



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 06:01 PM UTC

PDB ID : 4BTS / pdb_00004bts
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

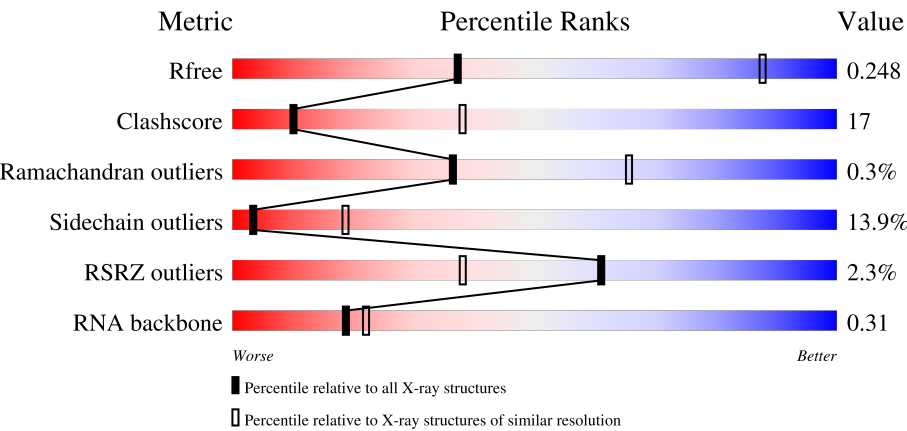
1 Overall quality at a glance i

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.



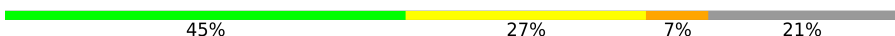
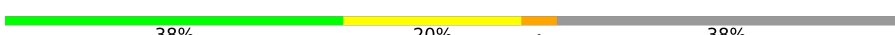
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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

Mol	Chain	Length	Quality of chain
1	A0	211	29% 16% . 53%
1	B0	211	28% 16% . 53%
1	C0	211	28% 16% . 53%
1	D0	211	30% 14% . 53%

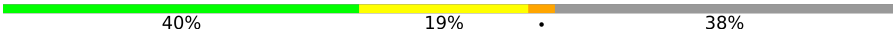
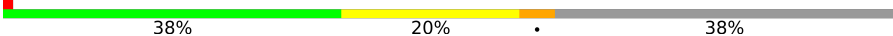
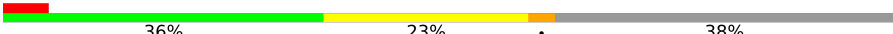
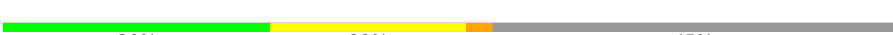
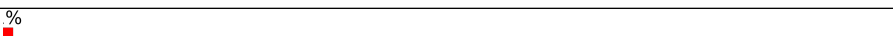
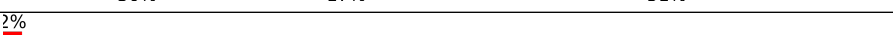
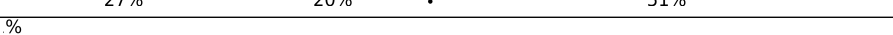
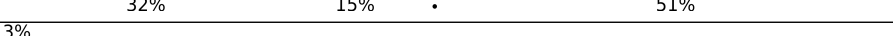
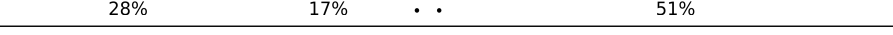
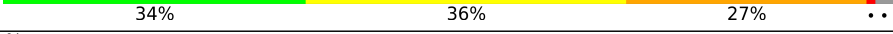
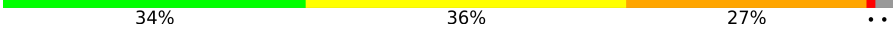
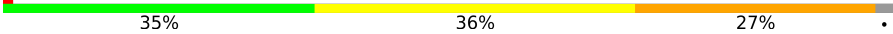
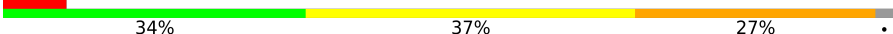
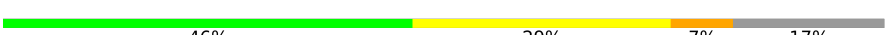
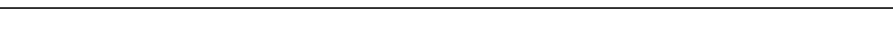
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Mol	Chain	Length	Quality of chain
2	A1	68	
2	B1	68	
2	C1	68	
2	D1	68	
3	A2	208	
3	B2	208	
3	C2	208	
3	D2	208	
4	A3	197	
4	B3	197	
4	C3	197	
4	D3	197	
5	A4	265	
5	B4	265	
5	C4	265	
5	D4	265	
6	A5	119	
6	B5	119	
6	C5	119	
6	D5	119	
7	A6	81	
7	B6	81	
7	C6	81	
7	D6	81	
8	A7	162	

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Mol	Chain	Length	Quality of chain
8	B7	162	
8	C7	162	
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	

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Mol	Chain	Length	Quality of chain
14	CD	181	
14	DD	181	
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	

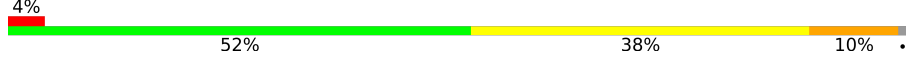
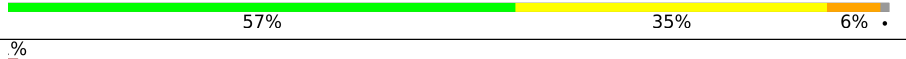
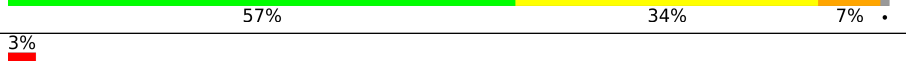
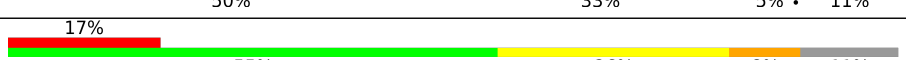
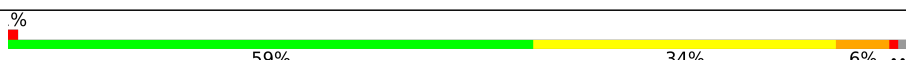
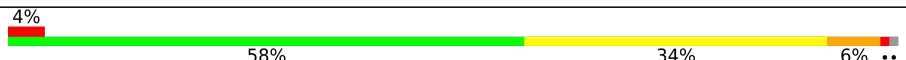
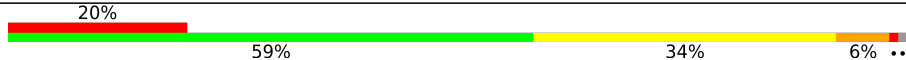
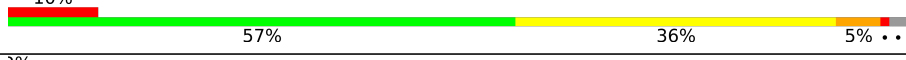
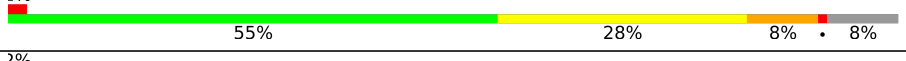
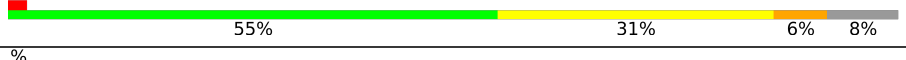
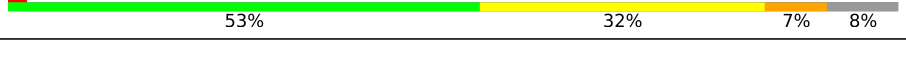
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Mol	Chain	Length	Quality of chain
20	DJ	120	
21	AK	151	
21	BK	151	
21	CK	151	
21	DK	151	
22	AL	142	
22	BL	142	
22	CL	142	
22	DL	142	
23	AM	155	
23	BM	155	
23	CM	155	
23	DM	155	
24	AN	55	
24	BN	55	
24	CN	55	
24	DN	55	
25	AO	153	
25	BO	153	
25	CO	153	
25	DO	153	
26	AP	149	
26	BP	149	
26	CP	149	
26	DP	149	

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Mol	Chain	Length	Quality of chain
27	AQ	157	
27	BQ	157	
27	CQ	157	
27	DQ	157	
28	AR	343	
28	BR	343	
28	CR	343	
28	DR	343	
29	AS	144	
29	BS	144	
29	CS	144	
29	DS	144	
30	AT	155	
30	BT	155	
30	CT	155	
30	DT	155	
31	AU	126	
31	BU	126	
31	CU	126	
31	DU	126	
32	AV	130	
32	BV	130	
32	CV	130	
32	DV	130	
33	AW	259	

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Mol	Chain	Length	Quality of chain
33	BW	259	
33	CW	259	
33	DW	259	
34	AX	80	
34	BX	80	
34	CX	80	
34	DX	80	
35	AY	293	
35	BY	293	
35	CY	293	
35	DY	293	
36	AZ	97	
36	BZ	97	
36	CZ	97	
36	DZ	97	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	MG	DA	5056	-	-	-	X

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	C	N	O	S	0	0	0
			511	308	103	96	4			
2	B1	66	Total	C	N	O	S	0	0	0
			511	308	103	96	4			
2	C1	66	Total	C	N	O	S	0	0	0
			511	308	103	96	4			
2	D1	66	Total	C	N	O	S	0	0	0
			511	308	103	96	4			

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

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

- 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 (CCD ID: 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	Zn	0	0
			1	1		
37	D6	1	Total	Zn	0	0
			1	1		
37	D9	1	Total	Zn	0	0
			1	1		
37	DN	1	Total	Zn	0	0
			1	1		

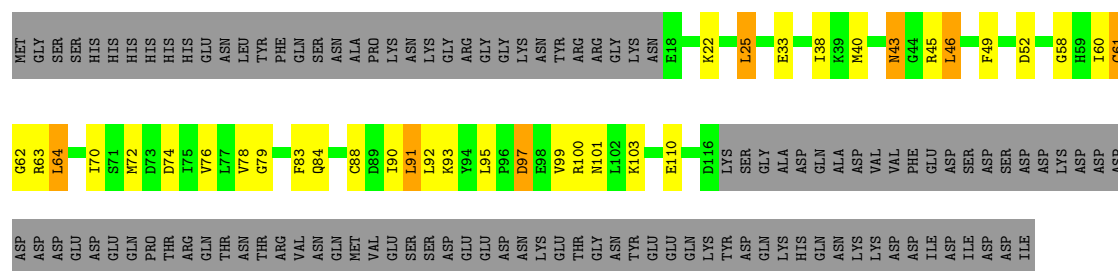
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 39 is water.

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

Chain D0:  30% 14% 53%



• Molecule 2: 40S RIBOSOMAL PROTEIN RPS28E

Chain A1:  53% 35% 9%



• Molecule 2: 40S RIBOSOMAL PROTEIN RPS28E

Chain B1:  56% 34% 7%



• Molecule 2: 40S RIBOSOMAL PROTEIN RPS28E

Chain C1:  51% 35% 10%



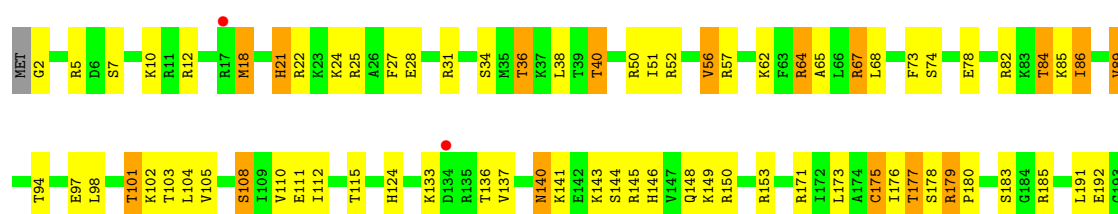
• Molecule 2: 40S RIBOSOMAL PROTEIN RPS28E

Chain D1:  3% 53% 34% 10%



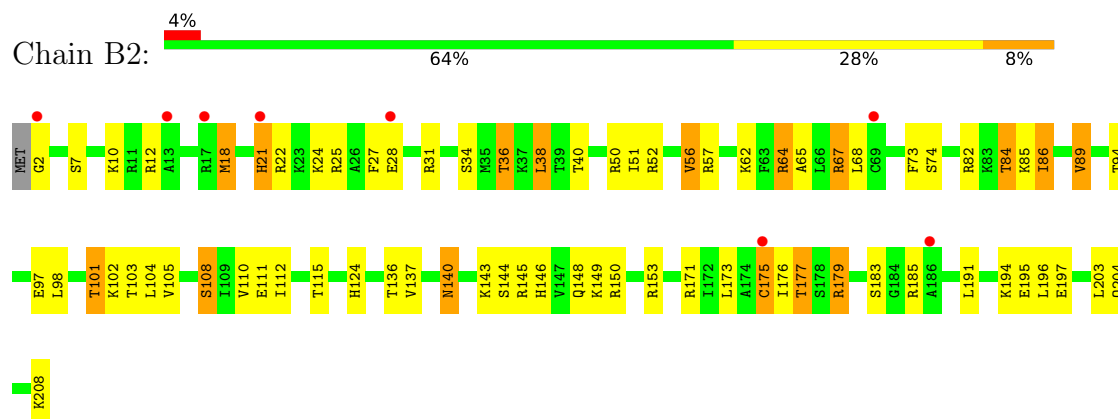
• Molecule 3: 40S RIBOSOMAL PROTEIN S8

Chain A2:  61% 31% 8%

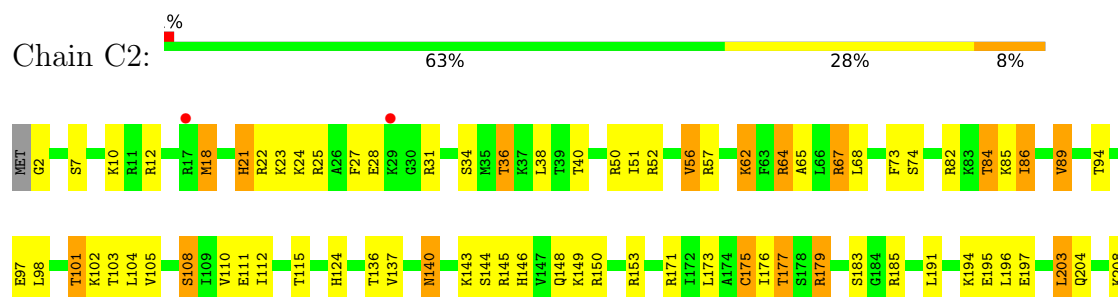




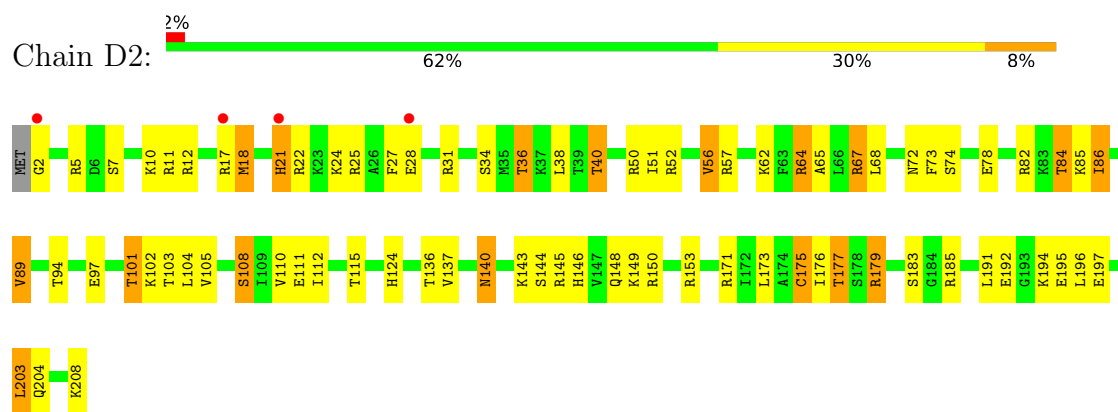
• Molecule 3: 40S RIBOSOMAL PROTEIN S8



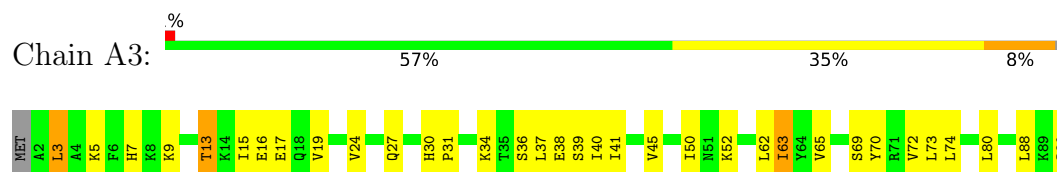
• Molecule 3: 40S RIBOSOMAL PROTEIN S8

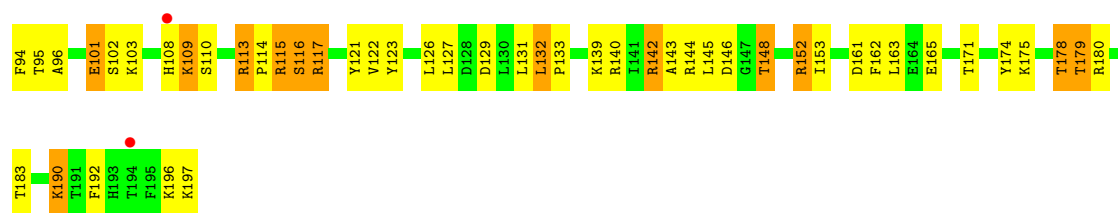


• Molecule 3: 40S RIBOSOMAL PROTEIN S8

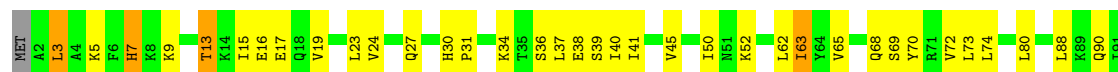


• Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E

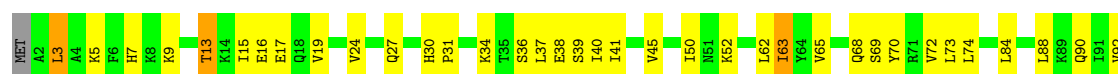




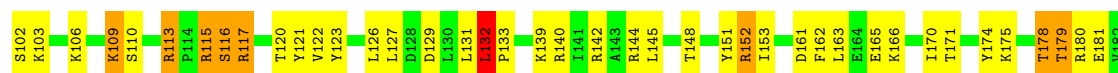
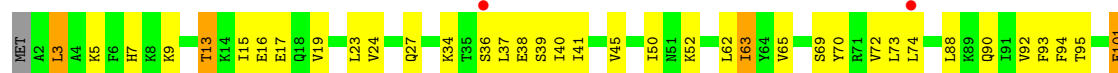
● Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E



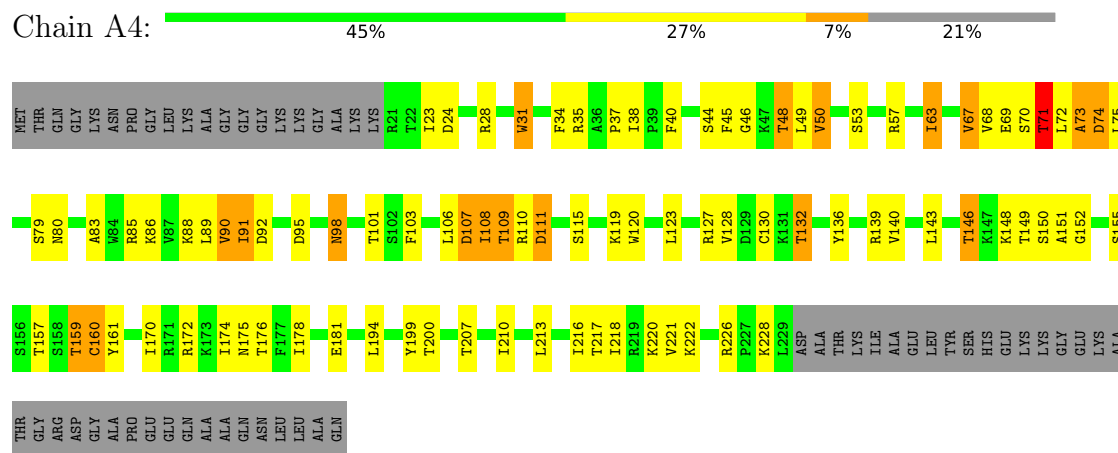
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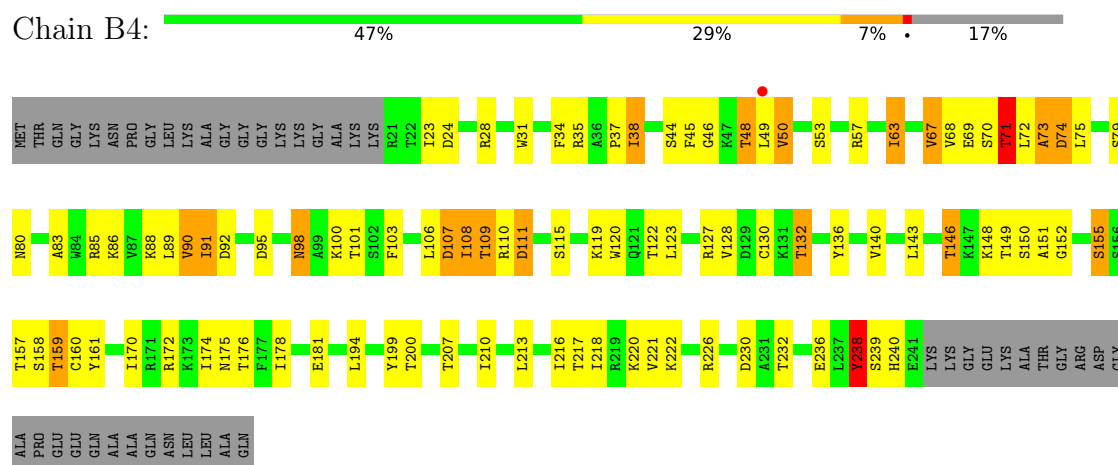
● Molecule 4: 40S RIBOSOMAL PROTEIN RPS7E



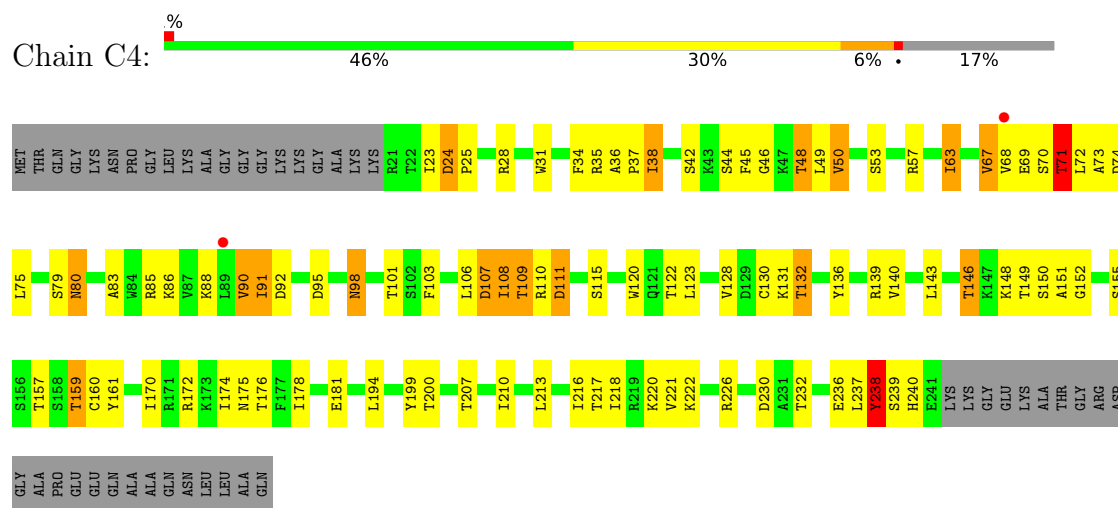
● Molecule 5: 40S RIBOSOMAL PROTEIN S3A



• Molecule 5: 40S RIBOSOMAL PROTEIN S3A

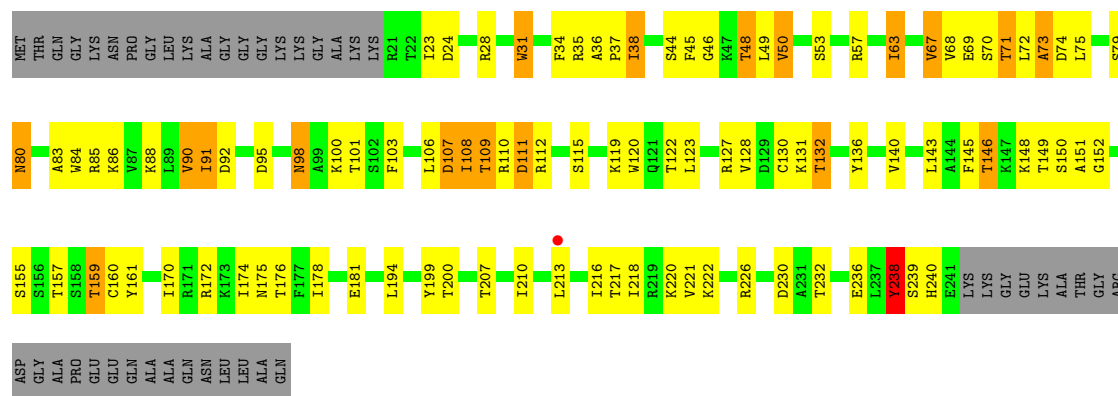


• Molecule 5: 40S RIBOSOMAL PROTEIN S3A



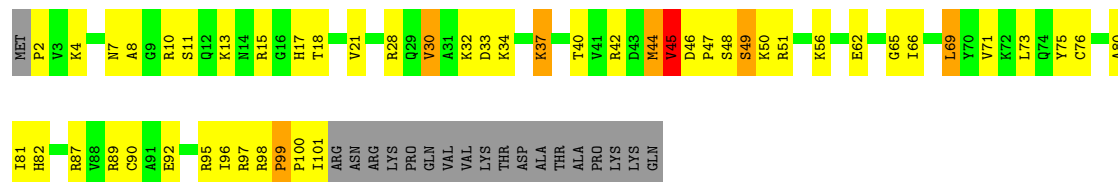
• Molecule 5: 40S RIBOSOMAL PROTEIN S3A





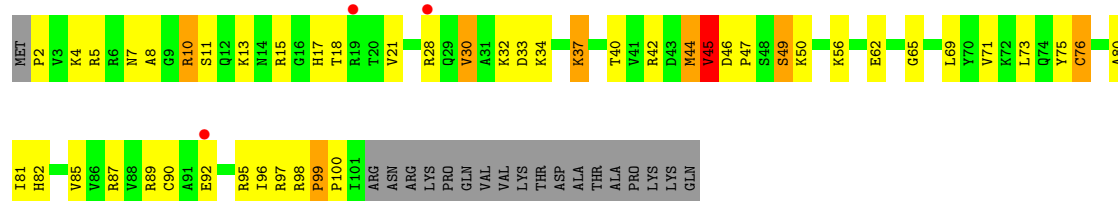
• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E

