



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2024 – 03:34 PM EDT

PDB ID : 4BTS
Title : THE CRYSTAL STRUCTURE OF THE EUKARYOTIC 40S RIBOSOMAL
SUBUNIT IN COMPLEX WITH EIF1 AND EIF1A
Authors : Weisser, M.; Voigts-Hoffmann, F.; Rabl, J.; Leibundgut, M.; Ban, N.
Deposited on : 2013-06-19
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

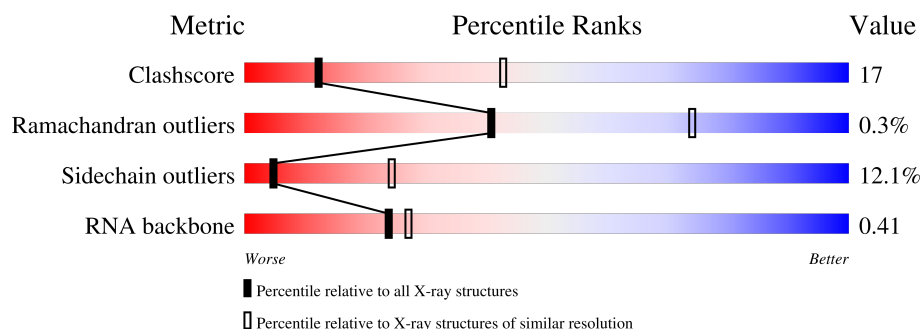
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RNA backbone	3102	1027 (4.40-3.00)











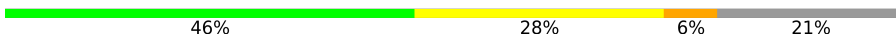

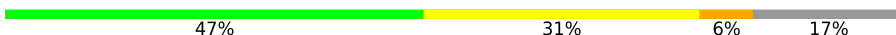









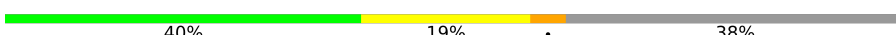
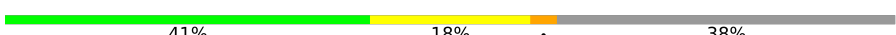
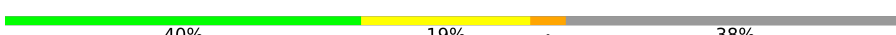
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A0	211	30% 14% • 53%
1	B0	211	28% 15% • 53%
1	C0	211	29% 15% • 53%
1	D0	211	31% 13% • 53%
2	A1	68	54% 38% • •
2	B1	68	57% 34% 6% •

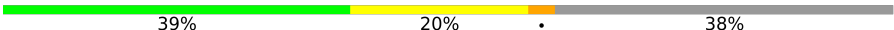


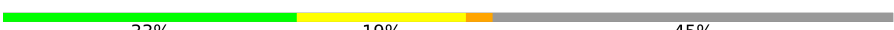






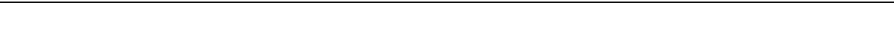

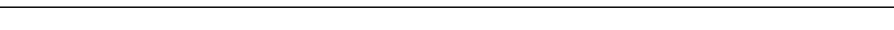
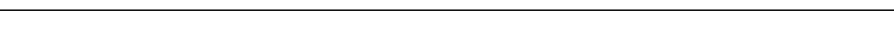











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Mol	Chain	Length	Quality of chain
2	C1	68	
2	D1	68	
3	A2	208	
3	B2	208	
3	C2	208	
3	D2	208	
4	A3	197	
4	B3	197	
4	C3	197	
4	D3	197	
5	A4	265	
5	B4	265	
5	C4	265	
5	D4	265	
6	A5	119	
6	B5	119	
6	C5	119	
6	D5	119	
7	A6	81	
7	B6	81	
7	C6	81	
7	D6	81	
8	A7	162	
8	B7	162	
8	C7	162	


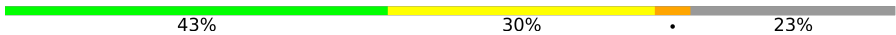
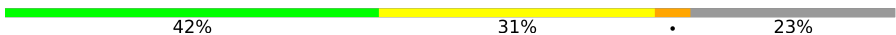








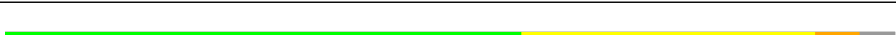

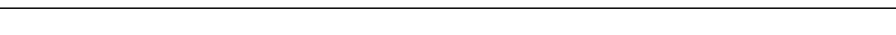
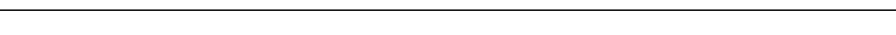
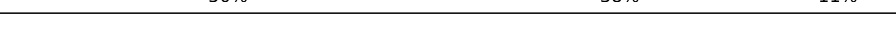

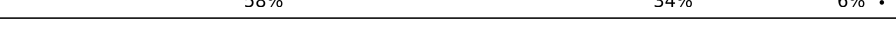







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Mol	Chain	Length	Quality of chain
8	D7	162	
9	A8	143	
9	B8	143	
9	C8	143	
9	D8	143	
10	A9	189	
10	B9	189	
10	C9	189	
10	D9	189	
11	AA	1753	
11	BA	1753	
11	CA	1753	
11	DA	1753	
12	AB	241	
12	BB	241	
12	CB	241	
12	DB	241	
13	AC	243	
13	BC	243	
13	CC	243	
13	DC	243	
14	AD	181	
14	BD	181	
14	CD	181	
14	DD	181	












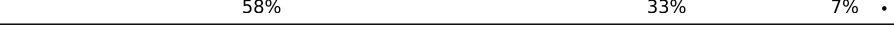







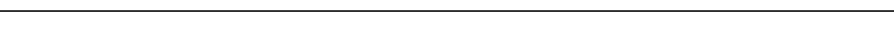

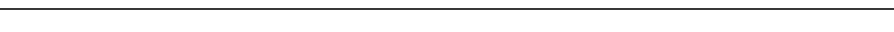
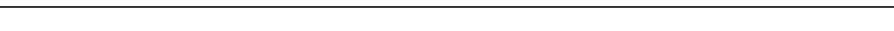


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Mol	Chain	Length	Quality of chain
15	AE	296	
15	BE	296	
15	CE	296	
15	DE	296	
16	AF	101	
16	BF	101	
16	CF	101	
16	DF	101	
17	AG	200	
17	BG	200	
17	CG	200	
17	DG	200	
18	AH	130	
18	BH	130	
18	CH	130	
18	DH	130	
19	AI	145	
19	BI	145	
19	CI	145	
19	DI	145	
20	AJ	120	
20	BJ	120	
20	CJ	120	
20	DJ	120	
21	AK	151	











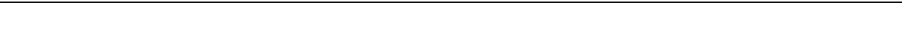

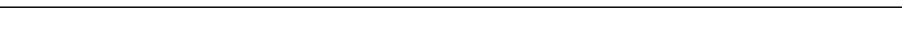
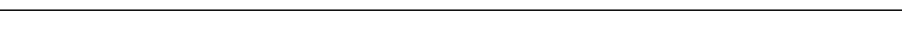











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Mol	Chain	Length	Quality of chain
21	BK	151	 54% 30% 9% 7%
21	CK	151	 52% 32% 9% 7%
21	DK	151	 50% 34% 9% 7%
22	AL	142	 61% 28% 9% .
22	BL	142	 59% 32% 8% .
22	CL	142	 58% 34% 7% .
22	DL	142	 59% 32% 8% .
23	AM	155	 59% 33% 7% .
23	BM	155	 59% 32% 8% .
23	CM	155	 61% 31% 7% .
23	DM	155	 51% 41% 7% .
24	AN	55	 58% 33% 7% .
24	BN	55	 62% 29% 7% .
24	CN	55	 58% 33% 7% .
24	DN	55	 58% 33% 7% .
25	AO	153	 59% 37% . .
25	BO	153	 58% 37% 5% .
25	CO	153	 59% 36% . .
25	DO	153	 58% 37% . .
26	AP	149	 60% 36% . .
26	BP	149	 60% 36% . .
26	CP	149	 60% 36% . .
26	DP	149	 62% 34% . .
27	AQ	157	 57% 34% 8% .
27	BQ	157	 55% 36% 8% .













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Mol	Chain	Length	Quality of chain
27	CQ	157	 59% 32% 9% .
27	DQ	157	 58% 32% 9% .
28	AR	343	 61% 33% . .
28	BR	343	 61% 33% . .
28	CR	343	 61% 33% 5% .
28	DR	343	 62% 32% . .
29	AS	144	 53% 33% . 11%
29	BS	144	 51% 35% . 11%
29	CS	144	 51% 35% . 11%
29	DS	144	 56% 28% 5% 11%
30	AT	155	 61% 33% 6% .
30	BT	155	 61% 32% 6% .
30	CT	155	 60% 33% 6% .
30	DT	155	 61% 33% 6% .
31	AU	126	 58% 36% . . .
31	BU	126	 60% 33% 5% . .
31	CU	126	 60% 33% 5% . .
31	DU	126	 60% 33% 5% . .
32	AV	130	 57% 30% 5% 8%
32	BV	130	 57% 31% . 8%
32	CV	130	 53% 35% . 8%
32	DV	130	 54% 32% 5% 8%
33	AW	259	 61% 33% 6%
33	BW	259	 57% 37% 6%
33	CW	259	 59% 35% 7%

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Mol	Chain	Length	Quality of chain
33	DW	259	 58%36%6%
34	AX	80	 66%22%•8%
34	BX	80	 62%26%•8%
34	CX	80	 64%25%•8%
34	DX	80	 66%21%5%8%
35	AY	293	 46%28%•22%
35	BY	293	 45%29%•22%
35	CY	293	 46%28%•22%
35	DY	293	 46%29%•22%
36	AZ	97	 61%35%•
36	BZ	97	 59%35%6%
36	CZ	97	 58%38%•
36	DZ	97	 62%34%•

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 315512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called TRANSLATION INITIATION FACTOR EIF-1A FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	99	Total	C	N	O	S	0	0	0
			817	517	142	152	6			
1	B0	99	Total	C	N	O	S	0	0	0
			817	517	142	152	6			
1	C0	99	Total	C	N	O	S	0	0	0
			817	517	142	152	6			
1	D0	99	Total	C	N	O	S	0	0	0
			817	517	142	152	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A0	-17	MET	-	expression tag	UNP I7MK25
A0	-16	GLY	-	expression tag	UNP I7MK25
A0	-15	SER	-	expression tag	UNP I7MK25
A0	-14	SER	-	expression tag	UNP I7MK25
A0	-13	HIS	-	expression tag	UNP I7MK25
A0	-12	HIS	-	expression tag	UNP I7MK25
A0	-11	HIS	-	expression tag	UNP I7MK25
A0	-10	HIS	-	expression tag	UNP I7MK25
A0	-9	HIS	-	expression tag	UNP I7MK25
A0	-8	HIS	-	expression tag	UNP I7MK25
A0	-7	GLU	-	expression tag	UNP I7MK25
A0	-6	ASN	-	expression tag	UNP I7MK25
A0	-5	LEU	-	expression tag	UNP I7MK25
A0	-4	TYR	-	expression tag	UNP I7MK25
A0	-3	PHE	-	expression tag	UNP I7MK25
A0	-2	GLN	-	expression tag	UNP I7MK25
A0	-1	SER	-	expression tag	UNP I7MK25
A0	0	ASN	-	expression tag	UNP I7MK25
A0	1	ALA	-	expression tag	UNP I7MK25
B0	-17	MET	-	expression tag	UNP I7MK25

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Chain	Residue	Modelled	Actual	Comment	Reference
B0	-16	GLY	-	expression tag	UNP I7MK25
B0	-15	SER	-	expression tag	UNP I7MK25
B0	-14	SER	-	expression tag	UNP I7MK25
B0	-13	HIS	-	expression tag	UNP I7MK25
B0	-12	HIS	-	expression tag	UNP I7MK25
B0	-11	HIS	-	expression tag	UNP I7MK25
B0	-10	HIS	-	expression tag	UNP I7MK25
B0	-9	HIS	-	expression tag	UNP I7MK25
B0	-8	HIS	-	expression tag	UNP I7MK25
B0	-7	GLU	-	expression tag	UNP I7MK25
B0	-6	ASN	-	expression tag	UNP I7MK25
B0	-5	LEU	-	expression tag	UNP I7MK25
B0	-4	TYR	-	expression tag	UNP I7MK25
B0	-3	PHE	-	expression tag	UNP I7MK25
B0	-2	GLN	-	expression tag	UNP I7MK25
B0	-1	SER	-	expression tag	UNP I7MK25
B0	0	ASN	-	expression tag	UNP I7MK25
B0	1	ALA	-	expression tag	UNP I7MK25
C0	-17	MET	-	expression tag	UNP I7MK25
C0	-16	GLY	-	expression tag	UNP I7MK25
C0	-15	SER	-	expression tag	UNP I7MK25
C0	-14	SER	-	expression tag	UNP I7MK25
C0	-13	HIS	-	expression tag	UNP I7MK25
C0	-12	HIS	-	expression tag	UNP I7MK25
C0	-11	HIS	-	expression tag	UNP I7MK25
C0	-10	HIS	-	expression tag	UNP I7MK25
C0	-9	HIS	-	expression tag	UNP I7MK25
C0	-8	HIS	-	expression tag	UNP I7MK25
C0	-7	GLU	-	expression tag	UNP I7MK25
C0	-6	ASN	-	expression tag	UNP I7MK25
C0	-5	LEU	-	expression tag	UNP I7MK25
C0	-4	TYR	-	expression tag	UNP I7MK25
C0	-3	PHE	-	expression tag	UNP I7MK25
C0	-2	GLN	-	expression tag	UNP I7MK25
C0	-1	SER	-	expression tag	UNP I7MK25
C0	0	ASN	-	expression tag	UNP I7MK25
C0	1	ALA	-	expression tag	UNP I7MK25
D0	-17	MET	-	expression tag	UNP I7MK25
D0	-16	GLY	-	expression tag	UNP I7MK25
D0	-15	SER	-	expression tag	UNP I7MK25
D0	-14	SER	-	expression tag	UNP I7MK25
D0	-13	HIS	-	expression tag	UNP I7MK25

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Chain	Residue	Modelled	Actual	Comment	Reference
D0	-12	HIS	-	expression tag	UNP I7MK25
D0	-11	HIS	-	expression tag	UNP I7MK25
D0	-10	HIS	-	expression tag	UNP I7MK25
D0	-9	HIS	-	expression tag	UNP I7MK25
D0	-8	HIS	-	expression tag	UNP I7MK25
D0	-7	GLU	-	expression tag	UNP I7MK25
D0	-6	ASN	-	expression tag	UNP I7MK25
D0	-5	LEU	-	expression tag	UNP I7MK25
D0	-4	TYR	-	expression tag	UNP I7MK25
D0	-3	PHE	-	expression tag	UNP I7MK25
D0	-2	GLN	-	expression tag	UNP I7MK25
D0	-1	SER	-	expression tag	UNP I7MK25
D0	0	ASN	-	expression tag	UNP I7MK25
D0	1	ALA	-	expression tag	UNP I7MK25

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN RPS28E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A1	66	Total 511	C 308	N 103	O 96	S 4	0	0	0
2	B1	66	Total 511	C 308	N 103	O 96	S 4	0	0	0
2	C1	66	Total 511	C 308	N 103	O 96	S 4	0	0	0
2	D1	66	Total 511	C 308	N 103	O 96	S 4	0	0	0

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	207	Total 1693	C 1057	N 336	O 296	S 4	0	0	0
3	B2	207	Total 1693	C 1057	N 336	O 296	S 4	0	0	0
3	C2	207	Total 1693	C 1057	N 336	O 296	S 4	0	0	0
3	D2	207	Total 1693	C 1057	N 336	O 296	S 4	0	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN RPS7E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			
4	B3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			
4	C3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			
4	D3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	209	Total	C	N	O	S	0	0	0
			1679	1061	304	310	4			
5	B4	221	Total	C	N	O	S	0	0	0
			1775	1121	319	331	4			
5	C4	221	Total	C	N	O	S	0	0	0
			1775	1121	319	331	4			
5	D4	221	Total	C	N	O	S	0	0	0
			1775	1121	319	331	4			

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN RPS26E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A5	100	Total	C	N	O	S	0	0	0
			812	496	172	138	6			
6	B5	100	Total	C	N	O	S	0	0	0
			812	496	172	138	6			
6	C5	100	Total	C	N	O	S	0	0	0
			812	496	172	138	6			
6	D5	100	Total	C	N	O	S	0	0	0
			812	496	172	138	6			

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			
7	B6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			
7	C6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN RPS10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	A7	101	Total	C	N	O	S	0	0	0
			833	546	139	146	2			
8	B7	101	Total	C	N	O	S	0	0	0
			833	546	139	146	2			
8	C7	101	Total	C	N	O	S	0	0	0
			833	546	139	146	2			
8	D7	101	Total	C	N	O	S	0	0	0
			833	546	139	146	2			

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN RPS25E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	A8	79	Total	C	N	O	S	0	0	0
			615	388	112	113	2			
9	B8	79	Total	C	N	O	S	0	0	0
			615	388	112	113	2			
9	C8	79	Total	C	N	O	S	0	0	0
			615	388	112	113	2			
9	D8	79	Total	C	N	O	S	0	0	0
			615	388	112	113	2			

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN RPS31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A9	93	Total	C	N	O	S	0	0	0
			751	477	143	126	5			
10	B9	93	Total	C	N	O	S	0	0	0
			751	477	143	126	5			
10	C9	93	Total	C	N	O	S	0	0	0
			751	477	143	126	5			
10	D9	93	Total	C	N	O	S	0	0	0
			751	477	143	126	5			

- Molecule 11 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AA	1717	Total	C	N	O	P	0	0	0
			36629	16385	6539	11988	1717			
11	BA	1717	Total	C	N	O	P	0	0	0
			36629	16385	6539	11988	1717			
11	CA	1717	Total	C	N	O	P	0	0	0
			36629	16385	6539	11988	1717			
11	DA	1717	Total	C	N	O	P	0	0	0
			36629	16385	6539	11988	1717			

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AB	201	Total	C	N	O	S	0	0	0
			1619	1023	285	301	10			
12	BB	201	Total	C	N	O	S	0	0	0
			1619	1023	285	301	10			
12	CB	201	Total	C	N	O	S	0	0	0
			1619	1023	285	301	10			
12	DB	201	Total	C	N	O	S	0	0	0
			1619	1023	285	301	10			

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN RPS3E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AC	228	Total	C	N	O	S	0	0	0
			1811	1167	318	318	8			
13	BC	228	Total	C	N	O	S	0	0	0
			1811	1167	318	318	8			
13	CC	228	Total	C	N	O	S	0	0	0
			1811	1167	318	318	8			
13	DC	228	Total	C	N	O	S	0	0	0
			1811	1167	318	318	8			

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN RPS9E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AD	180	Total	C	N	O	S	0	0	0
			1478	932	287	254	5			
14	BD	180	Total	C	N	O	S	0	0	0
			1478	932	287	254	5			
14	CD	180	Total	C	N	O	S	0	0	0
			1478	932	287	254	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	DD	180	Total	C	N	O	S	0	0	0
			1478	932	287	254	5			

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN RPS2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AE	229	Total	C	N	O	S	0	0	0
			1818	1171	321	323	3			
15	BE	229	Total	C	N	O	S	0	0	0
			1818	1171	321	323	3			
15	CE	229	Total	C	N	O	S	0	0	0
			1818	1171	321	323	3			
15	DE	229	Total	C	N	O	S	0	0	0
			1818	1171	321	323	3			

- Molecule 16 is a protein called EIF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			
16	BF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			
16	CF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			
16	DF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN RPS5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			
17	BG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			
17	CG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			
17	DG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN RPS22E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			
18	BH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			
18	CH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			
18	DH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN RPS16E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			
19	BI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			
19	CI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			
19	DI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN RPS20E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AJ	108	Total	C	N	O	S	0	0	0
			859	539	154	160	6			
20	BJ	108	Total	C	N	O	S	0	0	0
			859	539	154	160	6			
20	CJ	108	Total	C	N	O	S	0	0	0
			859	539	154	160	6			
20	DJ	108	Total	C	N	O	S	0	0	0
			859	539	154	160	6			

