



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:03 am 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

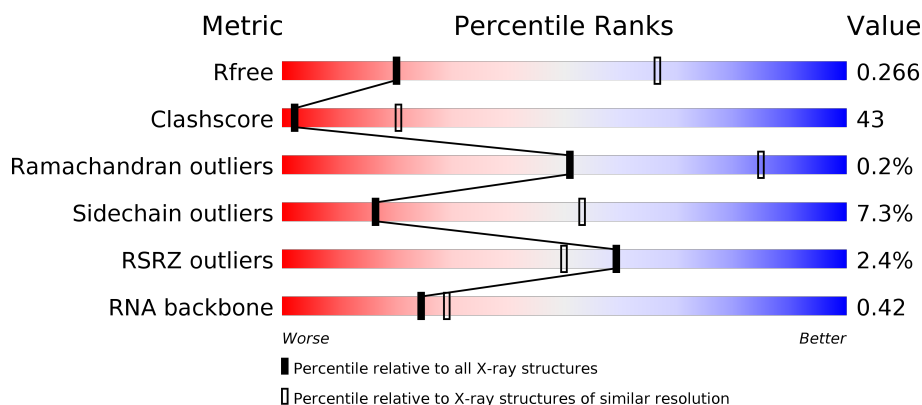
1 Overall quality at a glance

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.



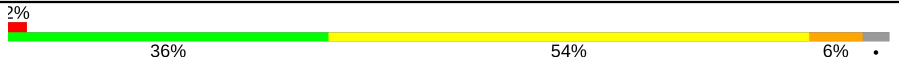
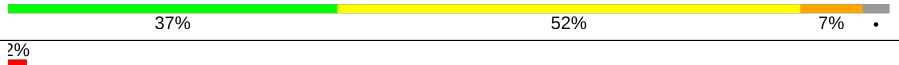
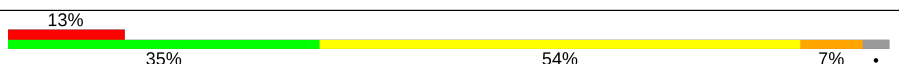
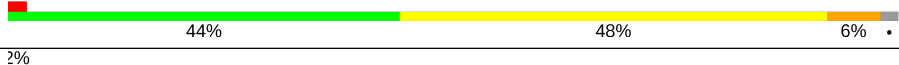
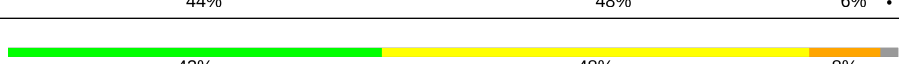
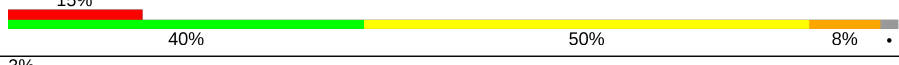



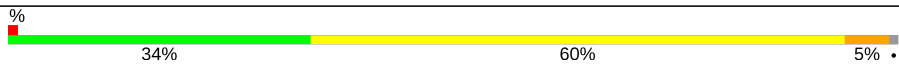

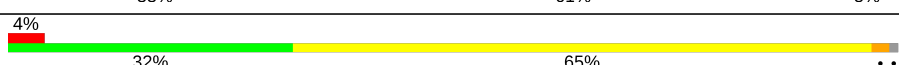
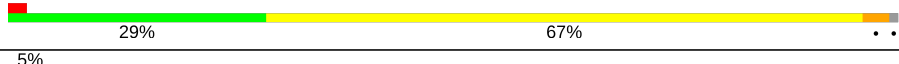
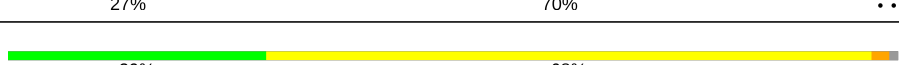
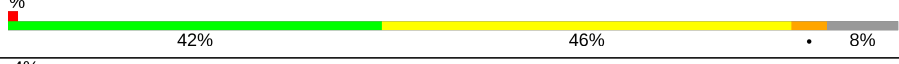
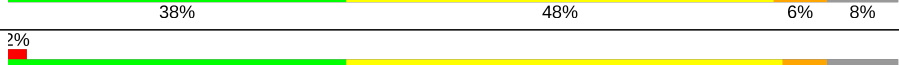




