



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 04:18 pm GMT

PDB ID : 4V8P  
Title : T.thermophila 60S ribosomal subunit in complex with initiation factor 6.  
Authors : Klinge, S.; Voigts-Hoffmann, F.; Leibundgut, M.; Arpagaus, S.; Ban, N.  
Deposited on : 2011-09-14  
Resolution : 3.52 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

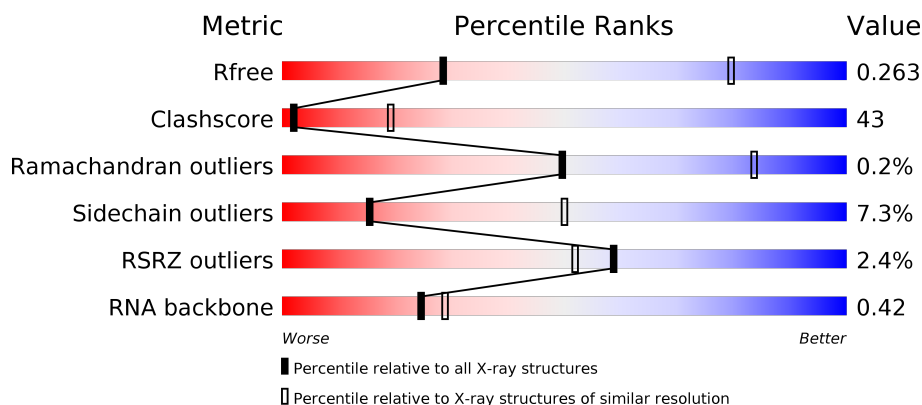
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




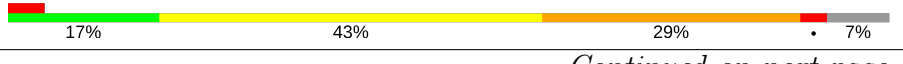
The reported resolution of this entry is 3.52 Å.

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))
$R_{free}$	111664	1052 (3.62-3.42)
Clashscore	122126	1048 (3.60-3.44)
Ramachandran outliers	120053	1014 (3.60-3.44)
Sidechain outliers	120020	1015 (3.60-3.44)
RSRZ outliers	108989	1353 (3.64-3.40)
RNA backbone	2636	1052 (4.10-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A1	3354	
1	D1	3354	
1	F1	3354	
1	H1	3354	

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Mol	Chain	Length	Quality of chain
2	AA	94	
2	DA	94	
2	FA	94	
2	HA	94	
3	AB	52	
3	DB	52	
3	FB	52	
3	HB	52	
4	AC	109	
4	DC	109	
4	FC	109	
4	HC	109	
5	AE	191	
5	DE	191	
5	FE	191	
5	HE	191	
6	AF	126	
6	DF	126	
6	FF	126	
6	HF	126	
7	AG	104	
7	DG	104	
7	FG	104	
7	HG	104	
8	AH	113	

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Mol	Chain	Length	Quality of chain
8	DH	113	
8	FH	113	
8	HH	113	
9	AJ	248	
9	DJ	248	
9	FJ	248	
9	HJ	248	
10	AK	129	
10	DK	129	
10	FK	129	
10	HK	129	
11	AL	123	
11	DL	123	
11	FL	123	
11	HL	123	
12	AM	118	
12	DM	118	
12	FM	118	
12	HM	118	
13	AN	144	
13	DN	144	
13	FN	144	
13	HN	144	
14	AO	134	
14	DO	134	

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Mol	Chain	Length	Quality of chain
14	FO	134	
14	HO	134	
15	AP	89	
15	DP	89	
15	FP	89	
15	HP	89	
16	AQ	104	
16	DQ	104	
16	FQ	104	
16	HQ	104	
17	AT	66	
17	DT	66	
17	FT	66	
17	HT	66	
18	AU	206	
18	DU	206	
18	FU	206	
18	HU	206	
19	AX	189	
19	DX	189	
19	FX	189	
19	HX	189	
20	B2	154	
20	C2	154	
20	E2	154	

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Mol	Chain	Length	Quality of chain
20	G2	154	
21	B3	120	
21	C3	120	
21	E3	120	
21	G3	120	
22	BA	264	
22	CA	264	
22	EA	264	
22	GA	264	
23	BB	391	
23	CB	391	
23	EB	391	
23	GB	391	
24	BC	410	
24	CC	410	
24	EC	410	
24	GC	410	
25	BD	172	
25	CD	172	
25	ED	172	
25	GD	172	
26	BE	188	
26	CE	188	
26	EE	188	
26	GE	188	


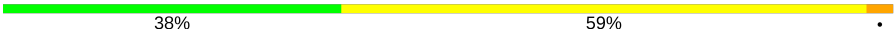


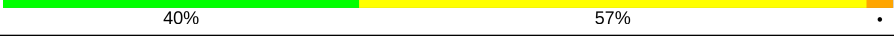
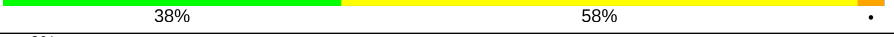
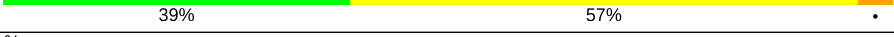

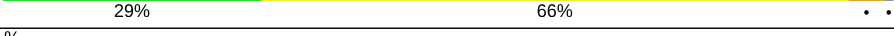


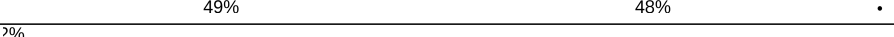

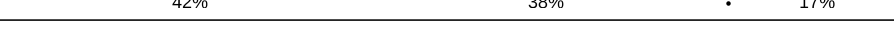


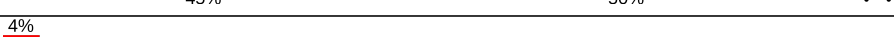

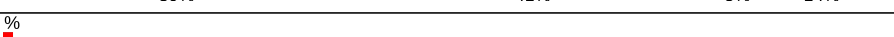
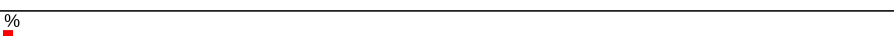

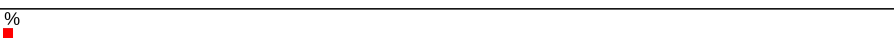
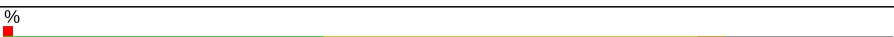
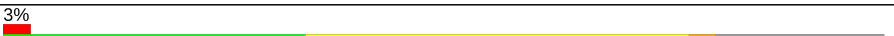

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Mol	Chain	Length	Quality of chain
27	BF	255	
27	CF	255	
27	EF	255	
27	GF	255	
28	BG	123	
28	CG	123	
28	EG	123	
28	GG	123	
29	BH	215	
29	CH	215	
29	EH	215	
29	GH	215	
30	BI	198	
30	CI	198	
30	EI	198	
30	GI	198	
31	BJ	141	
31	CJ	141	
31	EJ	141	
31	GJ	141	
32	BK	149	
32	CK	149	
32	EK	149	
32	GK	149	
33	BL	204	

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Mol	Chain	Length	Quality of chain
33	CL	204	
33	EL	204	
33	GL	204	
34	BM	301	
34	CM	301	
34	EM	301	
34	GM	301	
35	BN	181	
35	CN	181	
35	EN	181	
35	GN	181	
36	BO	185	
36	EO	185	
36	GO	185	
37	BP	157	
37	CP	157	
37	EP	157	
37	GP	157	
38	BQ	183	
38	CQ	183	
38	EQ	183	
38	GQ	183	
39	BR	150	
39	CR	150	
39	ER	150	

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Mol	Chain	Length	Quality of chain
39	GR	150	
40	BS	135	
40	CS	135	
40	ES	135	
40	GS	135	
41	BT	158	
41	CT	158	
41	ET	158	
41	GT	158	
42	BU	124	
42	CU	124	
42	EU	124	
42	GU	124	
43	BV	239	
43	CV	239	
43	EV	239	
43	GV	239	
44	BW	111	
44	CW	111	
44	EW	111	
44	GW	111	
45	BX	134	
45	CX	134	
45	EX	134	
45	GX	134	

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Mol	Chain	Length	Quality of chain
46	BY	103	
46	CY	103	
46	EY	103	
46	GY	103	
47	CO	185	

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
48	MG	A1	3422	-	-	-	X
48	MG	A1	3428	-	-	-	X
48	MG	A1	3430	-	-	-	X
48	MG	A1	3435	-	-	-	X
48	MG	A1	3437	-	-	-	X
48	MG	A1	3472	-	-	-	X
48	MG	A1	3522	-	-	-	X
48	MG	A1	3530	-	-	-	X
48	MG	A1	3555	-	-	-	X
48	MG	A1	3573	-	-	-	X
48	MG	A1	3579	-	-	-	X
48	MG	A1	3583	-	-	-	X
48	MG	A1	3585	-	-	-	X
48	MG	A1	3587	-	-	-	X
48	MG	A1	3593	-	-	-	X
48	MG	A1	3595	-	-	-	X
48	MG	C3	205	-	-	-	X
48	MG	C3	207	-	-	-	X
48	MG	D1	3424	-	-	-	X
48	MG	D1	3434	-	-	-	X
48	MG	D1	3446	-	-	-	X
48	MG	D1	3463	-	-	-	X
48	MG	D1	3497	-	-	-	X
48	MG	D1	3548	-	-	-	X
48	MG	D1	3550	-	-	-	X
48	MG	D1	3571	-	-	-	X
48	MG	D1	3576	-	-	-	X
48	MG	D1	3592	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	MG	D1	3596	-	-	-	X
48	MG	D1	3597	-	-	-	X
48	MG	D1	3600	-	-	-	X
48	MG	D1	3603	-	-	-	X
48	MG	D1	3606	-	-	-	X
48	MG	D1	3611	-	-	-	X
48	MG	D1	3624	-	-	-	X
48	MG	DJ	301	-	-	-	X
48	MG	E2	205	-	-	-	X
48	MG	E3	204	-	-	-	X
48	MG	F1	3411	-	-	-	X
48	MG	F1	3451	-	-	-	X
48	MG	F1	3493	-	-	-	X
48	MG	F1	3511	-	-	-	X
48	MG	F1	3515	-	-	-	X
48	MG	F1	3539	-	-	-	X
48	MG	F1	3560	-	-	-	X
48	MG	F1	3565	-	-	-	X
48	MG	F1	3566	-	-	-	X
48	MG	F1	3574	-	-	-	X
48	MG	F1	3576	-	-	-	X
48	MG	F1	3578	-	-	-	X
48	MG	G2	204	-	-	-	X
48	MG	G2	206	-	-	-	X
48	MG	G3	202	-	-	-	X
48	MG	G3	205	-	-	-	X
48	MG	GN	201	-	-	-	X
48	MG	GP	201	-	-	-	X
48	MG	H1	3409	-	-	-	X
48	MG	H1	3410	-	-	-	X
48	MG	H1	3412	-	-	-	X
48	MG	H1	3414	-	-	-	X
48	MG	H1	3450	-	-	-	X
48	MG	H1	3479	-	-	-	X
48	MG	H1	3489	-	-	-	X
48	MG	H1	3524	-	-	-	X
48	MG	H1	3531	-	-	-	X
48	MG	H1	3533	-	-	-	X
48	MG	H1	3534	-	-	-	X
48	MG	H1	3535	-	-	-	X
48	MG	H1	3536	-	-	-	X
48	MG	H1	3543	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	MG	H1	3544	-	-	-	X
48	MG	H1	3550	-	-	-	X
48	MG	H1	3551	-	-	-	X
48	MG	H1	3554	-	-	-	X

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 511395 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 RNA chain called 26S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	3119	Total	C	N	O	P	0	0	0
			66769	29861	12195	21594	3119			
1	D1	3119	Total	C	N	O	P	0	0	0
			66769	29861	12195	21594	3119			
1	F1	3119	Total	C	N	O	P	0	0	0
			66769	29861	12195	21594	3119			
1	H1	3119	Total	C	N	O	P	0	0	0
			66769	29861	12195	21594	3119			

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	91	Total	C	N	O	S	0	0	0
			721	440	158	116	7			
2	DA	91	Total	C	N	O	S	0	0	0
			721	440	158	116	7			
2	FA	91	Total	C	N	O	S	0	0	0
			721	440	158	116	7			
2	HA	91	Total	C	N	O	S	0	0	0
			721	440	158	116	7			

- Molecule 3 is a protein called RPL39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AB	51	Total	C	N	O	S	0	0	0
			456	288	97	70	1			
3	DB	51	Total	C	N	O	S	0	0	0
			456	288	97	70	1			
3	FB	51	Total	C	N	O	S	0	0	0
			456	288	97	70	1			
3	HB	51	Total	C	N	O	S	0	0	0
			456	288	97	70	1			

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AC	103	Total	C	N	O	S	0	0	0
			836	526	163	140	7			
4	DC	103	Total	C	N	O	S	0	0	0
			836	526	163	140	7			
4	FC	103	Total	C	N	O	S	0	0	0
			836	526	163	140	7			
4	HC	103	Total	C	N	O	S	0	0	0
			836	526	163	140	7			

- Molecule 5 is a protein called RPL6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	190	Total	C	N	O	S	0	0	0
			1525	966	286	272	1			
5	DE	190	Total	C	N	O	S	0	0	0
			1525	966	286	272	1			
5	FE	190	Total	C	N	O	S	0	0	0
			1525	966	286	272	1			
5	HE	190	Total	C	N	O	S	0	0	0
			1525	966	286	272	1			

- Molecule 6 is a protein called RPL14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	125	Total	C	N	O	S	0	0	0
			1021	659	192	169	1			
6	DF	125	Total	C	N	O	S	0	0	0
			1021	659	192	169	1			
6	FF	125	Total	C	N	O	S	0	0	0
			1021	659	192	169	1			
6	HF	125	Total	C	N	O	S	0	0	0
			1021	659	192	169	1			

- Molecule 7 is a protein called RPL30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	96	Total	C	N	O	S	0	0	0
			727	455	129	138	5			
7	DG	96	Total	C	N	O	S	0	0	0
			727	455	129	138	5			
7	FG	96	Total	C	N	O	S	0	0	0
			727	455	129	138	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	HG	96	Total	C	N	O	S	0	0	0
			727	455	129	138	5			

- Molecule 8 is a protein called RPL35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	107	Total	C	N	O	S	0	0	0
			850	540	167	142	1			
8	DH	107	Total	C	N	O	S	0	0	0
			850	540	167	142	1			
8	FH	107	Total	C	N	O	S	0	0	0
			850	540	167	142	1			
8	HH	107	Total	C	N	O	S	0	0	0
			850	540	167	142	1			

- Molecule 9 is a protein called TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	226	Total	C	N	O	S	0	0	0
			1716	1068	302	336	10			
9	DJ	226	Total	C	N	O	S	0	0	0
			1716	1068	302	336	10			
9	FJ	226	Total	C	N	O	S	0	0	0
			1716	1068	302	336	10			
9	HJ	226	Total	C	N	O	S	0	0	0
			1716	1068	302	336	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	-2	GLY	-	expression tag	UNP Q245F2
AJ	-1	THR	-	expression tag	UNP Q245F2
AJ	0	SER	-	expression tag	UNP Q245F2
DJ	-2	GLY	-	expression tag	UNP Q245F2
DJ	-1	THR	-	expression tag	UNP Q245F2
DJ	0	SER	-	expression tag	UNP Q245F2
FJ	-2	GLY	-	expression tag	UNP Q245F2
FJ	-1	THR	-	expression tag	UNP Q245F2
FJ	0	SER	-	expression tag	UNP Q245F2
HJ	-2	GLY	-	expression tag	UNP Q245F2
HJ	-1	THR	-	expression tag	UNP Q245F2

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Chain	Residue	Modelled	Actual	Comment	Reference
HJ	0	SER	-	expression tag	UNP Q245F2

- Molecule 10 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	52	Total	C	N	O	S	0	0	0
			415	257	83	69	6			
10	DK	52	Total	C	N	O	S	0	0	0
			415	257	83	69	6			
10	FK	52	Total	C	N	O	S	0	0	0
			415	257	83	69	6			
10	HK	52	Total	C	N	O	S	0	0	0
			415	257	83	69	6			

- Molecule 11 is a protein called RPL34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	108	Total	C	N	O	S	0	0	0
			852	529	170	147	6			
11	DL	108	Total	C	N	O	S	0	0	0
			852	529	170	147	6			
11	FL	108	Total	C	N	O	S	0	0	0
			852	529	170	147	6			
11	HL	108	Total	C	N	O	S	0	0	0
			852	529	170	147	6			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	100	Total	C	N	O	S	0	0	0
			819	530	137	151	1			
12	DM	100	Total	C	N	O	S	0	0	0
			819	530	137	151	1			
12	FM	100	Total	C	N	O	S	0	0	0
			819	530	137	151	1			
12	HM	100	Total	C	N	O	S	0	0	0
			819	530	137	151	1			

- Molecule 13 is a protein called RPL27.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	143	Total	C	N	O	S	0	0	0
			1170	755	213	199	3			
13	DN	143	Total	C	N	O	S	0	0	0
			1170	755	213	199	3			
13	FN	143	Total	C	N	O	S	0	0	0
			1170	755	213	199	3			
13	HN	143	Total	C	N	O	S	0	0	0
			1170	755	213	199	3			

- Molecule 14 is a protein called RPL28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	134	Total	C	N	O	S	0	0	0
			1034	650	204	179	1			
14	DO	134	Total	C	N	O	S	0	0	0
			1034	650	204	179	1			
14	FO	134	Total	C	N	O	S	0	0	0
			1034	650	204	179	1			
14	HO	134	Total	C	N	O	S	0	0	0
			1034	650	204	179	1			

- Molecule 15 is a protein called RPL38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	66	Total	C	N	O	S	0	0	0
			551	367	93	90	1			
15	DP	66	Total	C	N	O	S	0	0	0
			551	367	93	90	1			
15	FP	66	Total	C	N	O	S	0	0	0
			551	367	93	90	1			
15	HP	66	Total	C	N	O	S	0	0	0
			551	367	93	90	1			

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AQ	102	Total	C	N	O	0	0	0
			803	506	165	132			
16	DQ	102	Total	C	N	O	0	0	0
			803	506	165	132			
16	FQ	102	Total	C	N	O	0	0	0
			803	506	165	132			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	HQ	102	Total	C	N	O	0	0	0
			803	506	165	132			

- Molecule 17 is a protein called RPL29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AT	65	Total	C	N	O	0	0	0
			533	324	117	92			
17	DT	65	Total	C	N	O	0	0	0
			533	324	117	92			
17	FT	65	Total	C	N	O	0	0	0
			533	324	117	92			
17	HT	65	Total	C	N	O	0	0	0
			533	324	117	92			

- Molecule 18 is a protein called RPL13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AU	203	Total	C	N	O	S	0	0	0
			1624	1015	328	279	2			
18	DU	203	Total	C	N	O	S	0	0	0
			1624	1015	328	279	2			
18	FU	203	Total	C	N	O	S	0	0	0
			1624	1015	328	279	2			
18	HU	203	Total	C	N	O	S	0	0	0
			1624	1015	328	279	2			

- Molecule 19 is a protein called RPL18A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AX	188	Total	C	N	O	S	0	0	0
			1536	972	287	271	6			
19	DX	188	Total	C	N	O	S	0	0	0
			1536	972	287	271	6			
19	FX	188	Total	C	N	O	S	0	0	0
			1536	972	287	271	6			
19	HX	188	Total	C	N	O	S	0	0	0
			1536	972	287	271	6			

- Molecule 20 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	B2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			
20	C2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			
20	E2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			
20	G2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			

- Molecule 21 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	B3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			
21	C3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			
21	E3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			
21	G3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			

- Molecule 22 is a protein called RPL8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			
22	CA	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			
22	EA	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			
22	GA	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			
23	CB	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			
23	EB	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	GB	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			

- Molecule 24 is a protein called RPL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			
24	CC	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			
24	EC	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			
24	GC	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			
25	CD	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			
25	ED	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			
25	GD	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			
26	CE	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			
26	EE	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			
26	GE	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			

- Molecule 27 is a protein called RPL7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			
27	CF	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			
27	EF	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			
27	GF	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			

- Molecule 28 is a protein called RPLP0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	BG	123	Total	C	N	O	0	0	0
			711	465	123	123			
28	CG	123	Total	C	N	O	0	0	0
			711	465	123	123			
28	EG	123	Total	C	N	O	0	0	0
			711	465	123	123			
28	GG	123	Total	C	N	O	0	0	0
			711	465	123	123			

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			
29	CH	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			
29	EH	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			
29	GH	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			
30	CI	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			
30	EI	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	GI	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			

- Molecule 31 is a protein called RPL23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			
31	CJ	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			
31	EJ	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			
31	GJ	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			
32	CK	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			
32	EK	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			
32	GK	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			

- Molecule 33 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			
33	CL	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			
33	EL	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			
33	GL	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	298	Total	C	N	O	S	0	0	0
			2409	1530	445	430	4			
34	CM	300	Total	C	N	O	S	0	0	0
			2424	1541	447	432	4			
34	EM	300	Total	C	N	O	S	0	0	0
			2424	1541	447	432	4			
34	GM	300	Total	C	N	O	S	0	0	0
			2424	1541	447	432	4			

- Molecule 35 is a protein called RPL18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			
35	CN	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			
35	EN	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			
35	GN	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			

- Molecule 36 is a protein called RPL19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	184	Total	C	N	O	S	0	0	0
			1491	924	311	251	5			
36	EO	146	Total	C	N	O	S	0	0	0
			1192	745	249	193	5			
36	GO	153	Total	C	N	O	S	0	0	0
			1234	772	256	201	5			

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			
37	CP	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			
37	EP	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			
37	GP	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			

- Molecule 38 is a protein called RPL17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			
38	CQ	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			
38	EQ	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			
38	GQ	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			

- Molecule 39 is a protein called RPL23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			
39	CR	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			
39	ER	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			
39	GR	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			

- Molecule 40 is a protein called RPL26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			
40	CS	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			
40	ES	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			
40	GS	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			

- Molecule 41 is a protein called RPL24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			
41	CT	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			
41	ET	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	GT	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			

- Molecule 42 is a protein called RPL35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	123	Total	C	N	O		0	0	0
			990	629	196	165				
42	CU	123	Total	C	N	O		0	0	0
			990	629	196	165				
42	EU	123	Total	C	N	O		0	0	0
			990	629	196	165				
42	GU	123	Total	C	N	O		0	0	0
			990	629	196	165				

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			
43	CV	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			
43	EV	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			
43	GV	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			
44	CW	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			
44	EW	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			
44	GW	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			
45	CX	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			
45	EX	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			
45	GX	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			

- Molecule 46 is a protein called RPL37A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			
46	CY	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			
46	EY	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			
46	GY	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			

- Molecule 47 is a protein called RPL19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CO	175	Total	C	N	O	S	0	0	0
			1366	861	278	222	5			

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
48	DK	1	Total	Mg	0	0
			1	1		
48	AK	1	Total	Mg	0	0
			1	1		
48	DQ	1	Total	Mg	0	0
			1	1		
48	G3	5	Total	Mg	0	0
			5	5		
48	E3	6	Total	Mg	0	0
			6	6		
48	EN	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
48	BL	1	Total 1	Mg 1	0	0
48	GJ	1	Total 1	Mg 1	0	0
48	GA	1	Total 1	Mg 1	0	0
48	FK	1	Total 1	Mg 1	0	0
48	CD	1	Total 1	Mg 1	0	0
48	BP	1	Total 1	Mg 1	0	0
48	GN	1	Total 1	Mg 1	0	0
48	EQ	1	Total 1	Mg 1	0	0
48	CY	1	Total 1	Mg 1	0	0
48	G2	6	Total 6	Mg 6	0	0
48	E2	7	Total 7	Mg 7	0	0
48	B2	8	Total 8	Mg 8	0	0
48	AA	2	Total 2	Mg 2	0	0
48	BQ	2	Total 2	Mg 2	0	0
48	CQ	2	Total 2	Mg 2	0	0
48	BJ	1	Total 1	Mg 1	0	0
48	EW	2	Total 2	Mg 2	0	0
48	FA	2	Total 2	Mg 2	0	0
48	H1	155	Total 155	Mg 155	0	0
48	A1	200	Total 200	Mg 200	0	0
48	CN	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
48	BN	1	Total 1	Mg 1	0	0
48	GQ	1	Total 1	Mg 1	0	0
48	B3	3	Total 3	Mg 3	0	0
48	CJ	1	Total 1	Mg 1	0	0
48	GL	1	Total 1	Mg 1	0	0
48	DA	2	Total 2	Mg 2	0	0
48	HT	1	Total 1	Mg 1	0	0
48	C3	7	Total 7	Mg 7	0	0
48	GW	1	Total 1	Mg 1	0	0
48	EL	2	Total 2	Mg 2	0	0
48	D1	232	Total 232	Mg 232	0	0
48	DJ	1	Total 1	Mg 1	0	0
48	GP	2	Total 2	Mg 2	0	0
48	FT	1	Total 1	Mg 1	0	0
48	CW	1	Total 1	Mg 1	0	0
48	F1	184	Total 184	Mg 184	0	0
48	EJ	1	Total 1	Mg 1	0	0
48	C2	6	Total 6	Mg 6	0	0
48	BW	1	Total 1	Mg 1	0	0
48	GO	1	Total 1	Mg 1	0	0
48	CL	2	Total 2	Mg 2	0	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
49	FA	1	Total	Zn	0	0
			1	1		
49	HK	1	Total	Zn	0	0
			1	1		
49	DK	1	Total	Zn	0	0
			1	1		
49	AK	1	Total	Zn	0	0
			1	1		
49	DC	1	Total	Zn	0	0
			1	1		
49	BY	1	Total	Zn	0	0
			1	1		
49	AC	1	Total	Zn	0	0
			1	1		
49	DL	1	Total	Zn	0	0
			1	1		
49	HL	1	Total	Zn	0	0
			1	1		
49	FK	1	Total	Zn	0	0
			1	1		
49	AA	1	Total	Zn	0	0
			1	1		
49	DA	1	Total	Zn	0	0
			1	1		
49	EY	1	Total	Zn	0	0
			1	1		
49	HC	1	Total	Zn	0	0
			1	1		
49	GY	1	Total	Zn	0	0
			1	1		
49	FC	1	Total	Zn	0	0
			1	1		
49	FL	1	Total	Zn	0	0
			1	1		
49	AL	1	Total	Zn	0	0
			1	1		
49	CY	1	Total	Zn	0	0
			1	1		
49	HA	1	Total	Zn	0	0
			1	1		

- Molecule 50 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	A1	1134	Total 1134	O 1134	0	0
50	AA	8	Total 8	O 8	0	0
50	AB	5	Total 5	O 5	0	0
50	AH	1	Total 1	O 1	0	0
50	AK	3	Total 3	O 3	0	0
50	AM	1	Total 1	O 1	0	0
50	AP	2	Total 2	O 2	0	0
50	AT	3	Total 3	O 3	0	0
50	AU	4	Total 4	O 4	0	0
50	B2	54	Total 54	O 54	0	0
50	B3	23	Total 23	O 23	0	0
50	BA	12	Total 12	O 12	0	0
50	BB	4	Total 4	O 4	0	0
50	BC	7	Total 7	O 7	0	0
50	BE	1	Total 1	O 1	0	0
50	BI	3	Total 3	O 3	0	0
50	BJ	5	Total 5	O 5	0	0
50	BK	3	Total 3	O 3	0	0
50	BL	8	Total 8	O 8	0	0
50	BM	2	Total 2	O 2	0	0
50	BN	5	Total 5	O 5	0	0
50	BO	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	BP	5	Total	O	0	0
			5	5		
50	BQ	7	Total	O	0	0
			7	7		
50	BU	1	Total	O	0	0
			1	1		
50	BV	7	Total	O	0	0
			7	7		
50	BW	5	Total	O	0	0
			5	5		
50	BX	6	Total	O	0	0
			6	6		
50	BY	5	Total	O	0	0
			5	5		
50	C2	46	Total	O	0	0
			46	46		
50	C3	39	Total	O	0	0
			39	39		
50	CA	11	Total	O	0	0
			11	11		
50	CB	4	Total	O	0	0
			4	4		
50	CC	7	Total	O	0	0
			7	7		
50	CD	4	Total	O	0	0
			4	4		
50	CE	2	Total	O	0	0
			2	2		
50	CI	1	Total	O	0	0
			1	1		
50	CJ	4	Total	O	0	0
			4	4		
50	CK	3	Total	O	0	0
			3	3		
50	CL	12	Total	O	0	0
			12	12		
50	CM	6	Total	O	0	0
			6	6		
50	CN	7	Total	O	0	0
			7	7		
50	CO	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	CP	6	Total 6	O 6	0	0
50	CQ	7	Total 7	O 7	0	0
50	CU	1	Total 1	O 1	0	0
50	CV	4	Total 4	O 4	0	0
50	CW	5	Total 5	O 5	0	0
50	CX	6	Total 6	O 6	0	0
50	CY	5	Total 5	O 5	0	0
50	D1	1341	Total 1341	O 1341	0	0
50	DA	10	Total 10	O 10	0	0
50	DB	4	Total 4	O 4	0	0
50	DE	1	Total 1	O 1	0	0
50	DJ	2	Total 2	O 2	0	0
50	DK	2	Total 2	O 2	0	0
50	DP	1	Total 1	O 1	0	0
50	DQ	2	Total 2	O 2	0	0
50	DT	4	Total 4	O 4	0	0
50	DU	3	Total 3	O 3	0	0
50	DX	2	Total 2	O 2	0	0
50	E2	44	Total 44	O 44	0	0
50	E3	34	Total 34	O 34	0	0
50	EA	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	EB	3	Total 3	O 3	0	0
50	EC	2	Total 2	O 2	0	0
50	EE	2	Total 2	O 2	0	0
50	EJ	4	Total 4	O 4	0	0
50	EK	5	Total 5	O 5	0	0
50	EL	10	Total 10	O 10	0	0
50	EM	2	Total 2	O 2	0	0
50	EN	7	Total 7	O 7	0	0
50	EP	6	Total 6	O 6	0	0
50	EQ	4	Total 4	O 4	0	0
50	EV	6	Total 6	O 6	0	0
50	EW	7	Total 7	O 7	0	0
50	EX	5	Total 5	O 5	0	0
50	EY	5	Total 5	O 5	0	0
50	F1	1076	Total 1076	O 1076	0	0
50	FA	7	Total 7	O 7	0	0
50	FB	4	Total 4	O 4	0	0
50	FE	1	Total 1	O 1	0	0
50	FH	1	Total 1	O 1	0	0
50	FK	2	Total 2	O 2	0	0
50	FL	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	FP	2	Total	O	0	0
			2	2		
50	FT	4	Total	O	0	0
			4	4		
50	FU	4	Total	O	0	0
			4	4		
50	G2	34	Total	O	0	0
			34	34		
50	G3	26	Total	O	0	0
			26	26		
50	GA	6	Total	O	0	0
			6	6		
50	GB	3	Total	O	0	0
			3	3		
50	GC	2	Total	O	0	0
			2	2		
50	GE	2	Total	O	0	0
			2	2		
50	GI	1	Total	O	0	0
			1	1		
50	GJ	4	Total	O	0	0
			4	4		
50	GK	2	Total	O	0	0
			2	2		
50	GL	5	Total	O	0	0
			5	5		
50	GM	1	Total	O	0	0
			1	1		
50	GN	2	Total	O	0	0
			2	2		
50	GO	2	Total	O	0	0
			2	2		
50	GP	5	Total	O	0	0
			5	5		
50	GQ	4	Total	O	0	0
			4	4		
50	GV	3	Total	O	0	0
			3	3		
50	GW	4	Total	O	0	0
			4	4		
50	GX	5	Total	O	0	0
			5	5		

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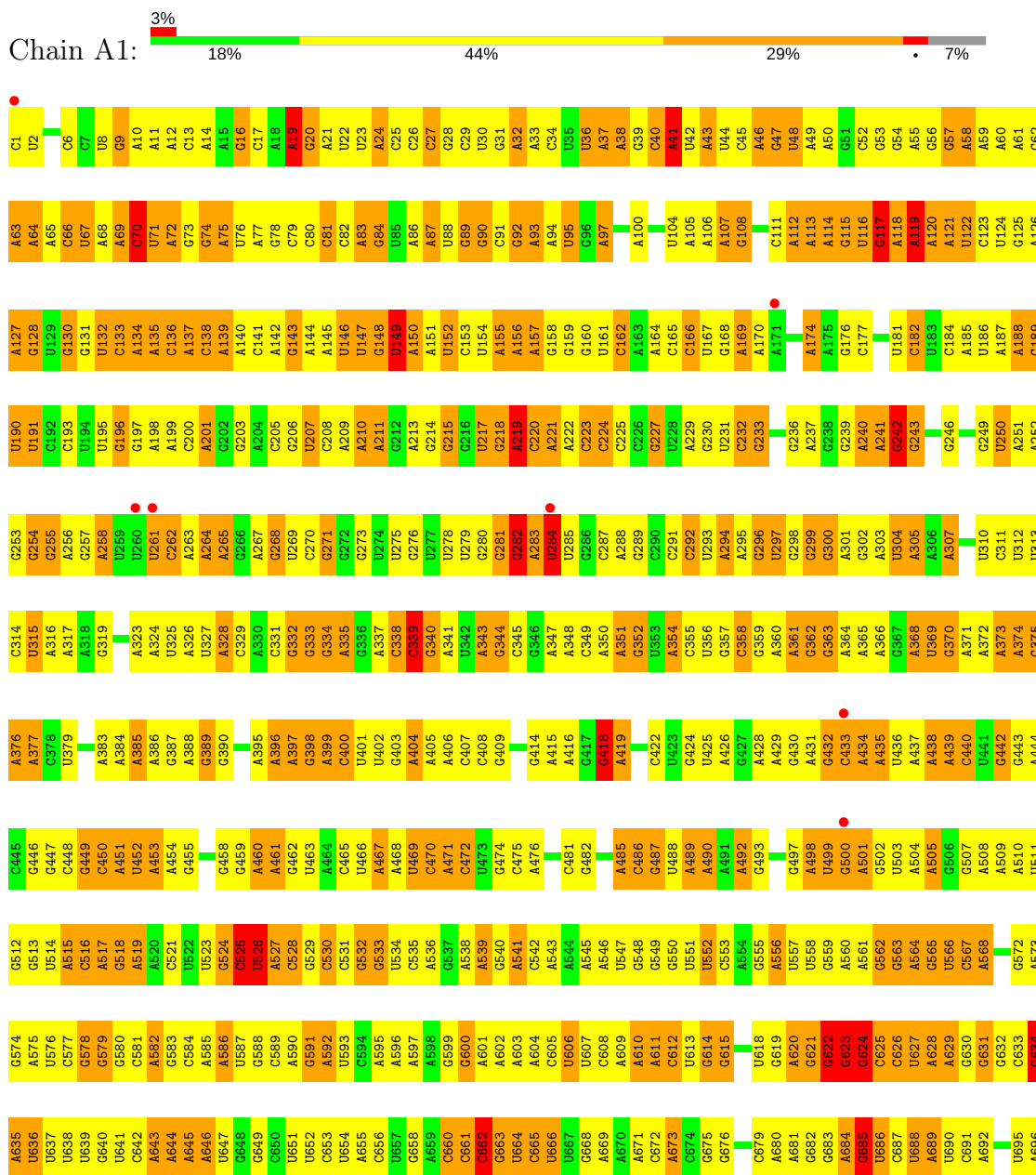
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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50	H1	924	Total 924	O 924	0	0
50	HA	4	Total 4	O 4	0	0
50	HB	4	Total 4	O 4	0	0
50	HJ	2	Total 2	O 2	0	0
50	HK	2	Total 2	O 2	0	0
50	HP	1	Total 1	O 1	0	0
50	HT	5	Total 5	O 5	0	0
50	HU	2	Total 2	O 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 26S rRNA









## Chain D1:

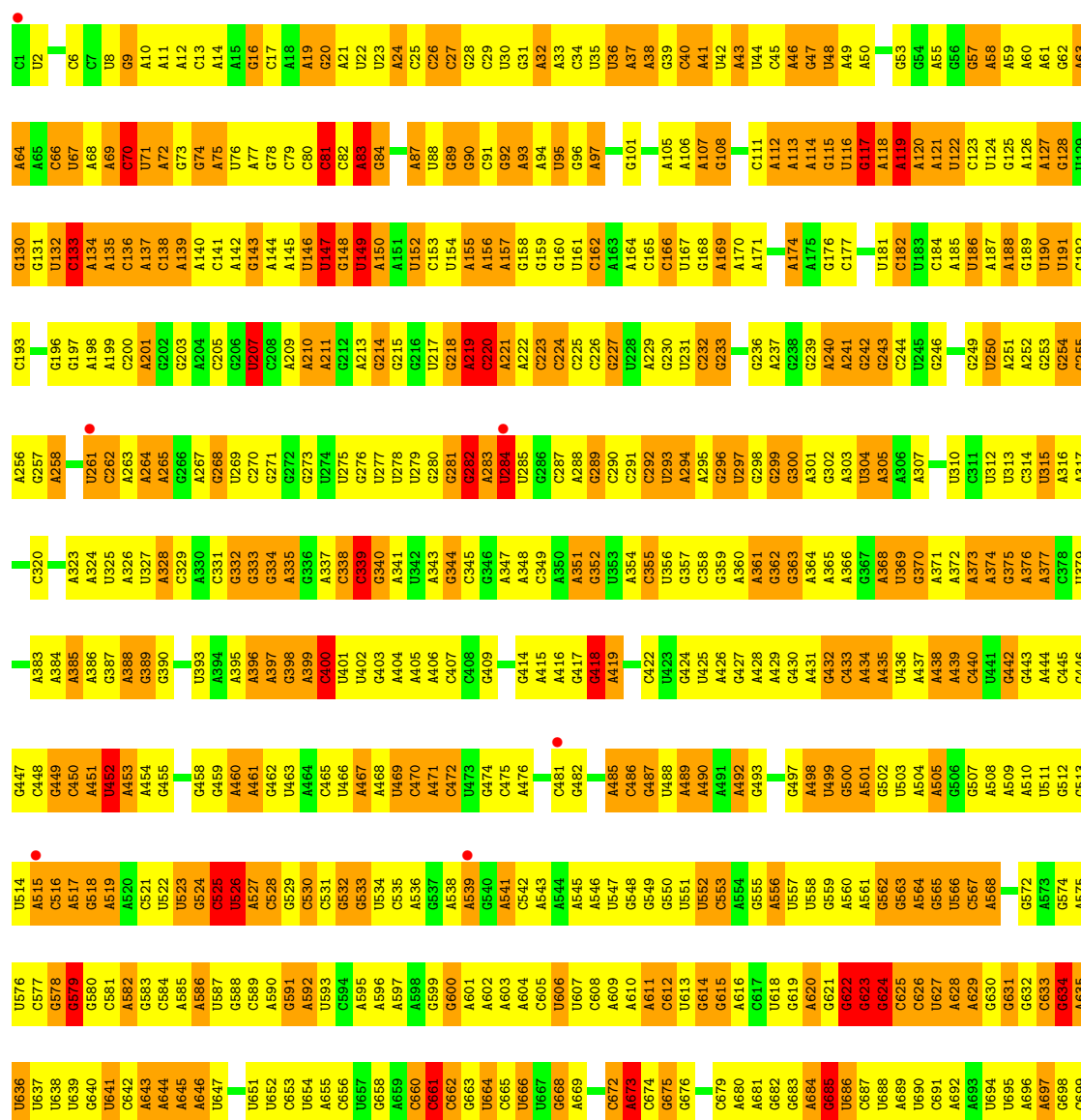
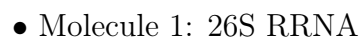


U1076	U1077	U1078	A1079	U1083	G1084	U1085	A1086	U1087	A1088	G1089	A1090	G1091	C1092	C1093	G1094	C1095	G1096	U1097	A1098	G1099	U1100	U1101	U1102	A1103	C1104	C1105	G1106	A1107	A1108	A1109	U1110	G1111	U1112	A1113	A1114	C1115	U1116	U1117	G1121	A1122	A1123	G1124	A1125	U1126	U1127	G1128	C1129	A1130	U1131	U1132	U1133	G1134	U1135	C1136	U1137	U1138	A1139																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U1011	U1012	U1013	U1016	U1017	A1018	G1019	U1020	U1021	A1022	U1023	A1024	G1025	U1026	G1027	A1028	U1034	A1035	A1036	U1037	G1038	U1039	A1040	U1041	C1042	C1043	G1044	U1045	U1046	U1047	U1048	U1049	U1050	C1051	C1052	A1053	A1054	A1055	U1056	U1057	C1058	A1059	C1060	G1061	A1062	U1063	C1064	U1065	A1066	U1067	U1068	C1069	U1070	U1071	A1072	U1073	U1074	C1075																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C948	G949	A950	A951	C952	C953	U957	A958	G959	U960	A961	U962	C963	U964	U965	U966	U967	U968	C969	C970	A971	U972	C973	C974	G975	A976	A977	C978	U979	U980	U981	C982	U983	C984	C985	C986	A987	G988	G989	A990	U991	A992	C993	C994	A995	A996	G997	A998	G999	U1002	G1003	U1004	A1005	A1006	C942	C943	U944	U945	A1008	A1009	G1010																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U191	C192	G193	U194	U195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347