Chain A5: 42% 36% 5% 16%



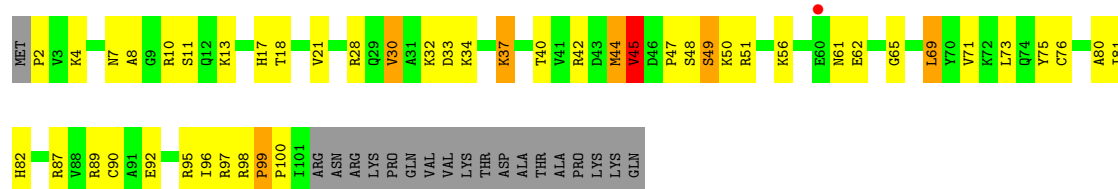
• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E

Chain B5: 3% 44% 34% 6% 16%



• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E

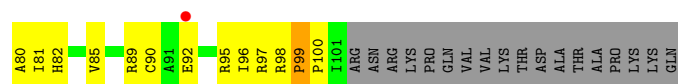
Chain C5: % 45% 34% 5% 16%



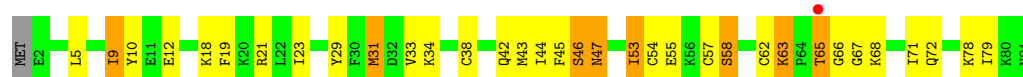
• Molecule 6: 40S RIBOSOMAL PROTEIN RPS26E

Chain D5: 4% 44% 35% 16%

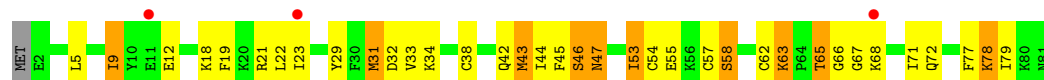




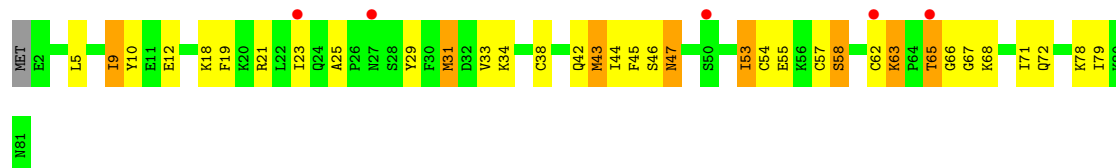
• Molecule 7: 40S RIBOSOMAL PROTEIN S27



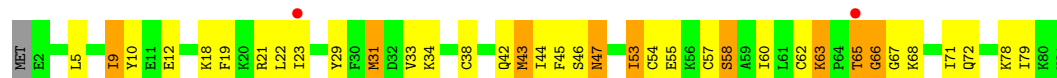
• Molecule 7: 40S RIBOSOMAL PROTEIN S27



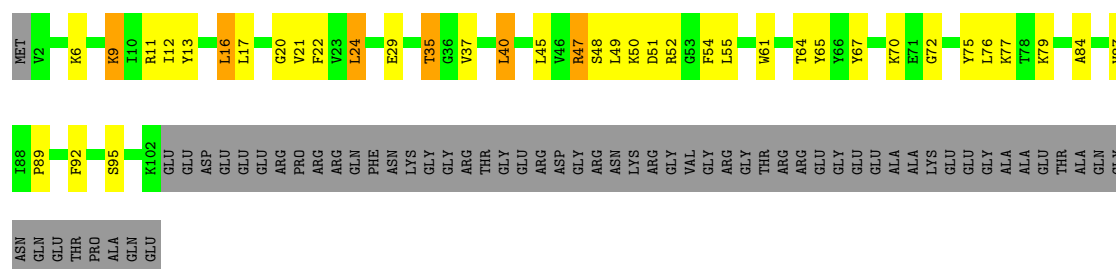
• Molecule 7: 40S RIBOSOMAL PROTEIN S27



• Molecule 7: 40S RIBOSOMAL PROTEIN S27

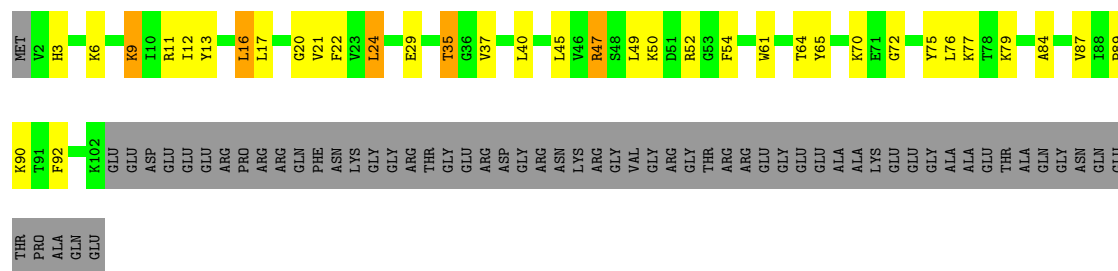


• Molecule 8: 40S RIBOSOMAL PROTEIN RPS10E

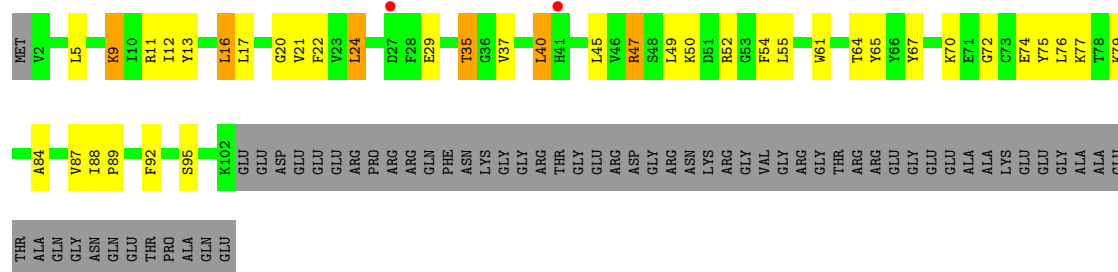


• Molecule 8: 40S RIBOSOMAL PROTEIN RPS10E

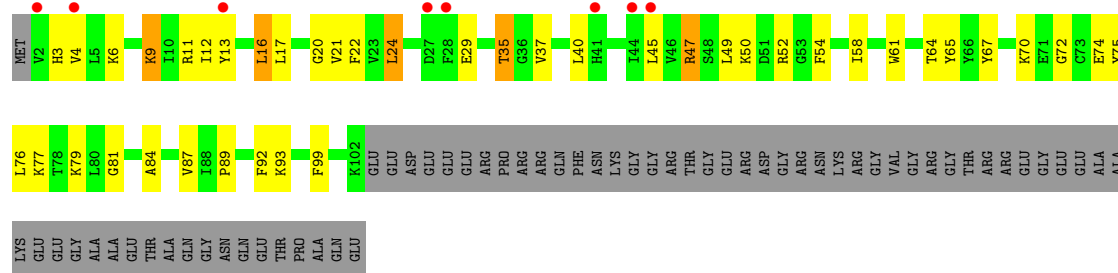




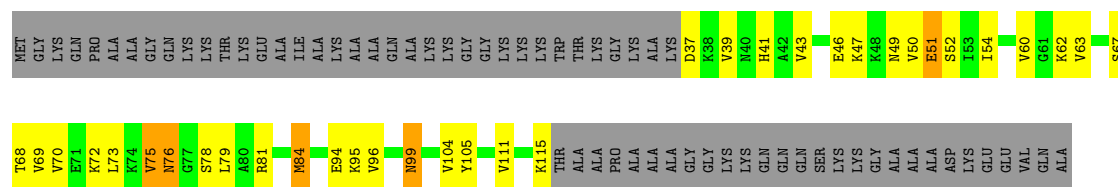
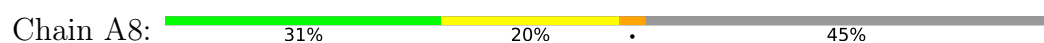
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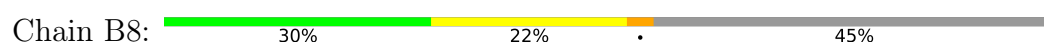
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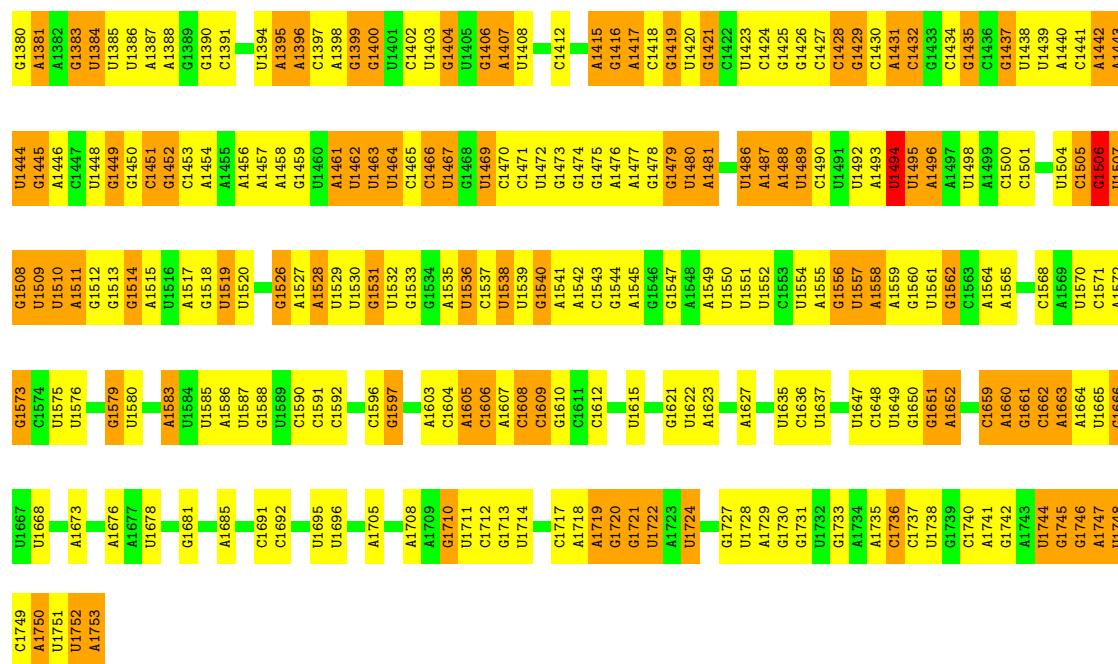
• Molecule 9: 40S RIBOSOMAL PROTEIN RPS25E



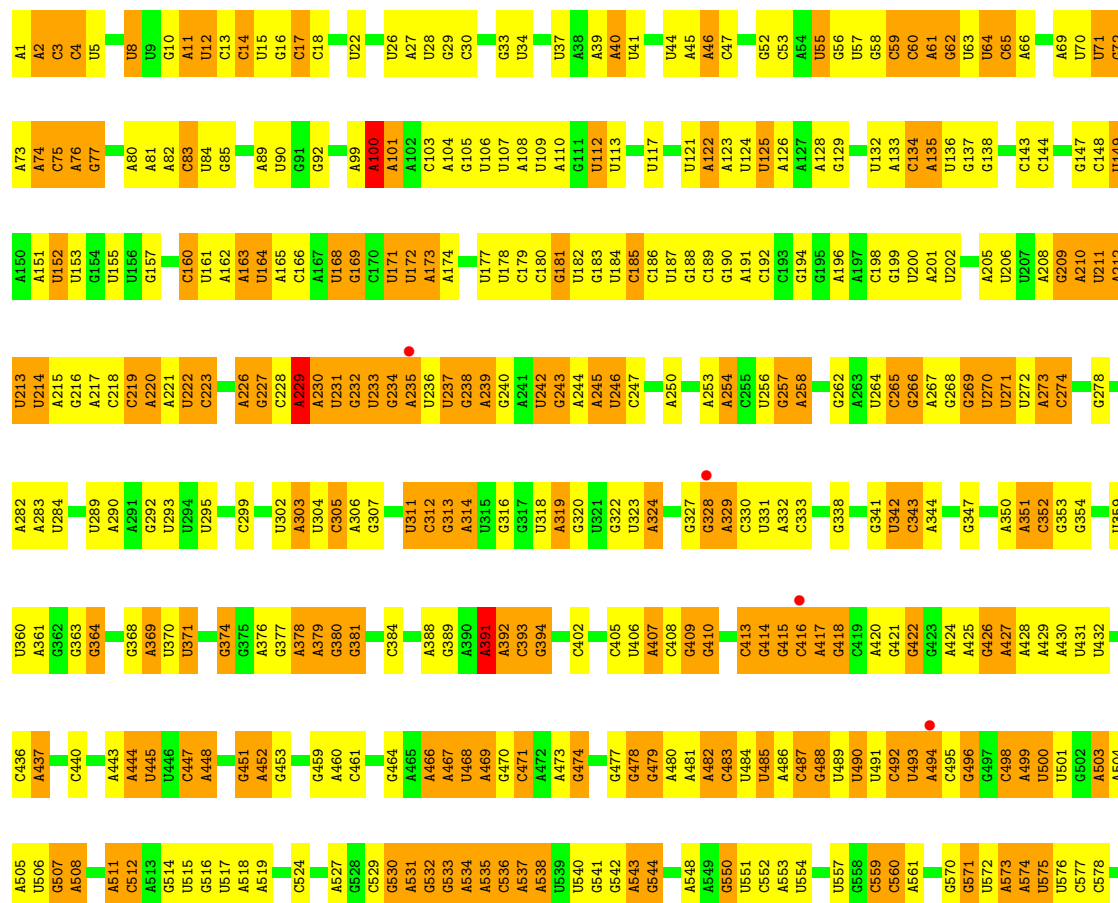
• Molecule 9: 40S RIBOSOMAL PROTEIN RPS25E



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A1316	C1246	A1174	G1113	G1025	G954	U981	A804	A723	G663	A593	G514	A444	A283
C1318	A1317	A1175	G1114	C1026	A955	A882	G905	C724	A664	A693	U515	U445	U284
U1319	U1248	A1176	A1115	U1027	A956	A883	C908	U725	A665	U594	U516	U446	U285
A1320	G1249	C1181	U1117	G1029	A957	A884	U811	U726	A666	U597	A517	U447	U286
G1321	G1250	A1180	A1118	A1030	G958	A885	U812	U727	C667	A598	A518	C447	A290
U1322	C1251	G1184	G1119	A1031	G962	U886	U813	U728	U668	A599	A448	U371	A291
C1323	C1252	C1185	A1120	U1032	G963	U887	U814	U729	G670	U603	G451	G374	G292
G1326	G1253	G1186	G1121	A1033	A966	U888	U815	C731	A671	G604	A452	A375	U293
U1327	C1256	A1187	G1122	A1034	G967	U889	U816	U738	C672	U605	G453	G376	U294
U1328	U1257	A1188	G1123	U1035	C968	G891	U817	A738	A673	G606	G459	G377	U295
G1329	U1258	G1189	G1124	U1036	C969	G892	G818	A739	U674	U606	A460	A378	C299
A1331	U1262	A1191	C1126	U1038	A970	U894	U819	U743	C676	C608	C461	A379	G389
A1332	G1263	G1192	G1127	G1042	A971	U895	U820	U749	G677	U611	A534	G381	U302
A1333	G1264	A1198	G1128	U1043	G972	U896	C821	U750	U678	U612	A535	C394	A303
U1334	U1265	G1199	C1131	C1044	A973	A897	U822	U751	U679	A613	C536	A388	U304
G1335	G1266	G1200	A1132	G1045	C974	U898	U823	U752	U680	A614	A537	A389	C305
G1339	A1268	G1201	C1133	U1046	G975	G902	G824	C753	G882	A615	U538	A467	A306
U1342	U1269	U1202	C1134	G1047	U977	G903	G825	C755	A	A616	U540	A468	G307
U1343	U1270	U1203	A1135	C1049	C978	A904	A833	G755	A	A617	U541	G470	U311
A1344	G1271	U1204	G1136	C1050	A981	C906	U834	A758	C	A618	A543	G474	G312
A1345	A1272	G1205	A1137	G1051	U982	U906	U835	G759	U		G544	C475	G313
C1346	U1273	C1207	A1138	U1052	A983	A907	U836	G760	A			C476	A314
U1347	U1274	U1208	G1139	A1053	C984	A908	A840	U761	A			C477	U315
U1348	U1275	G1209	C1140	G1055	C985	U910	A841	U762	A			C478	G316
U1349	G1276	U1210	G1141	G1056	G986	U911	U842	U763	A			C479	G317
U1350	U1277	U1211	A1143	A1059	G989	A912	A843	U764	U			C480	A319
A1351	U1278	U1212	A1144	A1060	G990	U913	G844	U765	C			C481	G320
C1352	U1279	G1213	C1145	U1061	C991	G914	G845	G766	G			C482	U323
A1353	G1281	A1214	U1146	C1062	U995	A919	A847	G770	C			U484	U324
G1354	U1282	U1215	G1147	A1063	U996	G920	A848	A771	U			U485	G327
G1355	U1283	C1216	C1148	A1064	A997	C921	C849	A772	U			C413	G328
U1356	U1284	U1217	G1149	A1065	A998	A922	G850	A776	U			C414	A329
A1357	U1285	U1218	U1150	U1069	U1000	U923	G854	U777	C			C415	U330
C1358	U1286	U1219	C1151	U1070	C928	C928	G857	C781	U			C416	U331
U1359	U1287	U1220	G1152	U1071	A1001	U1002	C858	G785	G			C417	A332
U1360	C1288	U1221	U1153	U1072	U1003	A1003	A859	A786	U			C418	C333
A1361	C1289	U1222	U1154	G1073	U1004	A1004	U860	A787	U			G421	G338
U1362	U1290	U1223	U1155	U1074	C1006	A1005	U861	U788	C			G422	G341
U1363	U1291	U1224	A1156	U1075	U1007	A933	A862	U789	G			G423	U342
C1364	C1292	U1225	U1157	G1076	U1008	U934	G863	A789	A			C424	C343
U1365	C1293	U1226	U1158	G1077	A1009	U935	U864	G792	U			C425	A344
U1366	C1294	U1227	U1159	G1078	U1010	U936	A865	G793	C			C426	
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U1369	U1298	U1230	C1162	G1083	G1013	A941	U868	A796	A			C429	A351
C1369	C1299	U1231	U1163	U1092	U1014	U942	A869	U797	G			C430	C352
U1370	U1300	U1232	C1164	A1093	A1015	U943	G872	U798	U			C431	G353
A1371	U1301	U1233	A1165	G1094	A1016	U944	U873	U799	G			C432	G354
U1372	G1235	U1234	C1166	A1095	C1017	A945	U874	G799	A			C433	
G1373	U1306	G1236	C1167	A1096	G1018	C947	C875	G800	G			C434	
A1377	U1307	G1237	C1168	U1097	G1019	A948	A876	G801	G			C435	
U1378	C1310	U1241	G1170	U1108	G1020	A949	A877	U802	A			C436	U359
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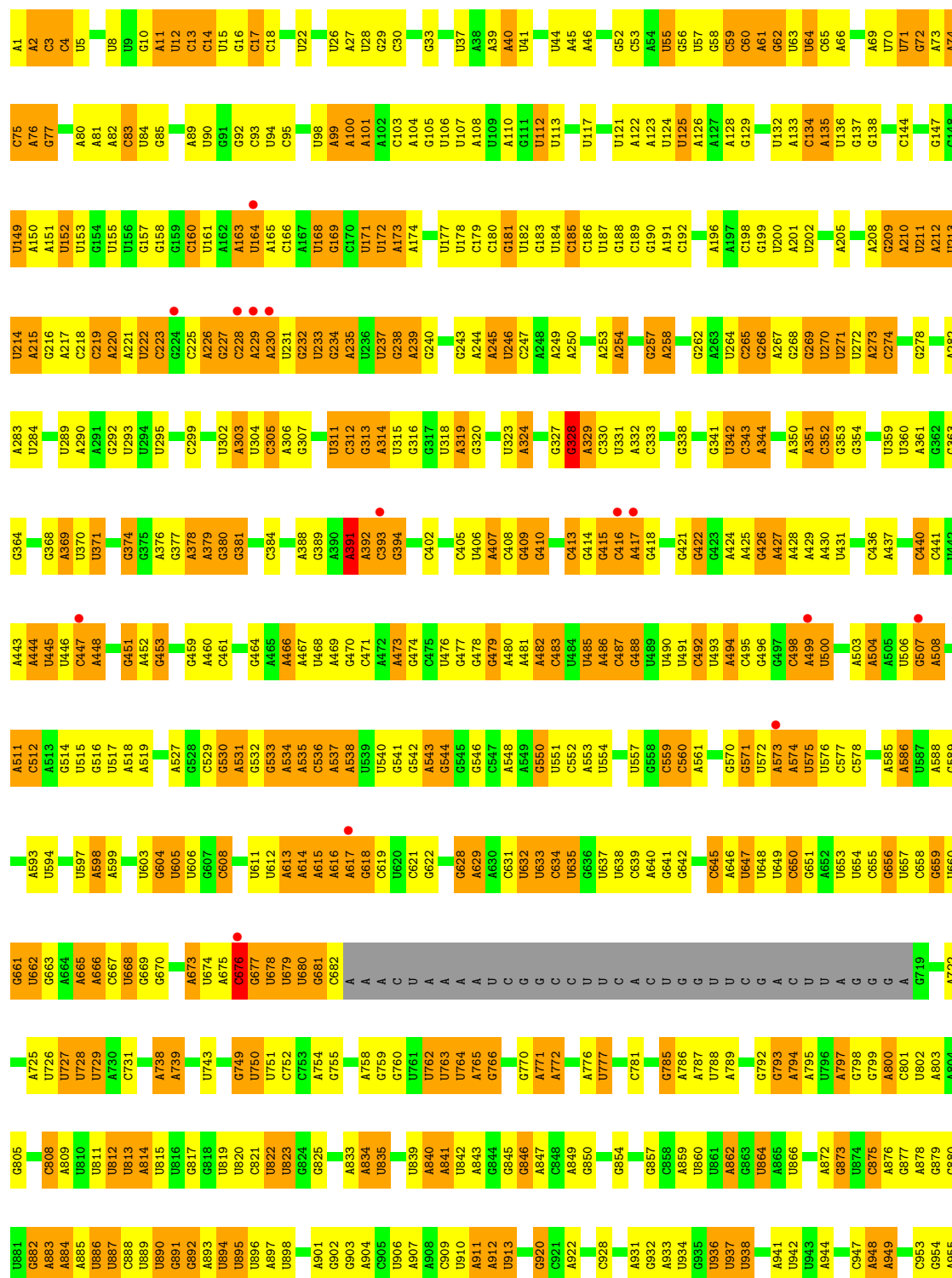
• Molecule 11: 18S ribosomal RNA