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN RPS14E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			
21	BK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			
21	CK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	DK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AL	140	Total	C	N	O	S	0	0	0
			1086	685	217	179	5			
22	BL	140	Total	C	N	O	S	0	0	0
			1086	685	217	179	5			
22	CL	140	Total	C	N	O	S	0	0	0
			1086	685	217	179	5			
22	DL	140	Total	C	N	O	S	0	0	0
			1086	685	217	179	5			

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN RPS18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AM	153	Total	C	N	O	S	0	0	0
			1231	775	236	215	5			
23	BM	153	Total	C	N	O	S	0	0	0
			1231	775	236	215	5			
23	CM	153	Total	C	N	O	S	0	0	0
			1231	775	236	215	5			
23	DM	153	Total	C	N	O	S	0	0	0
			1231	775	236	215	5			

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN RPS29E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AN	54	Total	C	N	O	S	0	0	0
			454	283	92	73	6			
24	BN	54	Total	C	N	O	S	0	0	0
			454	283	92	73	6			
24	CN	54	Total	C	N	O	S	0	0	0
			454	283	92	73	6			
24	DN	54	Total	C	N	O	S	0	0	0
			454	283	92	73	6			

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN RPS13E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AO	152	Total	C	N	O	S	0	0	0
			1229	790	233	202	4			
25	BO	152	Total	C	N	O	S	0	0	0
			1229	790	233	202	4			
25	CO	152	Total	C	N	O	S	0	0	0
			1229	790	233	202	4			
25	DO	152	Total	C	N	O	S	0	0	0
			1229	790	233	202	4			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AP	148	Total	C	N	O		0	0	0
			1197	763	221	213				
26	BP	148	Total	C	N	O		0	0	0
			1197	763	221	213				
26	CP	148	Total	C	N	O		0	0	0
			1197	763	221	213				
26	DP	148	Total	C	N	O		0	0	0
			1197	763	221	213				

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN RPS11E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AQ	156	Total	C	N	O	S	0	0	0
			1267	813	234	216	4			
27	BQ	156	Total	C	N	O	S	0	0	0
			1267	813	234	216	4			
27	CQ	156	Total	C	N	O	S	0	0	0
			1267	813	234	216	4			
27	DQ	156	Total	C	N	O	S	0	0	0
			1267	813	234	216	4			

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			
28	BR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			
28	CR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	DR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN RPS15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AS	128	Total	C	N	O	S	0	0	0
			1010	648	178	180	4			
29	BS	128	Total	C	N	O	S	0	0	0
			1010	648	178	180	4			
29	CS	128	Total	C	N	O	S	0	0	0
			1010	648	178	180	4			
29	DS	128	Total	C	N	O	S	0	0	0
			1010	648	178	180	4			

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN RPS19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AT	154	Total	C	N	O	S	0	0	0
			1242	785	234	221	2			
30	BT	154	Total	C	N	O	S	0	0	0
			1242	785	234	221	2			
30	CT	154	Total	C	N	O	S	0	0	0
			1242	785	234	221	2			
30	DT	154	Total	C	N	O	S	0	0	0
			1242	785	234	221	2			

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN RPS12E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			
31	BU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			
31	CU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			
31	DU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN RPS17E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AV	119	Total	C	N	O	S	0	0	0
			968	613	180	173	2			
32	BV	119	Total	C	N	O	S	0	0	0
			968	613	180	173	2			
32	CV	119	Total	C	N	O	S	0	0	0
			968	613	180	173	2			
32	DV	119	Total	C	N	O	S	0	0	0
			968	613	180	173	2			

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN RPS4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			
33	BW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			
33	CW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			
33	DW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN RPS30E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AX	74	Total	C	N	O	S	0	0	0
			599	376	124	96	3			
34	BX	74	Total	C	N	O	S	0	0	0
			599	376	124	96	3			
34	CX	74	Total	C	N	O	S	0	0	0
			599	376	124	96	3			
34	DX	74	Total	C	N	O	S	0	0	0
			599	376	124	96	3			

- Molecule 35 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AY	228	Total	C	N	O	S	0	0	0
			1826	1157	340	318	11			
35	BY	228	Total	C	N	O	S	0	0	0
			1826	1157	340	318	11			
35	CY	228	Total	C	N	O	S	0	0	0
			1826	1157	340	318	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DY	228	Total	C	N	O	S	0	0	0
			1826	1157	340	318	11			

- Molecule 36 is a protein called 40S RIBOSOMAL PROTEIN RPS21E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			
36	BZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			
36	CZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			
36	DZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A5	1	Total	Zn	0	0
			1	1		
37	A6	1	Total	Zn	0	0
			1	1		
37	A9	1	Total	Zn	0	0
			1	1		
37	AN	1	Total	Zn	0	0
			1	1		
37	B5	1	Total	Zn	0	0
			1	1		
37	B6	1	Total	Zn	0	0
			1	1		
37	B9	1	Total	Zn	0	0
			1	1		
37	BN	1	Total	Zn	0	0
			1	1		
37	C5	1	Total	Zn	0	0
			1	1		
37	C6	1	Total	Zn	0	0
			1	1		
37	C9	1	Total	Zn	0	0
			1	1		
37	CN	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	D5	1	Total 1	Zn 1	0	0
37	D6	1	Total 1	Zn 1	0	0
37	D9	1	Total 1	Zn 1	0	0
37	DN	1	Total 1	Zn 1	0	0

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

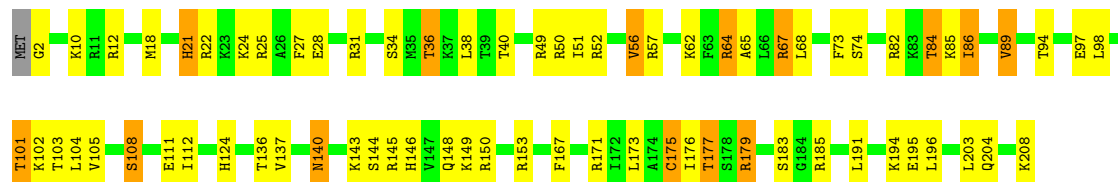
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	AA	79	Total 79	Mg 79	0	0
38	BA	79	Total 79	Mg 79	0	0
38	CA	79	Total 79	Mg 79	0	0
38	DA	79	Total 79	Mg 79	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	AA	474	Total 474	O 474	0	0
39	BA	474	Total 474	O 474	0	0
39	C2	2	Total 2	O 2	0	0
39	C4	2	Total 2	O 2	0	0
39	C5	3	Total 3	O 3	0	0
39	CA	467	Total 467	O 467	0	0
39	DA	474	Total 474	O 474	0	0

- Molecule 3: 40S RIBOSOMAL PROTEIN S8

Chain B2: 



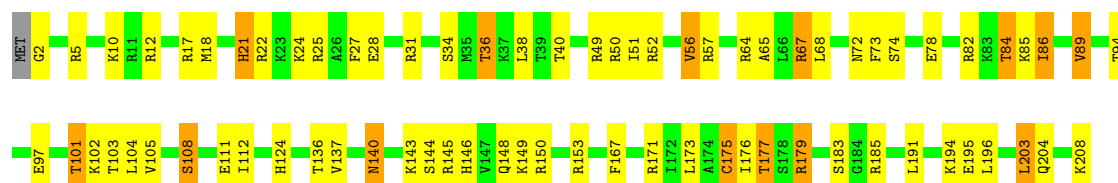
- Molecule 3: 40S RIBOSOMAL PROTEIN S8

Chain C2: 



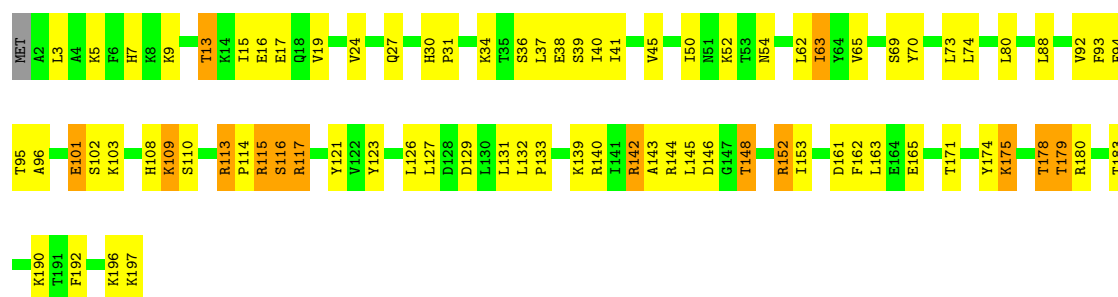
- Molecule 3: 40S RIBOSOMAL PROTEIN S8

Chain D2: 



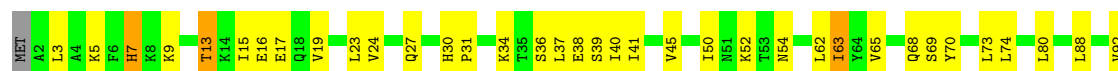
- Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E

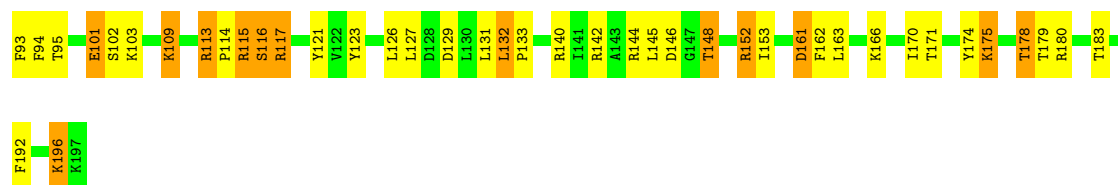
Chain A3: 



- Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E

Chain B3: 





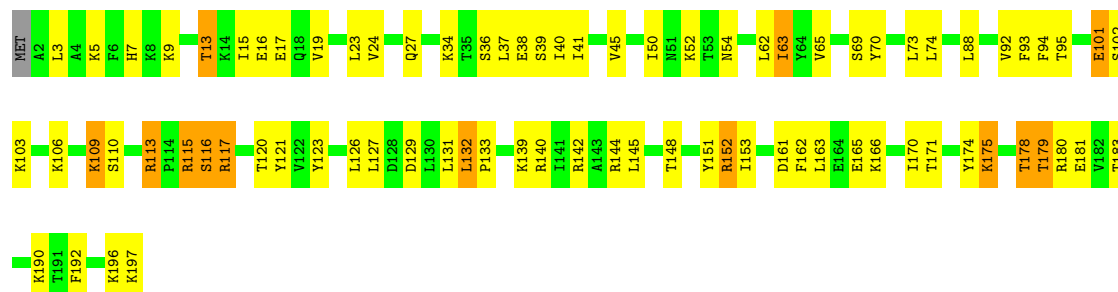
• Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E

Chain C3: 58% 35% 7%



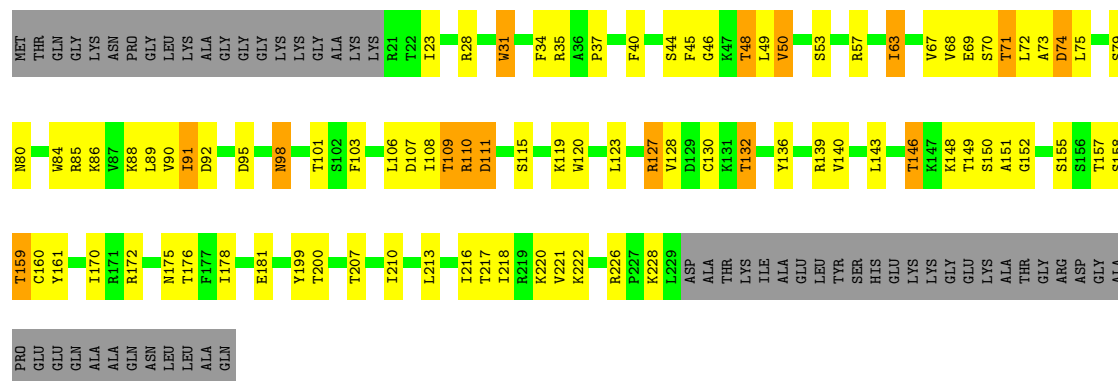
• Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E

Chain D3: 58% 35% 7%

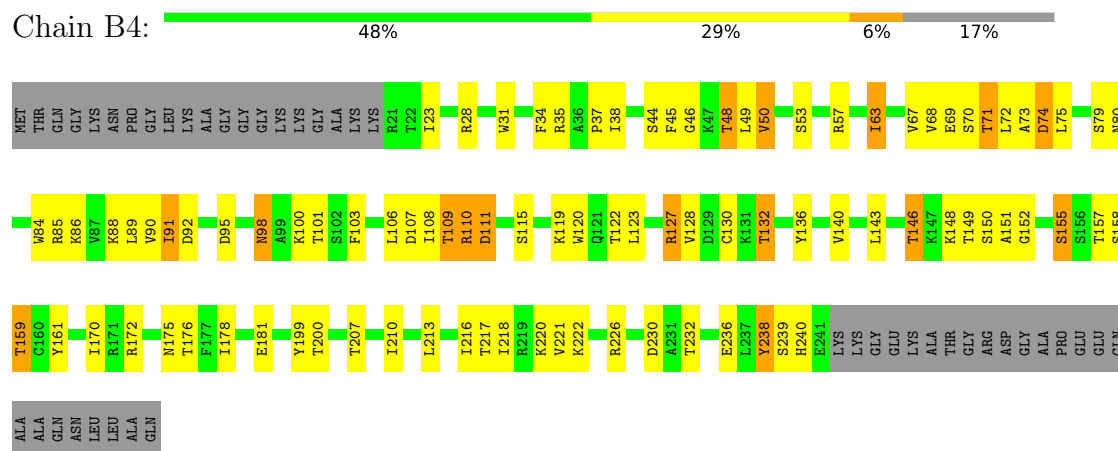


• Molecule 5: 40S RIBOSOMAL PROTEIN S3A

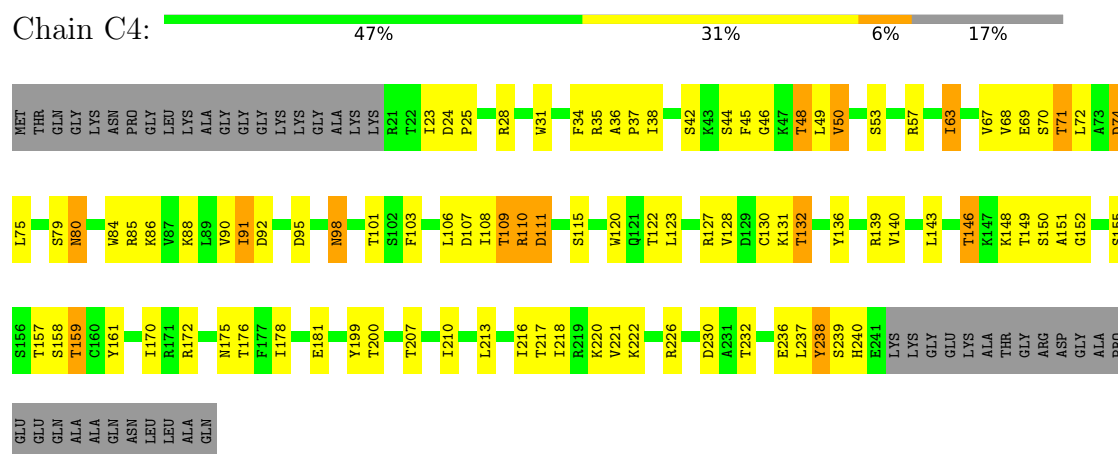
Chain A4: 46% 28% 6% 21%



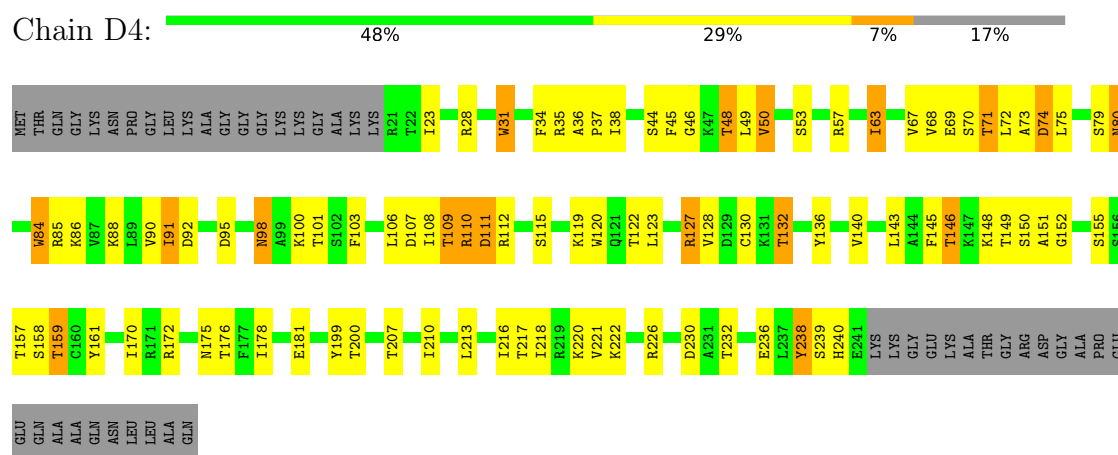
• Molecule 5: 40S RIBOSOMAL PROTEIN S3A



• Molecule 5: 40S RIBOSOMAL PROTEIN S3A

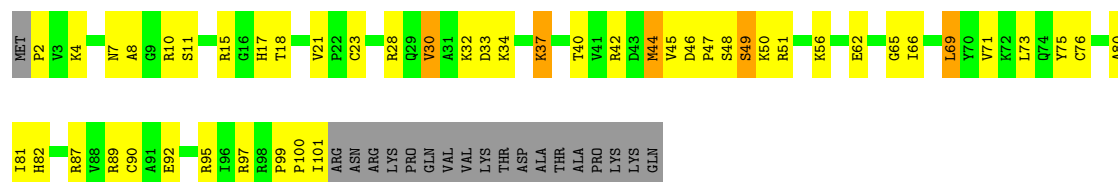


• Molecule 5: 40S RIBOSOMAL PROTEIN S3A

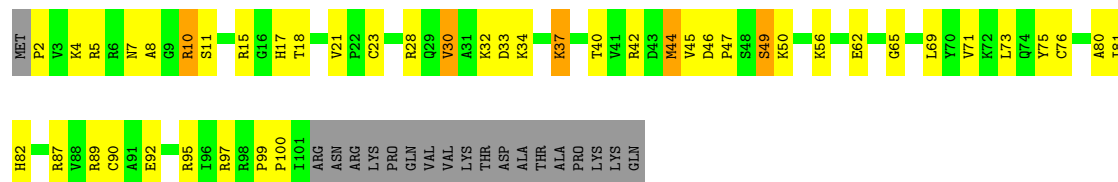


• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E

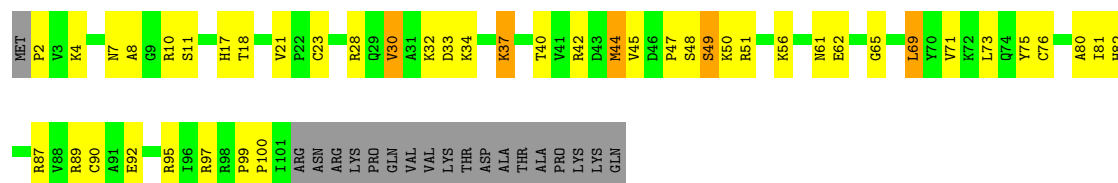




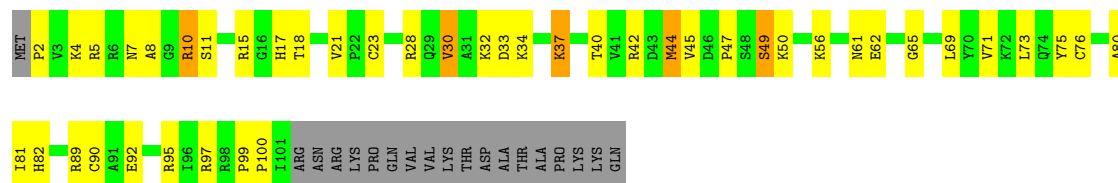
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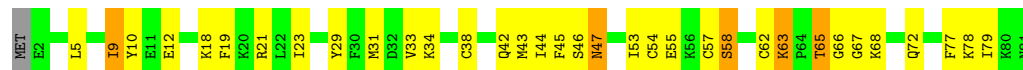
• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E