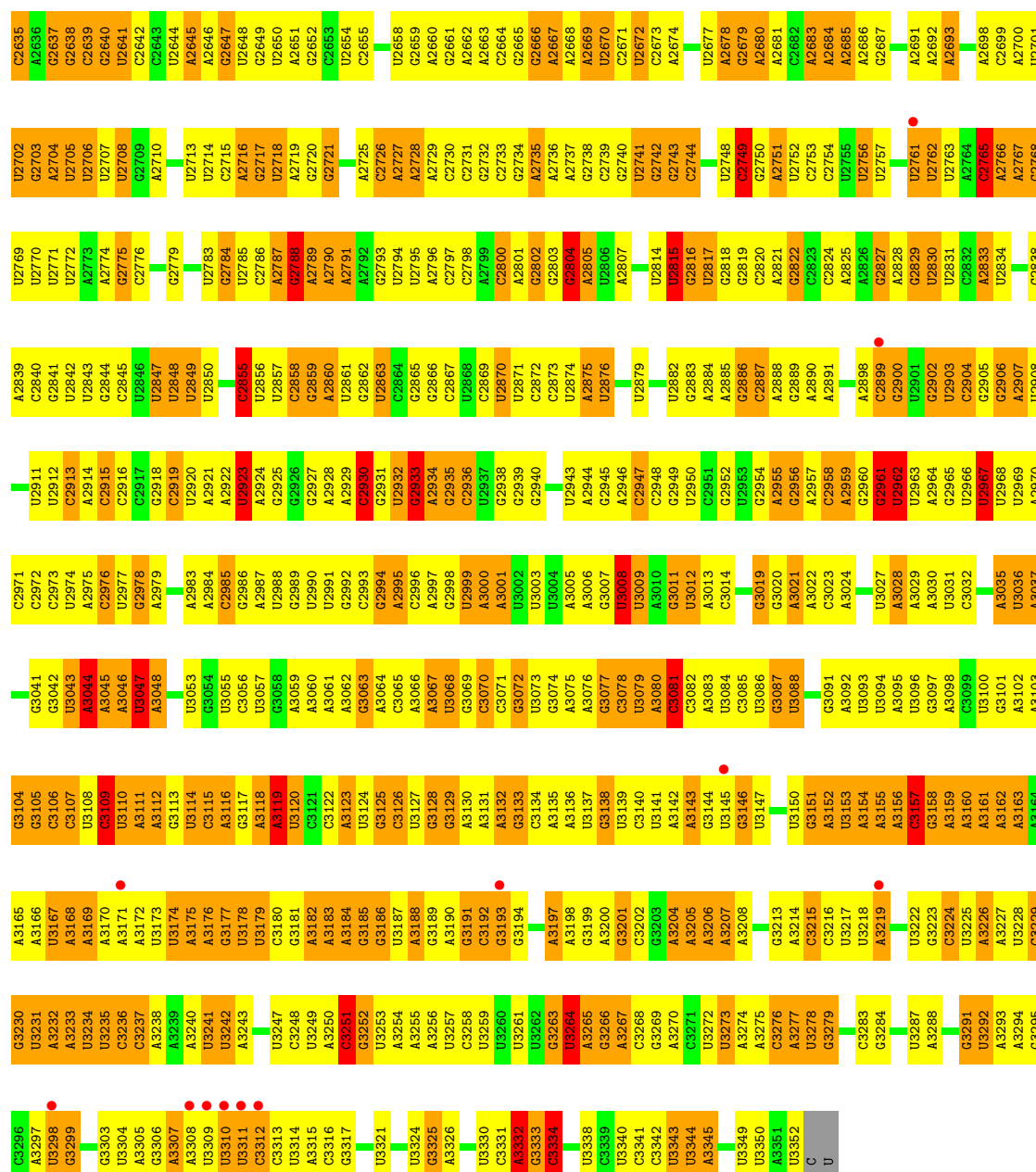
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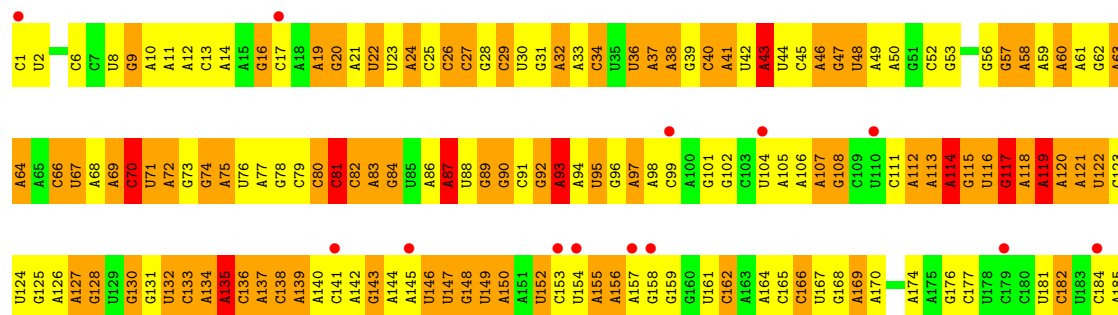
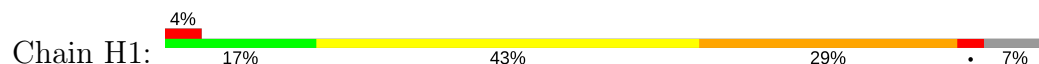


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	G1545	C1354	C1414	G	A1231	A1170	A1107	G1045	U982	G840	C775	U711
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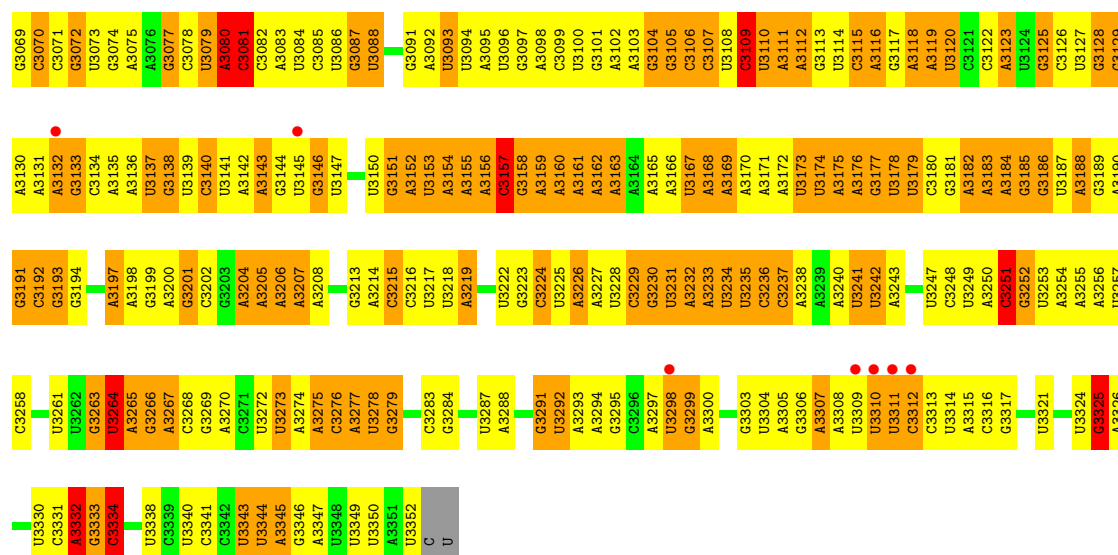


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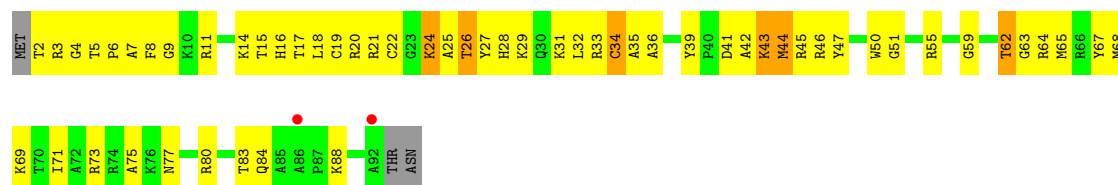
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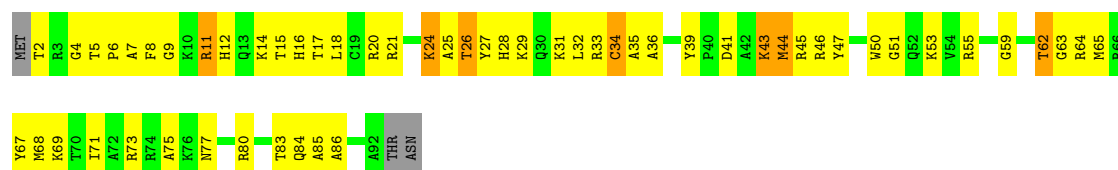
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A3013	A2885		G2817	C2749		U2620	C2557	C	U2431	A2368	G2306	G2245	U2171	G2109
G3014	G2886		U2817	A2750	A2683	G2621	U2558	C	A2432	A2369	A2307	G2246	G2172	G2110
	C2887		G2818	G2751	A2684	U2622	U2559	A	G2433	G2370	A2308	A2247	A2173	G2111
G3019	A2888			U2752	A2685	U2623	U2560	C	A2434	G2371	U2309	G2248		G2112
G3020	G2889		A2821	C2753	A2686	A2624	A2561	G	A2435		G2310	U2249		A2113
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C3065	G2931		G2865	A2729		A2663	U2601		A	A2414	A2351	C2288	U2220	U2151
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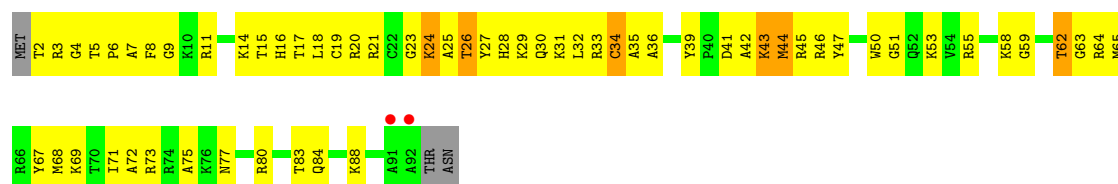
• Molecule 2: RIBOSOMAL PROTEIN L37



• Molecule 2: RIBOSOMAL PROTEIN L37

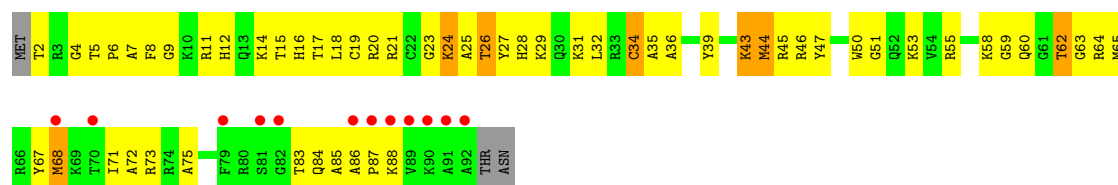


• Molecule 2: RIBOSOMAL PROTEIN L37



• Molecule 2: RIBOSOMAL PROTEIN L37





• Molecule 3: RPL39



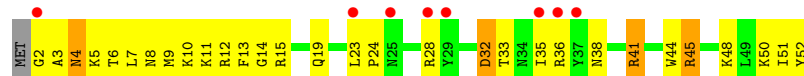
• Molecule 3: RPL39



• Molecule 3: RPL39



• Molecule 3: RPL39



• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



• Molecule 4: 60S RIBOSOMAL PROTEIN L36A

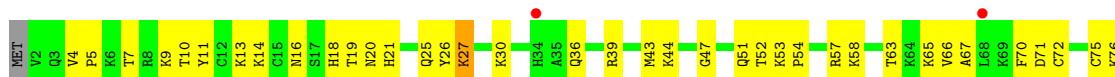




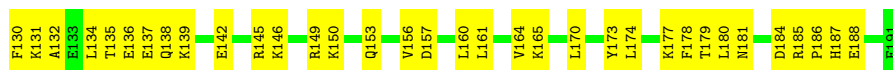
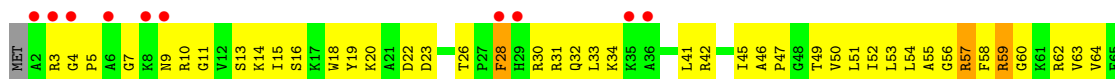
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



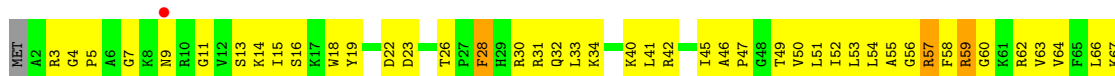
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



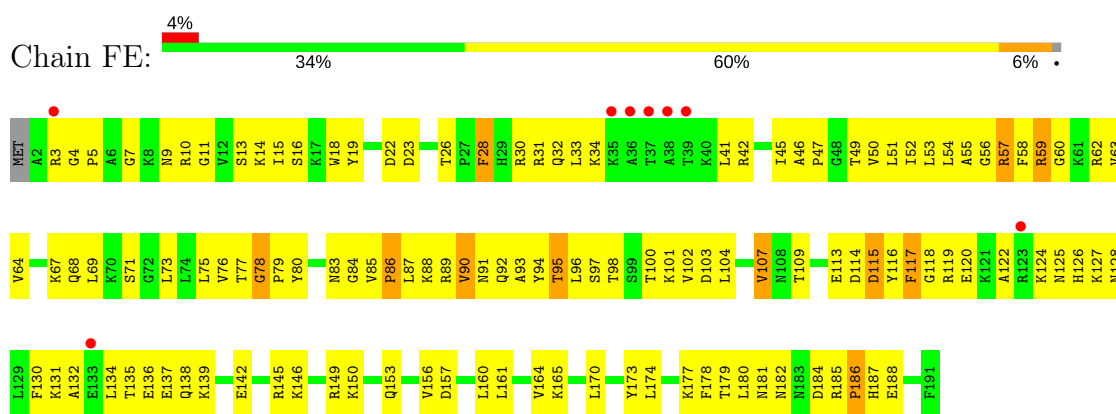
• Molecule 5: RPL6



• Molecule 5: RPL6



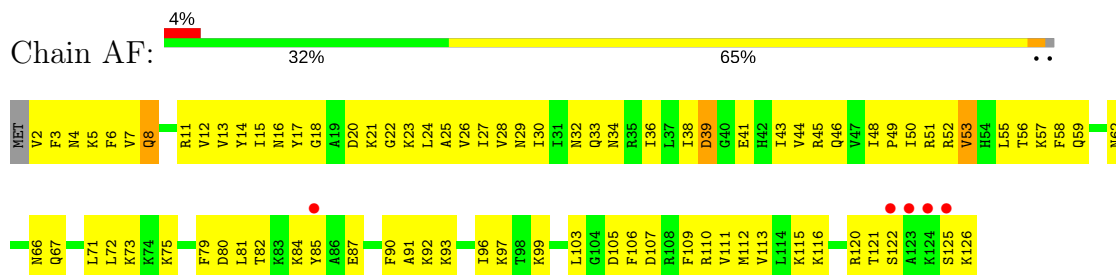
• Molecule 5: RPL6



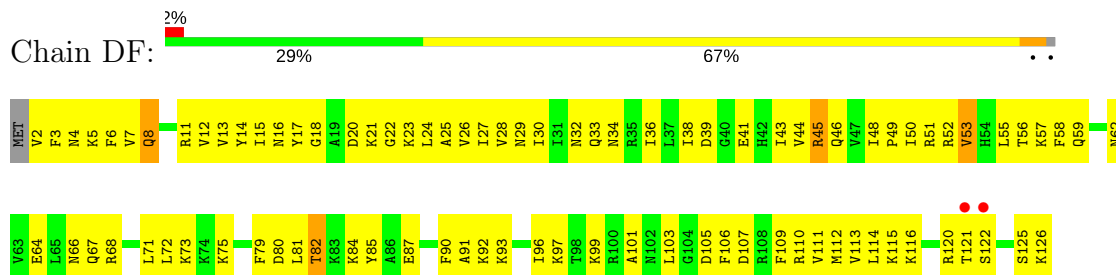
• Molecule 5: RPL6



• Molecule 6: RPL14

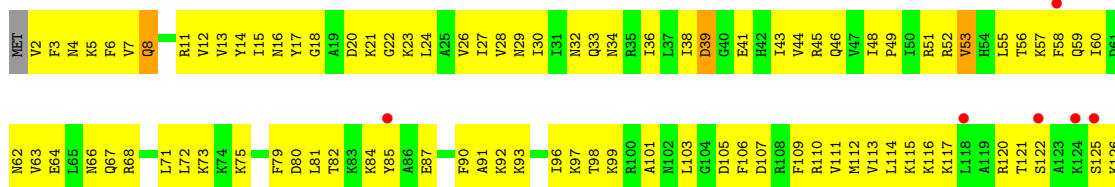


• Molecule 6: RPL14

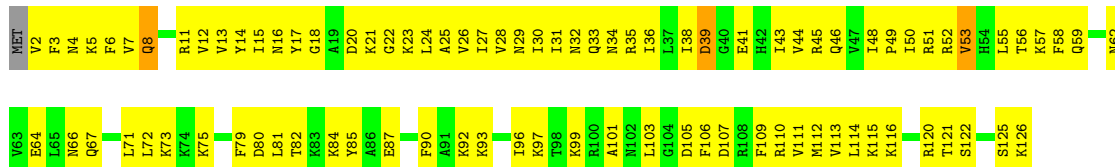
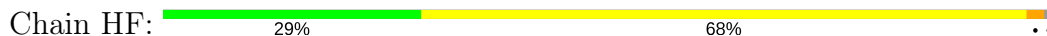


• Molecule 6: RPL14

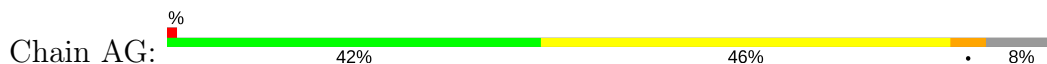




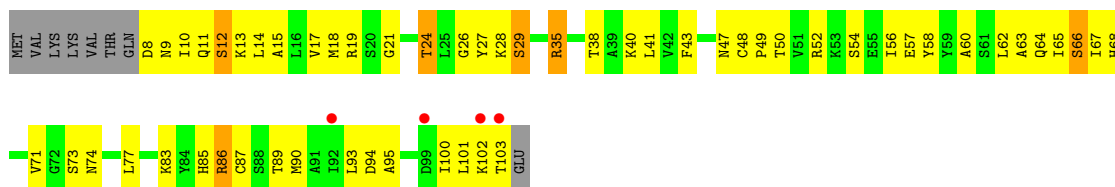
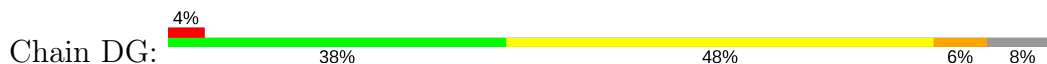
• Molecule 6: RPL14



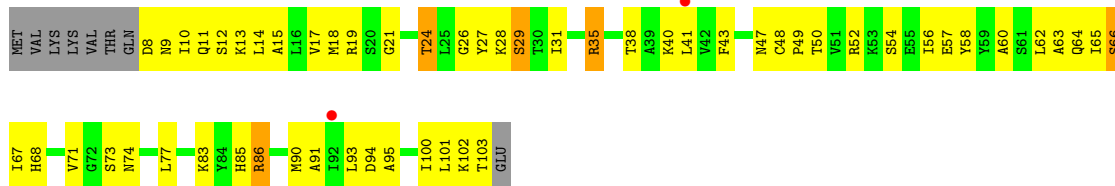
• Molecule 7: RPL30



• Molecule 7: RPL30

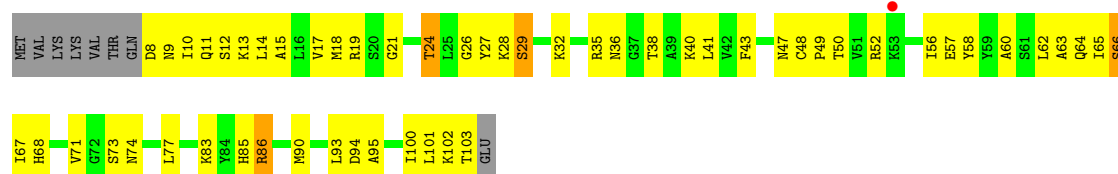


• Molecule 7: RPL30

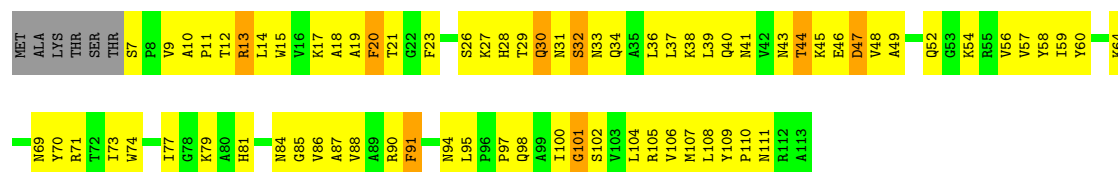


• Molecule 7: RPL30

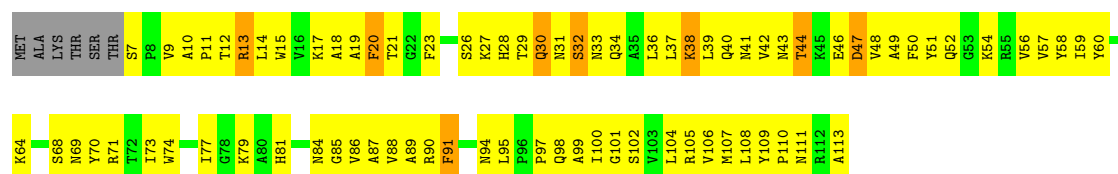
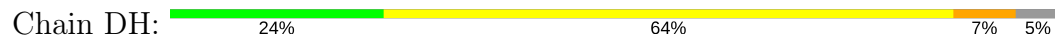




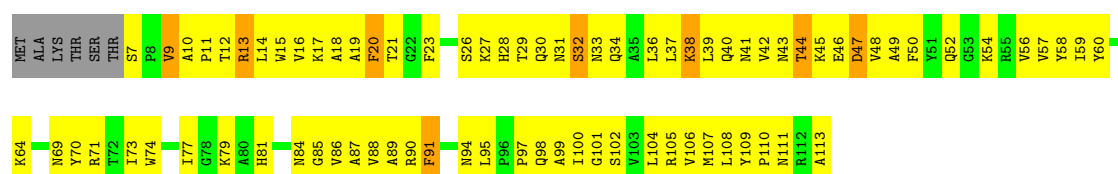
• Molecule 8: RPL35A



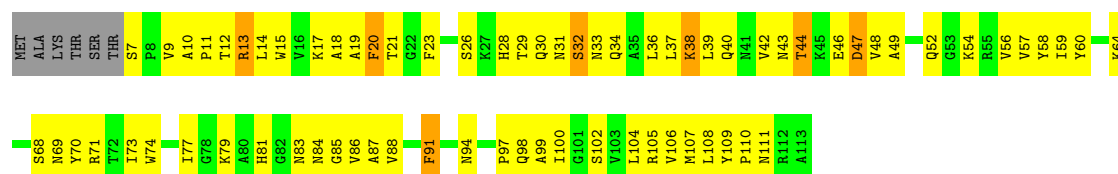
• Molecule 8: RPL35A



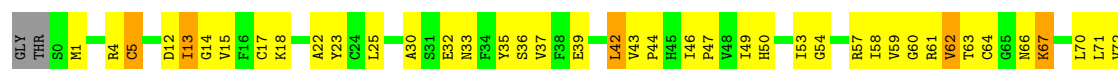
• Molecule 8: RPL35A

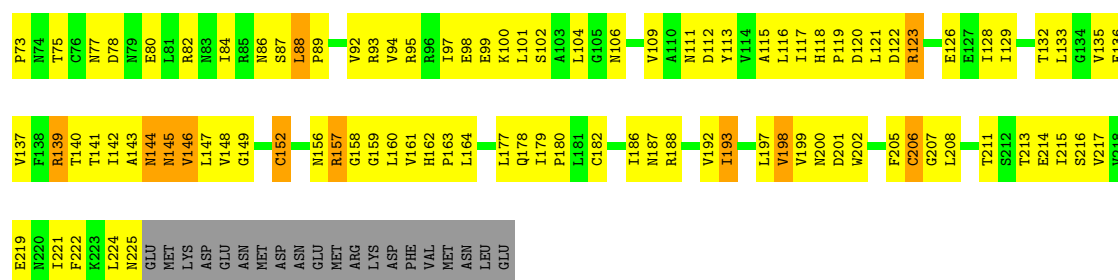


• Molecule 8: RPL35A



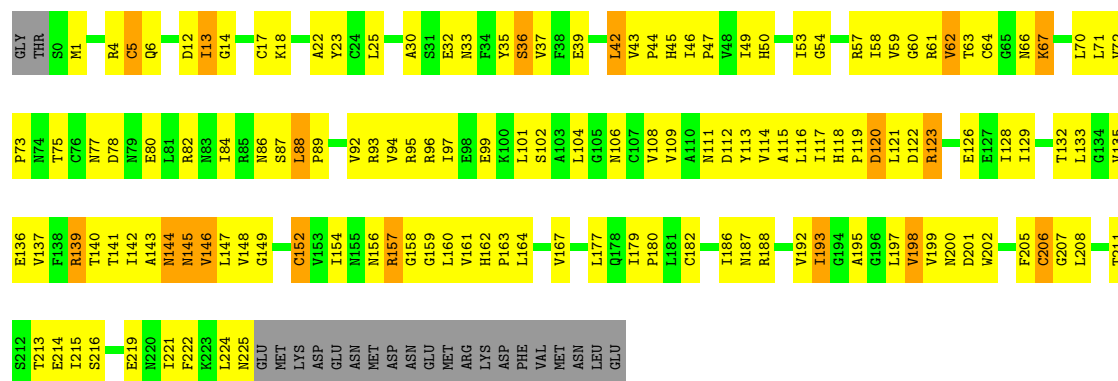
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN





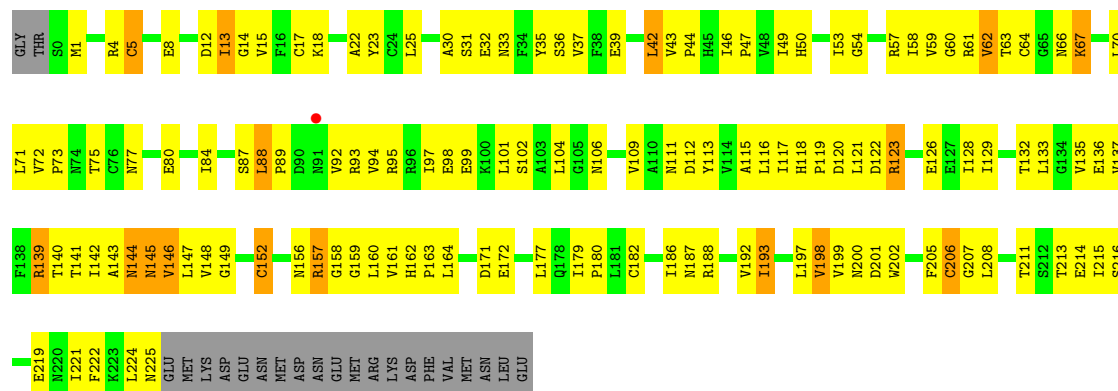
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain DJ: 35% 49% 7% 9%



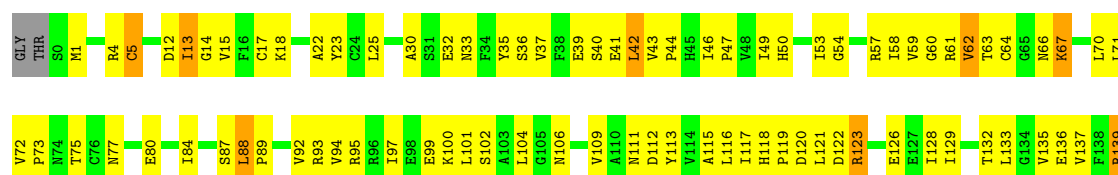
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain FJ: 37% 48% 6% 9%

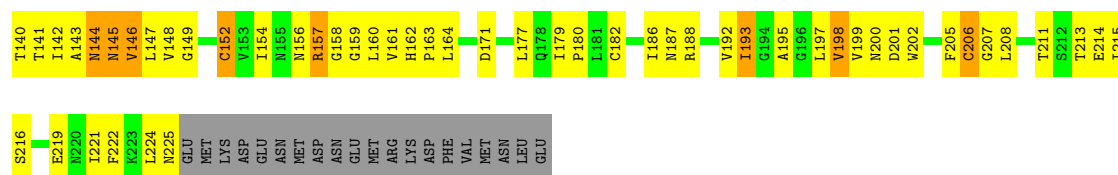


• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

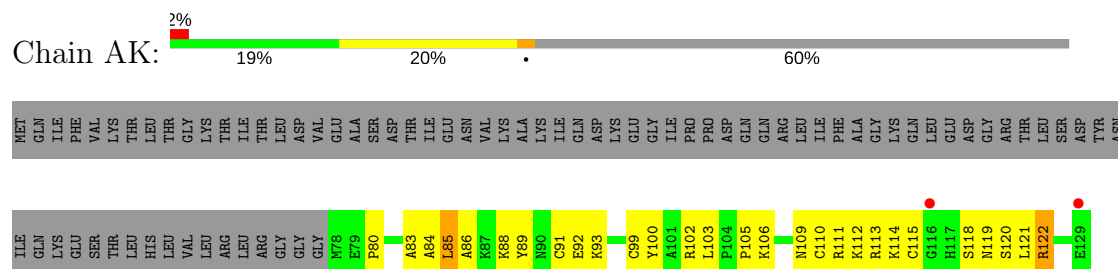
Chain HJ: 36% 48% 6% 9%



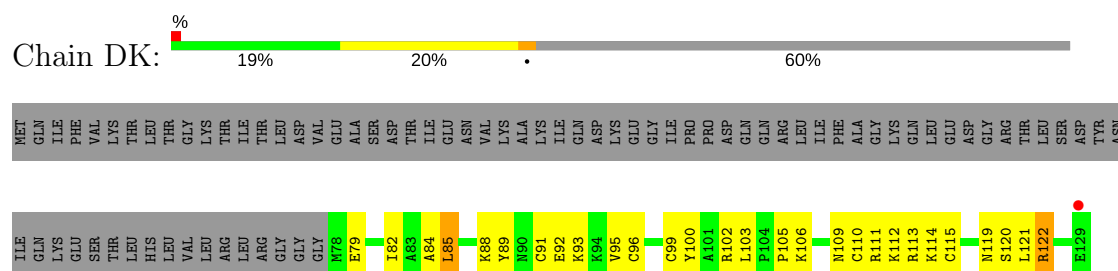




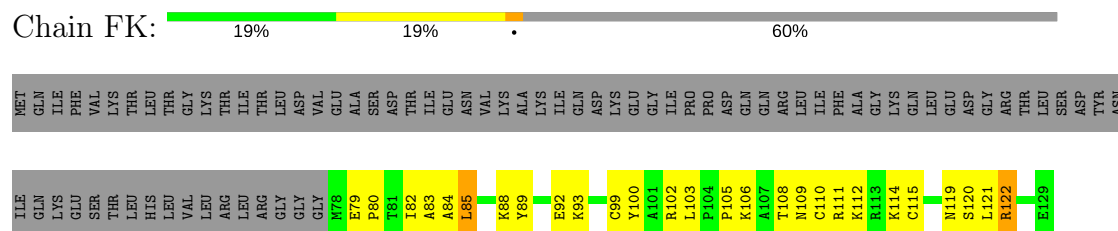
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



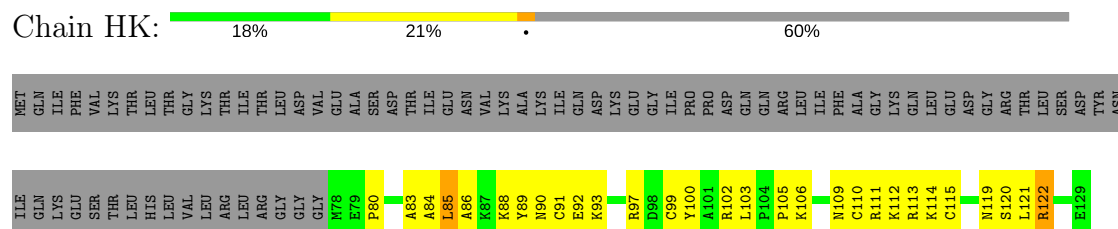
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



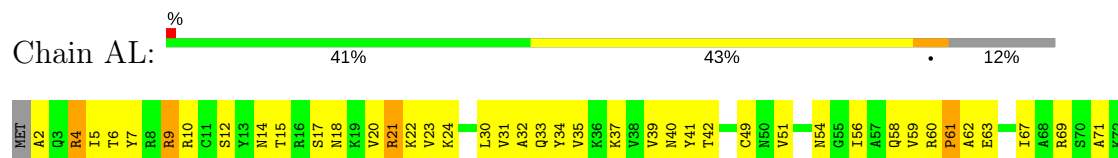
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

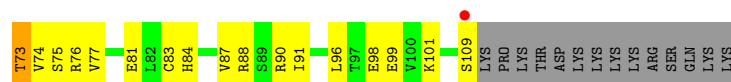


- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



- Molecule 11: RPL34





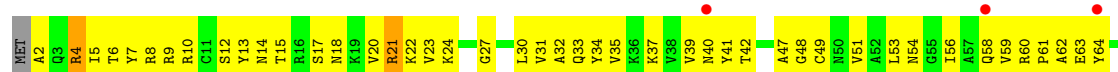
• Molecule 11: RPL34



• Molecule 11: RPL34



• Molecule 11: RPL34

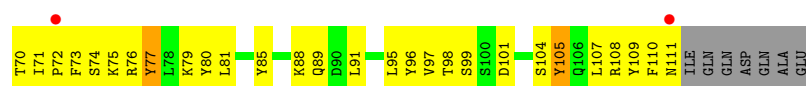


• Molecule 12: RIBOSOMAL PROTEIN L22

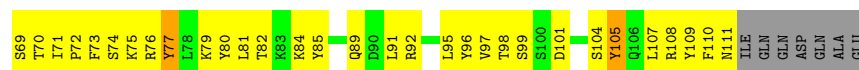


• Molecule 12: RIBOSOMAL PROTEIN L22





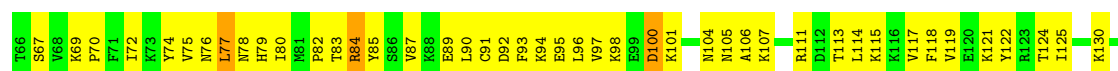
• Molecule 12: RIBOSOMAL PROTEIN L22



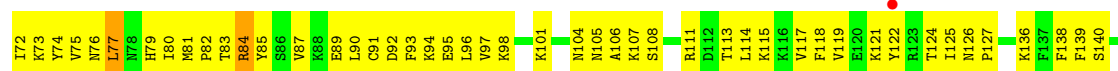
• Molecule 12: RIBOSOMAL PROTEIN L22



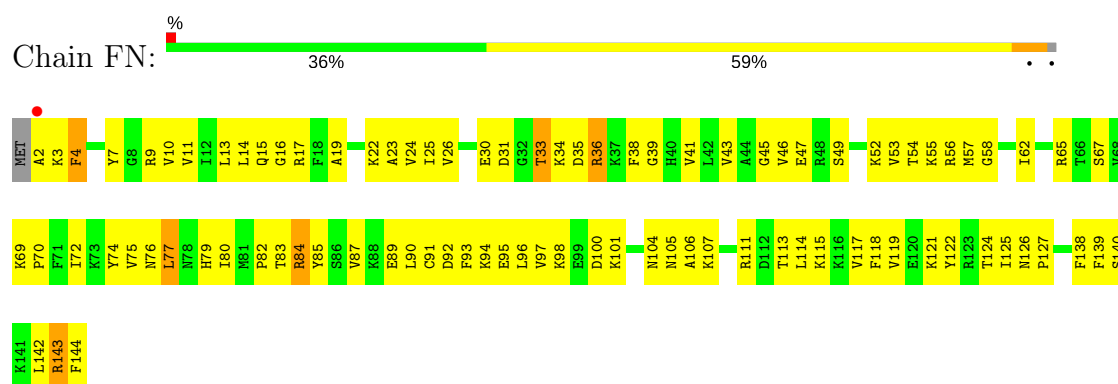
• Molecule 13: RPL27



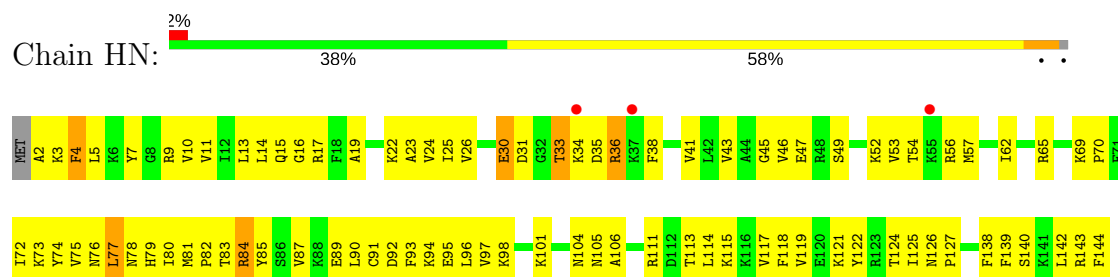
• Molecule 13: RPL27



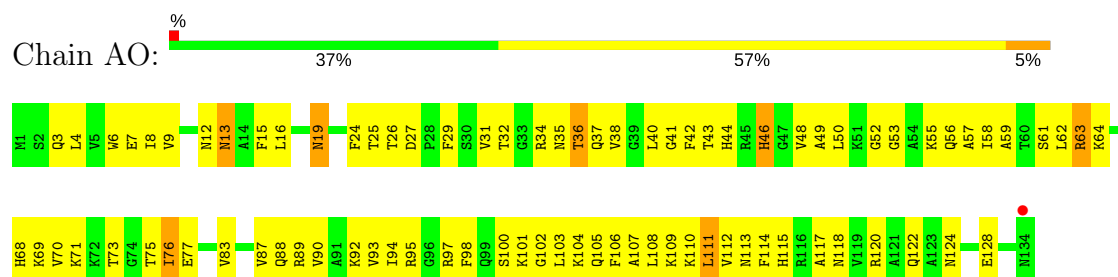
• Molecule 13: RPL27



• Molecule 13: RPL27



• Molecule 14: RPL28



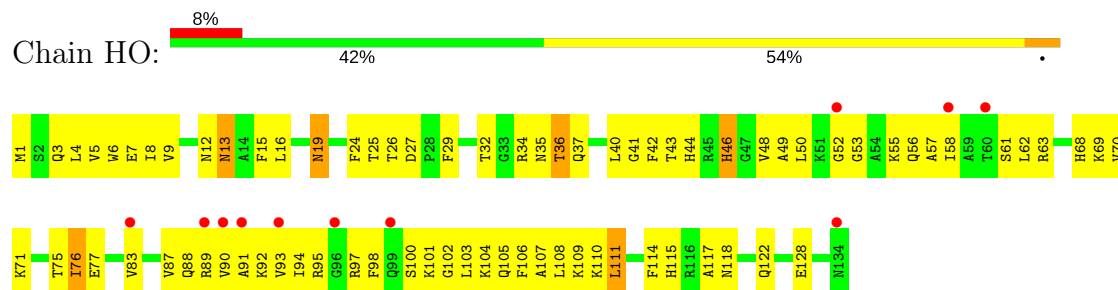
• Molecule 14: RPL28



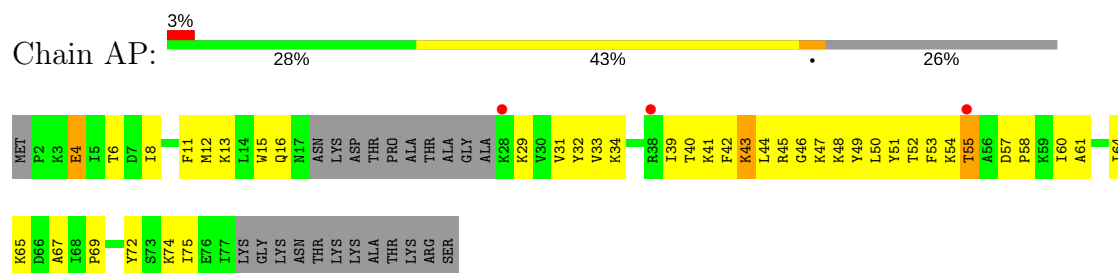
• Molecule 14: RPL28



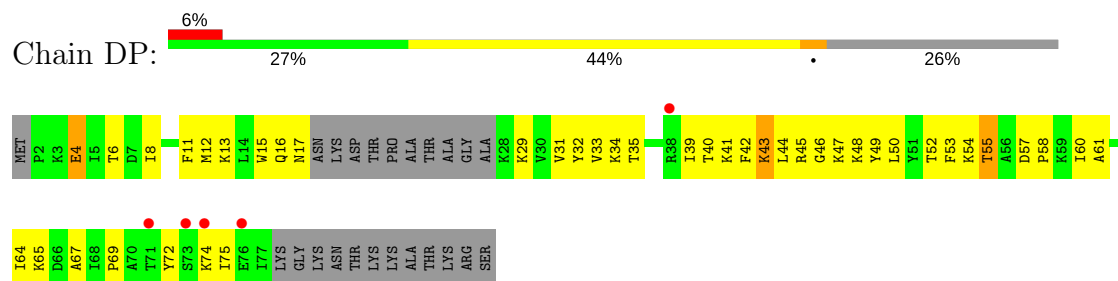
- Molecule 14: RPL28



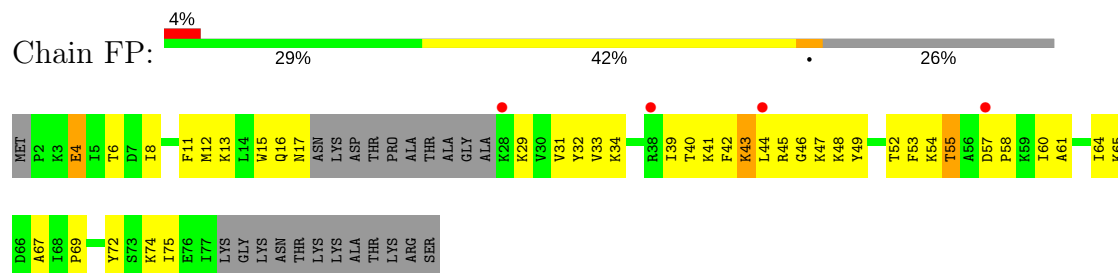
- Molecule 15: RPL38



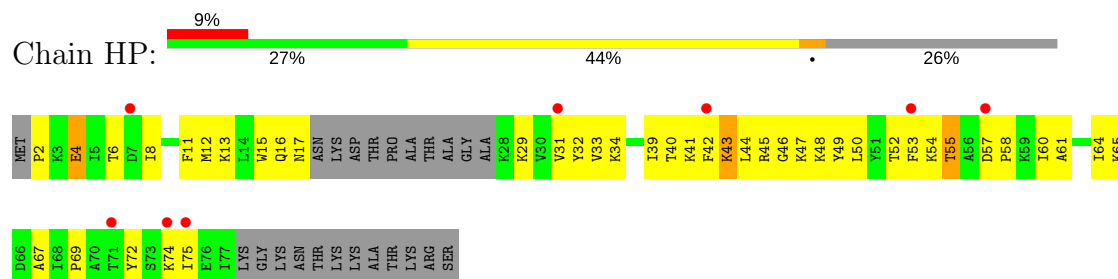
- Molecule 15: RPL38



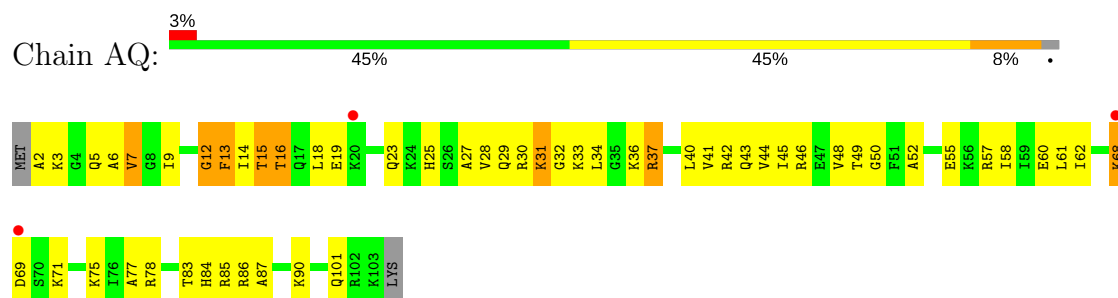
- Molecule 15: RPL38



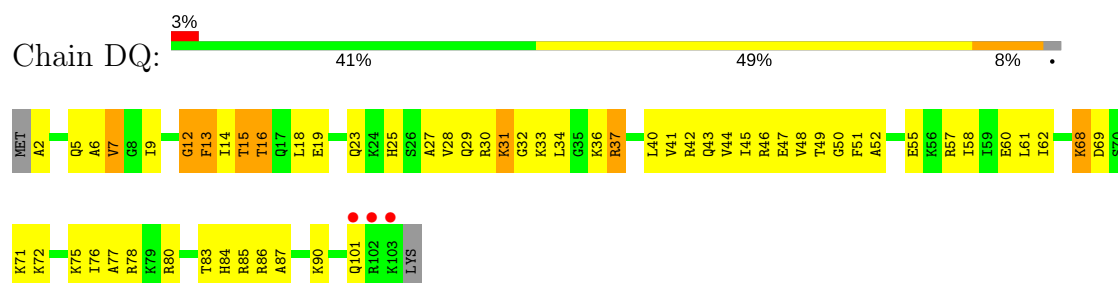
- Molecule 15: RPL38



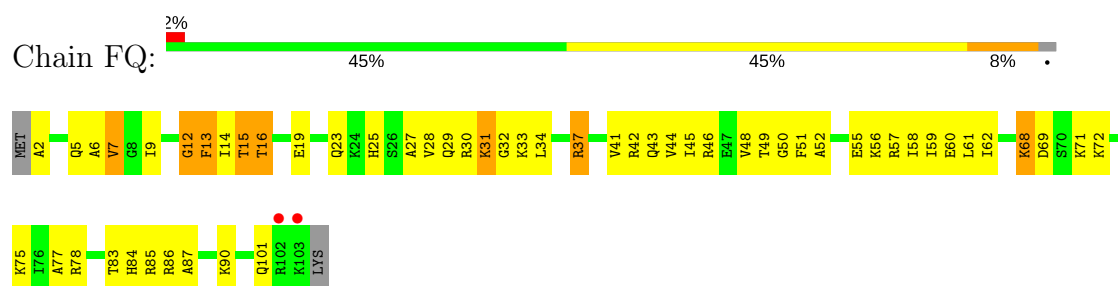
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