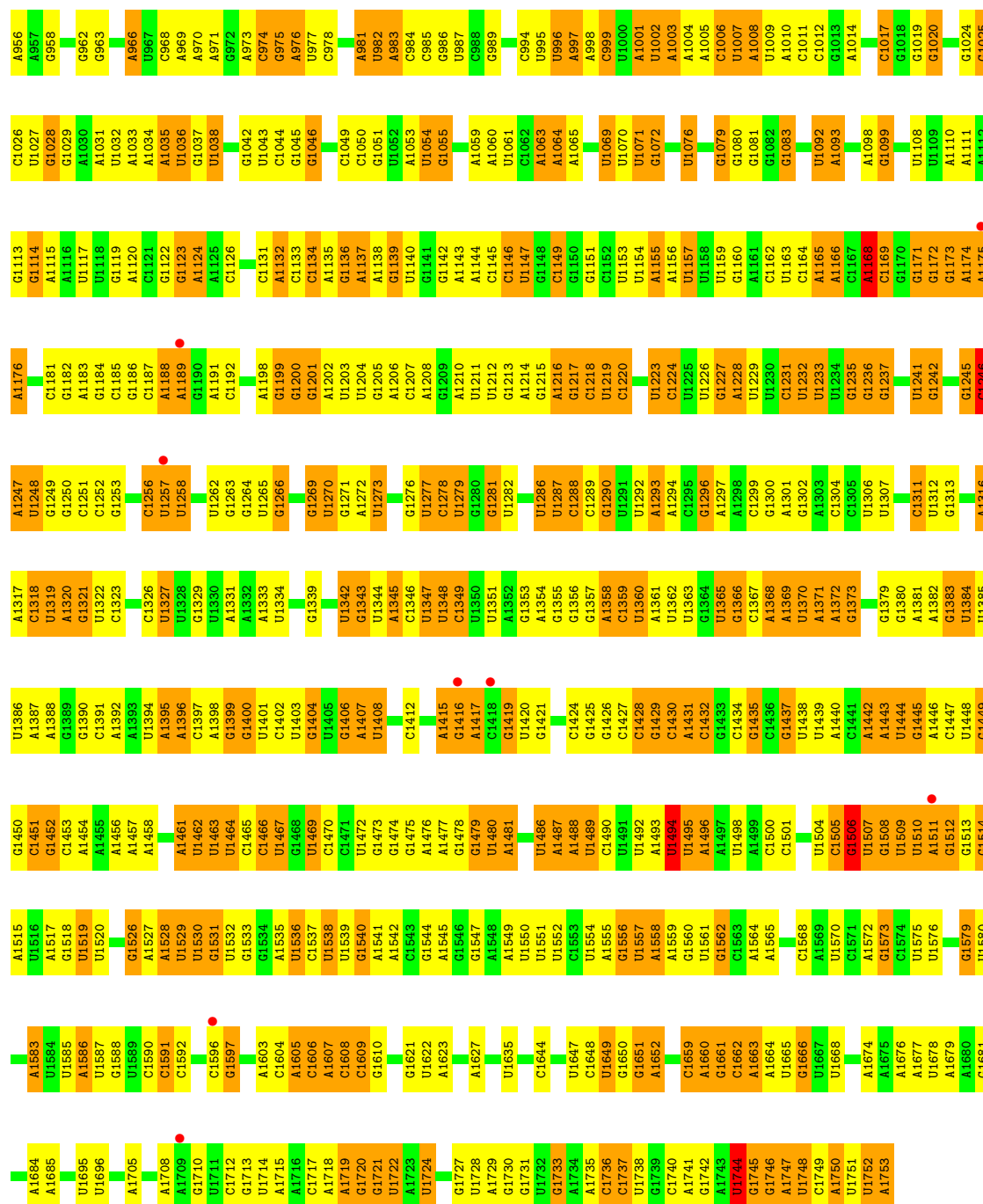




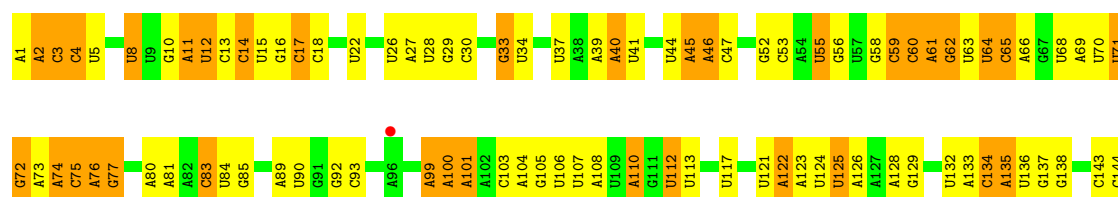


• Molecule 11: 18S ribosomal RNA

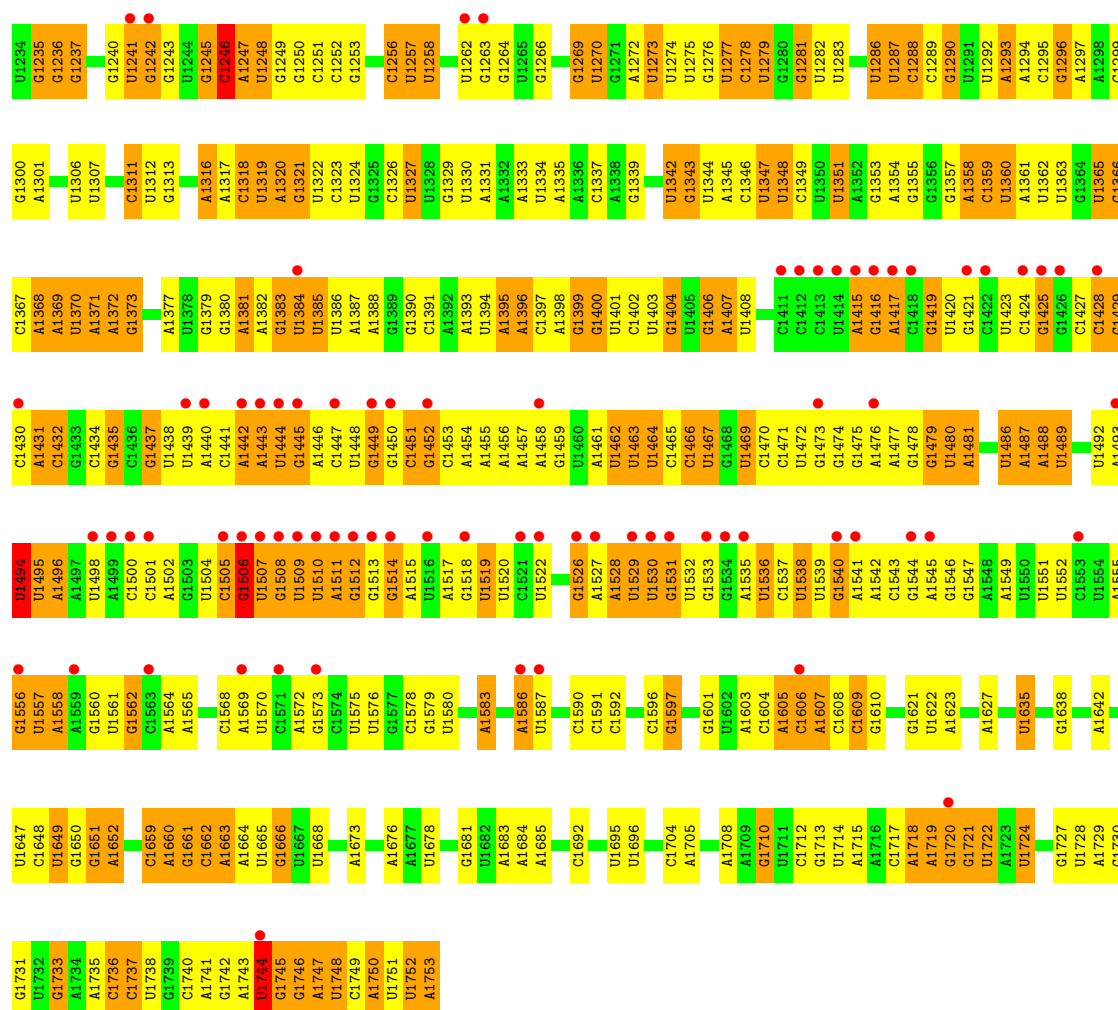




• Molecule 11: 18S ribosomal RNA

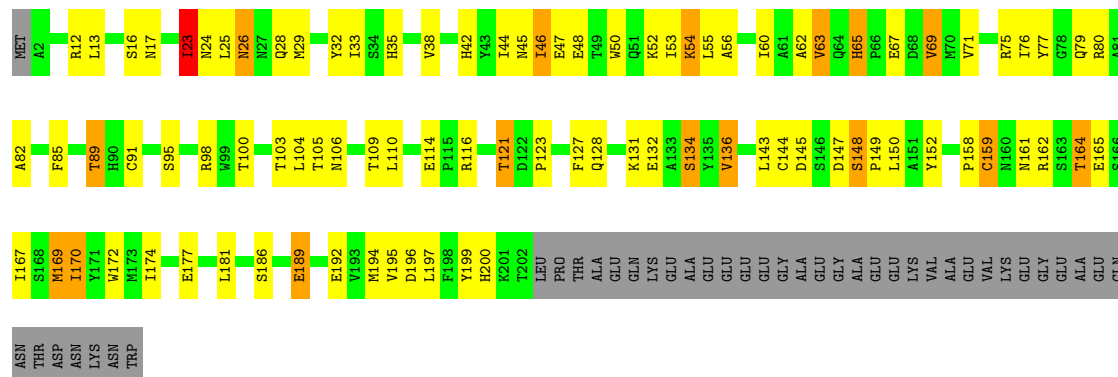


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G1170	A1098	G1019	A948	A876	A800	G	U657	C578	U500	A428	U359	G274	A212	A146
G1171	G1099	G1020	A949	G877	C801	A	G658	A585	A503	A429	U359	G278	U213	G147
A1172				A878	U802		G659	A586	A504	A430	U360		U214	C148
A1173	U1108	G1024	C953	G880	A804		U660	U587	A505	U431	A361	A282	U215	U149
A1175	A1110	C1026	A955	G881	G805		U662	A588	U506	U432	G364	A283	G216	A150
A1176	A1111	U1027	A956	G882			G663	G589	G507	C436		U284	A217	A151
C1177	A1112	G1028	A957	A883	C808		A664		A508	A437			C218	U152
C1178	G1113	A1030	G958	A884	U809		A665	A593	A369	U370		U289	C219	U153
C1179	G1114	A1031		A885	U810		A666	U594	A370	C440		A291	A220	G154
A1180	A1115	U1031	G962	U886	U811		C667	U597	C512	C441		G292	A221	U155
A1181	A1116	U1032		U887	U812		U668	A598	C513			U293	A222	U156
A1182	U1117	A1033	A966	C888	U813		G669	A599	G514	A444		U294	C223	G157
A1183	U1118	A1034	U967	U889	A814		G670	A599	U515	U445			G224	
A1184	G1119	A1035	C968	U890	U815		A671		U516	U446		U295	C225	C160
C1185	A1120	U1036	A969	G891	U816		C672	U603	G516	A447		G296	A226	U161
G1186	A1121	G1037	A970	G892	G817		U673	G604	U518	C447		U297	G227	A162
C1187	G1122	U1038	A971	A893	G818		U674	U605	A519	A448		G298	C228	A163
A1188	G1123		G972	U894	U819		A675	U606		G451		C298	A229	U164
A1189	A1124		A973	U895	U820		C676	G607	A527	A452		U302	A230	A165
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	C1134		C978		G825		G681	A613	G532	C461		G307	A235	G170
G1199	A1135	C1049	A979	A901			C682	A614	G533				U236	U171
G1200	G1136	C1050	G980	G902	A833			A615	A534	G464		U311	U237	U172
G1201	A1137	U1043	A981	G903	U835			A616	A535	A465		C312	G238	A173
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U1203	A1139	U1052	U906	G906	U839			G618	A537	A467		A314	G240	
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G1205		U1054	A908	A908	A841			U620	U539	G470		G316	G243	U178
A1206		G1055			U842			G621	U540	A471		G317	U244	C179
C1207					U843			A622	G541	U318		A319	A245	G180
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A1210					G846			A630	G544	C475		U323	A248	U184
U1211					C847			C631	A548	U476		A324	A249	C186
U1212					C848			U632	A549	G477			A250	U187
G1213					A849			U633	G550	G478		G327	A253	G188
A1214					G850			C634	U551	A480		A328	A254	C189
G1215								U635	C552	A481		C330	C255	G190
A1216					G854				A553	A482		U331	U256	A191
G1217								U638	U554	C483		U412	G257	C192
C1218					G857			C639		U484		A332	A258	
U1219					A859			A640	U557	U485		C333		A196
C1220					U860			G641	G558	A486		G338	G262	A197
U1222					U861			G642	C559	C487			A263	C198
U1223					U862				C560	G488		G338	U264	G199
C1224					A862			U647	A561				C265	U202
U1225					G863			U648	G570	U491		G341	G266	
U1226					U864			U649	G571	C492		U342	A267	
C1227					A865			C650	G572	U493		C343	A268	A205
A1228					U866			G651	U572	A494		A344	G269	U206
U1229								A852	A573	G495			U270	U207
U1230					A872			U653	A574	G496		A351	U271	A208
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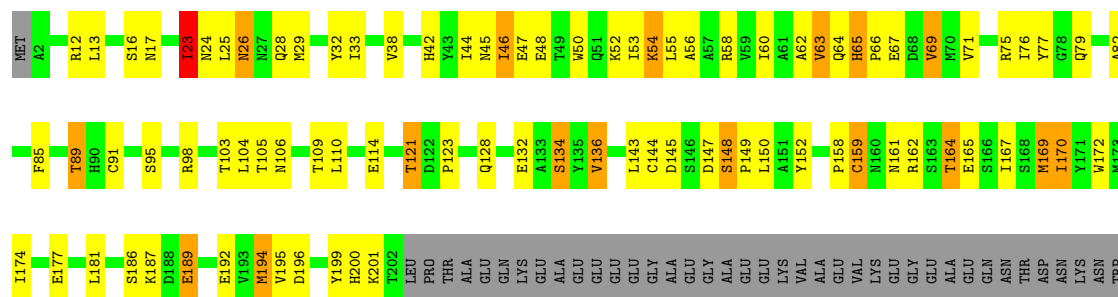
● Molecule 12: 40S RIBOSOMAL PROTEIN SA

Chain AB: 46% 31% 7% 17%



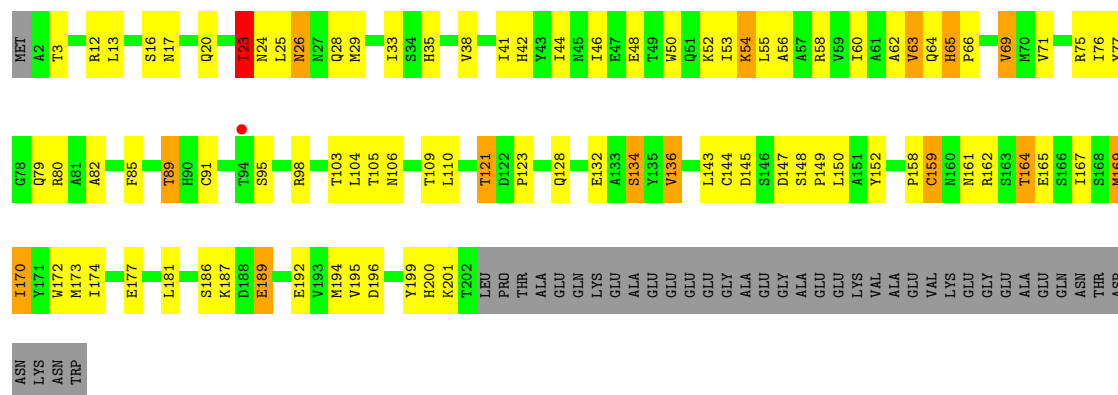
● Molecule 12: 40S RIBOSOMAL PROTEIN SA

Chain BB: 46% 29% 7% 17%



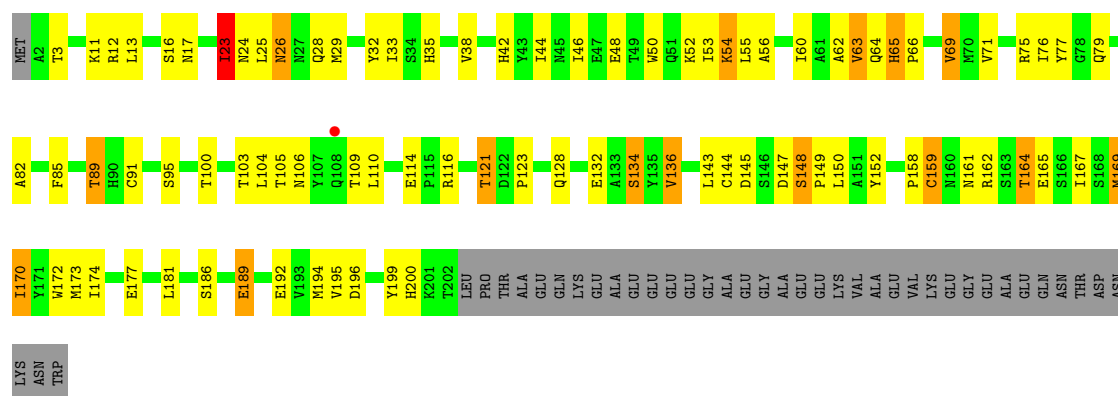
• Molecule 12: 40S RIBOSOMAL PROTEIN SA

Chain CB: 46% 31% 6% 17%



• Molecule 12: 40S RIBOSOMAL PROTEIN SA

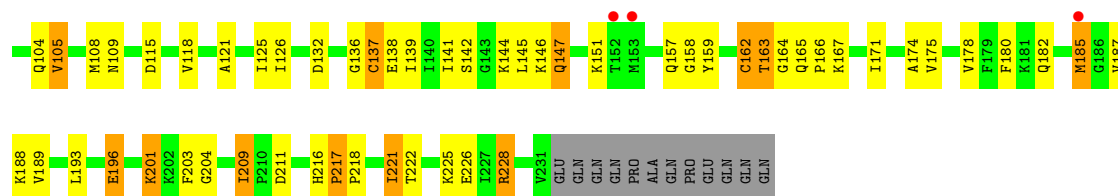
Chain DB: 47% 30% 6% 17%



• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

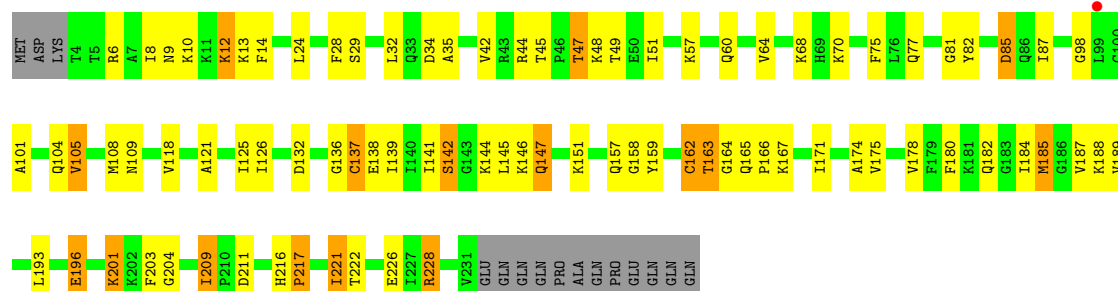
Chain AC: 58% 30% 6% 6%





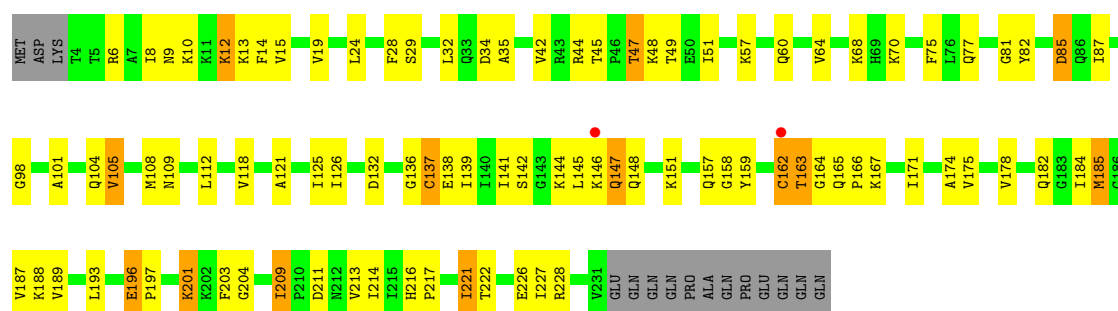
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain BC: 58% 29% 7% 6%



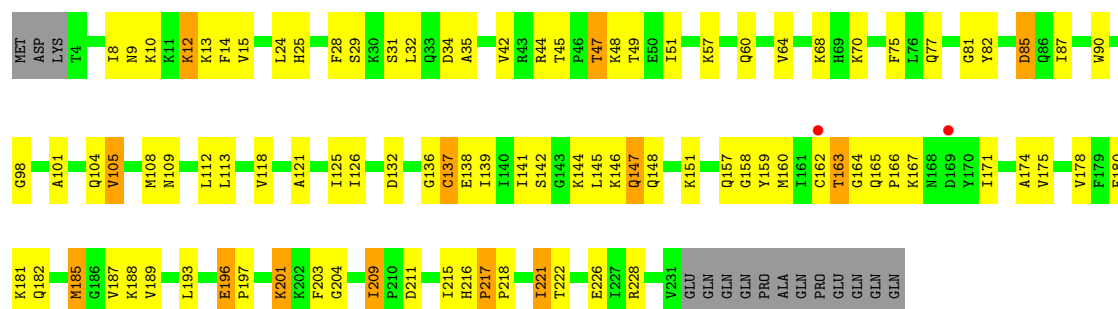
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain CC: 56% 33% 5% 6%



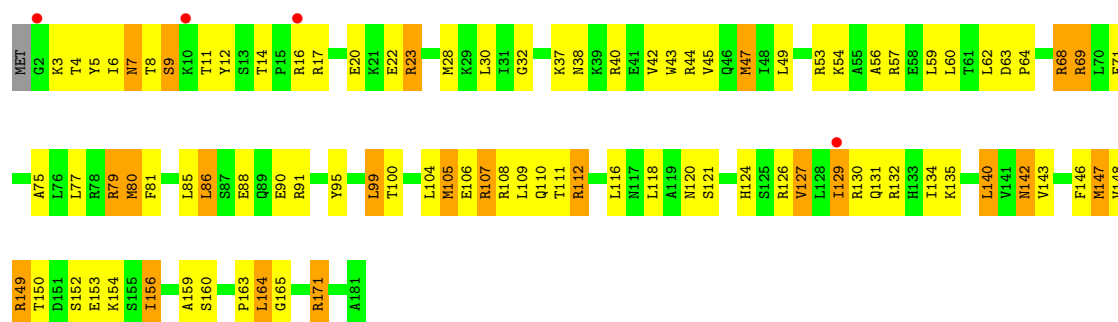
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain DC: 54% 34% 5% 6%

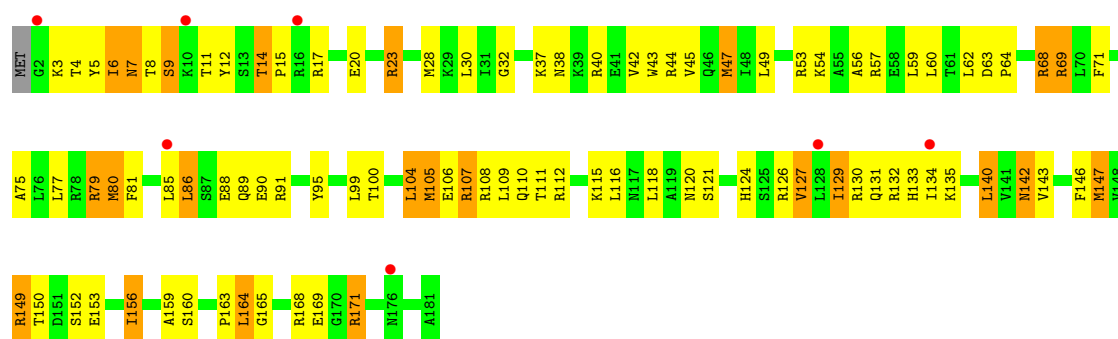


• Molecule 14: 40S RIBOSOMAL PROTEIN RPS9E

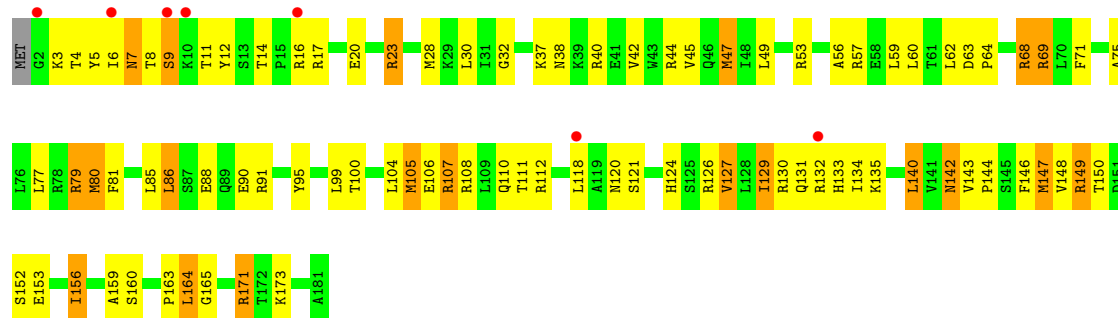
Chain AD: 2% 49% 39% 12%



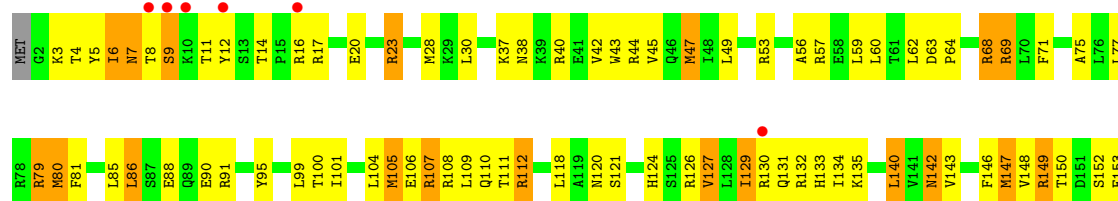
• Molecule 14: 40S RIBOSOMAL PROTEIN RPS9E