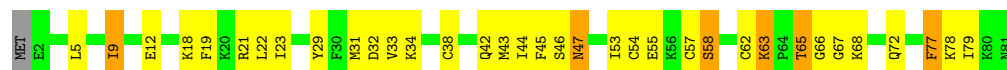
• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E



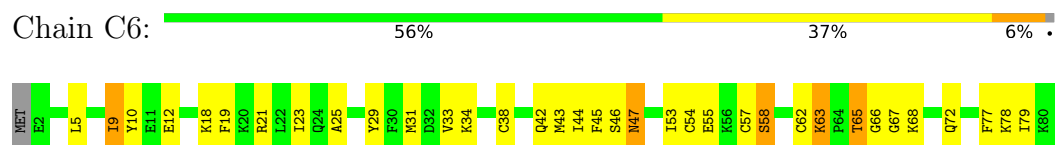
• Molecule 7: 40S RIBOSOMAL PROTEIN S27



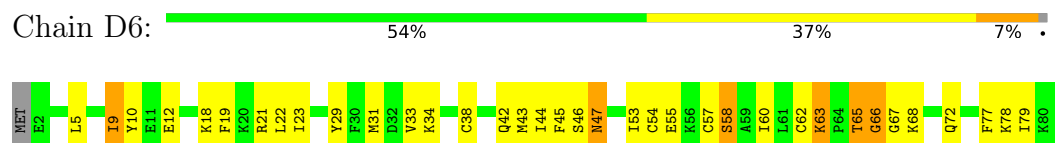
• Molecule 7: 40S RIBOSOMAL PROTEIN S27



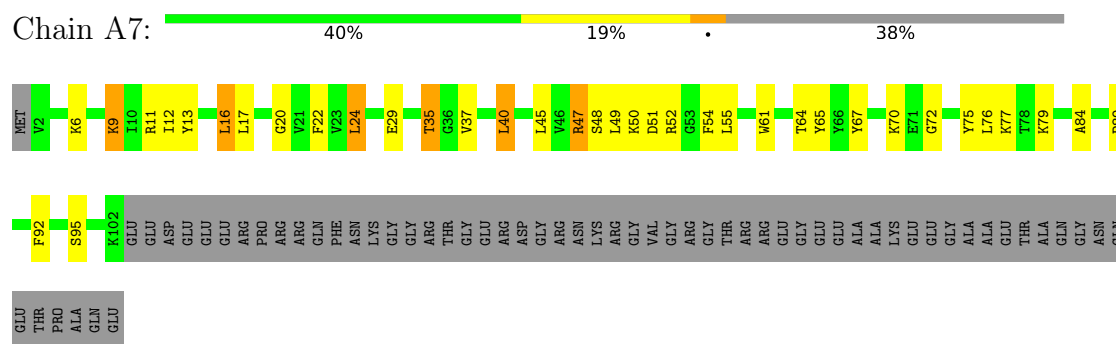
- Molecule 7: 40S RIBOSOMAL PROTEIN S27



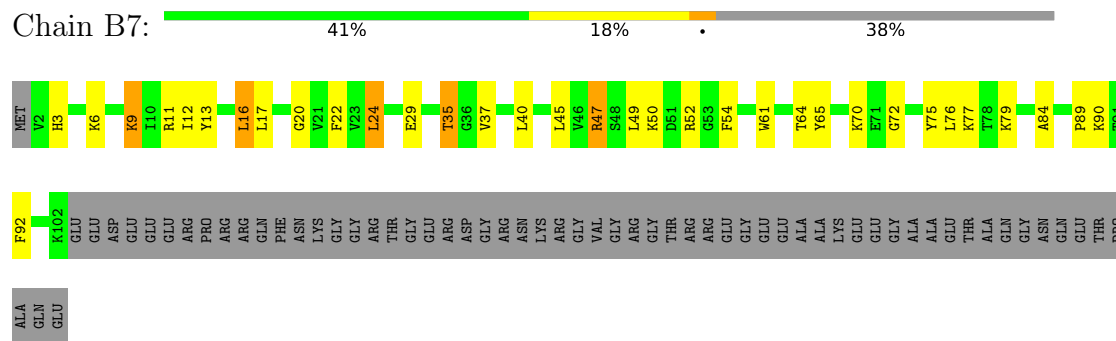
- Molecule 7: 40S RIBOSOMAL PROTEIN S27



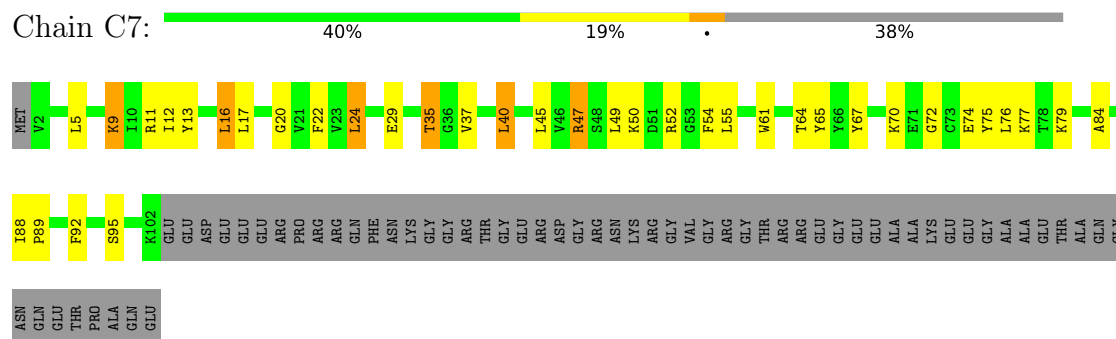
- Molecule 8: 40S RIBOSOMAL PROTEIN RPS10E

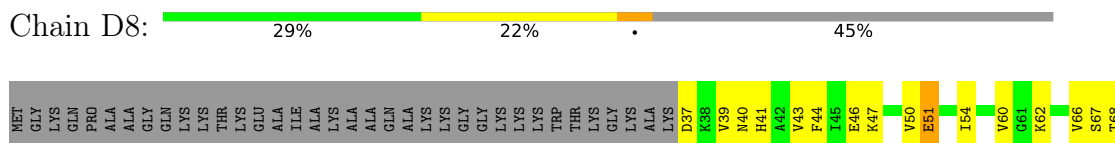


- Molecule 8: 40S RIBOSOMAL PROTEIN RPS10E



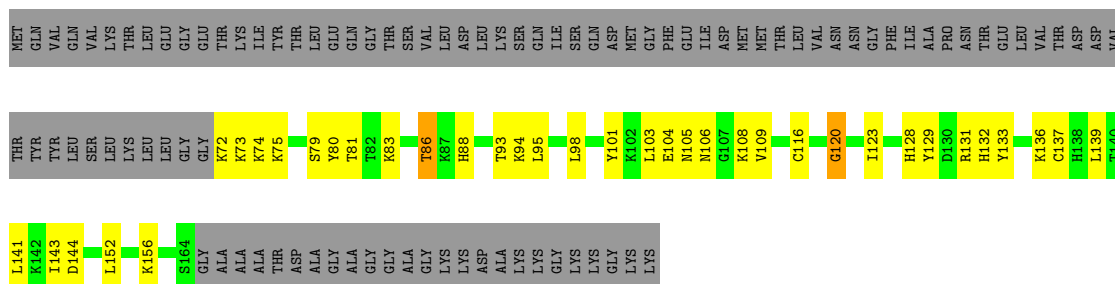
- Molecule 8: 40S RIBOSOMAL PROTEIN RPS10E



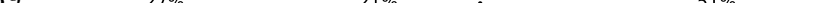


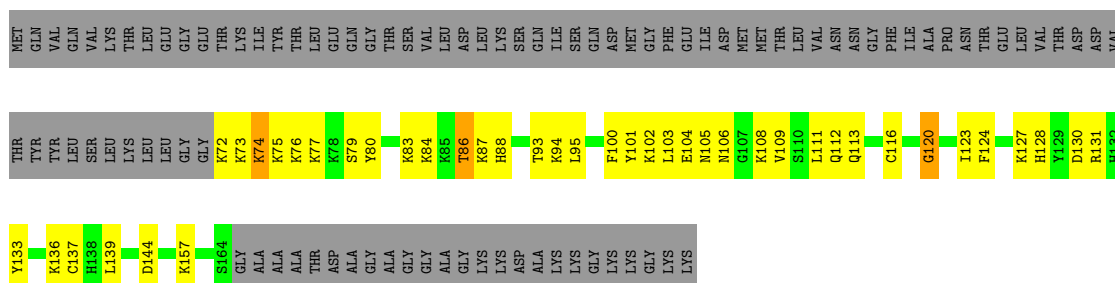
- Molecule 10: 40S RIBOSOMAL PROTEIN RPS31E

Chain A9: 30% 19% . 51%




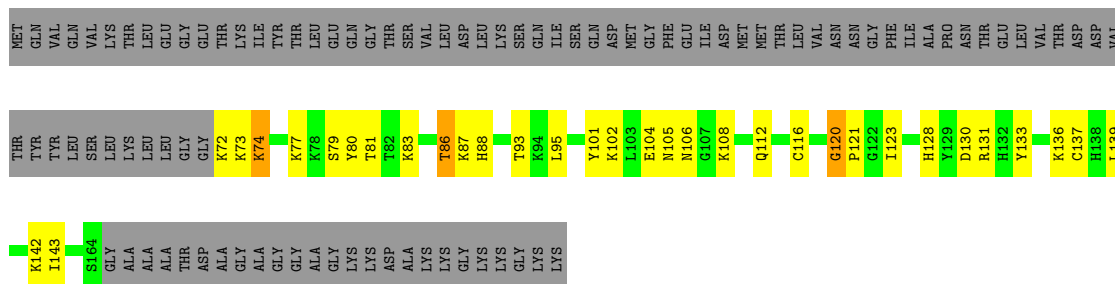
- Molecule 10: 40S RIBOSOMAL PROTEIN RPS31E

Chain B9:  27% 21% . 51%

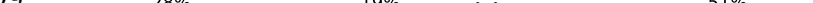


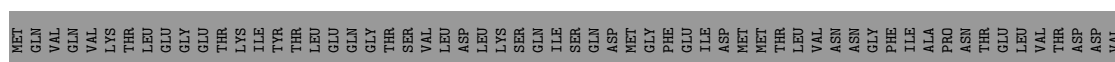
- Molecule 10: 40S RIBOSOMAL PROTEIN RPS31E

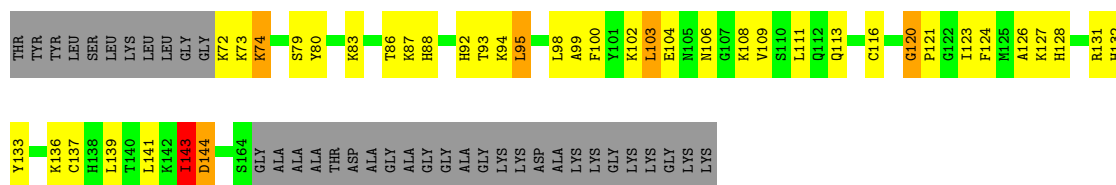
Chain C9:  32% 16% . 51%



- Molecule 10: 40S RIBOSOMAL PROTEIN RPS31E

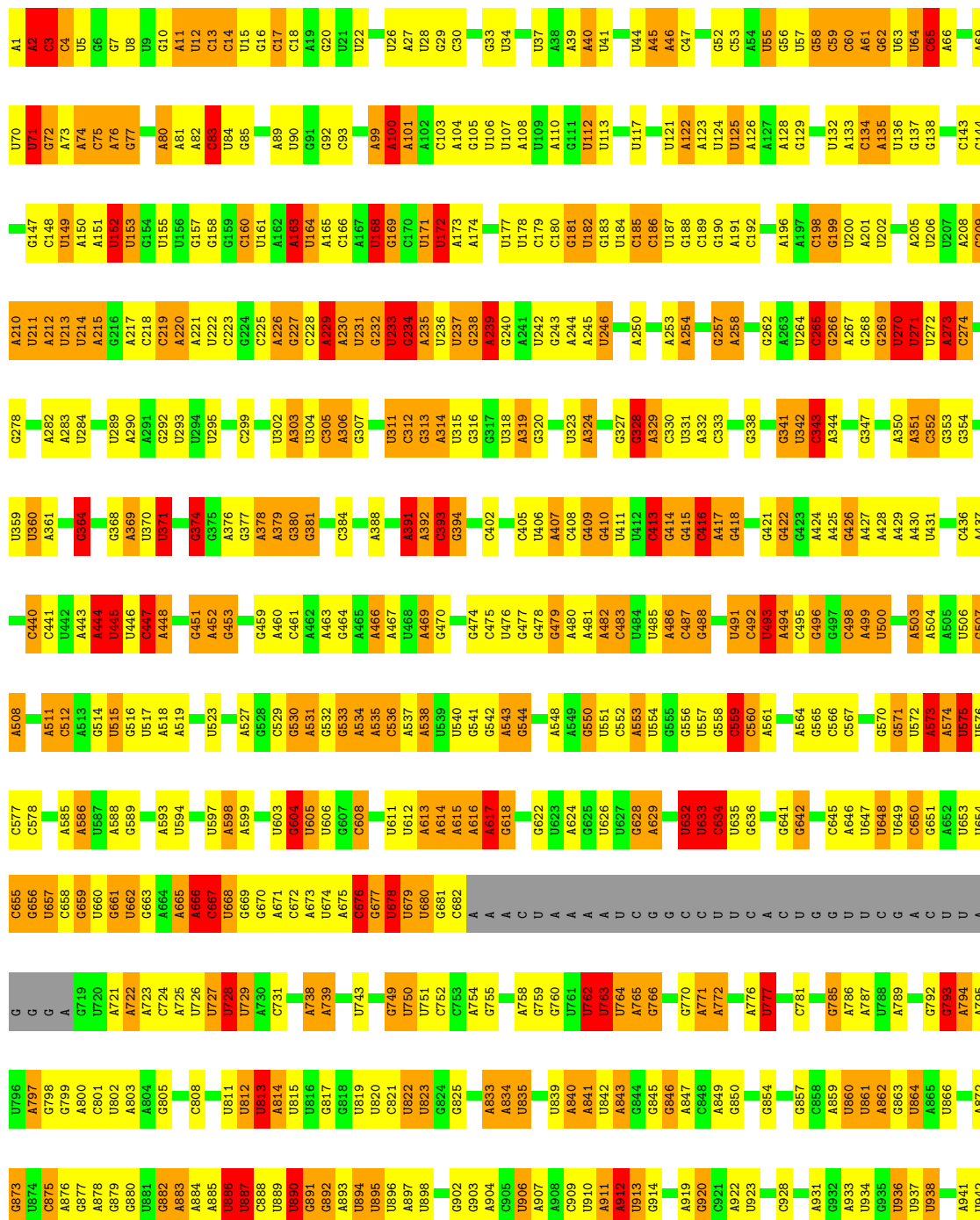
Chain D9: 

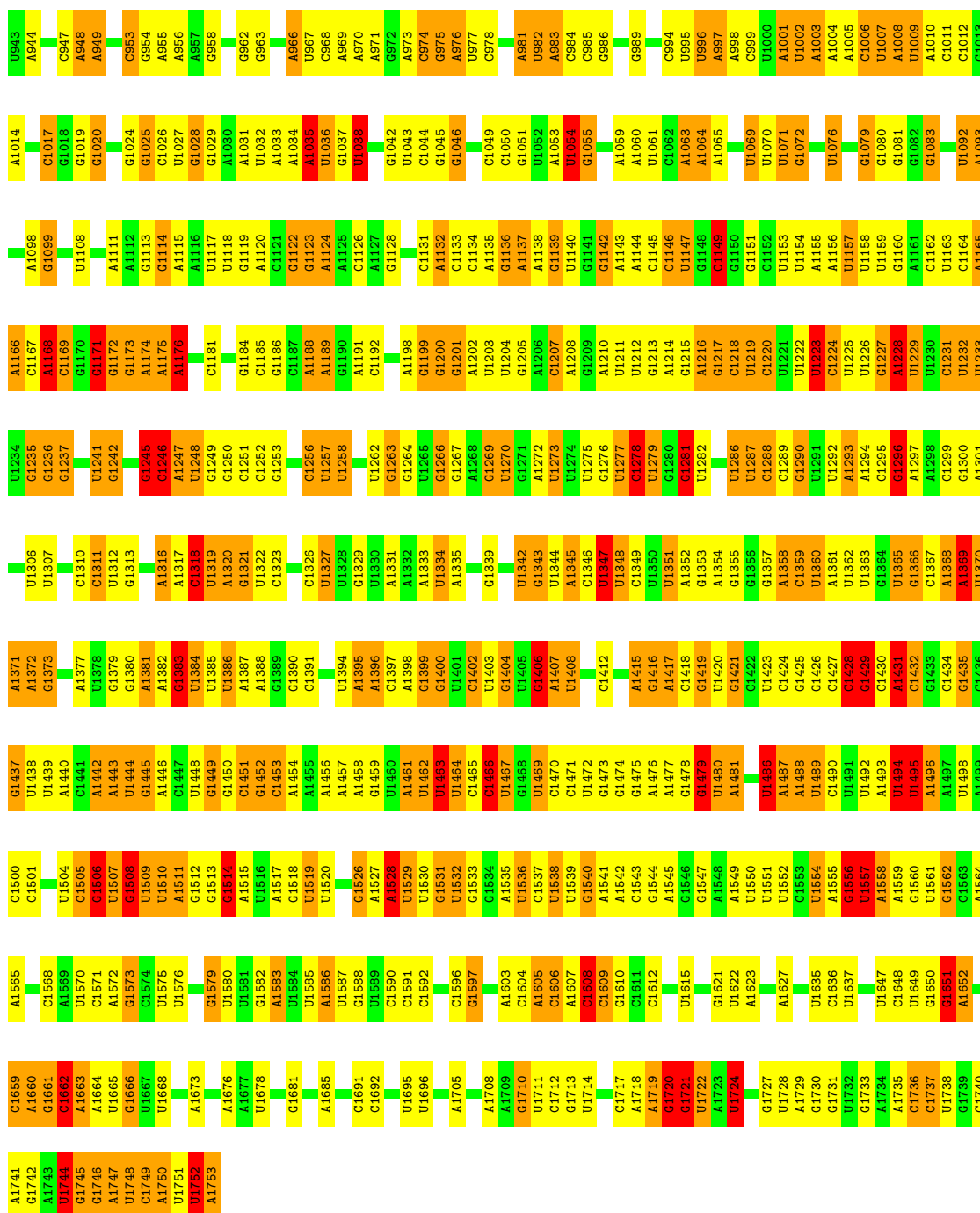




• Molecule 11: 18S ribosomal RNA

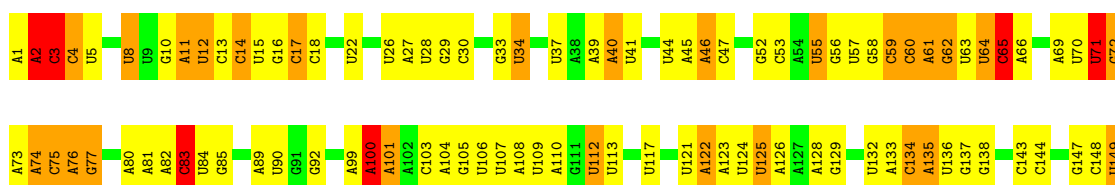
Chain AA: 34% 36% 23% 5% .