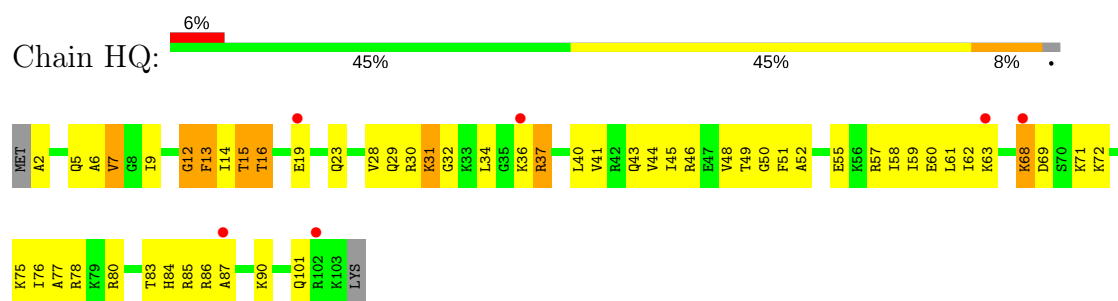
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



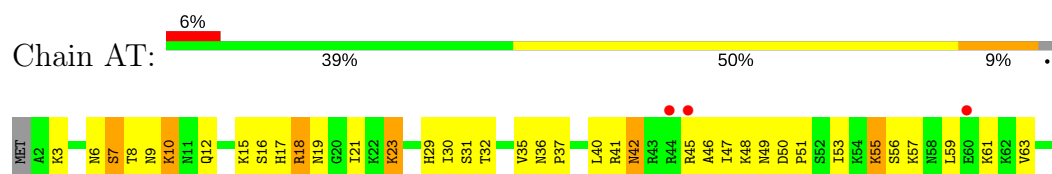
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



- Molecule 16: 60S RIBOSOMAL PROTEIN L36

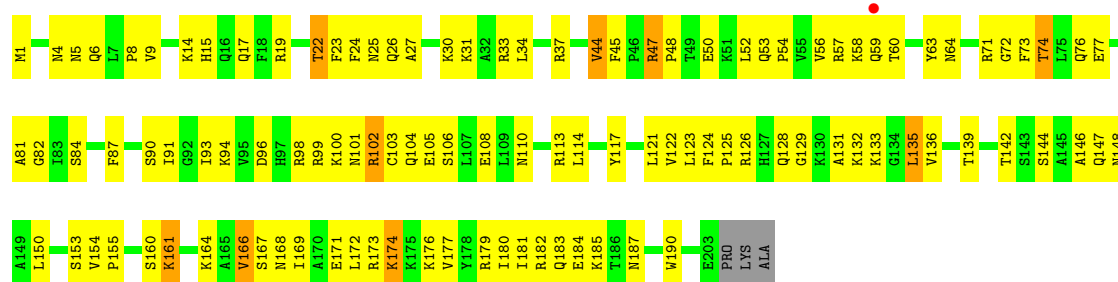


- Molecule 17: RPL29

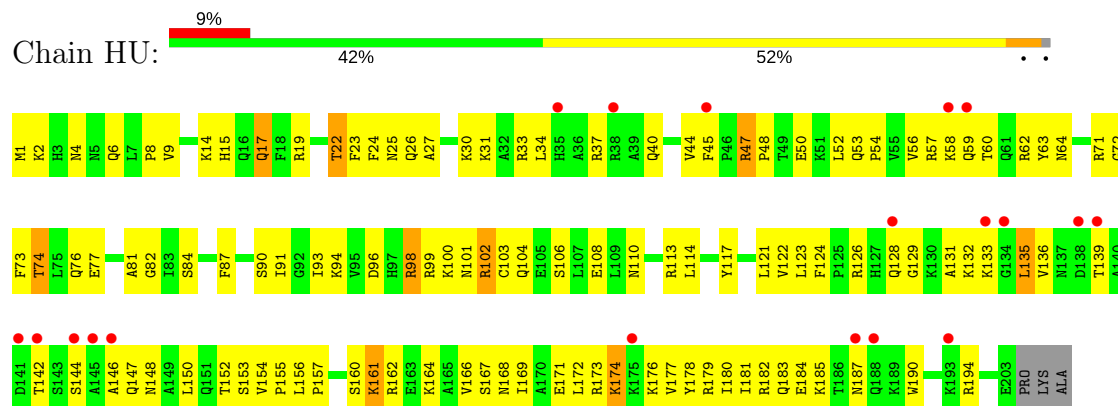


- Molecule 17: RPL29

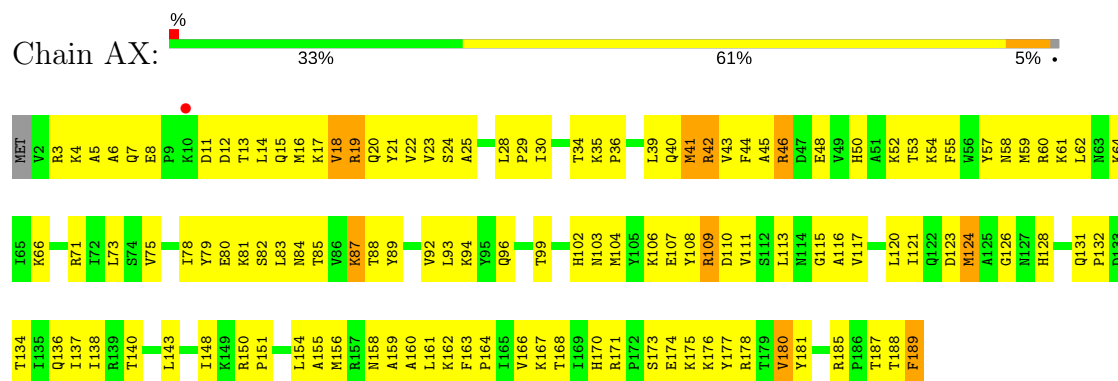




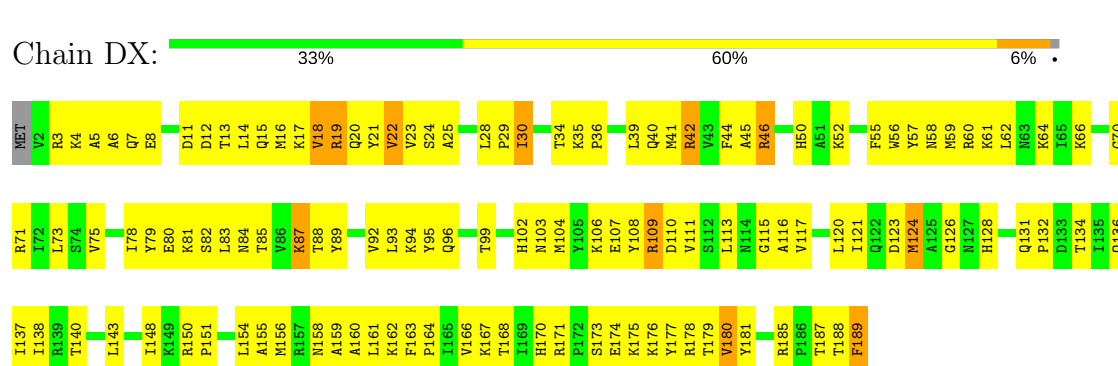
• Molecule 18: RPL13



• Molecule 19: RPL18A



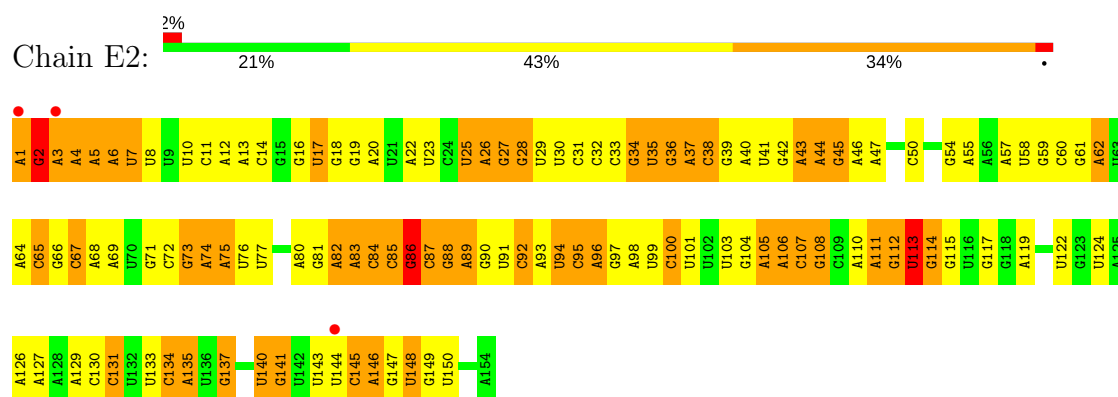
• Molecule 19: RPL18A



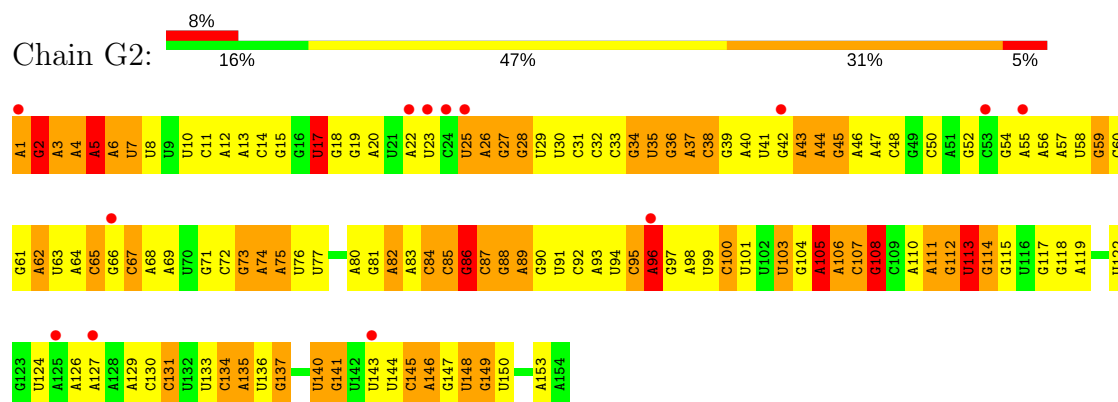
• Molecule 19: RPL18A



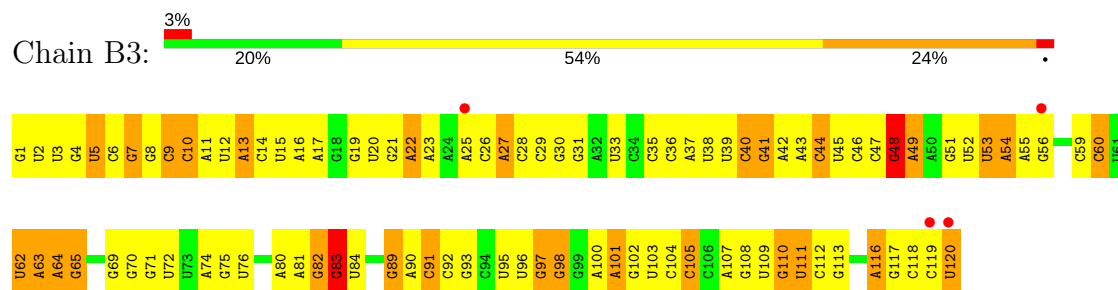




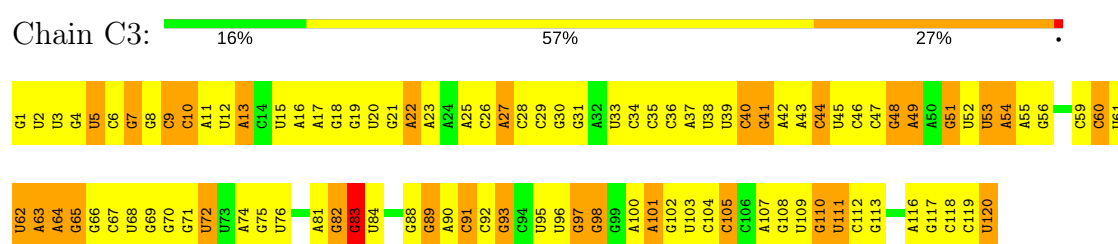
## ● Molecule 20: 5.8S RRNA



## ● Molecule 21: 5S RRNA

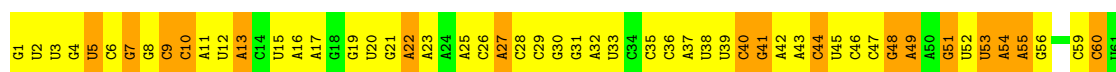


## ● Molecule 21: 5S RRNA

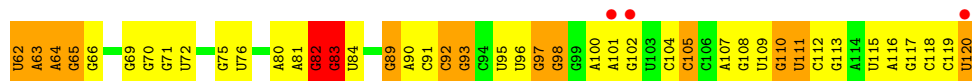
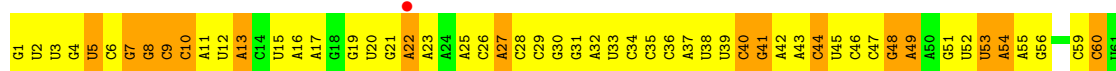


## ● Molecule 21: 5S RRNA

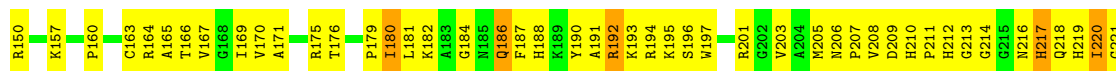
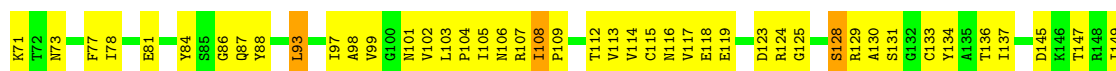




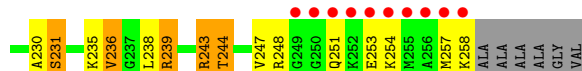
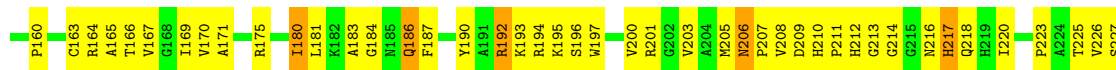
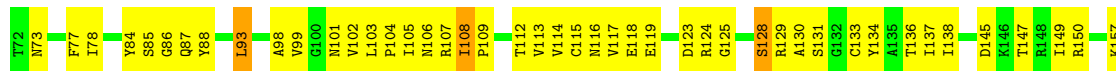
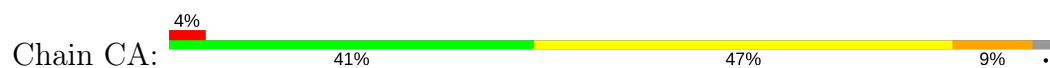
• Molecule 21: 5S rRNA



• Molecule 22: RPL8

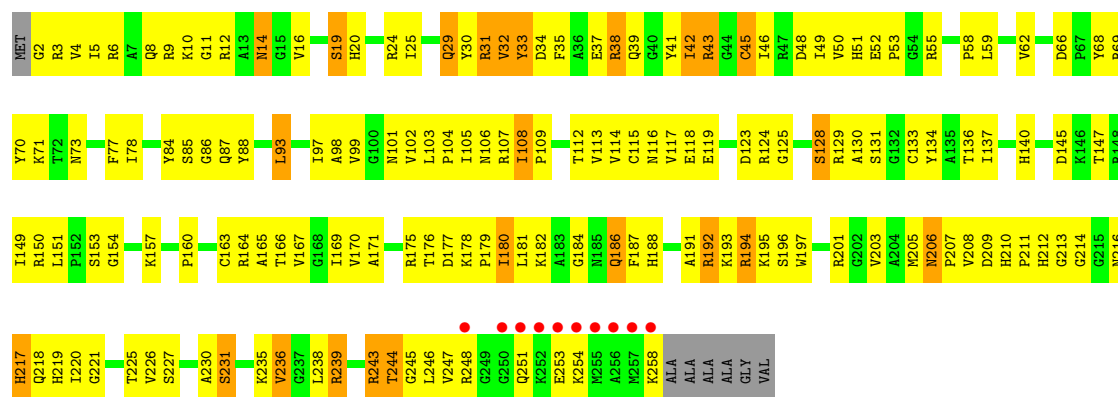


• Molecule 22: RPL8

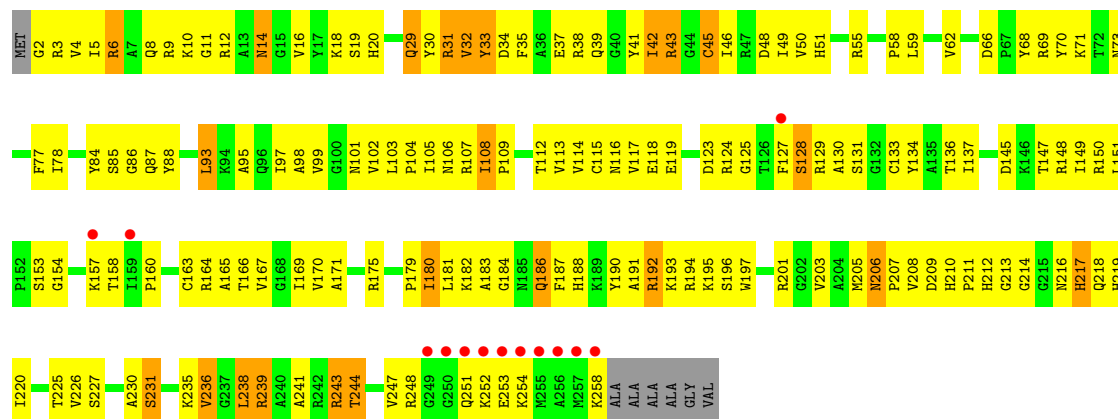
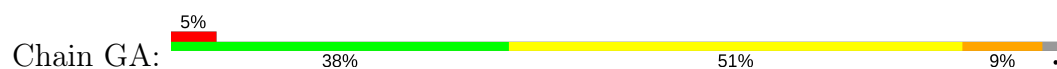


• Molecule 22: RPL8

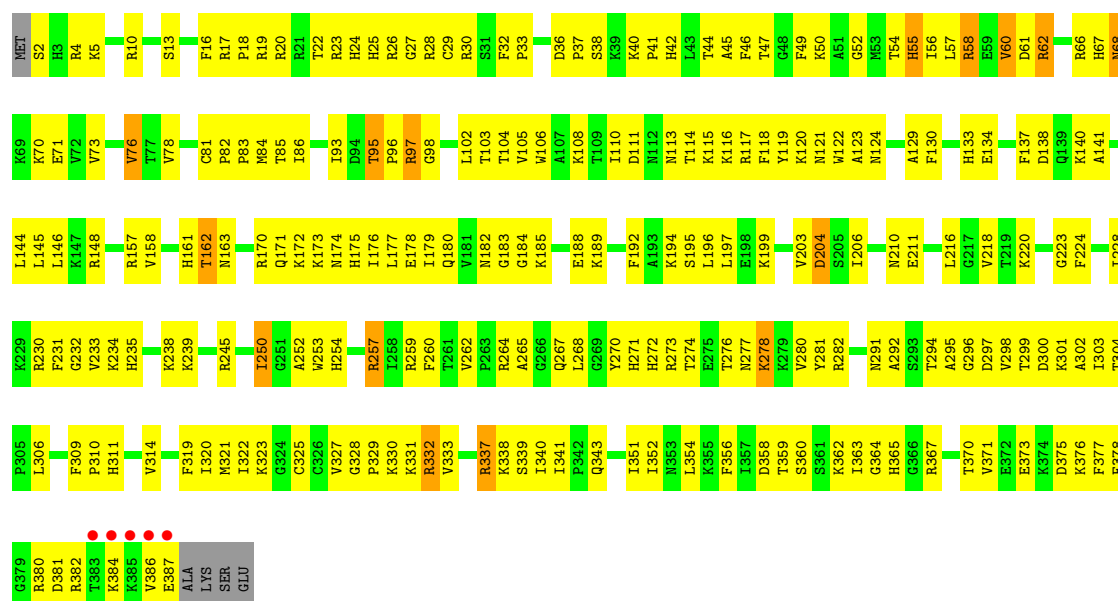
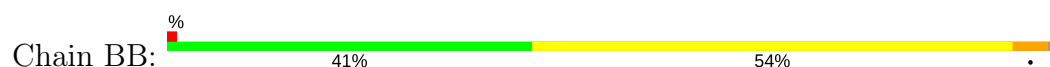




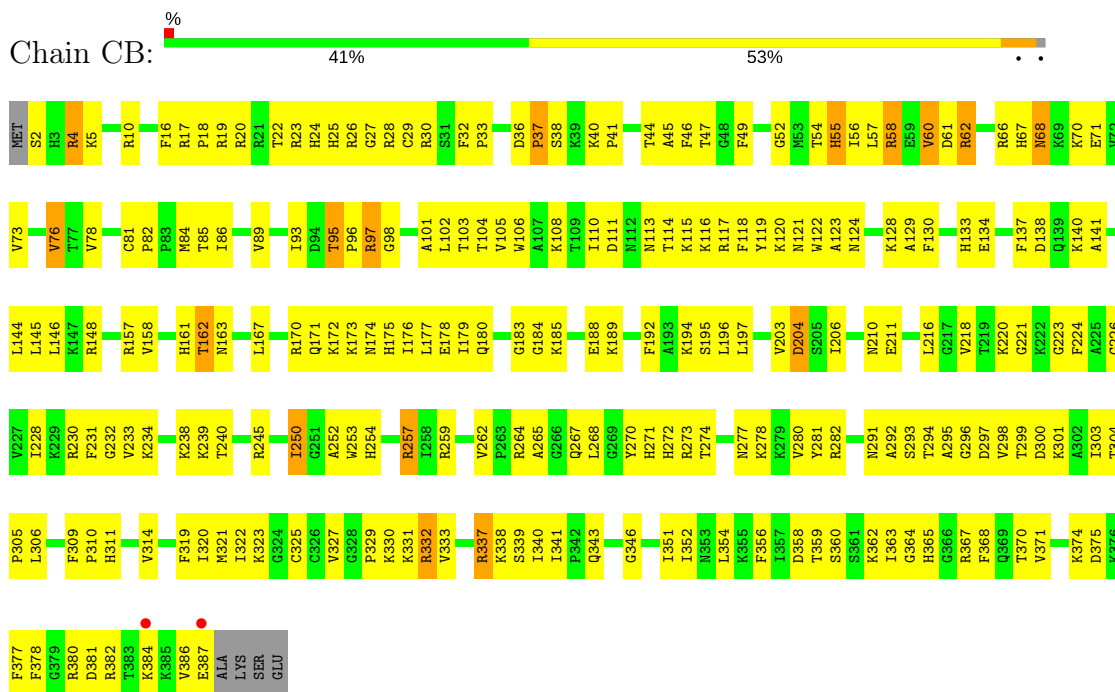
• Molecule 22: RPL8



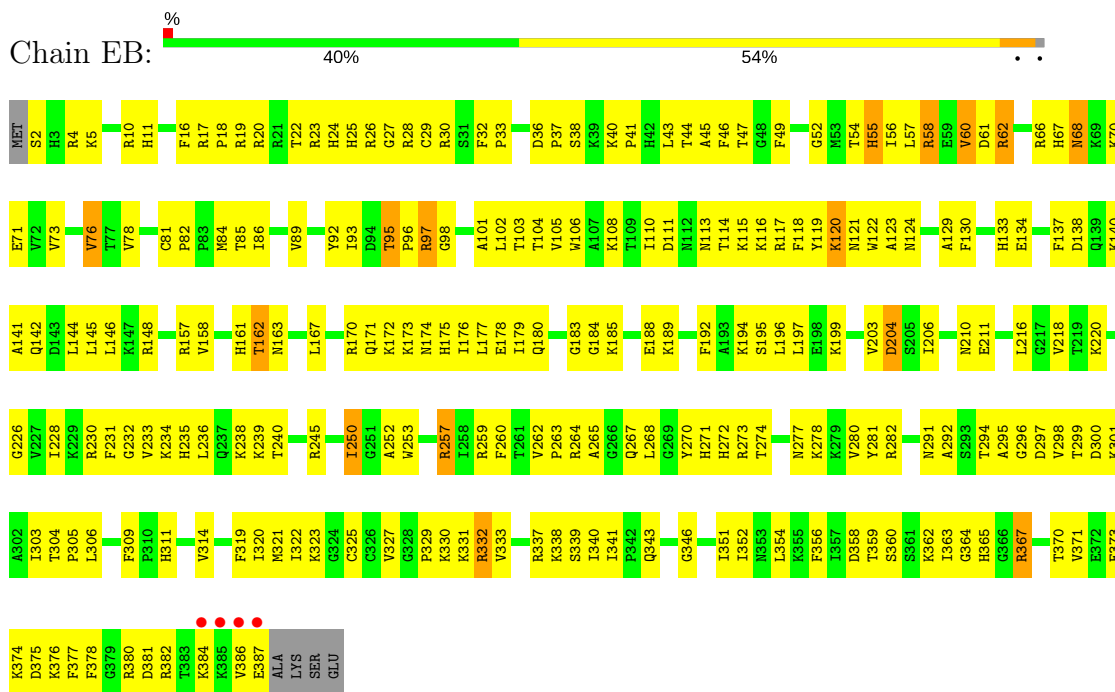
• Molecule 23: RIBOSOMAL PROTEIN L3



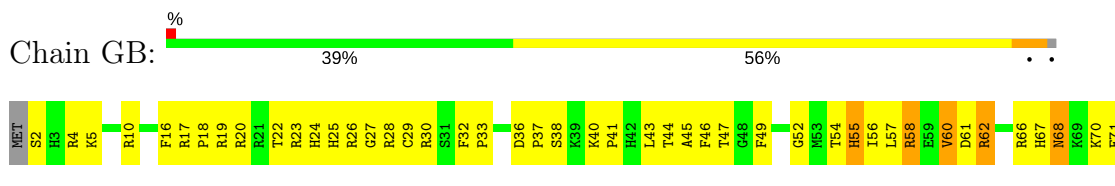
● Molecule 23: RIBOSOMAL PROTEIN L3

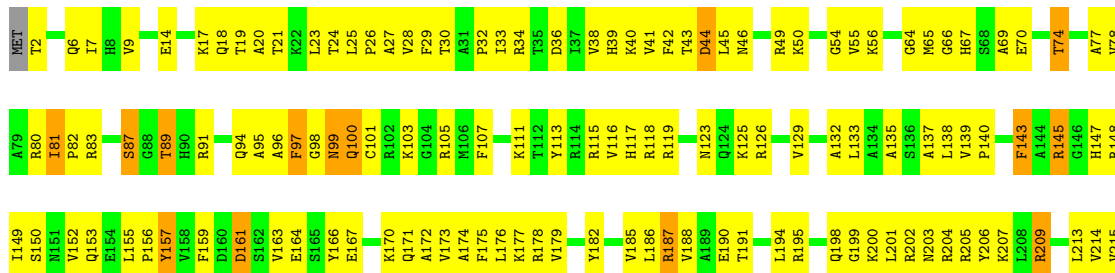


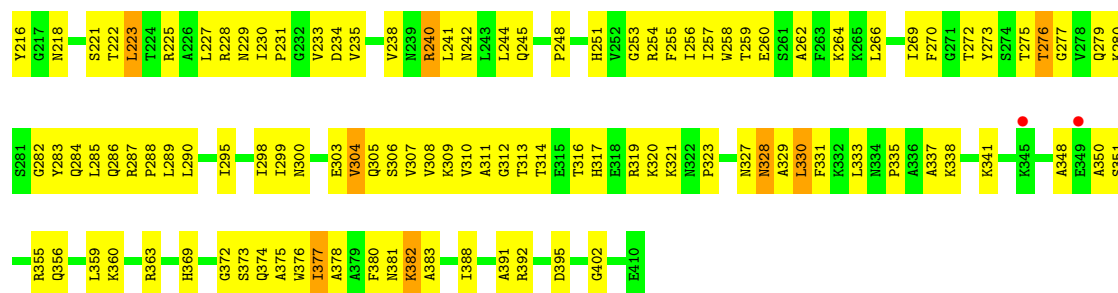
● Molecule 23: RIBOSOMAL PROTEIN L3



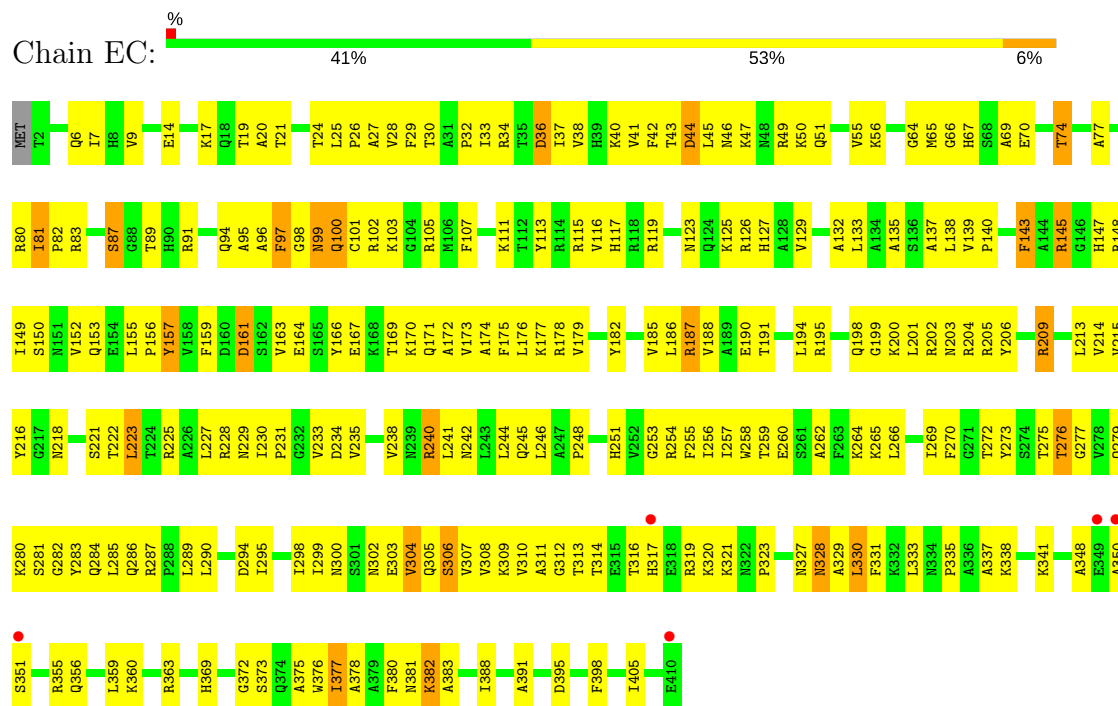
● Molecule 23: RIBOSOMAL PROTEIN L3



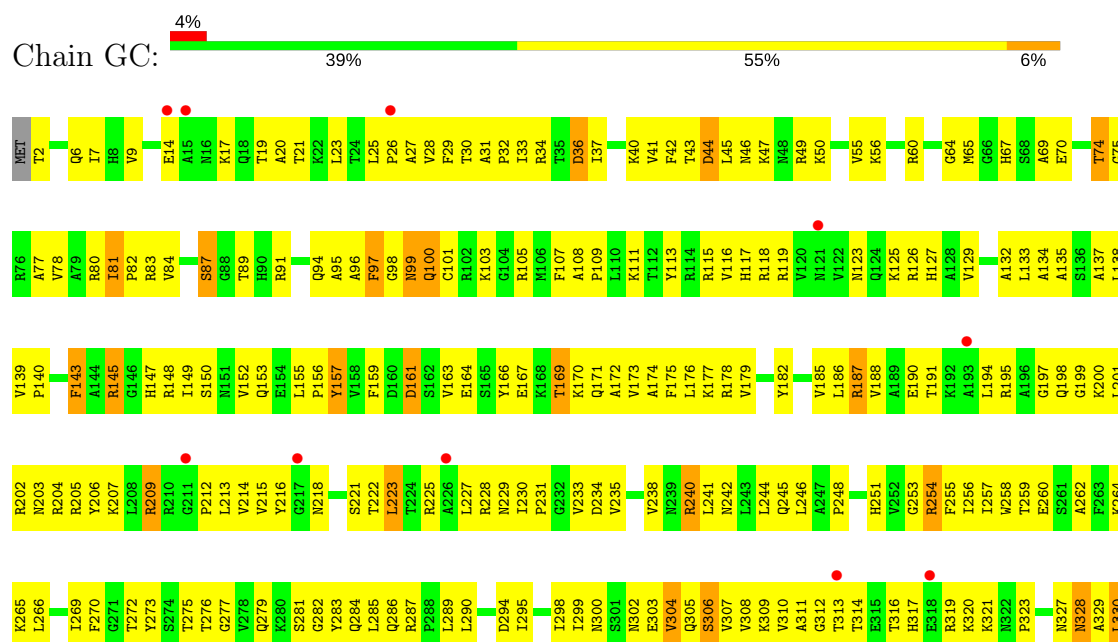




• Molecule 24: RPL4

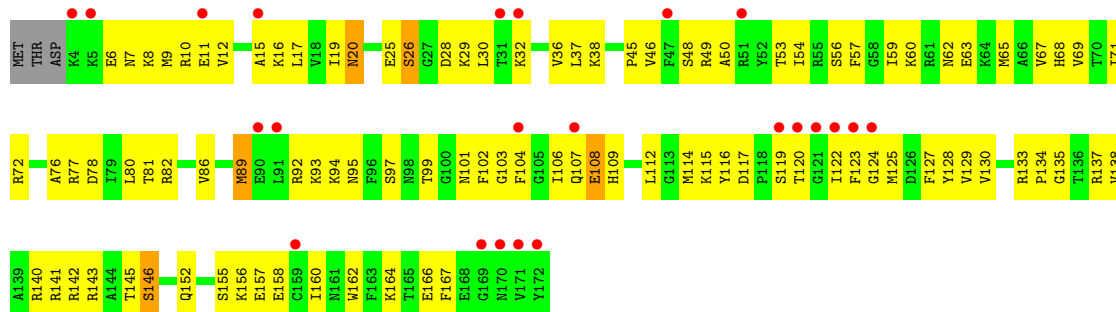


• Molecule 24: RPL4

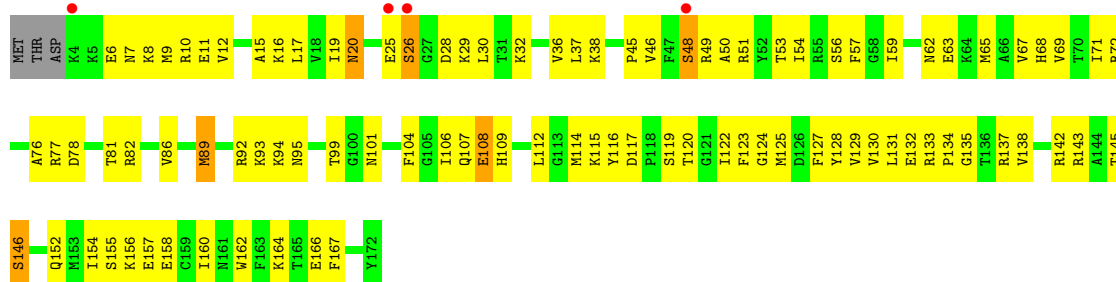
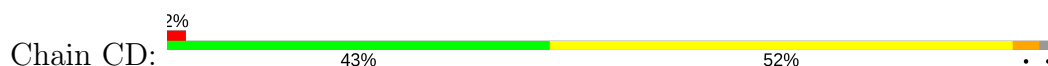




