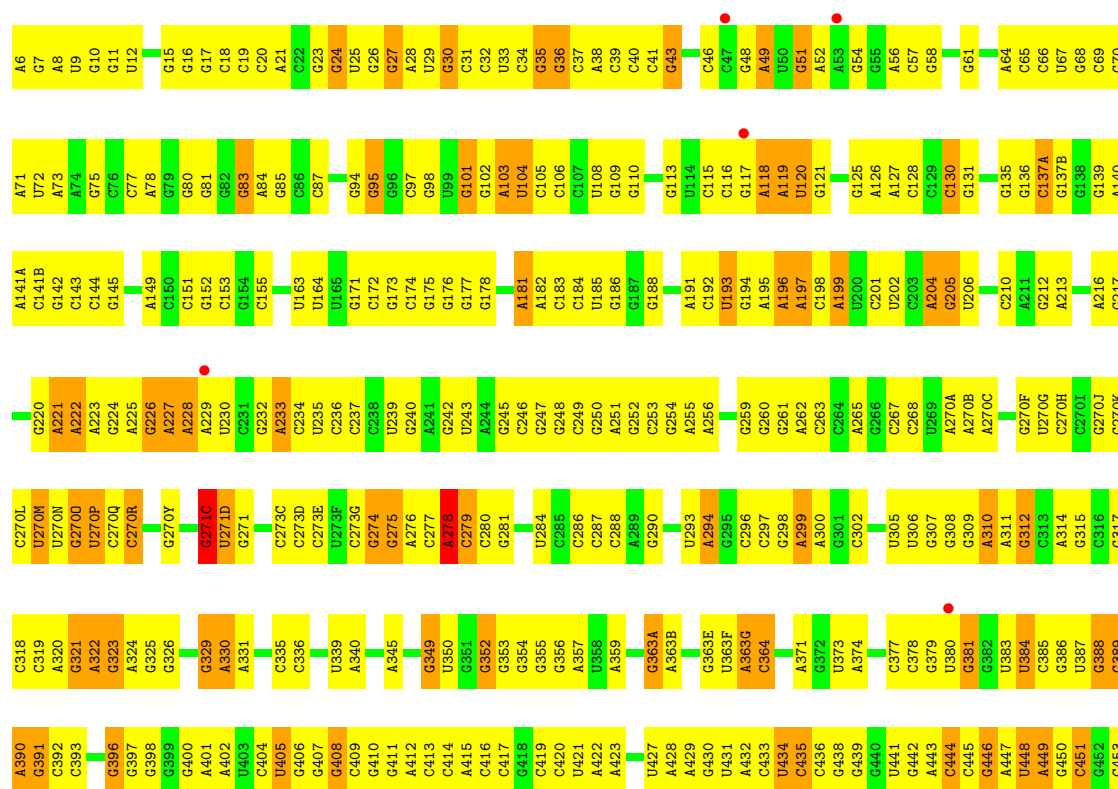
- Molecule 57: 50S ribosomal protein L31

Chain D4:



- Molecule 58: 23S ribosomal RNA

Chain BA:



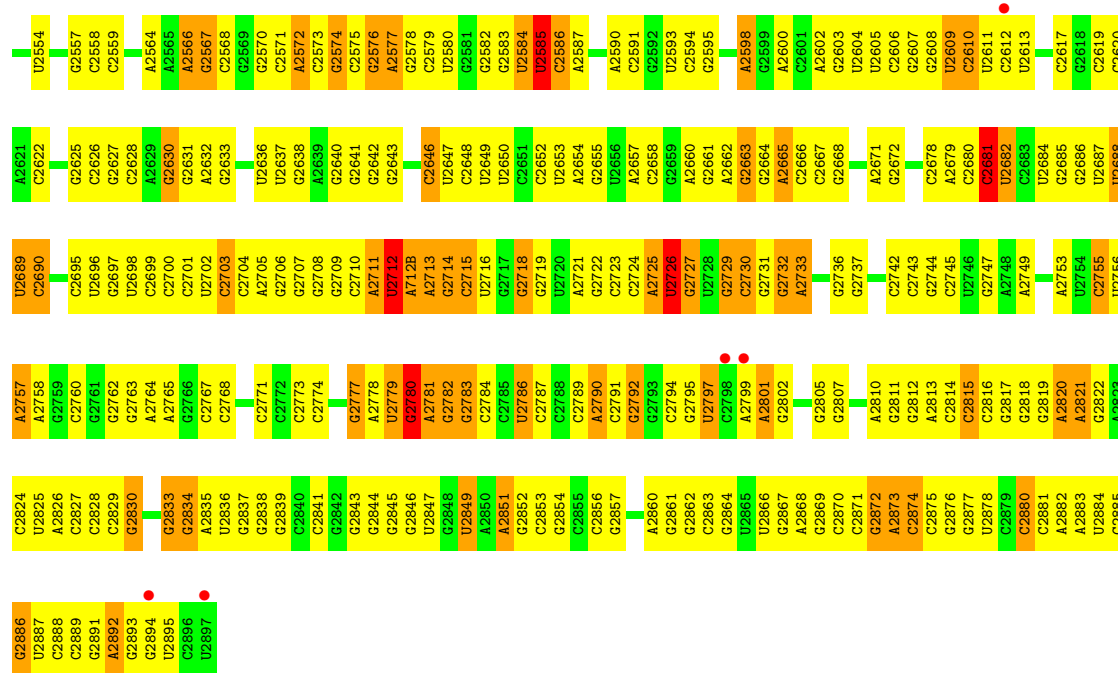
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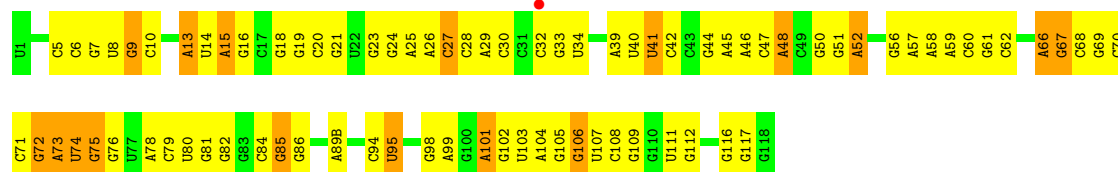
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	G1442	G1380	U1313	A1243	G1181	G1120	G1056		G931				G663	A603
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A1510	G1444	G1382	C1315	G1244	G1184	G1122	C995		G933				G665	C736
A1511	A144B	C1383		G1245			A996		A933					