• Molecule 14: 40S RIBOSOMAL PROTEIN RPS9E

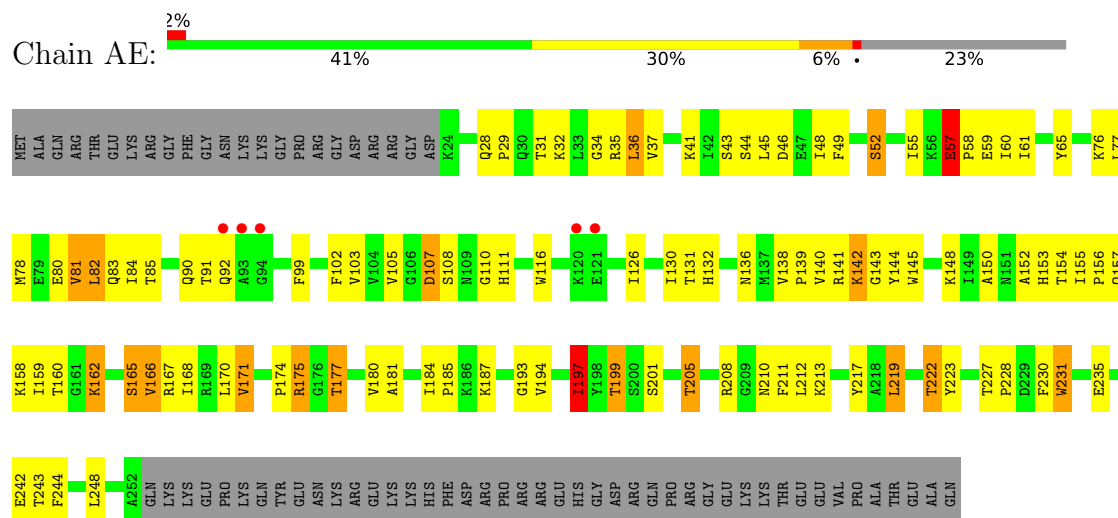


• Molecule 14: 40S RIBOSOMAL PROTEIN RPS9E

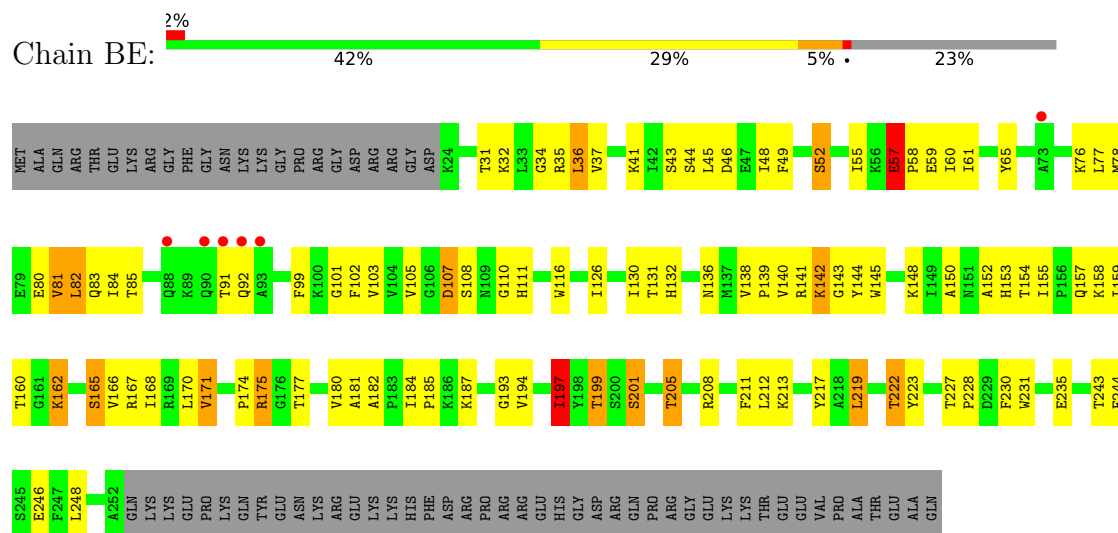




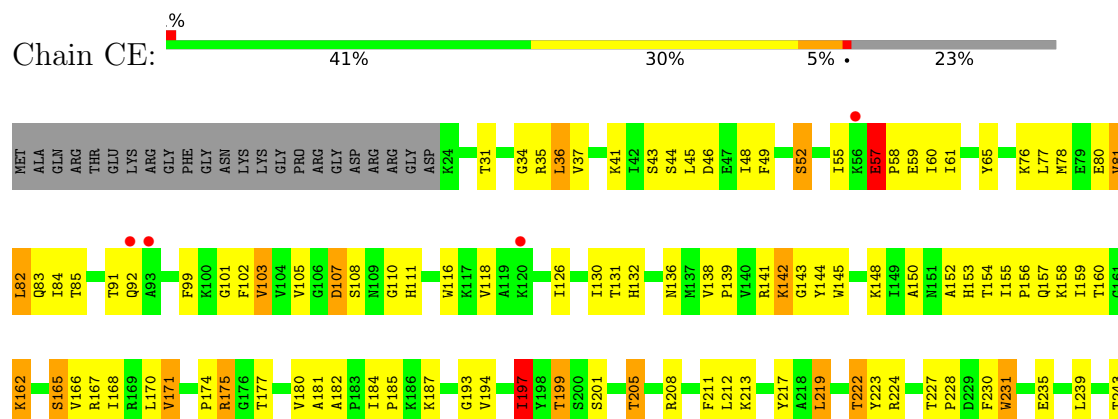
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

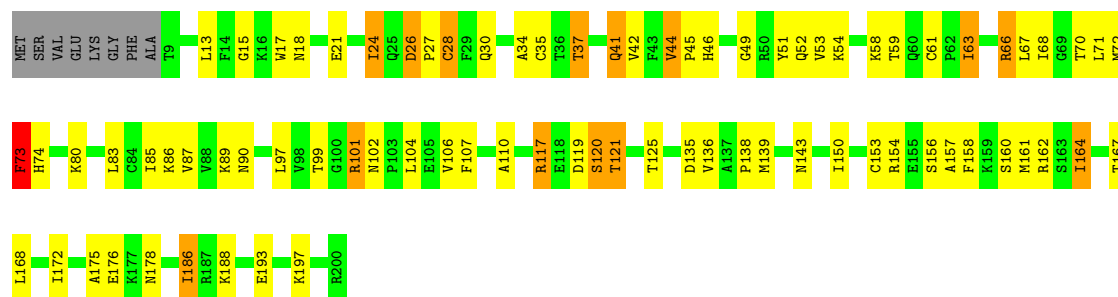


• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E



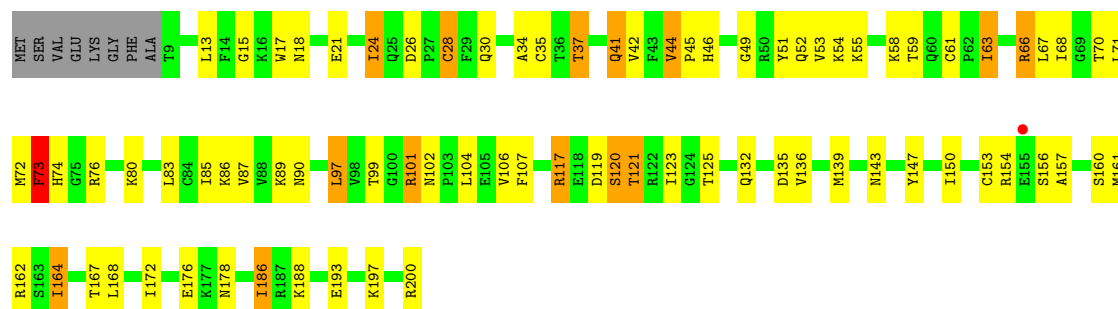
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E





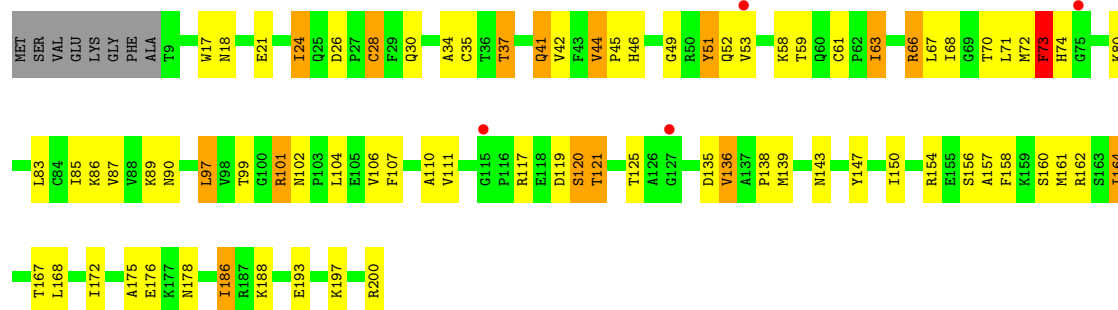
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain BG: 56% 33% 7%



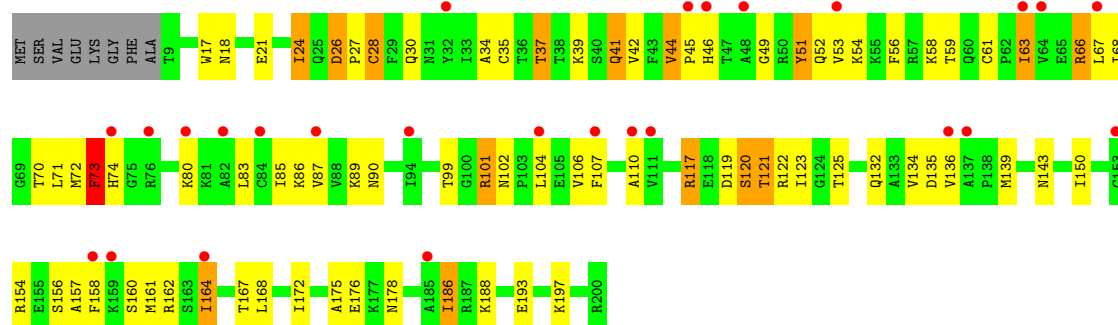
• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain CG: 2% 57% 31% 8%

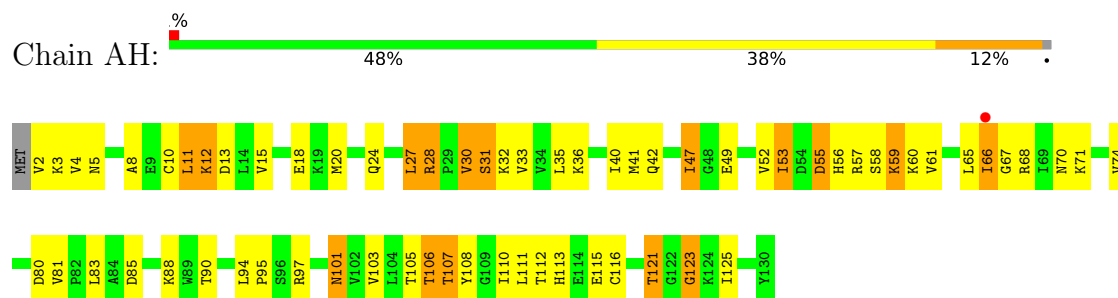


• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

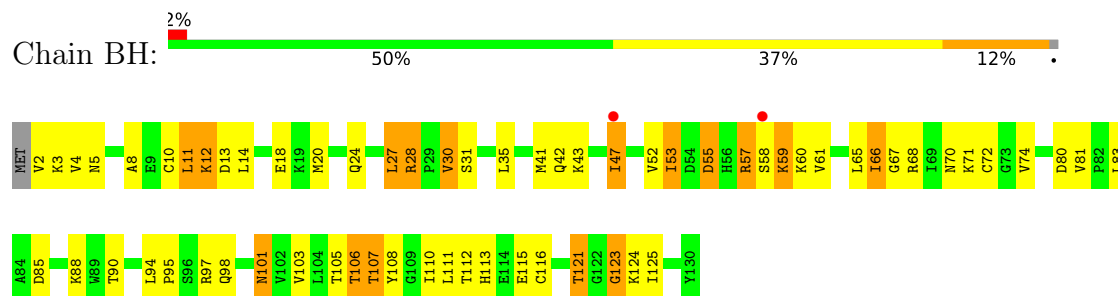
Chain DG: 13% 56% 32% 8%



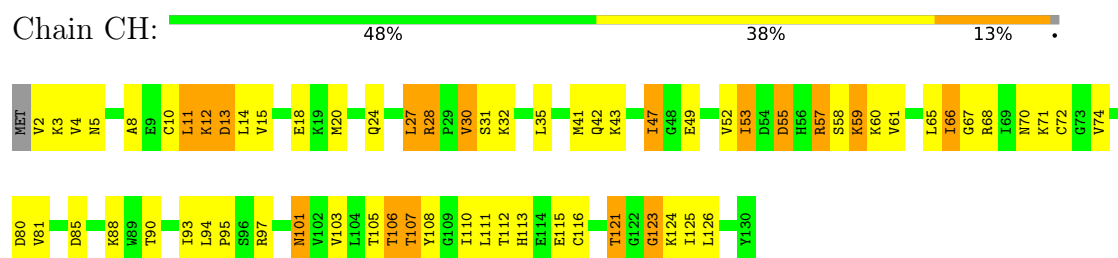
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E



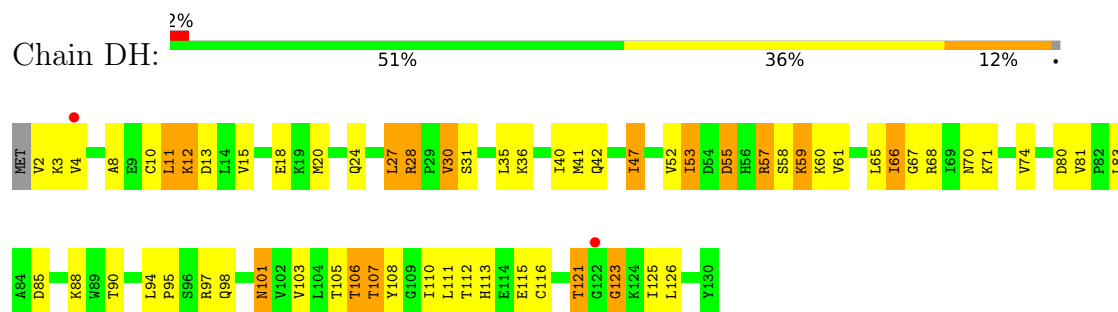
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E



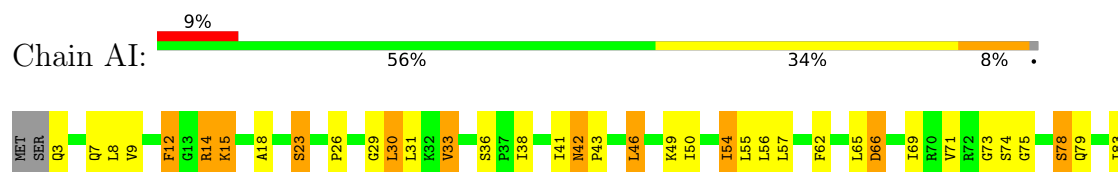
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E



- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

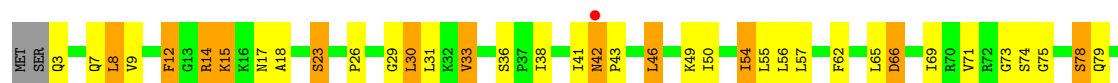


- Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E





• Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E



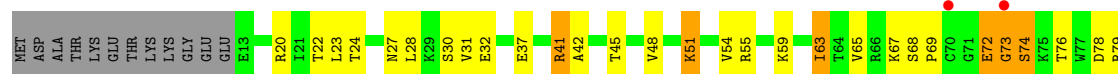
• Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E



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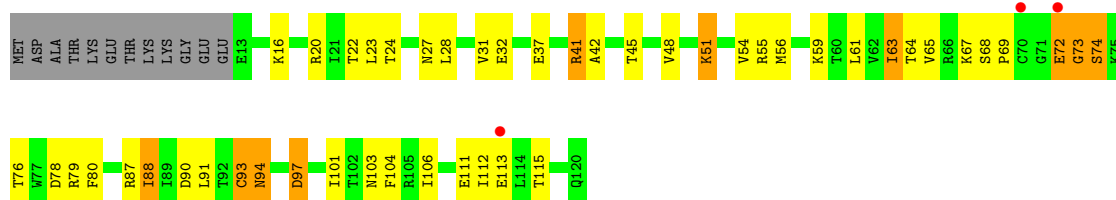


• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E



• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E





• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E



• Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E



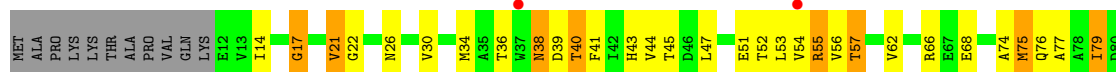
• Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E



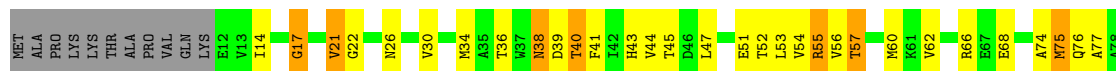
• Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E



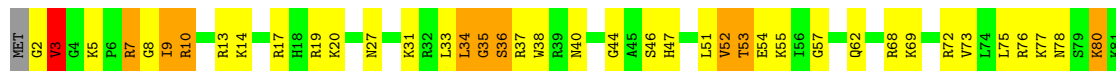
• Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E



• Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E



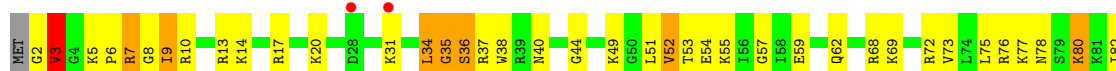
• Molecule 22: 40S RIBOSOMAL PROTEIN S12



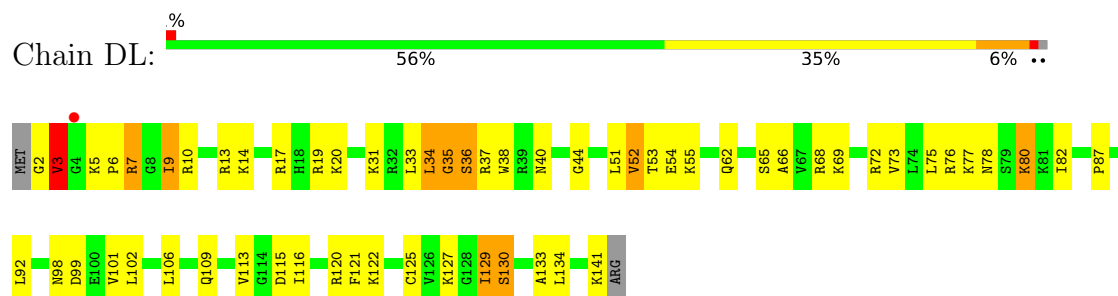
• Molecule 22: 40S RIBOSOMAL PROTEIN S12



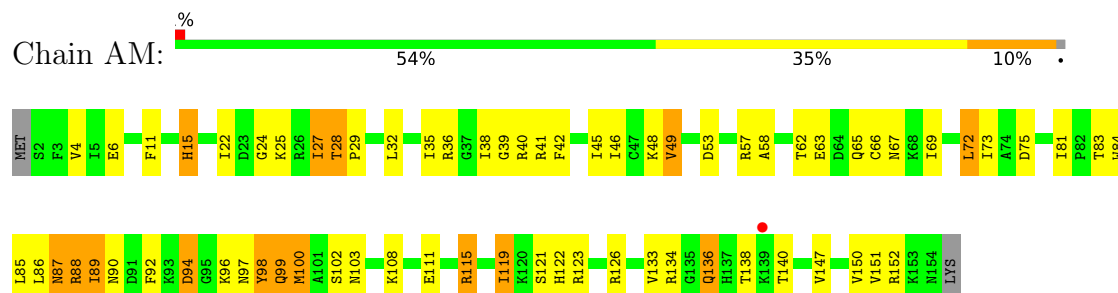
• Molecule 22: 40S RIBOSOMAL PROTEIN S12



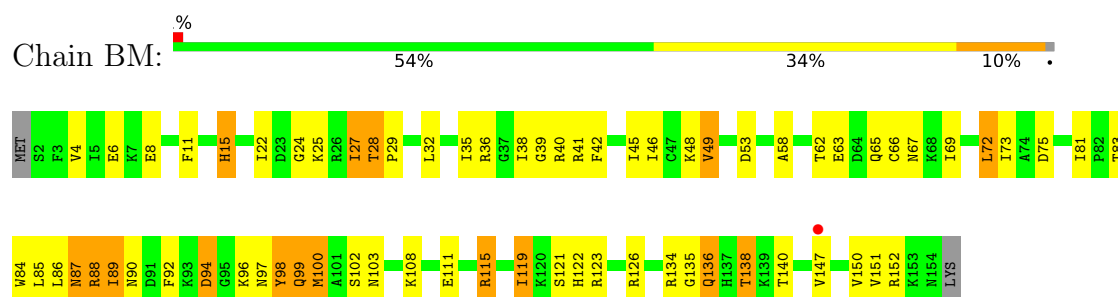
- Molecule 22: 40S RIBOSOMAL PROTEIN S12



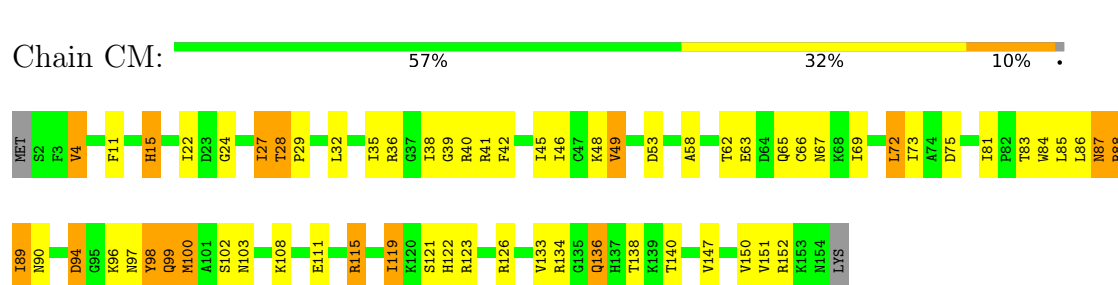
- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E



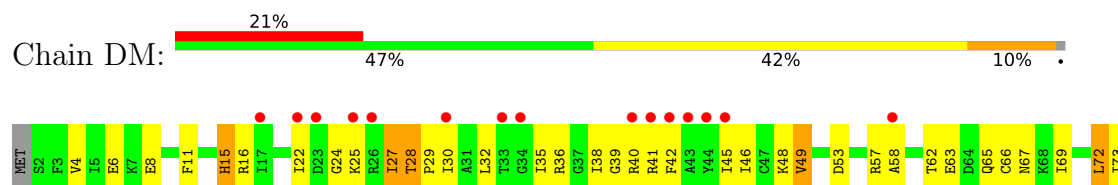
- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E



- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

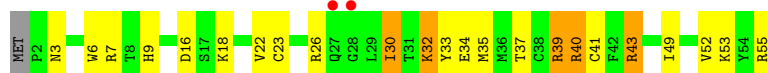


- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E





• Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E



• Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E



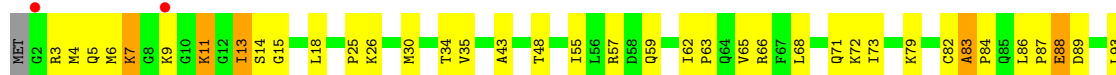
• Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E



• Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E

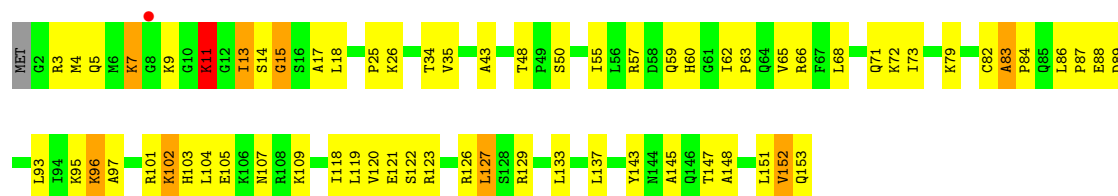


• Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E

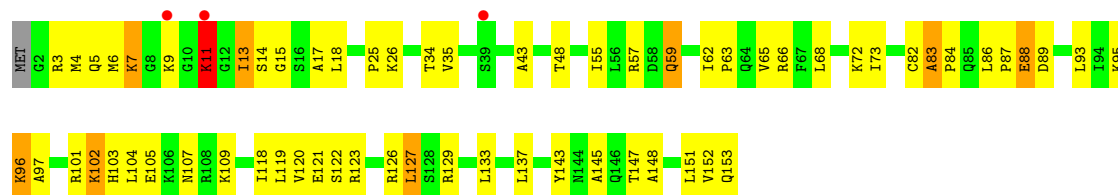


• Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E

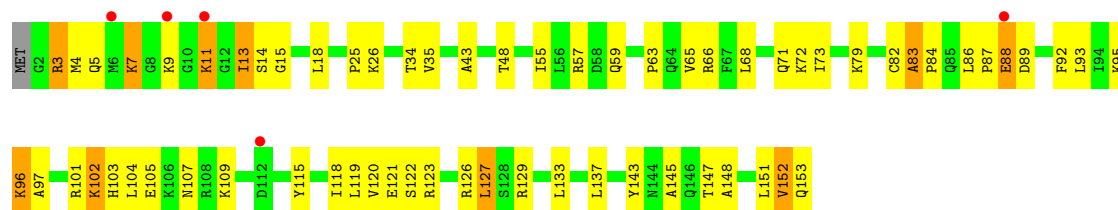




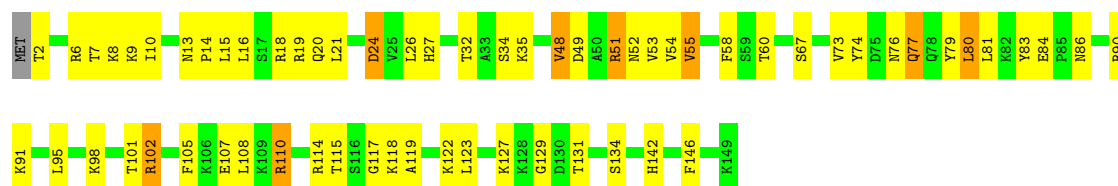
• Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E



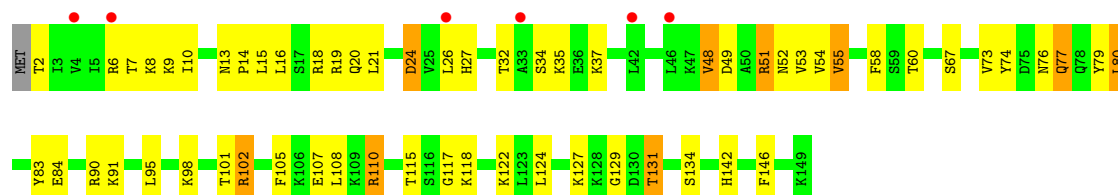
• Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E