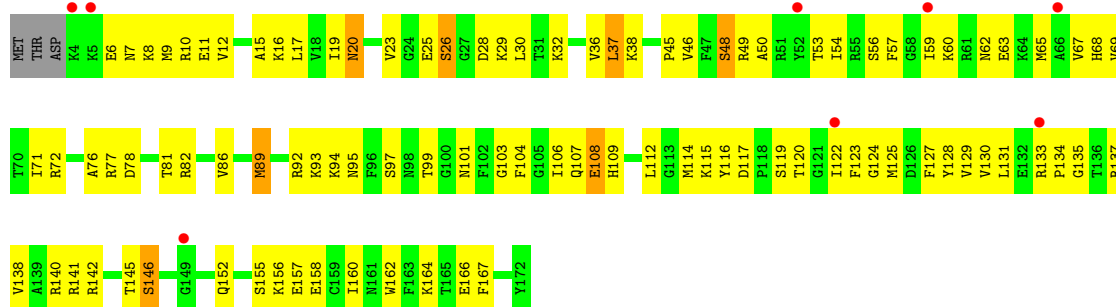
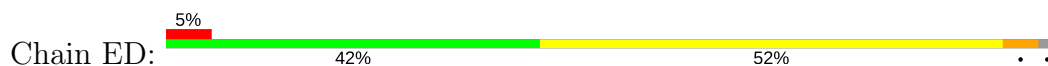
• Molecule 25: 60S RIBOSOMAL PROTEIN L11



• Molecule 25: 60S RIBOSOMAL PROTEIN L11



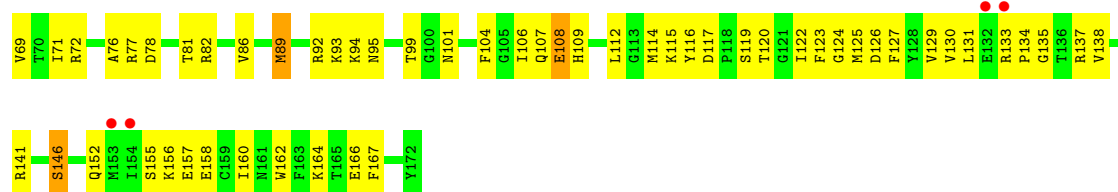
• Molecule 25: 60S RIBOSOMAL PROTEIN L11



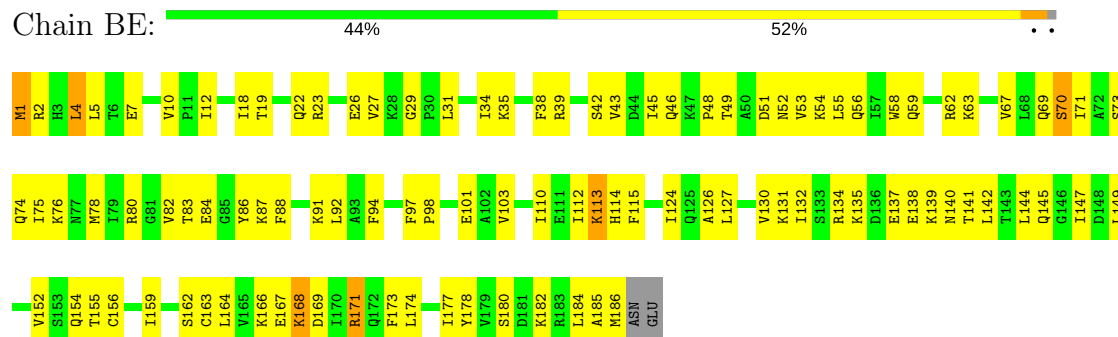
• Molecule 25: 60S RIBOSOMAL PROTEIN L11



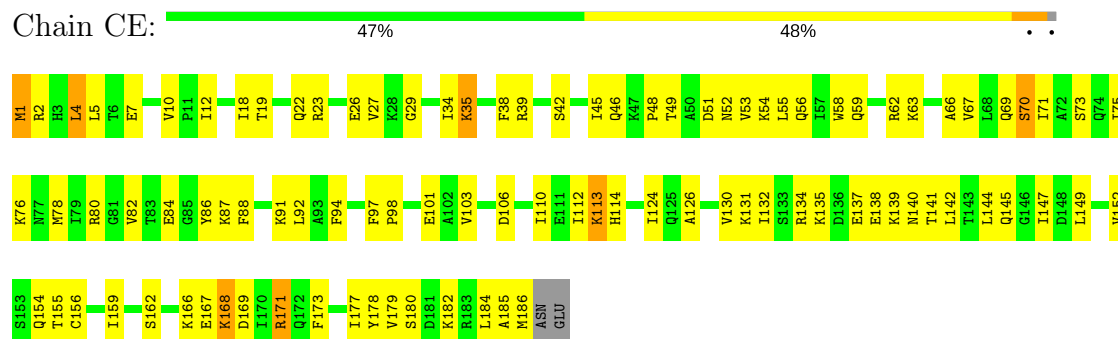




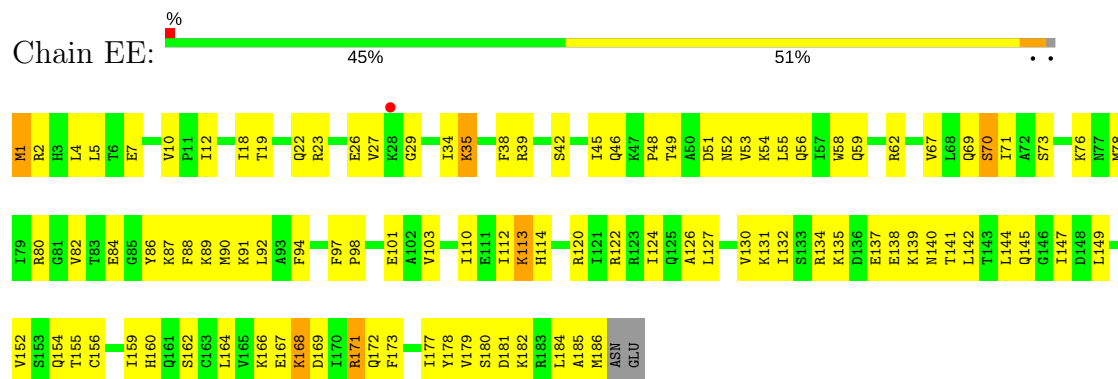
• Molecule 26: 60S RIBOSOMAL PROTEIN L9



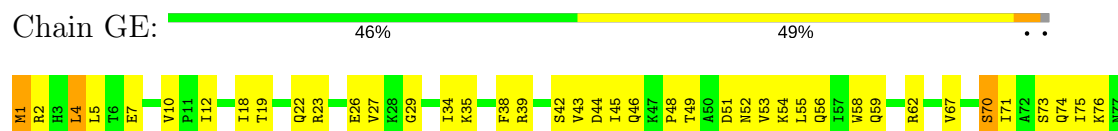
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

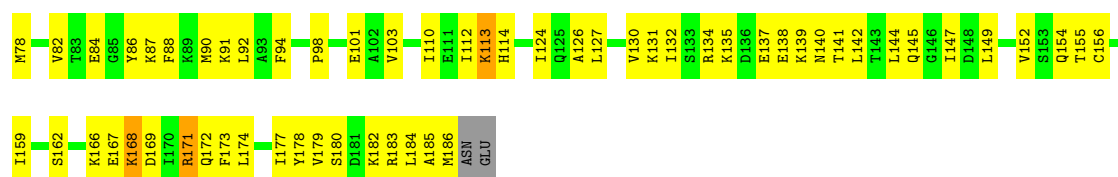


• Molecule 26: 60S RIBOSOMAL PROTEIN L9

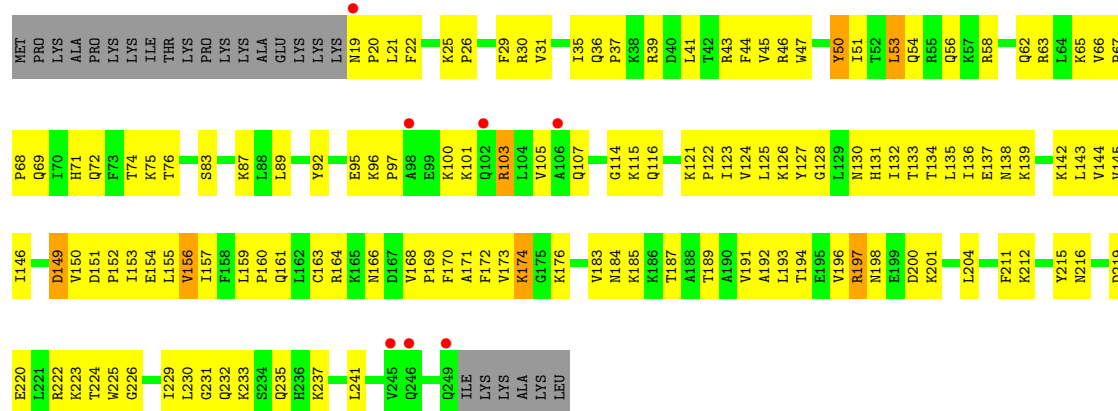
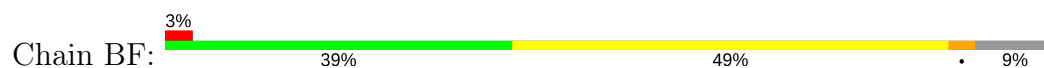


• Molecule 26: 60S RIBOSOMAL PROTEIN L9

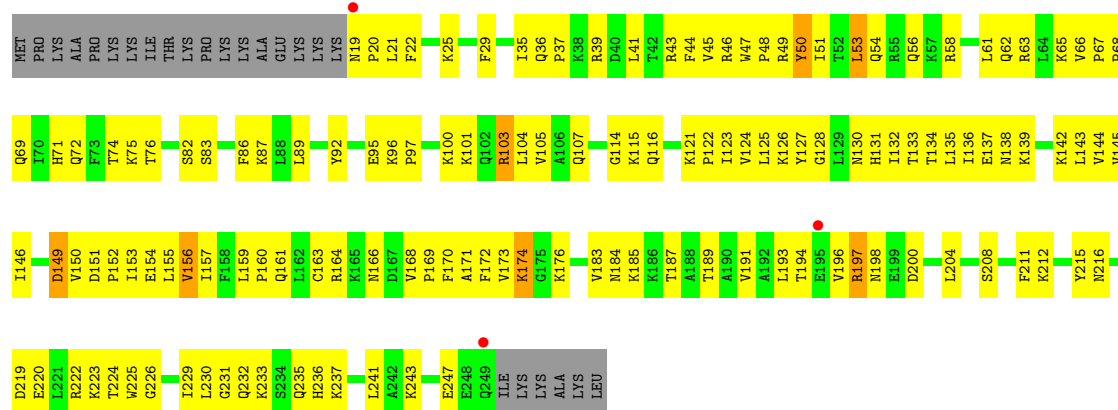




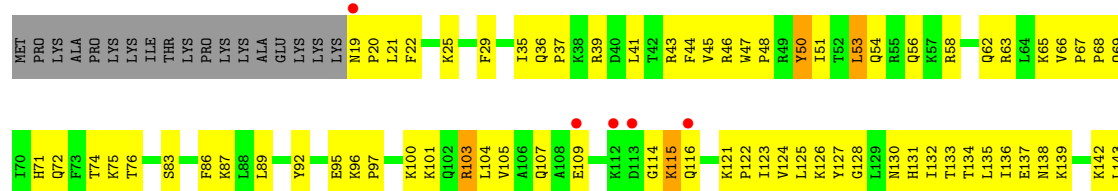
### • Molecule 27: RPL7A

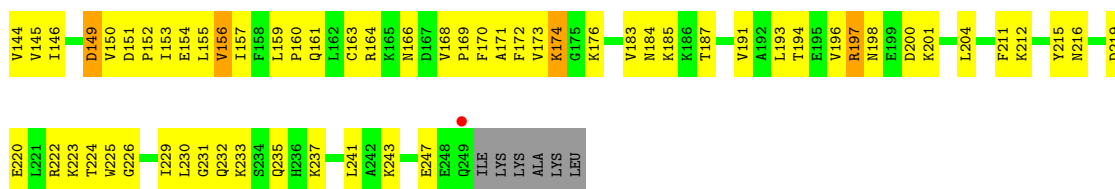


### • Molecule 27: RPL7A

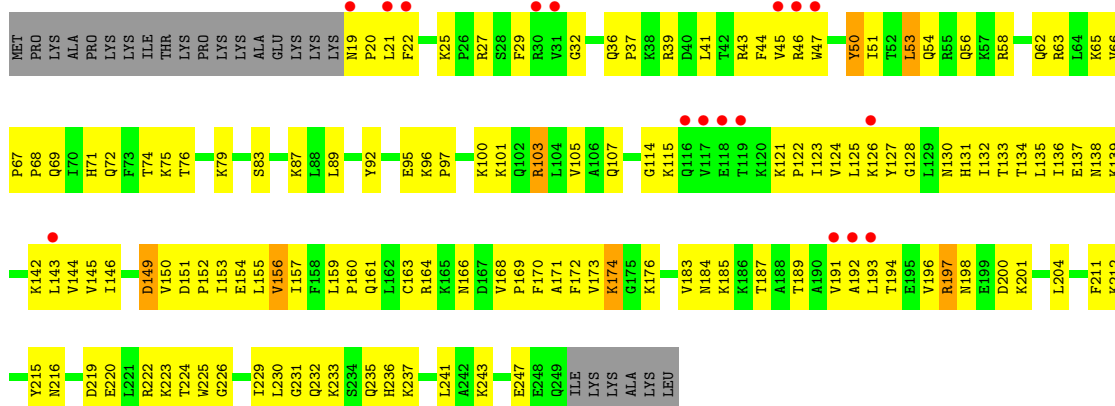


### • Molecule 27: RPL7A

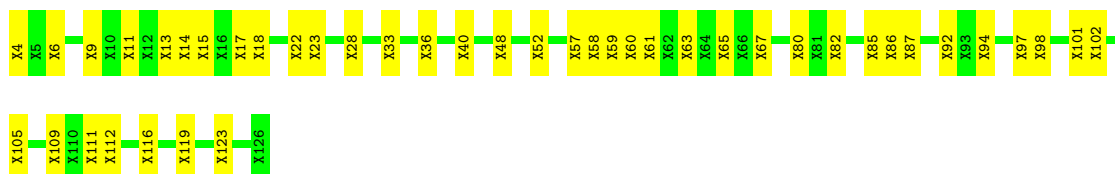




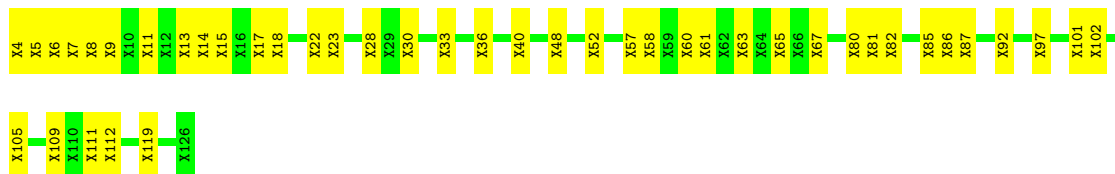
• Molecule 27: RPL7A



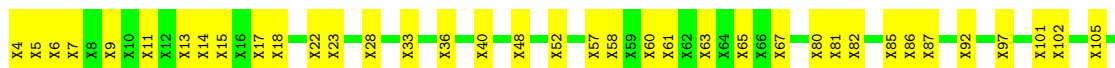
• Molecule 28: RPLP0

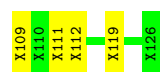


• Molecule 28: RPLP0



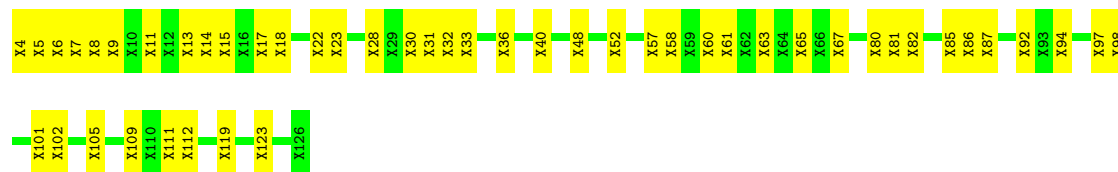
• Molecule 28: RPLP0





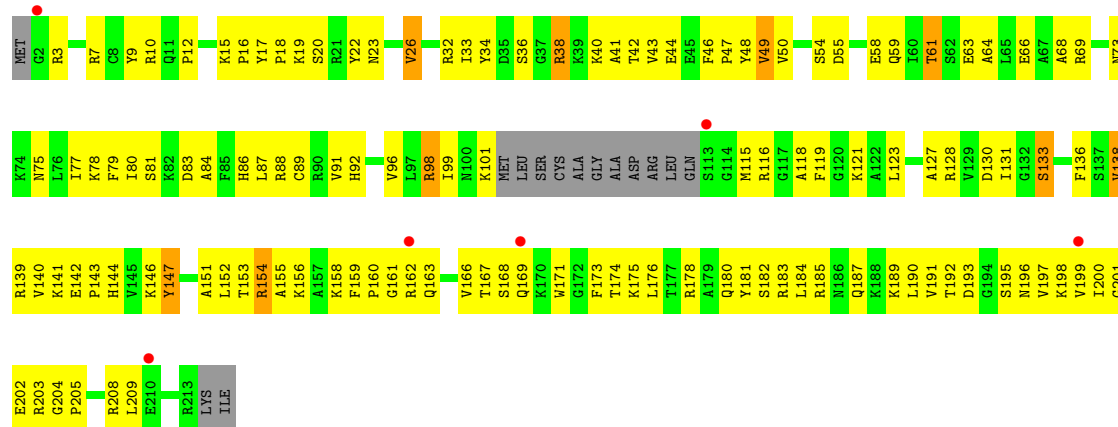
• Molecule 28: RPLP0

Chain GG: 61% 39%



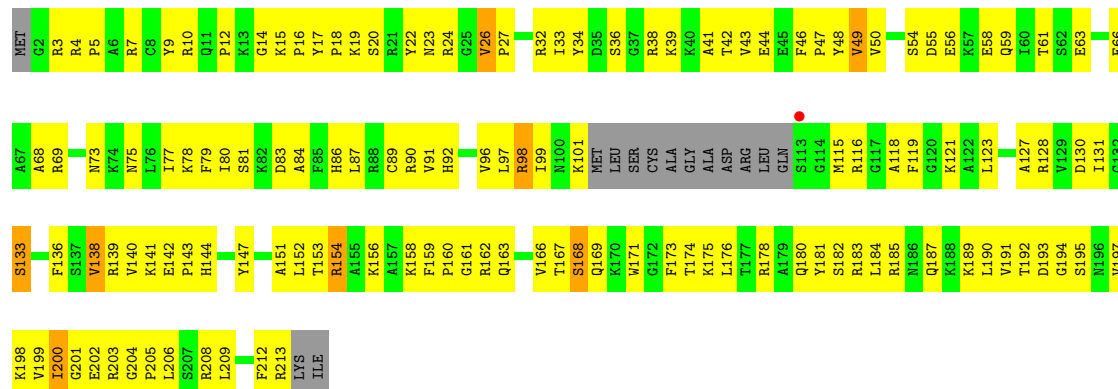
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain BH: 3% 35% 54% 7%



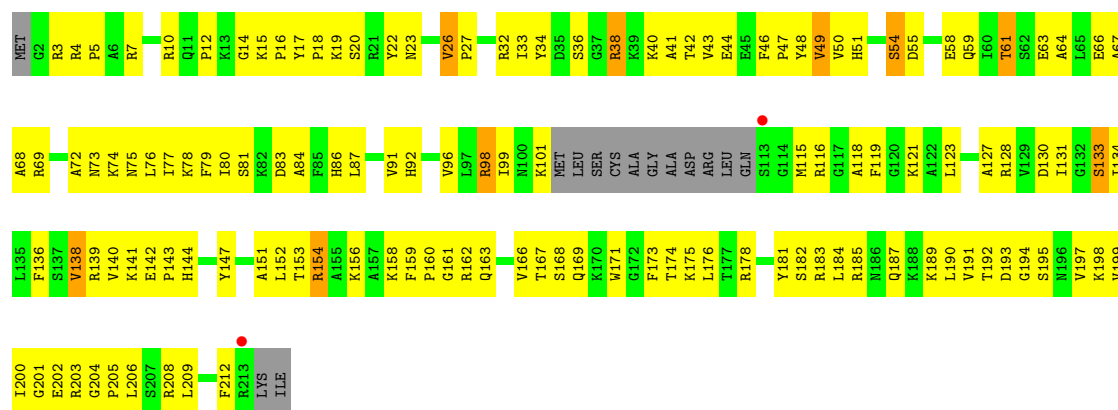
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain CH: 32% 58% 7%

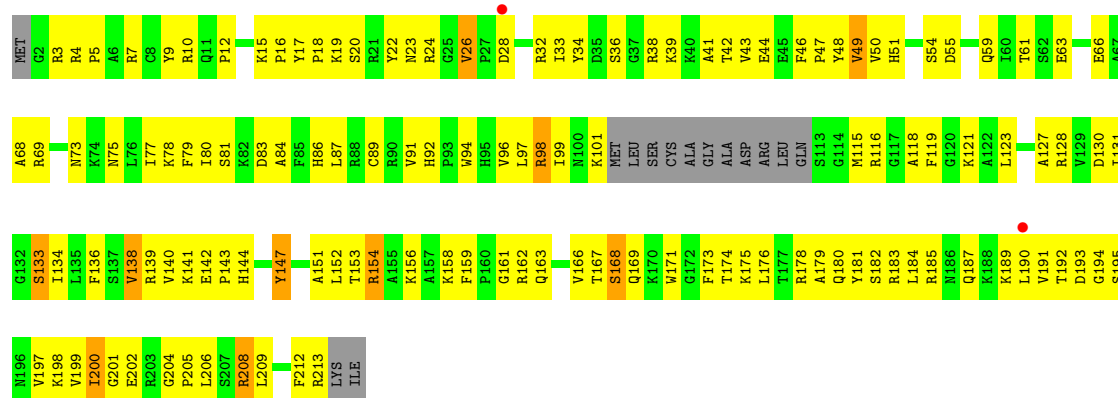


• Molecule 29: 60S RIBOSOMAL PROTEIN L10

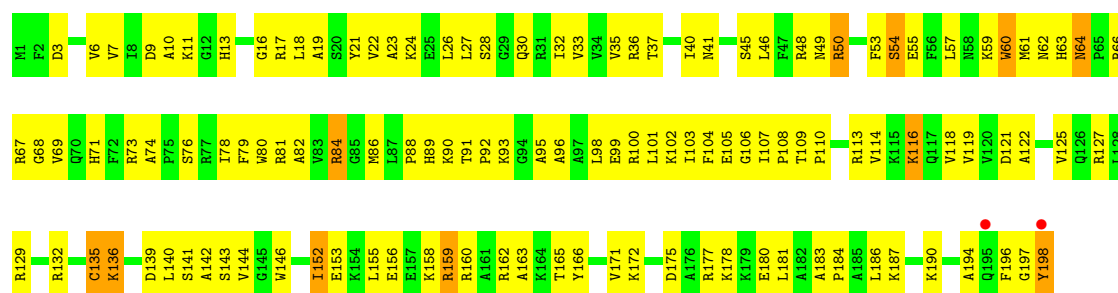
Chain EH: 32% 57% 7%



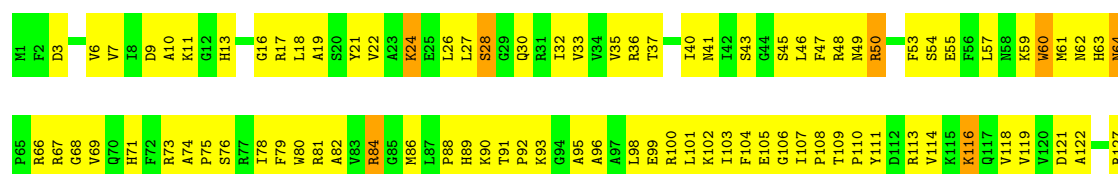
• Molecule 29: 60S RIBOSOMAL PROTEIN L10



• Molecule 30: 60S RIBOSOMAL PROTEIN L13A

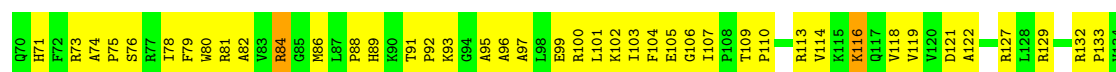


• Molecule 30: 60S RIBOSOMAL PROTEIN L13A

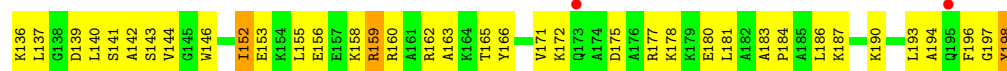
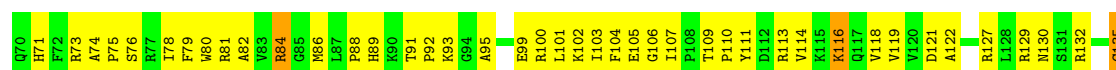




• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



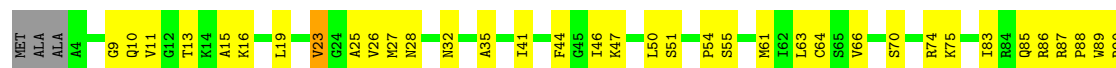
• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



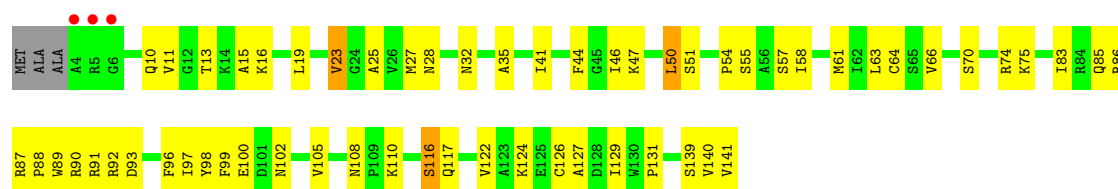
• Molecule 31: RPL23



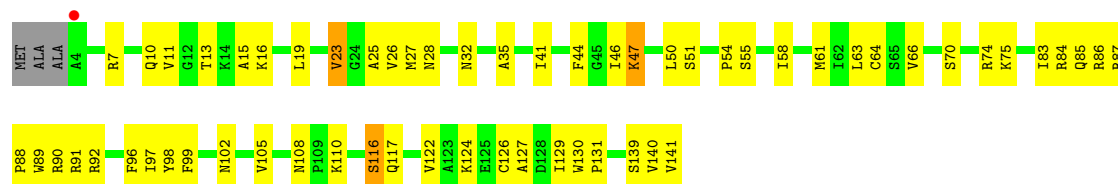
• Molecule 31: RPL23



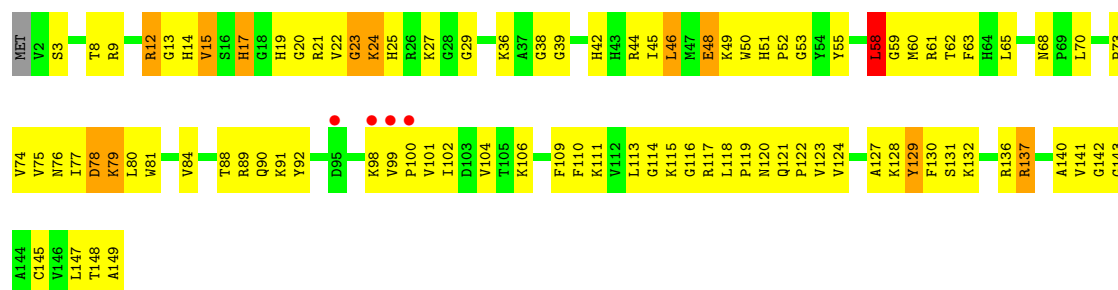
• Molecule 31: RPL23



• Molecule 31: RPL23



• Molecule 32: 60S RIBOSOMAL PROTEIN L27A

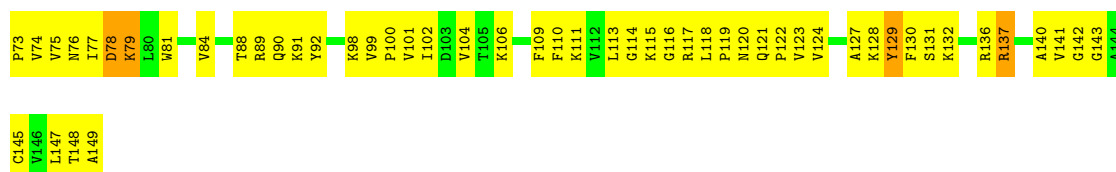


• Molecule 32: 60S RIBOSOMAL PROTEIN L27A

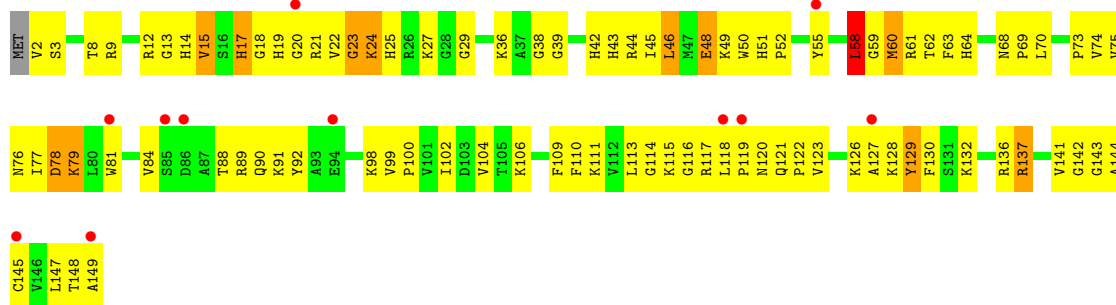


• Molecule 32: 60S RIBOSOMAL PROTEIN L27A





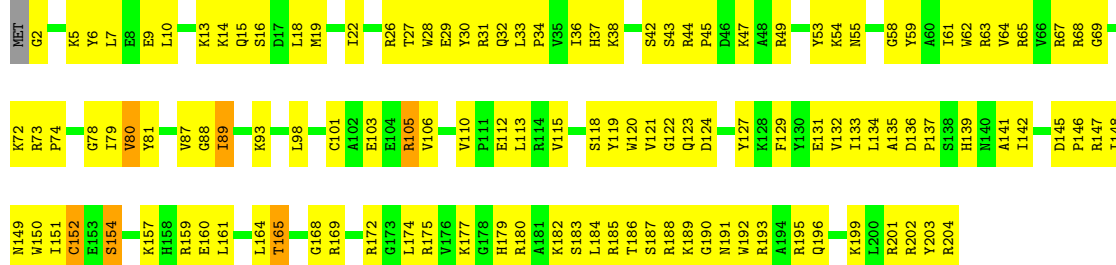
• Molecule 32: 60S RIBOSOMAL PROTEIN L27A