A2488	C2424	G2299	G2083	C2021	A1953	G1863	U1796	G1707	A1846	A1580	G1512
G2489	A2425	G2300	C2084	U2022	G1954	U1864	C1797	C1708	G1647	G1581	C1513
G2490	A2426	C2301	C2085	G2023	U1955	U1871	U1798	U1709	G1648	G1582	U1514
U2491	A2427	G2302	U2086	G2024	U1956	A1871	G1799	G1710	G1649	A1583	C1515
G2493	G2428	G2303	G2087	C2025	C1957	A1872	C1801	C1711	G1650	C1585	U1516
G2495	G2429	G2304	G2088	C2026	C1958	G1878	G1802	G1712	G1651	A1586	G1517
C2496	A2430	A2305	U2089	G2027	U1959	C1879	A1803	U1716	G1652	A1587	C1518
U2431	U2432	C2306	U2090	A2030	U1962	A1884	A1803	G1717	G1653	C1588	G1519
A2432	G2235	G2307	U2091	G2030	U1963	A1885	C1806	G1718	G1654	C1589	U1522
A2433	G2236	G2308	U2092	A2031	G1964	A1886	G1807	G1725	A1655	U1590	G1523
C2434	G2237	A2309	G2093	G2032	C1965	C1887	G1808	G1726	C1656	G1591	G1524
A2435	G2238	A2310	G2094	A2033	A1966	G1888	U1809	U1727	G1657	G1594	G1525
G2436	G2239	A2311	U2095	U2034	G1967	G1889	A1810	G1728	C1658	G1595	G1526
A2439	C2240	U2312	U2096	G2035	G1968	A1889	A1811	A1729	U1659		
C2440	A2241	U2313	C2097	G2036	G1969	A1890	G1812	U1730	G1661	A1529	
A2441	G2242	G2314	U2098	C2037	A1970	A1891	G1813	A1732	A1664	C1530	
A2443	G2243	G2315	A2170	G2038	A1971	G1892	G1814	A1733	A1665	C1531	
A2448	U2244	G2316	A2171	G2039	A1972	C1893	G1815	G1733	A1666	C1532	
C2449	U2245	G2317	U2172	C2040	G1973	A1900	G1816	C1741	G1667	C1533	
A2450	G2246	G2318	A2173	U2041	G1974	A1901	G1817	C1742	G1668	G1534	
A2451	A2247	G2319	C2174	A2042	G1975	A1902	U1818	G1743	A1669	A1536	
G2446	C2248	A2320	C2175	C2043	U1976	G1903	A1819	G1746	C1670	C1537	
G2452	U2249	G2321	A2176	C2044	A1977	G1904	U1820	G1747	U1671	G1538	
G2453	G2250	G2322	C2177	G2045	A1978	G1905	A1821	G1748	C1672	G1539	
A2454	G2251	G2323	C2178	G2046	A1979	G1906	G1822	U1672	A1610	G1540	
A2455	C2254	G2324	C2179	U2047	G1980		G1823	G1673	U1611	U1541	
G2445	G2255	G2325	U2180	G2048	A1981	U1911	G1824	G1674	C1612	G1542	
G2446	G2256	G2326	C2181	G2049	C1982	A1912	G1825	C1675	G1613	A1543	
G2454	U2257	A2327	G2182	C2050	U1976	A1913	G1826	A1676	G1614	C1544	
G2455	C2258	A2328	C2183	A2051	U1981	G1914	C1827	G1677	C1615	A1545	
G2456	G2259	G2329	C2184	G2052	U1991	U1915	G1828	G1678	A1616	A1546	
U2457	G2260	G2330	C2185	C2053	G1992	U1916	A1829	U1679	C1617	C1547	
G2458	U2262	G2331	G2186	A2054	U1993	A1917	C1830	G1681	C1548	C1549	
A2459	U2263	U2332	G2187	C2055	U1994	U1918	G1832	G1682	C1550	C1551	
U2462	A2266	A2333	U2189	G2056	U1995	U1923	U1833	G1683	G1622	G1552	
C2463	A2267	G2334	G2190	A2057	G1996	C1924	U1834	G1684	G1623		
C2464	A2268	G2335	G2191	A2058	U1997	U1927	U1841	C1685	G1626	G1556	
C2465	A2269	A2336	G2192	G2059	G1998	A1928	G1842	G1687	G1627	C1556	
G2466	G2270	G2337	G2193	A2060	G1999	G1929	C1843	U1688	G1628	C1557	
U2467	G2271	U2338	C2194	G2061	G2000	G1930	G1844	A1689	U1629	A1558	
C2468	U2272	G2339	A2196	A2062	A2001	C1931	G1845	C1691	G1630	G1559	
A2469	A2273	G2340	U2197	C2063	G2002	C1932	A1847	U1692	C1631	G1563	
G2470	A2274	A2341	A2198	C2064	G2003	G1933	A1848	C1693	A1632		
C2471	G2275	G2342	A2199	C2065	G2004	U1934	G1849	C1694	G1633		
U2472	A2276	C2343	U2130	C2066	A2005	A1935	U1851	G1695	A1634	G1568	
G2473	A2277	U2344	G2131	G2067	C2006	C1936	A1852	G1696	A1635	A1569	
A2474	G2278	G2345	U2132	U2068	C2007	C1937	A1853	G1697	C1636	A1570	
C2475	G2279	A2346	G2133	C2069	C2008	G1938	A1854	C1698	A1637	A1571	
U2476	G2280	A2347	A2134	G2070	G2009	A1939	G1855	G1699	C1638	A1572	
A2477	C2281	G2348	A2135	A2071	G2010	U1940	A1857	A1700	U1639		
G2478	G2282	U2349	G2136	G2072	U2011	A1938	G1856	G1788	A1701	C1575	
C2479	A2283	G2350	U2137	C2073	G2012	U1939	A1858	A1785	C1640	U1576	
A2480	G2284	A2351	C2138	U2074	A2013	G1947	A1859	G1786	A1641	U1577	
G2481	A2285	G2352	G2139	U2075	A2014	G1948	G1857	A1787	G1642	U1578	
A2482	C2286	U2353	C2140	U2076	A2015	G1949	G1858	G1788	G1705		
C2483	A2287	G2354	U2141	G2077	U2016	G1949	G1859	A1702	U1706	A1579	
G2484	G2288	A2355	G2142	U2078	U2017	G1949	G1860	G1703			
A2485	C2289	G2356	C2143	U2079	U2018	G1950		G1704			
G2486	U2290	U2357	U2144	G2079	G2019	A1952		G1792			
C2487	G2291	G2358	C2145	U2079	G2020						
G2488	C2292	A2359	C2146	G2080	A2019						
U2547	G2293	G2360	G2147	C2081	A2020						
G2548	C2294	G2361	G2148	A2082							



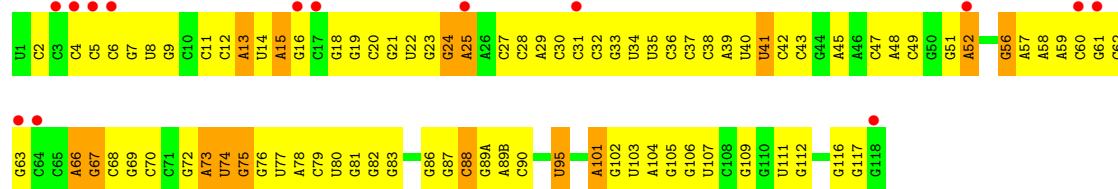
• Molecule 59: 5S ribosomal RNA

Chain BB:



• Molecule 59: 5S ribosomal RNA

Chain DB:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.21Å 670.44Å 350.40Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 145.85 – 3.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.00) 77.8 (145.85-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.329 0.280 , 0.294	Depositor DCC
R_{free} test set	25982 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , -3.0	EDS
Estimated twinning fraction	0.249 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 517738 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	308068	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: GDP, FUA