• Molecule 11: 18S ribosomal RNA

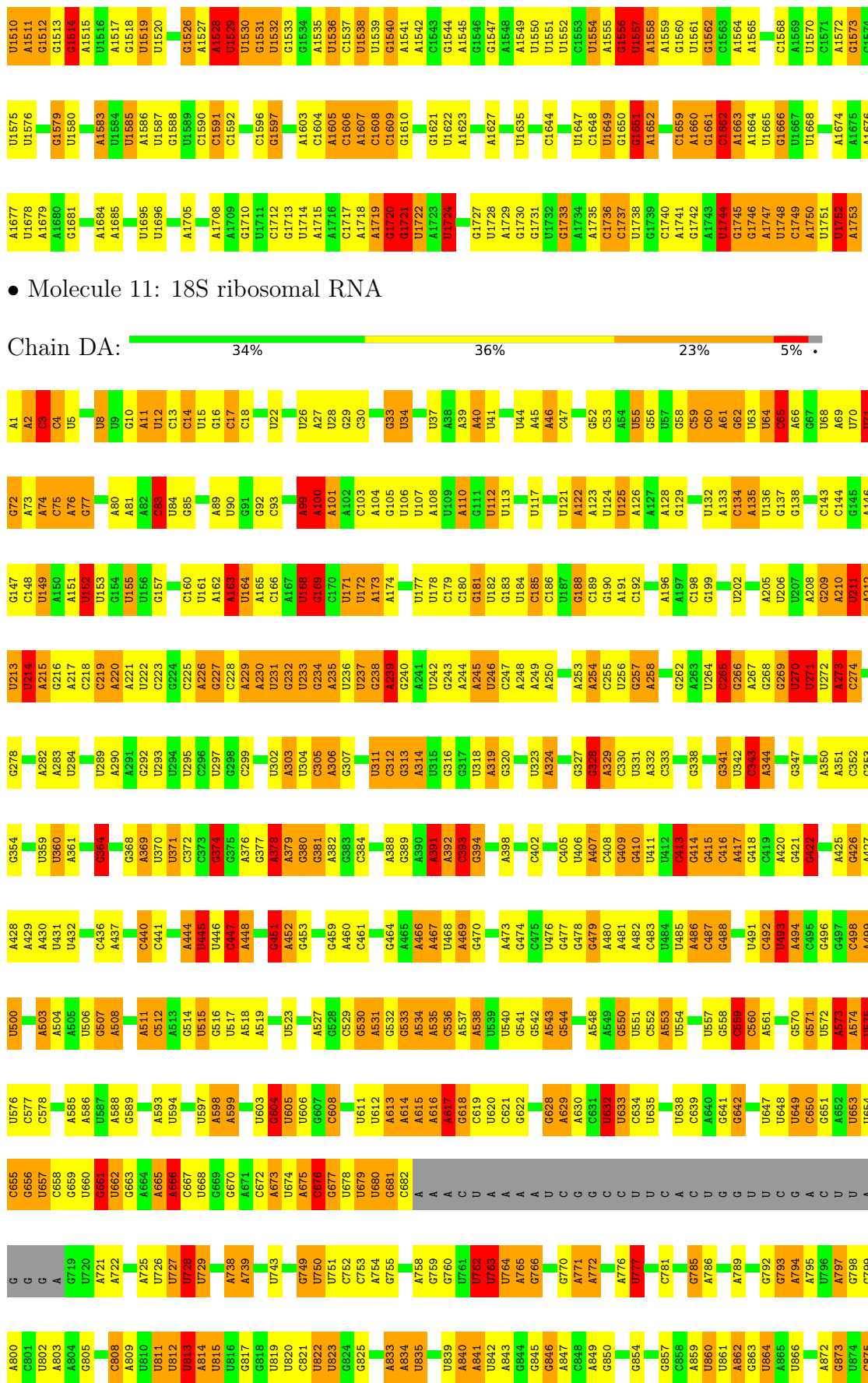
Chain BA: 34% 35% 24% 5% •







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			A1556	G1429	G1429	U1362	A1298	U1232	G1082	A1010	U937	
U1732	U1647		G1556	U1494	C1430	U1363	A1298	U1232	G1083	C1011	U938	
G1733	C1648		U1557	U1495	A1431	G1364	C1299	U1233	A1166	C1012		
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C1737	A1652		U1561	A1498	G1435	A1368	A1303	G1237	G1170	A1097	C1017	A944
			G1562	C1500	C1436	A1369			G1171	A1098	C1018	
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• Molecule 12: 40S RIBOSOMAL PROTEIN SA

Chain AB:

47%

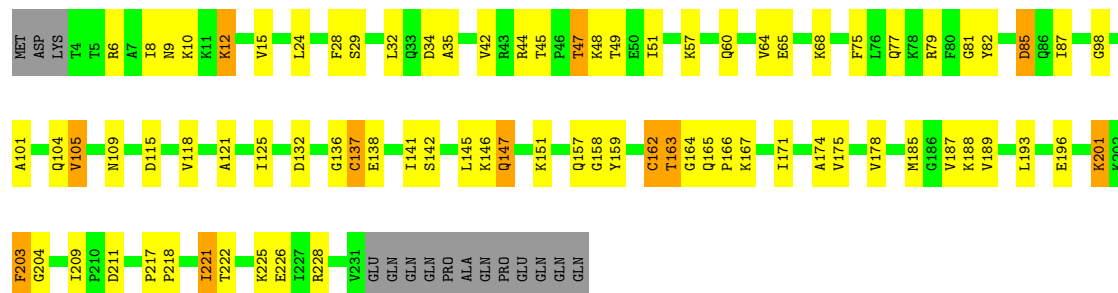
34%

17%

MET	A2	R12	S16	N17	I23	N24	L25	N26	N27	Q28	M29	Y32	I33	S34	H35	V38	H42	Y43	I44	N45	I46	E47	E48	A49	I50	H51	H52	H53	H54	H55	H56	I60	A61	A62	V63	Q64	H65	P66	E67	D68	V69	W70	V71	R75	I76	Y77	A78	G79	R80	A81	A82
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

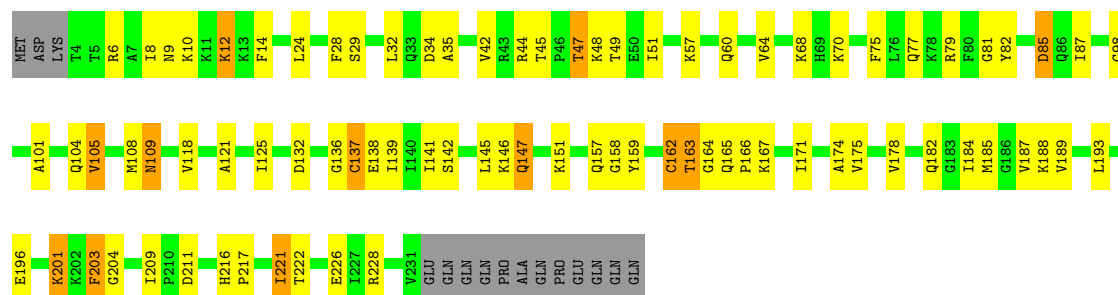
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain AC: 



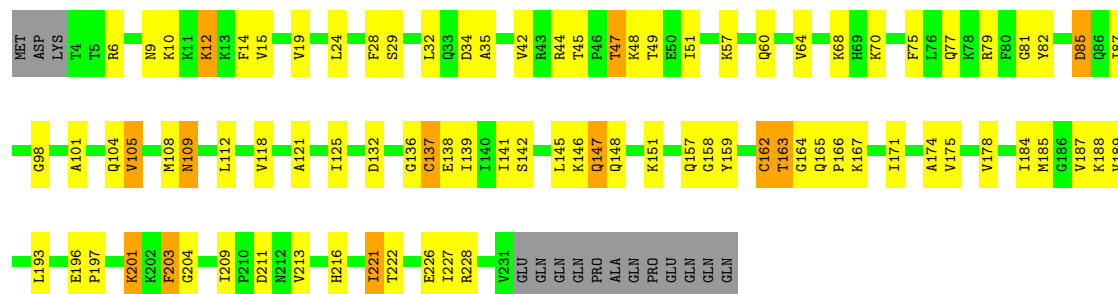
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain BC: 



• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

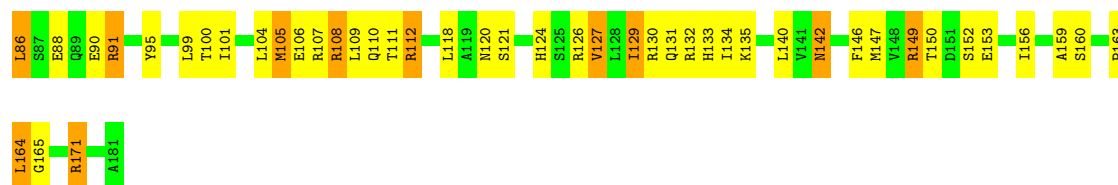
Chain CC: 



• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

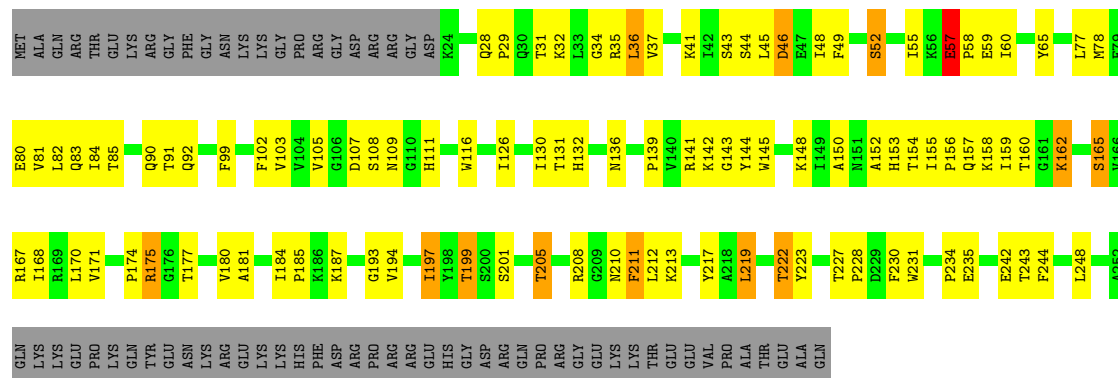
Chain DC: 





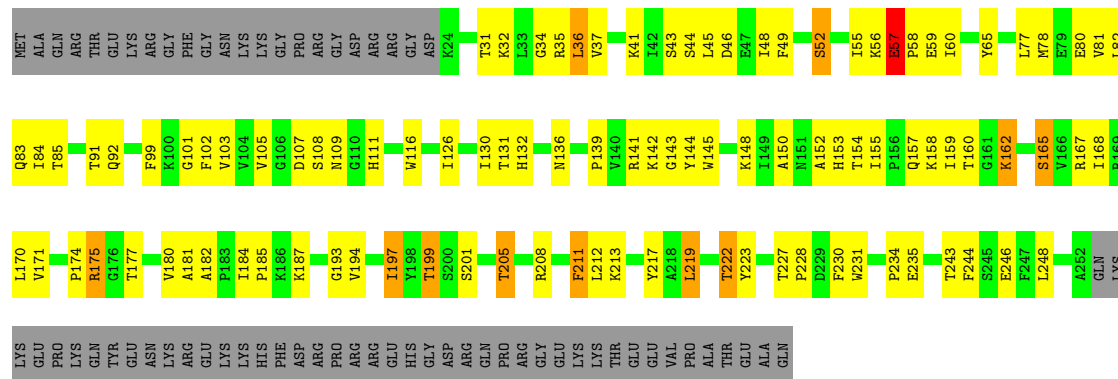
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

Chain AE: 43% 30% 23%



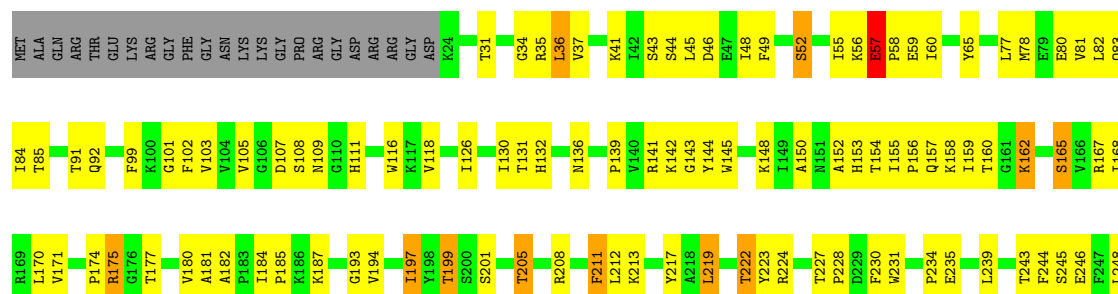
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

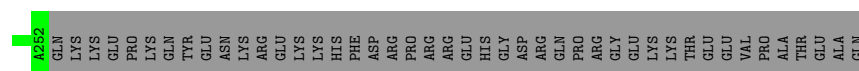
Chain BE: 43% 30% 23%



• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

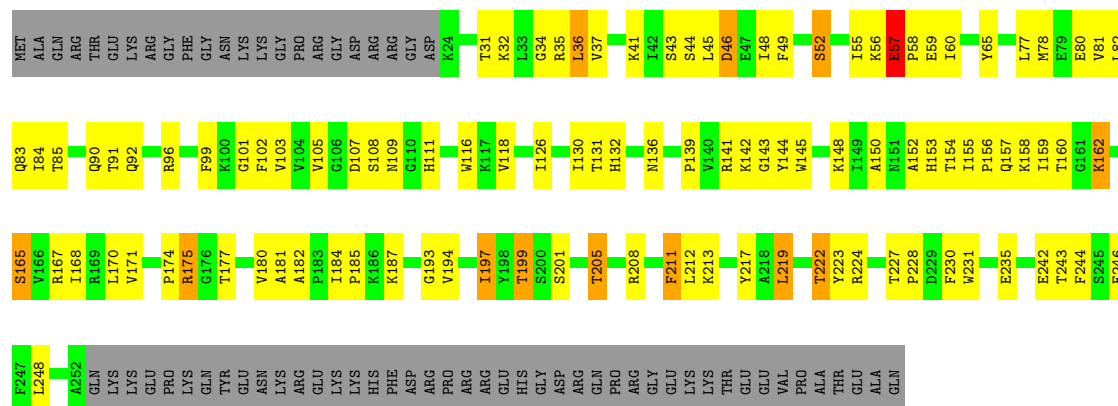
Chain CE: 42% 31% 23%





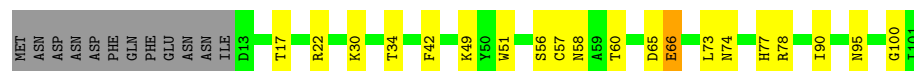
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

Chain DE: 42% 31% • 23%



• Molecule 16: EIF1

Chain AF: 68% 19% • 12%



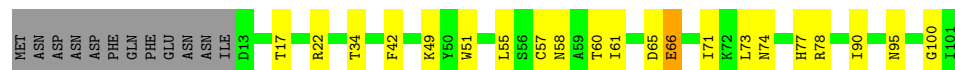
• Molecule 16: EIF1

Chain BF: 70% 17% • 12%



• Molecule 16: EIF1

Chain CF: 67% 20% • 12%



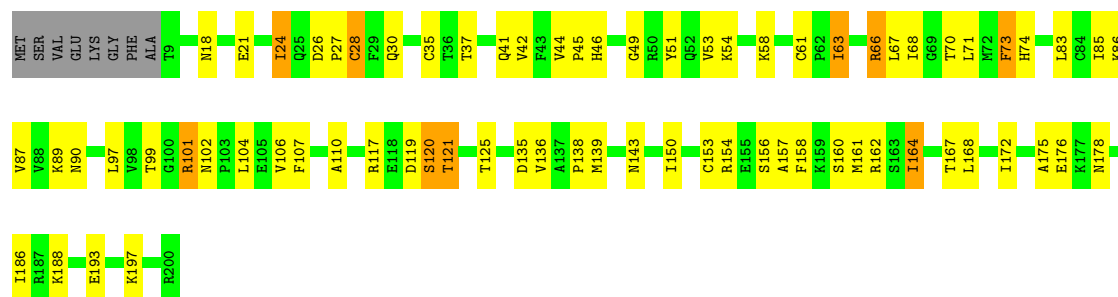
• Molecule 16: EIF1

Chain DF: 70% 17% • 12%



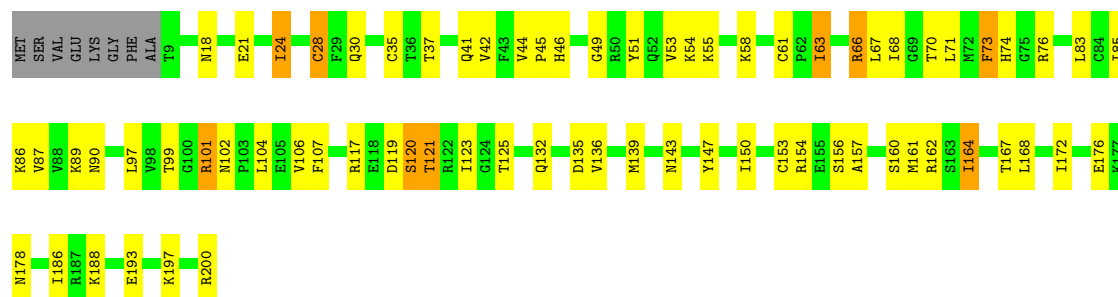
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain AG: 60% 32% • •



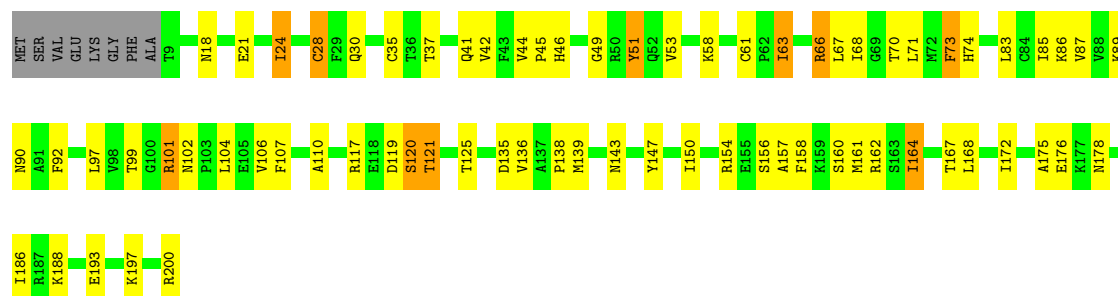
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain BG: 60% 32%



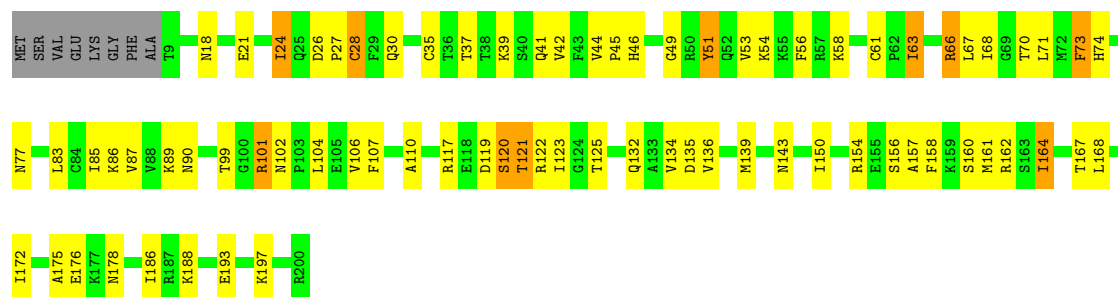
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain CG: 60% 30% 5%



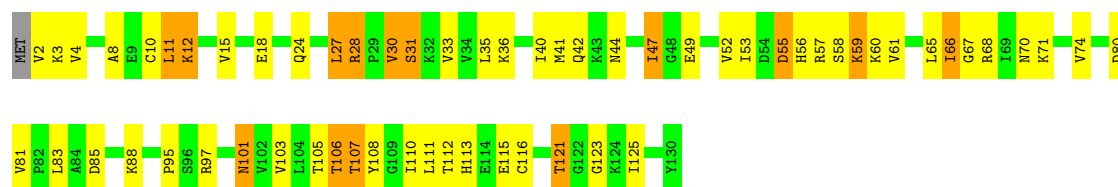
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain DG: 58% 33% 5%



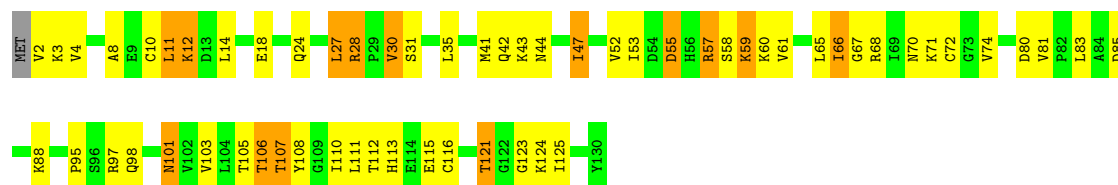
• Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

Chain AH:  52% 36% 11% .