• Molecule 33: RIBOSOMAL PROTEIN L15



• Molecule 33: RIBOSOMAL PROTEIN L15

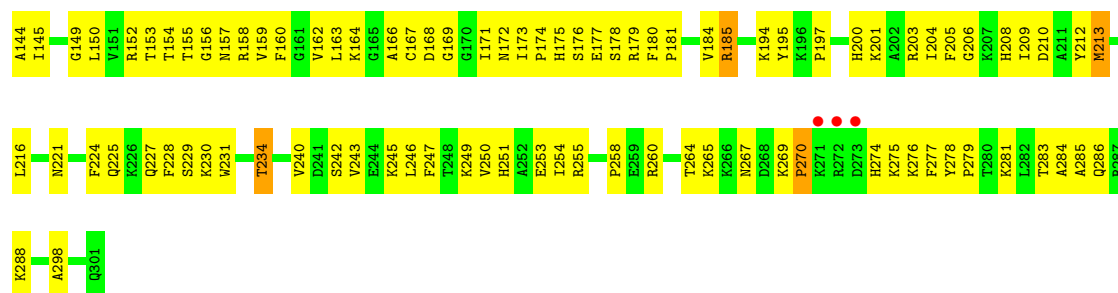


• Molecule 33: RIBOSOMAL PROTEIN L15

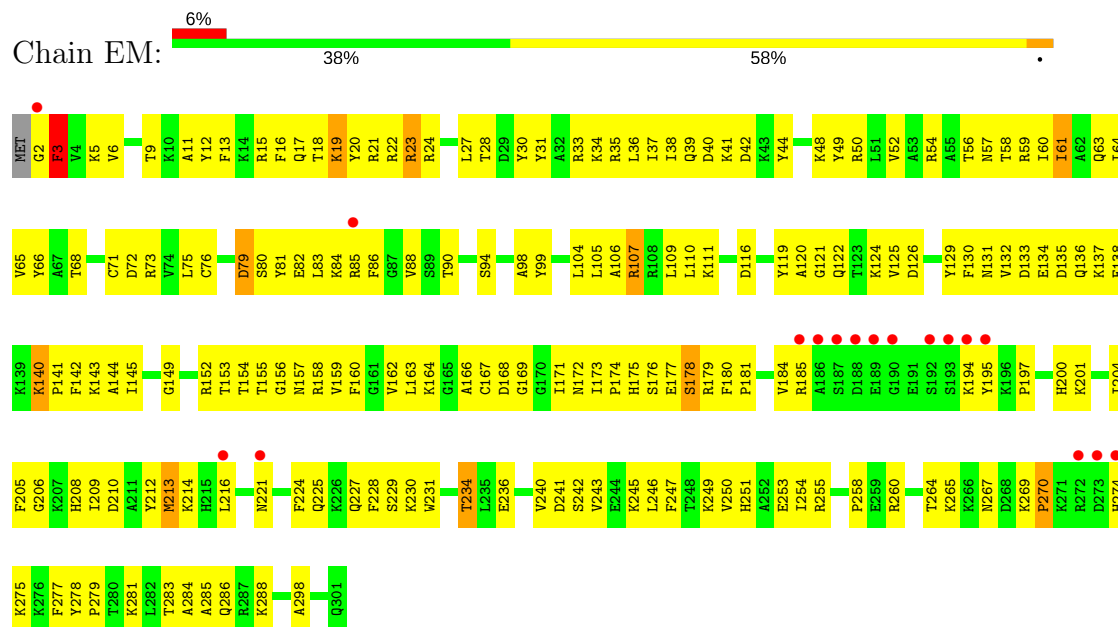




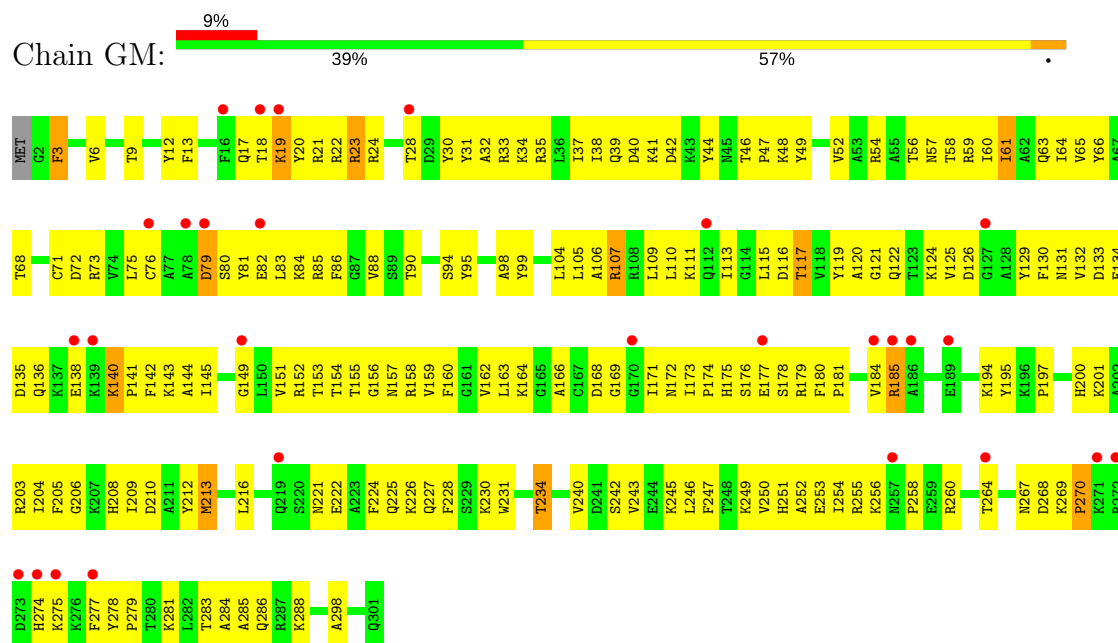




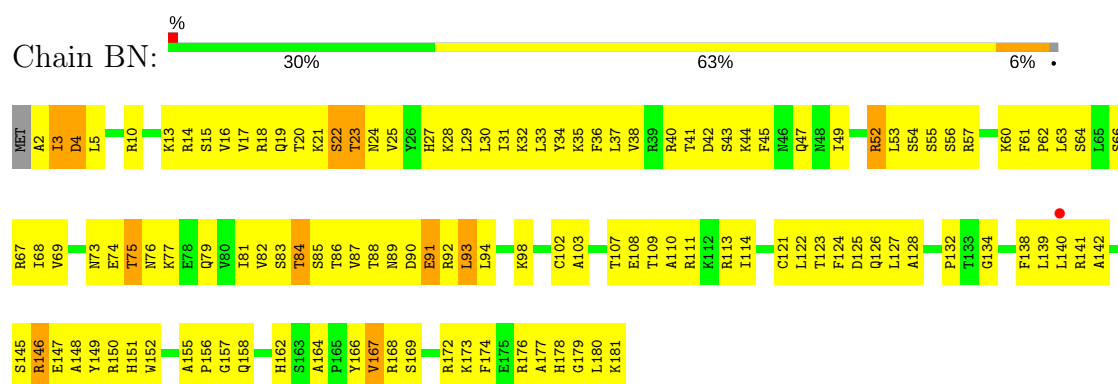
• Molecule 34: 60S RIBOSOMAL PROTEIN L5



• Molecule 34: 60S RIBOSOMAL PROTEIN L5



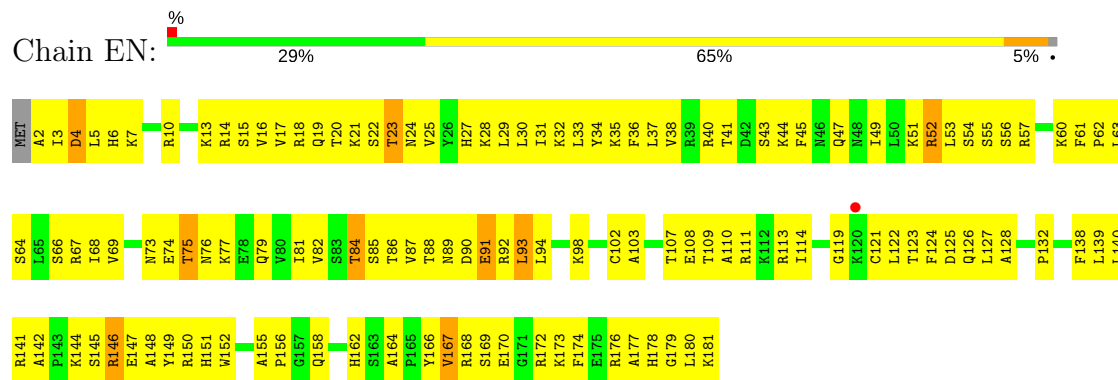
• Molecule 35: RPL18



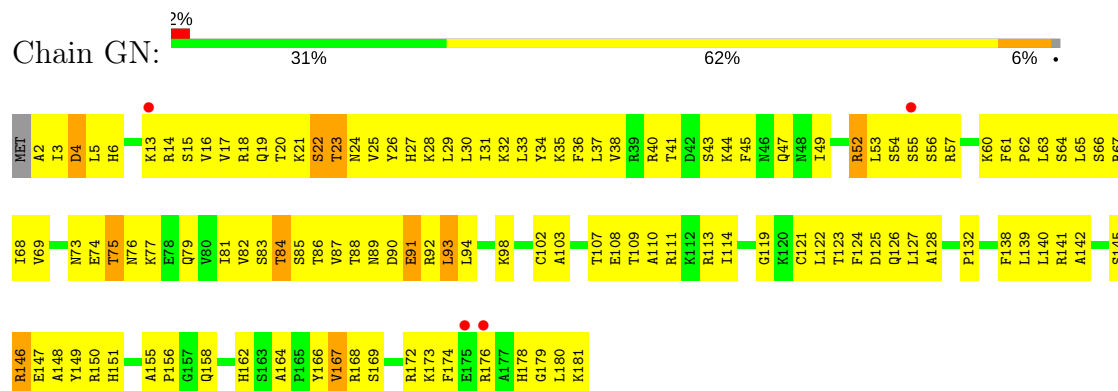
- Molecule 35: RPL18



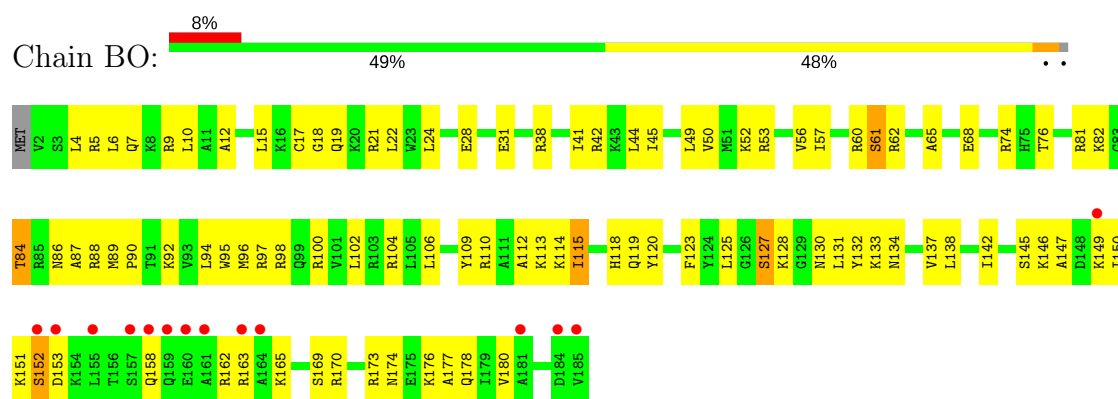
- Molecule 35: RPL18



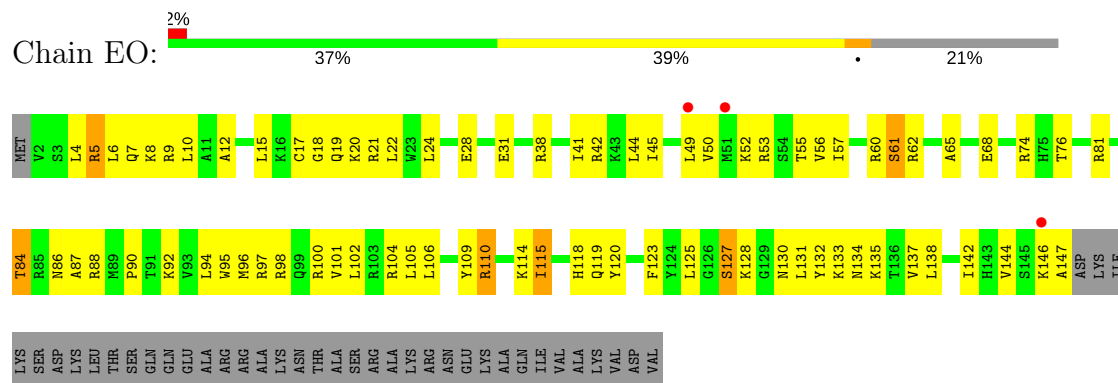
- Molecule 35: RPL18



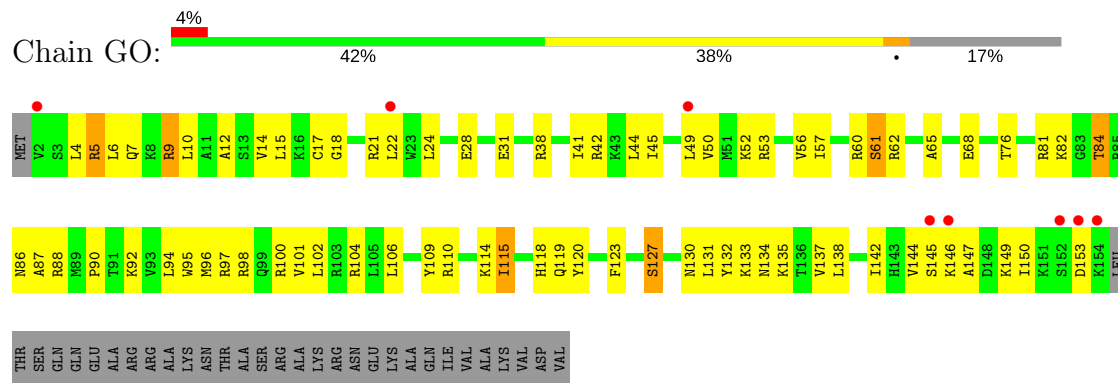
- Molecule 36: RPL19



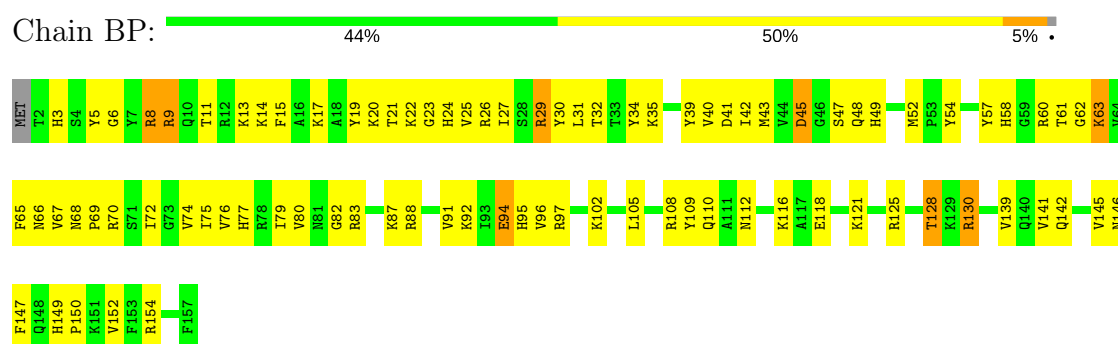
• Molecule 36: RPL19



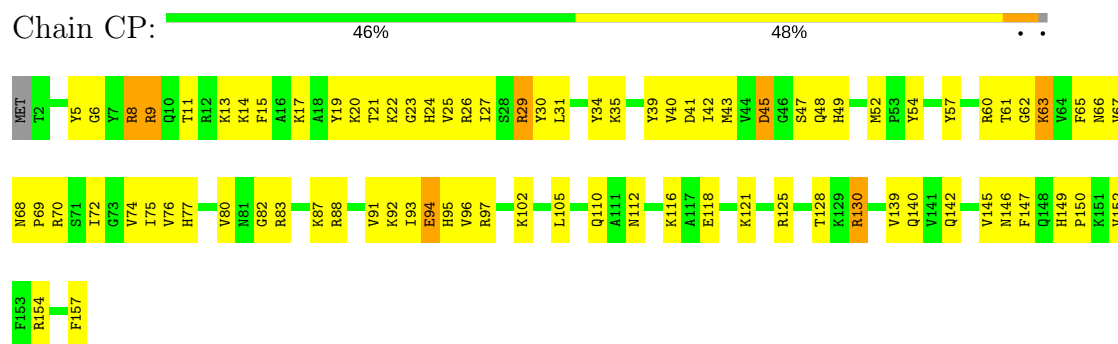
• Molecule 36: RPL19



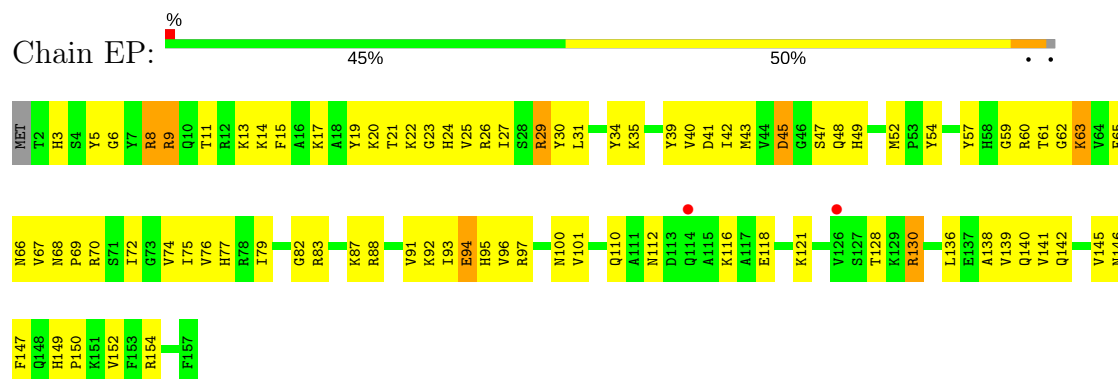
• Molecule 37: 60S RIBOSOMAL PROTEIN L21



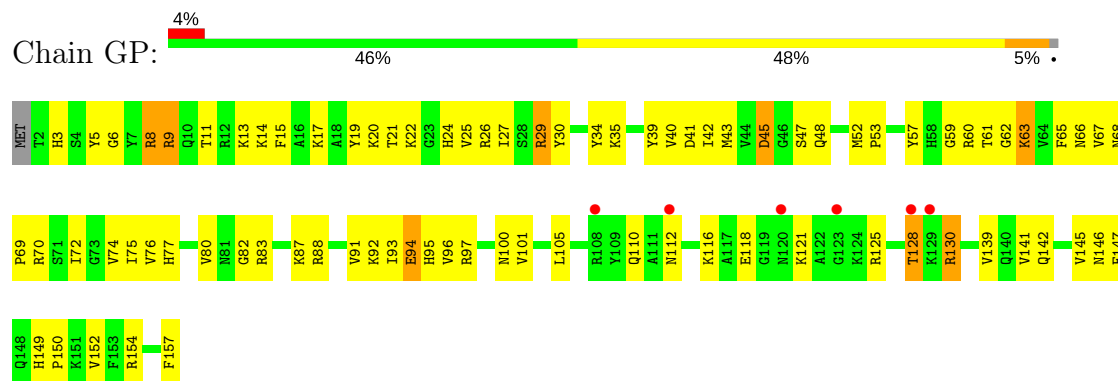
- Molecule 37: 60S RIBOSOMAL PROTEIN L21



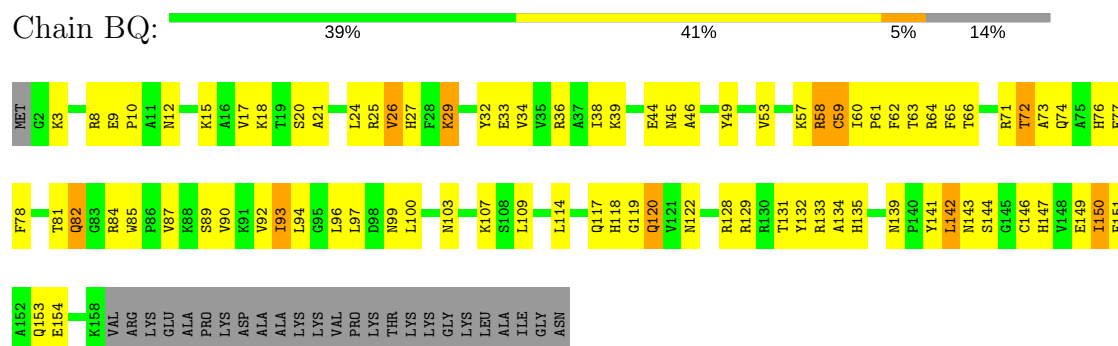
- Molecule 37: 60S RIBOSOMAL PROTEIN L21



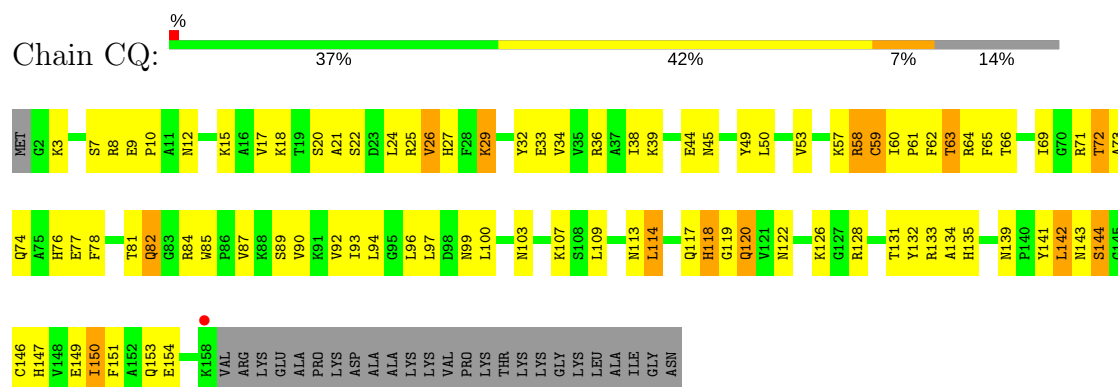
- Molecule 37: 60S RIBOSOMAL PROTEIN L21



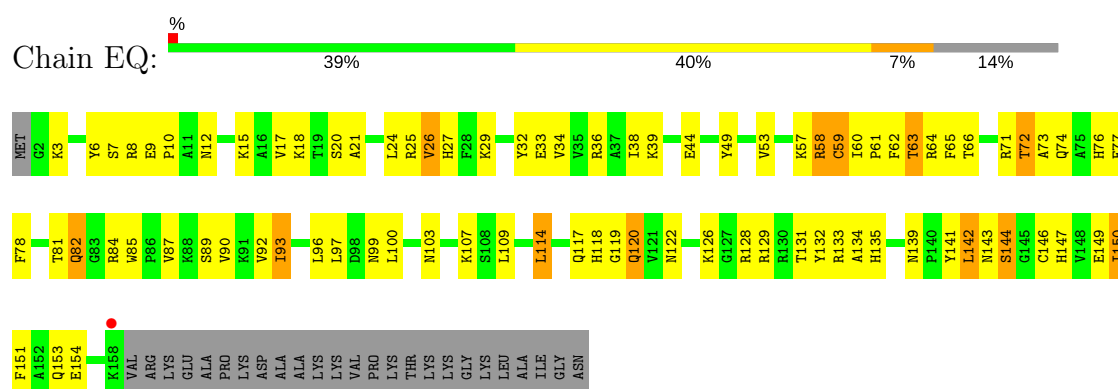
- Molecule 38: RPL17



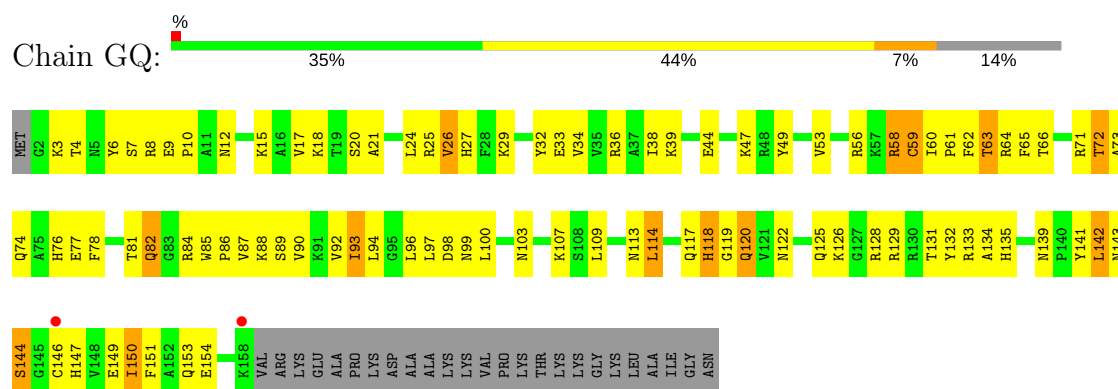
- Molecule 38: RPL17



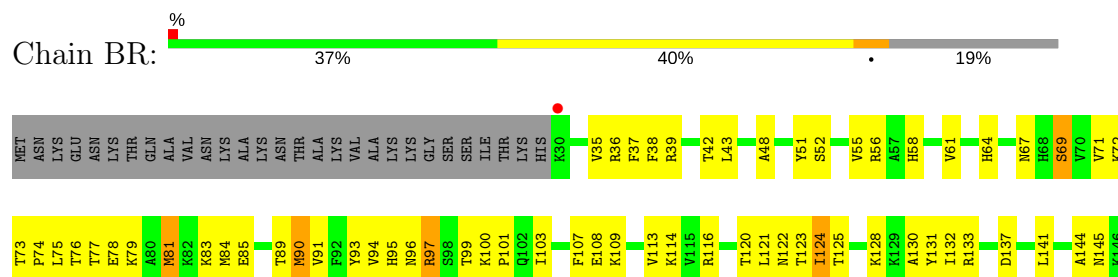
- Molecule 38: RPL17



- Molecule 38: RPL17



- Molecule 39: RPL23A



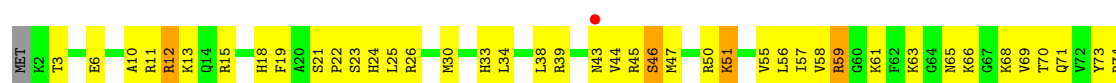
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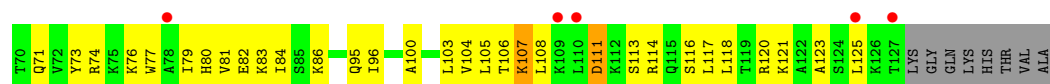
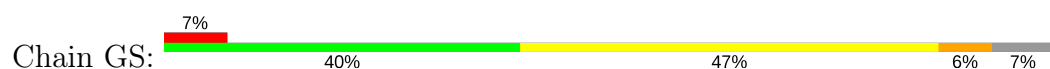
- Molecule 40: RPL26



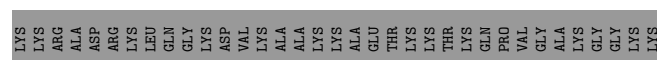
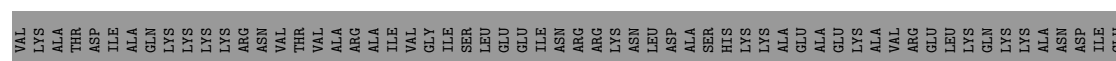
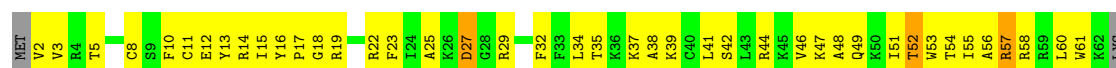
- Molecule 40: RPL26



- Molecule 40: RPL26



- Molecule 41: RPL24

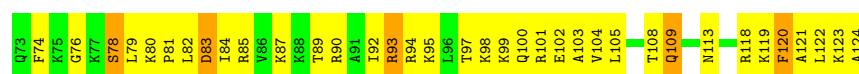


- Molecule 41: RPL24

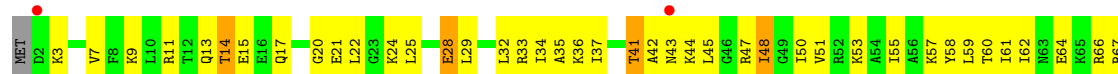




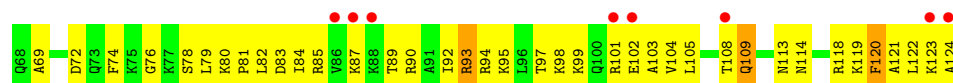
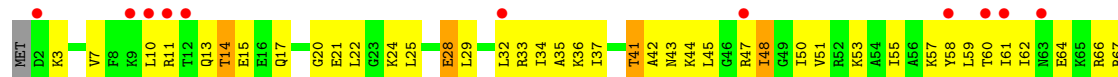




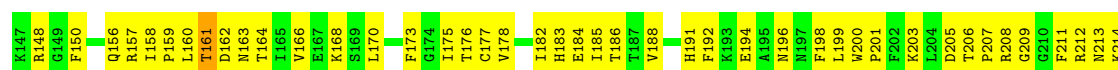
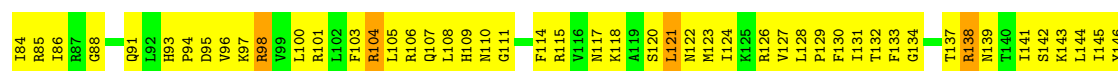
• Molecule 42: RPL35



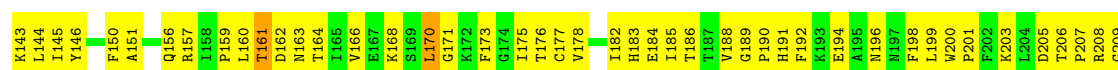
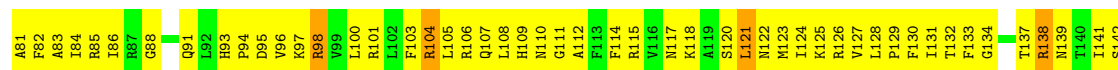
• Molecule 42: RPL35

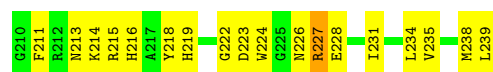


• Molecule 43: 60S RIBOSOMAL PROTEIN L7



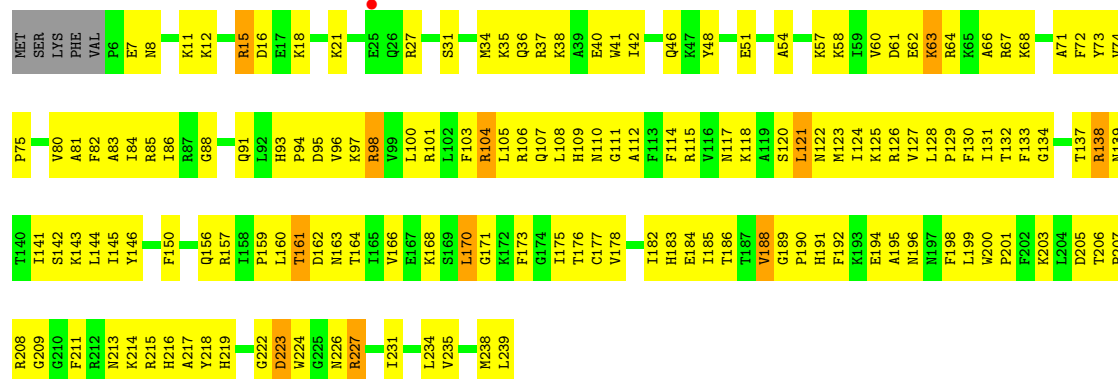
• Molecule 43: 60S RIBOSOMAL PROTEIN L7





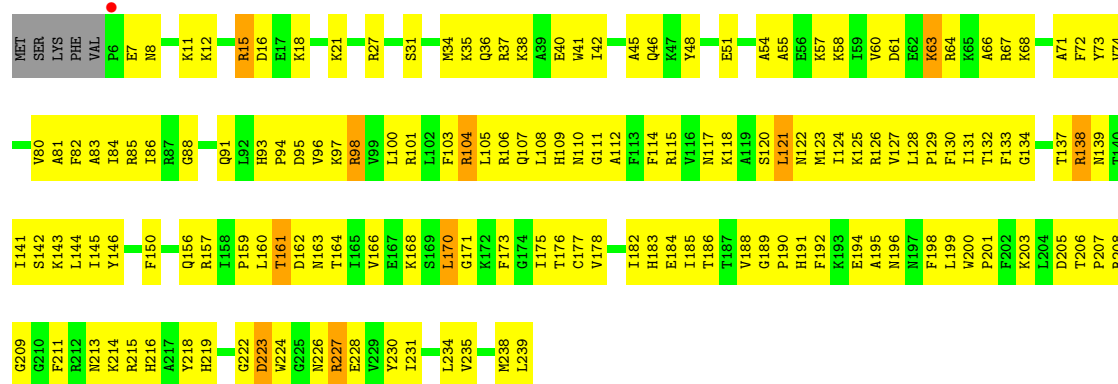
• Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain EV: 35% 59% 5%



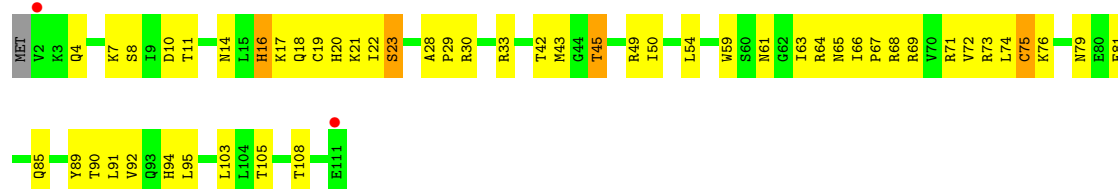
• Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain GV: 34% 59% 7%



• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain BW: 2% 53% 42%

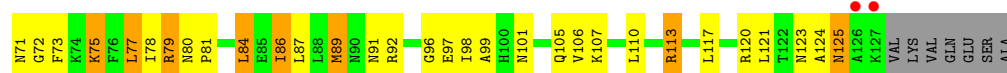


• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain CW: 50% 45% 5%







• Molecule 45: 60S RIBOSOMAL PROTEIN L32



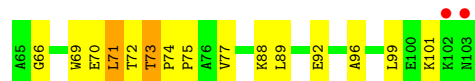
• Molecule 46: RPL37A



• Molecule 46: RPL37A



• Molecule 46: RPL37A



• Molecule 46: RPL37A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	320.19Å 289.25Å 535.04Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 39.96 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.52) 99.4 (39.96-3.52)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.216 , 0.244 0.238 , 0.263	Depositor DCC
$R_{free}$ test set	10000 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 73.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	511395	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A1	0.75	14/74792 (0.0%)	1.12	353/116594 (0.3%)
1	D1	0.82	60/74792 (0.1%)	1.14	368/116594 (0.3%)
1	F1	0.74	57/74792 (0.1%)	1.12	384/116594 (0.3%)
1	H1	0.78	8/74792 (0.0%)	1.15	436/116594 (0.4%)
2	AA	0.64	1/734 (0.1%)	0.77	0/972
2	DA	0.63	0/734	0.76	0/972
2	FA	0.61	1/734 (0.1%)	0.75	0/972
2	HA	0.63	0/734	0.77	0/972
3	AB	0.54	0/466	0.62	0/619
3	DB	0.46	0/466	0.62	0/619
3	FB	0.48	0/466	0.62	0/619
3	HB	0.51	0/466	0.62	0/619
4	AC	0.58	0/848	0.71	1/1123 (0.1%)
4	DC	0.53	0/848	0.69	0/1123
4	FC	0.54	0/848	0.70	0/1123
4	HC	0.57	0/848	0.71	1/1123 (0.1%)
5	AE	0.47	0/1550	0.74	2/2077 (0.1%)
5	DE	0.47	0/1550	0.74	2/2077 (0.1%)
5	FE	0.48	0/1550	0.75	2/2077 (0.1%)
5	HE	0.47	0/1550	0.75	2/2077 (0.1%)
6	AF	0.51	0/1033	0.71	0/1380
6	DF	0.51	0/1033	0.71	0/1380
6	FF	0.53	0/1033	0.71	0/1380
6	HF	0.53	0/1033	0.72	0/1380
7	AG	0.50	0/736	0.74	0/990
7	DG	0.47	0/736	0.73	0/990
7	FG	0.47	0/736	0.72	0/990
7	HG	0.46	0/736	0.72	0/990
8	AH	0.63	0/870	0.81	0/1175
8	DH	0.62	0/870	0.82	0/1175
8	FH	0.63	0/870	0.81	0/1175
8	HH	0.58	0/870	0.81	0/1175



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	AJ	0.51	0/1739	0.70	0/2368
9	DJ	0.49	0/1739	0.70	0/2368
9	FJ	0.53	0/1739	0.70	0/2368
9	HJ	0.54	0/1739	0.70	0/2368
10	AK	0.48	0/421	0.69	0/558
10	DK	0.45	0/421	0.70	0/558
10	FK	0.46	0/421	0.69	0/558
10	HK	0.48	0/421	0.71	0/558
11	AL	0.64	0/861	0.77	1/1154 (0.1%)
11	DL	0.57	0/861	0.72	0/1154
11	FL	0.51	0/861	0.73	0/1154
11	HL	0.51	0/861	0.74	0/1154
12	AM	0.41	0/832	0.67	0/1113
12	DM	0.41	0/832	0.67	0/1113
12	FM	0.41	0/832	0.67	0/1113
12	HM	0.42	0/832	0.66	0/1113
13	AN	0.43	0/1190	0.63	1/1582 (0.1%)
13	DN	0.38	0/1190	0.58	0/1582
13	FN	0.38	0/1190	0.58	0/1582
13	HN	0.38	0/1190	0.58	0/1582
14	AO	0.47	0/1047	0.77	1/1400 (0.1%)
14	DO	0.47	0/1047	0.77	1/1400 (0.1%)
14	FO	0.46	0/1047	0.76	1/1400 (0.1%)
14	HO	0.51	0/1047	0.78	1/1400 (0.1%)
15	AP	0.41	0/561	0.61	0/745
15	DP	0.38	0/561	0.62	0/745
15	FP	0.40	0/561	0.60	0/745
15	HP	0.40	0/561	0.62	0/745
16	AQ	0.48	0/808	0.70	0/1068
16	DQ	0.48	0/808	0.69	0/1068
16	FQ	0.49	0/808	0.73	0/1068
16	HQ	0.50	0/808	0.70	0/1068
17	AT	0.48	0/539	0.72	0/711
17	DT	0.48	0/539	0.72	0/711
17	FT	0.49	0/539	0.71	0/711
17	HT	0.52	0/539	0.72	0/711
18	AU	0.53	0/1647	0.74	1/2201 (0.0%)
18	DU	0.51	0/1647	0.74	1/2201 (0.0%)
18	FU	0.54	0/1647	0.74	1/2201 (0.0%)
18	HU	0.58	0/1647	0.74	1/2201 (0.0%)
19	AX	0.48	0/1563	0.74	0/2104
19	DX	0.50	0/1563	0.75	1/2104 (0.0%)
19	FX	0.49	0/1563	0.74	0/2104

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	HX	0.50	0/1563	0.74	2/2104 (0.1%)
20	B2	0.69	0/3696	1.06	10/5761 (0.2%)
20	C2	0.69	0/3696	1.07	7/5761 (0.1%)
20	E2	0.63	0/3696	1.07	10/5761 (0.2%)
20	G2	0.86	1/3696 (0.0%)	1.17	24/5761 (0.4%)
21	B3	0.70	0/2870	0.96	7/4473 (0.2%)
21	C3	0.61	0/2870	0.97	5/4473 (0.1%)
21	E3	0.59	0/2870	0.95	4/4473 (0.1%)
21	G3	0.63	0/2870	0.98	10/4473 (0.2%)
22	BA	0.63	0/2019	0.79	1/2712 (0.0%)
22	CA	0.61	0/2019	0.77	1/2712 (0.0%)
22	EA	0.61	0/2019	0.77	1/2712 (0.0%)
22	GA	0.60	0/2019	0.76	1/2712 (0.0%)
23	BB	0.56	0/3144	0.72	0/4213
23	CB	0.54	0/3144	0.71	0/4213
23	EB	0.54	0/3144	0.71	0/4213
23	GB	0.52	0/3144	0.72	0/4213
24	BC	0.47	0/3222	0.67	0/4338
24	CC	0.49	0/3222	0.68	0/4338
24	EC	0.49	0/3222	0.68	0/4338
24	GC	0.53	0/3222	0.69	1/4338 (0.0%)
25	BD	0.48	0/1376	0.66	0/1833
25	CD	0.45	0/1376	0.66	0/1833
25	ED	0.46	0/1376	0.66	0/1833
25	GD	0.47	0/1376	0.67	0/1833
26	BE	0.49	0/1501	0.72	2/2015 (0.1%)
26	CE	0.48	0/1501	0.72	2/2015 (0.1%)
26	EE	0.50	0/1501	0.72	1/2015 (0.0%)
26	GE	0.50	0/1501	0.74	2/2015 (0.1%)
27	BF	0.48	0/1893	0.66	0/2548
27	CF	0.48	0/1893	0.66	0/2548
27	EF	0.48	0/1893	0.65	0/2548
27	GF	0.49	0/1893	0.66	0/2548
29	BH	0.48	0/1652	0.68	0/2213
29	CH	0.48	0/1652	0.66	0/2213
29	EH	0.46	0/1652	0.66	0/2213
29	GH	0.46	0/1652	0.67	0/2213
30	BI	0.48	0/1624	0.66	0/2176
30	CI	0.49	0/1624	0.68	0/2176
30	EI	0.49	0/1624	0.66	0/2176
30	GI	0.87	6/1624 (0.4%)	0.92	7/2176 (0.3%)
31	BJ	0.64	1/1038 (0.1%)	0.77	0/1394
31	CJ	0.67	1/1038 (0.1%)	0.77	1/1394 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	EJ	0.64	1/1038 (0.1%)	0.76	0/1394
31	GJ	0.68	1/1038 (0.1%)	0.77	2/1394 (0.1%)
32	BK	0.53	0/1189	0.71	0/1589
32	CK	0.53	0/1189	0.73	1/1589 (0.1%)
32	EK	0.52	0/1189	0.73	1/1589 (0.1%)
32	GK	0.58	0/1189	0.74	0/1589
33	BL	0.53	0/1727	0.71	0/2308
33	CL	0.53	0/1727	0.71	0/2308
33	EL	0.53	0/1727	0.72	0/2308
33	GL	0.59	0/1727	0.73	0/2308
34	BM	0.49	0/2453	0.70	1/3285 (0.0%)
34	CM	0.48	0/2469	0.69	1/3306 (0.0%)
34	EM	0.54	1/2469 (0.0%)	0.71	1/3306 (0.0%)
34	GM	0.53	1/2469 (0.0%)	0.72	1/3306 (0.0%)
35	BN	0.54	0/1464	0.77	1/1965 (0.1%)
35	CN	0.52	0/1464	0.77	0/1965
35	EN	0.53	0/1464	0.76	0/1965
35	GN	0.60	0/1464	0.78	1/1965 (0.1%)
36	BO	0.58	0/1507	0.67	0/2001
36	EO	0.44	0/1208	0.62	0/1604
36	GO	0.50	0/1250	0.65	0/1660
37	BP	0.53	0/1300	0.64	0/1743
37	CP	0.49	0/1300	0.62	0/1743
37	EP	0.50	0/1300	0.63	0/1743
37	GP	0.54	0/1300	0.64	0/1743
38	BQ	0.60	0/1259	0.77	0/1693
38	CQ	0.57	0/1259	0.75	1/1693 (0.1%)
38	EQ	0.55	0/1259	0.75	1/1693 (0.1%)
38	GQ	0.56	0/1259	0.78	1/1693 (0.1%)
39	BR	0.52	0/981	0.67	0/1320
39	CR	0.47	0/981	0.66	0/1320
39	ER	0.46	0/981	0.66	0/1320
39	GR	0.52	0/981	0.67	0/1320
40	BS	0.44	0/1028	0.62	0/1372
40	CS	0.42	0/1028	0.61	0/1372
40	ES	0.44	0/1028	0.61	0/1372
40	GS	0.50	0/1028	0.63	0/1372
41	BT	0.60	0/521	0.72	0/693
41	CT	0.57	0/521	0.69	0/693
41	ET	0.55	0/521	0.71	0/693
41	GT	0.53	0/521	0.70	0/693
42	BU	0.44	0/995	0.65	0/1318
42	CU	0.44	0/995	0.64	0/1318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
42	EU	0.44	0/995	0.65	0/1318
42	GU	0.51	0/995	0.66	0/1318
43	BV	0.48	0/1950	0.66	0/2614
43	CV	0.49	0/1950	0.67	1/2614 (0.0%)
43	EV	0.50	0/1950	0.67	1/2614 (0.0%)
43	GV	0.49	0/1950	0.66	1/2614 (0.0%)
44	BW	0.60	0/913	0.68	0/1222
44	CW	0.55	0/913	0.68	0/1222
44	EW	0.51	0/913	0.67	0/1222
44	GW	0.51	0/913	0.68	0/1222
45	BX	0.48	0/1028	0.67	0/1371
45	CX	0.51	0/1028	0.67	0/1371
45	EX	0.47	0/1028	0.67	0/1371
45	GX	0.56	0/1028	0.68	0/1371
46	BY	0.60	0/799	0.79	0/1069
46	CY	0.60	0/799	0.75	0/1069
46	EY	0.57	0/799	0.76	0/1069
46	GY	0.55	0/799	0.75	0/1069
47	CO	0.46	0/1208	0.63	0/1604
All	All	0.68	154/540737 (0.0%)	0.99	1677/795620 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AA	0	1
2	DA	0	1
2	FA	0	1
2	HA	0	1
8	AH	0	1
12	AM	0	1
12	DM	0	1
12	FM	0	1
12	HM	0	1
16	AQ	0	1
16	DQ	0	1
16	FQ	0	1
16	HQ	0	1
18	FU	0	1
27	BF	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
27	CF	0	1
27	EF	0	1
27	GF	0	1
32	BK	0	2
32	CK	0	2
32	EK	0	2
32	GK	0	2
38	CQ	0	1
38	GQ	0	1
42	CU	0	1
45	GX	0	1
All	All	0	30

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F1	2239	A	O3'-P	25.66	1.92	1.61
30	GI	60	TRP	NE1-CE2	-18.39	1.13	1.37
1	D1	2254	A	C5-C4	17.31	1.50	1.38
1	D1	2254	A	N7-C5	15.90	1.48	1.39
1	D1	2254	A	N3-C4	15.68	1.44	1.34

The worst 5 of 1677 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F1	2253	U	C5-C6-N1	-21.57	111.92	122.70
30	GI	60	TRP	CE2-CD2-CG	-18.64	92.39	107.30
1	D1	284	U	C6-N1-C2	-15.54	111.67	121.00
1	F1	119	A	N1-C6-N6	15.41	127.85	118.60
1	H1	1053	A	C6-N1-C2	-15.06	109.57	118.60