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)
RNA backbone	2435	1027 (4.18-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>18% 45% 28% 7%</div> </div>
1	D1	3354	<div> <div>%</div> <div>18% 45% 27% 7%</div> </div>
1	F1	3354	<div> <div>2%</div> <div>18% 45% 27% 7%</div> </div>
1	H1	3354	<div> <div>4%</div> <div>17% 45% 28% 7%</div> </div>

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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	




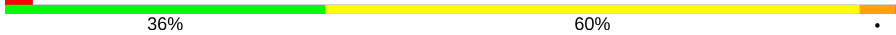
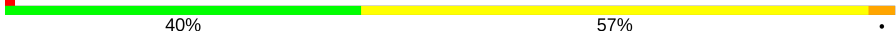
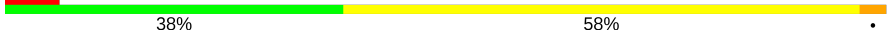
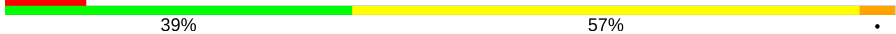
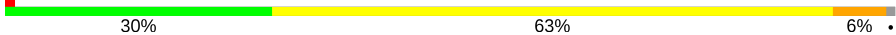
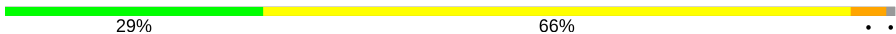
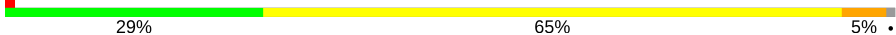
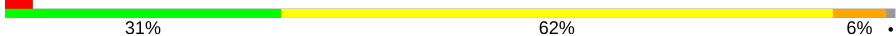

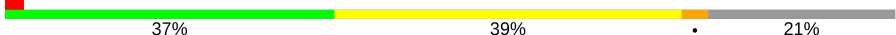












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Mol	Chain	Length	Quality of chain
27	BF	255	
27	CF	255	
27	EF	255	
27	GF	255	
28	BG	123	
28	CG	123	
28	EG	123	
28	GG	123	
29	BH	215	
29	CH	215	
29	EH	215	
29	GH	215	
30	BI	198	
30	CI	198	
30	EI	198	
30	GI	198	
31	BJ	141	
31	CJ	141	
31	EJ	141	
31	GJ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

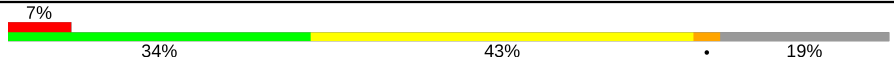

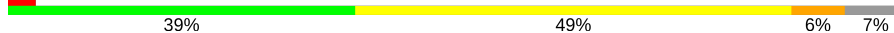
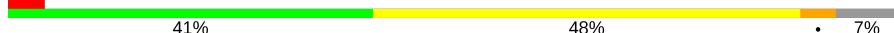





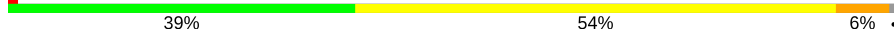
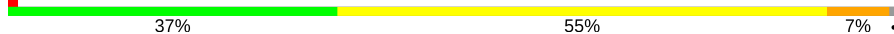
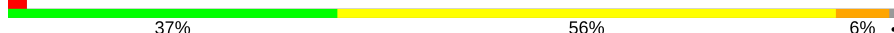