• Molecule 26: 40S RIBOSOMAL PROTEIN S24



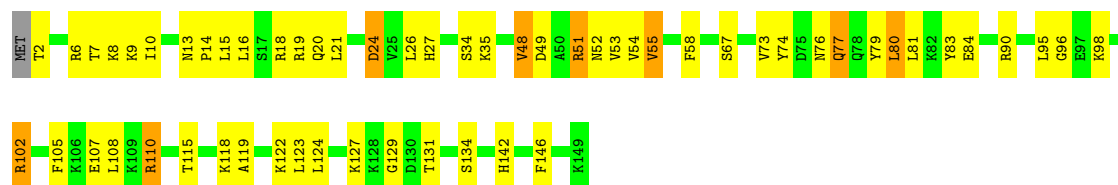
• Molecule 26: 40S RIBOSOMAL PROTEIN S24



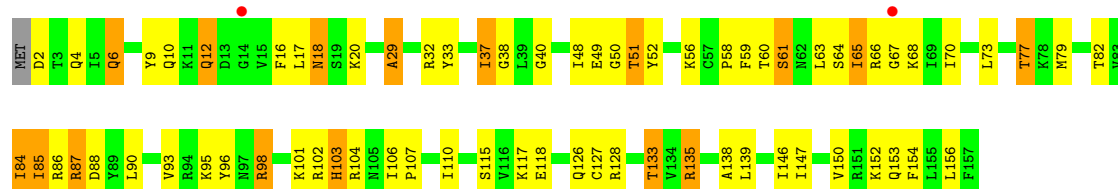
• Molecule 26: 40S RIBOSOMAL PROTEIN S24



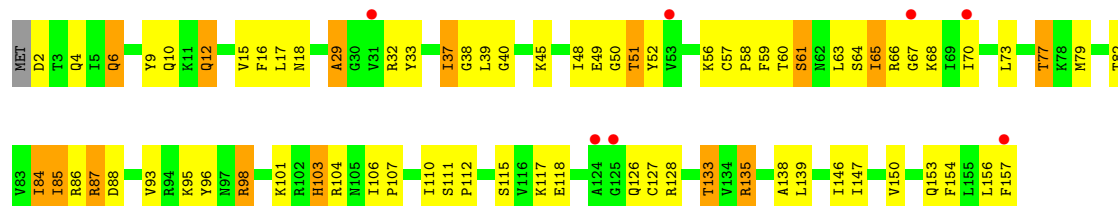
• Molecule 26: 40S RIBOSOMAL PROTEIN S24



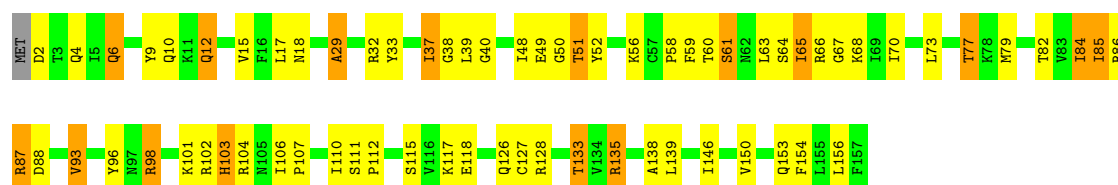
• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



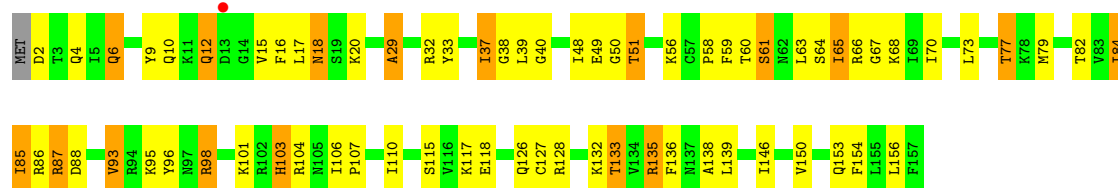
• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



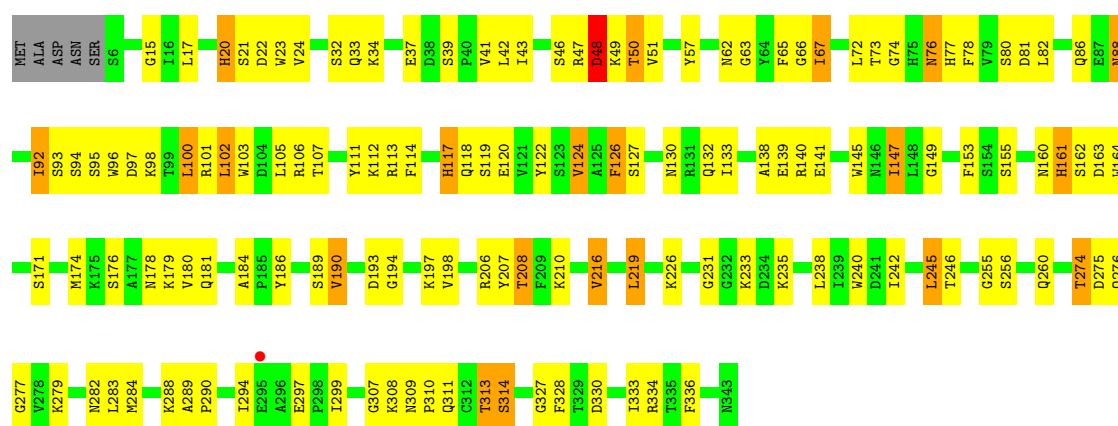
• Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



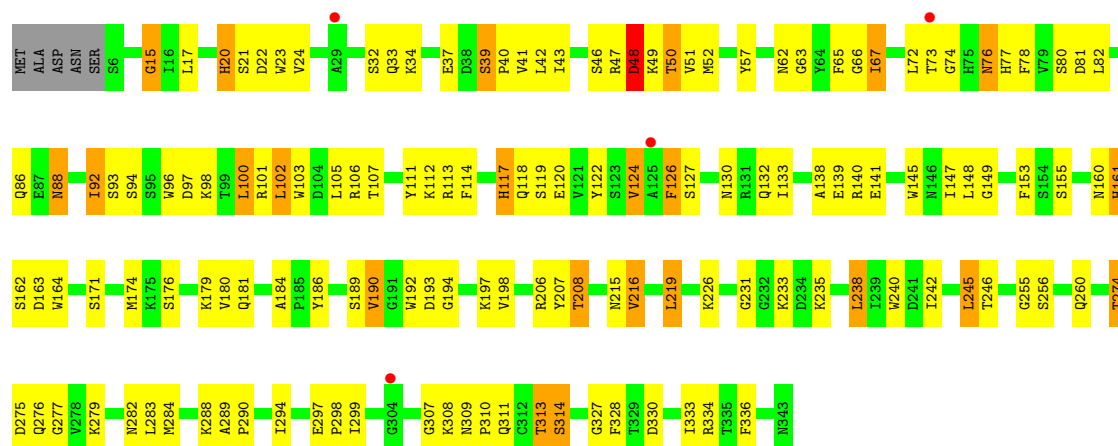
- Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E



- Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

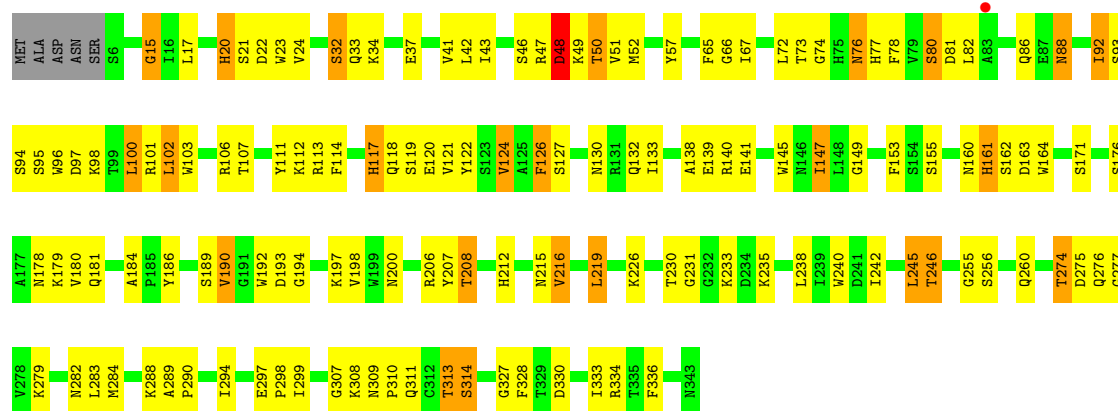


- Molecule 28: 40S RIBOSOMAL PROTEIN RACK1



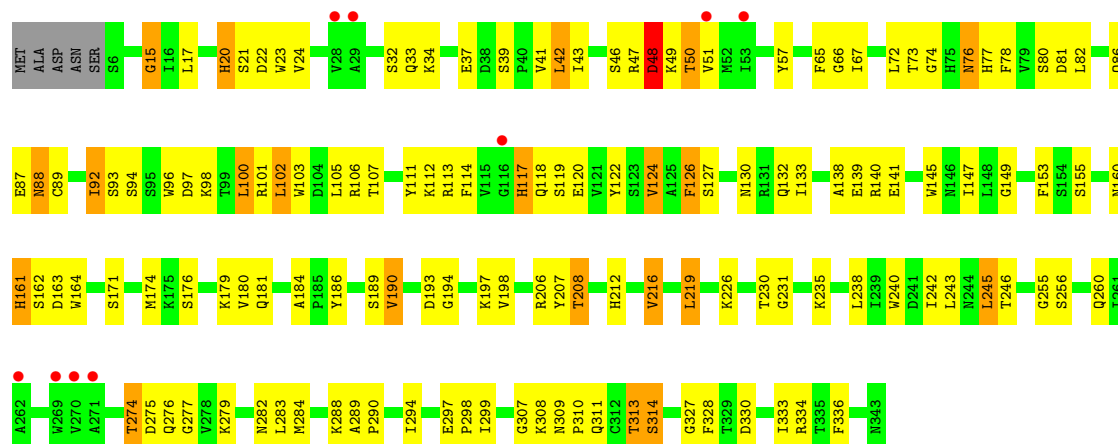
- Molecule 28: 40S RIBOSOMAL PROTEIN RACK1





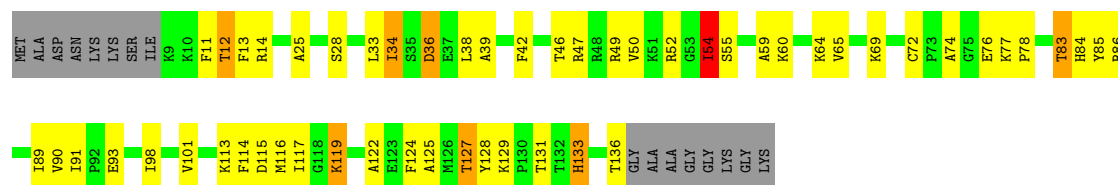
• Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

Chain DR: 3% 57% 35% 6% •



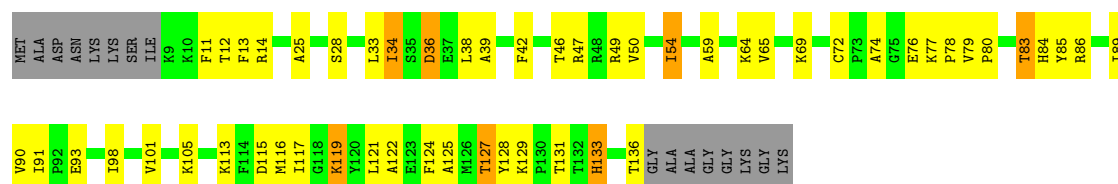
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain AS: 51% 32% 5% 11% •

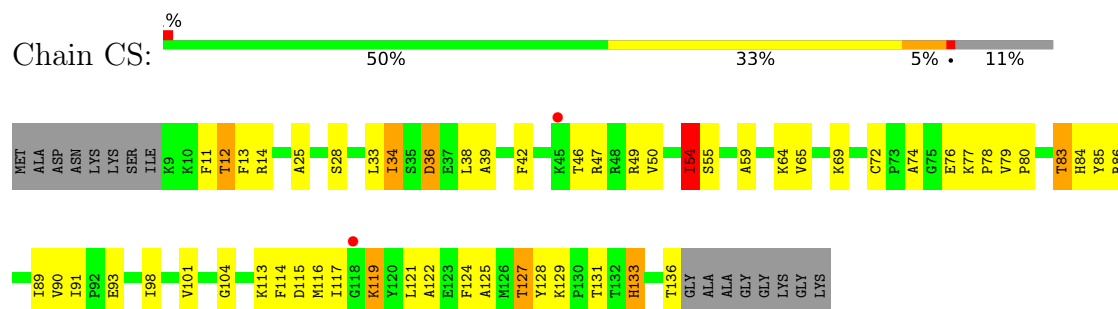


• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

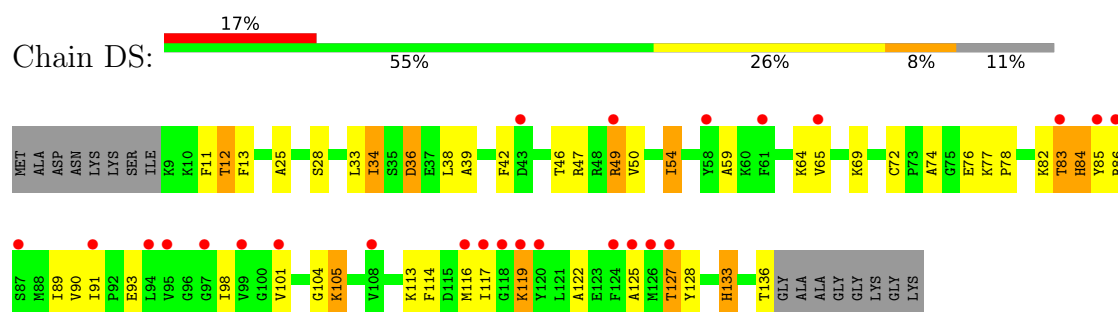
Chain BS: 51% 33% 5% 11% •



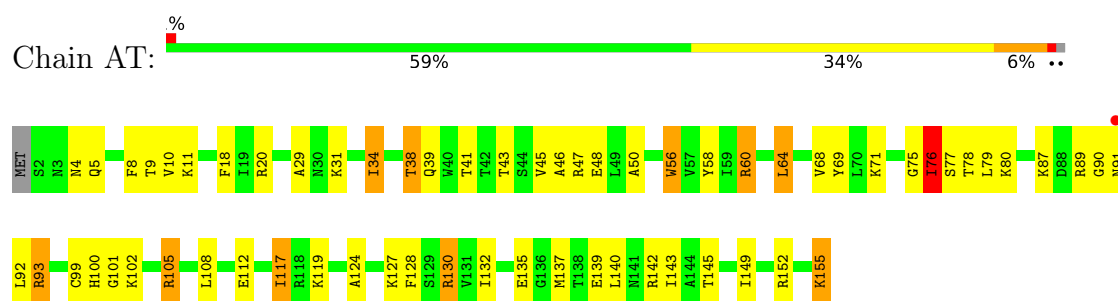
- Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E



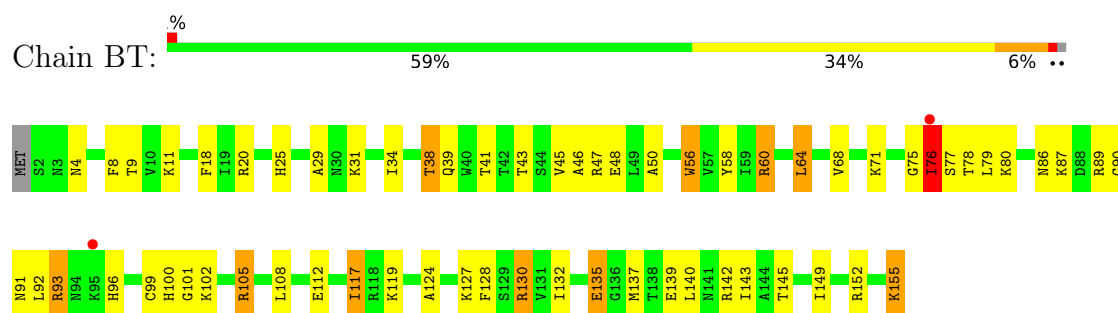
- Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E



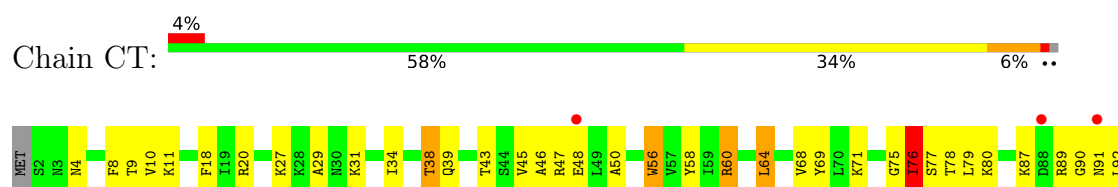
- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

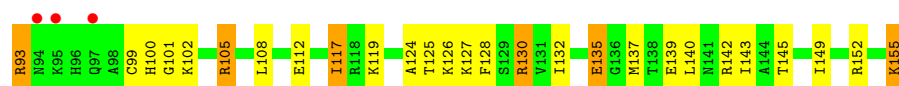


- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

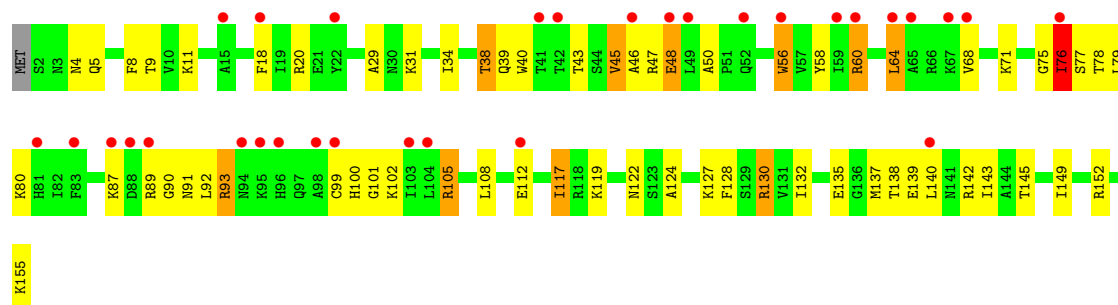


- Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

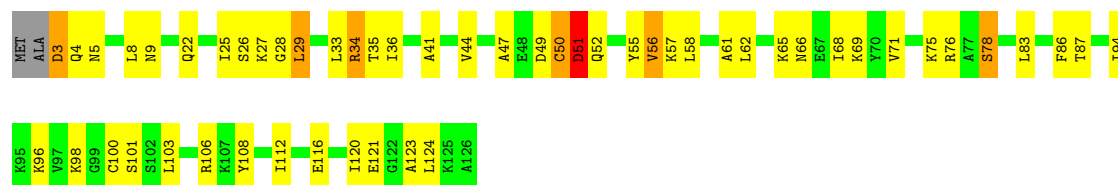




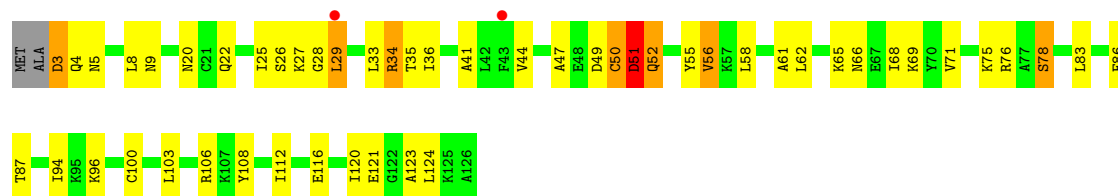
• Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E



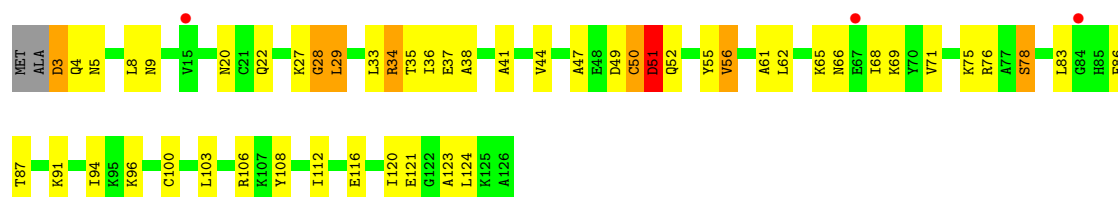
• Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E



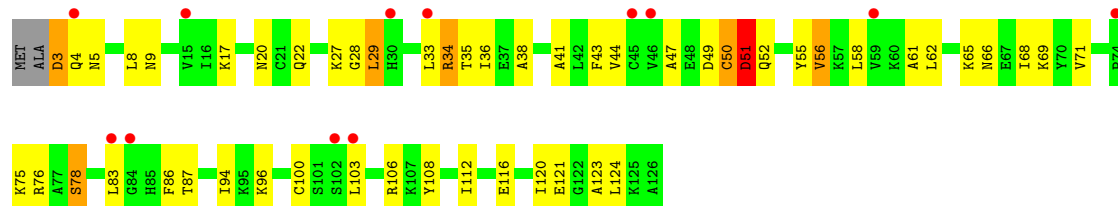
• Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E



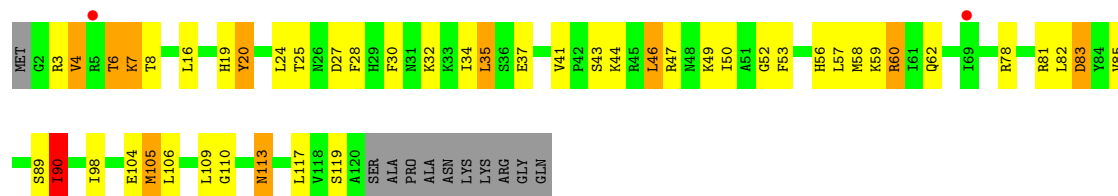
• Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E



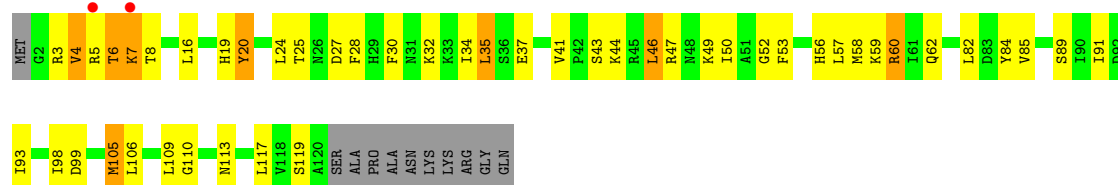
• Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E



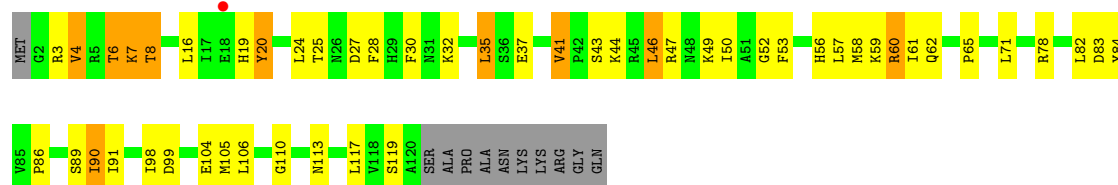
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E



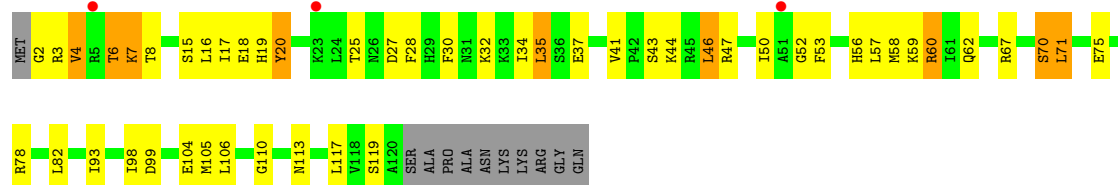
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E



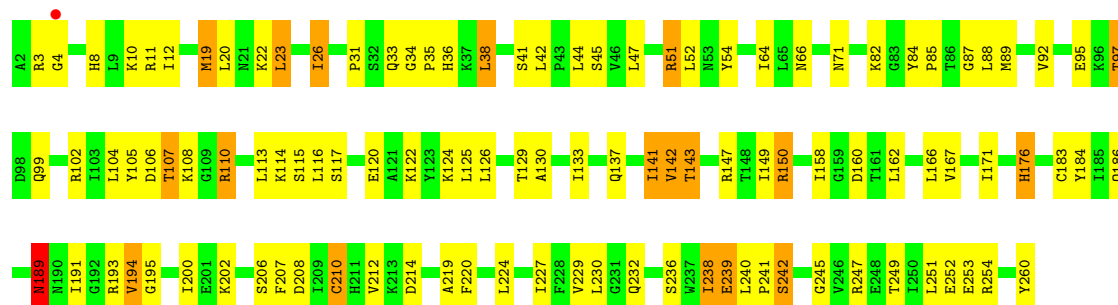
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E



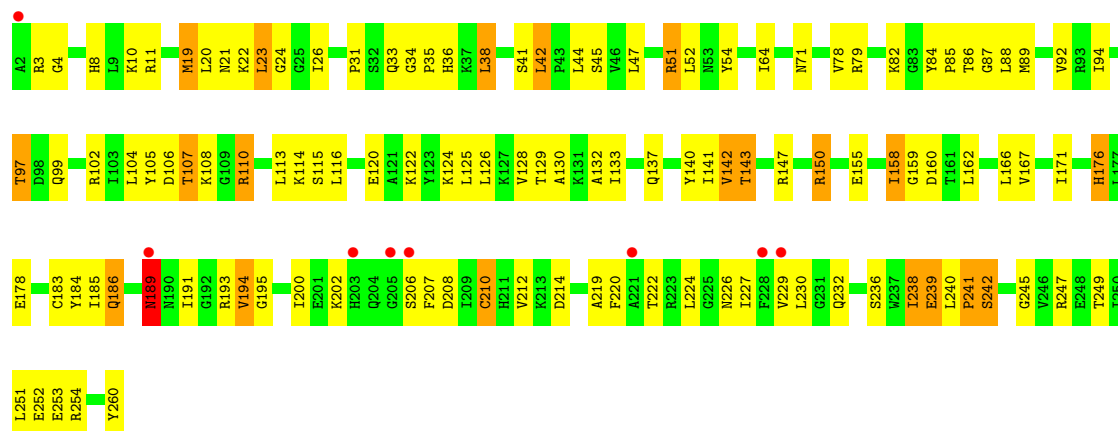
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E