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	AB	0.37	0/1945	0.70	1/2621 (0.0%)
1	CB	0.37	0/1945	0.70	1/2621 (0.0%)
2	AC	0.27	0/1645	0.53	0/2216
2	CC	0.27	0/1645	0.55	0/2216
3	AD	0.29	0/1733	0.61	1/2318 (0.0%)
3	CD	0.29	0/1733	0.57	0/2318
4	AE	0.28	0/1172	0.58	1/1576 (0.1%)
4	CE	0.30	0/1172	0.57	1/1576 (0.1%)
5	AF	0.28	0/856	0.59	1/1154 (0.1%)
5	CF	0.29	0/856	0.57	1/1154 (0.1%)
6	AG	0.27	0/1276	0.52	0/1709
6	CG	0.28	0/1276	0.53	0/1709
7	AH	0.29	0/1136	0.61	0/1527
7	CH	0.28	0/1136	0.58	0/1527
8	AI	0.28	0/1029	0.51	0/1379
8	CI	0.26	0/1029	0.52	0/1379
9	AJ	0.25	0/815	0.56	1/1095 (0.1%)
9	CJ	0.27	0/815	0.58	1/1095 (0.1%)
10	AK	0.33	0/900	0.66	1/1213 (0.1%)
10	CK	0.35	0/900	0.63	0/1213
11	AL	0.39	0/992	0.86	1/1327 (0.1%)
11	CL	0.38	0/992	0.83	1/1327 (0.1%)
12	AM	0.28	0/1008	0.62	1/1347 (0.1%)
12	CM	0.25	0/1008	0.55	0/1347
13	AN	0.28	0/501	0.49	0/664
13	CN	0.28	0/501	0.47	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.28	0/745	0.56	0/992
15	AP	0.28	0/722	0.51	0/970
15	CP	0.26	0/722	0.50	0/970
16	AQ	0.37	0/848	0.71	0/1131
16	CQ	0.36	0/848	0.72	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/579	0.60	0/768
17	CR	0.27	0/579	0.62	0/768
18	AS	0.28	0/647	0.60	1/870 (0.1%)
18	CS	0.28	0/647	0.64	0/870
19	AT	0.32	0/765	0.57	0/1007
19	CT	0.31	0/765	0.57	0/1007
20	AA	0.35	0/36351	1.03	78/56736 (0.1%)
20	CA	0.34	0/36351	1.01	66/56736 (0.1%)
21	AW	0.35	0/1827	1.09	6/2845 (0.2%)
21	CW	0.36	0/1827	1.10	8/2845 (0.3%)
22	AV	0.26	0/568	0.83	0/886
22	CV	0.28	0/568	0.90	0/886
23	AY	0.33	1/5317 (0.0%)	0.70	10/7198 (0.1%)
23	CY	0.34	1/5317 (0.0%)	0.71	6/7198 (0.1%)
24	BC	0.39	0/1774	0.75	0/2391
24	DC	0.41	0/1774	0.75	1/2391 (0.0%)
25	BD	0.33	0/2195	0.68	2/2955 (0.1%)
25	DD	0.34	0/2195	0.67	1/2955 (0.0%)
26	BE	0.31	0/1602	0.66	0/2160
26	DE	0.31	0/1602	0.67	0/2160
27	BF	0.34	0/1663	0.74	2/2249 (0.1%)
27	DF	0.35	0/1663	0.76	2/2249 (0.1%)
28	BG	0.27	0/1499	0.56	0/2016
28	DG	0.33	1/1499 (0.1%)	0.63	3/2016 (0.1%)
29	BH	0.29	0/1298	0.61	0/1751
29	DH	0.31	0/1298	0.59	0/1751
31	BK	0.26	0/1054	0.50	0/1427
31	DK	0.26	0/1054	0.49	0/1427
32	BN	0.34	0/1131	0.66	0/1525
32	DN	0.34	0/1131	0.66	0/1525
33	BO	0.29	0/943	0.57	0/1269
33	DO	0.27	0/943	0.55	0/1269
34	BP	0.29	0/1131	0.61	0/1504
34	DP	0.29	0/1131	0.66	0/1504
35	BQ	0.32	0/1143	0.64	0/1527
35	DQ	0.32	0/1143	0.61	0/1527
36	BR	0.30	0/974	0.63	0/1302
36	DR	0.31	0/974	0.65	0/1302
37	BS	0.33	0/783	0.69	0/1041
37	DS	0.34	0/783	0.73	0/1041
38	BT	0.34	0/1161	0.70	1/1549 (0.1%)
38	DT	0.33	0/1161	0.66	0/1549
39	BU	0.37	0/982	0.62	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.37	0/982	0.62	1/1306 (0.1%)
40	BV	0.34	0/790	0.71	0/1057
40	DV	0.36	0/790	0.70	0/1057
41	BW	0.30	0/911	0.60	0/1220
41	DW	0.31	0/911	0.65	2/1220 (0.2%)
42	BX	0.27	0/748	0.55	0/1004
42	DX	0.29	0/748	0.58	0/1004
43	BY	0.31	0/831	0.60	0/1108
43	DY	0.30	0/831	0.65	0/1108
44	BZ	0.27	0/1505	0.60	0/2042
44	DZ	0.28	0/1505	0.60	0/2042
45	B0	0.25	0/671	0.51	0/892
45	D0	0.26	0/671	0.56	0/892
46	B2	0.32	0/600	0.59	0/793
46	D2	0.31	0/600	0.61	0/793
47	B3	0.26	0/482	0.54	0/646
47	D3	0.24	0/482	0.54	0/646
48	B5	0.27	0/473	0.55	0/639
48	D5	0.26	0/473	0.58	0/639
49	B6	0.31	0/440	0.72	1/586 (0.2%)
49	D6	0.31	0/440	0.68	1/586 (0.2%)
50	B7	0.32	0/438	0.64	0/575
50	D7	0.30	0/438	0.59	0/575
51	B8	0.31	0/525	0.67	0/691
51	D8	0.29	0/525	0.63	2/691 (0.3%)
52	B9	0.27	0/310	0.55	0/407
52	D9	0.27	0/310	0.50	0/407
53	Be	0.45	1/538 (0.2%)	0.55	0/715
53	De	0.26	0/538	0.51	0/715
56	B1	0.46	0/739	0.84	0/981
56	D1	0.46	0/739	0.86	0/981
57	B4	0.33	0/276	0.62	0/372
57	D4	0.34	0/276	0.58	0/372
58	BA	0.37	3/69437 (0.0%)	1.06	184/108401 (0.2%)
58	DA	0.37	1/69437 (0.0%)	1.05	153/108401 (0.1%)
59	BB	0.35	0/2853	1.07	9/4451 (0.2%)
59	DB	0.34	0/2853	1.03	11/4451 (0.2%)
All	All	0.35	8/330554 (0.0%)	0.94	564/492202 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	2
1	CB	0	3
11	CL	0	1
23	AY	0	5
23	CY	0	1
24	BC	0	2
24	DC	0	3
25	BD	0	2
27	BF	0	2
27	DF	0	2
30	BJ	0	1
30	DJ	0	1
37	BS	0	2
37	DS	0	4
41	BW	0	1
41	DW	0	1
56	B1	0	1
56	D1	0	2
All	All	0	36

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	1914	C	O3'-P	-10.49	1.48	1.61
53	Be	87	LYS	C-N	8.65	1.53	1.34
58	BA	1911	U	O3'-P	-6.43	1.53	1.61
58	BA	1006	C	N1-C2	5.82	1.46	1.40
58	DA	1911	U	O3'-P	-5.77	1.54	1.61