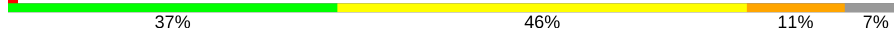



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Mol	Chain	Length	Quality of chain
33	CL	204	
33	EL	204	
33	GL	204	
34	BM	301	
34	CM	301	
34	EM	301	
34	GM	301	
35	BN	181	
35	CN	181	
35	EN	181	
35	GN	181	
36	BO	185	
36	EO	185	
36	GO	185	
37	BP	157	
37	CP	157	
37	EP	157	
37	GP	157	
38	BQ	183	
38	CQ	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	3412	-	-	-	X
48	MG	A1	3500	-	-	-	X
48	MG	A1	3579	-	-	-	X
48	MG	D1	3412	-	-	-	X
48	MG	D1	3481	-	-	-	X
48	MG	D1	3484	-	-	-	X
48	MG	D1	3497	-	-	-	X
48	MG	D1	3504	-	-	-	X
48	MG	D1	3511	-	-	-	X
48	MG	D1	3516	-	-	-	X
48	MG	D1	3517	-	-	-	X
48	MG	D1	3589	-	-	-	X
48	MG	D1	3603	-	-	-	X
48	MG	D1	3607	-	-	-	X
48	MG	DJ	301	-	-	-	X
48	MG	F1	3479	-	-	-	X
48	MG	F1	3483	-	-	-	X
48	MG	F1	3493	-	-	-	X
48	MG	F1	3506	-	-	-	X
48	MG	F1	3538	-	-	-	X
48	MG	F1	3566	-	-	-	X
48	MG	G2	202	-	-	-	X
48	MG	G3	204	-	-	-	X
48	MG	GO	201	-	-	-	X
48	MG	H1	3409	-	-	-	X
48	MG	H1	3469	-	-	-	X
48	MG	H1	3519	-	-	-	X
48	MG	H1	3529	-	-	-	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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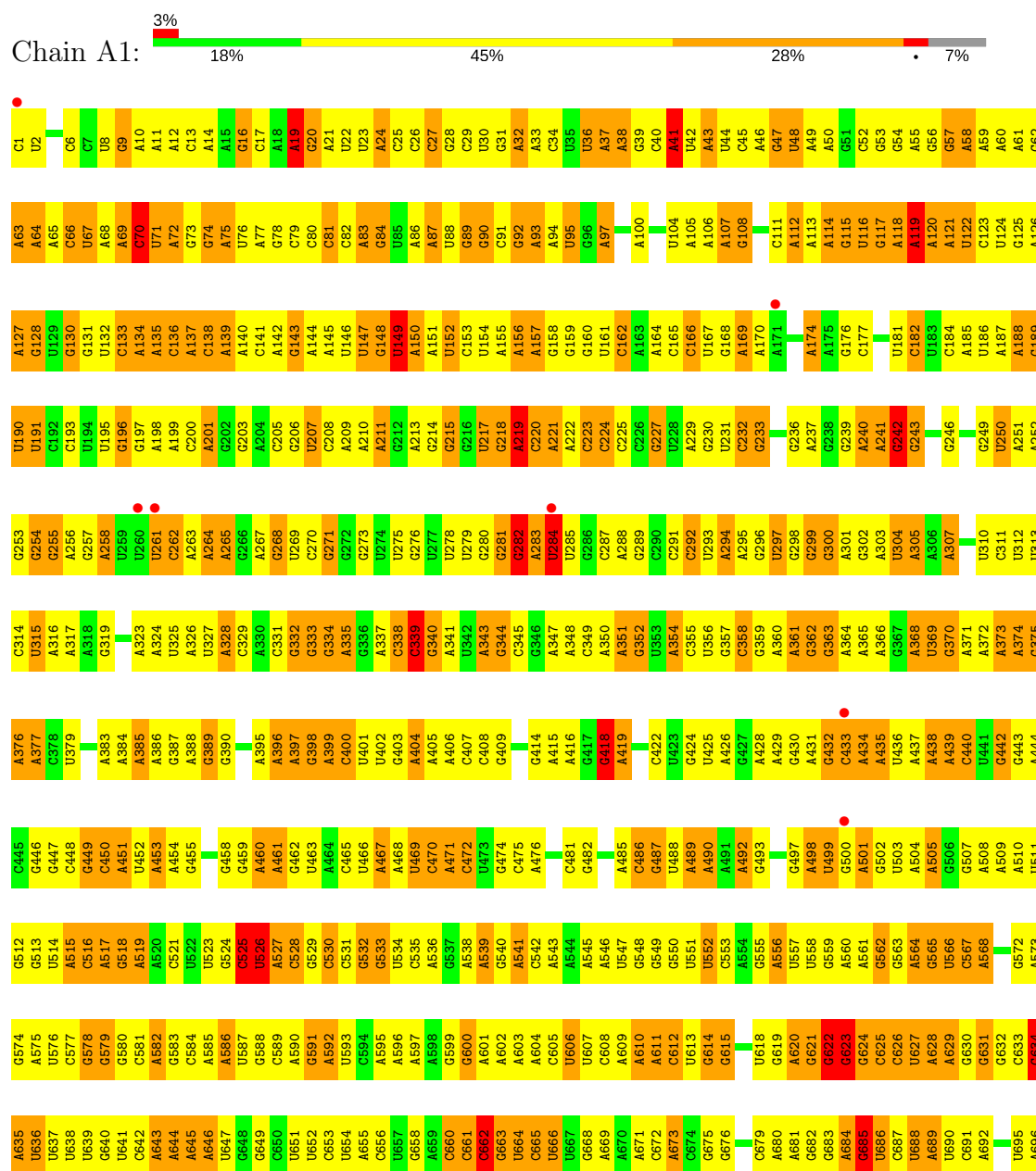
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	GY	1	Total	O	0	0
			1	1		
50	H1	924	Total	O	0	0
			924	924		
50	HA	4	Total	O	0	0
			4	4		
50	HB	4	Total	O	0	0
			4	4		
50	HJ	2	Total	O	0	0
			2	2		
50	HK	2	Total	O	0	0
			2	2		
50	HP	1	Total	O	0	0
			1	1		
50	HT	5	Total	O	0	0
			5	5		
50	HU	2	Total	O	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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