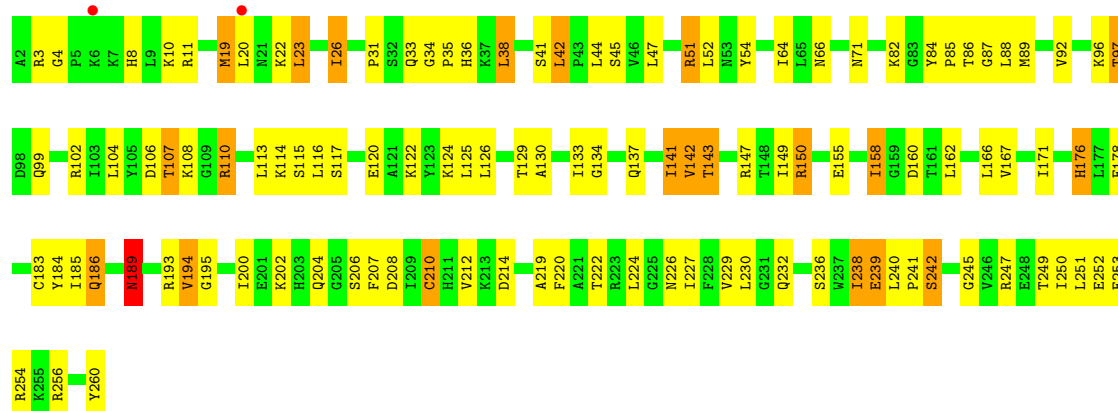
● Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

Chain AW: 

● Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

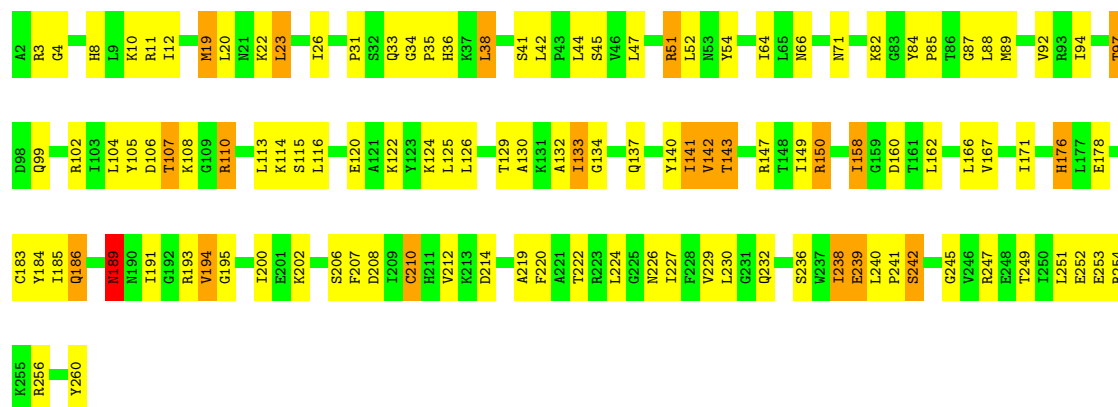
Chain BW: 

● Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

Chain CW: 

● Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

Chain DW: 



• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E



• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E



• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

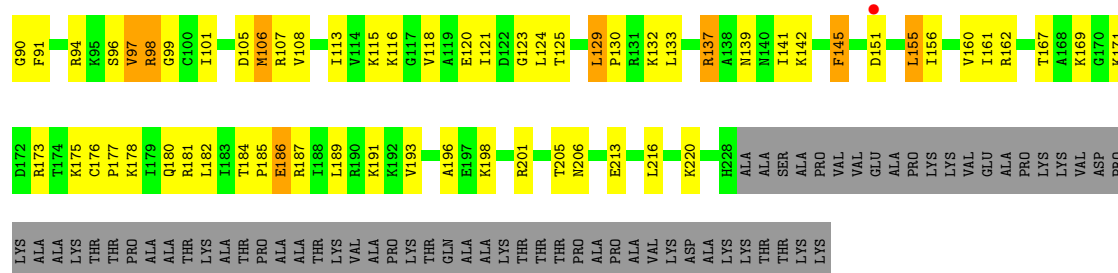


• Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E



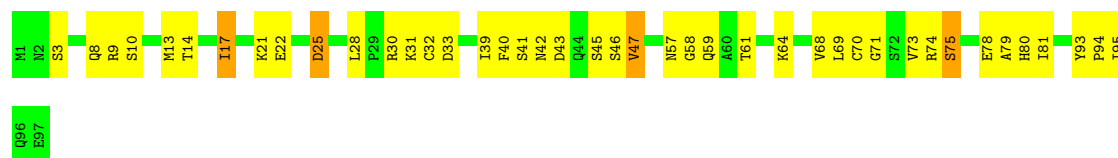
• Molecule 35: 40S RIBOSOMAL PROTEIN S6





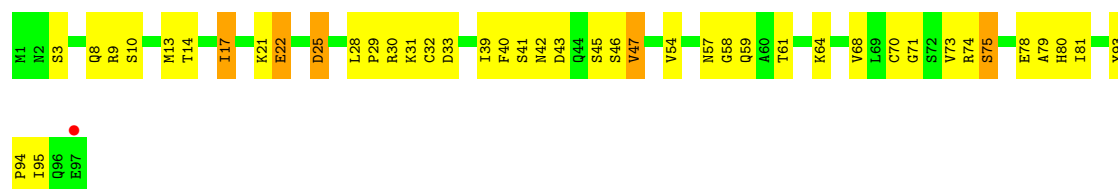
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain AZ: 57% 39%



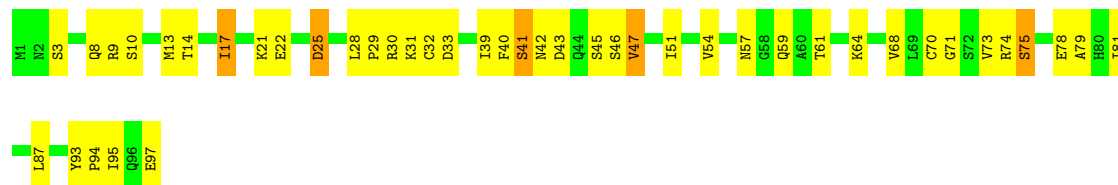
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain BZ: 56% 39% 5%



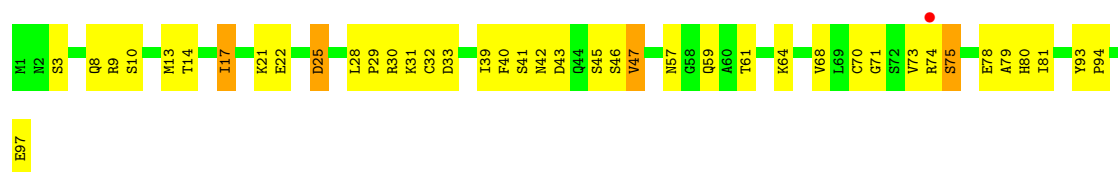
• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain CZ: 55% 40% 5%



• Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain DZ: 58% 38%



4 Data and refinement statistics

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 49.75 – 3.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.75-3.70) 90.8 (49.75-3.70)	Depositor EDS
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 0.222 , 0.248	Depositor DCC
R_{free} test set	5823 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	97.6	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 117.2	EDS
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
F_o, F_c correlation	0.92	EDS
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	0.35	0/827	0.90	1/1103 (0.1%)
1	B0	0.36	0/827	0.91	0/1103
1	C0	0.35	0/827	0.91	1/1103 (0.1%)
1	D0	0.35	0/827	0.90	0/1103
2	A1	0.41	0/510	1.03	1/677 (0.1%)
2	B1	0.39	0/510	1.01	1/677 (0.1%)
2	C1	0.41	0/510	1.04	1/677 (0.1%)
2	D1	0.37	0/510	1.02	1/677 (0.1%)
3	A2	0.45	0/1717	0.99	3/2288 (0.1%)
3	B2	0.44	0/1717	0.98	2/2288 (0.1%)
3	C2	0.43	0/1717	0.98	3/2288 (0.1%)
3	D2	0.42	0/1717	0.97	3/2288 (0.1%)
4	A3	0.43	0/1656	0.94	4/2223 (0.2%)
4	B3	0.43	0/1656	0.95	4/2223 (0.2%)
4	C3	0.41	0/1656	0.93	4/2223 (0.2%)
4	D3	0.39	0/1656	0.93	4/2223 (0.2%)
5	A4	0.54	0/1703	1.12	12/2284 (0.5%)
5	B4	0.49	0/1801	1.09	11/2417 (0.5%)
5	C4	0.43	0/1801	1.07	11/2417 (0.5%)
5	D4	0.58	4/1801 (0.2%)	1.09	10/2417 (0.4%)
6	A5	0.56	0/823	1.14	4/1100 (0.4%)
6	B5	0.54	0/823	1.14	6/1100 (0.5%)
6	C5	0.52	0/823	1.14	4/1100 (0.4%)
6	D5	0.48	0/823	1.12	4/1100 (0.4%)
7	A6	0.46	0/640	0.95	2/855 (0.2%)
7	B6	0.49	0/640	0.95	2/855 (0.2%)
7	C6	0.42	0/640	0.92	0/855
7	D6	0.41	0/640	0.92	0/855
8	A7	0.40	0/853	0.95	1/1148 (0.1%)
8	B7	0.43	0/853	0.94	1/1148 (0.1%)
8	C7	0.42	0/853	0.95	1/1148 (0.1%)
8	D7	0.40	0/853	0.96	1/1148 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	A8	0.41	0/620	1.00	0/831
9	B8	0.47	0/620	1.04	2/831 (0.2%)
9	C8	0.42	0/620	1.01	0/831
9	D8	0.41	0/620	1.00	0/831
10	A9	0.35	0/764	0.90	3/1007 (0.3%)
10	B9	0.35	0/764	0.92	4/1007 (0.4%)
10	C9	0.43	0/764	0.89	3/1007 (0.3%)
10	D9	0.43	0/764	1.12	7/1007 (0.7%)
11	AA	0.28	0/40993	0.59	12/63880 (0.0%)
11	BA	0.28	0/40993	0.58	13/63880 (0.0%)
11	CA	0.26	0/40993	0.58	14/63880 (0.0%)
11	DA	0.25	1/40993 (0.0%)	0.57	13/63880 (0.0%)
12	AB	0.43	0/1652	0.97	8/2240 (0.4%)
12	BB	0.42	0/1652	0.98	8/2240 (0.4%)
12	CB	0.42	0/1652	0.98	6/2240 (0.3%)
12	DB	0.40	0/1652	0.97	8/2240 (0.4%)
13	AC	0.42	0/1846	0.99	8/2479 (0.3%)
13	BC	0.43	0/1846	0.99	8/2479 (0.3%)
13	CC	0.44	0/1846	0.98	8/2479 (0.3%)
13	DC	0.40	0/1846	0.98	8/2479 (0.3%)
14	AD	0.44	0/1501	1.06	7/2003 (0.3%)
14	BD	0.43	0/1501	1.05	6/2003 (0.3%)
14	CD	0.42	0/1501	1.05	7/2003 (0.3%)
14	DD	0.43	0/1501	1.05	7/2003 (0.3%)
15	AE	0.50	0/1864	1.01	7/2521 (0.3%)
15	BE	0.48	0/1864	1.01	6/2521 (0.2%)
15	CE	0.46	0/1864	1.01	6/2521 (0.2%)
15	DE	0.46	0/1864	1.00	6/2521 (0.2%)
16	AF	0.40	0/751	0.94	2/1010 (0.2%)
16	BF	0.40	0/751	0.93	2/1010 (0.2%)
16	CF	0.38	0/751	0.93	3/1010 (0.3%)
16	DF	0.40	0/751	0.94	3/1010 (0.3%)
17	AG	0.43	0/1546	1.06	10/2079 (0.5%)
17	BG	0.43	0/1546	1.06	10/2079 (0.5%)
17	CG	0.42	0/1546	1.06	10/2079 (0.5%)
17	DG	0.40	0/1546	1.07	10/2079 (0.5%)
18	AH	0.52	0/1058	1.14	8/1421 (0.6%)
18	BH	0.53	0/1058	1.14	7/1421 (0.5%)
18	CH	0.48	0/1058	1.14	8/1421 (0.6%)
18	DH	0.45	0/1058	1.12	6/1421 (0.4%)
19	AI	0.45	0/1151	1.01	4/1540 (0.3%)
19	BI	0.45	0/1151	1.00	5/1540 (0.3%)
19	CI	0.46	0/1151	1.03	7/1540 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	DI	0.42	0/1151	1.01	6/1540 (0.4%)
20	AJ	0.46	0/868	1.03	2/1168 (0.2%)
20	BJ	0.48	0/868	1.03	4/1168 (0.3%)
20	CJ	0.44	0/868	1.02	4/1168 (0.3%)
20	DJ	0.44	0/868	1.02	2/1168 (0.2%)
21	AK	0.51	0/1078	1.14	7/1452 (0.5%)
21	BK	0.48	0/1078	1.12	7/1452 (0.5%)
21	CK	0.46	0/1078	1.12	7/1452 (0.5%)
21	DK	0.44	0/1078	1.12	7/1452 (0.5%)
22	AL	0.46	0/1103	1.02	3/1471 (0.2%)
22	BL	0.47	0/1103	1.03	2/1471 (0.1%)
22	CL	0.45	0/1103	0.99	1/1471 (0.1%)
22	DL	0.44	0/1103	1.02	2/1471 (0.1%)
23	AM	0.38	0/1252	1.01	5/1680 (0.3%)
23	BM	0.39	0/1252	1.01	5/1680 (0.3%)
23	CM	0.37	0/1252	1.00	5/1680 (0.3%)
23	DM	0.37	0/1252	1.00	5/1680 (0.3%)
24	AN	0.39	0/465	0.92	1/619 (0.2%)
24	BN	0.41	0/465	0.92	1/619 (0.2%)
24	CN	0.37	0/465	0.90	1/619 (0.2%)
24	DN	0.38	0/465	0.92	1/619 (0.2%)
25	AO	0.47	0/1253	1.02	5/1677 (0.3%)
25	BO	0.46	0/1253	1.01	6/1677 (0.4%)
25	CO	0.43	0/1253	1.00	5/1677 (0.3%)
25	DO	0.42	0/1253	1.00	5/1677 (0.3%)
26	AP	0.39	0/1215	0.95	1/1626 (0.1%)
26	BP	0.39	0/1215	0.91	0/1626
26	CP	0.39	0/1215	0.91	0/1626
26	DP	0.39	0/1215	0.92	1/1626 (0.1%)
27	AQ	0.48	0/1290	1.05	7/1731 (0.4%)
27	BQ	0.45	0/1290	1.05	7/1731 (0.4%)
27	CQ	0.45	0/1290	1.04	7/1731 (0.4%)
27	DQ	0.41	0/1290	1.03	6/1731 (0.3%)
28	AR	0.39	0/2750	1.00	12/3726 (0.3%)
28	BR	0.39	0/2750	1.00	13/3726 (0.3%)
28	CR	0.39	0/2750	1.00	11/3726 (0.3%)
28	DR	0.37	0/2750	0.99	13/3726 (0.3%)
29	AS	0.35	0/1028	0.86	1/1374 (0.1%)
29	BS	0.36	0/1028	0.86	1/1374 (0.1%)
29	CS	0.37	0/1028	0.87	1/1374 (0.1%)
29	DS	0.36	0/1028	0.87	1/1374 (0.1%)
30	AT	0.44	0/1264	0.92	3/1698 (0.2%)
30	BT	0.45	0/1264	0.94	3/1698 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CT	0.40	0/1264	0.93	3/1698 (0.2%)
30	DT	0.41	0/1264	0.93	3/1698 (0.2%)
31	AU	0.38	0/961	0.92	1/1288 (0.1%)
31	BU	0.39	0/961	0.92	2/1288 (0.2%)
31	CU	0.38	0/961	0.92	2/1288 (0.2%)
31	DU	0.39	0/961	0.92	1/1288 (0.1%)
32	AV	0.44	0/981	1.01	7/1311 (0.5%)
32	BV	0.41	0/981	0.96	4/1311 (0.3%)
32	CV	0.43	0/981	0.97	4/1311 (0.3%)
32	DV	0.41	0/981	0.96	4/1311 (0.3%)
33	AW	0.46	0/2119	0.97	12/2849 (0.4%)
33	BW	0.42	0/2119	0.97	12/2849 (0.4%)
33	CW	0.42	0/2119	0.96	12/2849 (0.4%)
33	DW	0.43	0/2119	0.97	12/2849 (0.4%)
34	AX	0.39	0/612	1.01	3/812 (0.4%)
34	BX	0.37	0/612	1.01	3/812 (0.4%)
34	CX	0.36	0/612	1.01	3/812 (0.4%)
34	DX	0.36	0/612	1.02	3/812 (0.4%)
35	AY	0.38	0/1852	0.90	2/2462 (0.1%)
35	BY	0.39	0/1852	0.90	3/2462 (0.1%)
35	CY	0.38	0/1852	0.90	2/2462 (0.1%)
35	DY	0.38	0/1852	0.90	2/2462 (0.1%)
36	AZ	0.48	0/755	0.97	2/1013 (0.2%)
36	BZ	0.48	0/755	0.98	2/1013 (0.2%)
36	CZ	0.46	0/755	0.98	3/1013 (0.3%)
36	DZ	0.44	0/755	0.97	2/1013 (0.2%)
All	All	0.36	5/333578 (0.0%)	0.80	679/482983 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D4	31	TRP	NE1-CE2	-12.55	1.23	1.37
5	D4	31	TRP	CD1-NE1	6.91	1.52	1.37
11	DA	1586	A	O3'-P	6.08	1.70	1.61
5	D4	31	TRP	CG-CD2	6.05	1.54	1.43
5	D4	31	TRP	CD2-CE2	5.36	1.50	1.41

The worst 5 of 679 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B9	120	GLY	N-CA-C	12.22	130.00	115.09
6	C5	99	PRO	N-CA-C	10.61	123.64	110.70
6	A5	99	PRO	N-CA-C	10.54	123.55	110.70
6	B5	99	PRO	N-CA-C	10.46	123.46	110.70
5	A4	73	ALA	N-CA-C	-10.46	100.00	113.17

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 ⓘ

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	26	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	34	0
1	D0	817	0	829	31	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	76	1
3	B2	1693	0	1795	61	0
3	C2	1693	0	1795	66	0
3	D2	1693	0	1795	68	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	57	0
5	A4	1679	0	1762	59	0
5	B4	1775	0	1851	64	0
5	C4	1775	0	1851	58	0
5	D4	1775	0	1851	66	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	30	0
7	B6	632	0	646	34	1
7	C6	632	0	646	32	0
7	D6	632	0	646	36	0
8	A7	833	0	844	37	0
8	B7	833	0	844	29	0
8	C7	833	0	844	36	0
8	D7	833	0	844	48	0
9	A8	615	0	660	26	0
9	B8	615	0	660	29	1
9	C8	615	0	660	21	0
9	D8	615	0	660	36	0
10	A9	751	0	807	54	0
10	B9	751	0	809	74	0
10	C9	751	0	809	41	0
10	D9	751	0	809	56	0
11	AA	36629	0	18413	1089	0
11	BA	36629	0	18413	1125	3
11	CA	36629	0	18413	1066	2
11	DA	36629	0	18413	1116	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AB	1619	0	1623	73	0
12	BB	1619	0	1623	81	0
12	CB	1619	0	1623	69	0
12	DB	1619	0	1623	62	0
13	AC	1811	0	1907	69	0
13	BC	1811	0	1907	68	0
13	CC	1811	0	1907	80	0
13	DC	1811	0	1907	88	0
14	AD	1478	0	1569	76	0
14	BD	1478	0	1569	76	0
14	CD	1478	0	1569	69	0
14	DD	1478	0	1569	68	0
15	AE	1818	0	1853	77	0
15	BE	1818	0	1853	76	0
15	CE	1818	0	1853	82	0
15	DE	1818	0	1853	79	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	61	0
17	BG	1520	0	1572	60	0
17	CG	1520	0	1572	56	0
17	DG	1520	0	1572	56	0
18	AH	1040	0	1096	42	0
18	BH	1040	0	1096	43	0
18	CH	1040	0	1096	50	0
18	DH	1040	0	1096	43	0
19	AI	1135	0	1204	47	0
19	BI	1135	0	1204	50	0
19	CI	1135	0	1204	49	0
19	DI	1135	0	1204	51	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	50	0
22	BL	1086	0	1156	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CL	1086	0	1156	49	0
22	DL	1086	0	1156	46	0
23	AM	1231	0	1276	59	0
23	BM	1231	0	1276	62	0
23	CM	1231	0	1276	56	0
23	DM	1231	0	1276	78	0
24	AN	454	0	453	34	0
24	BN	454	0	453	32	0
24	CN	454	0	453	28	0
24	DN	454	0	453	33	0
25	AO	1229	0	1338	50	0
25	BO	1229	0	1338	50	0
25	CO	1229	0	1338	49	0
25	DO	1229	0	1338	50	0
26	AP	1197	0	1285	47	0
26	BP	1197	0	1285	52	0
26	CP	1197	0	1285	45	1
26	DP	1197	0	1285	45	0
27	AQ	1267	0	1342	62	0
27	BQ	1267	0	1342	61	0
27	CQ	1267	0	1342	55	0
27	DQ	1267	0	1342	59	0
28	AR	2682	0	2629	106	0
28	BR	2682	0	2629	108	0
28	CR	2682	0	2629	120	0
28	DR	2682	0	2629	103	0
29	AS	1010	0	1059	45	0
29	BS	1010	0	1059	41	0
29	CS	1010	0	1059	41	0
29	DS	1010	0	1059	41	0
30	AT	1242	0	1290	52	0
30	BT	1242	0	1290	58	0
30	CT	1242	0	1290	50	0
30	DT	1242	0	1290	53	1
31	AU	952	0	993	51	0
31	BU	952	0	993	44	0
31	CU	952	0	993	38	0
31	DU	952	0	993	47	0
32	AV	968	0	1031	41	0
32	BV	968	0	1031	45	0
32	CV	968	0	1031	43	0
32	DV	968	0	1031	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AW	2079	0	2151	89	0
33	BW	2079	0	2151	96	0
33	CW	2079	0	2151	93	0
33	DW	2079	0	2151	91	0
34	AX	599	0	651	19	0
34	BX	599	0	651	22	0
34	CX	599	0	651	22	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	68	0
35	DY	1826	0	1954	81	0
36	AZ	747	0	758	31	0
36	BZ	747	0	758	33	0
36	CZ	747	0	758	32	0
36	DZ	747	0	758	29	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	9661	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 9661 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%)	12	43
5	B4	219/265 (83%)	202 (92%)	14 (6%)	3 (1%)	9	37
5	C4	219/265 (83%)	203 (93%)	13 (6%)	3 (1%)	9	37
5	D4	219/265 (83%)	203 (93%)	13 (6%)	3 (1%)	9	37
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%)	9	38
7	B6	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	9	38
7	C6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	9	38
7	D6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	9	38
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%)	11	42
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%)	30	60
15	BE	227/296 (77%)	212 (93%)	14 (6%)	1 (0%)	30	60
15	CE	227/296 (77%)	211 (93%)	15 (7%)	1 (0%)	30	60
15	DE	227/296 (77%)	212 (93%)	14 (6%)	1 (0%)	30	60
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%)	24	56
17	BG	190/200 (95%)	178 (94%)	12 (6%)	0	100	100
17	CG	190/200 (95%)	179 (94%)	9 (5%)	2 (1%)	11	42
17	DG	190/200 (95%)	178 (94%)	10 (5%)	2 (1%)	11	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	16	48
18	BH	127/130 (98%)	111 (87%)	15 (12%)	1 (1%)	16	48
18	CH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	16	48
18	DH	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	16	48
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%)	9	37
22	BL	138/142 (97%)	126 (91%)	10 (7%)	2 (1%)	9	37
22	CL	138/142 (97%)	127 (92%)	9 (6%)	2 (1%)	9	37
22	DL	138/142 (97%)	125 (91%)	11 (8%)	2 (1%)	9	37
23	AM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	9	38
23	BM	151/155 (97%)	139 (92%)	10 (7%)	2 (1%)	9	38
23	CM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	9	38
23	DM	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	9	38
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%)	18	50
25	BO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	18	50
25	CO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	18	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	DO	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	18	50
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%)	21	52
28	BR	336/343 (98%)	308 (92%)	26 (8%)	2 (1%)	21	52
28	CR	336/343 (98%)	308 (92%)	26 (8%)	2 (1%)	21	52
28	DR	336/343 (98%)	307 (91%)	27 (8%)	2 (1%)	21	52
29	AS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	16	48
29	BS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	16	48
29	CS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	16	48
29	DS	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	16	48
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%)	14	45
32	DV	117/130 (90%)	115 (98%)	1 (1%)	1 (1%)	14	45
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%)	30	60
35	BY	226/293 (77%)	214 (95%)	10 (4%)	2 (1%)	14	45
35	CY	226/293 (77%)	214 (95%)	11 (5%)	1 (0%)	30	60
35	DY	226/293 (77%)	215 (95%)	10 (4%)	1 (0%)	30	60
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%)	36	65