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AA	51	GLY	Peptide
8	AH	101	GLY	Peptide
12	AM	53	GLY	Peptide
16	AQ	12	GLY	Peptide
27	BF	174	LYS	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	A1	66769	0	33570	4643	2
1	D1	66769	0	33568	4655	1
1	F1	66769	0	33568	4661	3
1	H1	66769	0	33570	4682	4
2	AA	721	0	744	102	0
2	DA	721	0	744	103	0
2	FA	721	0	744	110	0
2	HA	721	0	744	114	0
3	AB	456	0	483	51	0
3	DB	456	0	483	52	0
3	FB	456	0	483	53	0
3	HB	456	0	483	51	0
4	AC	836	0	912	64	0
4	DC	836	0	911	62	0
4	FC	836	0	911	65	0
4	HC	836	0	911	67	0
5	AE	1525	0	1600	230	0
5	DE	1525	0	1600	225	0
5	FE	1525	0	1600	221	0
5	HE	1525	0	1600	231	0
6	AF	1021	0	1119	147	0
6	DF	1021	0	1119	152	0
6	FF	1021	0	1119	152	0
6	HF	1021	0	1119	152	0
7	AG	727	0	747	103	0
7	DG	727	0	747	92	0
7	FG	727	0	747	88	0
7	HG	727	0	747	88	0
8	AH	850	0	870	134	0
8	DH	850	0	870	139	0
8	FH	850	0	870	139	0
8	HH	850	0	870	129	0
9	AJ	1716	0	1712	162	0
9	DJ	1716	0	1712	181	0
9	FJ	1716	0	1712	178	0
9	HJ	1716	0	1712	176	0
10	AK	415	0	446	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	DK	415	0	446	38	0
10	FK	415	0	446	36	0
10	HK	415	0	446	35	0
11	AL	852	0	906	90	0
11	DL	852	0	906	94	0
11	FL	852	0	906	88	0
11	HL	852	0	906	90	0
12	AM	819	0	855	75	0
12	DM	819	0	855	73	0
12	FM	819	0	855	77	0
12	HM	819	0	855	74	0
13	AN	1170	0	1259	156	0
13	DN	1170	0	1259	134	0
13	FN	1170	0	1259	155	0
13	HN	1170	0	1259	134	0
14	AO	1034	0	1101	143	0
14	DO	1034	0	1101	127	0
14	FO	1034	0	1101	130	0
14	HO	1034	0	1101	119	0
15	AP	551	0	614	53	0
15	DP	551	0	614	57	2
15	FP	551	0	614	49	0
15	HP	551	0	614	58	0
16	AQ	803	0	907	87	2
16	DQ	803	0	907	98	0
16	FQ	803	0	907	100	0
16	HQ	803	0	907	82	0
17	AT	533	0	578	65	0
17	DT	533	0	578	55	0
17	FT	533	0	578	56	0
17	HT	533	0	578	62	0
18	AU	1624	0	1733	210	0
18	DU	1624	0	1733	215	0
18	FU	1624	0	1733	209	0
18	HU	1624	0	1733	236	0
19	AX	1536	0	1613	221	0
19	DX	1536	0	1613	220	0
19	FX	1536	0	1613	222	0
19	HX	1536	0	1613	211	0
20	B2	3300	0	1657	219	1
20	C2	3300	0	1657	225	0
20	E2	3300	0	1657	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G2	3300	0	1657	234	0
21	B3	2566	0	1294	179	0
21	C3	2566	0	1294	195	0
21	E3	2566	0	1294	191	0
21	G3	2566	0	1294	187	0
22	BA	1977	0	2000	233	0
22	CA	1977	0	2000	221	0
22	EA	1977	0	2000	240	0
22	GA	1977	0	2000	247	0
23	BB	3080	0	3187	338	0
23	CB	3080	0	3187	332	0
23	EB	3080	0	3187	364	0
23	GB	3080	0	3187	361	0
24	BC	3172	0	3274	422	0
24	CC	3172	0	3274	428	0
24	EC	3172	0	3274	438	0
24	GC	3172	0	3274	443	0
25	BD	1357	0	1400	124	0
25	CD	1357	0	1400	123	0
25	ED	1357	0	1400	125	0
25	GD	1357	0	1400	127	0
26	BE	1481	0	1574	124	0
26	CE	1481	0	1574	119	0
26	EE	1481	0	1574	124	0
26	GE	1481	0	1574	123	0
27	BF	1860	0	1968	208	0
27	CF	1860	0	1968	217	0
27	EF	1860	0	1968	197	1
27	GF	1860	0	1968	208	0
28	BG	711	0	644	56	0
28	CG	711	0	644	44	0
28	EG	711	0	644	46	0
28	GG	711	0	644	86	0
29	BH	1620	0	1701	159	0
29	CH	1620	0	1701	155	0
29	EH	1620	0	1701	165	0
29	GH	1620	0	1701	160	0
30	BI	1594	0	1701	172	0
30	CI	1594	0	1701	179	0
30	EI	1594	0	1701	170	0
30	GI	1594	0	1701	179	0
31	BJ	1022	0	1078	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	CJ	1022	0	1079	64	0
31	EJ	1022	0	1079	70	0
31	GJ	1022	0	1078	71	0
32	BK	1161	0	1227	189	0
32	CK	1161	0	1227	180	0
32	EK	1161	0	1227	183	0
32	GK	1161	0	1227	195	0
33	BL	1691	0	1762	183	0
33	CL	1691	0	1762	187	0
33	EL	1691	0	1762	195	0
33	GL	1691	0	1762	203	0
34	BM	2409	0	2497	327	0
34	CM	2424	0	2509	312	1
34	EM	2424	0	2509	311	4
34	GM	2424	0	2509	286	2
35	BN	1441	0	1534	218	0
35	CN	1441	0	1534	232	0
35	EN	1441	0	1534	223	0
35	GN	1441	0	1534	234	0
36	BO	1491	0	1618	106	0
36	EO	1192	0	1296	87	0
36	GO	1234	0	1323	87	0
37	BP	1272	0	1310	136	0
37	CP	1272	0	1310	129	0
37	EP	1272	0	1310	137	0
37	GP	1272	0	1310	126	0
38	BQ	1239	0	1276	126	0
38	CQ	1239	0	1276	132	0
38	EQ	1239	0	1276	125	0
38	GQ	1239	0	1276	133	0
39	BR	965	0	1020	96	0
39	CR	965	0	1020	82	0
39	ER	965	0	1020	90	0
39	GR	965	0	1020	97	0
40	BS	1013	0	1101	90	0
40	CS	1013	0	1101	96	1
40	ES	1013	0	1101	94	0
40	GS	1013	0	1101	92	0
41	BT	510	0	546	51	0
41	CT	510	0	546	51	0
41	ET	510	0	546	59	0
41	GT	510	0	546	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BU	990	0	1123	98	0
42	CU	990	0	1123	106	0
42	EU	990	0	1123	109	0
42	GU	990	0	1123	117	0
43	BV	1910	0	1983	203	0
43	CV	1910	0	1983	202	0
43	EV	1910	0	1983	212	0
43	GV	1910	0	1983	199	0
44	BW	901	0	937	65	0
44	CW	901	0	937	68	0
44	EW	901	0	937	70	0
44	GW	901	0	937	69	0
45	BX	1012	0	1079	110	0
45	CX	1012	0	1079	108	0
45	EX	1012	0	1079	114	0
45	GX	1012	0	1079	120	0
46	BY	786	0	851	83	0
46	CY	786	0	849	90	0
46	EY	786	0	851	105	0
46	GY	786	0	851	94	0
47	CO	1366	0	1470	140	0
48	A1	200	0	0	0	0
48	AA	2	0	0	0	0
48	AK	1	0	0	0	0
48	B2	8	0	0	0	0
48	B3	3	0	0	0	0
48	BJ	1	0	0	0	0
48	BL	1	0	0	0	0
48	BN	1	0	0	0	0
48	BP	1	0	0	0	0
48	BQ	2	0	0	0	0
48	BW	1	0	0	0	0
48	C2	6	0	0	0	0
48	C3	7	0	0	0	0
48	CD	1	0	0	0	0
48	CJ	1	0	0	0	0
48	CL	2	0	0	0	0
48	CN	1	0	0	0	0
48	CQ	2	0	0	0	0
48	CW	1	0	0	0	0
48	CY	1	0	0	0	0
48	D1	232	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	DA	2	0	0	0	0
48	DJ	1	0	0	0	0
48	DK	1	0	0	0	0
48	DQ	1	0	0	0	0
48	E2	7	0	0	0	0
48	E3	6	0	0	0	0
48	EJ	1	0	0	0	0
48	EL	2	0	0	0	0
48	EN	2	0	0	0	0
48	EQ	1	0	0	0	0
48	EW	2	0	0	0	0
48	F1	184	0	0	0	0
48	FA	2	0	0	0	0
48	FK	1	0	0	0	0
48	FT	1	0	0	0	0
48	G2	6	0	0	0	0
48	G3	5	0	0	0	0
48	GA	1	0	0	0	0
48	GJ	1	0	0	0	0
48	GL	1	0	0	0	0
48	GN	1	0	0	0	0
48	GO	1	0	0	0	0
48	GP	2	0	0	0	0
48	GQ	1	0	0	0	0
48	GW	1	0	0	0	0
48	H1	155	0	0	0	0
48	HT	1	0	0	0	0
49	AA	1	0	0	0	0
49	AC	1	0	0	0	0
49	AK	1	0	0	0	0
49	AL	1	0	0	0	0
49	BY	1	0	0	0	0
49	CY	1	0	0	0	0
49	DA	1	0	0	0	0
49	DC	1	0	0	0	0
49	DK	1	0	0	0	0
49	DL	1	0	0	0	0
49	EY	1	0	0	0	0
49	FA	1	0	0	0	0
49	FC	1	0	0	0	0
49	FK	1	0	0	0	0
49	FL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	GY	1	0	0	0	0
49	HA	1	0	0	0	0
49	HC	1	0	0	0	0
49	HK	1	0	0	0	0
49	HL	1	0	0	0	0
50	A1	1134	0	0	292	0
50	AA	8	0	0	2	0
50	AB	5	0	0	2	0
50	AH	1	0	0	0	0
50	AK	3	0	0	1	0
50	AM	1	0	0	0	0
50	AP	2	0	0	0	0
50	AT	3	0	0	3	0
50	AU	4	0	0	3	0
50	B2	54	0	0	5	0
50	B3	23	0	0	6	0
50	BA	12	0	0	3	0
50	BB	4	0	0	1	0
50	BC	7	0	0	0	0
50	BE	1	0	0	0	0
50	BI	3	0	0	1	0
50	BJ	5	0	0	1	0
50	BK	3	0	0	1	0
50	BL	8	0	0	0	0
50	BM	2	0	0	1	0
50	BN	5	0	0	0	0
50	BO	2	0	0	2	0
50	BP	5	0	0	2	0
50	BQ	7	0	0	3	0
50	BU	1	0	0	0	0
50	BV	7	0	0	1	0
50	BW	5	0	0	0	0
50	BX	6	0	0	1	0
50	BY	5	0	0	0	0
50	C2	46	0	0	3	0
50	C3	39	0	0	10	0
50	CA	11	0	0	3	0
50	CB	4	0	0	0	0
50	CC	7	0	0	0	0
50	CD	4	0	0	0	0
50	CE	2	0	0	1	0
50	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	CJ	4	0	0	3	0
50	CK	3	0	0	1	0
50	CL	12	0	0	2	0
50	CM	6	0	0	1	0
50	CN	7	0	0	5	0
50	CO	2	0	0	1	0
50	CP	6	0	0	1	0
50	CQ	7	0	0	5	0
50	CU	1	0	0	0	0
50	CV	4	0	0	1	0
50	CW	5	0	0	0	0
50	CX	6	0	0	0	0
50	CY	5	0	0	0	0
50	D1	1341	0	0	313	0
50	DA	10	0	0	1	0
50	DB	4	0	0	2	0
50	DE	1	0	0	0	0
50	DJ	2	0	0	1	0
50	DK	2	0	0	0	0
50	DP	1	0	0	0	0
50	DQ	2	0	0	2	0
50	DT	4	0	0	3	0
50	DU	3	0	0	0	0
50	DX	2	0	0	0	0
50	E2	44	0	0	8	0
50	E3	34	0	0	4	0
50	EA	4	0	0	4	0
50	EB	3	0	0	0	0
50	EC	2	0	0	0	0
50	EE	2	0	0	0	0
50	EJ	4	0	0	1	0
50	EK	5	0	0	1	0
50	EL	10	0	0	1	0
50	EM	2	0	0	0	0
50	EN	7	0	0	6	0
50	EP	6	0	0	1	0
50	EQ	4	0	0	4	0
50	EV	6	0	0	1	0
50	EW	7	0	0	0	0
50	EX	5	0	0	2	0
50	EY	5	0	0	0	0
50	F1	1076	0	0	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	FA	7	0	0	2	0
50	FB	4	0	0	1	0
50	FE	1	0	0	0	0
50	FH	1	0	0	0	0
50	FK	2	0	0	0	0
50	FL	3	0	0	1	0
50	FP	2	0	0	0	0
50	FT	4	0	0	4	0
50	FU	4	0	0	0	0
50	G2	34	0	0	2	0
50	G3	26	0	0	9	0
50	GA	6	0	0	6	0
50	GB	3	0	0	0	0
50	GC	2	0	0	0	0
50	GE	2	0	0	0	0
50	GI	1	0	0	0	0
50	GJ	4	0	0	2	0
50	GK	2	0	0	2	0
50	GL	5	0	0	1	0
50	GM	1	0	0	1	0
50	GN	2	0	0	1	0
50	GO	2	0	0	1	0
50	GP	5	0	0	0	0
50	GQ	4	0	0	2	0
50	GV	3	0	0	0	0
50	GW	4	0	0	0	0
50	GX	5	0	0	1	0
50	GY	1	0	0	0	0
50	H1	924	0	0	217	0
50	HA	4	0	0	1	0
50	HB	4	0	0	2	0
50	HJ	2	0	0	0	0
50	HK	2	0	0	0	0
50	HP	1	0	0	0	0
50	HT	5	0	0	5	0
50	HU	2	0	0	0	0
All	All	511395	0	371708	37500	12

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 43.

The worst 5 of 37500 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)
28:GG:8:UNK:CG	1:H1:1248:G:N2	1.82	1.41
28:GG:8:UNK:HG3	1:H1:1248:G:N2	1.34	1.40
1:F1:452:U:H5'	14:FO:56:GLN:NE2	1.41	1.35
13:AN:130:LYS:HG2	1:H1:2664:C:OP1	1.22	1.33
46:CY:28:LYS:NZ	1:F1:2252:C:OP1	1.60	1.33

The worst 5 of 12 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)
34:CM:276:LYS:NZ	1:D1:259:U:O3'[2_546]	1.54	0.66
34:GM:117:THR:OG1	1:H1:192:C:C4'[2_445]	1.57	0.63
34:EM:214:LYS:NZ	1:F1:171:A:O4'[2_456]	1.76	0.44
20:B2:87:C:N4	40:CS:82:GLU:OE2[1_545]	1.84	0.36
1:A1:1840:U:O4	15:DP:74:LYS:N[1_545]	1.88	0.32

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
2	DA	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
2	FA	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
2	HA	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	AB	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
3	DB	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
3	FB	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
3	HB	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
4	AC	101/109 (93%)	99 (98%)	2 (2%)	0	100	100
4	DC	101/109 (93%)	99 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	FC	101/109 (93%)	99 (98%)	2 (2%)	0	100	100
4	HC	101/109 (93%)	99 (98%)	2 (2%)	0	100	100
5	AE	188/191 (98%)	178 (95%)	9 (5%)	1 (0%)	31	72
5	DE	188/191 (98%)	176 (94%)	11 (6%)	1 (0%)	31	72
5	FE	188/191 (98%)	178 (95%)	9 (5%)	1 (0%)	31	72
5	HE	188/191 (98%)	177 (94%)	10 (5%)	1 (0%)	31	72
6	AF	123/126 (98%)	115 (94%)	8 (6%)	0	100	100
6	DF	123/126 (98%)	116 (94%)	7 (6%)	0	100	100
6	FF	123/126 (98%)	115 (94%)	8 (6%)	0	100	100
6	HF	123/126 (98%)	114 (93%)	9 (7%)	0	100	100
7	AG	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
7	DG	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
7	FG	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
7	HG	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
8	AH	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
8	DH	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
8	FH	105/113 (93%)	100 (95%)	4 (4%)	1 (1%)	17	59
8	HH	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
9	AJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	19	62
9	DJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	19	62
9	FJ	224/248 (90%)	212 (95%)	10 (4%)	2 (1%)	19	62
9	HJ	224/248 (90%)	213 (95%)	9 (4%)	2 (1%)	19	62
10	AK	50/129 (39%)	43 (86%)	7 (14%)	0	100	100
10	DK	50/129 (39%)	44 (88%)	6 (12%)	0	100	100
10	FK	50/129 (39%)	44 (88%)	6 (12%)	0	100	100
10	HK	50/129 (39%)	43 (86%)	7 (14%)	0	100	100
11	AL	106/123 (86%)	98 (92%)	8 (8%)	0	100	100
11	DL	106/123 (86%)	98 (92%)	8 (8%)	0	100	100
11	FL	106/123 (86%)	98 (92%)	8 (8%)	0	100	100
11	HL	106/123 (86%)	98 (92%)	8 (8%)	0	100	100
12	AM	98/118 (83%)	92 (94%)	5 (5%)	1 (1%)	17	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	DM	98/118 (83%)	94 (96%)	3 (3%)	1 (1%)	17	59
12	FM	98/118 (83%)	93 (95%)	4 (4%)	1 (1%)	17	59
12	HM	98/118 (83%)	92 (94%)	5 (5%)	1 (1%)	17	59
13	AN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	24	67
13	DN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	24	67
13	FN	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
13	HN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	24	67
14	AO	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
14	DO	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
14	FO	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
14	HO	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
15	AP	62/89 (70%)	58 (94%)	4 (6%)	0	100	100
15	DP	62/89 (70%)	58 (94%)	4 (6%)	0	100	100
15	FP	62/89 (70%)	58 (94%)	4 (6%)	0	100	100
15	HP	62/89 (70%)	58 (94%)	4 (6%)	0	100	100
16	AQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	8	46
16	DQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	8	46
16	FQ	100/104 (96%)	88 (88%)	10 (10%)	2 (2%)	8	46
16	HQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	8	46
17	AT	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	11	49
17	DT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	49
17	FT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	49
17	HT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	49
18	AU	201/206 (98%)	188 (94%)	12 (6%)	1 (0%)	31	72
18	DU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	31	72
18	FU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	31	72
18	HU	201/206 (98%)	189 (94%)	11 (6%)	1 (0%)	31	72
19	AX	186/189 (98%)	177 (95%)	8 (4%)	1 (0%)	31	72
19	DX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	16	58
19	FX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	16	58
19	HX	186/189 (98%)	177 (95%)	7 (4%)	2 (1%)	16	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	BA	255/264 (97%)	236 (92%)	19 (8%)	0	100	100
22	CA	255/264 (97%)	235 (92%)	20 (8%)	0	100	100
22	EA	255/264 (97%)	234 (92%)	21 (8%)	0	100	100
22	GA	255/264 (97%)	237 (93%)	18 (7%)	0	100	100
23	BB	384/391 (98%)	371 (97%)	13 (3%)	0	100	100
23	CB	384/391 (98%)	371 (97%)	13 (3%)	0	100	100
23	EB	384/391 (98%)	371 (97%)	13 (3%)	0	100	100
23	GB	384/391 (98%)	370 (96%)	14 (4%)	0	100	100
24	BC	407/410 (99%)	383 (94%)	24 (6%)	0	100	100
24	CC	407/410 (99%)	387 (95%)	20 (5%)	0	100	100
24	EC	407/410 (99%)	384 (94%)	23 (6%)	0	100	100
24	GC	407/410 (99%)	386 (95%)	21 (5%)	0	100	100
25	BD	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
25	CD	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
25	ED	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
25	GD	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
26	BE	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
26	CE	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
26	EE	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
26	GE	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
27	BF	229/255 (90%)	219 (96%)	10 (4%)	0	100	100
27	CF	229/255 (90%)	219 (96%)	10 (4%)	0	100	100
27	EF	229/255 (90%)	219 (96%)	9 (4%)	1 (0%)	36	75
27	GF	229/255 (90%)	219 (96%)	10 (4%)	0	100	100
29	BH	197/215 (92%)	186 (94%)	11 (6%)	0	100	100
29	CH	197/215 (92%)	187 (95%)	10 (5%)	0	100	100
29	EH	197/215 (92%)	186 (94%)	11 (6%)	0	100	100
29	GH	197/215 (92%)	186 (94%)	11 (6%)	0	100	100
30	BI	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
30	CI	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
30	EI	196/198 (99%)	189 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	GI	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
31	BJ	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
31	CJ	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
31	EJ	136/141 (96%)	131 (96%)	5 (4%)	0	100	100
31	GJ	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
32	BK	146/149 (98%)	136 (93%)	8 (6%)	2 (1%)	12	52
32	CK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	8	44
32	EK	146/149 (98%)	137 (94%)	7 (5%)	2 (1%)	12	52
32	GK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	8	44
33	BL	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
33	CL	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
33	EL	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
33	GL	201/204 (98%)	193 (96%)	7 (4%)	1 (0%)	31	72
34	BM	296/301 (98%)	282 (95%)	13 (4%)	1 (0%)	43	78
34	CM	298/301 (99%)	282 (95%)	15 (5%)	1 (0%)	43	78
34	EM	298/301 (99%)	283 (95%)	14 (5%)	1 (0%)	43	78
34	GM	298/301 (99%)	285 (96%)	12 (4%)	1 (0%)	43	78
35	BN	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
35	CN	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
35	EN	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
35	GN	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
36	BO	182/185 (98%)	170 (93%)	11 (6%)	1 (0%)	31	72
36	EO	144/185 (78%)	137 (95%)	7 (5%)	0	100	100
36	GO	151/185 (82%)	143 (95%)	8 (5%)	0	100	100
37	BP	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
37	CP	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
37	EP	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
37	GP	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
38	BQ	155/183 (85%)	146 (94%)	9 (6%)	0	100	100
38	CQ	155/183 (85%)	147 (95%)	8 (5%)	0	100	100
38	EQ	155/183 (85%)	147 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	GQ	155/183 (85%)	147 (95%)	8 (5%)	0	100	100
39	BR	119/150 (79%)	115 (97%)	4 (3%)	0	100	100
39	CR	119/150 (79%)	116 (98%)	3 (2%)	0	100	100
39	ER	119/150 (79%)	115 (97%)	4 (3%)	0	100	100
39	GR	119/150 (79%)	114 (96%)	5 (4%)	0	100	100
40	BS	124/135 (92%)	119 (96%)	5 (4%)	0	100	100
40	CS	124/135 (92%)	119 (96%)	5 (4%)	0	100	100
40	ES	124/135 (92%)	119 (96%)	5 (4%)	0	100	100
40	GS	124/135 (92%)	118 (95%)	6 (5%)	0	100	100
41	BT	59/158 (37%)	57 (97%)	2 (3%)	0	100	100
41	CT	59/158 (37%)	56 (95%)	3 (5%)	0	100	100
41	ET	59/158 (37%)	57 (97%)	2 (3%)	0	100	100
41	GT	59/158 (37%)	57 (97%)	2 (3%)	0	100	100
42	BU	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
42	CU	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
42	EU	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
42	GU	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
43	BV	232/239 (97%)	216 (93%)	16 (7%)	0	100	100
43	CV	232/239 (97%)	216 (93%)	16 (7%)	0	100	100
43	EV	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	36	75
43	GV	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	36	75
44	BW	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
44	CW	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
44	EW	108/111 (97%)	101 (94%)	7 (6%)	0	100	100
44	GW	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
45	BX	123/134 (92%)	119 (97%)	4 (3%)	0	100	100
45	CX	123/134 (92%)	117 (95%)	6 (5%)	0	100	100
45	EX	123/134 (92%)	118 (96%)	5 (4%)	0	100	100
45	GX	123/134 (92%)	117 (95%)	6 (5%)	0	100	100
46	BY	100/103 (97%)	91 (91%)	9 (9%)	0	100	100
46	CY	100/103 (97%)	90 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	EY	100/103 (97%)	90 (90%)	10 (10%)	0	100	100
46	GY	100/103 (97%)	90 (90%)	10 (10%)	0	100	100
47	CO	145/185 (78%)	138 (95%)	7 (5%)	0	100	100
All	All	26160/28348 (92%)	24720 (94%)	1378 (5%)	62 (0%)	49	83

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	AQ	7	VAL
32	BK	24	LYS
32	CK	24	LYS
16	DQ	7	VAL
32	EK	24	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	69/72 (96%)	58 (84%)	11 (16%)	3	17
2	DA	69/72 (96%)	58 (84%)	11 (16%)	3	17
2	FA	69/72 (96%)	59 (86%)	10 (14%)	3	21
2	HA	69/72 (96%)	58 (84%)	11 (16%)	3	17
3	AB	48/49 (98%)	44 (92%)	4 (8%)	12	44
3	DB	48/49 (98%)	44 (92%)	4 (8%)	12	44
3	FB	48/49 (98%)	44 (92%)	4 (8%)	12	44
3	HB	48/49 (98%)	44 (92%)	4 (8%)	12	44
4	AC	95/101 (94%)	92 (97%)	3 (3%)	42	74
4	DC	95/101 (94%)	92 (97%)	3 (3%)	42	74
4	FC	95/101 (94%)	92 (97%)	3 (3%)	42	74
4	HC	95/101 (94%)	92 (97%)	3 (3%)	42	74
5	AE	162/163 (99%)	152 (94%)	10 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	DE	162/163 (99%)	152 (94%)	10 (6%)	20	56
5	FE	162/163 (99%)	151 (93%)	11 (7%)	17	53
5	HE	162/163 (99%)	151 (93%)	11 (7%)	17	53
6	AF	111/112 (99%)	107 (96%)	4 (4%)	38	71
6	DF	111/112 (99%)	106 (96%)	5 (4%)	30	66
6	FF	111/112 (99%)	107 (96%)	4 (4%)	38	71
6	HF	111/112 (99%)	107 (96%)	4 (4%)	38	71
7	AG	80/88 (91%)	76 (95%)	4 (5%)	27	63
7	DG	80/88 (91%)	74 (92%)	6 (8%)	15	49
7	FG	80/88 (91%)	75 (94%)	5 (6%)	20	56
7	HG	80/88 (91%)	76 (95%)	4 (5%)	27	63
8	AH	87/92 (95%)	78 (90%)	9 (10%)	8	36
8	DH	87/92 (95%)	78 (90%)	9 (10%)	8	36
8	FH	87/92 (95%)	78 (90%)	9 (10%)	8	36
8	HH	87/92 (95%)	78 (90%)	9 (10%)	8	36
9	AJ	195/216 (90%)	177 (91%)	18 (9%)	10	40
9	DJ	195/216 (90%)	176 (90%)	19 (10%)	9	38
9	FJ	195/216 (90%)	177 (91%)	18 (9%)	10	40
9	HJ	195/216 (90%)	177 (91%)	18 (9%)	10	40
10	AK	46/113 (41%)	43 (94%)	3 (6%)	19	55
10	DK	46/113 (41%)	43 (94%)	3 (6%)	19	55
10	FK	46/113 (41%)	43 (94%)	3 (6%)	19	55
10	HK	46/113 (41%)	43 (94%)	3 (6%)	19	55
11	AL	92/107 (86%)	87 (95%)	5 (5%)	24	60
11	DL	92/107 (86%)	87 (95%)	5 (5%)	24	60
11	FL	92/107 (86%)	88 (96%)	4 (4%)	32	67
11	HL	92/107 (86%)	87 (95%)	5 (5%)	24	60
12	AM	93/110 (84%)	90 (97%)	3 (3%)	42	74
12	DM	93/110 (84%)	90 (97%)	3 (3%)	42	74
12	FM	93/110 (84%)	90 (97%)	3 (3%)	42	74
12	HM	93/110 (84%)	90 (97%)	3 (3%)	42	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AN	130/131 (99%)	123 (95%)	7 (5%)	24	60
13	DN	130/131 (99%)	122 (94%)	8 (6%)	20	56
13	FN	130/131 (99%)	123 (95%)	7 (5%)	24	60
13	HN	130/131 (99%)	123 (95%)	7 (5%)	24	60
14	AO	108/108 (100%)	102 (94%)	6 (6%)	23	59
14	DO	108/108 (100%)	102 (94%)	6 (6%)	23	59
14	FO	108/108 (100%)	100 (93%)	8 (7%)	15	49
14	HO	108/108 (100%)	102 (94%)	6 (6%)	23	59
15	AP	60/77 (78%)	56 (93%)	4 (7%)	18	54
15	DP	60/77 (78%)	56 (93%)	4 (7%)	18	54
15	FP	60/77 (78%)	56 (93%)	4 (7%)	18	54
15	HP	60/77 (78%)	56 (93%)	4 (7%)	18	54
16	AQ	81/83 (98%)	75 (93%)	6 (7%)	15	49
16	DQ	81/83 (98%)	75 (93%)	6 (7%)	15	49
16	FQ	81/83 (98%)	75 (93%)	6 (7%)	15	49
16	HQ	81/83 (98%)	75 (93%)	6 (7%)	15	49
17	AT	61/62 (98%)	55 (90%)	6 (10%)	9	37
17	DT	61/62 (98%)	57 (93%)	4 (7%)	18	54
17	FT	61/62 (98%)	57 (93%)	4 (7%)	18	54
17	HT	61/62 (98%)	57 (93%)	4 (7%)	18	54
18	AU	169/171 (99%)	159 (94%)	10 (6%)	21	58
18	DU	169/171 (99%)	161 (95%)	8 (5%)	29	65
18	FU	169/171 (99%)	160 (95%)	9 (5%)	25	61
18	HU	169/171 (99%)	161 (95%)	8 (5%)	29	65
19	AX	167/168 (99%)	153 (92%)	14 (8%)	12	44
19	DX	167/168 (99%)	152 (91%)	15 (9%)	10	42
19	FX	167/168 (99%)	151 (90%)	16 (10%)	9	39
19	HX	167/168 (99%)	154 (92%)	13 (8%)	14	47
22	BA	196/198 (99%)	165 (84%)	31 (16%)	3	18
22	CA	196/198 (99%)	164 (84%)	32 (16%)	2	16
22	EA	196/198 (99%)	164 (84%)	32 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	GA	196/198 (99%)	165 (84%)	31 (16%)	3	18
23	BB	330/334 (99%)	306 (93%)	24 (7%)	15	50
23	CB	330/334 (99%)	307 (93%)	23 (7%)	16	52
23	EB	330/334 (99%)	308 (93%)	22 (7%)	18	54
23	GB	330/334 (99%)	306 (93%)	24 (7%)	15	50
24	BC	325/326 (100%)	302 (93%)	23 (7%)	16	51
24	CC	325/326 (100%)	302 (93%)	23 (7%)	16	51
24	EC	325/326 (100%)	300 (92%)	25 (8%)	14	47
24	GC	325/326 (100%)	300 (92%)	25 (8%)	14	47
25	BD	146/149 (98%)	136 (93%)	10 (7%)	17	53
25	CD	146/149 (98%)	136 (93%)	10 (7%)	17	53
25	ED	146/149 (98%)	135 (92%)	11 (8%)	15	49
25	GD	146/149 (98%)	136 (93%)	10 (7%)	17	53
26	BE	163/165 (99%)	157 (96%)	6 (4%)	37	70
26	CE	163/165 (99%)	157 (96%)	6 (4%)	37	70
26	EE	163/165 (99%)	157 (96%)	6 (4%)	37	70
26	GE	163/165 (99%)	157 (96%)	6 (4%)	37	70
27	BF	201/222 (90%)	194 (96%)	7 (4%)	39	72
27	CF	201/222 (90%)	194 (96%)	7 (4%)	39	72
27	EF	201/222 (90%)	194 (96%)	7 (4%)	39	72
27	GF	201/222 (90%)	194 (96%)	7 (4%)	39	72
29	BH	169/180 (94%)	155 (92%)	14 (8%)	12	44
29	CH	169/180 (94%)	155 (92%)	14 (8%)	12	44
29	EH	169/180 (94%)	156 (92%)	13 (8%)	14	47
29	GH	169/180 (94%)	153 (90%)	16 (10%)	9	39
30	BI	166/166 (100%)	150 (90%)	16 (10%)	9	39
30	CI	166/166 (100%)	149 (90%)	17 (10%)	8	36
30	EI	166/166 (100%)	150 (90%)	16 (10%)	9	39
30	GI	166/166 (100%)	150 (90%)	16 (10%)	9	39
31	BJ	107/108 (99%)	98 (92%)	9 (8%)	12	44
31	CJ	107/108 (99%)	99 (92%)	8 (8%)	15	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	EJ	107/108 (99%)	99 (92%)	8 (8%)	15	49
31	GJ	107/108 (99%)	99 (92%)	8 (8%)	15	49
32	BK	120/121 (99%)	110 (92%)	10 (8%)	12	44
32	CK	120/121 (99%)	111 (92%)	9 (8%)	15	49
32	EK	120/121 (99%)	110 (92%)	10 (8%)	12	44
32	GK	120/121 (99%)	110 (92%)	10 (8%)	12	44
33	BL	174/175 (99%)	165 (95%)	9 (5%)	25	62
33	CL	174/175 (99%)	165 (95%)	9 (5%)	25	62
33	EL	174/175 (99%)	165 (95%)	9 (5%)	25	62
33	GL	174/175 (99%)	166 (95%)	8 (5%)	29	65
34	BM	252/254 (99%)	239 (95%)	13 (5%)	25	62
34	CM	253/254 (100%)	242 (96%)	11 (4%)	32	67
34	EM	253/254 (100%)	242 (96%)	11 (4%)	32	67
34	GM	253/254 (100%)	240 (95%)	13 (5%)	26	62
35	BN	159/160 (99%)	145 (91%)	14 (9%)	11	43
35	CN	159/160 (99%)	146 (92%)	13 (8%)	12	45
35	EN	159/160 (99%)	145 (91%)	14 (9%)	11	43
35	GN	159/160 (99%)	146 (92%)	13 (8%)	12	45
36	BO	158/159 (99%)	148 (94%)	10 (6%)	20	56
36	EO	126/159 (79%)	116 (92%)	10 (8%)	13	46
36	GO	127/159 (80%)	117 (92%)	10 (8%)	13	46
37	BP	134/135 (99%)	124 (92%)	10 (8%)	15	49
37	CP	134/135 (99%)	126 (94%)	8 (6%)	21	57
37	EP	134/135 (99%)	125 (93%)	9 (7%)	18	54
37	GP	134/135 (99%)	125 (93%)	9 (7%)	18	54
38	BQ	128/148 (86%)	115 (90%)	13 (10%)	8	36
38	CQ	128/148 (86%)	115 (90%)	13 (10%)	8	36
38	EQ	128/148 (86%)	115 (90%)	13 (10%)	8	36
38	GQ	128/148 (86%)	115 (90%)	13 (10%)	8	36
39	BR	108/132 (82%)	101 (94%)	7 (6%)	19	55
39	CR	108/132 (82%)	101 (94%)	7 (6%)	19	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	ER	108/132 (82%)	102 (94%)	6 (6%)	23	59
39	GR	108/132 (82%)	103 (95%)	5 (5%)	29	65
40	BS	113/120 (94%)	105 (93%)	8 (7%)	16	51
40	CS	113/120 (94%)	104 (92%)	9 (8%)	13	46
40	ES	113/120 (94%)	105 (93%)	8 (7%)	16	51
40	GS	113/120 (94%)	104 (92%)	9 (8%)	13	46
41	BT	52/130 (40%)	46 (88%)	6 (12%)	6	31
41	CT	52/130 (40%)	46 (88%)	6 (12%)	6	31
41	ET	52/130 (40%)	46 (88%)	6 (12%)	6	31
41	GT	52/130 (40%)	46 (88%)	6 (12%)	6	31
42	BU	105/106 (99%)	96 (91%)	9 (9%)	11	43
42	CU	105/106 (99%)	96 (91%)	9 (9%)	11	43
42	EU	105/106 (99%)	96 (91%)	9 (9%)	11	43
42	GU	105/106 (99%)	96 (91%)	9 (9%)	11	43
43	BV	197/202 (98%)	186 (94%)	11 (6%)	23	59
43	CV	197/202 (98%)	187 (95%)	10 (5%)	26	62
43	EV	197/202 (98%)	188 (95%)	9 (5%)	29	65
43	GV	197/202 (98%)	187 (95%)	10 (5%)	26	62
44	BW	100/101 (99%)	96 (96%)	4 (4%)	34	69
44	CW	100/101 (99%)	95 (95%)	5 (5%)	27	63
44	EW	100/101 (99%)	95 (95%)	5 (5%)	27	63
44	GW	100/101 (99%)	96 (96%)	4 (4%)	34	69
45	BX	104/111 (94%)	88 (85%)	16 (15%)	3	19
45	CX	104/111 (94%)	87 (84%)	17 (16%)	2	16
45	EX	104/111 (94%)	88 (85%)	16 (15%)	3	19
45	GX	104/111 (94%)	88 (85%)	16 (15%)	3	19
46	BY	79/80 (99%)	72 (91%)	7 (9%)	11	42
46	CY	79/80 (99%)	71 (90%)	8 (10%)	8	36
46	EY	79/80 (99%)	71 (90%)	8 (10%)	8	36
46	GY	79/80 (99%)	73 (92%)	6 (8%)	14	48
47	CO	126/127 (99%)	116 (92%)	10 (8%)	13	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	22468/23988 (94%)	20823 (93%)	1645 (7%)	15 50

5 of 1645 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	DH	47	ASP
26	EE	113	LYS
46	GY	71	LEU
10	DK	85	LEU
22	EA	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 750 such sidechains are listed below:

Mol	Chain	Res	Type
14	DO	56	GLN
27	EF	107	GLN
6	HF	67	GLN
18	DU	3	HIS
23	EB	163	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	3114/3354 (92%)	1118 (35%)	209 (6%)
1	D1	3114/3354 (92%)	1113 (35%)	215 (6%)
1	F1	3114/3354 (92%)	1113 (35%)	211 (6%)
1	H1	3114/3354 (92%)	1113 (35%)	210 (6%)
20	B2	154/154 (100%)	58 (37%)	13 (8%)
20	C2	154/154 (100%)	60 (38%)	13 (8%)
20	E2	154/154 (100%)	60 (38%)	13 (8%)
20	G2	154/154 (100%)	60 (38%)	13 (8%)
21	B3	119/120 (99%)	38 (31%)	1 (0%)
21	C3	119/120 (99%)	39 (32%)	1 (0%)
21	E3	119/120 (99%)	38 (31%)	1 (0%)
21	G3	119/120 (99%)	38 (31%)	1 (0%)
All	All	13548/14512 (93%)	4848 (35%)	901 (6%)

5 of 4848 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	9	G
1	A1	16	G
1	A1	17	C
1	A1	19	A
1	A1	20	G

5 of 901 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D1	2741	U
1	F1	500	G
1	H1	2300	G
1	D1	3035	A
20	E2	43	A

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 885 ligands modelled in this entry, 885 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F1	2239:A	O3'	2240:C	P	1.91