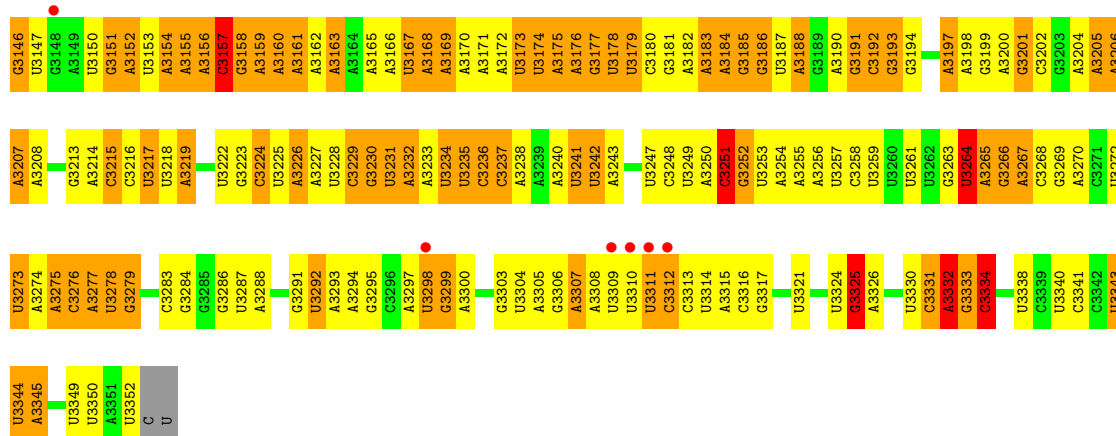
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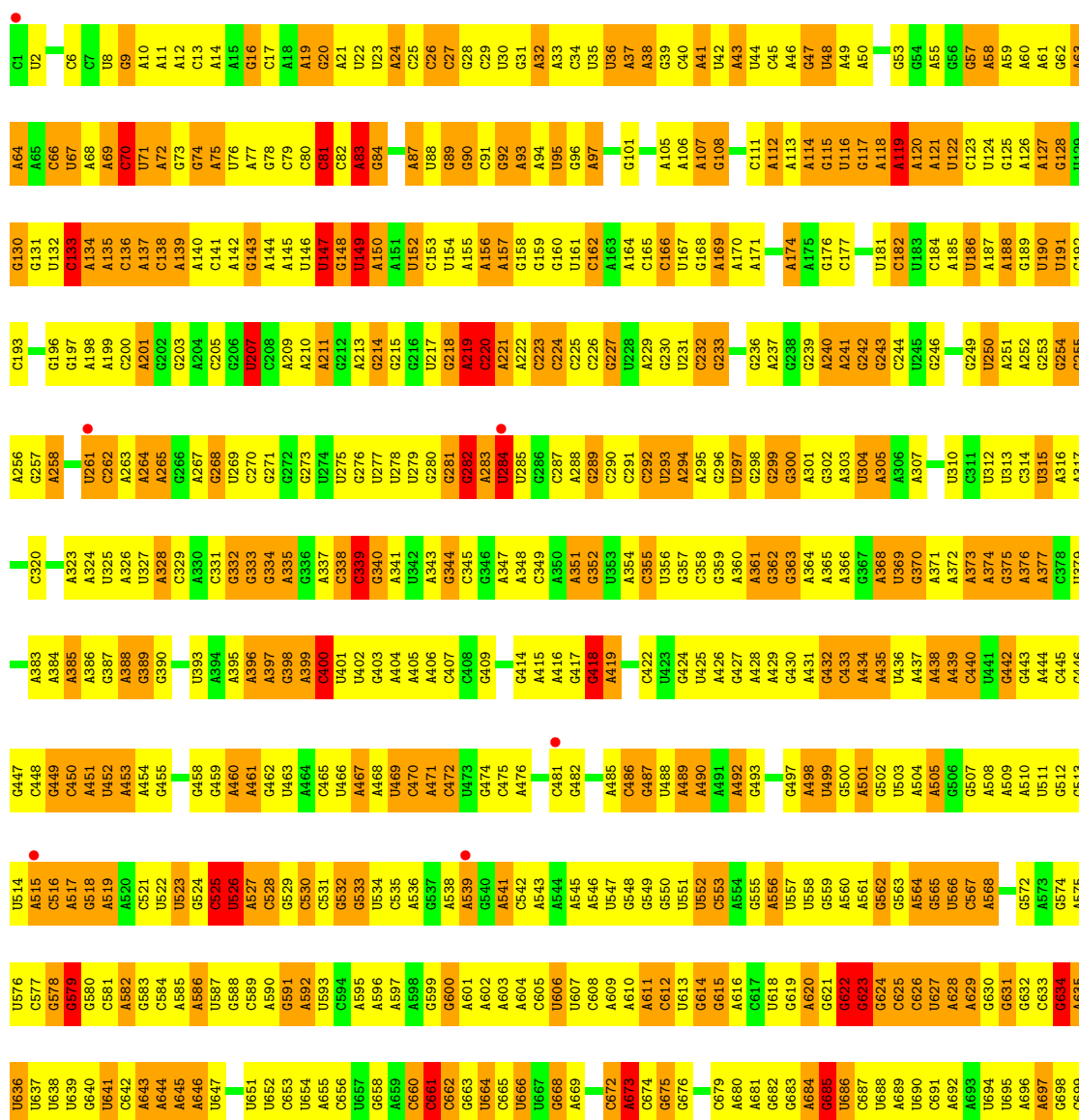
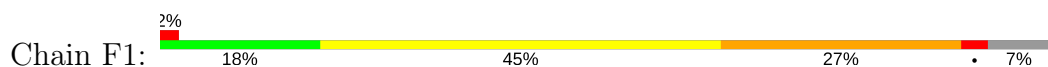
U1076	U1011	C948	G879	A816	C751	A889	A629	C567	G507	A444	C378	A316	G954	U191	G128
U1077	U1012	G949	U880	A817	C752	U890	G630	A868	A508	C445	U379	A317	G255	G192	U129
U1078	U1013	A950	G882	U818	A753	C891	G631	A869	A509	G447	A383	G131	A256	C193	G130
A1079	U1016	A951	A883	U819	A754	A892	G632	G572	A510	G448	A322	U121	G257	G196	U132
U1083	U1017	C952	A884	U821	C755	U895	G633	A574	A511	G449	A385	A323	A258	G197	G133
G1084	A1018	C953	G885	U822	C757	A896	G634	A575	A512	G450	A386	A324	U259	A198	A134
U1085	G1019	U957	C886	A823	A761	A897	U636	U576	A513	A451	A387	U325	U261	A199	A135
U1086	G1020	A958	G889	G824	A762	G898	U637	U577	A514	U452	A388	U326	U262	C200	C136
A1087	U1021	G959	G894	A825	G762	C699	U638	G578	C516	A453	G387	U327	A263	C209	A137
U1088	A1022	U960	G895	G826	G763	G700	U639	G579	A517	A454	G389	A328	A264	G202	C138
G1089	U1023	A961	U896	C827	U764	G701	G640	G580	A518	G455	U393	A329	A265	G203	A139
U1090	A1024	G962	A897	C828	A765	G702	U641	G581	A519	G456	A394	A330	G266	A204	A140
G1091	G1025	C963	C898	C829	G766	U703	G642	A882	A520	G458	A395	C331	A267	C205	C141
C1092	U1026	U964	U899	G830	C767	G704	A643	A583	C521	A459	A396	G332	G268	G206	A142
G1094	G1027	G965	C902	A831	A768	A705	A644	C584	U522	G460	A397	G333	U269	U207	G143
U1095	U1028	U966	C903	A832	G769	U706	A645	A585	U523	A461	G398	A334	C270	C208	A144
C1096	U1032	U967	G904	A833	G771	A707	A646	A586	C524	G462	A399	A335	G271	A209	A145
G1096	U1034	U968	U903	G834	U772	G708	U647	U587	C525	U463	C400	A336	G272	A210	U146