The worst 5 of 564 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	500	GLN	CA-C-N	17.19	155.01	117.20
58	BA	1006	C	C6-N1-C2	-16.88	113.55	120.30
58	BA	1006	C	N3-C2-O2	-14.80	111.54	121.90
23	CY	500	GLN	C-N-CA	14.70	158.44	121.70
58	BA	1006	C	N1-C2-O2	13.47	126.98	118.90

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
1	AB	170	GLU	Peptide
23	AY	133	ILE	Peptide
23	AY	135	PHE	Mainchain
23	AY	499	ARG	Mainchain

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	AB	1910	0	1957	137	0
1	CB	1910	0	1957	134	0
2	AC	1621	0	1688	88	0
2	CC	1621	0	1688	70	0
3	AD	1703	0	1763	134	0
3	CD	1703	0	1763	105	0
4	AE	1156	0	1213	66	0
4	CE	1156	0	1213	71	0
5	AF	843	0	857	45	0
5	CF	843	0	857	43	0
6	AG	1257	0	1296	49	0
6	CG	1257	0	1296	49	0
7	AH	1116	0	1177	71	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	56	0
8	CI	1010	0	1037	60	0
9	AJ	802	0	849	52	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	56	0
10	CK	885	0	904	55	0
11	AL	976	0	1062	97	0
11	CL	976	0	1062	110	0
12	AM	997	0	1072	55	0
12	CM	997	0	1072	56	0
13	AN	492	0	529	37	0
13	CN	492	0	529	29	0
14	AO	734	0	771	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CO	734	0	771	41	0
15	AP	706	0	725	42	0
15	CP	706	0	725	37	0
16	AQ	835	0	904	60	0
16	CQ	835	0	904	65	0
17	AR	574	0	644	35	0
17	CR	574	0	644	43	0
18	AS	634	0	655	38	0
18	CS	634	0	655	43	0
19	AT	763	0	861	43	0
19	CT	763	0	861	45	0
20	AA	32474	0	16393	1058	0
20	CA	32474	0	16393	1056	0
21	AW	1635	0	831	68	0
21	CW	1635	0	831	51	0
22	AV	503	0	252	13	0
22	CV	503	0	252	16	0
23	AY	5219	0	5290	335	0
23	CY	5219	0	5290	319	0
24	BC	1742	0	1798	162	0
24	DC	1742	0	1798	172	0
25	BD	2145	0	2234	214	0
25	DD	2145	0	2234	202	0
26	BE	1569	0	1634	132	0
26	DE	1569	0	1634	142	0
27	BF	1628	0	1680	141	0
27	DF	1628	0	1680	141	0
28	BG	1474	0	1535	96	0
28	DG	1474	0	1535	80	0
29	BH	1274	0	1342	79	0
29	DH	1274	0	1342	66	0
30	BJ	851	0	196	31	0
30	DJ	851	0	196	41	0
31	BK	1035	0	1082	53	0
31	DK	1035	0	1082	51	0
32	BN	1104	0	1179	205	0
32	DN	1104	0	1180	217	0
33	BO	933	0	996	62	0
33	DO	933	0	996	69	0
34	BP	1114	0	1187	96	0
34	DP	1114	0	1187	97	0
35	BQ	1122	0	1179	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DQ	1122	0	1179	69	0
36	BR	960	0	1021	72	0
36	DR	960	0	1021	79	0
37	BS	775	0	835	77	0
37	DS	775	0	835	68	0
38	BT	1147	0	1207	107	0
38	DT	1147	0	1207	90	0
39	BU	964	0	1020	95	0
39	DU	964	0	1022	103	1
40	BV	779	0	852	70	0
40	DV	779	0	852	72	0
41	BW	900	0	964	53	0
41	DW	900	0	964	56	0
42	BX	734	0	789	42	0
42	DX	734	0	789	50	0
43	BY	818	0	908	59	0
43	DY	818	0	908	53	0
44	BZ	1473	0	1497	83	0
44	DZ	1473	0	1497	76	0
45	B0	662	0	688	41	0
45	D0	662	0	688	42	0
46	B2	598	0	653	30	0
46	D2	598	0	653	38	0
47	B3	477	0	529	19	0
47	D3	477	0	529	30	0
48	B5	459	0	477	27	0
48	D5	459	0	477	45	0
49	B6	433	0	461	27	0
49	D6	433	0	461	29	0
50	B7	430	0	480	37	0
50	D7	430	0	480	30	0
51	B8	517	0	582	49	0
51	D8	517	0	582	43	0
52	B9	307	0	338	22	0
52	D9	307	0	335	14	0
53	Be	686	0	617	0	0
53	De	686	0	615	0	0
54	Bf	156	0	41	0	0
54	Bg	156	0	38	0	0
54	Df	156	0	42	0	0
54	Dg	156	0	40	0	0
55	Bh	151	0	41	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Dh	151	0	40	0	0
56	B1	732	0	808	72	0
56	D1	732	0	808	78	0
57	B4	271	0	284	17	0
57	D4	271	0	284	15	0
58	BA	61997	0	31250	2049	1
58	DA	61997	0	31250	2317	0
59	BB	2551	0	1295	93	0
59	DB	2551	0	1295	94	0
60	AY	37	0	47	13	0
60	CY	37	0	47	10	0
61	AY	28	0	12	6	0
61	CY	28	0	12	6	0
All	All	308068	0	213012	12886	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 25.

The worst 5 of 12886 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:CA:1494:G:C5'	58:DA:1913:A:N6	1.79	1.45
32:BN:1:MET:HG2	40:BV:13:ARG:NH1	1.30	1.39
58:BA:2681:C:N4	58:BA:2725:A:H62	1.22	1.35
23:AY:580:MET:HE2	58:BA:1913:A:N1	1.37	1.35
23:AY:580:MET:CE	58:BA:1913:A:N1	1.91	1.34