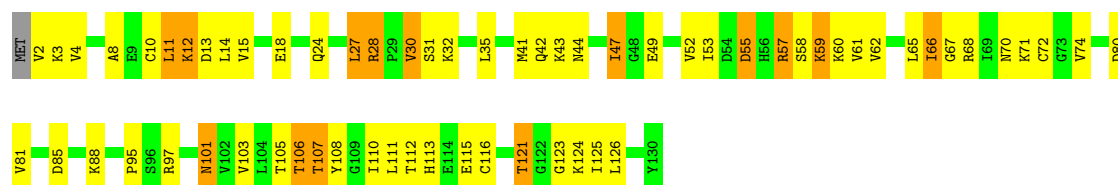
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

Chain BH:  53% 35% 11% .



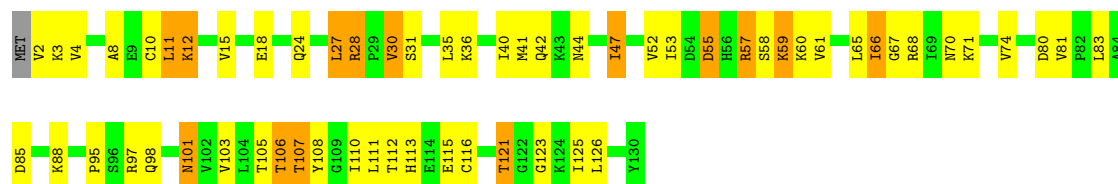
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

Chain CH:  50% 38% 11% .



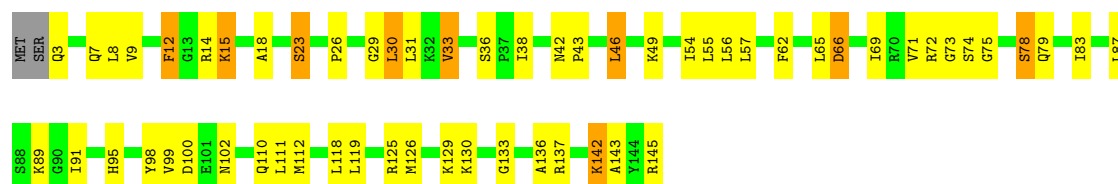
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

Chain DH:  53% 35% 11% .

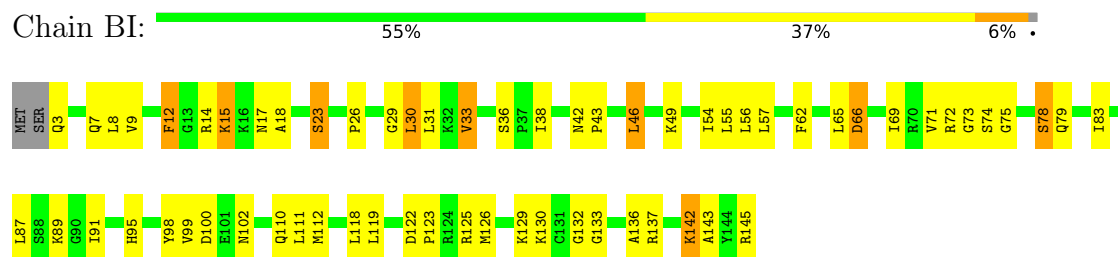


- Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E

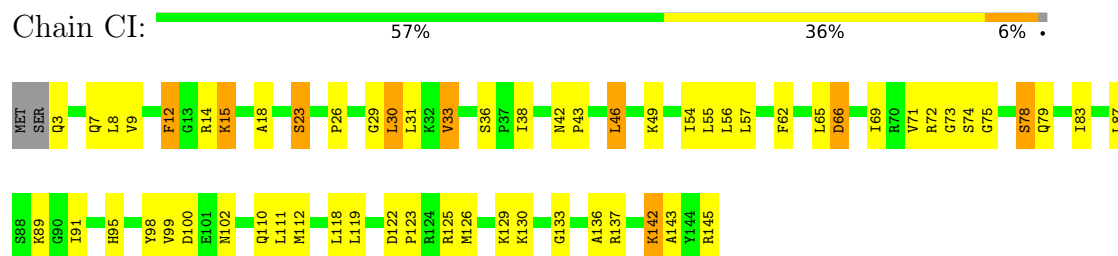
Chain AI:  58% 34% 6% .



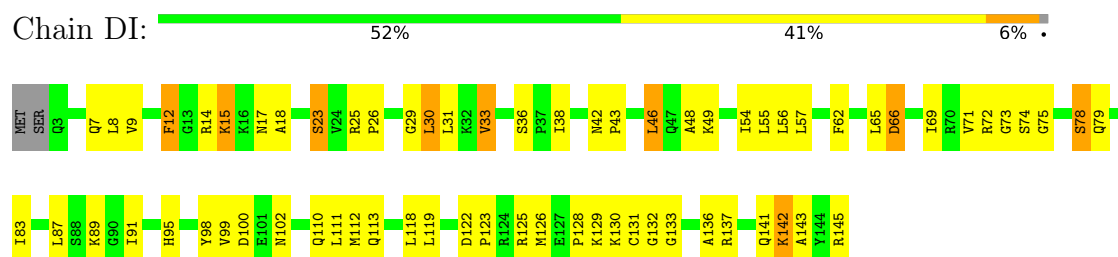
- Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E



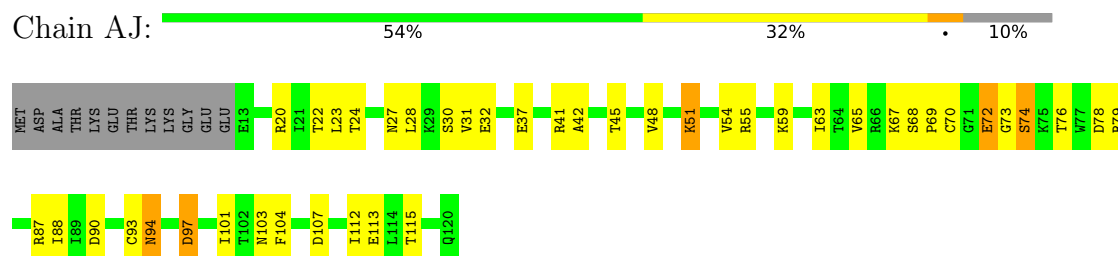
• Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E



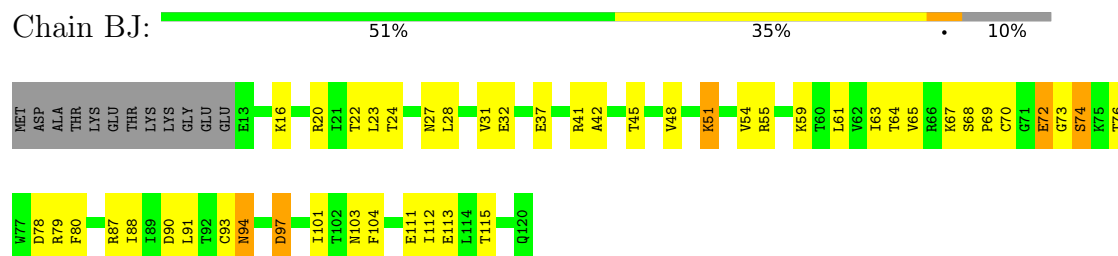
• Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E



• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E

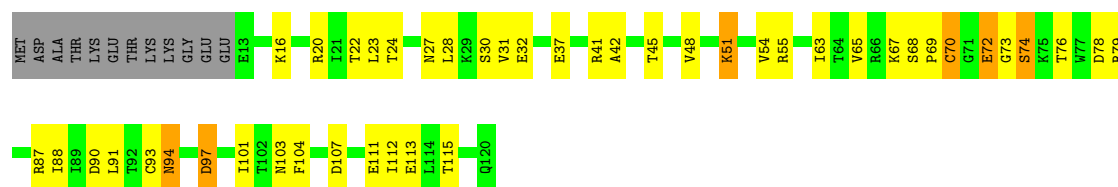


• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E



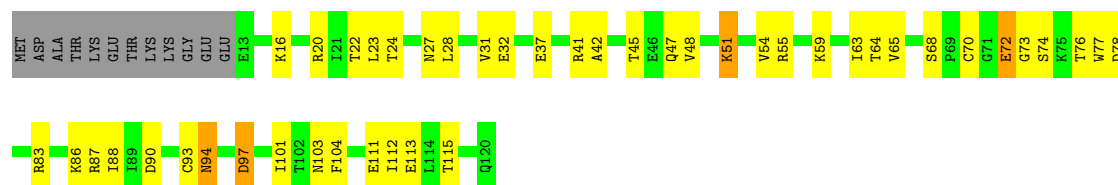
• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E

Chain CJ: 



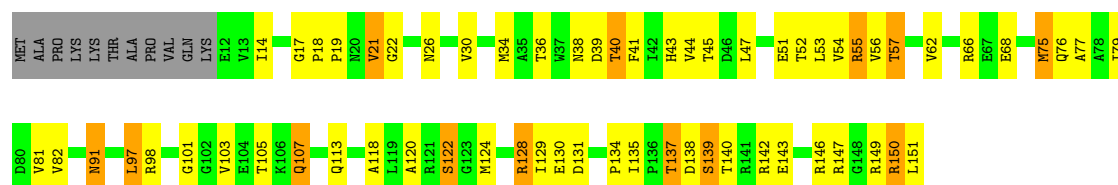
- Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E

Chain DJ: 



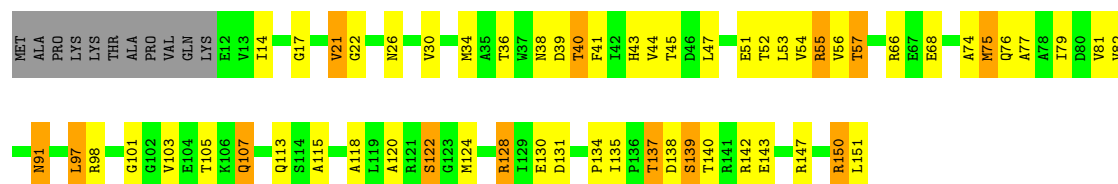
- Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E

Chain AK: 



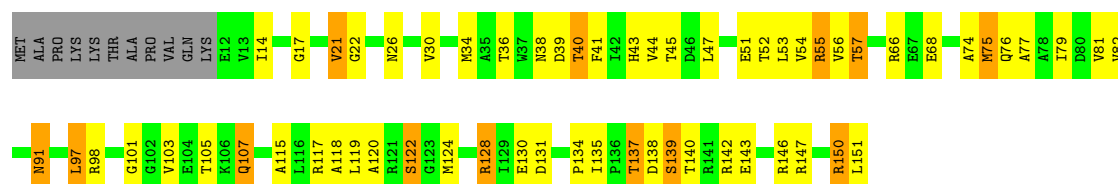
- Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E

Chain BK: 



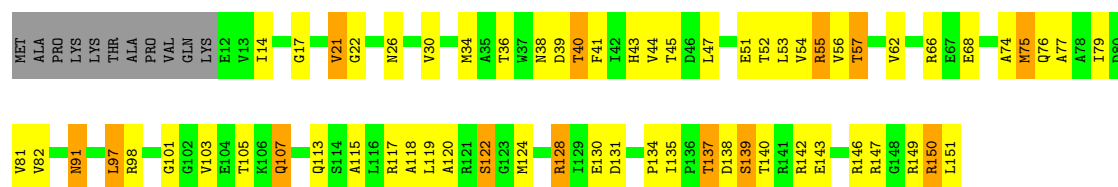
- Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E

Chain CK: 



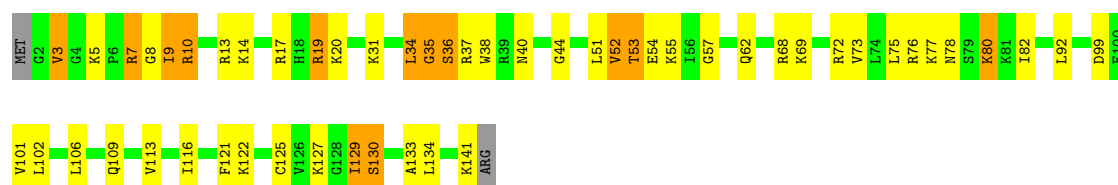
- Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E

Chain DK: 



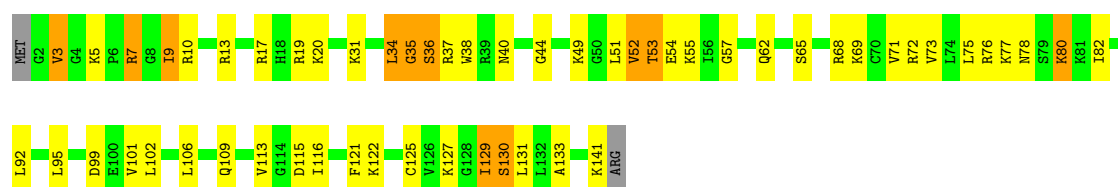
• Molecule 22: 40S RIBOSOMAL PROTEIN S12

Chain AL: 



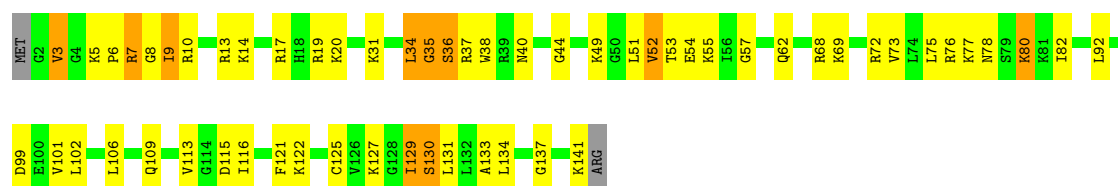
• Molecule 22: 40S RIBOSOMAL PROTEIN S12

Chain BL: 



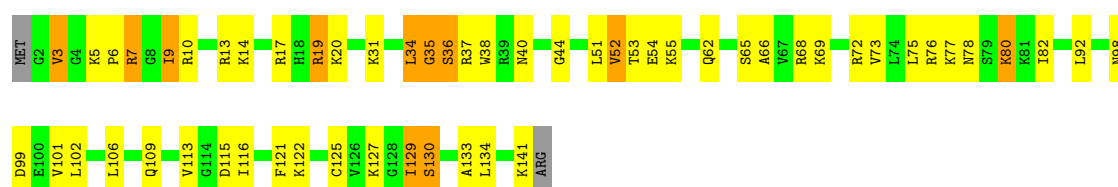
• Molecule 22: 40S RIBOSOMAL PROTEIN S12

Chain CL: 



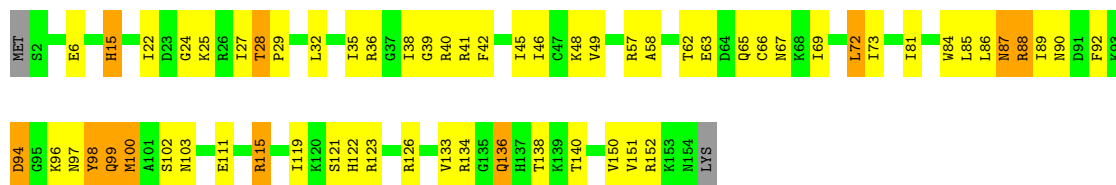
• Molecule 22: 40S RIBOSOMAL PROTEIN S12

Chain DL: 



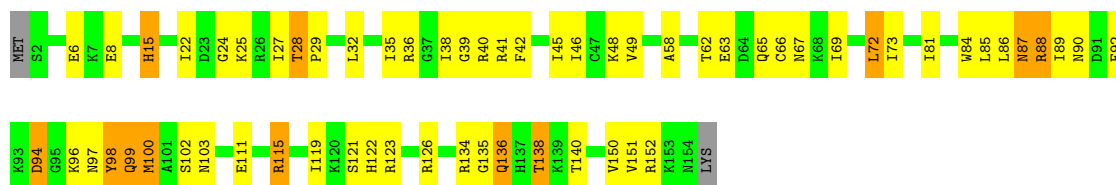
• Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

Chain AM:  59% 33% 7% .



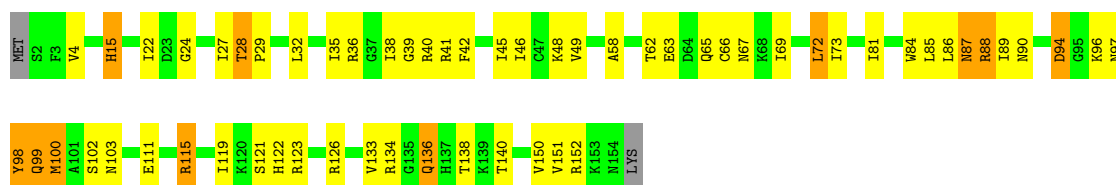
- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

Chain BM:  59% 32% 8% .



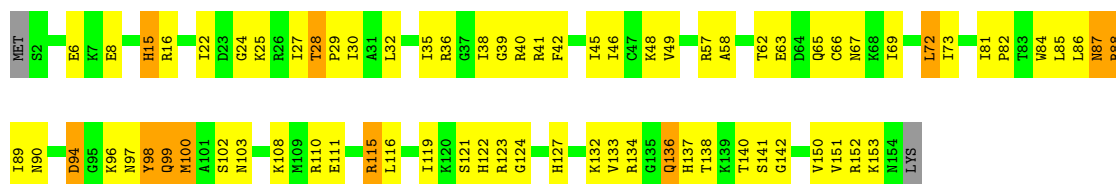
- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

Chain CM:  61% 31% 7% .



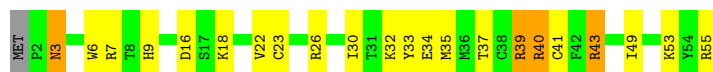
- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

Chain DM:  51% 41% 7% .



- Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E

Chain AN:  58% 33% 7% .



- Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E

Chain BN:  62% 29% 7% .



- Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E



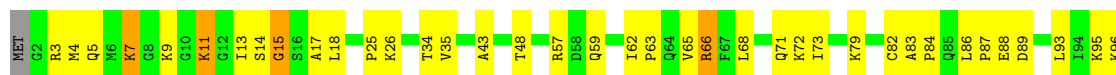
- Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E



- Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E



- Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E

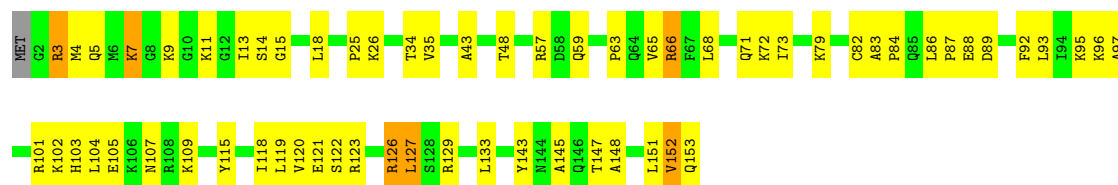


- Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E



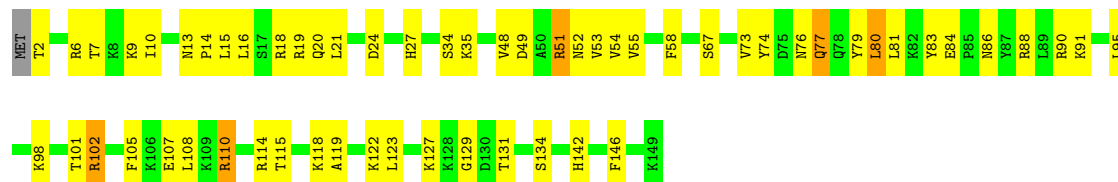
- Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E





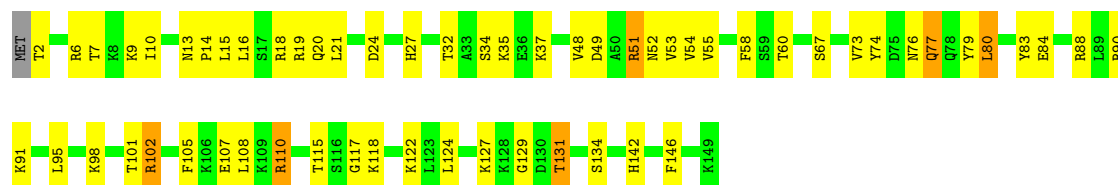
• Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain AP: 60% 36% ..