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A1	3119/3354 (92%)	0.13	90 (2%) 51 45	42, 91, 187, 390	0
1	D1	3119/3354 (92%)	0.05	34 (1%) 80 75	40, 79, 164, 330	0
1	F1	3119/3354 (92%)	0.18	62 (1%) 65 59	51, 94, 176, 357	0
1	H1	3119/3354 (92%)	0.49	136 (4%) 34 29	54, 121, 213, 367	0
2	AA	91/94 (96%)	-0.16	2 (2%) 62 55	29, 65, 120, 243	0
2	DA	91/94 (96%)	-0.09	0 100 100	34, 66, 123, 226	0
2	FA	91/94 (96%)	0.21	2 (2%) 62 55	47, 83, 132, 204	0
2	HA	91/94 (96%)	0.86	12 (13%) 3 4	74, 119, 186, 243	0
3	AB	51/52 (98%)	-0.20	1 (1%) 65 59	44, 63, 110, 148	0
3	DB	51/52 (98%)	-0.13	1 (1%) 65 59	49, 69, 111, 146	0
3	FB	51/52 (98%)	0.09	0 100 100	59, 86, 118, 167	0
3	HB	51/52 (98%)	0.79	8 (15%) 2 2	90, 114, 144, 197	0
4	AC	103/109 (94%)	0.37	3 (2%) 51 45	73, 117, 154, 228	0
4	DC	103/109 (94%)	-0.01	0 100 100	46, 84, 135, 194	0
4	FC	103/109 (94%)	0.01	1 (0%) 82 77	58, 96, 156, 192	0
4	HC	103/109 (94%)	0.32	3 (2%) 51 45	81, 130, 176, 199	0
5	AE	190/191 (99%)	0.19	12 (6%) 20 17	69, 122, 171, 214	0
5	DE	190/191 (99%)	0.08	1 (0%) 90 88	74, 124, 169, 226	0
5	FE	190/191 (99%)	0.20	8 (4%) 36 31	60, 123, 176, 227	0
5	HE	190/191 (99%)	0.35	14 (7%) 14 14	76, 141, 194, 227	0
6	AF	125/126 (99%)	0.02	5 (4%) 38 33	71, 111, 156, 213	0
6	DF	125/126 (99%)	-0.22	2 (1%) 72 66	70, 106, 157, 190	0
6	FF	125/126 (99%)	0.01	6 (4%) 30 26	63, 109, 166, 245	0
6	HF	125/126 (99%)	0.02	0 100 100	74, 113, 163, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AG	96/104 (92%)	0.08	1 (1%) 82 77	62, 103, 188, 218	0
7	DG	96/104 (92%)	0.06	4 (4%) 36 31	57, 114, 179, 222	0
7	FG	96/104 (92%)	0.18	2 (2%) 63 57	81, 112, 176, 199	0
7	HG	96/104 (92%)	0.21	1 (1%) 82 77	94, 134, 183, 218	0
8	AH	107/113 (94%)	-0.11	0 100 100	61, 91, 127, 159	0
8	DH	107/113 (94%)	-0.12	0 100 100	54, 89, 127, 138	0
8	FH	107/113 (94%)	-0.04	0 100 100	57, 89, 122, 164	0
8	HH	107/113 (94%)	0.14	0 100 100	68, 109, 141, 181	0
9	AJ	226/248 (91%)	-0.40	0 100 100	52, 90, 138, 190	0
9	DJ	226/248 (91%)	-0.36	0 100 100	51, 89, 136, 206	0
9	FJ	226/248 (91%)	-0.41	1 (0%) 92 90	38, 82, 130, 183	0
9	HJ	226/248 (91%)	-0.49	0 100 100	40, 78, 123, 155	0
10	AK	52/129 (40%)	0.12	2 (3%) 40 35	73, 101, 146, 182	0
10	DK	52/129 (40%)	-0.32	1 (1%) 66 60	53, 79, 134, 151	0
10	FK	52/129 (40%)	-0.40	0 100 100	56, 81, 139, 189	0
10	HK	52/129 (40%)	-0.27	0 100 100	61, 77, 118, 158	0
11	AL	108/123 (87%)	-0.12	1 (0%) 84 79	38, 73, 130, 165	0
11	DL	108/123 (87%)	-0.10	1 (0%) 84 79	47, 85, 144, 217	0
11	FL	108/123 (87%)	0.13	1 (0%) 84 79	66, 98, 135, 174	0
11	HL	108/123 (87%)	0.51	5 (4%) 32 27	90, 117, 156, 183	0
12	AM	100/118 (84%)	0.20	3 (3%) 50 44	72, 121, 155, 185	0
12	DM	100/118 (84%)	0.16	4 (4%) 38 33	73, 126, 179, 199	0
12	FM	100/118 (84%)	0.29	2 (2%) 65 59	93, 144, 196, 208	0
12	HM	100/118 (84%)	0.06	2 (2%) 65 59	98, 151, 195, 214	0
13	AN	143/144 (99%)	-0.20	1 (0%) 87 83	59, 97, 163, 189	0
13	DN	143/144 (99%)	-0.06	1 (0%) 87 83	73, 121, 179, 214	0
13	FN	143/144 (99%)	-0.02	1 (0%) 87 83	72, 122, 175, 208	0
13	HN	143/144 (99%)	0.30	3 (2%) 63 57	92, 148, 189, 217	0
14	AO	134/134 (100%)	-0.20	1 (0%) 87 83	66, 116, 162, 202	0
14	DO	134/134 (100%)	-0.11	1 (0%) 87 83	52, 99, 151, 209	0
14	FO	134/134 (100%)	0.04	2 (1%) 73 68	65, 118, 167, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	HO	134/134 (100%)	0.48	11 (8%) 11 12	96, 143, 197, 227	0
15	AP	66/89 (74%)	0.39	3 (4%) 33 28	55, 128, 209, 241	0
15	DP	66/89 (74%)	0.32	5 (7%) 14 13	73, 116, 176, 245	0
15	FP	66/89 (74%)	0.56	4 (6%) 21 18	99, 143, 202, 214	0
15	HP	66/89 (74%)	1.03	8 (12%) 4 5	99, 149, 219, 247	0
16	AQ	102/104 (98%)	0.09	3 (2%) 51 45	72, 122, 172, 208	0
16	DQ	102/104 (98%)	-0.01	3 (2%) 51 45	63, 105, 151, 186	0
16	FQ	102/104 (98%)	0.01	2 (1%) 65 59	72, 114, 166, 190	0
16	HQ	102/104 (98%)	0.57	6 (5%) 22 19	110, 154, 195, 203	0
17	AT	65/66 (98%)	0.37	4 (6%) 20 18	76, 121, 156, 193	0
17	DT	65/66 (98%)	0.11	1 (1%) 73 68	51, 87, 122, 211	0
17	FT	65/66 (98%)	0.26	1 (1%) 73 68	51, 107, 144, 201	0
17	HT	65/66 (98%)	0.76	4 (6%) 20 18	69, 136, 171, 222	0
18	AU	203/206 (98%)	0.09	4 (1%) 65 59	74, 122, 179, 233	0
18	DU	203/206 (98%)	-0.13	0 100 100	48, 98, 158, 198	0
18	FU	203/206 (98%)	-0.07	1 (0%) 90 88	67, 116, 174, 203	0
18	HU	203/206 (98%)	0.54	19 (9%) 8 9	102, 155, 206, 240	0
19	AX	188/189 (99%)	-0.20	1 (0%) 90 88	72, 105, 145, 201	0
19	DX	188/189 (99%)	-0.29	0 100 100	54, 89, 128, 170	0
19	FX	188/189 (99%)	-0.09	1 (0%) 90 88	62, 98, 141, 179	0
19	HX	188/189 (99%)	-0.03	0 100 100	74, 106, 135, 193	0
20	B2	154/154 (100%)	-0.11	2 (1%) 77 71	61, 80, 118, 192	0
20	C2	154/154 (100%)	-0.03	0 100 100	54, 80, 120, 186	0
20	E2	154/154 (100%)	0.16	3 (1%) 66 60	74, 105, 142, 189	0
20	G2	154/154 (100%)	0.73	13 (8%) 11 11	98, 146, 182, 210	0
21	B3	120/120 (100%)	0.46	4 (3%) 46 41	90, 150, 184, 217	0
21	C3	120/120 (100%)	-0.10	0 100 100	64, 98, 116, 161	0
21	E3	120/120 (100%)	0.03	0 100 100	72, 120, 147, 172	0
21	G3	120/120 (100%)	0.45	4 (3%) 46 41	95, 138, 175, 235	0
22	BA	257/264 (97%)	-0.02	9 (3%) 44 38	30, 70, 134, 233	0
22	CA	257/264 (97%)	-0.18	10 (3%) 39 34	31, 75, 139, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
22	EA	257/264 (97%)	-0.16	10 (3%) 39 34	40, 79, 136, 217	0
22	GA	257/264 (97%)	0.22	13 (5%) 28 24	60, 106, 157, 242	0
23	BB	386/391 (98%)	-0.32	5 (1%) 77 71	33, 69, 120, 227	0
23	CB	386/391 (98%)	-0.44	2 (0%) 90 88	34, 75, 123, 222	0
23	EB	386/391 (98%)	-0.36	4 (1%) 82 77	38, 75, 123, 230	0
23	GB	386/391 (98%)	-0.35	4 (1%) 82 77	51, 82, 132, 217	0
24	BC	409/410 (99%)	-0.01	12 (2%) 51 45	37, 107, 173, 241	0
24	CC	409/410 (99%)	-0.20	2 (0%) 90 88	40, 91, 151, 206	0
24	EC	409/410 (99%)	-0.07	5 (1%) 79 73	54, 107, 162, 237	0
24	GC	409/410 (99%)	0.34	17 (4%) 36 31	77, 143, 195, 252	0
25	BD	169/172 (98%)	0.96	23 (13%) 3 4	116, 159, 200, 225	0
25	CD	169/172 (98%)	0.12	4 (2%) 59 52	70, 110, 151, 188	0
25	ED	169/172 (98%)	0.49	8 (4%) 31 27	89, 133, 179, 209	0
25	GD	169/172 (98%)	0.66	19 (11%) 5 6	96, 139, 182, 216	0
26	BE	186/188 (98%)	-0.08	0 100 100	65, 109, 150, 194	0
26	CE	186/188 (98%)	-0.19	0 100 100	59, 94, 131, 171	0
26	EE	186/188 (98%)	-0.08	1 (0%) 90 88	60, 94, 139, 195	0
26	GE	186/188 (98%)	-0.12	0 100 100	53, 91, 135, 220	0
27	BF	231/255 (90%)	0.18	7 (3%) 50 44	70, 122, 176, 252	0
27	CF	231/255 (90%)	-0.14	3 (1%) 77 71	71, 115, 175, 233	0
27	EF	231/255 (90%)	0.00	6 (2%) 56 49	76, 120, 187, 241	0
27	GF	231/255 (90%)	0.60	17 (7%) 14 14	112, 166, 210, 233	0
28	BG	0/123	-	-	-	-
28	CG	0/123	-	-	-	-
28	EG	0/123	-	-	-	-
28	GG	0/123	-	-	-	-
29	BH	201/215 (93%)	0.18	6 (2%) 50 44	79, 133, 181, 221	0
29	CH	201/215 (93%)	-0.24	1 (0%) 90 88	42, 93, 139, 153	0
29	EH	201/215 (93%)	-0.15	2 (0%) 82 77	50, 105, 158, 202	0
29	GH	201/215 (93%)	0.08	2 (0%) 82 77	71, 118, 171, 203	0
30	BI	198/198 (100%)	-0.21	2 (1%) 82 77	51, 85, 152, 185	0
30	CI	198/198 (100%)	-0.36	0 100 100	48, 78, 149, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	EI	198/198 (100%)	-0.26	2 (1%) 82 77	47, 79, 152, 174	0
30	GI	198/198 (100%)	-0.20	2 (1%) 82 77	53, 91, 151, 195	0
31	BJ	138/141 (97%)	-0.43	0 100 100	42, 68, 112, 160	0
31	CJ	138/141 (97%)	-0.47	0 100 100	40, 65, 108, 150	0
31	EJ	138/141 (97%)	-0.44	3 (2%) 62 55	40, 65, 108, 202	0
31	GJ	138/141 (97%)	-0.41	1 (0%) 87 83	30, 60, 98, 186	0
32	BK	148/149 (99%)	0.01	4 (2%) 54 48	50, 105, 158, 221	0
32	CK	148/149 (99%)	-0.27	0 100 100	36, 74, 124, 184	0
32	EK	148/149 (99%)	-0.10	0 100 100	50, 95, 140, 228	0
32	GK	148/149 (99%)	0.53	11 (7%) 14 14	78, 129, 181, 208	0
33	BL	203/204 (99%)	-0.26	1 (0%) 90 88	57, 83, 120, 153	0
33	CL	203/204 (99%)	-0.36	0 100 100	37, 74, 106, 180	0
33	EL	203/204 (99%)	-0.10	0 100 100	51, 89, 121, 160	0
33	GL	203/204 (99%)	0.39	7 (3%) 45 40	89, 133, 165, 205	0
34	BM	298/301 (99%)	0.35	10 (3%) 45 40	87, 152, 201, 240	0
34	CM	300/301 (99%)	-0.12	3 (1%) 82 77	61, 110, 166, 208	0
34	EM	300/301 (99%)	0.23	17 (5%) 24 20	76, 127, 183, 233	0
34	GM	300/301 (99%)	0.69	28 (9%) 8 9	98, 157, 204, 233	0
35	BN	180/181 (99%)	0.04	1 (0%) 89 85	68, 110, 150, 224	0
35	CN	180/181 (99%)	-0.33	0 100 100	47, 82, 125, 185	0
35	EN	180/181 (99%)	-0.10	1 (0%) 89 85	63, 101, 142, 187	0
35	GN	180/181 (99%)	0.28	4 (2%) 62 55	94, 139, 188, 248	0
36	BO	184/185 (99%)	0.27	14 (7%) 14 13	29, 78, 184, 207	0
36	EO	146/185 (78%)	0.19	3 (2%) 63 57	57, 95, 128, 194	0
36	GO	153/185 (82%)	0.39	8 (5%) 27 24	67, 109, 153, 262	0
37	BP	156/157 (99%)	0.16	0 100 100	70, 116, 169, 203	0
37	CP	156/157 (99%)	-0.27	0 100 100	42, 79, 136, 152	0
37	EP	156/157 (99%)	-0.09	2 (1%) 77 71	56, 100, 148, 183	0
37	GP	156/157 (99%)	0.46	6 (3%) 40 35	69, 122, 163, 222	0
38	BQ	157/183 (85%)	-0.34	0 100 100	31, 68, 121, 173	0
38	CQ	157/183 (85%)	-0.32	1 (0%) 89 85	26, 70, 124, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
38	EQ	157/183 (85%)	-0.18	1 (0%) 89 85	48, 86, 141, 177	0
38	GQ	157/183 (85%)	0.16	2 (1%) 77 71	60, 106, 157, 200	0
39	BR	121/150 (80%)	-0.20	1 (0%) 86 80	42, 78, 129, 185	0
39	CR	121/150 (80%)	0.05	1 (0%) 86 80	54, 88, 129, 172	0
39	ER	121/150 (80%)	0.18	5 (4%) 37 32	65, 112, 146, 172	0
39	GR	121/150 (80%)	0.45	9 (7%) 14 14	97, 138, 175, 191	0
40	BS	126/135 (93%)	-0.17	0 100 100	62, 98, 133, 177	0
40	CS	126/135 (93%)	0.02	4 (3%) 47 42	46, 89, 127, 152	0
40	ES	126/135 (93%)	0.16	5 (3%) 38 33	74, 112, 151, 184	0
40	GS	126/135 (93%)	0.58	9 (7%) 16 15	101, 143, 186, 218	0
41	BT	61/158 (38%)	-0.38	0 100 100	39, 73, 127, 158	0
41	CT	61/158 (38%)	-0.31	0 100 100	37, 73, 105, 137	0
41	ET	61/158 (38%)	-0.35	0 100 100	45, 78, 113, 147	0
41	GT	61/158 (38%)	-0.20	0 100 100	42, 76, 115, 138	0
42	BU	123/124 (99%)	-0.12	1 (0%) 86 80	59, 101, 139, 204	0
42	CU	123/124 (99%)	-0.22	1 (0%) 86 80	49, 92, 143, 163	0
42	EU	123/124 (99%)	-0.06	2 (1%) 72 66	79, 114, 157, 220	0
42	GU	123/124 (99%)	0.80	19 (15%) 2 2	113, 157, 193, 233	0
43	BV	234/239 (97%)	-0.32	0 100 100	61, 107, 160, 213	0
43	CV	234/239 (97%)	-0.44	0 100 100	47, 87, 145, 213	0
43	EV	234/239 (97%)	-0.36	1 (0%) 92 90	53, 102, 159, 232	0
43	GV	234/239 (97%)	-0.15	1 (0%) 92 90	75, 121, 173, 239	0
44	BW	110/111 (99%)	-0.21	2 (1%) 68 62	36, 64, 155, 204	0
44	CW	110/111 (99%)	-0.19	0 100 100	43, 76, 138, 178	0
44	EW	110/111 (99%)	-0.00	1 (0%) 84 79	56, 88, 170, 227	0
44	GW	110/111 (99%)	0.09	1 (0%) 84 79	63, 102, 183, 216	0
45	BX	125/134 (93%)	-0.01	2 (1%) 72 66	53, 89, 128, 202	0
45	CX	125/134 (93%)	-0.27	1 (0%) 86 80	40, 78, 116, 196	0
45	EX	125/134 (93%)	-0.13	2 (1%) 72 66	49, 88, 129, 233	0
45	GX	125/134 (93%)	0.34	4 (3%) 47 42	73, 117, 162, 215	0
46	BY	102/103 (99%)	-0.11	4 (3%) 39 34	40, 74, 164, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	CY	102/103 (99%)	-0.21	4 (3%) 39 34	41, 83, 173, 196	0
46	EY	102/103 (99%)	-0.08	3 (2%) 51 45	45, 84, 156, 193	0
46	GY	102/103 (99%)	0.05	4 (3%) 39 34	53, 102, 189, 222	0
47	CO	146/185 (78%)	-0.08	0 100 100	45, 79, 115, 148	0
All	All	40083/43352 (92%)	0.07	964 (2%) 59 52	26, 101, 177, 390	0

The worst 5 of 964 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HA	92	ALA	14.8
1	A1	2500	C	11.2
1	H1	1597	U	11.2
1	A1	1597	U	10.4
23	BB	387	GLU	10.1