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
58:BA:1015:G:O2'	39:DU:118:GLY:O[3_545]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	155 (66%)	52 (22%)	26 (11%)	1	16
1	CB	233/235 (99%)	152 (65%)	55 (24%)	26 (11%)	1	16
2	AC	205/207 (99%)	156 (76%)	33 (16%)	16 (8%)	1	28
2	CC	205/207 (99%)	148 (72%)	41 (20%)	16 (8%)	1	28
3	AD	206/208 (99%)	145 (70%)	37 (18%)	24 (12%)	1	15
3	CD	206/208 (99%)	150 (73%)	32 (16%)	24 (12%)	1	15
4	AE	149/151 (99%)	124 (83%)	17 (11%)	8 (5%)	3	41
4	CE	149/151 (99%)	116 (78%)	25 (17%)	8 (5%)	3	41
5	AF	99/101 (98%)	73 (74%)	20 (20%)	6 (6%)	2	37
5	CF	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	37
6	AG	153/155 (99%)	122 (80%)	23 (15%)	8 (5%)	3	42
6	CG	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	2	38
7	AH	136/138 (99%)	93 (68%)	29 (21%)	14 (10%)	1	19
7	CH	136/138 (99%)	101 (74%)	22 (16%)	13 (10%)	1	21
8	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	6	57
8	CI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	4	44
9	AJ	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	1	19
9	CJ	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	37
10	AK	117/119 (98%)	85 (73%)	16 (14%)	16 (14%)	0	11
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	9
11	AL	123/125 (98%)	42 (34%)	45 (37%)	36 (29%)	0	1
11	CL	123/125 (98%)	43 (35%)	41 (33%)	39 (32%)	0	0
12	AM	123/125 (98%)	88 (72%)	24 (20%)	11 (9%)	1	25
12	CM	123/125 (98%)	90 (73%)	24 (20%)	9 (7%)	2	31
13	AN	58/60 (97%)	43 (74%)	8 (14%)	7 (12%)	1	14
13	CN	58/60 (97%)	44 (76%)	8 (14%)	6 (10%)	1	19
14	AO	86/88 (98%)	62 (72%)	15 (17%)	9 (10%)	1	18
14	CO	86/88 (98%)	62 (72%)	20 (23%)	4 (5%)	4	45
15	AP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	44
15	CP	82/84 (98%)	62 (76%)	16 (20%)	4 (5%)	3	44
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	19
16	CQ	98/100 (98%)	68 (69%)	21 (21%)	9 (9%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AR	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	2	31
17	CR	68/70 (97%)	47 (69%)	19 (28%)	2 (3%)	7	59
18	AS	77/79 (98%)	41 (53%)	24 (31%)	12 (16%)	0	7
18	CS	77/79 (98%)	50 (65%)	11 (14%)	16 (21%)	0	3
19	AT	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	2	37
19	CT	97/99 (98%)	76 (78%)	17 (18%)	4 (4%)	4	49
23	AY	663/687 (96%)	436 (66%)	147 (22%)	80 (12%)	1	14
23	CY	663/687 (96%)	454 (68%)	139 (21%)	70 (11%)	1	17
24	BC	226/228 (99%)	106 (47%)	70 (31%)	50 (22%)	0	2
24	DC	226/228 (99%)	114 (50%)	68 (30%)	44 (20%)	0	4
25	BD	273/275 (99%)	177 (65%)	52 (19%)	44 (16%)	0	7
25	DD	273/275 (99%)	171 (63%)	56 (20%)	46 (17%)	0	6
26	BE	203/205 (99%)	127 (63%)	45 (22%)	31 (15%)	0	8
26	DE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	6
27	BF	206/208 (99%)	132 (64%)	53 (26%)	21 (10%)	1	19
27	DF	206/208 (99%)	131 (64%)	42 (20%)	33 (16%)	0	7
28	BG	179/181 (99%)	126 (70%)	40 (22%)	13 (7%)	2	31
28	DG	179/181 (99%)	131 (73%)	35 (20%)	13 (7%)	2	31
29	BH	165/167 (99%)	113 (68%)	32 (19%)	20 (12%)	1	14
29	DH	165/167 (99%)	102 (62%)	42 (26%)	21 (13%)	0	13
31	BK	138/140 (99%)	98 (71%)	30 (22%)	10 (7%)	2	32
31	DK	138/140 (99%)	100 (72%)	31 (22%)	7 (5%)	3	42
32	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	1	14
32	DN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	1	14
33	BO	120/122 (98%)	84 (70%)	20 (17%)	16 (13%)	0	12
33	DO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	27
34	BP	144/146 (99%)	82 (57%)	36 (25%)	26 (18%)	0	5
34	DP	144/146 (99%)	81 (56%)	35 (24%)	28 (19%)	0	4
35	BQ	139/141 (99%)	94 (68%)	33 (24%)	12 (9%)	1	25
35	DQ	139/141 (99%)	99 (71%)	30 (22%)	10 (7%)	2	32
36	BR	115/117 (98%)	80 (70%)	21 (18%)	14 (12%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DR	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	18
37	BS	97/99 (98%)	57 (59%)	18 (19%)	22 (23%)	0	2
37	DS	97/99 (98%)	48 (50%)	26 (27%)	23 (24%)	0	2
38	BT	136/138 (99%)	85 (62%)	22 (16%)	29 (21%)	0	3
38	DT	136/138 (99%)	90 (66%)	22 (16%)	24 (18%)	0	5
39	BU	115/117 (98%)	91 (79%)	18 (16%)	6 (5%)	3	42
39	DU	115/117 (98%)	90 (78%)	21 (18%)	4 (4%)	6	55
40	BV	99/101 (98%)	65 (66%)	16 (16%)	18 (18%)	0	5
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	10
41	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	24
41	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	1	17
42	BX	91/93 (98%)	66 (72%)	19 (21%)	6 (7%)	2	35
42	DX	91/93 (98%)	70 (77%)	15 (16%)	6 (7%)	2	35
43	BY	105/107 (98%)	44 (42%)	38 (36%)	23 (22%)	0	2
43	DY	105/107 (98%)	47 (45%)	28 (27%)	30 (29%)	0	1
44	BZ	183/185 (99%)	129 (70%)	34 (19%)	20 (11%)	1	17
44	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	1	21
45	B0	82/84 (98%)	58 (71%)	17 (21%)	7 (8%)	1	26
45	D0	82/84 (98%)	51 (62%)	24 (29%)	7 (8%)	1	26
46	B2	69/71 (97%)	50 (72%)	13 (19%)	6 (9%)	1	25
46	D2	69/71 (97%)	50 (72%)	16 (23%)	3 (4%)	4	48
47	B3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	3	42
47	D3	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	3	42
48	B5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	2	32
48	D5	57/59 (97%)	36 (63%)	18 (32%)	3 (5%)	3	41
49	B6	48/50 (96%)	27 (56%)	13 (27%)	8 (17%)	0	6
49	D6	48/50 (96%)	28 (58%)	11 (23%)	9 (19%)	0	4
50	B7	47/49 (96%)	31 (66%)	14 (30%)	2 (4%)	4	48
50	D7	47/49 (96%)	36 (77%)	6 (13%)	5 (11%)	1	17
51	B8	62/64 (97%)	32 (52%)	22 (36%)	8 (13%)	0	12
51	D8	62/64 (97%)	38 (61%)	14 (23%)	10 (16%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B9	35/37 (95%)	23 (66%)	7 (20%)	5 (14%)	0	10
52	D9	35/37 (95%)	26 (74%)	8 (23%)	1 (3%)	7	59
53	Be	70/102 (69%)	35 (50%)	28 (40%)	7 (10%)	1	20
53	De	70/102 (69%)	39 (56%)	24 (34%)	7 (10%)	1	20
56	B1	91/93 (98%)	53 (58%)	19 (21%)	19 (21%)	0	3
56	D1	91/93 (98%)	57 (63%)	15 (16%)	19 (21%)	0	3
57	B4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	8
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	1
All	All	13256/13564 (98%)	8908 (67%)	2779 (21%)	1569 (12%)	1	14

5 of 1569 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	94	ASN
1	AB	95	GLN
1	AB	165	VAL
1	AB	194	PRO