G1097	A1035	C969	G905	A835	C773	G709	G648	G588	U526	A464	U401	A337	U274	A211	U147
A1098	U1036	G970	C906	U836	A774	G710	G649	C589	A527	G465	U402	A338	U275	G212	G148
G1099	A1037	A907	A907	G837	C775	U711	C650	A590	C528	U466	G403	A339	U276	A213	U149
U1100	G1038	U972	A908	G838	C776	G712	U651	G591	C529	U467	A404	G340	U277	G214	A150
U1101	U1039	C973	A909	U839	C777	G713	U652	A592	C530	U468	A405	A341	U278	G215	A151
U1102	A1040	C974	U910	G840	G778	G714	C653	U593	C531	U469	A406	U342	U279	G216	U152
A1103	C1041	G975	C911	A841	A779	A715	U654	C594	C532	C470	C407	A343	G280	U217	C153
C1104	U1042	A976	G912	A842	C780	A716	C655	A595	C533	A471	C408	G344	G281	G218	U154
U1105	C1043	A977	U913	C846	G784	A717	C656	A596	U534	C472	G409	G345	G282	A219	A155
G1106	U1044	G978	U914	C847	C785	A718	U657	A597	C535	U473	G346	A347	A283	C220	A156
A1107	G1045	U979	C915	G848	A785	C719	C658	A598	A536	G474	A348	A347	U284	A221	A157
U1108	U1046	U980	G916	U849	G786	G720	C659	G599	C537	C475	U349	A350	U285	A222	G158
A1109	G1047	U981	U917	U849	U787	C728	U660	G600	A538	A476	A415	C355	G286	C223	G159
U1110	U1048	C982	C918	U850	C788	U723	C661	A601	A539	A485	A416	U356	C287	C224	G160
G1111	U1049	U983	A919	G851	C789	C724	C662	A602	C540	G479	G417	A351	C287	C225	U161
A1112	C1050	C984	A920	A852	C790	C725	G663	A603	A541	U480	G418	A352	G289	C226	C162
U1113	C1051	U985	A921	A853	C791	G726	U664	A604	C542	C481	A419	U353	C290	G227	A163
C1114	A1052	C986	A922	U854	G792	C727	C665	C605	A543	G482	A420	A354	C291	U228	A164
U1115	U1053	A987	G925	A855	A793	G728	U666	U606	A544	G485	G421	C355	C292	A229	C165
C1116	G1054	G988	A926	G858	C794	A729	U667	U607	A545	A486	G422	U356	C293	G230	C166
U1117	U1055	C989	G927	U859	G795	A730	G668	C608	A546	C486	U423	G357	A294	U231	U167