## 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 carbohydrates 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
48	MG	D1	3463	1/1	-0.16	1.03	176,176,176,176	0
48	MG	G2	204	1/1	-0.14	0.92	181,181,181,181	0
48	MG	EW	201	1/1	-0.02	0.33	172,172,172,172	0
48	MG	H1	3529	1/1	0.04	0.33	214,214,214,214	0
48	MG	F1	3411	1/1	0.09	0.65	142,142,142,142	0
48	MG	H1	3489	1/1	0.10	0.45	206,206,206,206	0
48	MG	H1	3551	1/1	0.12	3.30	202,202,202,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3534	1/1	0.16	1.54	221,221,221,221	0
48	MG	G3	202	1/1	0.20	0.62	136,136,136,136	0
48	MG	H1	3519	1/1	0.21	0.31	151,151,151,151	0
48	MG	A1	3527	1/1	0.28	0.30	119,119,119,119	0
48	MG	F1	3561	1/1	0.30	0.24	167,167,167,167	0
48	MG	A1	3568	1/1	0.34	0.36	173,173,173,173	0
48	MG	F1	3415	1/1	0.35	0.32	118,118,118,118	0
48	MG	E3	204	1/1	0.36	1.60	199,199,199,199	0
48	MG	D1	3528	1/1	0.39	0.26	123,123,123,123	0
48	MG	H1	3548	1/1	0.40	0.38	188,188,188,188	0
48	MG	F1	3515	1/1	0.40	0.42	143,143,143,143	0
48	MG	D1	3611	1/1	0.41	0.63	205,205,205,205	0
48	MG	H1	3406	1/1	0.42	0.16	143,143,143,143	0
48	MG	H1	3525	1/1	0.42	0.39	157,157,157,157	0
48	MG	H1	3547	1/1	0.44	0.31	175,175,175,175	0
48	MG	F1	3575	1/1	0.44	0.25	130,130,130,130	0
48	MG	H1	3481	1/1	0.44	0.29	134,134,134,134	0
48	MG	A1	3422	1/1	0.44	0.58	144,144,144,144	0
48	MG	H1	3544	1/1	0.45	0.99	146,146,146,146	0
48	MG	H1	3541	1/1	0.46	0.35	154,154,154,154	0
48	MG	F1	3539	1/1	0.46	1.11	187,187,187,187	0
48	MG	A1	3585	1/1	0.47	0.45	152,152,152,152	0
48	MG	D1	3437	1/1	0.50	0.32	148,148,148,148	0
48	MG	E2	206	1/1	0.51	0.32	151,151,151,151	0
48	MG	A1	3428	1/1	0.52	0.60	159,159,159,159	0
48	MG	D1	3608	1/1	0.52	0.23	115,115,115,115	0
48	MG	H1	3543	1/1	0.52	0.46	183,183,183,183	0
48	MG	F1	3540	1/1	0.53	0.21	111,111,111,111	0
48	MG	E2	205	1/1	0.53	0.60	140,140,140,140	0
48	MG	D1	3401	1/1	0.53	0.25	109,109,109,109	0
48	MG	H1	3450	1/1	0.53	0.73	156,156,156,156	0
48	MG	H1	3479	1/1	0.53	0.43	132,132,132,132	0
48	MG	H1	3409	1/1	0.54	0.55	193,193,193,193	0
48	MG	A1	3573	1/1	0.54	0.47	186,186,186,186	0
48	MG	D1	3606	1/1	0.55	1.19	157,157,157,157	0
48	MG	F1	3490	1/1	0.55	0.22	139,139,139,139	0
48	MG	F1	3419	1/1	0.56	0.11	124,124,124,124	0
48	MG	D1	3624	1/1	0.57	0.61	162,162,162,162	0
48	MG	F1	3522	1/1	0.58	0.18	111,111,111,111	0
48	MG	A1	3430	1/1	0.58	0.50	146,146,146,146	0
48	MG	D1	3470	1/1	0.58	0.38	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	B3	201	1/1	0.59	0.29	129,129,129,129	0
48	MG	F1	3421	1/1	0.59	0.35	174,174,174,174	0
48	MG	H1	3414	1/1	0.59	0.54	169,169,169,169	0
48	MG	A1	3556	1/1	0.59	0.18	124,124,124,124	0
48	MG	H1	3538	1/1	0.59	0.27	140,140,140,140	0
48	MG	H1	3412	1/1	0.59	0.89	173,173,173,173	0
48	MG	F1	3578	1/1	0.60	0.79	161,161,161,161	0
48	MG	H1	3536	1/1	0.60	0.86	168,168,168,168	0
48	MG	D1	3598	1/1	0.61	0.24	159,159,159,159	0
48	MG	A1	3588	1/1	0.61	0.26	144,144,144,144	0
48	MG	F1	3496	1/1	0.61	0.24	122,122,122,122	0
48	MG	D1	3616	1/1	0.61	0.20	150,150,150,150	0
48	MG	F1	3430	1/1	0.61	0.15	128,128,128,128	0
48	MG	A1	3427	1/1	0.61	0.26	152,152,152,152	0
48	MG	A1	3402	1/1	0.62	0.31	143,143,143,143	0
48	MG	A1	3578	1/1	0.62	0.18	117,117,117,117	0
48	MG	H1	3554	1/1	0.62	0.68	128,128,128,128	0
48	MG	H1	3533	1/1	0.63	1.06	153,153,153,153	0
48	MG	D1	3592	1/1	0.63	0.97	159,159,159,159	0
48	MG	A1	3522	1/1	0.63	1.27	146,146,146,146	0
48	MG	H1	3540	1/1	0.63	0.20	136,136,136,136	0
48	MG	H1	3470	1/1	0.63	0.16	140,140,140,140	0
48	MG	G2	205	1/1	0.64	0.18	146,146,146,146	0
48	MG	H1	3535	1/1	0.64	0.99	150,150,150,150	0
48	MG	A1	3583	1/1	0.64	0.44	112,112,112,112	0
48	MG	G3	205	1/1	0.64	0.94	171,171,171,171	0
48	MG	F1	3509	1/1	0.65	0.34	144,144,144,144	0
48	MG	F1	3414	1/1	0.65	0.20	123,123,123,123	0
48	MG	H1	3401	1/1	0.65	0.12	146,146,146,146	0
48	MG	H1	3516	1/1	0.66	0.28	129,129,129,129	0
48	MG	D1	3521	1/1	0.66	0.28	129,129,129,129	0
48	MG	GN	201	1/1	0.66	0.52	212,212,212,212	0
48	MG	A1	3417	1/1	0.66	0.28	150,150,150,150	0
48	MG	H1	3415	1/1	0.66	0.13	133,133,133,133	0
48	MG	H1	3511	1/1	0.66	0.27	140,140,140,140	0
48	MG	F1	3469	1/1	0.66	0.16	112,112,112,112	0
48	MG	D1	3605	1/1	0.66	0.13	108,108,108,108	0
48	MG	D1	3446	1/1	0.66	0.83	176,176,176,176	0
48	MG	A1	3436	1/1	0.66	0.23	110,110,110,110	0
48	MG	B2	207	1/1	0.66	0.38	149,149,149,149	0
48	MG	BQ	201	1/1	0.66	0.21	122,122,122,122	0
48	MG	H1	3402	1/1	0.66	0.23	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	A1	3593	1/1	0.66	0.72	158,158,158,158	0
48	MG	D1	3497	1/1	0.67	0.53	151,151,151,151	0
48	MG	F1	3493	1/1	0.67	0.51	145,145,145,145	0
48	MG	A1	3515	1/1	0.67	0.25	111,111,111,111	0
48	MG	F1	3570	1/1	0.67	0.27	113,113,113,113	0
48	MG	G2	206	1/1	0.67	0.90	174,174,174,174	0
48	MG	EN	201	1/1	0.67	0.17	111,111,111,111	0
48	MG	H1	3550	1/1	0.68	0.44	152,152,152,152	0
48	MG	F1	3566	1/1	0.68	1.27	146,146,146,146	0
48	MG	A1	3592	1/1	0.68	0.30	134,134,134,134	0
48	MG	F1	3577	1/1	0.68	0.26	152,152,152,152	0
48	MG	D1	3548	1/1	0.68	0.96	183,183,183,183	0
48	MG	H1	3532	1/1	0.68	0.39	162,162,162,162	0
48	MG	B3	203	1/1	0.68	0.23	160,160,160,160	0
48	MG	A1	3580	1/1	0.68	0.21	130,130,130,130	0
48	MG	H1	3477	1/1	0.68	0.30	103,103,103,103	0
48	MG	E2	202	1/1	0.69	0.18	89,89,89,89	0
48	MG	F1	3583	1/1	0.69	0.18	104,104,104,104	0
48	MG	H1	3542	1/1	0.69	0.36	137,137,137,137	0
48	MG	C3	207	1/1	0.69	0.62	160,160,160,160	0
48	MG	H1	3420	1/1	0.69	0.26	113,113,113,113	0
48	MG	D1	3597	1/1	0.70	0.83	158,158,158,158	0
48	MG	F1	3555	1/1	0.70	0.27	168,168,168,168	0
48	MG	A1	3507	1/1	0.70	0.20	129,129,129,129	0
48	MG	H1	3531	1/1	0.70	0.59	157,157,157,157	0
48	MG	D1	3547	1/1	0.71	0.28	109,109,109,109	0
48	MG	A1	3451	1/1	0.71	0.16	146,146,146,146	0
48	MG	D1	3550	1/1	0.71	0.59	136,136,136,136	0
48	MG	A1	3435	1/1	0.71	0.54	151,151,151,151	0
48	MG	D1	3603	1/1	0.72	0.44	125,125,125,125	0
48	MG	A1	3401	1/1	0.72	0.12	108,108,108,108	0
48	MG	A1	3483	1/1	0.72	0.14	83,83,83,83	0
48	MG	F1	3489	1/1	0.72	0.10	85,85,85,85	0
48	MG	F1	3574	1/1	0.72	0.70	161,161,161,161	0
48	MG	D1	3418	1/1	0.72	0.16	114,114,114,114	0
48	MG	D1	3576	1/1	0.72	0.54	150,150,150,150	0
48	MG	D1	3579	1/1	0.72	0.10	97,97,97,97	0
48	MG	D1	3467	1/1	0.72	0.18	123,123,123,123	0
48	MG	F1	3488	1/1	0.73	0.37	110,110,110,110	0
48	MG	A1	3595	1/1	0.73	1.09	151,151,151,151	0
48	MG	D1	3541	1/1	0.73	0.34	114,114,114,114	0
48	MG	F1	3563	1/1	0.73	0.18	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	B2	201	1/1	0.73	0.20	119,119,119,119	0
48	MG	H1	3410	1/1	0.73	0.44	192,192,192,192	0
48	MG	D1	3600	1/1	0.73	0.40	123,123,123,123	0
48	MG	A1	3454	1/1	0.73	0.18	101,101,101,101	0
48	MG	D1	3596	1/1	0.73	0.66	165,165,165,165	0
48	MG	H1	3524	1/1	0.74	0.57	139,139,139,139	0
48	MG	F1	3462	1/1	0.74	0.15	118,118,118,118	0
48	MG	D1	3424	1/1	0.74	0.43	150,150,150,150	0
48	MG	H1	3526	1/1	0.74	0.22	94,94,94,94	0
48	MG	A1	3416	1/1	0.74	0.23	140,140,140,140	0
48	MG	A1	3491	1/1	0.74	0.24	125,125,125,125	0
48	MG	E3	206	1/1	0.74	0.35	132,132,132,132	0
48	MG	H1	3521	1/1	0.74	0.29	123,123,123,123	0
48	MG	H1	3418	1/1	0.74	0.21	141,141,141,141	0
48	MG	D1	3429	1/1	0.74	0.23	113,113,113,113	0
48	MG	A1	3420	1/1	0.75	0.30	155,155,155,155	0
48	MG	A1	3587	1/1	0.75	1.09	182,182,182,182	0
48	MG	A1	3582	1/1	0.75	0.19	110,110,110,110	0
48	MG	GA	301	1/1	0.75	0.24	142,142,142,142	0
48	MG	F1	3560	1/1	0.75	0.47	169,169,169,169	0
48	MG	C3	205	1/1	0.75	1.45	175,175,175,175	0
48	MG	H1	3408	1/1	0.75	0.30	111,111,111,111	0
48	MG	EW	202	1/1	0.75	0.20	121,121,121,121	0
48	MG	A1	3437	1/1	0.75	0.48	141,141,141,141	0
48	MG	D1	3625	1/1	0.75	0.39	164,164,164,164	0
48	MG	A1	3449	1/1	0.75	0.23	115,115,115,115	0
48	MG	D1	3434	1/1	0.75	0.63	144,144,144,144	0
48	MG	A1	3408	1/1	0.76	0.27	122,122,122,122	0
48	MG	A1	3567	1/1	0.76	0.30	144,144,144,144	0
48	MG	F1	3451	1/1	0.76	0.49	122,122,122,122	0
48	MG	A1	3547	1/1	0.76	0.16	81,81,81,81	0
48	MG	D1	3593	1/1	0.76	0.36	180,180,180,180	0
48	MG	D1	3551	1/1	0.76	0.18	142,142,142,142	0
48	MG	H1	3539	1/1	0.76	0.34	128,128,128,128	0
48	MG	F1	3564	1/1	0.76	0.38	143,143,143,143	0
48	MG	H1	3537	1/1	0.76	0.18	152,152,152,152	0
48	MG	A1	3414	1/1	0.76	0.19	142,142,142,142	0
48	MG	F1	3554	1/1	0.76	0.18	131,131,131,131	0
48	MG	D1	3583	1/1	0.76	0.32	139,139,139,139	0
48	MG	A1	3576	1/1	0.76	0.40	122,122,122,122	0
48	MG	E3	205	1/1	0.76	0.17	127,127,127,127	0
48	MG	A1	3579	1/1	0.76	0.52	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3580	1/1	0.76	0.21	147,147,147,147	0
48	MG	DJ	301	1/1	0.77	0.45	150,150,150,150	0
48	MG	F1	3511	1/1	0.77	0.71	154,154,154,154	0
48	MG	F1	3576	1/1	0.77	0.46	142,142,142,142	0
48	MG	D1	3514	1/1	0.77	0.20	128,128,128,128	0
48	MG	A1	3503	1/1	0.77	0.16	95,95,95,95	0
48	MG	F1	3468	1/1	0.77	0.16	103,103,103,103	0
48	MG	H1	3446	1/1	0.77	0.34	120,120,120,120	0
48	MG	D1	3571	1/1	0.77	0.43	130,130,130,130	0
48	MG	D1	3588	1/1	0.77	0.18	156,156,156,156	0
48	MG	F1	3519	1/1	0.77	0.16	65,65,65,65	0
48	MG	B2	202	1/1	0.78	0.12	103,103,103,103	0
48	MG	D1	3448	1/1	0.78	0.22	125,125,125,125	0
48	MG	H1	3478	1/1	0.78	0.10	114,114,114,114	0
48	MG	H1	3413	1/1	0.78	0.20	117,117,117,117	0
48	MG	A1	3577	1/1	0.78	0.14	104,104,104,104	0
48	MG	H1	3473	1/1	0.78	0.19	123,123,123,123	0
48	MG	A1	3530	1/1	0.78	0.48	149,149,149,149	0
48	MG	A1	3431	1/1	0.78	0.12	90,90,90,90	0
48	MG	H1	3492	1/1	0.78	0.13	96,96,96,96	0
48	MG	F1	3503	1/1	0.78	0.18	129,129,129,129	0
48	MG	D1	3442	1/1	0.79	0.35	126,126,126,126	0
48	MG	F1	3550	1/1	0.79	0.21	154,154,154,154	0
48	MG	GP	201	1/1	0.79	0.47	109,109,109,109	0
48	MG	F1	3448	1/1	0.79	0.15	126,126,126,126	0
48	MG	A1	3433	1/1	0.79	0.10	84,84,84,84	0
48	MG	A1	3555	1/1	0.79	0.58	128,128,128,128	0
48	MG	F1	3572	1/1	0.79	0.36	155,155,155,155	0
48	MG	GP	202	1/1	0.79	0.24	137,137,137,137	0
48	MG	F1	3483	1/1	0.79	0.32	129,129,129,129	0
48	MG	FT	101	1/1	0.79	0.11	124,124,124,124	0
48	MG	D1	3427	1/1	0.79	0.26	153,153,153,153	0
48	MG	C3	202	1/1	0.80	0.15	135,135,135,135	0
48	MG	A1	3419	1/1	0.80	0.14	100,100,100,100	0
48	MG	F1	3565	1/1	0.80	0.86	168,168,168,168	0
48	MG	H1	3486	1/1	0.80	0.15	105,105,105,105	0
48	MG	B3	202	1/1	0.80	0.15	113,113,113,113	0
48	MG	A1	3472	1/1	0.80	0.63	149,149,149,149	0
48	MG	A1	3591	1/1	0.80	0.27	121,121,121,121	0
48	MG	A1	3551	1/1	0.80	0.33	123,123,123,123	0
48	MG	D1	3516	1/1	0.80	0.36	82,82,82,82	0
48	MG	H1	3549	1/1	0.80	0.47	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3417	1/1	0.80	0.20	132,132,132,132	0
48	MG	D1	3604	1/1	0.81	0.44	141,141,141,141	0
48	MG	H1	3503	1/1	0.81	0.26	91,91,91,91	0
48	MG	H1	3434	1/1	0.81	0.18	93,93,93,93	0
48	MG	CD	201	1/1	0.81	0.16	93,93,93,93	0
48	MG	A1	3586	1/1	0.81	0.72	177,177,177,177	0
48	MG	H1	3433	1/1	0.81	0.19	132,132,132,132	0
48	MG	D1	3627	1/1	0.81	0.08	119,119,119,119	0
48	MG	D1	3586	1/1	0.81	0.16	109,109,109,109	0
48	MG	A1	3425	1/1	0.81	0.16	107,107,107,107	0
48	MG	D1	3626	1/1	0.81	0.20	137,137,137,137	0
48	MG	C2	206	1/1	0.81	0.31	123,123,123,123	0
48	MG	F1	3501	1/1	0.81	0.16	116,116,116,116	0
48	MG	H1	3553	1/1	0.81	0.39	146,146,146,146	0
48	MG	HT	101	1/1	0.81	0.35	174,174,174,174	0
48	MG	F1	3548	1/1	0.81	0.12	106,106,106,106	0
48	MG	A1	3589	1/1	0.81	0.13	113,113,113,113	0
48	MG	H1	3443	1/1	0.82	0.42	157,157,157,157	0
48	MG	H1	3411	1/1	0.82	0.32	120,120,120,120	0
48	MG	D1	3565	1/1	0.82	0.33	114,114,114,114	0
48	MG	H1	3448	1/1	0.82	0.15	98,98,98,98	0
48	MG	H1	3530	1/1	0.82	0.34	154,154,154,154	0
48	MG	H1	3436	1/1	0.82	0.43	146,146,146,146	0
48	MG	D1	3557	1/1	0.82	0.13	116,116,116,116	0
48	MG	F1	3447	1/1	0.82	0.30	156,156,156,156	0
48	MG	F1	3425	1/1	0.82	0.33	115,115,115,115	0
48	MG	F1	3422	1/1	0.82	0.29	149,149,149,149	0
48	MG	A1	3499	1/1	0.82	0.16	117,117,117,117	0
48	MG	F1	3428	1/1	0.82	0.30	111,111,111,111	0
48	MG	F1	3506	1/1	0.82	0.32	114,114,114,114	0
48	MG	D1	3594	1/1	0.82	0.23	106,106,106,106	0
48	MG	A1	3461	1/1	0.82	0.14	67,67,67,67	0
48	MG	F1	3567	1/1	0.82	0.42	128,128,128,128	0
48	MG	F1	3498	1/1	0.82	0.22	141,141,141,141	0
48	MG	A1	3444	1/1	0.83	0.13	126,126,126,126	0
48	MG	F1	3482	1/1	0.83	0.21	130,130,130,130	0
48	MG	H1	3482	1/1	0.83	0.61	162,162,162,162	0
48	MG	H1	3509	1/1	0.83	0.18	143,143,143,143	0
48	MG	H1	3422	1/1	0.83	0.46	151,151,151,151	0
48	MG	D1	3435	1/1	0.83	0.14	108,108,108,108	0
48	MG	D1	3615	1/1	0.83	0.24	132,132,132,132	0
48	MG	D1	3574	1/1	0.83	0.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	E2	201	1/1	0.83	0.34	156,156,156,156	0
48	MG	F1	3549	1/1	0.83	0.20	125,125,125,125	0
48	MG	G3	204	1/1	0.83	0.36	143,143,143,143	0
48	MG	D1	3609	1/1	0.83	0.67	120,120,120,120	0
48	MG	D1	3540	1/1	0.83	0.20	139,139,139,139	0
48	MG	A1	3453	1/1	0.83	0.72	184,184,184,184	0
48	MG	D1	3613	1/1	0.83	0.23	120,120,120,120	0
48	MG	F1	3453	1/1	0.83	0.23	131,131,131,131	0
48	MG	F1	3461	1/1	0.83	0.49	106,106,106,106	0
48	MG	D1	3425	1/1	0.83	0.59	123,123,123,123	0
48	MG	D1	3485	1/1	0.83	0.17	120,120,120,120	0
48	MG	D1	3484	1/1	0.83	0.31	96,96,96,96	0
48	MG	H1	3552	1/1	0.83	0.18	131,131,131,131	0
48	MG	H1	3438	1/1	0.83	0.29	120,120,120,120	0
48	MG	D1	3433	1/1	0.83	0.14	149,149,149,149	0
48	MG	F1	3573	1/1	0.83	0.08	84,84,84,84	0
48	MG	BN	201	1/1	0.84	0.22	147,147,147,147	0
48	MG	A1	3565	1/1	0.84	0.13	132,132,132,132	0
48	MG	GO	201	1/1	0.84	0.44	141,141,141,141	0
48	MG	D1	3582	1/1	0.84	0.19	93,93,93,93	0
48	MG	D1	3614	1/1	0.84	0.19	129,129,129,129	0
48	MG	H1	3490	1/1	0.84	0.55	122,122,122,122	0
48	MG	A1	3409	1/1	0.84	0.14	87,87,87,87	0
48	MG	H1	3441	1/1	0.84	0.15	102,102,102,102	0
48	MG	A1	3412	1/1	0.84	0.33	117,117,117,117	0
48	MG	A1	3553	1/1	0.84	0.16	108,108,108,108	0
48	MG	F1	3424	1/1	0.84	0.31	114,114,114,114	0
48	MG	F1	3464	1/1	0.84	0.23	120,120,120,120	0
48	MG	H1	3465	1/1	0.84	0.42	143,143,143,143	0
48	MG	E3	203	1/1	0.84	0.17	104,104,104,104	0
48	MG	H1	3462	1/1	0.84	0.36	131,131,131,131	0
48	MG	D1	3607	1/1	0.84	0.30	89,89,89,89	0
48	MG	H1	3417	1/1	0.84	0.11	114,114,114,114	0
48	MG	H1	3426	1/1	0.84	0.15	105,105,105,105	0
48	MG	B2	208	1/1	0.84	0.42	138,138,138,138	0
48	MG	F1	3558	1/1	0.84	0.17	144,144,144,144	0
48	MG	A1	3513	1/1	0.84	0.33	133,133,133,133	0
48	MG	C2	205	1/1	0.84	0.19	127,127,127,127	0
48	MG	D1	3530	1/1	0.84	0.16	94,94,94,94	0
48	MG	H1	3528	1/1	0.84	0.23	119,119,119,119	0
48	MG	D1	3542	1/1	0.85	0.13	71,71,71,71	0
48	MG	F1	3413	1/1	0.85	0.38	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3580	1/1	0.85	0.11	95,95,95,95	0
48	MG	H1	3487	1/1	0.85	0.19	122,122,122,122	0
48	MG	A1	3571	1/1	0.85	0.24	100,100,100,100	0
48	MG	D1	3534	1/1	0.85	0.20	98,98,98,98	0
48	MG	G2	201	1/1	0.85	0.14	141,141,141,141	0
48	MG	A1	3594	1/1	0.85	0.28	150,150,150,150	0
48	MG	F1	3403	1/1	0.85	0.11	96,96,96,96	0
48	MG	A1	3569	1/1	0.85	0.09	91,91,91,91	0
48	MG	D1	3513	1/1	0.85	0.16	89,89,89,89	0
48	MG	H1	3546	1/1	0.85	0.27	120,120,120,120	0
48	MG	A1	3528	1/1	0.85	0.37	120,120,120,120	0
48	MG	D1	3499	1/1	0.85	0.14	118,118,118,118	0
48	MG	F1	3545	1/1	0.85	0.21	137,137,137,137	0
48	MG	EN	202	1/1	0.85	1.14	238,238,238,238	0
48	MG	D1	3631	1/1	0.85	0.08	78,78,78,78	0
48	MG	D1	3482	1/1	0.85	0.15	106,106,106,106	0
48	MG	A1	3450	1/1	0.85	0.20	133,133,133,133	0
48	MG	F1	3433	1/1	0.85	0.64	95,95,95,95	0
48	MG	D1	3426	1/1	0.85	0.38	143,143,143,143	0
48	MG	H1	3512	1/1	0.86	0.31	121,121,121,121	0
48	MG	D1	3561	1/1	0.86	0.19	57,57,57,57	0
48	MG	F1	3529	1/1	0.86	0.71	140,140,140,140	0
48	MG	F1	3477	1/1	0.86	0.68	146,146,146,146	0
48	MG	F1	3569	1/1	0.86	0.40	130,130,130,130	0
48	MG	F1	3408	1/1	0.86	0.14	82,82,82,82	0
48	MG	D1	3504	1/1	0.86	0.27	98,98,98,98	0
48	MG	CQ	201	1/1	0.86	0.18	127,127,127,127	0
48	MG	A1	3552	1/1	0.86	0.10	97,97,97,97	0
48	MG	F1	3495	1/1	0.86	0.12	83,83,83,83	0
48	MG	D1	3622	1/1	0.86	0.30	133,133,133,133	0
48	MG	H1	3484	1/1	0.86	0.24	166,166,166,166	0
48	MG	D1	3421	1/1	0.86	0.22	126,126,126,126	0
48	MG	DQ	201	1/1	0.86	0.32	118,118,118,118	0
48	MG	F1	3542	1/1	0.86	0.13	107,107,107,107	0
48	MG	F1	3463	1/1	0.86	0.19	100,100,100,100	0
48	MG	D1	3444	1/1	0.86	0.22	139,139,139,139	0
48	MG	A1	3584	1/1	0.86	0.23	125,125,125,125	0
48	MG	D1	3522	1/1	0.86	0.64	162,162,162,162	0
48	MG	GQ	201	1/1	0.86	0.30	102,102,102,102	0
48	MG	F1	3544	1/1	0.86	0.13	97,97,97,97	0
48	MG	D1	3515	1/1	0.86	0.15	106,106,106,106	0
48	MG	F1	3527	1/1	0.87	0.30	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3422	1/1	0.87	0.22	150,150,150,150	0
48	MG	A1	3574	1/1	0.87	0.15	119,119,119,119	0
48	MG	F1	3491	1/1	0.87	0.18	96,96,96,96	0
48	MG	F1	3538	1/1	0.87	0.36	113,113,113,113	0
48	MG	H1	3545	1/1	0.87	0.19	156,156,156,156	0
48	MG	D1	3623	1/1	0.87	0.26	151,151,151,151	0
48	MG	D1	3525	1/1	0.87	0.34	113,113,113,113	0
48	MG	D1	3618	1/1	0.87	0.09	95,95,95,95	0
48	MG	F1	3473	1/1	0.87	0.42	156,156,156,156	0
48	MG	A1	3474	1/1	0.87	0.13	88,88,88,88	0
48	MG	F1	3434	1/1	0.87	0.13	83,83,83,83	0
48	MG	A1	3531	1/1	0.87	0.28	128,128,128,128	0
48	MG	D1	3532	1/1	0.87	0.14	119,119,119,119	0
48	MG	D1	3575	1/1	0.87	0.13	124,124,124,124	0
48	MG	A1	3497	1/1	0.87	0.12	116,116,116,116	0
48	MG	D1	3439	1/1	0.87	0.38	146,146,146,146	0
48	MG	D1	3563	1/1	0.87	0.12	93,93,93,93	0
48	MG	A1	3566	1/1	0.87	0.11	75,75,75,75	0
48	MG	D1	3595	1/1	0.87	0.23	94,94,94,94	0
48	MG	D1	3475	1/1	0.87	0.51	120,120,120,120	0
48	MG	F1	3532	1/1	0.87	0.19	87,87,87,87	0
48	MG	DA	102	1/1	0.87	0.20	115,115,115,115	0
48	MG	F1	3401	1/1	0.87	0.35	101,101,101,101	0
48	MG	F1	3492	1/1	0.87	0.20	78,78,78,78	0
48	MG	H1	3459	1/1	0.87	0.10	97,97,97,97	0
48	MG	D1	3445	1/1	0.87	0.19	126,126,126,126	0
48	MG	F1	3423	1/1	0.87	0.08	56,56,56,56	0
48	MG	A1	3455	1/1	0.87	0.13	111,111,111,111	0
48	MG	D1	3621	1/1	0.87	0.15	110,110,110,110	0
48	MG	F1	3500	1/1	0.88	0.17	105,105,105,105	0
48	MG	H1	3504	1/1	0.88	0.11	111,111,111,111	0
48	MG	A1	3415	1/1	0.88	0.20	120,120,120,120	0
48	MG	B2	206	1/1	0.88	0.45	139,139,139,139	0
48	MG	A1	3542	1/1	0.88	0.22	96,96,96,96	0
48	MG	H1	3472	1/1	0.88	0.32	104,104,104,104	0
48	MG	A1	3424	1/1	0.88	0.37	150,150,150,150	0
48	MG	BP	200	1/1	0.88	0.10	123,123,123,123	0
48	MG	D1	3498	1/1	0.88	0.47	99,99,99,99	0
48	MG	A1	3512	1/1	0.88	0.10	90,90,90,90	0
48	MG	F1	3485	1/1	0.88	0.16	117,117,117,117	0
48	MG	A1	3536	1/1	0.88	0.14	104,104,104,104	0
48	MG	D1	3505	1/1	0.88	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3425	1/1	0.88	0.31	108,108,108,108	0
48	MG	D1	3496	1/1	0.88	0.16	78,78,78,78	0
48	MG	A1	3554	1/1	0.88	0.14	76,76,76,76	0
48	MG	F1	3516	1/1	0.88	0.30	121,121,121,121	0
48	MG	CW	201	1/1	0.88	0.29	90,90,90,90	0
48	MG	H1	3485	1/1	0.88	0.12	104,104,104,104	0
48	MG	A1	3404	1/1	0.88	0.12	94,94,94,94	0
48	MG	D1	3602	1/1	0.88	0.19	118,118,118,118	0
48	MG	D1	3599	1/1	0.88	0.27	126,126,126,126	0
48	MG	F1	3556	1/1	0.88	0.08	90,90,90,90	0
48	MG	A1	3516	1/1	0.88	0.23	88,88,88,88	0
48	MG	D1	3620	1/1	0.88	0.15	106,106,106,106	0
48	MG	H1	3510	1/1	0.88	0.24	120,120,120,120	0
48	MG	H1	3407	1/1	0.88	0.20	105,105,105,105	0
48	MG	G3	201	1/1	0.88	0.12	119,119,119,119	0
48	MG	H1	3452	1/1	0.88	0.10	108,108,108,108	0
48	MG	A1	3532	1/1	0.89	0.07	74,74,74,74	0
48	MG	F1	3484	1/1	0.89	0.17	78,78,78,78	0
48	MG	A1	3423	1/1	0.89	0.21	115,115,115,115	0
48	MG	A1	3479	1/1	0.89	0.22	120,120,120,120	0
48	MG	H1	3404	1/1	0.89	0.11	132,132,132,132	0
48	MG	A1	3590	1/1	0.89	0.26	142,142,142,142	0
48	MG	F1	3431	1/1	0.89	0.17	103,103,103,103	0
48	MG	A1	3438	1/1	0.89	0.23	148,148,148,148	0
48	MG	H1	3501	1/1	0.89	0.30	110,110,110,110	0
48	MG	A1	3563	1/1	0.89	0.13	100,100,100,100	0
48	MG	A1	3492	1/1	0.89	0.28	127,127,127,127	0
48	MG	H1	3555	1/1	0.89	0.15	123,123,123,123	0
48	MG	H1	3496	1/1	0.89	0.44	141,141,141,141	0
48	MG	F1	3559	1/1	0.89	0.10	133,133,133,133	0
48	MG	D1	3577	1/1	0.89	0.22	121,121,121,121	0
48	MG	F1	3456	1/1	0.89	0.07	62,62,62,62	0
48	MG	H1	3468	1/1	0.89	0.23	121,121,121,121	0
48	MG	D1	3523	1/1	0.89	0.10	105,105,105,105	0
48	MG	A1	3500	1/1	0.89	0.30	89,89,89,89	0
48	MG	C2	201	1/1	0.89	0.15	121,121,121,121	0
48	MG	H1	3499	1/1	0.89	0.11	75,75,75,75	0
48	MG	F1	3502	1/1	0.89	0.26	108,108,108,108	0
48	MG	D1	3440	1/1	0.89	0.12	99,99,99,99	0
48	MG	A1	3470	1/1	0.89	0.32	164,164,164,164	0
48	MG	H1	3464	1/1	0.89	0.15	108,108,108,108	0
48	MG	F1	3446	1/1	0.89	0.20	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3468	1/1	0.89	0.13	75,75,75,75	0
48	MG	D1	3549	1/1	0.90	0.13	99,99,99,99	0
48	MG	F1	3541	1/1	0.90	0.23	112,112,112,112	0
48	MG	H1	3442	1/1	0.90	0.09	79,79,79,79	0
48	MG	F1	3439	1/1	0.90	0.09	62,62,62,62	0
48	MG	D1	3511	1/1	0.90	0.24	118,118,118,118	0
48	MG	D1	3481	1/1	0.90	0.39	114,114,114,114	0
48	MG	F1	3475	1/1	0.90	0.17	93,93,93,93	0
48	MG	H1	3435	1/1	0.90	0.17	116,116,116,116	0
48	MG	F1	3440	1/1	0.90	0.11	82,82,82,82	0
48	MG	H1	3488	1/1	0.90	0.19	108,108,108,108	0
48	MG	H1	3449	1/1	0.90	0.62	118,118,118,118	0
48	MG	F1	3457	1/1	0.90	0.27	91,91,91,91	0
48	MG	A1	3443	1/1	0.90	0.14	90,90,90,90	0
48	MG	E2	207	1/1	0.90	0.41	147,147,147,147	0
49	ZN	HC	201	1/1	0.90	0.04	168,168,168,168	0
48	MG	F1	3535	1/1	0.90	0.11	58,58,58,58	0
48	MG	D1	3535	1/1	0.90	0.17	86,86,86,86	0
48	MG	F1	3581	1/1	0.90	0.38	144,144,144,144	0
48	MG	A1	3529	1/1	0.90	0.10	96,96,96,96	0
48	MG	C3	203	1/1	0.90	0.08	69,69,69,69	0
48	MG	H1	3430	1/1	0.90	0.20	82,82,82,82	0
48	MG	C2	202	1/1	0.90	0.23	112,112,112,112	0
48	MG	H1	3523	1/1	0.90	0.12	167,167,167,167	0
48	MG	CL	301	1/1	0.90	0.15	109,109,109,109	0
48	MG	H1	3518	1/1	0.90	0.15	110,110,110,110	0
48	MG	D1	3472	1/1	0.90	0.10	82,82,82,82	0
48	MG	A1	3575	1/1	0.90	0.62	143,143,143,143	0
48	MG	A1	3596	1/1	0.90	0.30	163,163,163,163	0
48	MG	F1	3553	1/1	0.90	0.09	68,68,68,68	0
48	MG	A1	3471	1/1	0.90	0.31	88,88,88,88	0
48	MG	H1	3457	1/1	0.90	0.56	147,147,147,147	0
48	MG	A1	3600	1/1	0.90	0.11	111,111,111,111	0
48	MG	EL	302	1/1	0.90	0.09	68,68,68,68	0
48	MG	F1	3579	1/1	0.90	0.12	166,166,166,166	0
48	MG	F1	3472	1/1	0.90	0.15	111,111,111,111	0
48	MG	F1	3537	1/1	0.90	0.21	136,136,136,136	0
48	MG	F1	3513	1/1	0.90	0.17	79,79,79,79	0
48	MG	D1	3538	1/1	0.90	0.10	119,119,119,119	0
48	MG	F1	3534	1/1	0.90	0.08	79,79,79,79	0
48	MG	A1	3510	1/1	0.90	0.21	109,109,109,109	0
48	MG	D1	3628	1/1	0.90	0.07	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3520	1/1	0.91	0.19	85,85,85,85	0
48	MG	F1	3568	1/1	0.91	0.13	98,98,98,98	0
48	MG	A1	3447	1/1	0.91	0.13	58,58,58,58	0
48	MG	A1	3519	1/1	0.91	0.10	113,113,113,113	0
48	MG	E3	202	1/1	0.91	0.20	122,122,122,122	0
48	MG	D1	3512	1/1	0.91	0.14	101,101,101,101	0
48	MG	H1	3455	1/1	0.91	0.14	113,113,113,113	0
48	MG	A1	3572	1/1	0.91	0.23	121,121,121,121	0
48	MG	D1	3506	1/1	0.91	0.30	132,132,132,132	0
48	MG	A1	3403	1/1	0.91	0.13	96,96,96,96	0
48	MG	D1	3545	1/1	0.91	0.15	88,88,88,88	0
48	MG	D1	3572	1/1	0.91	0.23	69,69,69,69	0
48	MG	CY	201	1/1	0.91	0.20	99,99,99,99	0
48	MG	F1	3571	1/1	0.91	0.29	132,132,132,132	0
48	MG	FK	201	1/1	0.91	0.50	168,168,168,168	0
48	MG	D1	3568	1/1	0.91	0.17	105,105,105,105	0
48	MG	D1	3416	1/1	0.91	0.24	110,110,110,110	0
48	MG	H1	3432	1/1	0.91	0.09	91,91,91,91	0
48	MG	F1	3497	1/1	0.91	0.12	93,93,93,93	0
48	MG	G2	202	1/1	0.91	0.34	122,122,122,122	0
48	MG	FA	101	1/1	0.91	0.11	97,97,97,97	0
48	MG	F1	3466	1/1	0.91	0.34	140,140,140,140	0
48	MG	D1	3507	1/1	0.91	0.10	75,75,75,75	0
48	MG	D1	3441	1/1	0.91	0.15	75,75,75,75	0
48	MG	A1	3467	1/1	0.91	0.19	106,106,106,106	0
48	MG	D1	3573	1/1	0.91	0.14	126,126,126,126	0
48	MG	D1	3409	1/1	0.91	0.13	57,57,57,57	0
48	MG	D1	3447	1/1	0.91	0.23	101,101,101,101	0
48	MG	D1	3406	1/1	0.91	0.14	67,67,67,67	0
48	MG	F1	3429	1/1	0.91	0.17	73,73,73,73	0
48	MG	H1	3429	1/1	0.91	0.14	87,87,87,87	0
48	MG	D1	3543	1/1	0.91	0.27	127,127,127,127	0
48	MG	GW	201	1/1	0.91	0.22	114,114,114,114	0
48	MG	H1	3416	1/1	0.91	0.66	113,113,113,113	0
48	MG	A1	3496	1/1	0.91	0.24	137,137,137,137	0
48	MG	A1	3498	1/1	0.91	0.11	116,116,116,116	0
48	MG	D1	3476	1/1	0.91	0.08	43,43,43,43	0
48	MG	H1	3456	1/1	0.91	0.76	145,145,145,145	0
48	MG	H1	3505	1/1	0.92	0.11	95,95,95,95	0
48	MG	F1	3517	1/1	0.92	0.11	62,62,62,62	0
48	MG	A1	3509	1/1	0.92	0.12	128,128,128,128	0
48	MG	H1	3447	1/1	0.92	0.25	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3562	1/1	0.92	0.40	140,140,140,140	0
48	MG	D1	3451	1/1	0.92	0.42	115,115,115,115	0
48	MG	AK	202	1/1	0.92	0.72	179,179,179,179	0
48	MG	H1	3431	1/1	0.92	0.25	94,94,94,94	0
48	MG	D1	3452	1/1	0.92	0.15	106,106,106,106	0
48	MG	D1	3443	1/1	0.92	0.48	112,112,112,112	0
48	MG	D1	3403	1/1	0.92	0.07	89,89,89,89	0
48	MG	D1	3552	1/1	0.92	0.06	55,55,55,55	0
48	MG	D1	3562	1/1	0.92	0.22	93,93,93,93	0
48	MG	D1	3491	1/1	0.92	0.15	97,97,97,97	0
48	MG	F1	3442	1/1	0.92	0.27	109,109,109,109	0
48	MG	H1	3474	1/1	0.92	0.09	123,123,123,123	0
48	MG	A1	3548	1/1	0.92	0.17	124,124,124,124	0
48	MG	B2	204	1/1	0.92	0.08	85,85,85,85	0
48	MG	A1	3521	1/1	0.92	0.12	105,105,105,105	0
48	MG	D1	3537	1/1	0.92	0.28	121,121,121,121	0
48	MG	H1	3480	1/1	0.92	0.14	81,81,81,81	0
48	MG	A1	3490	1/1	0.92	0.21	105,105,105,105	0
48	MG	F1	3402	1/1	0.92	0.09	83,83,83,83	0
48	MG	A1	3501	1/1	0.92	0.22	102,102,102,102	0
48	MG	A1	3429	1/1	0.92	0.11	122,122,122,122	0
48	MG	G3	203	1/1	0.92	0.13	86,86,86,86	0
48	MG	D1	3407	1/1	0.92	0.09	70,70,70,70	0
48	MG	A1	3518	1/1	0.92	0.24	109,109,109,109	0
48	MG	H1	3424	1/1	0.92	0.08	96,96,96,96	0
48	MG	A1	3468	1/1	0.92	0.18	109,109,109,109	0
48	MG	D1	3610	1/1	0.92	0.21	66,66,66,66	0
48	MG	H1	3508	1/1	0.92	0.16	80,80,80,80	0
48	MG	D1	3517	1/1	0.92	0.31	127,127,127,127	0
48	MG	F1	3470	1/1	0.92	0.09	49,49,49,49	0
48	MG	H1	3467	1/1	0.92	0.11	95,95,95,95	0
48	MG	D1	3581	1/1	0.92	0.08	68,68,68,68	0
48	MG	H1	3403	1/1	0.92	0.14	111,111,111,111	0
48	MG	A1	3511	1/1	0.92	0.08	90,90,90,90	0
48	MG	EL	301	1/1	0.92	0.12	119,119,119,119	0
48	MG	F1	3407	1/1	0.92	0.10	111,111,111,111	0
48	MG	F1	3543	1/1	0.92	0.09	71,71,71,71	0
48	MG	A1	3581	1/1	0.92	0.32	126,126,126,126	0
48	MG	A1	3464	1/1	0.92	0.06	64,64,64,64	0
48	MG	F1	3444	1/1	0.92	0.42	155,155,155,155	0
48	MG	D1	3432	1/1	0.92	0.17	118,118,118,118	0
48	MG	H1	3405	1/1	0.93	0.25	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	A1	3559	1/1	0.93	0.06	89,89,89,89	0
48	MG	A1	3562	1/1	0.93	0.20	91,91,91,91	0
48	MG	H1	3451	1/1	0.93	0.13	78,78,78,78	0
48	MG	F1	3479	1/1	0.93	0.29	81,81,81,81	0
48	MG	H1	3495	1/1	0.93	0.06	65,65,65,65	0
48	MG	D1	3412	1/1	0.93	0.35	95,95,95,95	0
48	MG	F1	3405	1/1	0.93	0.13	79,79,79,79	0
48	MG	A1	3439	1/1	0.93	0.08	106,106,106,106	0
48	MG	D1	3527	1/1	0.93	0.28	106,106,106,106	0
48	MG	A1	3488	1/1	0.93	0.17	91,91,91,91	0
48	MG	A1	3493	1/1	0.93	0.21	113,113,113,113	0
48	MG	D1	3585	1/1	0.93	0.08	108,108,108,108	0
48	MG	H1	3419	1/1	0.93	0.17	62,62,62,62	0
48	MG	A1	3441	1/1	0.93	0.50	127,127,127,127	0
48	MG	C3	204	1/1	0.93	0.11	85,85,85,85	0
48	MG	A1	3564	1/1	0.93	0.07	141,141,141,141	0
48	MG	F1	3551	1/1	0.93	0.24	91,91,91,91	0
48	MG	A1	3599	1/1	0.93	0.12	103,103,103,103	0
48	MG	A1	3475	1/1	0.93	0.22	80,80,80,80	0
48	MG	F1	3420	1/1	0.93	0.09	88,88,88,88	0
48	MG	D1	3458	1/1	0.93	0.06	51,51,51,51	0
48	MG	F1	3436	1/1	0.93	0.10	70,70,70,70	0
48	MG	F1	3458	1/1	0.93	0.09	95,95,95,95	0
48	MG	D1	3414	1/1	0.93	0.15	96,96,96,96	0
48	MG	H1	3527	1/1	0.93	0.14	99,99,99,99	0
48	MG	A1	3570	1/1	0.93	0.08	70,70,70,70	0
48	MG	F1	3455	1/1	0.93	0.09	65,65,65,65	0
48	MG	H1	3461	1/1	0.93	0.15	134,134,134,134	0
48	MG	D1	3487	1/1	0.93	0.09	65,65,65,65	0
48	MG	H1	3520	1/1	0.93	0.17	114,114,114,114	0
48	MG	D1	3494	1/1	0.93	0.13	78,78,78,78	0
48	MG	D1	3531	1/1	0.93	0.08	87,87,87,87	0
48	MG	BL	301	1/1	0.93	0.09	71,71,71,71	0
48	MG	H1	3517	1/1	0.93	0.16	79,79,79,79	0
48	MG	A1	3541	1/1	0.93	0.35	86,86,86,86	0
48	MG	F1	3494	1/1	0.93	0.12	97,97,97,97	0
48	MG	D1	3520	1/1	0.93	0.11	93,93,93,93	0
48	MG	F1	3406	1/1	0.93	0.08	83,83,83,83	0
48	MG	FA	102	1/1	0.93	0.10	84,84,84,84	0
48	MG	D1	3454	1/1	0.93	0.14	64,64,64,64	0
48	MG	A1	3560	1/1	0.93	0.45	138,138,138,138	0
48	MG	H1	3522	1/1	0.93	0.16	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3513	1/1	0.93	0.11	87,87,87,87	0
48	MG	A1	3549	1/1	0.93	0.13	54,54,54,54	0
48	MG	F1	3478	1/1	0.94	0.12	73,73,73,73	0
48	MG	E2	203	1/1	0.94	0.07	77,77,77,77	0
48	MG	F1	3507	1/1	0.94	0.17	87,87,87,87	0
48	MG	F1	3530	1/1	0.94	0.15	107,107,107,107	0
48	MG	A1	3469	1/1	0.94	0.17	113,113,113,113	0
48	MG	H1	3471	1/1	0.94	0.21	124,124,124,124	0
48	MG	F1	3437	1/1	0.94	0.17	100,100,100,100	0
48	MG	H1	3469	1/1	0.94	0.34	119,119,119,119	0
48	MG	F1	3536	1/1	0.94	0.20	67,67,67,67	0
48	MG	AA	102	1/1	0.94	0.08	98,98,98,98	0
48	MG	H1	3440	1/1	0.94	0.08	73,73,73,73	0
48	MG	F1	3471	1/1	0.94	0.17	90,90,90,90	0
48	MG	F1	3531	1/1	0.94	0.09	95,95,95,95	0
48	MG	A1	3405	1/1	0.94	0.08	65,65,65,65	0
48	MG	C3	201	1/1	0.94	0.34	123,123,123,123	0
48	MG	EJ	201	1/1	0.94	0.12	69,69,69,69	0
48	MG	BJ	201	1/1	0.94	0.17	66,66,66,66	0
48	MG	A1	3504	1/1	0.94	0.49	138,138,138,138	0
48	MG	F1	3480	1/1	0.94	0.12	59,59,59,59	0
48	MG	D1	3589	1/1	0.94	0.26	107,107,107,107	0
48	MG	A1	3533	1/1	0.94	0.22	73,73,73,73	0
48	MG	H1	3428	1/1	0.94	0.12	77,77,77,77	0
48	MG	D1	3508	1/1	0.94	0.05	86,86,86,86	0
48	MG	D1	3423	1/1	0.94	0.17	67,67,67,67	0
48	MG	D1	3478	1/1	0.94	0.12	81,81,81,81	0
48	MG	F1	3533	1/1	0.94	0.18	101,101,101,101	0
48	MG	D1	3413	1/1	0.94	0.09	51,51,51,51	0
48	MG	H1	3475	1/1	0.94	0.10	70,70,70,70	0
48	MG	A1	3505	1/1	0.94	0.12	137,137,137,137	0
48	MG	A1	3481	1/1	0.94	0.16	88,88,88,88	0
48	MG	F1	3557	1/1	0.94	0.15	84,84,84,84	0
48	MG	F1	3418	1/1	0.94	0.12	126,126,126,126	0
48	MG	D1	3431	1/1	0.94	0.19	95,95,95,95	0
48	MG	A1	3407	1/1	0.94	0.11	83,83,83,83	0
48	MG	A1	3494	1/1	0.94	0.07	98,98,98,98	0
48	MG	H1	3454	1/1	0.94	0.12	111,111,111,111	0
48	MG	D1	3601	1/1	0.94	0.22	124,124,124,124	0
48	MG	DA	101	1/1	0.94	0.07	82,82,82,82	0
48	MG	D1	3558	1/1	0.94	0.07	56,56,56,56	0
48	MG	F1	3417	1/1	0.94	0.17	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3492	1/1	0.94	0.34	125,125,125,125	0
48	MG	AA	103	1/1	0.94	0.08	56,56,56,56	0
48	MG	A1	3448	1/1	0.94	0.14	78,78,78,78	0
48	MG	F1	3443	1/1	0.94	0.06	104,104,104,104	0
48	MG	B2	205	1/1	0.94	0.09	81,81,81,81	0
48	MG	H1	3427	1/1	0.94	0.14	83,83,83,83	0
48	MG	D1	3584	1/1	0.94	0.13	101,101,101,101	0
48	MG	D1	3612	1/1	0.94	0.23	123,123,123,123	0
48	MG	D1	3564	1/1	0.94	0.21	92,92,92,92	0
48	MG	F1	3410	1/1	0.94	0.17	42,42,42,42	0
48	MG	D1	3455	1/1	0.94	0.09	80,80,80,80	0
48	MG	A1	3558	1/1	0.94	0.10	91,91,91,91	0
48	MG	D1	3617	1/1	0.94	0.34	113,113,113,113	0
48	MG	D1	3553	1/1	0.94	0.07	90,90,90,90	0
48	MG	A1	3485	1/1	0.95	0.15	137,137,137,137	0
48	MG	A1	3482	1/1	0.95	0.06	62,62,62,62	0
48	MG	H1	3476	1/1	0.95	0.08	52,52,52,52	0
48	MG	D1	3591	1/1	0.95	0.10	55,55,55,55	0
48	MG	A1	3487	1/1	0.95	0.23	121,121,121,121	0
48	MG	F1	3524	1/1	0.95	0.14	56,56,56,56	0
48	MG	D1	3524	1/1	0.95	0.06	69,69,69,69	0
48	MG	D1	3449	1/1	0.95	0.09	68,68,68,68	0
48	MG	D1	3566	1/1	0.95	0.14	80,80,80,80	0
48	MG	D1	3477	1/1	0.95	0.09	60,60,60,60	0
48	MG	F1	3452	1/1	0.95	0.10	50,50,50,50	0
48	MG	A1	3506	1/1	0.95	0.12	77,77,77,77	0
48	MG	CN	201	1/1	0.95	0.29	175,175,175,175	0
48	MG	GJ	201	1/1	0.95	0.13	69,69,69,69	0
48	MG	F1	3552	1/1	0.95	0.15	139,139,139,139	0
48	MG	D1	3590	1/1	0.95	0.20	89,89,89,89	0
48	MG	D1	3474	1/1	0.95	0.10	58,58,58,58	0
48	MG	A1	3508	1/1	0.95	0.12	89,89,89,89	0
48	MG	H1	3507	1/1	0.95	0.07	64,64,64,64	0
48	MG	H1	3463	1/1	0.95	0.11	78,78,78,78	0
48	MG	H1	3491	1/1	0.95	0.13	111,111,111,111	0
48	MG	A1	3411	1/1	0.95	0.17	83,83,83,83	0
48	MG	F1	3412	1/1	0.95	0.11	60,60,60,60	0
48	MG	A1	3535	1/1	0.95	0.09	99,99,99,99	0
48	MG	A1	3480	1/1	0.95	0.31	120,120,120,120	0
48	MG	D1	3483	1/1	0.95	0.09	88,88,88,88	0
48	MG	A1	3459	1/1	0.95	0.20	90,90,90,90	0
48	MG	A1	3418	1/1	0.95	0.10	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	A1	3434	1/1	0.95	0.16	74,74,74,74	0
48	MG	H1	3483	1/1	0.95	0.14	108,108,108,108	0
48	MG	D1	3419	1/1	0.95	0.10	92,92,92,92	0
48	MG	F1	3504	1/1	0.95	0.13	84,84,84,84	0
48	MG	D1	3488	1/1	0.95	0.18	97,97,97,97	0
48	MG	D1	3402	1/1	0.95	0.08	52,52,52,52	0
48	MG	A1	3550	1/1	0.95	0.04	69,69,69,69	0
48	MG	E3	201	1/1	0.95	0.09	90,90,90,90	0
48	MG	H1	3423	1/1	0.95	0.11	98,98,98,98	0
48	MG	F1	3481	1/1	0.95	0.13	45,45,45,45	0
48	MG	F1	3584	1/1	0.95	0.16	97,97,97,97	0
48	MG	D1	3510	1/1	0.95	0.19	81,81,81,81	0
48	MG	A1	3544	1/1	0.95	0.48	135,135,135,135	0
48	MG	F1	3416	1/1	0.95	0.45	116,116,116,116	0
48	MG	D1	3408	1/1	0.95	0.30	106,106,106,106	0
48	MG	A1	3484	1/1	0.95	0.13	108,108,108,108	0
48	MG	A1	3445	1/1	0.95	0.18	88,88,88,88	0
48	MG	H1	3460	1/1	0.95	0.13	69,69,69,69	0
48	MG	H1	3500	1/1	0.95	0.16	82,82,82,82	0
48	MG	A1	3406	1/1	0.95	0.10	75,75,75,75	0
48	MG	D1	3567	1/1	0.95	0.26	60,60,60,60	0
48	MG	D1	3555	1/1	0.95	0.39	119,119,119,119	0
48	MG	D1	3450	1/1	0.95	0.07	49,49,49,49	0
48	MG	GL	301	1/1	0.95	0.11	113,113,113,113	0
48	MG	A1	3477	1/1	0.95	0.13	62,62,62,62	0
48	MG	A1	3545	1/1	0.95	0.30	71,71,71,71	0
48	MG	D1	3457	1/1	0.95	0.12	34,34,34,34	0
48	MG	F1	3582	1/1	0.95	0.20	77,77,77,77	0
48	MG	H1	3466	1/1	0.95	0.08	107,107,107,107	0
48	MG	D1	3415	1/1	0.95	0.11	117,117,117,117	0
48	MG	A1	3478	1/1	0.95	0.08	79,79,79,79	0
48	MG	DK	201	1/1	0.95	0.29	101,101,101,101	0
48	MG	D1	3629	1/1	0.95	0.11	121,121,121,121	0
48	MG	A1	3486	1/1	0.95	0.15	93,93,93,93	0
48	MG	D1	3529	1/1	0.96	0.10	80,80,80,80	0
48	MG	A1	3463	1/1	0.96	0.10	59,59,59,59	0
48	MG	F1	3512	1/1	0.96	0.11	94,94,94,94	0
48	MG	D1	3438	1/1	0.96	0.08	39,39,39,39	0
48	MG	A1	3523	1/1	0.96	0.12	91,91,91,91	0
48	MG	H1	3453	1/1	0.96	0.11	66,66,66,66	0
48	MG	A1	3520	1/1	0.96	0.16	70,70,70,70	0
48	MG	H1	3514	1/1	0.96	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3445	1/1	0.96	0.14	68,68,68,68	0
48	MG	D1	3578	1/1	0.96	0.07	88,88,88,88	0
48	MG	H1	3502	1/1	0.96	0.07	82,82,82,82	0
48	MG	F1	3476	1/1	0.96	0.16	99,99,99,99	0
48	MG	D1	3526	1/1	0.96	0.05	54,54,54,54	0
48	MG	F1	3521	1/1	0.96	0.09	65,65,65,65	0
48	MG	D1	3465	1/1	0.96	0.09	65,65,65,65	0
48	MG	D1	3459	1/1	0.96	0.07	63,63,63,63	0
48	MG	D1	3519	1/1	0.96	0.08	72,72,72,72	0
49	ZN	AC	201	1/1	0.96	0.08	143,143,143,143	0
48	MG	D1	3473	1/1	0.96	0.11	63,63,63,63	0
48	MG	A1	3557	1/1	0.96	0.20	104,104,104,104	0
48	MG	A1	3462	1/1	0.96	0.10	46,46,46,46	0
48	MG	D1	3539	1/1	0.96	0.14	57,57,57,57	0
48	MG	F1	3465	1/1	0.96	0.26	101,101,101,101	0
48	MG	A1	3537	1/1	0.96	0.12	54,54,54,54	0
48	MG	A1	3442	1/1	0.96	0.10	52,52,52,52	0
48	MG	D1	3518	1/1	0.96	0.21	92,92,92,92	0
48	MG	D1	3466	1/1	0.96	0.22	132,132,132,132	0
49	ZN	FL	201	1/1	0.96	0.09	86,86,86,86	0
48	MG	G2	203	1/1	0.96	0.10	112,112,112,112	0
48	MG	CJ	201	1/1	0.96	0.14	64,64,64,64	0
48	MG	F1	3487	1/1	0.96	0.09	60,60,60,60	0
48	MG	F1	3445	1/1	0.96	0.16	78,78,78,78	0
48	MG	F1	3526	1/1	0.96	0.14	72,72,72,72	0
48	MG	D1	3493	1/1	0.96	0.33	128,128,128,128	0
48	MG	D1	3495	1/1	0.96	0.07	88,88,88,88	0
48	MG	H1	3498	1/1	0.96	0.07	60,60,60,60	0
48	MG	F1	3508	1/1	0.96	0.24	127,127,127,127	0
48	MG	D1	3461	1/1	0.96	0.10	86,86,86,86	0
48	MG	D1	3619	1/1	0.96	0.07	101,101,101,101	0
48	MG	F1	3409	1/1	0.96	0.16	60,60,60,60	0
48	MG	EQ	201	1/1	0.96	0.18	88,88,88,88	0
48	MG	D1	3404	1/1	0.96	0.11	55,55,55,55	0
48	MG	D1	3544	1/1	0.96	0.09	50,50,50,50	0
48	MG	A1	3546	1/1	0.96	0.23	51,51,51,51	0
48	MG	A1	3514	1/1	0.96	0.14	59,59,59,59	0
48	MG	F1	3514	1/1	0.96	0.13	70,70,70,70	0
48	MG	H1	3494	1/1	0.96	0.14	56,56,56,56	0
48	MG	F1	3486	1/1	0.96	0.11	90,90,90,90	0
48	MG	C3	206	1/1	0.96	0.15	120,120,120,120	0
48	MG	F1	3518	1/1	0.96	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	A1	3465	1/1	0.96	0.08	54,54,54,54	0
48	MG	D1	3460	1/1	0.96	0.09	85,85,85,85	0
48	MG	F1	3547	1/1	0.96	0.10	112,112,112,112	0
48	MG	D1	3500	1/1	0.96	0.09	44,44,44,44	0
48	MG	A1	3539	1/1	0.96	0.08	46,46,46,46	0
48	MG	D1	3436	1/1	0.96	0.16	78,78,78,78	0
48	MG	A1	3597	1/1	0.97	0.38	133,133,133,133	0
48	MG	D1	3503	1/1	0.97	0.14	82,82,82,82	0
48	MG	D1	3420	1/1	0.97	0.08	105,105,105,105	0
48	MG	H1	3437	1/1	0.97	0.11	93,93,93,93	0
48	MG	A1	3466	1/1	0.97	0.12	40,40,40,40	0
48	MG	F1	3441	1/1	0.97	0.19	111,111,111,111	0
48	MG	CL	302	1/1	0.97	0.10	68,68,68,68	0
48	MG	A1	3540	1/1	0.97	0.15	66,66,66,66	0
48	MG	A1	3452	1/1	0.97	0.10	90,90,90,90	0
48	MG	F1	3525	1/1	0.97	0.09	73,73,73,73	0
48	MG	H1	3444	1/1	0.97	0.06	65,65,65,65	0
48	MG	CQ	202	1/1	0.97	0.06	62,62,62,62	0
48	MG	D1	3479	1/1	0.97	0.04	50,50,50,50	0
48	MG	A1	3538	1/1	0.97	0.08	49,49,49,49	0
48	MG	D1	3464	1/1	0.97	0.08	44,44,44,44	0
48	MG	D1	3509	1/1	0.97	0.09	41,41,41,41	0
48	MG	C2	204	1/1	0.97	0.07	75,75,75,75	0
48	MG	D1	3632	1/1	0.97	0.12	83,83,83,83	0
48	MG	D1	3456	1/1	0.97	0.11	70,70,70,70	0
48	MG	D1	3453	1/1	0.97	0.11	54,54,54,54	0
48	MG	F1	3432	1/1	0.97	0.08	68,68,68,68	0
48	MG	D1	3490	1/1	0.97	0.16	92,92,92,92	0
48	MG	A1	3457	1/1	0.97	0.35	94,94,94,94	0
48	MG	D1	3570	1/1	0.97	0.20	54,54,54,54	0
48	MG	D1	3501	1/1	0.97	0.13	51,51,51,51	0
48	MG	A1	3526	1/1	0.97	0.10	48,48,48,48	0
48	MG	D1	3462	1/1	0.97	0.19	116,116,116,116	0
48	MG	D1	3559	1/1	0.97	0.08	55,55,55,55	0
48	MG	D1	3536	1/1	0.97	0.10	73,73,73,73	0
48	MG	A1	3598	1/1	0.97	0.21	111,111,111,111	0
48	MG	D1	3546	1/1	0.97	0.10	49,49,49,49	0
48	MG	F1	3449	1/1	0.97	0.10	90,90,90,90	0
48	MG	F1	3459	1/1	0.97	0.07	79,79,79,79	0
48	MG	C2	203	1/1	0.97	0.06	63,63,63,63	0
48	MG	F1	3427	1/1	0.97	0.16	51,51,51,51	0
48	MG	H1	3493	1/1	0.97	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	B2	203	1/1	0.97	0.06	81,81,81,81	0
48	MG	D1	3630	1/1	0.97	0.14	71,71,71,71	0
48	MG	A1	3458	1/1	0.97	0.10	59,59,59,59	0
48	MG	A1	3517	1/1	0.97	0.08	74,74,74,74	0
48	MG	A1	3446	1/1	0.97	0.19	64,64,64,64	0
48	MG	BW	201	1/1	0.97	0.09	67,67,67,67	0
48	MG	H1	3439	1/1	0.97	0.12	75,75,75,75	0
48	MG	F1	3426	1/1	0.97	0.24	110,110,110,110	0
48	MG	BQ	202	1/1	0.97	0.07	53,53,53,53	0
48	MG	H1	3506	1/1	0.97	0.12	75,75,75,75	0
48	MG	H1	3515	1/1	0.97	0.09	73,73,73,73	0
48	MG	F1	3510	1/1	0.97	0.10	95,95,95,95	0
48	MG	D1	3560	1/1	0.97	0.10	64,64,64,64	0
48	MG	A1	3426	1/1	0.97	0.09	73,73,73,73	0
48	MG	D1	3587	1/1	0.97	0.14	93,93,93,93	0
48	MG	E2	204	1/1	0.97	0.06	75,75,75,75	0
48	MG	A1	3495	1/1	0.97	0.06	70,70,70,70	0
48	MG	F1	3404	1/1	0.97	0.10	75,75,75,75	0
48	MG	D1	3486	1/1	0.97	0.13	47,47,47,47	0
48	MG	F1	3474	1/1	0.97	0.13	64,64,64,64	0
48	MG	A1	3456	1/1	0.97	0.12	49,49,49,49	0
48	MG	F1	3454	1/1	0.98	0.15	56,56,56,56	0
48	MG	F1	3460	1/1	0.98	0.14	36,36,36,36	0
48	MG	F1	3528	1/1	0.98	0.06	75,75,75,75	0
48	MG	A1	3524	1/1	0.98	0.12	63,63,63,63	0
48	MG	A1	3432	1/1	0.98	0.07	45,45,45,45	0
48	MG	H1	3458	1/1	0.98	0.06	90,90,90,90	0
49	ZN	DC	201	1/1	0.98	0.07	89,89,89,89	0
48	MG	A1	3421	1/1	0.98	0.06	71,71,71,71	0
49	ZN	GY	201	1/1	0.98	0.10	116,116,116,116	0
48	MG	D1	3430	1/1	0.98	0.08	59,59,59,59	0
48	MG	F1	3499	1/1	0.98	0.04	57,57,57,57	0
48	MG	A1	3440	1/1	0.98	0.04	78,78,78,78	0
48	MG	F1	3523	1/1	0.98	0.09	55,55,55,55	0
48	MG	D1	3480	1/1	0.98	0.09	32,32,32,32	0
48	MG	D1	3411	1/1	0.98	0.11	44,44,44,44	0
48	MG	F1	3450	1/1	0.98	0.09	59,59,59,59	0
48	MG	D1	3489	1/1	0.98	0.07	44,44,44,44	0
48	MG	D1	3405	1/1	0.98	0.10	59,59,59,59	0
48	MG	D1	3569	1/1	0.98	0.09	48,48,48,48	0
48	MG	F1	3546	1/1	0.98	0.07	59,59,59,59	0
48	MG	D1	3469	1/1	0.98	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
49	ZN	DL	201	1/1	0.98	0.17	86,86,86,86	0
48	MG	A1	3476	1/1	0.98	0.07	59,59,59,59	0
48	MG	F1	3505	1/1	0.98	0.10	83,83,83,83	0
48	MG	A1	3543	1/1	0.98	0.08	96,96,96,96	0
48	MG	A1	3561	1/1	0.98	0.14	60,60,60,60	0
49	ZN	HA	101	1/1	0.98	0.14	112,112,112,112	0
48	MG	H1	3421	1/1	0.98	0.13	97,97,97,97	0
49	ZN	BY	201	1/1	0.98	0.10	59,59,59,59	0
49	ZN	FC	201	1/1	0.98	0.04	108,108,108,108	0
49	ZN	HL	201	1/1	0.98	0.08	118,118,118,118	0
49	ZN	AK	201	1/1	0.98	0.10	89,89,89,89	0
48	MG	D1	3428	1/1	0.98	0.06	106,106,106,106	0
48	MG	A1	3525	1/1	0.98	0.08	51,51,51,51	0
48	MG	D1	3556	1/1	0.98	0.07	76,76,76,76	0
49	ZN	EY	201	1/1	0.98	0.10	77,77,77,77	0
48	MG	A1	3410	1/1	0.98	0.21	62,62,62,62	0
49	ZN	AA	101	1/1	0.98	0.14	64,64,64,64	0
48	MG	A1	3460	1/1	0.99	0.13	61,61,61,61	0
48	MG	D1	3502	1/1	0.99	0.07	38,38,38,38	0
48	MG	D1	3471	1/1	0.99	0.20	40,40,40,40	0
49	ZN	AL	201	1/1	0.99	0.09	70,70,70,70	0
48	MG	A1	3473	1/1	0.99	0.08	55,55,55,55	0
48	MG	D1	3410	1/1	0.99	0.12	39,39,39,39	0
48	MG	F1	3467	1/1	0.99	0.10	57,57,57,57	0
49	ZN	CY	202	1/1	0.99	0.08	70,70,70,70	0
48	MG	F1	3438	1/1	0.99	0.14	58,58,58,58	0
49	ZN	FA	103	1/1	0.99	0.12	80,80,80,80	0
48	MG	H1	3497	1/1	0.99	0.13	50,50,50,50	0
49	ZN	HK	201	1/1	0.99	0.11	70,70,70,70	0
48	MG	D1	3554	1/1	0.99	0.12	59,59,59,59	0
49	ZN	DK	202	1/1	0.99	0.11	68,68,68,68	0
49	ZN	DA	103	1/1	0.99	0.14	69,69,69,69	0
48	MG	D1	3533	1/1	0.99	0.07	41,41,41,41	0
48	MG	F1	3435	1/1	0.99	0.11	44,44,44,44	0
48	MG	A1	3502	1/1	0.99	0.10	80,80,80,80	0
48	MG	A1	3534	1/1	0.99	0.13	62,62,62,62	0
49	ZN	FK	202	1/1	0.99	0.12	74,74,74,74	0
48	MG	A1	3413	1/1	0.99	0.18	136,136,136,136	0
48	MG	A1	3489	1/1	0.99	0.07	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.