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	2	13
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	11
2	AC	161/161 (100%)	136 (84%)	25 (16%)	4	28
2	CC	161/161 (100%)	136 (84%)	25 (16%)	4	28
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	12
3	CD	180/180 (100%)	150 (83%)	30 (17%)	3	24
4	AE	116/116 (100%)	95 (82%)	21 (18%)	2	19
4	CE	116/116 (100%)	92 (79%)	24 (21%)	2	13
5	AF	90/90 (100%)	80 (89%)	10 (11%)	9	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	90/90 (100%)	85 (94%)	5 (6%)	30	77
6	AG	126/126 (100%)	112 (89%)	14 (11%)	9	46
6	CG	126/126 (100%)	114 (90%)	12 (10%)	12	54
7	AH	119/119 (100%)	97 (82%)	22 (18%)	2	18
7	CH	119/119 (100%)	104 (87%)	15 (13%)	7	39
8	AI	98/98 (100%)	83 (85%)	15 (15%)	4	29
8	CI	98/98 (100%)	82 (84%)	16 (16%)	3	26
9	AJ	89/89 (100%)	73 (82%)	16 (18%)	2	19
9	CJ	89/89 (100%)	70 (79%)	19 (21%)	1	12
10	AK	90/90 (100%)	76 (84%)	14 (16%)	4	28
10	CK	90/90 (100%)	71 (79%)	19 (21%)	1	12
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	12
11	CL	104/104 (100%)	74 (71%)	30 (29%)	0	5
12	AM	100/100 (100%)	81 (81%)	19 (19%)	2	16
12	CM	100/100 (100%)	88 (88%)	12 (12%)	7	41
13	AN	49/49 (100%)	40 (82%)	9 (18%)	2	18
13	CN	49/49 (100%)	42 (86%)	7 (14%)	5	33
14	AO	79/79 (100%)	70 (89%)	9 (11%)	8	44
14	CO	79/79 (100%)	68 (86%)	11 (14%)	5	34
15	AP	72/72 (100%)	65 (90%)	7 (10%)	12	53
15	CP	72/72 (100%)	69 (96%)	3 (4%)	40	83
16	AQ	95/95 (100%)	78 (82%)	17 (18%)	2	19
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	5	35
17	AR	61/61 (100%)	53 (87%)	8 (13%)	6	37
17	CR	61/61 (100%)	51 (84%)	10 (16%)	3	25
18	AS	69/69 (100%)	53 (77%)	16 (23%)	1	9
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	9
19	AT	76/76 (100%)	64 (84%)	12 (16%)	4	28
19	CT	76/76 (100%)	69 (91%)	7 (9%)	13	56
23	AY	563/579 (97%)	466 (83%)	97 (17%)	3	22
23	CY	563/579 (97%)	460 (82%)	103 (18%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	180/180 (100%)	135 (75%)	45 (25%)	1	8
24	DC	180/180 (100%)	139 (77%)	41 (23%)	1	10
25	BD	217/217 (100%)	173 (80%)	44 (20%)	2	14
25	DD	217/217 (100%)	171 (79%)	46 (21%)	1	12
26	BE	165/165 (100%)	134 (81%)	31 (19%)	2	17
26	DE	165/165 (100%)	133 (81%)	32 (19%)	2	15
27	BF	165/165 (100%)	127 (77%)	38 (23%)	1	10
27	DF	165/165 (100%)	133 (81%)	32 (19%)	2	15
28	BG	155/155 (100%)	126 (81%)	29 (19%)	2	17
28	DG	155/155 (100%)	127 (82%)	28 (18%)	2	19
29	BH	136/136 (100%)	111 (82%)	25 (18%)	2	18
29	DH	136/136 (100%)	120 (88%)	16 (12%)	8	42
31	BK	105/105 (100%)	85 (81%)	20 (19%)	2	16
31	DK	105/105 (100%)	88 (84%)	17 (16%)	3	26
32	BN	117/117 (100%)	100 (86%)	17 (14%)	5	31
32	DN	117/117 (100%)	100 (86%)	17 (14%)	5	31
33	BO	100/100 (100%)	84 (84%)	16 (16%)	3	27
33	DO	100/100 (100%)	87 (87%)	13 (13%)	6	38
34	BP	112/112 (100%)	92 (82%)	20 (18%)	2	19
34	DP	112/112 (100%)	88 (79%)	24 (21%)	1	12
35	BQ	111/111 (100%)	88 (79%)	23 (21%)	2	13
35	DQ	111/111 (100%)	87 (78%)	24 (22%)	1	11
36	BR	100/100 (100%)	83 (83%)	17 (17%)	3	23
36	DR	100/100 (100%)	83 (83%)	17 (17%)	3	23
37	BS	77/77 (100%)	63 (82%)	14 (18%)	2	18
37	DS	77/77 (100%)	59 (77%)	18 (23%)	1	9
38	BT	120/120 (100%)	95 (79%)	25 (21%)	2	13
38	DT	120/120 (100%)	91 (76%)	29 (24%)	1	8
39	BU	93/93 (100%)	71 (76%)	22 (24%)	1	9
39	DU	93/93 (100%)	75 (81%)	18 (19%)	2	15
40	BV	82/82 (100%)	65 (79%)	17 (21%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DV	82/82 (100%)	62 (76%)	20 (24%)	1	8
41	BW	92/92 (100%)	71 (77%)	21 (23%)	1	10
41	DW	92/92 (100%)	76 (83%)	16 (17%)	3	21
42	BX	75/75 (100%)	61 (81%)	14 (19%)	2	17
42	DX	75/75 (100%)	60 (80%)	15 (20%)	2	14
43	BY	88/88 (100%)	65 (74%)	23 (26%)	1	7
43	DY	88/88 (100%)	71 (81%)	17 (19%)	2	15
44	BZ	162/162 (100%)	132 (82%)	30 (18%)	2	18
44	DZ	162/162 (100%)	134 (83%)	28 (17%)	3	21
45	B0	66/66 (100%)	52 (79%)	14 (21%)	1	12
45	D0	66/66 (100%)	53 (80%)	13 (20%)	2	15
46	B2	66/66 (100%)	59 (89%)	7 (11%)	10	48
46	D2	66/66 (100%)	60 (91%)	6 (9%)	14	56
47	B3	52/52 (100%)	42 (81%)	10 (19%)	2	16
47	D3	52/52 (100%)	48 (92%)	4 (8%)	18	65
48	B5	51/51 (100%)	41 (80%)	10 (20%)	2	15
48	D5	51/51 (100%)	40 (78%)	11 (22%)	1	11
49	B6	49/49 (100%)	43 (88%)	6 (12%)	7	41
49	D6	49/49 (100%)	38 (78%)	11 (22%)	1	11
50	B7	42/42 (100%)	36 (86%)	6 (14%)	5	33
50	D7	42/42 (100%)	36 (86%)	6 (14%)	5	33
51	B8	54/54 (100%)	37 (68%)	17 (32%)	0	4
51	D8	54/54 (100%)	40 (74%)	14 (26%)	1	7
52	B9	34/34 (100%)	30 (88%)	4 (12%)	8	42
52	D9	34/34 (100%)	32 (94%)	2 (6%)	28	75
53	Be	54/54 (100%)	47 (87%)	7 (13%)	6	38
53	De	54/54 (100%)	46 (85%)	8 (15%)	4	31
56	B1	78/78 (100%)	64 (82%)	14 (18%)	2	19
56	D1	78/78 (100%)	59 (76%)	19 (24%)	1	8
57	B4	31/31 (100%)	26 (84%)	5 (16%)	3	27
57	D4	31/31 (100%)	25 (81%)	6 (19%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11138/11170 (100%)	9124 (82%)	2014 (18%)	2 19

5 of 2014 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BZ	112	ARG
4	CE	31	LEU
42	DX	57	LEU
45	B0	67	VAL
57	B4	23	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
42	BX	58	HIS
11	CL	8	ASN
40	DV	64	HIS
44	BZ	30	ASN
3	CD	116	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	291 (19%)	17 (1%)
20	CA	1510/1511 (99%)	294 (19%)	16 (1%)
21	AW	76/77 (98%)	21 (27%)	2 (2%)
21	CW	76/77 (98%)	24 (31%)	2 (2%)
22	AV	22/23 (95%)	11 (50%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
58	BA	2878/2879 (99%)	665 (23%)	22 (0%)
58	DA	2878/2879 (99%)	658 (22%)	23 (0%)
59	BB	118/119 (99%)	17 (14%)	2 (1%)
59	DB	118/119 (99%)	14 (11%)	1 (0%)
All	All	9208/9218 (99%)	2003 (21%)	88 (0%)