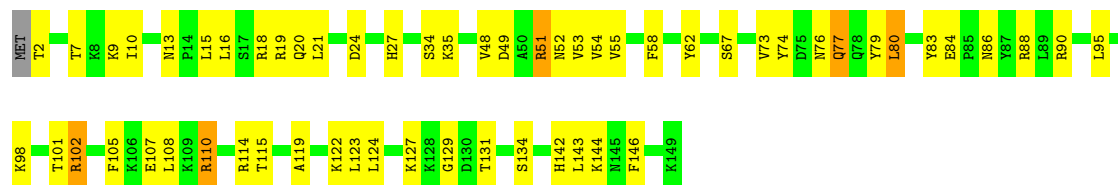
• Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain BP: 60% 36% ..



• Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain CP: 60% 36% ..



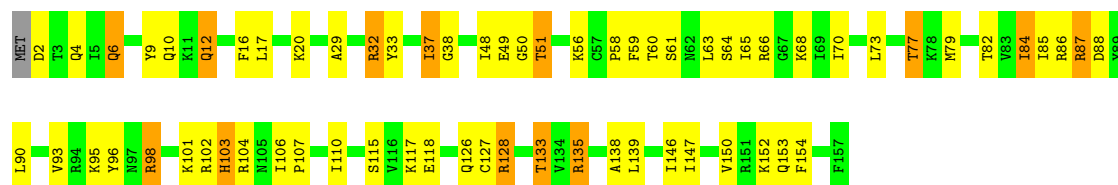
• Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain DP: 62% 34% ..

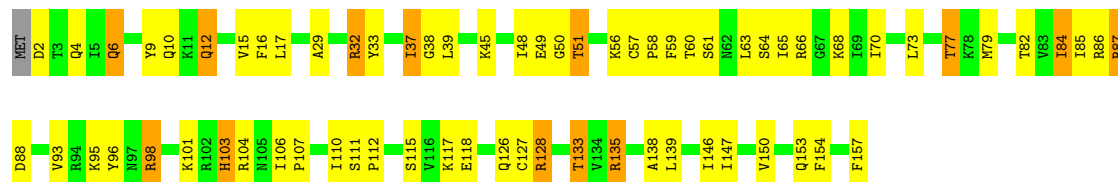


• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E

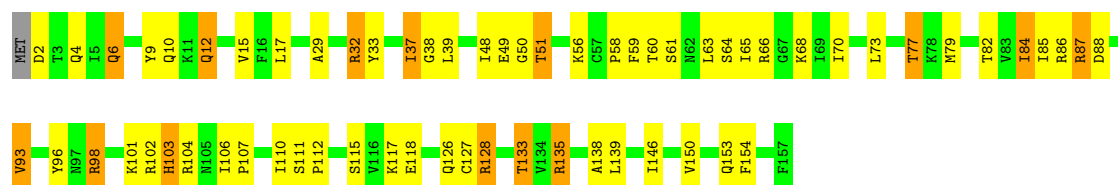
Chain AQ: 57% 34% 8% .



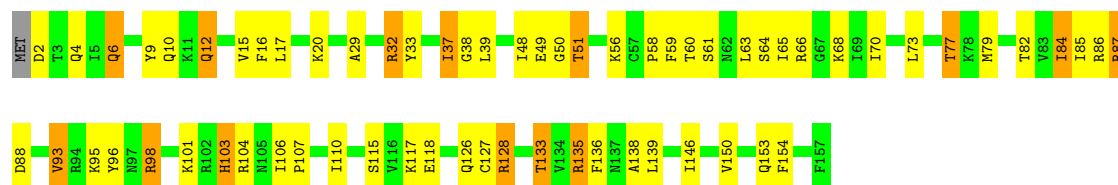
• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



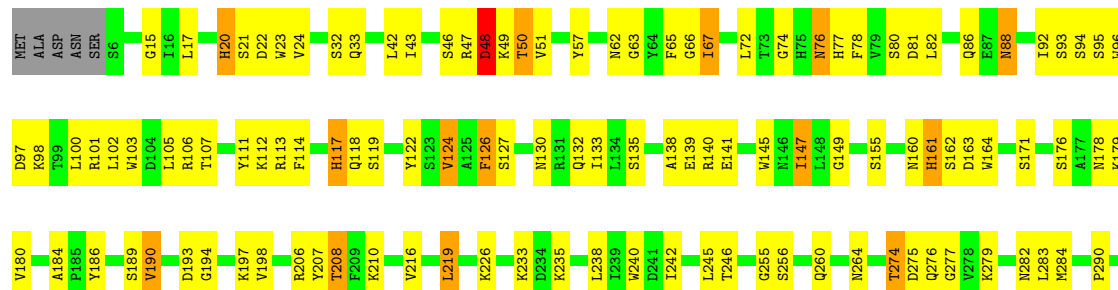
• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



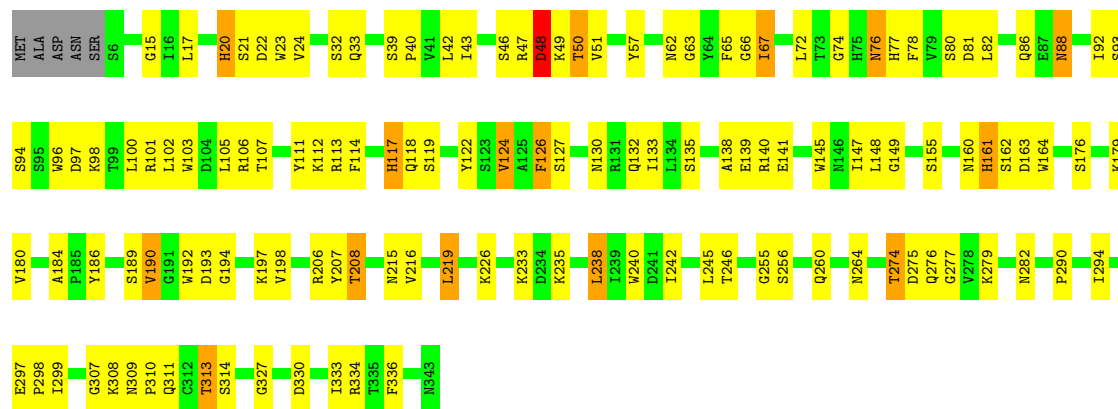
• Molecule 28: 40S RIBOSOMAL PROTEIN RACK1





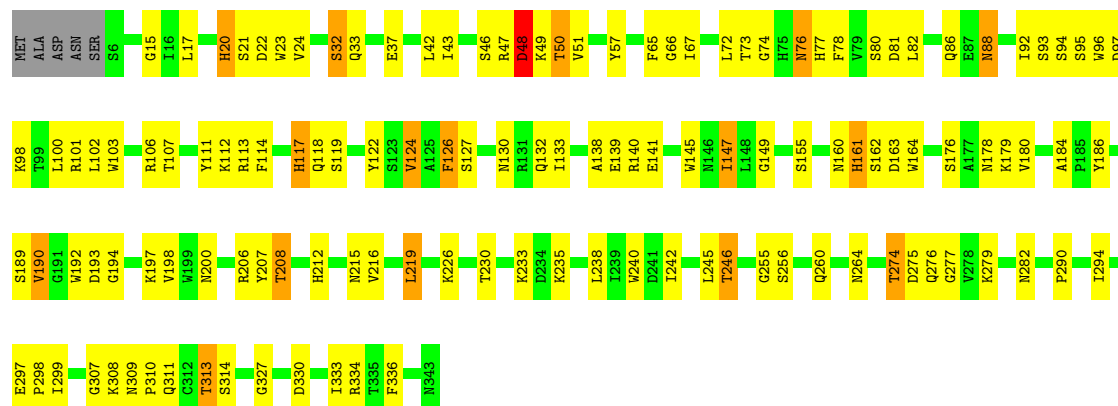
• Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

Chain BR: 61% 33%



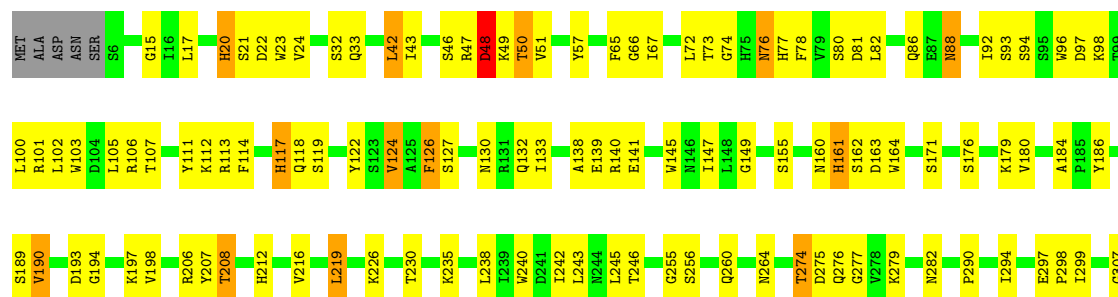
• Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

Chain CR: 61% 33% 5%



• Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

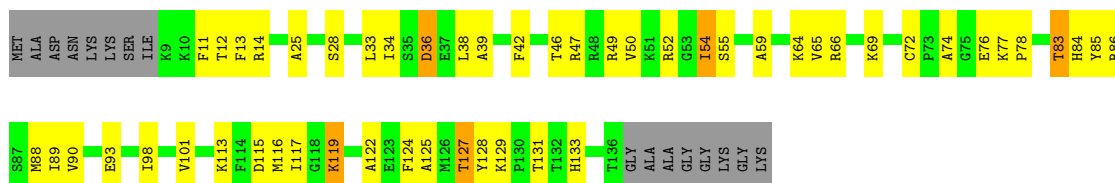
Chain DR: 62% 32%





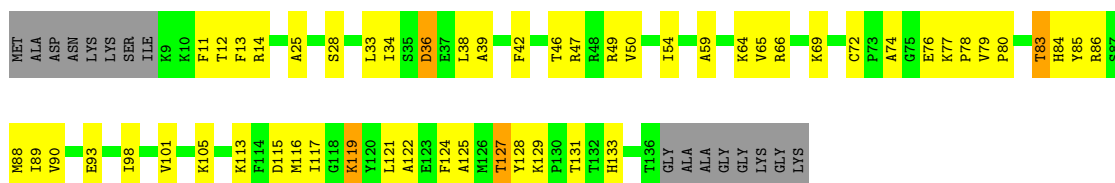
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain AS: 53% 33% 11%



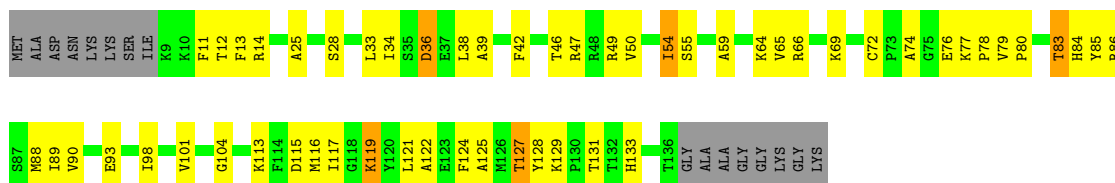
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain BS: 51% 35% 11%



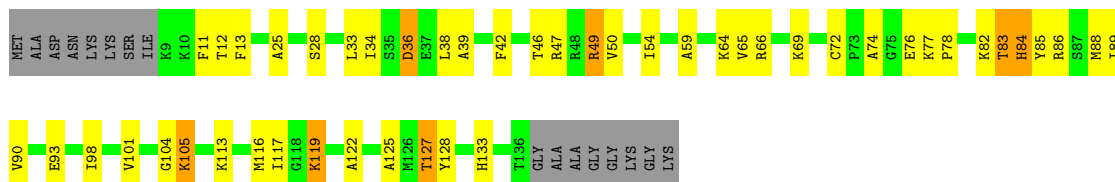
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain CS: 51% 35% 11%



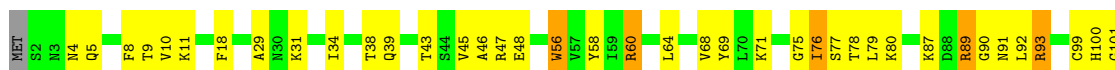
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain DS: 56% 28% 5% 11%



• Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

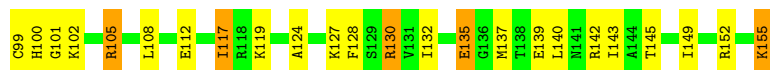
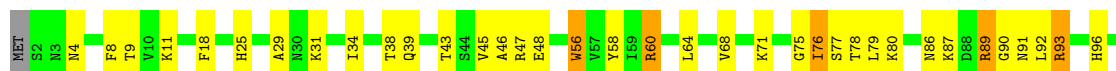
Chain AT: 61% 33% 6%





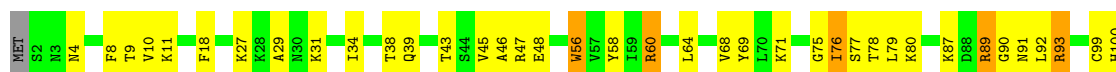
- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

Chain BT: 61% 32% 6% .



- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

Chain CT: 60% 33% 6% .



- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

Chain DT: 61% 33% 6% .



- Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E

Chain AU: 58% 36% . . .



- Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E

Chain BU: 60% 33% 5% . .





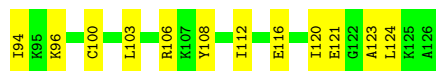
- Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E

Chain CU: 60% 33% 5% ..



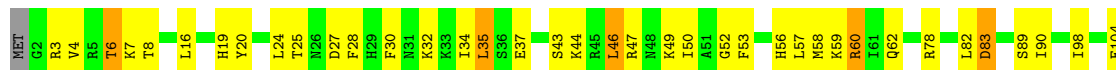
- Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E

Chain DU: 60% 33% 5% ..



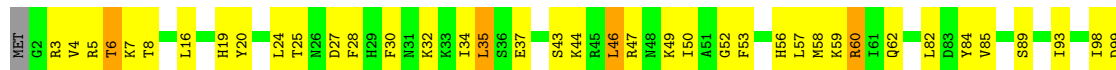
- Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E

Chain AV: 57% 30% 5% 8%



- Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E

Chain BV: 57% 31% 8%



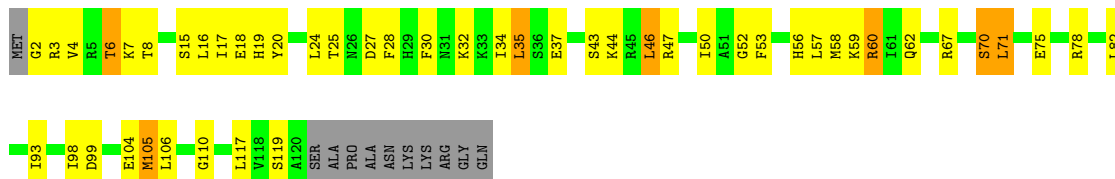
- Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E

Chain CV: 53% 35% 8%

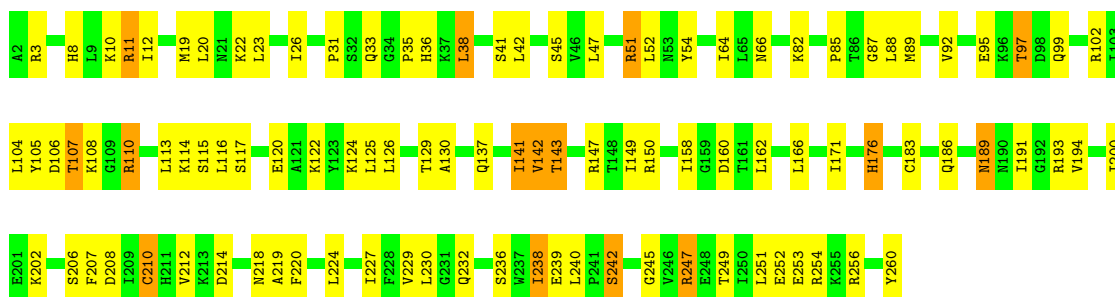




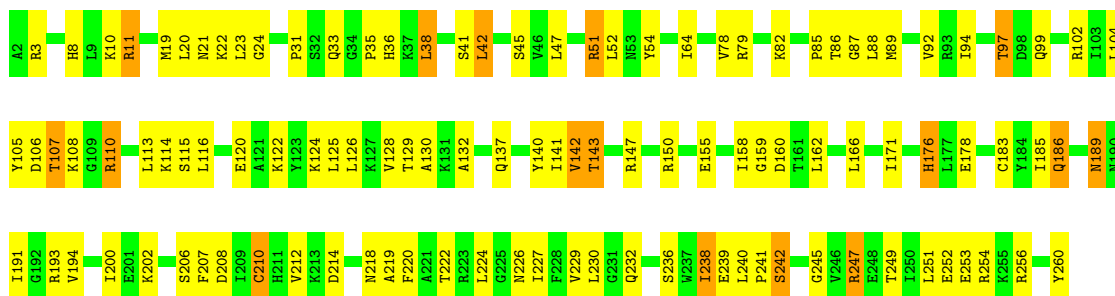
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E



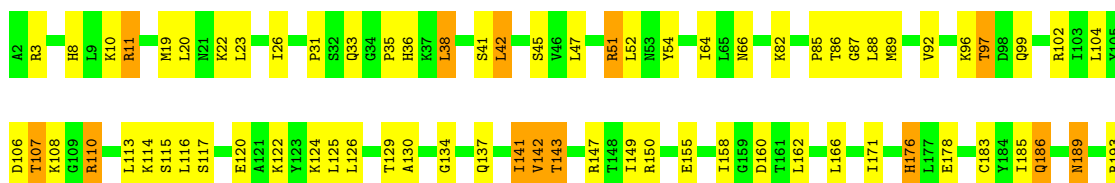
• Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E



• Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E



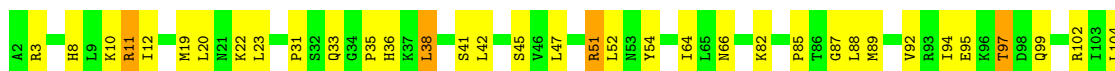
• Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E





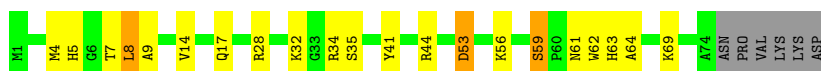
• Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

Chain DW: 58% 36% 6%



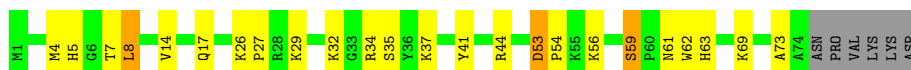
• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

Chain AX: 66% 22% 8%



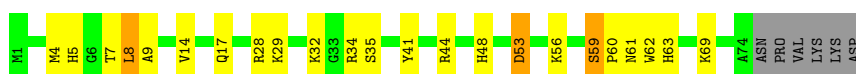
• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

Chain BX: 62% 26% 8%



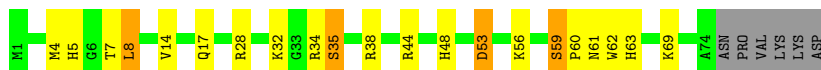
• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

Chain CX: 64% 25% 8%



• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

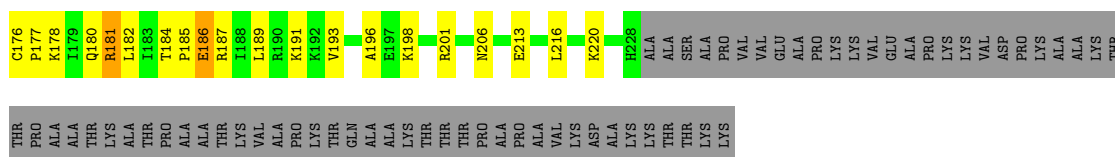
Chain DX: 66% 21% 5% 8%



• Molecule 35: 40S RIBOSOMAL PROTEIN S6

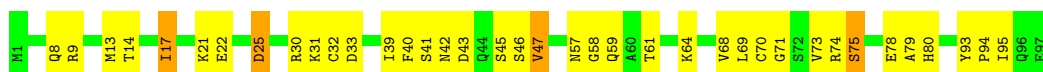
Chain AY: 46% 28% 22%





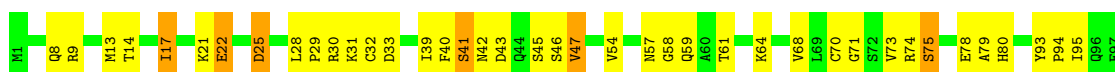
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain AZ: 61% 35% .