G1121	A1056	A990	U928	U859	A796	A731	A669	A609	U547	G487	G424	C358	A295	G232	G168
A1122	U1057	U991	G929	G860	A797	C732	A670	A610	C548	U488	U425	C359	G296	C233	A169
U1123	C1058	A992	U930	A861	G798	G733	A671	A611	C549	A489	A426	A360	U297	G234	A170
G1124	U1059	C993	A931	A862	G799	A734	C672	C612	C550	A490	G427	A361	G298	G236	A174
A1125	C1060	C994	G932	G863	G800	A735	A673	U613	U551	A491	A428	G362	G299	A237	A175
U1127	U1061	A995	G933	C864	U801	A736	C674	G614	U552	A492	A429	C363	G300	G238	G176
G1128	A1062	A996	G934	C865	U802	G737	G675	G615	C553	G493	G430	A364	A301	G239	G177
U1129	C1063	G997	G935	A866	C803	U738	G676	A616	A554	G494	A431	A365	G302	A240	C177
C1129	U1064	A998	C936	G867	G804	G739	A677	C617	G555	U495	G432	A366	A303	A241	U178
U1130	U1065	G999	G937	G868	A805	A740	C678	U618	A556	C496	C433	A367	U304	G242	G179
G1131	A1066	G1002	A938	G869	G806	G741	C679	G619	U557	G497	A434	G368	A305	G243	U181
U1132	U1067	U1003	A939	G870	G807	G742	A680	A620	U558	A498	A435	U369	A306	C244	U182
C1133	A1068	A1004	A940	A871	A808	A743	A681	G621	C559	U499	A436	U370	A307	G245	U183
U1134	C1069	G1005	G941	A872	A809	C744	G682	G622	A560	G500	A437	A371	G307	U246	C184
C1135	U1070	A1006	A942	A873	C810	C745	G683	G623	A561	A501	A438	A372	U310	G247	G178
U1136	C1071	C943	C943	C874	A811	A746	A684	G624	G562	G502	A439	A373	C311	G249	U186
C1137	A1072	U944	U944	U875	G812	G747	G685	C625	G563	U503	C440	A374	U312	U250	A187
U1137	U1073	A945	C876	U876	C813	G748	U686	C626	A564	A504	U441	G375	U313	A251	A188
U1138	A1074	A1009	U877	U877	U814	G749	C687	U627	G565	A505	G442	A376	U314	A252	G189
A1139	C1075	G1010	U947	G878	U815	G750	U688	A628	U566	G506	G443	A377	U315	G253	U190