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%)	81 (90%)	9 (10%)	7	30
1	B0	90/192 (47%)	81 (90%)	9 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C0	90/192 (47%)	81 (90%)	9 (10%)	7	30
1	D0	90/192 (47%)	81 (90%)	9 (10%)	7	30
2	A1	55/57 (96%)	43 (78%)	12 (22%)	1	7
2	B1	55/57 (96%)	44 (80%)	11 (20%)	1	9
2	C1	55/57 (96%)	43 (78%)	12 (22%)	1	7
2	D1	55/57 (96%)	43 (78%)	12 (22%)	1	7
3	A2	184/185 (100%)	154 (84%)	30 (16%)	2	14
3	B2	184/185 (100%)	154 (84%)	30 (16%)	2	14
3	C2	184/185 (100%)	155 (84%)	29 (16%)	2	15
3	D2	184/185 (100%)	154 (84%)	30 (16%)	2	14
4	A3	182/183 (100%)	151 (83%)	31 (17%)	2	13
4	B3	182/183 (100%)	151 (83%)	31 (17%)	2	13
4	C3	182/183 (100%)	151 (83%)	31 (17%)	2	13
4	D3	182/183 (100%)	151 (83%)	31 (17%)	2	13
5	A4	187/225 (83%)	155 (83%)	32 (17%)	2	13
5	B4	197/225 (88%)	165 (84%)	32 (16%)	2	14
5	C4	197/225 (88%)	164 (83%)	33 (17%)	2	13
5	D4	197/225 (88%)	164 (83%)	33 (17%)	2	13
6	A5	90/107 (84%)	74 (82%)	16 (18%)	2	12
6	B5	90/107 (84%)	74 (82%)	16 (18%)	2	12
6	C5	90/107 (84%)	74 (82%)	16 (18%)	2	12
6	D5	90/107 (84%)	73 (81%)	17 (19%)	1	10
7	A6	71/72 (99%)	60 (84%)	11 (16%)	2	15
7	B6	71/72 (99%)	59 (83%)	12 (17%)	2	13
7	C6	71/72 (99%)	60 (84%)	11 (16%)	2	15
7	D6	71/72 (99%)	60 (84%)	11 (16%)	2	15
8	A7	91/136 (67%)	82 (90%)	9 (10%)	7	30
8	B7	91/136 (67%)	82 (90%)	9 (10%)	7	30
8	C7	91/136 (67%)	82 (90%)	9 (10%)	7	30
8	D7	91/136 (67%)	82 (90%)	9 (10%)	7	30
9	A8	70/109 (64%)	59 (84%)	11 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B8	70/109 (64%)	59 (84%)	11 (16%)	2	15
9	C8	70/109 (64%)	59 (84%)	11 (16%)	2	15
9	D8	70/109 (64%)	59 (84%)	11 (16%)	2	15
10	A9	81/156 (52%)	75 (93%)	6 (7%)	13	39
10	B9	81/156 (52%)	77 (95%)	4 (5%)	22	48
10	C9	81/156 (52%)	75 (93%)	6 (7%)	13	39
10	D9	81/156 (52%)	71 (88%)	10 (12%)	4	22
12	AB	180/211 (85%)	159 (88%)	21 (12%)	5	24
12	BB	180/211 (85%)	159 (88%)	21 (12%)	5	24
12	CB	180/211 (85%)	159 (88%)	21 (12%)	5	24
12	DB	180/211 (85%)	159 (88%)	21 (12%)	5	24
13	AC	196/210 (93%)	178 (91%)	18 (9%)	8	32
13	BC	196/210 (93%)	178 (91%)	18 (9%)	8	32
13	CC	196/210 (93%)	179 (91%)	17 (9%)	9	34
13	DC	196/210 (93%)	179 (91%)	17 (9%)	9	34
14	AD	161/162 (99%)	126 (78%)	35 (22%)	1	7
14	BD	161/162 (99%)	126 (78%)	35 (22%)	1	7
14	CD	161/162 (99%)	126 (78%)	35 (22%)	1	7
14	DD	161/162 (99%)	126 (78%)	35 (22%)	1	7
15	AE	193/250 (77%)	164 (85%)	29 (15%)	3	16
15	BE	193/250 (77%)	165 (86%)	28 (14%)	3	17
15	CE	193/250 (77%)	165 (86%)	28 (14%)	3	17
15	DE	193/250 (77%)	166 (86%)	27 (14%)	3	18
16	AF	80/92 (87%)	73 (91%)	7 (9%)	9	33
16	BF	80/92 (87%)	73 (91%)	7 (9%)	9	33
16	CF	80/92 (87%)	73 (91%)	7 (9%)	9	33
16	DF	80/92 (87%)	73 (91%)	7 (9%)	9	33
17	AG	163/169 (96%)	141 (86%)	22 (14%)	4	20
17	BG	163/169 (96%)	140 (86%)	23 (14%)	3	18
17	CG	163/169 (96%)	139 (85%)	24 (15%)	3	17
17	DG	163/169 (96%)	141 (86%)	22 (14%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AH	116/117 (99%)	94 (81%)	22 (19%)	1	10
18	BH	116/117 (99%)	94 (81%)	22 (19%)	1	10
18	CH	116/117 (99%)	94 (81%)	22 (19%)	1	10
18	DH	116/117 (99%)	94 (81%)	22 (19%)	1	10
19	AI	120/122 (98%)	102 (85%)	18 (15%)	3	16
19	BI	120/122 (98%)	102 (85%)	18 (15%)	3	16
19	CI	120/122 (98%)	102 (85%)	18 (15%)	3	16
19	DI	120/122 (98%)	102 (85%)	18 (15%)	3	16
20	AJ	101/111 (91%)	87 (86%)	14 (14%)	3	19
20	BJ	101/111 (91%)	87 (86%)	14 (14%)	3	19
20	CJ	101/111 (91%)	87 (86%)	14 (14%)	3	19
20	DJ	101/111 (91%)	87 (86%)	14 (14%)	3	19
21	AK	112/121 (93%)	97 (87%)	15 (13%)	4	20
21	BK	112/121 (93%)	96 (86%)	16 (14%)	3	18
21	CK	112/121 (93%)	96 (86%)	16 (14%)	3	18
21	DK	112/121 (93%)	97 (87%)	15 (13%)	4	20
22	AL	112/114 (98%)	95 (85%)	17 (15%)	3	16
22	BL	112/114 (98%)	95 (85%)	17 (15%)	3	16
22	CL	112/114 (98%)	95 (85%)	17 (15%)	3	16
22	DL	112/114 (98%)	96 (86%)	16 (14%)	3	18
23	AM	133/135 (98%)	113 (85%)	20 (15%)	3	16
23	BM	133/135 (98%)	113 (85%)	20 (15%)	3	16
23	CM	133/135 (98%)	113 (85%)	20 (15%)	3	16
23	DM	133/135 (98%)	113 (85%)	20 (15%)	3	16
24	AN	48/49 (98%)	41 (85%)	7 (15%)	3	17
24	BN	48/49 (98%)	41 (85%)	7 (15%)	3	17
24	CN	48/49 (98%)	40 (83%)	8 (17%)	2	14
24	DN	48/49 (98%)	40 (83%)	8 (17%)	2	14
25	AO	135/136 (99%)	115 (85%)	20 (15%)	3	17
25	BO	135/136 (99%)	115 (85%)	20 (15%)	3	17
25	CO	135/136 (99%)	115 (85%)	20 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	DO	135/136 (99%)	115 (85%)	20 (15%)	3	17
26	AP	133/134 (99%)	115 (86%)	18 (14%)	4	20
26	BP	133/134 (99%)	114 (86%)	19 (14%)	3	18
26	CP	133/134 (99%)	115 (86%)	18 (14%)	4	20
26	DP	133/134 (99%)	115 (86%)	18 (14%)	4	20
27	AQ	140/141 (99%)	122 (87%)	18 (13%)	4	21
27	BQ	140/141 (99%)	122 (87%)	18 (13%)	4	21
27	CQ	140/141 (99%)	122 (87%)	18 (13%)	4	21
27	DQ	140/141 (99%)	122 (87%)	18 (13%)	4	21
28	AR	291/295 (99%)	259 (89%)	32 (11%)	6	26
28	BR	291/295 (99%)	260 (89%)	31 (11%)	6	27
28	CR	291/295 (99%)	260 (89%)	31 (11%)	6	27
28	DR	291/295 (99%)	260 (89%)	31 (11%)	6	27
29	AS	108/117 (92%)	95 (88%)	13 (12%)	5	23
29	BS	108/117 (92%)	95 (88%)	13 (12%)	5	23
29	CS	108/117 (92%)	95 (88%)	13 (12%)	5	23
29	DS	108/117 (92%)	95 (88%)	13 (12%)	5	23
30	AT	133/134 (99%)	115 (86%)	18 (14%)	4	20
30	BT	133/134 (99%)	116 (87%)	17 (13%)	4	21
30	CT	133/134 (99%)	117 (88%)	16 (12%)	5	23
30	DT	133/134 (99%)	116 (87%)	17 (13%)	4	21
31	AU	103/104 (99%)	93 (90%)	10 (10%)	8	31
31	BU	103/104 (99%)	93 (90%)	10 (10%)	8	31
31	CU	103/104 (99%)	93 (90%)	10 (10%)	8	31
31	DU	103/104 (99%)	93 (90%)	10 (10%)	8	31
32	AV	107/115 (93%)	93 (87%)	14 (13%)	4	20
32	BV	107/115 (93%)	95 (89%)	12 (11%)	6	25
32	CV	107/115 (93%)	95 (89%)	12 (11%)	6	25
32	DV	107/115 (93%)	96 (90%)	11 (10%)	7	29
33	AW	226/226 (100%)	190 (84%)	36 (16%)	2	15
33	BW	226/226 (100%)	189 (84%)	37 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	CW	226/226 (100%)	188 (83%)	38 (17%)	2	13
33	DW	226/226 (100%)	188 (83%)	38 (17%)	2	13
34	AX	61/67 (91%)	53 (87%)	8 (13%)	4	20
34	BX	61/67 (91%)	53 (87%)	8 (13%)	4	20
34	CX	61/67 (91%)	53 (87%)	8 (13%)	4	20
34	DX	61/67 (91%)	53 (87%)	8 (13%)	4	20
35	AY	197/244 (81%)	173 (88%)	24 (12%)	5	22
35	BY	197/244 (81%)	173 (88%)	24 (12%)	5	22
35	CY	197/244 (81%)	173 (88%)	24 (12%)	5	22
35	DY	197/244 (81%)	173 (88%)	24 (12%)	5	22
36	AZ	82/82 (100%)	73 (89%)	9 (11%)	6	26
36	BZ	82/82 (100%)	73 (89%)	9 (11%)	6	26
36	CZ	82/82 (100%)	73 (89%)	9 (11%)	6	26
36	DZ	82/82 (100%)	73 (89%)	9 (11%)	6	26
All	All	18158/20320 (89%)	15634 (86%)	2524 (14%)	3	19

5 of 2524 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	CX	8	LEU
23	DM	100	MET
2	D1	36	GLU
33	CW	256	ARG
12	DB	159	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 460 such sidechains are listed below:

Mol	Chain	Res	Type
36	BZ	57	ASN
30	DT	3	ASN
17	CG	102	ASN
28	DR	160	ASN
15	DE	237	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	1716/1753 (97%)	653 (38%)	149 (8%)
11	BA	1716/1753 (97%)	657 (38%)	148 (8%)
11	CA	1716/1753 (97%)	654 (38%)	149 (8%)
11	DA	1716/1753 (97%)	652 (37%)	149 (8%)
All	All	6864/7012 (97%)	2616 (38%)	595 (8%)

5 of 2616 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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A0	99/211 (46%)	-0.13	0 100 100	88, 142, 216, 291	0
1	B0	99/211 (46%)	0.20	1 (1%) 79 55	85, 127, 207, 282	0
1	C0	99/211 (46%)	0.29	0 100 100	106, 156, 225, 248	0
1	D0	99/211 (46%)	-0.05	0 100 100	92, 149, 224, 274	0
2	A1	66/68 (97%)	0.03	0 100 100	92, 140, 222, 249	0
2	B1	66/68 (97%)	0.14	0 100 100	89, 134, 206, 234	0
2	C1	66/68 (97%)	0.07	0 100 100	81, 112, 181, 215	0
2	D1	66/68 (97%)	0.54	2 (3%) 52 32	203, 261, 324, 343	0
3	A2	207/208 (99%)	-0.02	2 (0%) 79 55	66, 90, 157, 218	0
3	B2	207/208 (99%)	0.50	8 (3%) 43 28	80, 126, 196, 251	0
3	C2	207/208 (99%)	0.08	2 (0%) 79 55	61, 97, 172, 255	0
3	D2	207/208 (99%)	0.22	4 (1%) 66 42	71, 144, 216, 259	0
4	A3	196/197 (99%)	-0.01	2 (1%) 79 55	73, 125, 204, 261	0
4	B3	196/197 (99%)	0.10	1 (0%) 87 69	66, 113, 185, 234	0
4	C3	196/197 (99%)	0.19	1 (0%) 87 69	92, 164, 230, 267	0
4	D3	196/197 (99%)	0.23	2 (1%) 79 55	116, 179, 252, 285	0
5	A4	209/265 (78%)	0.01	0 100 100	56, 92, 164, 235	0
5	B4	221/265 (83%)	0.01	1 (0%) 87 69	59, 105, 175, 263	0
5	C4	221/265 (83%)	0.22	2 (0%) 81 58	86, 139, 217, 254	0
5	D4	221/265 (83%)	0.21	1 (0%) 87 69	103, 155, 208, 245	0
6	A5	100/119 (84%)	0.09	0 100 100	49, 81, 197, 247	0
6	B5	100/119 (84%)	0.13	3 (3%) 52 32	58, 85, 201, 233	0
6	C5	100/119 (84%)	0.26	1 (1%) 79 55	65, 100, 205, 287	0
6	D5	100/119 (84%)	0.38	5 (5%) 34 22	86, 134, 219, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	A6	80/81 (98%)	-0.03	1 (1%) 75 50	62, 104, 165, 180	0
7	B6	80/81 (98%)	0.19	3 (3%) 44 28	62, 95, 150, 209	0
7	C6	80/81 (98%)	0.37	5 (6%) 26 18	80, 144, 188, 218	0
7	D6	80/81 (98%)	0.33	2 (2%) 58 36	117, 170, 216, 228	0
8	A7	101/162 (62%)	0.02	0 100 100	126, 182, 218, 252	0
8	B7	101/162 (62%)	0.03	0 100 100	94, 132, 192, 242	0
8	C7	101/162 (62%)	0.17	2 (1%) 65 41	109, 147, 199, 248	0
8	D7	101/162 (62%)	0.60	8 (7%) 18 15	130, 187, 230, 255	0
9	A8	79/143 (55%)	-0.22	0 100 100	118, 159, 233, 299	0
9	B8	79/143 (55%)	0.10	0 100 100	98, 134, 208, 242	0
9	C8	79/143 (55%)	0.13	0 100 100	90, 144, 211, 272	0
9	D8	79/143 (55%)	0.79	4 (5%) 33 22	252, 277, 348, 437	0
10	A9	93/189 (49%)	0.23	2 (2%) 62 39	172, 238, 339, 370	0
10	B9	93/189 (49%)	0.31	3 (3%) 50 31	124, 171, 239, 269	0
10	C9	93/189 (49%)	0.27	1 (1%) 78 53	148, 195, 256, 286	0
10	D9	93/189 (49%)	0.69	6 (6%) 25 18	197, 257, 314, 331	0
11	AA	1717/1753 (97%)	-0.12	3 (0%) 91 80	54, 98, 250, 465	0
11	BA	1717/1753 (97%)	0.13	11 (0%) 85 66	52, 98, 270, 521	0
11	CA	1717/1753 (97%)	0.22	22 (1%) 75 50	58, 111, 256, 459	0
11	DA	1717/1753 (97%)	0.46	122 (7%) 22 16	79, 137, 297, 532	0
12	AB	201/241 (83%)	-0.18	0 100 100	64, 116, 167, 234	0
12	BB	201/241 (83%)	0.04	0 100 100	60, 107, 164, 201	0
12	CB	201/241 (83%)	0.11	1 (0%) 87 69	84, 128, 181, 226	0
12	DB	201/241 (83%)	0.19	1 (0%) 87 69	102, 168, 221, 256	0
13	AC	228/243 (93%)	-0.04	3 (1%) 75 50	80, 144, 214, 246	0
13	BC	228/243 (93%)	0.08	1 (0%) 88 72	74, 133, 210, 254	0
13	CC	228/243 (93%)	0.10	2 (0%) 81 58	77, 132, 210, 272	0
13	DC	228/243 (93%)	0.02	2 (0%) 81 58	89, 156, 238, 280	0
14	AD	180/181 (99%)	0.16	4 (2%) 62 39	69, 103, 167, 214	0
14	BD	180/181 (99%)	0.72	7 (3%) 43 28	80, 142, 207, 289	0
14	CD	180/181 (99%)	0.43	7 (3%) 43 28	81, 124, 187, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
14	DD	180/181 (99%)	0.35	6 (3%)	49	31	86, 115, 180, 234	0
15	AE	229/296 (77%)	-0.02	5 (2%)	62	39	58, 99, 205, 259	0
15	BE	229/296 (77%)	0.15	6 (2%)	57	35	43, 95, 202, 258	0
15	CE	229/296 (77%)	0.14	4 (1%)	69	43	64, 109, 228, 260	0
15	DE	229/296 (77%)	0.19	2 (0%)	81	58	81, 123, 226, 266	0
16	AF	89/101 (88%)	-0.17	0	100	100	86, 133, 211, 281	0
16	BF	89/101 (88%)	0.03	0	100	100	84, 130, 216, 319	0
16	CF	89/101 (88%)	-0.04	0	100	100	116, 161, 252, 292	0
16	DF	89/101 (88%)	-0.02	0	100	100	93, 146, 216, 259	0
17	AG	192/200 (96%)	0.01	0	100	100	82, 127, 195, 248	0
17	BG	192/200 (96%)	0.14	1 (0%)	87	69	65, 116, 187, 227	0
17	CG	192/200 (96%)	0.08	4 (2%)	63	40	69, 107, 180, 237	0
17	DG	192/200 (96%)	1.01	26 (13%)	7	8	198, 256, 315, 346	0
18	AH	129/130 (99%)	-0.02	1 (0%)	82	60	51, 76, 118, 163	0
18	BH	129/130 (99%)	0.00	2 (1%)	70	45	47, 67, 118, 151	0
18	CH	129/130 (99%)	0.19	0	100	100	65, 88, 129, 160	0
18	DH	129/130 (99%)	0.29	2 (1%)	70	45	76, 117, 156, 179	0
19	AI	143/145 (98%)	0.37	13 (9%)	15	13	69, 111, 212, 248	0
19	BI	143/145 (98%)	0.39	9 (6%)	26	18	65, 109, 197, 284	0
19	CI	143/145 (98%)	0.54	13 (9%)	15	13	77, 114, 215, 266	0
19	DI	143/145 (98%)	1.00	23 (16%)	4	6	152, 218, 272, 312	0
20	AJ	108/120 (90%)	-0.06	2 (1%)	66	42	70, 123, 225, 295	0
20	BJ	108/120 (90%)	0.15	3 (2%)	55	34	61, 112, 220, 250	0
20	CJ	108/120 (90%)	0.13	1 (0%)	81	58	81, 125, 238, 303	0
20	DJ	108/120 (90%)	0.23	5 (4%)	37	24	89, 145, 231, 248	0
21	AK	140/151 (92%)	-0.09	0	100	100	58, 86, 152, 222	0
21	BK	140/151 (92%)	0.10	3 (2%)	63	40	60, 97, 160, 214	0
21	CK	140/151 (92%)	0.43	5 (3%)	46	29	77, 126, 200, 233	0
21	DK	140/151 (92%)	0.36	3 (2%)	63	40	89, 147, 206, 225	0
22	AL	140/142 (98%)	0.09	0	100	100	47, 92, 129, 193	0
22	BL	140/142 (98%)	0.17	1 (0%)	84	63	52, 83, 125, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
22	CL	140/142 (98%)	0.44	3 (2%) 63 40	56, 100, 153, 185	0
22	DL	140/142 (98%)	0.24	1 (0%) 84 63	77, 105, 148, 213	0
23	AM	153/155 (98%)	0.07	1 (0%) 84 63	105, 156, 208, 238	0
23	BM	153/155 (98%)	0.23	1 (0%) 84 63	80, 122, 181, 217	0
23	CM	153/155 (98%)	0.26	0 100 100	101, 149, 205, 238	0
23	DM	153/155 (98%)	1.33	33 (21%) 2 3	198, 260, 333, 366	0
24	AN	54/55 (98%)	0.27	2 (3%) 45 28	77, 115, 174, 210	0
24	BN	54/55 (98%)	0.27	2 (3%) 45 28	60, 92, 133, 168	0
24	CN	54/55 (98%)	0.63	4 (7%) 20 15	87, 116, 142, 171	0
24	DN	54/55 (98%)	0.94	8 (14%) 5 7	95, 135, 203, 233	0
25	AO	152/153 (99%)	-0.03	4 (2%) 57 35	58, 88, 169, 229	0
25	BO	152/153 (99%)	0.05	1 (0%) 84 63	53, 94, 177, 244	0
25	CO	152/153 (99%)	0.39	3 (1%) 65 41	73, 124, 196, 280	0
25	DO	152/153 (99%)	0.31	5 (3%) 49 31	91, 153, 215, 269	0
26	AP	148/149 (99%)	0.02	0 100 100	86, 125, 168, 232	0
26	BP	148/149 (99%)	0.63	6 (4%) 41 26	84, 143, 190, 226	0
26	CP	148/149 (99%)	0.51	4 (2%) 56 35	101, 155, 212, 242	0
26	DP	148/149 (99%)	0.01	0 100 100	92, 125, 170, 225	0
27	AQ	156/157 (99%)	0.04	2 (1%) 75 50	49, 83, 196, 262	0
27	BQ	156/157 (99%)	0.67	7 (4%) 38 24	69, 126, 206, 274	0
27	CQ	156/157 (99%)	0.01	0 100 100	56, 93, 190, 227	0
27	DQ	156/157 (99%)	0.19	1 (0%) 85 66	80, 129, 223, 275	0
28	AR	338/343 (98%)	0.02	1 (0%) 90 76	94, 157, 239, 316	0
28	BR	338/343 (98%)	0.29	4 (1%) 76 51	106, 171, 250, 317	0
28	CR	338/343 (98%)	0.05	1 (0%) 90 76	91, 140, 226, 297	0
28	DR	338/343 (98%)	0.34	9 (2%) 56 35	172, 250, 315, 352	0
29	AS	128/144 (88%)	0.06	0 100 100	127, 185, 235, 293	0
29	BS	128/144 (88%)	0.15	0 100 100	86, 132, 204, 236	0
29	CS	128/144 (88%)	0.23	2 (1%) 70 45	117, 163, 226, 260	0
29	DS	128/144 (88%)	1.16	25 (19%) 3 4	231, 263, 309, 342	0
30	AT	154/155 (99%)	0.21	1 (0%) 85 66	78, 115, 186, 268	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	BT	154/155 (99%)	0.14	2 (1%) 75 50	60, 97, 181, 264	0
30	CT	154/155 (99%)	0.35	6 (3%) 43 28	87, 126, 181, 222	0
30	DT	154/155 (99%)	1.29	31 (20%) 3 3	169, 226, 303, 354	0
31	AU	124/126 (98%)	-0.01	0 100 100	191, 241, 287, 311	0
31	BU	124/126 (98%)	0.28	2 (1%) 70 45	140, 196, 236, 257	0
31	CU	124/126 (98%)	0.39	3 (2%) 59 37	142, 191, 234, 269	0
31	DU	124/126 (98%)	0.93	12 (9%) 13 13	210, 259, 325, 375	0
32	AV	119/130 (91%)	-0.02	2 (1%) 69 43	77, 129, 196, 215	0
32	BV	119/130 (91%)	0.03	2 (1%) 69 43	76, 139, 211, 238	0
32	CV	119/130 (91%)	0.17	1 (0%) 82 60	74, 135, 220, 246	0
32	DV	119/130 (91%)	0.26	3 (2%) 58 36	135, 188, 258, 292	0
33	AW	259/259 (100%)	-0.09	1 (0%) 88 72	63, 92, 133, 174	0
33	BW	259/259 (100%)	0.53	8 (3%) 51 32	83, 139, 195, 234	0
33	CW	259/259 (100%)	0.27	2 (0%) 82 60	72, 119, 168, 230	0
33	DW	259/259 (100%)	0.09	0 100 100	76, 118, 164, 211	0
34	AX	74/80 (92%)	0.16	1 (1%) 73 48	87, 141, 227, 272	0
34	BX	74/80 (92%)	0.48	0 100 100	86, 139, 242, 277	0
34	CX	74/80 (92%)	0.29	1 (1%) 73 48	101, 159, 222, 277	0
34	DX	74/80 (92%)	0.20	1 (1%) 73 48	84, 141, 259, 292	0
35	AY	228/293 (77%)	0.19	3 (1%) 75 50	91, 149, 211, 251	0
35	BY	228/293 (77%)	0.45	1 (0%) 88 72	88, 150, 229, 308	0
35	CY	228/293 (77%)	0.46	7 (3%) 51 32	91, 157, 227, 259	0
35	DY	228/293 (77%)	0.22	1 (0%) 88 72	99, 163, 225, 282	0
36	AZ	97/97 (100%)	-0.20	0 100 100	70, 97, 167, 203	0
36	BZ	97/97 (100%)	-0.03	1 (1%) 79 55	63, 94, 165, 205	0
36	CZ	97/97 (100%)	0.02	0 100 100	79, 116, 189, 207	0
36	DZ	97/97 (100%)	0.23	1 (1%) 79 55	106, 143, 197, 210	0
All	All	27676/30568 (90%)	0.21	624 (2%) 61 38	43, 129, 254, 532	0

The worst 5 of 624 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	AI	134	ARG	7.2