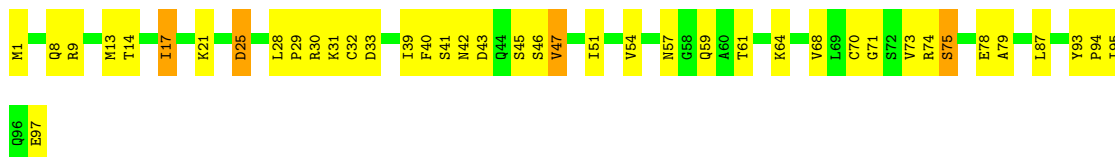
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain BZ: 59% 35% 6% .



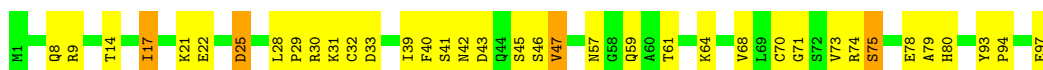
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain CZ: 58% 38% .



• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain DZ: 62% 34% .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	209.99Å 471.55Å 298.54Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70	Depositor
% Data completeness (in resolution range)	91.0 (49.75-3.70)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.202 , 0.229	Depositor
Wilson B-factor (Å ²)	97.6	Xtriage
Anisotropy	0.570	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
Total number of atoms	315512	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A0	0.31	0/827	0.56	0/1103
1	B0	0.31	0/827	0.56	0/1103
1	C0	0.31	0/827	0.56	0/1103
1	D0	0.31	0/827	0.57	0/1103
2	A1	0.31	0/510	0.66	0/677
2	B1	0.30	0/510	0.65	0/677
2	C1	0.31	0/510	0.66	0/677
2	D1	0.28	0/510	0.65	0/677
3	A2	0.35	0/1717	0.62	0/2288
3	B2	0.33	0/1717	0.61	0/2288
3	C2	0.34	0/1717	0.61	0/2288
3	D2	0.32	0/1717	0.61	0/2288
4	A3	0.34	0/1656	0.60	0/2223
4	B3	0.34	0/1656	0.61	0/2223
4	C3	0.33	0/1656	0.60	0/2223
4	D3	0.32	0/1656	0.60	0/2223
5	A4	0.49	2/1703 (0.1%)	0.75	4/2284 (0.2%)
5	B4	0.42	0/1801	0.68	0/2417
5	C4	0.34	0/1801	0.67	0/2417
5	D4	0.54	4/1801 (0.2%)	0.70	2/2417 (0.1%)
6	A5	0.42	0/823	0.68	0/1100
6	B5	0.41	0/823	0.68	0/1100
6	C5	0.39	0/823	0.67	0/1100
6	D5	0.35	0/823	0.67	0/1100
7	A6	0.36	0/640	0.56	0/855
7	B6	0.39	0/640	0.56	0/855
7	C6	0.34	0/640	0.54	0/855
7	D6	0.32	0/640	0.55	0/855
8	A7	0.31	0/853	0.55	0/1148
8	B7	0.32	0/853	0.55	0/1148
8	C7	0.32	0/853	0.55	0/1148
8	D7	0.30	0/853	0.56	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	A8	0.32	0/620	0.61	0/831
9	B8	0.36	0/620	0.62	0/831
9	C8	0.32	0/620	0.61	0/831
9	D8	0.31	0/620	0.62	0/831
10	A9	0.28	0/764	0.56	1/1007 (0.1%)
10	B9	0.29	0/764	0.54	1/1007 (0.1%)
10	C9	0.31	0/764	0.57	1/1007 (0.1%)
10	D9	0.31	0/764	0.67	1/1007 (0.1%)
11	AA	0.51	3/40993 (0.0%)	1.15	225/63880 (0.4%)
11	BA	0.51	1/40993 (0.0%)	1.14	222/63880 (0.3%)
11	CA	0.47	1/40993 (0.0%)	1.13	221/63880 (0.3%)
11	DA	0.44	1/40993 (0.0%)	1.12	219/63880 (0.3%)
12	AB	0.32	0/1652	0.59	0/2240
12	BB	0.31	0/1652	0.59	0/2240
12	CB	0.31	0/1652	0.59	0/2240
12	DB	0.29	0/1652	0.58	0/2240
13	AC	0.33	0/1846	0.59	1/2479 (0.0%)
13	BC	0.34	0/1846	0.59	1/2479 (0.0%)
13	CC	0.34	0/1846	0.59	1/2479 (0.0%)
13	DC	0.31	0/1846	0.58	1/2479 (0.0%)
14	AD	0.33	0/1501	0.65	0/2003
14	BD	0.33	0/1501	0.64	0/2003
14	CD	0.33	0/1501	0.64	0/2003
14	DD	0.33	0/1501	0.65	0/2003
15	AE	0.38	0/1864	0.63	0/2521
15	BE	0.37	0/1864	0.63	0/2521
15	CE	0.35	0/1864	0.62	0/2521
15	DE	0.35	0/1864	0.62	0/2521
16	AF	0.31	0/751	0.60	0/1010
16	BF	0.32	0/751	0.59	0/1010
16	CF	0.29	0/751	0.59	0/1010
16	DF	0.30	0/751	0.60	0/1010
17	AG	0.34	0/1546	0.63	1/2079 (0.0%)
17	BG	0.34	0/1546	0.63	1/2079 (0.0%)
17	CG	0.34	0/1546	0.63	1/2079 (0.0%)
17	DG	0.31	0/1546	0.62	1/2079 (0.0%)
18	AH	0.42	0/1058	0.74	1/1421 (0.1%)
18	BH	0.42	0/1058	0.75	1/1421 (0.1%)
18	CH	0.39	0/1058	0.74	1/1421 (0.1%)
18	DH	0.36	0/1058	0.73	1/1421 (0.1%)
19	AI	0.34	0/1151	0.62	0/1540
19	BI	0.34	0/1151	0.61	0/1540
19	CI	0.34	0/1151	0.62	0/1540

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	DI	0.31	0/1151	0.61	0/1540
20	AJ	0.38	1/868 (0.1%)	0.63	0/1168
20	BJ	0.39	1/868 (0.1%)	0.64	1/1168 (0.1%)
20	CJ	0.37	1/868 (0.1%)	0.63	0/1168
20	DJ	0.37	1/868 (0.1%)	0.63	0/1168
21	AK	0.38	0/1078	0.72	0/1452
21	BK	0.36	0/1078	0.71	0/1452
21	CK	0.34	0/1078	0.70	0/1452
21	DK	0.33	0/1078	0.70	0/1452
22	AL	0.36	0/1103	0.65	0/1471
22	BL	0.36	0/1103	0.66	0/1471
22	CL	0.35	0/1103	0.64	0/1471
22	DL	0.34	0/1103	0.64	0/1471
23	AM	0.29	0/1252	0.61	0/1680
23	BM	0.30	0/1252	0.61	0/1680
23	CM	0.29	0/1252	0.60	0/1680
23	DM	0.28	0/1252	0.60	0/1680
24	AN	0.36	0/465	0.63	0/619
24	BN	0.37	0/465	0.64	0/619
24	CN	0.32	0/465	0.62	0/619
24	DN	0.34	0/465	0.63	0/619
25	AO	0.36	0/1253	0.63	0/1677
25	BO	0.36	0/1253	0.64	0/1677
25	CO	0.34	0/1253	0.63	0/1677
25	DO	0.32	0/1253	0.62	0/1677
26	AP	0.31	0/1215	0.60	0/1626
26	BP	0.32	0/1215	0.61	0/1626
26	CP	0.30	0/1215	0.60	0/1626
26	DP	0.31	0/1215	0.60	0/1626
27	AQ	0.39	0/1290	0.66	0/1731
27	BQ	0.36	0/1290	0.67	0/1731
27	CQ	0.36	0/1290	0.66	0/1731
27	DQ	0.33	0/1290	0.65	0/1731
28	AR	0.31	0/2750	0.60	0/3726
28	BR	0.30	0/2750	0.61	0/3726
28	CR	0.30	0/2750	0.61	0/3726
28	DR	0.29	0/2750	0.60	0/3726
29	AS	0.27	0/1028	0.54	0/1374
29	BS	0.29	0/1028	0.55	0/1374
29	CS	0.28	0/1028	0.54	0/1374
29	DS	0.27	0/1028	0.54	0/1374
30	AT	0.34	0/1264	0.58	0/1698
30	BT	0.35	0/1264	0.58	0/1698

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CT	0.32	0/1264	0.57	0/1698
30	DT	0.33	0/1264	0.57	0/1698
31	AU	0.28	0/961	0.56	0/1288
31	BU	0.29	0/961	0.56	0/1288
31	CU	0.29	0/961	0.56	0/1288
31	DU	0.30	0/961	0.58	0/1288
32	AV	0.32	0/981	0.59	0/1311
32	BV	0.30	0/981	0.56	0/1311
32	CV	0.32	0/981	0.56	0/1311
32	DV	0.30	0/981	0.57	0/1311
33	AW	0.36	0/2119	0.62	0/2849
33	BW	0.34	0/2119	0.62	0/2849
33	CW	0.34	0/2119	0.62	0/2849
33	DW	0.34	0/2119	0.62	0/2849
34	AX	0.29	0/612	0.54	0/812
34	BX	0.29	0/612	0.55	0/812
34	CX	0.28	0/612	0.54	0/812
34	DX	0.28	0/612	0.54	0/812
35	AY	0.31	0/1852	0.55	0/2462
35	BY	0.31	0/1852	0.55	0/2462
35	CY	0.31	0/1852	0.55	0/2462
35	DY	0.31	0/1852	0.55	0/2462
36	AZ	0.36	0/755	0.61	0/1013
36	BZ	0.35	0/755	0.61	0/1013
36	CZ	0.34	0/755	0.60	0/1013
36	DZ	0.33	0/755	0.61	0/1013
All	All	0.41	16/333578 (0.0%)	0.93	910/482983 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A3	0	1
4	B3	0	1
4	C3	0	1
4	D3	0	1
5	A4	0	1
5	B4	0	2
5	C4	0	2
5	D4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	A6	0	1
7	B6	0	1
7	C6	0	1
7	D6	0	1
9	A8	0	1
9	B8	0	1
9	C8	0	1
9	D8	0	1
17	AG	0	1
17	BG	0	1
17	CG	0	1
17	DG	0	1
18	AH	0	2
18	BH	0	2
18	CH	0	2
18	DH	0	2
20	AJ	0	1
20	BJ	0	1
20	CJ	0	1
20	DJ	0	1
21	AK	0	1
21	BK	0	1
21	CK	0	1
21	DK	0	1
24	CN	0	1
25	AO	0	1
25	BO	0	1
25	CO	0	1
25	DO	0	1
29	AS	0	1
29	BS	0	1
29	CS	0	1
29	DS	0	2
31	AU	0	2
31	BU	0	2
31	CU	0	2
31	DU	0	2
32	DV	0	1
33	AW	0	1
33	BW	0	1
33	CW	0	1
33	DW	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	62

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D4	31	TRP	NE1-CE2	-10.69	1.23	1.37
5	D4	31	TRP	CD1-NE1	8.48	1.52	1.38
5	A4	31	TRP	CG-CD1	7.86	1.47	1.36
11	DA	1586	A	O3'-P	7.60	1.70	1.61
5	D4	31	TRP	CD2-CE2	7.60	1.50	1.41

The worst 5 of 910 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	515	U	N1-C2-O2	12.79	131.75	122.80
11	BA	515	U	N1-C2-O2	12.46	131.52	122.80
11	DA	515	U	N1-C2-O2	12.24	131.37	122.80
11	CA	515	U	N1-C2-O2	12.05	131.23	122.80
11	BA	1296	G	N3-C2-N2	-11.69	111.72	119.90

There are no chirality outliers.

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A3	131	LEU	Peptide
5	A4	71	THR	Peptide
7	A6	65	THR	Peptide
9	A8	99	ASN	Peptide
17	AG	73	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	817	0	829	24	0
1	B0	817	0	829	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C0	817	0	829	33	0
1	D0	817	0	829	29	0
2	A1	511	0	544	24	0
2	B1	511	0	544	18	0
2	C1	511	0	544	23	1
2	D1	511	0	544	22	0
3	A2	1693	0	1795	75	1
3	B2	1693	0	1795	61	0
3	C2	1693	0	1795	65	0
3	D2	1693	0	1795	67	0
4	A3	1629	0	1708	63	0
4	B3	1629	0	1708	63	0
4	C3	1629	0	1708	64	0
4	D3	1629	0	1708	58	0
5	A4	1679	0	1762	60	0
5	B4	1775	0	1851	64	0
5	C4	1775	0	1851	60	0
5	D4	1775	0	1851	68	0
6	A5	812	0	854	46	0
6	B5	812	0	854	41	0
6	C5	812	0	854	40	0
6	D5	812	0	854	39	0
7	A6	632	0	646	28	0
7	B6	632	0	646	31	1
7	C6	632	0	646	29	0
7	D6	632	0	646	33	0
8	A7	833	0	844	37	0
8	B7	833	0	844	28	0
8	C7	833	0	844	36	0
8	D7	833	0	844	47	0
9	A8	615	0	660	25	0
9	B8	615	0	660	27	1
9	C8	615	0	660	20	0
9	D8	615	0	660	36	0
10	A9	751	0	807	55	0
10	B9	751	0	809	76	0
10	C9	751	0	809	41	0
10	D9	751	0	809	56	0
11	AA	36629	0	18413	1084	0
11	BA	36629	0	18413	1119	3
11	CA	36629	0	18413	1052	2
11	DA	36629	0	18413	1110	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AB	1619	0	1623	70	0
12	BB	1619	0	1623	75	0
12	CB	1619	0	1623	66	0
12	DB	1619	0	1623	61	0
13	AC	1811	0	1907	64	0
13	BC	1811	0	1907	68	0
13	CC	1811	0	1907	78	0
13	DC	1811	0	1907	84	0
14	AD	1478	0	1569	74	0
14	BD	1478	0	1569	72	0
14	CD	1478	0	1569	65	0
14	DD	1478	0	1569	64	0
15	AE	1818	0	1853	76	0
15	BE	1818	0	1853	75	0
15	CE	1818	0	1853	80	0
15	DE	1818	0	1853	78	0
16	AF	736	0	722	16	0
16	BF	736	0	722	13	0
16	CF	736	0	722	14	0
16	DF	736	0	722	12	0
17	AG	1520	0	1572	58	0
17	BG	1520	0	1572	57	0
17	CG	1520	0	1572	52	0
17	DG	1520	0	1572	54	0
18	AH	1040	0	1096	42	0
18	BH	1040	0	1096	42	0
18	CH	1040	0	1096	49	0
18	DH	1040	0	1096	43	0
19	AI	1135	0	1204	46	0
19	BI	1135	0	1204	48	0
19	CI	1135	0	1204	47	0
19	DI	1135	0	1204	50	0
20	AJ	859	0	921	36	0
20	BJ	859	0	921	41	0
20	CJ	859	0	921	39	0
20	DJ	859	0	921	39	0
21	AK	1063	0	1088	62	0
21	BK	1063	0	1088	59	0
21	CK	1063	0	1088	57	0
21	DK	1063	0	1088	61	0
22	AL	1086	0	1156	46	0
22	BL	1086	0	1156	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CL	1086	0	1156	48	0
22	DL	1086	0	1156	44	0
23	AM	1231	0	1276	57	0
23	BM	1231	0	1276	60	0
23	CM	1231	0	1276	55	0
23	DM	1231	0	1276	78	0
24	AN	454	0	453	32	0
24	BN	454	0	453	30	0
24	CN	454	0	453	27	0
24	DN	454	0	453	32	0
25	AO	1229	0	1338	47	0
25	BO	1229	0	1338	49	0
25	CO	1229	0	1338	48	0
25	DO	1229	0	1338	50	0
26	AP	1197	0	1285	45	0
26	BP	1197	0	1285	51	0
26	CP	1197	0	1285	41	1
26	DP	1197	0	1285	44	0
27	AQ	1267	0	1342	60	0
27	BQ	1267	0	1342	60	0
27	CQ	1267	0	1342	55	0
27	DQ	1267	0	1342	56	0
28	AR	2682	0	2629	104	0
28	BR	2682	0	2629	103	0
28	CR	2682	0	2629	116	0
28	DR	2682	0	2629	100	0
29	AS	1010	0	1059	42	0
29	BS	1010	0	1059	40	0
29	CS	1010	0	1059	39	0
29	DS	1010	0	1059	39	0
30	AT	1242	0	1290	52	0
30	BT	1242	0	1290	57	0
30	CT	1242	0	1290	50	0
30	DT	1242	0	1290	53	1
31	AU	952	0	993	50	0
31	BU	952	0	993	42	0
31	CU	952	0	993	37	0
31	DU	952	0	993	48	0
32	AV	968	0	1031	41	0
32	BV	968	0	1031	44	0
32	CV	968	0	1031	44	0
32	DV	968	0	1031	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AW	2079	0	2151	85	0
33	BW	2079	0	2151	91	0
33	CW	2079	0	2151	87	0
33	DW	2079	0	2151	86	0
34	AX	599	0	651	19	0
34	BX	599	0	651	22	0
34	CX	599	0	651	21	0
34	DX	599	0	651	18	0
35	AY	1826	0	1954	72	0
35	BY	1826	0	1954	80	0
35	CY	1826	0	1954	67	0
35	DY	1826	0	1954	80	0
36	AZ	747	0	758	31	0
36	BZ	747	0	758	33	0
36	CZ	747	0	758	33	0
36	DZ	747	0	758	28	0
37	A5	1	0	0	0	0
37	A6	1	0	0	0	0
37	A9	1	0	0	0	0
37	AN	1	0	0	0	0
37	B5	1	0	0	0	0
37	B6	1	0	0	0	0
37	B9	1	0	0	0	0
37	BN	1	0	0	0	0
37	C5	1	0	0	0	0
37	C6	1	0	0	0	0
37	C9	1	0	0	0	0
37	CN	1	0	0	0	0
37	D5	1	0	0	0	0
37	D6	1	0	0	0	0
37	D9	1	0	0	0	0
37	DN	1	0	0	0	0
38	AA	79	0	0	0	0
38	BA	79	0	0	0	0
38	CA	79	0	0	0	0
38	DA	79	0	0	0	0
39	AA	474	0	0	51	0
39	BA	474	0	0	48	0
39	C2	2	0	0	0	0
39	C4	2	0	0	0	0
39	C5	3	0	0	1	0
39	CA	467	0	0	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DA	474	0	0	54	0
All	All	315512	0	247405	9487	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 9487 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B9:87:LYS:NZ	11:BA:1187:C:OP2	1.62	1.32
11:DA:1377:A:OP2	17:DG:54:LYS:NZ	1.65	1.29
11:BA:1377:A:OP2	17:BG:54:LYS:NZ	1.67	1.25
11:DA:1214:A:OP1	29:DS:64:LYS:NZ	1.71	1.23
9:D8:81:ARG:NH2	11:DA:1505:C:OP2	1.73	1.20