U	A	A1973	A1905	A1837	G1773	A1638	C1576	H1510	A1447	G1384	U1320	G	C1200	G1140
C	U	U1974	G1906	A1838	C1774	G1639	C1577	G1511	G1448	C1385	A1321	G	G1201	U1141
A	A	A	A1907	A1839	A1775	C1640	U1578	A1512	G1449	U1386	G1322	U	C1202	G1142
A	G	G	U1776	U1770	G1776	U1641	U1579	A1513		U1387	G1323	G	C1203	G1143
A	G	A	U1840	U1809	G1777	G1642	U1580	A1514	U1453	U1388	A1204	C	C1204	G1144
C	C	G	U1711	U1712	G1778	G1643	C1581	A1515	U1454	G1389	A1328	C	A1205	G1145
U	U	U	U1713	U1713	U1713	A1644	A1582	A1516	G1455	A1390	A1329	U	A1206	C1146
U	U	A	C1714	C1714	C1714	C1645	A1583	G1517	U1456	U1391		A	A1207	A1147
G	G	A	U1715	U1715	U1715	G1646	A1584	G1518	G1457	G1392	U1332	U	U1208	U1148
C	A	A	U1716	U1716	U1716	U1647	A1585	G1519	U1458	A1393	G1333	G	G1209	U1149
C	A	A	U1717	U1717	U1717	G1648	C1586	U1520	A1459	G1394	G1334	G	C1210	U1150
C	A	A	U1783	U1783	U1783	G1649	A1587	U1521	G1460	U1395	A1335	A	A1211	U1151
A	A	A	U1718	U1718	U1718	G1650	A1588	C1522	A1461	A1396	U1336	A	A1212	U1152
A	A	A	U1719	U1719	U1719	A1651	G1589	G1523	U1462	G1397	G1337	G	G1213	U1153
C	C	C	A1720	A1720	A1720	U1652	A1590	A1524	U1463	G1398	U1338	U	C1214	G1154
G	G	A	A1721	A1721	A1721	A1653	A1591	U1525	U1464	A1399	U1339	U	U1215	U1155
A	U	U	U1724	U1724	U1724	G1654	G1592	G1526	U1465	G1400	G1340	A	C1216	A1156