5 of 2003 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	9	G
20	AA	13	U

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Mol	Chain	Res	Type
20	AA	32	A
20	AA	39	G
20	AA	47	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
58	BA	2750	A
20	CA	484	G
58	DA	2212	A
58	BA	2780	G
20	CA	115	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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$
60	FUA	AY	701	-	40,40,40	1.66	9 (22%)	64,64,64	2.19	15 (23%)
61	GDP	AY	702	-	30,30,30	1.40	5 (16%)	45,47,47	2.08	9 (20%)
60	FUA	CY	701	-	40,40,40	1.72	6 (15%)	64,64,64	2.39	19 (29%)
61	GDP	CY	702	-	30,30,30	1.41	5 (16%)	45,47,47	2.07	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FUA	AY	701	-	-	1/18/92/92	0/4/4/4
61	GDP	AY	702	-	-	0/16/32/32	0/3/3/3
60	FUA	CY	701	-	-	4/18/92/92	0/4/4/4
61	GDP	CY	702	-	-	0/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CY	701	FUA	C29-C22	4.57	1.53	1.47
60	AY	701	FUA	C29-C22	4.36	1.53	1.47
60	CY	701	FUA	C23-C22	-4.25	1.39	1.51
60	AY	701	FUA	C23-C22	-4.15	1.40	1.51
60	CY	701	FUA	C23-C24	-4.10	1.39	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CY	701	FUA	C13-C12-C11	-8.05	101.03	112.00
60	AY	701	FUA	C13-C12-C11	-8.01	101.09	112.00
61	AY	702	GDP	C6-C5-N7	-7.14	133.18	134.14
61	CY	702	GDP	C6-C5-N7	-7.04	133.19	134.14
60	CY	701	FUA	C5-C4-C3	-7.02	98.38	110.13

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CY	701	FUA	C16-C17-C22-C29
60	CY	701	FUA	C13-C17-C22-C29
60	AY	701	FUA	C16-C17-C22-C29
60	CY	701	FUA	C13-C17-C22-C23
60	CY	701	FUA	C16-C17-C22-C23

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
53	Be	1
53	De	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	37.61
1	Be	30:UNK	C	51:ALA	N	36.82