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B8:47:LYS:NZ	11:BA:270:U:O2[2_556]	1.96	0.24
7:B6:32:ASP:OD2	2:C1:35:LYS:NZ[1_556]	1.99	0.21
11:CA:891:G:OP2	30:DT:122:ASN:ND2[1_455]	2.07	0.13
3:A2:133:LYS:NZ	11:BA:1730:G:OP1[1_655]	2.10	0.10
11:BA:229:A:OP2	26:CP:146:PHE:N[2_546]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	97/211 (46%)	92 (95%)	5 (5%)	0	100	100
1	B0	97/211 (46%)	92 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C0	97/211 (46%)	92 (95%)	5 (5%)	0	100	100
1	D0	97/211 (46%)	91 (94%)	6 (6%)	0	100	100
2	A1	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
2	B1	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
2	C1	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
2	D1	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
3	A2	205/208 (99%)	197 (96%)	8 (4%)	0	100	100
3	B2	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
3	C2	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
3	D2	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
4	A3	194/197 (98%)	187 (96%)	7 (4%)	0	100	100
4	B3	194/197 (98%)	187 (96%)	7 (4%)	0	100	100
4	C3	194/197 (98%)	188 (97%)	6 (3%)	0	100	100
4	D3	194/197 (98%)	187 (96%)	7 (4%)	0	100	100
5	A4	207/265 (78%)	191 (92%)	14 (7%)	2 (1%)	15	51
5	B4	219/265 (83%)	202 (92%)	14 (6%)	3 (1%)	11	45
5	C4	219/265 (83%)	203 (93%)	13 (6%)	3 (1%)	11	45
5	D4	219/265 (83%)	203 (93%)	13 (6%)	3 (1%)	11	45
6	A5	98/119 (82%)	98 (100%)	0	0	100	100
6	B5	98/119 (82%)	98 (100%)	0	0	100	100
6	C5	98/119 (82%)	97 (99%)	1 (1%)	0	100	100
6	D5	98/119 (82%)	98 (100%)	0	0	100	100
7	A6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	12	47
7	B6	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	12	47
7	C6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	12	47
7	D6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	12	47
8	A7	99/162 (61%)	94 (95%)	5 (5%)	0	100	100
8	B7	99/162 (61%)	96 (97%)	3 (3%)	0	100	100
8	C7	99/162 (61%)	95 (96%)	4 (4%)	0	100	100
8	D7	99/162 (61%)	95 (96%)	4 (4%)	0	100	100
9	A8	77/143 (54%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	B8	77/143 (54%)	73 (95%)	4 (5%)	0	100	100
9	C8	77/143 (54%)	73 (95%)	4 (5%)	0	100	100
9	D8	77/143 (54%)	73 (95%)	4 (5%)	0	100	100
10	A9	91/189 (48%)	90 (99%)	1 (1%)	0	100	100
10	B9	91/189 (48%)	89 (98%)	2 (2%)	0	100	100
10	C9	91/189 (48%)	89 (98%)	2 (2%)	0	100	100
10	D9	91/189 (48%)	89 (98%)	1 (1%)	1 (1%)	14	50
12	AB	199/241 (83%)	197 (99%)	2 (1%)	0	100	100
12	BB	199/241 (83%)	197 (99%)	2 (1%)	0	100	100
12	CB	199/241 (83%)	197 (99%)	2 (1%)	0	100	100
12	DB	199/241 (83%)	197 (99%)	2 (1%)	0	100	100
13	AC	226/243 (93%)	213 (94%)	13 (6%)	0	100	100
13	BC	226/243 (93%)	214 (95%)	12 (5%)	0	100	100
13	CC	226/243 (93%)	214 (95%)	12 (5%)	0	100	100
13	DC	226/243 (93%)	214 (95%)	12 (5%)	0	100	100
14	AD	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
14	BD	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
14	CD	178/181 (98%)	175 (98%)	3 (2%)	0	100	100
14	DD	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
15	AE	227/296 (77%)	211 (93%)	15 (7%)	1 (0%)	34	69
15	BE	227/296 (77%)	212 (93%)	14 (6%)	1 (0%)	34	69
15	CE	227/296 (77%)	211 (93%)	15 (7%)	1 (0%)	34	69
15	DE	227/296 (77%)	212 (93%)	14 (6%)	1 (0%)	34	69
16	AF	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
16	BF	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
16	CF	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
16	DF	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
17	AG	190/200 (95%)	178 (94%)	11 (6%)	1 (0%)	29	66
17	BG	190/200 (95%)	178 (94%)	12 (6%)	0	100	100
17	CG	190/200 (95%)	179 (94%)	9 (5%)	2 (1%)	14	50
17	DG	190/200 (95%)	178 (94%)	10 (5%)	2 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	19	56
18	BH	127/130 (98%)	111 (87%)	15 (12%)	1 (1%)	19	56
18	CH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	19	56
18	DH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	19	56
19	AI	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
19	BI	141/145 (97%)	131 (93%)	10 (7%)	0	100	100
19	CI	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
19	DI	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
20	AJ	106/120 (88%)	104 (98%)	2 (2%)	0	100	100
20	BJ	106/120 (88%)	105 (99%)	1 (1%)	0	100	100
20	CJ	106/120 (88%)	104 (98%)	2 (2%)	0	100	100
20	DJ	106/120 (88%)	104 (98%)	2 (2%)	0	100	100
21	AK	138/151 (91%)	133 (96%)	5 (4%)	0	100	100
21	BK	138/151 (91%)	134 (97%)	4 (3%)	0	100	100
21	CK	138/151 (91%)	133 (96%)	5 (4%)	0	100	100
21	DK	138/151 (91%)	133 (96%)	5 (4%)	0	100	100
22	AL	138/142 (97%)	126 (91%)	10 (7%)	2 (1%)	11	45
22	BL	138/142 (97%)	126 (91%)	10 (7%)	2 (1%)	11	45
22	CL	138/142 (97%)	127 (92%)	9 (6%)	2 (1%)	11	45
22	DL	138/142 (97%)	125 (91%)	11 (8%)	2 (1%)	11	45
23	AM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	12	47
23	BM	151/155 (97%)	139 (92%)	10 (7%)	2 (1%)	12	47
23	CM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	12	47
23	DM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	12	47
24	AN	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
24	BN	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
24	CN	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
24	DN	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
25	AO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	22	59
25	BO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	22	59
25	CO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	DO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	22	59
26	AP	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
26	BP	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
26	CP	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
26	DP	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
27	AQ	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
27	BQ	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
27	CQ	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
27	DQ	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
28	AR	336/343 (98%)	309 (92%)	25 (7%)	2 (1%)	25	62
28	BR	336/343 (98%)	308 (92%)	26 (8%)	2 (1%)	25	62
28	CR	336/343 (98%)	308 (92%)	26 (8%)	2 (1%)	25	62
28	DR	336/343 (98%)	307 (91%)	27 (8%)	2 (1%)	25	62
29	AS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	19	56
29	BS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	19	56
29	CS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	19	56
29	DS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	19	56
30	AT	152/155 (98%)	145 (95%)	7 (5%)	0	100	100
30	BT	152/155 (98%)	144 (95%)	8 (5%)	0	100	100
30	CT	152/155 (98%)	145 (95%)	7 (5%)	0	100	100
30	DT	152/155 (98%)	144 (95%)	8 (5%)	0	100	100
31	AU	122/126 (97%)	112 (92%)	10 (8%)	0	100	100
31	BU	122/126 (97%)	113 (93%)	9 (7%)	0	100	100
31	CU	122/126 (97%)	112 (92%)	10 (8%)	0	100	100
31	DU	122/126 (97%)	112 (92%)	10 (8%)	0	100	100
32	AV	117/130 (90%)	115 (98%)	2 (2%)	0	100	100
32	BV	117/130 (90%)	116 (99%)	1 (1%)	0	100	100
32	CV	117/130 (90%)	114 (97%)	2 (2%)	1 (1%)	17	54
32	DV	117/130 (90%)	115 (98%)	1 (1%)	1 (1%)	17	54
33	AW	257/259 (99%)	246 (96%)	11 (4%)	0	100	100
33	BW	257/259 (99%)	248 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	CW	257/259 (99%)	247 (96%)	10 (4%)	0	100	100
33	DW	257/259 (99%)	247 (96%)	10 (4%)	0	100	100
34	AX	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
34	BX	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
34	CX	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
34	DX	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
35	AY	226/293 (77%)	214 (95%)	11 (5%)	1 (0%)	34	69
35	BY	226/293 (77%)	214 (95%)	10 (4%)	2 (1%)	17	54
35	CY	226/293 (77%)	214 (95%)	11 (5%)	1 (0%)	34	69
35	DY	226/293 (77%)	215 (95%)	10 (4%)	1 (0%)	34	69
36	AZ	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
36	BZ	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
36	CZ	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
36	DZ	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
All	All	20528/23556 (87%)	19447 (95%)	1013 (5%)	68 (0%)	41	74

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	AL	3	VAL
25	AO	152	VAL
28	AR	48	ASP
22	BL	3	VAL
25	BO	152	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	90/192 (47%)	82 (91%)	8 (9%)	9	37
1	B0	90/192 (47%)	82 (91%)	8 (9%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C0	90/192 (47%)	82 (91%)	8 (9%)	9	37
1	D0	90/192 (47%)	83 (92%)	7 (8%)	12	42
2	A1	55/57 (96%)	46 (84%)	9 (16%)	2	15
2	B1	55/57 (96%)	45 (82%)	10 (18%)	1	11
2	C1	55/57 (96%)	45 (82%)	10 (18%)	1	11
2	D1	55/57 (96%)	44 (80%)	11 (20%)	1	8
3	A2	184/185 (100%)	157 (85%)	27 (15%)	3	18
3	B2	184/185 (100%)	157 (85%)	27 (15%)	3	18
3	C2	184/185 (100%)	157 (85%)	27 (15%)	3	18
3	D2	184/185 (100%)	158 (86%)	26 (14%)	3	20
4	A3	182/183 (100%)	153 (84%)	29 (16%)	2	16
4	B3	182/183 (100%)	154 (85%)	28 (15%)	2	17
4	C3	182/183 (100%)	154 (85%)	28 (15%)	2	17
4	D3	182/183 (100%)	153 (84%)	29 (16%)	2	16
5	A4	187/225 (83%)	157 (84%)	30 (16%)	2	15
5	B4	197/225 (88%)	167 (85%)	30 (15%)	3	17
5	C4	197/225 (88%)	166 (84%)	31 (16%)	2	16
5	D4	197/225 (88%)	167 (85%)	30 (15%)	3	17
6	A5	90/107 (84%)	76 (84%)	14 (16%)	2	17
6	B5	90/107 (84%)	76 (84%)	14 (16%)	2	17
6	C5	90/107 (84%)	76 (84%)	14 (16%)	2	17
6	D5	90/107 (84%)	76 (84%)	14 (16%)	2	17
7	A6	71/72 (99%)	60 (84%)	11 (16%)	2	17
7	B6	71/72 (99%)	60 (84%)	11 (16%)	2	17
7	C6	71/72 (99%)	60 (84%)	11 (16%)	2	17
7	D6	71/72 (99%)	60 (84%)	11 (16%)	2	17
8	A7	91/136 (67%)	83 (91%)	8 (9%)	10	38
8	B7	91/136 (67%)	83 (91%)	8 (9%)	10	38
8	C7	91/136 (67%)	83 (91%)	8 (9%)	10	38
8	D7	91/136 (67%)	83 (91%)	8 (9%)	10	38
9	A8	70/109 (64%)	59 (84%)	11 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B8	70/109 (64%)	59 (84%)	11 (16%)	2	16
9	C8	70/109 (64%)	59 (84%)	11 (16%)	2	16
9	D8	70/109 (64%)	59 (84%)	11 (16%)	2	16
10	A9	81/156 (52%)	75 (93%)	6 (7%)	13	44
10	B9	81/156 (52%)	76 (94%)	5 (6%)	18	49
10	C9	81/156 (52%)	75 (93%)	6 (7%)	13	44
10	D9	81/156 (52%)	72 (89%)	9 (11%)	6	28
12	AB	180/211 (85%)	164 (91%)	16 (9%)	9	37
12	BB	180/211 (85%)	164 (91%)	16 (9%)	9	37
12	CB	180/211 (85%)	164 (91%)	16 (9%)	9	37
12	DB	180/211 (85%)	164 (91%)	16 (9%)	9	37
13	AC	196/210 (93%)	178 (91%)	18 (9%)	9	36
13	BC	196/210 (93%)	179 (91%)	17 (9%)	10	38
13	CC	196/210 (93%)	179 (91%)	17 (9%)	10	38
13	DC	196/210 (93%)	178 (91%)	18 (9%)	9	36
14	AD	161/162 (99%)	129 (80%)	32 (20%)	1	8
14	BD	161/162 (99%)	128 (80%)	33 (20%)	1	7
14	CD	161/162 (99%)	129 (80%)	32 (20%)	1	8
14	DD	161/162 (99%)	128 (80%)	33 (20%)	1	7
15	AE	193/250 (77%)	169 (88%)	24 (12%)	4	24
15	BE	193/250 (77%)	169 (88%)	24 (12%)	4	24
15	CE	193/250 (77%)	169 (88%)	24 (12%)	4	24
15	DE	193/250 (77%)	168 (87%)	25 (13%)	4	22
16	AF	80/92 (87%)	76 (95%)	4 (5%)	24	55
16	BF	80/92 (87%)	76 (95%)	4 (5%)	24	55
16	CF	80/92 (87%)	76 (95%)	4 (5%)	24	55
16	DF	80/92 (87%)	76 (95%)	4 (5%)	24	55
17	AG	163/169 (96%)	145 (89%)	18 (11%)	6	29
17	BG	163/169 (96%)	145 (89%)	18 (11%)	6	29
17	CG	163/169 (96%)	144 (88%)	19 (12%)	5	26
17	DG	163/169 (96%)	145 (89%)	18 (11%)	6	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AH	116/117 (99%)	97 (84%)	19 (16%)	2	15
18	BH	116/117 (99%)	97 (84%)	19 (16%)	2	15
18	CH	116/117 (99%)	97 (84%)	19 (16%)	2	15
18	DH	116/117 (99%)	97 (84%)	19 (16%)	2	15
19	AI	120/122 (98%)	105 (88%)	15 (12%)	4	23
19	BI	120/122 (98%)	105 (88%)	15 (12%)	4	23
19	CI	120/122 (98%)	105 (88%)	15 (12%)	4	23
19	DI	120/122 (98%)	105 (88%)	15 (12%)	4	23
20	AJ	101/111 (91%)	91 (90%)	10 (10%)	8	32
20	BJ	101/111 (91%)	91 (90%)	10 (10%)	8	32
20	CJ	101/111 (91%)	91 (90%)	10 (10%)	8	32
20	DJ	101/111 (91%)	91 (90%)	10 (10%)	8	32
21	AK	112/121 (93%)	97 (87%)	15 (13%)	4	21
21	BK	112/121 (93%)	98 (88%)	14 (12%)	4	23
21	CK	112/121 (93%)	98 (88%)	14 (12%)	4	23
21	DK	112/121 (93%)	97 (87%)	15 (13%)	4	21
22	AL	112/114 (98%)	96 (86%)	16 (14%)	3	19
22	BL	112/114 (98%)	96 (86%)	16 (14%)	3	19
22	CL	112/114 (98%)	96 (86%)	16 (14%)	3	19
22	DL	112/114 (98%)	96 (86%)	16 (14%)	3	19
23	AM	133/135 (98%)	120 (90%)	13 (10%)	8	33
23	BM	133/135 (98%)	120 (90%)	13 (10%)	8	33
23	CM	133/135 (98%)	120 (90%)	13 (10%)	8	33
23	DM	133/135 (98%)	120 (90%)	13 (10%)	8	33
24	AN	48/49 (98%)	42 (88%)	6 (12%)	4	23
24	BN	48/49 (98%)	42 (88%)	6 (12%)	4	23
24	CN	48/49 (98%)	42 (88%)	6 (12%)	4	23
24	DN	48/49 (98%)	41 (85%)	7 (15%)	3	18
25	AO	135/136 (99%)	118 (87%)	17 (13%)	4	23
25	BO	135/136 (99%)	118 (87%)	17 (13%)	4	23
25	CO	135/136 (99%)	118 (87%)	17 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	DO	135/136 (99%)	118 (87%)	17 (13%)	4	23
26	AP	133/134 (99%)	117 (88%)	16 (12%)	5	25
26	BP	133/134 (99%)	116 (87%)	17 (13%)	4	23
26	CP	133/134 (99%)	116 (87%)	17 (13%)	4	23
26	DP	133/134 (99%)	117 (88%)	16 (12%)	5	25
27	AQ	140/141 (99%)	122 (87%)	18 (13%)	4	22
27	BQ	140/141 (99%)	122 (87%)	18 (13%)	4	22
27	CQ	140/141 (99%)	122 (87%)	18 (13%)	4	22
27	DQ	140/141 (99%)	122 (87%)	18 (13%)	4	22
28	AR	291/295 (99%)	264 (91%)	27 (9%)	9	35
28	BR	291/295 (99%)	265 (91%)	26 (9%)	9	37
28	CR	291/295 (99%)	264 (91%)	27 (9%)	9	35
28	DR	291/295 (99%)	264 (91%)	27 (9%)	9	35
29	AS	108/117 (92%)	97 (90%)	11 (10%)	7	31
29	BS	108/117 (92%)	97 (90%)	11 (10%)	7	31
29	CS	108/117 (92%)	97 (90%)	11 (10%)	7	31
29	DS	108/117 (92%)	97 (90%)	11 (10%)	7	31
30	AT	133/134 (99%)	119 (90%)	14 (10%)	7	30
30	BT	133/134 (99%)	119 (90%)	14 (10%)	7	30
30	CT	133/134 (99%)	120 (90%)	13 (10%)	8	33
30	DT	133/134 (99%)	120 (90%)	13 (10%)	8	33
31	AU	103/104 (99%)	93 (90%)	10 (10%)	8	33
31	BU	103/104 (99%)	93 (90%)	10 (10%)	8	33
31	CU	103/104 (99%)	93 (90%)	10 (10%)	8	33
31	DU	103/104 (99%)	93 (90%)	10 (10%)	8	33
32	AV	107/115 (93%)	97 (91%)	10 (9%)	9	35
32	BV	107/115 (93%)	97 (91%)	10 (9%)	9	35
32	CV	107/115 (93%)	98 (92%)	9 (8%)	11	40
32	DV	107/115 (93%)	98 (92%)	9 (8%)	11	40
33	AW	226/226 (100%)	194 (86%)	32 (14%)	3	20
33	BW	226/226 (100%)	194 (86%)	32 (14%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	CW	226/226 (100%)	194 (86%)	32 (14%)	3	20
33	DW	226/226 (100%)	194 (86%)	32 (14%)	3	20
34	AX	61/67 (91%)	54 (88%)	7 (12%)	5	27
34	BX	61/67 (91%)	54 (88%)	7 (12%)	5	27
34	CX	61/67 (91%)	55 (90%)	6 (10%)	8	33
34	DX	61/67 (91%)	54 (88%)	7 (12%)	5	27
35	AY	197/244 (81%)	177 (90%)	20 (10%)	7	31
35	BY	197/244 (81%)	178 (90%)	19 (10%)	8	34
35	CY	197/244 (81%)	177 (90%)	20 (10%)	7	31
35	DY	197/244 (81%)	177 (90%)	20 (10%)	7	31
36	AZ	82/82 (100%)	74 (90%)	8 (10%)	8	33
36	BZ	82/82 (100%)	73 (89%)	9 (11%)	6	29
36	CZ	82/82 (100%)	75 (92%)	7 (8%)	10	40
36	DZ	82/82 (100%)	74 (90%)	8 (10%)	8	33
All	All	18158/20320 (89%)	15963 (88%)	2195 (12%)	5	24

5 of 2195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	DD	107	ARG
17	DG	139	MET
14	DD	104	LEU
28	DR	238	LEU
15	BE	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 397 such sidechains are listed below:

Mol	Chain	Res	Type
15	CE	75	HIS
32	CV	56	HIS
17	CG	90	ASN
26	CP	20	GLN
36	CZ	80	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	1716/1753 (97%)	647 (37%)	149 (8%)
11	BA	1716/1753 (97%)	652 (37%)	148 (8%)
11	CA	1716/1753 (97%)	649 (37%)	149 (8%)
11	DA	1716/1753 (97%)	647 (37%)	149 (8%)
All	All	6864/7012 (97%)	2595 (37%)	595 (8%)

5 of 2595 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	2	A
11	AA	3	C
11	AA	4	C
11	AA	8	U
11	AA	11	A

5 of 595 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	DA	213	U
11	DA	1462	U
11	DA	312	C
11	DA	211	U
11	DA	882	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 332 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.