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Mol	Chain	Res	Type	RSRZ
19	AI	140	MET	6.5
15	BE	93	ALA	5.7
23	DM	146	VAL	5.6
19	BI	134	ARG	5.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	DA	5016	1/1	0.24	0.10	191,191,191,191	0
38	MG	DA	5029	1/1	0.25	0.24	217,217,217,217	0
38	MG	DA	5071	1/1	0.25	0.15	238,238,238,238	0
38	MG	CA	5053	1/1	0.27	0.23	246,246,246,246	0
38	MG	DA	5078	1/1	0.27	0.28	241,241,241,241	0
38	MG	AA	5073	1/1	0.28	0.24	205,205,205,205	0
38	MG	DA	5070	1/1	0.32	0.21	251,251,251,251	0
38	MG	DA	5013	1/1	0.33	0.16	218,218,218,218	0
38	MG	BA	5071	1/1	0.33	0.25	215,215,215,215	0
38	MG	DA	5006	1/1	0.34	0.21	159,159,159,159	0
38	MG	DA	5048	1/1	0.37	0.19	222,222,222,222	0
38	MG	DA	5066	1/1	0.39	0.24	251,251,251,251	0
38	MG	CA	5077	1/1	0.43	0.20	222,222,222,222	0
38	MG	CA	5016	1/1	0.44	0.17	195,195,195,195	0
38	MG	BA	5013	1/1	0.44	0.17	182,182,182,182	0
38	MG	AA	5071	1/1	0.44	0.25	212,212,212,212	0
38	MG	DA	5053	1/1	0.46	0.18	256,256,256,256	0
38	MG	BA	5067	1/1	0.47	0.18	227,227,227,227	0
38	MG	BA	5078	1/1	0.49	0.29	232,232,232,232	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	CA	5014	1/1	0.51	0.31	232,232,232,232	0
38	MG	DA	5077	1/1	0.51	0.13	235,235,235,235	0
38	MG	AA	5067	1/1	0.51	0.15	194,194,194,194	0
38	MG	DA	5034	1/1	0.52	0.17	220,220,220,220	0
38	MG	BA	5031	1/1	0.52	0.15	205,205,205,205	0
38	MG	AA	5014	1/1	0.53	0.22	220,220,220,220	0
38	MG	CA	5021	1/1	0.53	0.23	201,201,201,201	0
38	MG	CA	5010	1/1	0.53	0.11	212,212,212,212	0
38	MG	AA	5077	1/1	0.53	0.20	198,198,198,198	0
38	MG	DA	5056	1/1	0.54	0.81	238,238,238,238	0
38	MG	CA	5073	1/1	0.54	0.19	208,208,208,208	0
38	MG	CA	5071	1/1	0.55	0.21	190,190,190,190	0
38	MG	BA	5073	1/1	0.57	0.18	179,179,179,179	0
38	MG	AA	5013	1/1	0.57	0.14	222,222,222,222	0
38	MG	BA	5059	1/1	0.57	0.11	206,206,206,206	0
38	MG	DA	5035	1/1	0.57	0.13	196,196,196,196	0
38	MG	AA	5059	1/1	0.58	0.13	220,220,220,220	0
38	MG	DA	5031	1/1	0.58	0.19	218,218,218,218	0
38	MG	CA	5013	1/1	0.58	0.13	174,174,174,174	0
38	MG	BA	5029	1/1	0.59	0.16	231,231,231,231	0
38	MG	AA	5078	1/1	0.59	0.20	207,207,207,207	0
38	MG	CA	5029	1/1	0.59	0.16	206,206,206,206	0
38	MG	BA	5014	1/1	0.59	0.15	192,192,192,192	0
38	MG	BA	5075	1/1	0.59	0.13	176,176,176,176	0
38	MG	DA	5019	1/1	0.59	0.25	184,184,184,184	0
38	MG	DA	5052	1/1	0.60	0.07	218,218,218,218	0
38	MG	DA	5043	1/1	0.60	0.22	197,197,197,197	0
38	MG	BA	5032	1/1	0.61	0.24	175,175,175,175	0
38	MG	BA	5056	1/1	0.61	0.39	200,200,200,200	0
38	MG	BA	5016	1/1	0.61	0.12	237,237,237,237	0
38	MG	DA	5058	1/1	0.62	0.20	227,227,227,227	0
38	MG	CA	5067	1/1	0.62	0.14	199,199,199,199	0
38	MG	DA	5014	1/1	0.63	0.13	206,206,206,206	0
38	MG	BA	5043	1/1	0.64	0.17	200,200,200,200	0
38	MG	DA	5076	1/1	0.64	0.13	201,201,201,201	0
38	MG	CA	5028	1/1	0.65	0.19	184,184,184,184	0
38	MG	BA	5058	1/1	0.65	0.17	169,169,169,169	0
38	MG	BA	5017	1/1	0.65	0.33	197,197,197,197	0
38	MG	AA	5043	1/1	0.65	0.13	174,174,174,174	0
38	MG	CA	5057	1/1	0.66	0.23	191,191,191,191	0
38	MG	DA	5020	1/1	0.66	0.20	199,199,199,199	0
38	MG	DA	5037	1/1	0.67	0.17	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	DA	5062	1/1	0.67	0.12	213,213,213,213	0
38	MG	BA	5062	1/1	0.67	0.18	219,219,219,219	0
38	MG	DA	5032	1/1	0.67	0.17	174,174,174,174	0
38	MG	CA	5008	1/1	0.69	0.14	179,179,179,179	0
38	MG	AA	5058	1/1	0.69	0.16	160,160,160,160	0
38	MG	DA	5017	1/1	0.69	0.20	192,192,192,192	0
38	MG	DA	5075	1/1	0.69	0.14	239,239,239,239	0
38	MG	CA	5078	1/1	0.69	0.28	199,199,199,199	0
38	MG	CA	5031	1/1	0.69	0.12	231,231,231,231	0
38	MG	CA	5038	1/1	0.69	0.17	173,173,173,173	0
38	MG	CA	5076	1/1	0.70	0.10	172,172,172,172	0
38	MG	DA	5045	1/1	0.70	0.20	197,197,197,197	0
38	MG	CA	5035	1/1	0.70	0.12	158,158,158,158	0
38	MG	DA	5026	1/1	0.70	0.20	208,208,208,208	0
38	MG	DA	5042	1/1	0.70	0.14	177,177,177,177	0
38	MG	BA	5046	1/1	0.71	0.18	182,182,182,182	0
38	MG	CA	5043	1/1	0.71	0.22	218,218,218,218	0
38	MG	CA	5048	1/1	0.71	0.14	208,208,208,208	0
38	MG	DA	5068	1/1	0.71	0.17	169,169,169,169	0
38	MG	AA	5030	1/1	0.71	0.19	271,271,271,271	0
38	MG	DA	5049	1/1	0.72	0.23	207,207,207,207	0
38	MG	CA	5061	1/1	0.72	0.17	136,136,136,136	0
38	MG	DA	5038	1/1	0.72	0.18	191,191,191,191	0
38	MG	DA	5073	1/1	0.72	0.14	221,221,221,221	0
38	MG	CA	5037	1/1	0.72	0.15	178,178,178,178	0
38	MG	CA	5032	1/1	0.72	0.10	186,186,186,186	0
38	MG	CA	5056	1/1	0.72	0.37	200,200,200,200	0
38	MG	CA	5006	1/1	0.72	0.10	170,170,170,170	0
38	MG	BA	5001	1/1	0.73	0.15	135,135,135,135	0
38	MG	CA	5036	1/1	0.73	0.09	193,193,193,193	0
38	MG	BA	5053	1/1	0.74	0.39	231,231,231,231	0
38	MG	AA	5048	1/1	0.74	0.26	213,213,213,213	0
38	MG	BA	5034	1/1	0.74	0.12	174,174,174,174	0
38	MG	BA	5077	1/1	0.74	0.16	199,199,199,199	0
38	MG	DA	5059	1/1	0.74	0.11	205,205,205,205	0
38	MG	DA	5069	1/1	0.75	0.20	199,199,199,199	0
38	MG	CA	5062	1/1	0.75	0.10	188,188,188,188	0
38	MG	BA	5021	1/1	0.75	0.18	191,191,191,191	0
38	MG	BA	5049	1/1	0.75	0.17	210,210,210,210	0
38	MG	AA	5049	1/1	0.75	0.22	167,167,167,167	0
38	MG	BA	5069	1/1	0.75	0.18	123,123,123,123	0
38	MG	AA	5053	1/1	0.75	0.24	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	BA	5045	1/1	0.75	0.12	164,164,164,164	0
38	MG	DA	5011	1/1	0.76	0.12	187,187,187,187	0
38	MG	CA	5059	1/1	0.76	0.10	206,206,206,206	0
38	MG	CA	5030	1/1	0.76	0.16	224,224,224,224	0
38	MG	BA	5070	1/1	0.76	0.15	143,143,143,143	0
38	MG	AA	5027	1/1	0.76	0.13	208,208,208,208	0
38	MG	AA	5056	1/1	0.76	0.29	163,163,163,163	0
38	MG	CA	5004	1/1	0.77	0.20	203,203,203,203	0
38	MG	AA	5055	1/1	0.77	0.13	150,150,150,150	0
38	MG	CA	5026	1/1	0.77	0.14	177,177,177,177	0
38	MG	AA	5029	1/1	0.77	0.12	161,161,161,161	0
38	MG	CA	5034	1/1	0.77	0.13	178,178,178,178	0
38	MG	CA	5045	1/1	0.77	0.11	207,207,207,207	0
38	MG	DA	5054	1/1	0.77	0.12	169,169,169,169	0
38	MG	CA	5017	1/1	0.78	0.19	165,165,165,165	0
38	MG	DA	5001	1/1	0.78	0.14	159,159,159,159	0
38	MG	BA	5030	1/1	0.78	0.29	252,252,252,252	0
38	MG	AA	5076	1/1	0.78	0.11	189,189,189,189	0
38	MG	AA	5034	1/1	0.79	0.18	186,186,186,186	0
38	MG	AA	5045	1/1	0.79	0.10	186,186,186,186	0
38	MG	AA	5069	1/1	0.79	0.13	147,147,147,147	0
38	MG	CA	5070	1/1	0.79	0.13	134,134,134,134	0
38	MG	BA	5074	1/1	0.79	0.18	153,153,153,153	0
38	MG	CA	5042	1/1	0.79	0.12	183,183,183,183	0
38	MG	CA	5058	1/1	0.79	0.14	178,178,178,178	0
38	MG	CA	5005	1/1	0.79	0.14	153,153,153,153	0
38	MG	BA	5004	1/1	0.80	0.25	234,234,234,234	0
38	MG	DA	5063	1/1	0.80	0.10	141,141,141,141	0
38	MG	DA	5021	1/1	0.80	0.23	189,189,189,189	0
38	MG	CA	5049	1/1	0.80	0.29	201,201,201,201	0
38	MG	DA	5067	1/1	0.81	0.17	220,220,220,220	0
38	MG	DA	5008	1/1	0.81	0.10	170,170,170,170	0
38	MG	CA	5012	1/1	0.81	0.12	123,123,123,123	0
38	MG	BA	5037	1/1	0.81	0.12	185,185,185,185	0
38	MG	CA	5022	1/1	0.81	0.11	135,135,135,135	0
38	MG	DA	5030	1/1	0.81	0.08	229,229,229,229	0
38	MG	AA	5046	1/1	0.81	0.12	135,135,135,135	0
38	MG	DA	5046	1/1	0.81	0.14	148,148,148,148	0
38	MG	CA	5027	1/1	0.81	0.09	185,185,185,185	0
38	MG	BA	5020	1/1	0.81	0.12	200,200,200,200	0
38	MG	DA	5057	1/1	0.82	0.15	178,178,178,178	0
38	MG	BA	5054	1/1	0.82	0.15	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	AA	5062	1/1	0.82	0.10	160,160,160,160	0
38	MG	CA	5075	1/1	0.82	0.11	157,157,157,157	0
38	MG	DA	5064	1/1	0.83	0.10	186,186,186,186	0
38	MG	BA	5011	1/1	0.83	0.14	136,136,136,136	0
38	MG	BA	5042	1/1	0.83	0.08	210,210,210,210	0
38	MG	DA	5036	1/1	0.84	0.12	199,199,199,199	0
38	MG	AA	5032	1/1	0.84	0.12	170,170,170,170	0
38	MG	CA	5069	1/1	0.84	0.11	129,129,129,129	0
38	MG	AA	5004	1/1	0.84	0.15	194,194,194,194	0
38	MG	BA	5006	1/1	0.84	0.11	175,175,175,175	0
38	MG	DA	5010	1/1	0.84	0.10	201,201,201,201	0
38	MG	DA	5004	1/1	0.85	0.14	167,167,167,167	0
38	MG	BA	5048	1/1	0.85	0.20	151,151,151,151	0
38	MG	BA	5061	1/1	0.85	0.12	132,132,132,132	0
38	MG	BA	5039	1/1	0.85	0.08	110,110,110,110	0
38	MG	AA	5016	1/1	0.85	0.07	167,167,167,167	0
38	MG	AA	5057	1/1	0.85	0.10	170,170,170,170	0
38	MG	DA	5074	1/1	0.85	0.11	198,198,198,198	0
38	MG	AA	5010	1/1	0.85	0.09	184,184,184,184	0
38	MG	DA	5015	1/1	0.85	0.12	118,118,118,118	0
38	MG	CA	5052	1/1	0.85	0.07	146,146,146,146	0
38	MG	AA	5031	1/1	0.85	0.10	190,190,190,190	0
38	MG	AA	5020	1/1	0.86	0.27	171,171,171,171	0
38	MG	AA	5022	1/1	0.86	0.11	128,128,128,128	0
38	MG	DA	5003	1/1	0.86	0.15	175,175,175,175	0
38	MG	AA	5070	1/1	0.86	0.14	144,144,144,144	0
38	MG	AA	5036	1/1	0.86	0.09	176,176,176,176	0
38	MG	CA	5074	1/1	0.86	0.08	148,148,148,148	0
38	MG	AA	5040	1/1	0.86	0.09	121,121,121,121	0
38	MG	BA	5005	1/1	0.86	0.13	146,146,146,146	0
38	MG	BA	5033	1/1	0.86	0.11	146,146,146,146	0
38	MG	BA	5076	1/1	0.87	0.13	172,172,172,172	0
38	MG	CA	5009	1/1	0.87	0.10	127,127,127,127	0
38	MG	AA	5037	1/1	0.87	0.11	173,173,173,173	0
38	MG	AA	5006	1/1	0.87	0.08	128,128,128,128	0
38	MG	BA	5064	1/1	0.87	0.10	134,134,134,134	0
37	ZN	D9	500	1/1	0.87	0.08	278,278,278,278	0
38	MG	AA	5028	1/1	0.87	0.12	176,176,176,176	0
38	MG	AA	5005	1/1	0.88	0.18	131,131,131,131	0
38	MG	CA	5060	1/1	0.88	0.22	170,170,170,170	0
38	MG	BA	5052	1/1	0.88	0.09	144,144,144,144	0
38	MG	AA	5017	1/1	0.88	0.25	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	AA	5019	1/1	0.88	0.12	136,136,136,136	0
38	MG	AA	5042	1/1	0.88	0.06	200,200,200,200	0
38	MG	CA	5020	1/1	0.88	0.11	154,154,154,154	0
38	MG	BA	5057	1/1	0.88	0.14	144,144,144,144	0
38	MG	AA	5035	1/1	0.88	0.13	137,137,137,137	0
38	MG	BA	5026	1/1	0.88	0.09	159,159,159,159	0
38	MG	BA	5035	1/1	0.88	0.10	153,153,153,153	0
38	MG	DA	5065	1/1	0.88	0.11	146,146,146,146	0
38	MG	CA	5039	1/1	0.89	0.11	123,123,123,123	0
38	MG	CA	5040	1/1	0.89	0.08	139,139,139,139	0
38	MG	BA	5022	1/1	0.89	0.14	115,115,115,115	0
38	MG	AA	5023	1/1	0.89	0.09	122,122,122,122	0
38	MG	DA	5060	1/1	0.89	0.14	148,148,148,148	0
38	MG	AA	5021	1/1	0.89	0.13	177,177,177,177	0
38	MG	DA	5007	1/1	0.89	0.09	142,142,142,142	0
38	MG	DA	5028	1/1	0.90	0.19	163,163,163,163	0
38	MG	DA	5040	1/1	0.90	0.13	161,161,161,161	0
38	MG	AA	5061	1/1	0.90	0.10	108,108,108,108	0
38	MG	AA	5008	1/1	0.90	0.13	154,154,154,154	0
38	MG	DA	5044	1/1	0.90	0.10	134,134,134,134	0
38	MG	AA	5066	1/1	0.90	0.08	172,172,172,172	0
38	MG	CA	5051	1/1	0.90	0.08	126,126,126,126	0
38	MG	BA	5047	1/1	0.90	0.12	115,115,115,115	0
38	MG	BA	5038	1/1	0.90	0.13	165,165,165,165	0
38	MG	AA	5011	1/1	0.90	0.08	137,137,137,137	0
38	MG	BA	5027	1/1	0.90	0.08	161,161,161,161	0
38	MG	CA	5050	1/1	0.91	0.08	135,135,135,135	0
38	MG	CA	5024	1/1	0.91	0.08	123,123,123,123	0
38	MG	BA	5041	1/1	0.91	0.18	119,119,119,119	0
38	MG	DA	5061	1/1	0.91	0.09	132,132,132,132	0
38	MG	AA	5075	1/1	0.91	0.10	155,155,155,155	0
38	MG	AA	5054	1/1	0.91	0.11	112,112,112,112	0
38	MG	DA	5041	1/1	0.91	0.12	162,162,162,162	0
38	MG	CA	5063	1/1	0.91	0.11	101,101,101,101	0
38	MG	CA	5065	1/1	0.91	0.09	158,158,158,158	0
38	MG	CA	5023	1/1	0.91	0.09	110,110,110,110	0
38	MG	BA	5051	1/1	0.92	0.10	130,130,130,130	0
38	MG	BA	5036	1/1	0.92	0.05	177,177,177,177	0
38	MG	DA	5025	1/1	0.92	0.08	105,105,105,105	0
38	MG	AA	5065	1/1	0.92	0.07	170,170,170,170	0
38	MG	CA	5011	1/1	0.92	0.06	128,128,128,128	0
38	MG	AA	5026	1/1	0.92	0.08	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	AA	5063	1/1	0.93	0.12	112,112,112,112	0
38	MG	BA	5024	1/1	0.93	0.07	106,106,106,106	0
38	MG	DA	5018	1/1	0.93	0.08	104,104,104,104	0
38	MG	CA	5019	1/1	0.93	0.09	114,114,114,114	0
38	MG	CA	5054	1/1	0.93	0.09	120,120,120,120	0
38	MG	DA	5072	1/1	0.93	0.10	146,146,146,146	0
38	MG	CA	5064	1/1	0.93	0.09	133,133,133,133	0
38	MG	BA	5008	1/1	0.93	0.17	125,125,125,125	0
38	MG	DA	5050	1/1	0.93	0.11	123,123,123,123	0
38	MG	AA	5041	1/1	0.93	0.09	127,127,127,127	0
38	MG	BA	5012	1/1	0.93	0.09	90,90,90,90	0
38	MG	AA	5003	1/1	0.93	0.19	120,120,120,120	0
38	MG	CA	5033	1/1	0.94	0.11	123,123,123,123	0
38	MG	CA	5046	1/1	0.94	0.08	138,138,138,138	0
38	MG	CA	5047	1/1	0.94	0.08	169,169,169,169	0
38	MG	AA	5060	1/1	0.94	0.20	137,137,137,137	0
38	MG	CA	5001	1/1	0.94	0.13	116,116,116,116	0
38	MG	DA	5051	1/1	0.94	0.07	162,162,162,162	0
38	MG	AA	5038	1/1	0.94	0.11	162,162,162,162	0
38	MG	DA	5000	1/1	0.94	0.06	107,107,107,107	0
38	MG	BA	5010	1/1	0.94	0.07	156,156,156,156	0
38	MG	BA	5028	1/1	0.94	0.06	159,159,159,159	0
38	MG	AA	5052	1/1	0.94	0.06	141,141,141,141	0
38	MG	AA	5068	1/1	0.94	0.13	112,112,112,112	0
38	MG	DA	5023	1/1	0.94	0.07	127,127,127,127	0
38	MG	DA	5024	1/1	0.94	0.07	144,144,144,144	0
38	MG	BA	5066	1/1	0.94	0.07	104,104,104,104	0
38	MG	AA	5001	1/1	0.94	0.09	106,106,106,106	0
38	MG	CA	5068	1/1	0.95	0.09	98,98,98,98	0
38	MG	DA	5039	1/1	0.95	0.07	120,120,120,120	0
38	MG	DA	5027	1/1	0.95	0.05	162,162,162,162	0
38	MG	AA	5025	1/1	0.95	0.23	96,96,96,96	0
38	MG	DA	5055	1/1	0.95	0.05	152,152,152,152	0
38	MG	AA	5051	1/1	0.95	0.06	111,111,111,111	0
38	MG	AA	5064	1/1	0.95	0.05	153,153,153,153	0
38	MG	CA	5015	1/1	0.95	0.07	80,80,80,80	0
38	MG	DA	5012	1/1	0.95	0.07	118,118,118,118	0
38	MG	DA	5022	1/1	0.95	0.05	108,108,108,108	0
38	MG	DA	5047	1/1	0.95	0.06	128,128,128,128	0
38	MG	CA	5066	1/1	0.95	0.07	130,130,130,130	0
38	MG	BA	5000	1/1	0.95	0.09	91,91,91,91	0
38	MG	DA	5005	1/1	0.95	0.19	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	AA	5015	1/1	0.96	0.07	88,88,88,88	0
38	MG	BA	5019	1/1	0.96	0.15	163,163,163,163	0
38	MG	AA	5050	1/1	0.96	0.07	104,104,104,104	0
38	MG	AA	5012	1/1	0.96	0.07	102,102,102,102	0
38	MG	CA	5025	1/1	0.96	0.06	100,100,100,100	0
38	MG	DA	5033	1/1	0.96	0.06	122,122,122,122	0
38	MG	AA	5033	1/1	0.96	0.08	143,143,143,143	0
38	MG	DA	5002	1/1	0.96	0.11	111,111,111,111	0
38	MG	CA	5003	1/1	0.96	0.07	135,135,135,135	0
38	MG	AA	5074	1/1	0.96	0.08	113,113,113,113	0
38	MG	BA	5040	1/1	0.96	0.07	121,121,121,121	0
38	MG	BA	5060	1/1	0.96	0.16	158,158,158,158	0
38	MG	CA	5044	1/1	0.96	0.06	105,105,105,105	0
38	MG	CA	5072	1/1	0.96	0.06	110,110,110,110	0
38	MG	DA	5009	1/1	0.96	0.05	110,110,110,110	0
38	MG	CA	5007	1/1	0.96	0.07	97,97,97,97	0
38	MG	BA	5009	1/1	0.96	0.07	96,96,96,96	0
38	MG	BA	5068	1/1	0.97	0.08	82,82,82,82	0
38	MG	AA	5047	1/1	0.97	0.06	112,112,112,112	0
38	MG	BA	5023	1/1	0.97	0.06	115,115,115,115	0
38	MG	BA	5007	1/1	0.97	0.06	106,106,106,106	0
38	MG	BA	5025	1/1	0.97	0.13	93,93,93,93	0
37	ZN	D6	500	1/1	0.97	0.04	173,173,173,173	0
37	ZN	C9	1165	1/1	0.97	0.05	159,159,159,159	0
38	MG	BA	5018	1/1	0.97	0.15	90,90,90,90	0
38	MG	BA	5050	1/1	0.97	0.06	123,123,123,123	0
38	MG	BA	5003	1/1	0.97	0.19	138,138,138,138	0
38	MG	CA	5041	1/1	0.97	0.08	130,130,130,130	0
38	MG	CA	5000	1/1	0.97	0.07	85,85,85,85	0
38	MG	AA	5018	1/1	0.97	0.08	85,85,85,85	0
37	ZN	DN	500	1/1	0.97	0.04	132,132,132,132	0
38	MG	BA	5072	1/1	0.98	0.05	91,91,91,91	0
37	ZN	A9	500	1/1	0.98	0.04	218,218,218,218	0
38	MG	BA	5063	1/1	0.98	0.07	82,82,82,82	0
38	MG	BA	5055	1/1	0.98	0.06	88,88,88,88	0
38	MG	CA	5018	1/1	0.98	0.05	95,95,95,95	0
38	MG	AA	5072	1/1	0.98	0.07	113,113,113,113	0
37	ZN	B9	500	1/1	0.98	0.04	148,148,148,148	0
38	MG	AA	5000	1/1	0.98	0.04	78,78,78,78	0
38	MG	BA	5015	1/1	0.98	0.07	87,87,87,87	0
38	MG	AA	5009	1/1	0.98	0.05	104,104,104,104	0
38	MG	AA	5039	1/1	0.98	0.09	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	MG	AA	5044	1/1	0.99	0.04	93,93,93,93	0
37	ZN	AN	500	1/1	0.99	0.02	124,124,124,124	0
38	MG	CA	5055	1/1	0.99	0.04	126,126,126,126	0
38	MG	BA	5065	1/1	0.99	0.06	89,89,89,89	0
38	MG	AA	5002	1/1	0.99	0.07	86,86,86,86	0
37	ZN	CN	1056	1/1	0.99	0.02	94,94,94,94	0
38	MG	CA	5002	1/1	0.99	0.03	88,88,88,88	0
37	ZN	B5	500	1/1	0.99	0.02	71,71,71,71	0
38	MG	BA	5044	1/1	0.99	0.07	88,88,88,88	0
37	ZN	A6	500	1/1	0.99	0.03	114,114,114,114	0
37	ZN	C5	1102	1/1	0.99	0.03	87,87,87,87	0
38	MG	BA	5002	1/1	0.99	0.05	85,85,85,85	0
38	MG	AA	5007	1/1	0.99	0.05	90,90,90,90	0
38	MG	AA	5024	1/1	0.99	0.04	100,100,100,100	0
37	ZN	C6	1082	1/1	0.99	0.03	179,179,179,179	0
37	ZN	D5	500	1/1	1.00	0.02	117,117,117,117	0
37	ZN	A5	500	1/1	1.00	0.01	70,70,70,70	0
37	ZN	BN	500	1/1	1.00	0.02	94,94,94,94	0
37	ZN	B6	500	1/1	1.00	0.02	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.