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	AB	235/235 (100%)	-0.08	3 (1%) 74 59	41, 81, 119, 159	0
1	CB	235/235 (100%)	0.00	6 (2%) 53 42	38, 80, 117, 178	0
2	AC	207/207 (100%)	0.76	31 (14%) 3 5	34, 76, 116, 152	0
2	CC	207/207 (100%)	0.77	36 (17%) 2 4	44, 78, 121, 158	0
3	AD	208/208 (100%)	-0.09	5 (2%) 56 43	37, 71, 125, 178	0
3	CD	208/208 (100%)	0.01	7 (3%) 43 35	51, 83, 120, 165	0
4	AE	151/151 (100%)	1.23	44 (29%) 1 2	30, 57, 93, 133	0
4	CE	151/151 (100%)	1.17	47 (31%) 1 2	31, 61, 99, 185	0
5	AF	101/101 (100%)	-0.28	0 100 100	31, 52, 87, 115	0
5	CF	101/101 (100%)	-0.34	0 100 100	25, 52, 78, 129	0
6	AG	155/155 (100%)	0.77	19 (12%) 5 7	54, 100, 147, 205	0
6	CG	155/155 (100%)	1.20	30 (19%) 2 3	57, 99, 155, 218	0
7	AH	138/138 (100%)	0.45	8 (5%) 22 21	28, 49, 83, 117	0
7	CH	138/138 (100%)	0.81	16 (11%) 5 8	29, 57, 101, 142	0
8	AI	127/127 (100%)	0.92	17 (13%) 4 6	48, 87, 128, 163	0
8	CI	127/127 (100%)	0.79	22 (17%) 2 4	51, 91, 136, 195	0
9	AJ	99/99 (100%)	0.53	12 (12%) 5 7	46, 74, 108, 114	0
9	CJ	99/99 (100%)	0.37	14 (14%) 3 5	37, 82, 121, 145	0
10	AK	119/119 (100%)	0.54	12 (10%) 7 10	41, 71, 114, 157	0
10	CK	119/119 (100%)	0.35	7 (5%) 22 20	22, 59, 106, 135	0
11	AL	125/125 (100%)	0.91	22 (17%) 2 4	31, 63, 97, 178	0
11	CL	125/125 (100%)	0.78	20 (16%) 3 5	29, 68, 109, 136	0
12	AM	125/125 (100%)	0.83	18 (14%) 3 5	61, 101, 139, 150	0
12	CM	125/125 (100%)	1.39	32 (25%) 1 3	52, 106, 160, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	1.34	15 (25%) 1 3	42, 64, 97, 106	0
13	CN	60/60 (100%)	0.63	3 (5%) 28 24	47, 67, 112, 156	0
14	AO	88/88 (100%)	-0.03	3 (3%) 43 35	32, 61, 102, 172	0
14	CO	88/88 (100%)	-0.00	1 (1%) 77 63	29, 61, 108, 215	0
15	AP	84/84 (100%)	2.40	49 (58%) 0 2	47, 80, 118, 187	0
15	CP	84/84 (100%)	2.03	46 (54%) 0 2	53, 81, 118, 174	0
16	AQ	100/100 (100%)	0.96	24 (24%) 1 3	33, 56, 100, 124	0
16	CQ	100/100 (100%)	0.61	14 (14%) 3 5	30, 58, 89, 139	0
17	AR	70/70 (100%)	0.39	4 (5%) 23 21	30, 55, 101, 156	0
17	CR	70/70 (100%)	0.36	6 (8%) 11 13	32, 46, 123, 186	0
18	AS	79/79 (100%)	0.88	14 (17%) 2 4	68, 90, 148, 159	0
18	CS	79/79 (100%)	1.15	15 (18%) 2 3	59, 92, 146, 215	0
19	AT	99/99 (100%)	0.37	9 (9%) 9 12	58, 86, 116, 146	0
19	CT	99/99 (100%)	0.65	13 (13%) 4 6	42, 81, 114, 147	0
20	AA	1511/1511 (100%)	-0.02	107 (7%) 16 16	25, 78, 180, 324	0
20	CA	1511/1511 (100%)	-0.07	92 (6%) 21 20	19, 82, 182, 332	0
21	AW	77/77 (100%)	-0.47	1 (1%) 74 59	55, 121, 189, 218	0
21	CW	77/77 (100%)	-0.66	0 100 100	58, 118, 230, 278	0
22	AV	23/23 (100%)	1.74	10 (43%) 1 2	70, 138, 188, 222	0
22	CV	23/23 (100%)	3.15	13 (56%) 0 2	88, 142, 211, 231	0
23	AY	667/687 (97%)	0.26	48 (7%) 15 16	29, 79, 132, 191	0
23	CY	667/687 (97%)	0.21	43 (6%) 19 19	32, 84, 131, 188	0
24	BC	228/228 (100%)	0.98	45 (19%) 2 3	91, 147, 211, 238	0
24	DC	228/228 (100%)	0.71	27 (11%) 5 8	89, 175, 227, 263	0
25	BD	275/275 (100%)	0.79	43 (15%) 3 5	24, 52, 90, 160	0
25	DD	275/275 (100%)	0.60	36 (13%) 4 6	23, 50, 94, 155	0
26	BE	205/205 (100%)	0.32	5 (2%) 56 43	25, 52, 97, 202	0
26	DE	205/205 (100%)	0.36	8 (3%) 37 31	28, 60, 135, 173	0
27	BF	208/208 (100%)	0.69	31 (14%) 3 5	32, 67, 126, 195	0
27	DF	208/208 (100%)	0.93	42 (20%) 2 3	34, 86, 165, 230	0
28	BG	181/181 (100%)	1.41	61 (33%) 1 2	52, 103, 150, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/181 (100%)	1.31	46 (25%) 1 3	73, 110, 158, 205	0
29	BH	167/167 (100%)	0.51	16 (9%) 8 11	38, 64, 111, 161	0
29	DH	167/167 (100%)	0.43	15 (8%) 10 12	40, 74, 130, 167	0
30	BJ	0/170	-	-	-	-
30	DJ	0/170	-	-	-	-
31	BK	140/140 (100%)	0.59	22 (15%) 3 5	67, 118, 175, 206	0
31	DK	140/140 (100%)	0.56	20 (14%) 3 5	66, 132, 200, 220	0
32	BN	138/138 (100%)	0.75	16 (11%) 5 8	58, 85, 106, 118	0
32	DN	138/138 (100%)	0.62	15 (10%) 6 9	63, 87, 111, 121	0
33	BO	122/122 (100%)	0.40	5 (4%) 35 29	24, 49, 67, 114	0
33	DO	122/122 (100%)	0.48	12 (9%) 8 10	30, 56, 88, 125	0
34	BP	146/146 (100%)	0.28	14 (9%) 8 11	28, 73, 113, 171	0
34	DP	146/146 (100%)	0.12	5 (3%) 43 35	31, 84, 130, 202	0
35	BQ	141/141 (100%)	-0.10	5 (3%) 42 34	40, 66, 100, 164	0
35	DQ	141/141 (100%)	0.02	9 (6%) 19 19	36, 64, 104, 161	0
36	BR	117/117 (100%)	-0.21	0 100 100	29, 53, 85, 105	0
36	DR	117/117 (100%)	-0.19	0 100 100	21, 53, 88, 156	0
37	BS	99/99 (100%)	0.56	14 (14%) 3 5	60, 111, 172, 189	0
37	DS	99/99 (100%)	1.56	30 (30%) 1 2	38, 128, 194, 220	0
38	BT	138/138 (100%)	0.10	6 (4%) 34 28	36, 64, 106, 201	0
38	DT	138/138 (100%)	0.22	10 (7%) 15 16	32, 71, 115, 216	0
39	BU	117/117 (100%)	0.17	5 (4%) 34 28	26, 44, 83, 132	0
39	DU	117/117 (100%)	0.22	9 (7%) 13 14	6, 45, 90, 155	0
40	BV	101/101 (100%)	0.84	18 (17%) 2 4	31, 51, 79, 104	0
40	DV	101/101 (100%)	0.32	7 (6%) 17 17	38, 70, 111, 124	0
41	BW	113/113 (100%)	0.66	16 (14%) 3 5	22, 51, 104, 120	0
41	DW	113/113 (100%)	0.94	19 (16%) 2 4	30, 49, 105, 202	0
42	BX	93/93 (100%)	0.66	9 (9%) 8 11	31, 59, 93, 113	0
42	DX	93/93 (100%)	0.45	6 (6%) 18 19	29, 63, 111, 175	0
43	BY	107/107 (100%)	-0.02	4 (3%) 39 32	35, 71, 133, 156	0
43	DY	107/107 (100%)	-0.04	7 (6%) 18 19	55, 87, 133, 209	0
44	BZ	185/185 (100%)	-0.00	5 (2%) 52 41	42, 78, 126, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	0.14	10 (5%) 25 22	36, 75, 123, 161	0
45	B0	84/84 (100%)	0.35	4 (4%) 29 25	38, 70, 99, 162	0
45	D0	84/84 (100%)	0.68	8 (9%) 8 11	33, 67, 139, 212	0
46	B2	71/71 (100%)	0.01	1 (1%) 72 57	44, 71, 114, 167	0
46	D2	71/71 (100%)	-0.07	0 100 100	53, 76, 129, 183	0
47	B3	60/60 (100%)	-0.14	0 100 100	26, 43, 74, 113	0
47	D3	60/60 (100%)	0.27	3 (5%) 28 24	27, 57, 99, 111	0
48	B5	59/59 (100%)	0.06	0 100 100	22, 56, 142, 156	0
48	D5	59/59 (100%)	0.25	2 (3%) 43 35	18, 67, 175, 198	0
49	B6	50/50 (100%)	0.28	2 (4%) 36 30	65, 91, 124, 176	0
49	D6	50/50 (100%)	1.09	14 (28%) 1 2	66, 106, 136, 139	0
50	B7	49/49 (100%)	2.14	22 (44%) 1 2	30, 48, 107, 132	0
50	D7	49/49 (100%)	2.68	26 (53%) 0 2	38, 51, 125, 168	0
51	B8	64/64 (100%)	0.80	8 (12%) 5 6	30, 62, 80, 89	0
51	D8	64/64 (100%)	1.06	18 (28%) 1 2	38, 70, 114, 148	0
52	B9	37/37 (100%)	1.91	17 (45%) 1 2	41, 63, 116, 166	0
52	D9	37/37 (100%)	0.75	6 (16%) 2 4	36, 55, 111, 148	0
53	Be	72/102 (70%)	2.08	31 (43%) 1 2	69, 117, 170, 201	0
53	De	72/102 (70%)	1.88	21 (29%) 1 2	82, 121, 212, 249	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	1.71	30 (32%) 1 2	40, 87, 151, 208	0
56	D1	93/93 (100%)	1.98	39 (41%) 1 2	42, 84, 174, 216	0
57	B4	35/35 (100%)	1.61	12 (34%) 1 2	96, 160, 227, 248	0
57	D4	35/35 (100%)	2.70	19 (54%) 0 2	116, 170, 265, 282	0
58	BA	2879/2879 (100%)	-0.39	36 (1%) 74 59	17, 60, 166, 304	0
58	DA	2879/2879 (100%)	-0.42	28 (0%) 79 65	17, 62, 182, 341	0
59	BB	119/119 (100%)	-0.34	1 (0%) 83 70	32, 114, 187, 214	0
59	DB	119/119 (100%)	0.26	14 (11%) 5 8	53, 104, 162, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22682/23306 (97%)	0.23	1993 (8%) 10 13	6, 73, 161, 341	0

The worst 5 of 1993 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	D7	48	LYS	11.4
56	D1	42	GLN	11.0
22	CV	12	A	10.3
24	DC	227	PRO	9.9
53	Be	122	VAL	9.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	GDP	CY	702	28/28	0.16	-	58,90,102,118	0
60	FUA	CY	701	37/37	0.22	-	125,150,161,166	0
60	FUA	AY	701	37/37	0.62	-	119,146,161,162	0
61	GDP	AY	702	28/28	0.23	-	58,89,106,121	0

6.5 Other polymers ⓘ

There are no such residues in this entry.