C	U	U	A1725	A1725	A1725	A1655	A1593	A1527	G1466	G1401	G1341	G	A1217	A1157
C	A	A	C1726	C1726	C1726	G1656	C1594	G1528	G1467	U1342	U1218	A	U1218	G1158
A	A	A	U1727	U1727	U1727	C1657	A1595		U1468	G1403		A	U1219	C1159
U	U	U	A1728	A1728	A1728	G1658	U1596	C1531	U1469	G1404	G1343	U	A1220	A1160
U	U	U	U1729	U1729	U1729	G1659	U1597	A1532	G1470	U1405	A1344	U	G1221	G1161
U	U	U	G1730	G1730	G1730	U1660	C1598	G1533	U1471	G1406	G1346	C	A1222	A1162
G	G	G	U1731	U1731	U1731	A1661	G1599	C1534	A1472	A1407	G1347	G	U1223	A1163
C	C	C	G1732	G1732	G1732	A1662	U1600	A1535	G1473	U1408	U1224	C	A1224	C1164
C	U	U	C1733	C1733	C1733	C1663	U1601	A1536	U1474	C1409		U	G1225	U1165
A	A	A	A1734	A1734	A1734	G1664	U1602	U1537	U1475	G1410	G1350	A	C1226	G1166
U	U	U	U1735	U1735	U1735	C1665	U1603	U1538	G1476	U1411	U1351	A	A1227	G1167
U	U	U	G1736	G1736	G1736	A1666	U1604	G1539	G1477	U1412	U1352	G	C1228	C1168
C	C	C	U1737	U1737	U1737	A1667	G1605	U1540	A1478	G1413	G1353	G	A1229	G1169
C	A	A	A1738	A1738	A1738	A1668	U1606	U1541	A1479	C1414	C1354	A	A1230	U1170
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U	U	U	G1742	G1742	G1742	G1675	C1610	G1545	U1483	G1418	U1358	U	G1234	G1174
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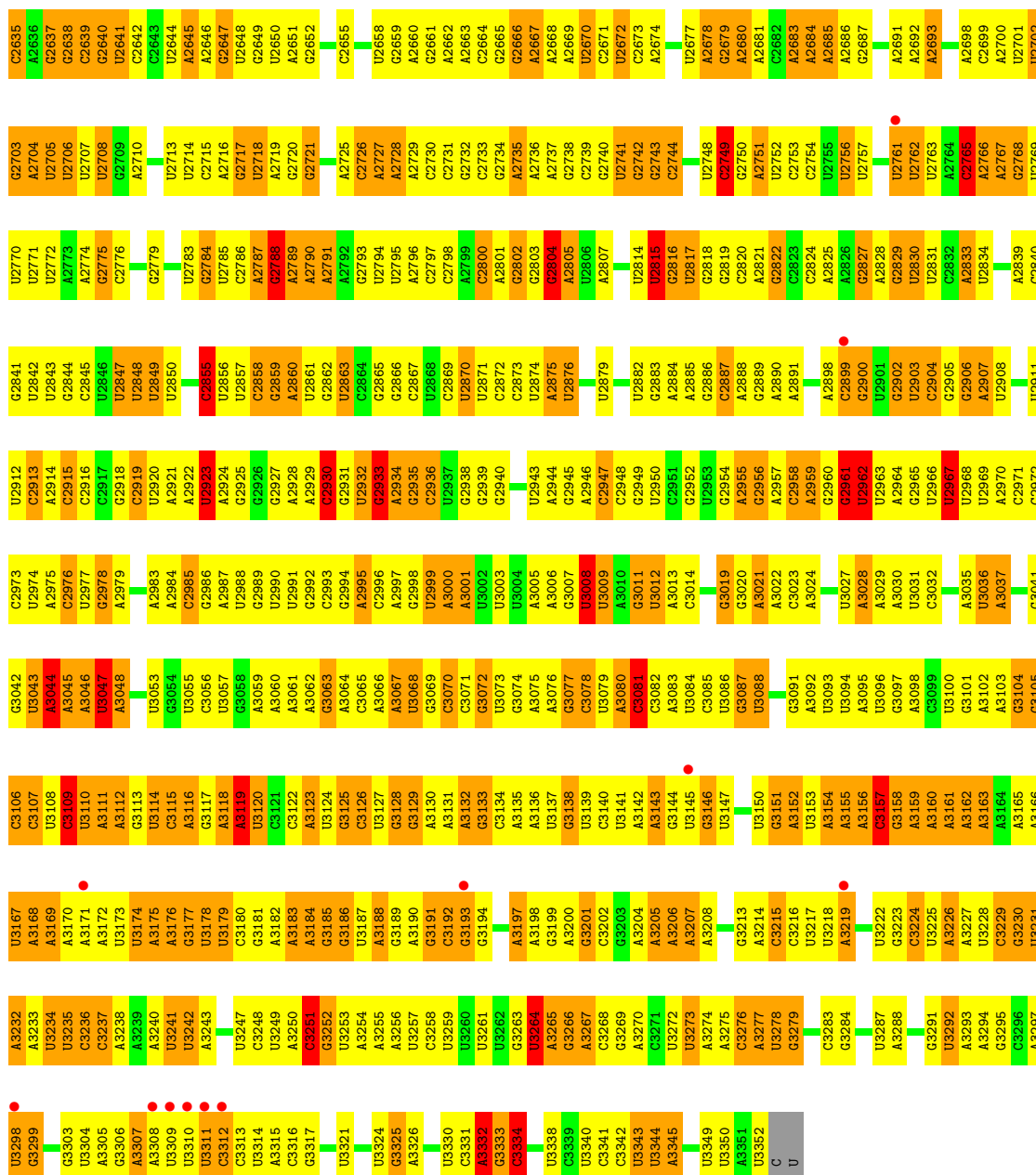


● Molecule 1: 26S rRNA

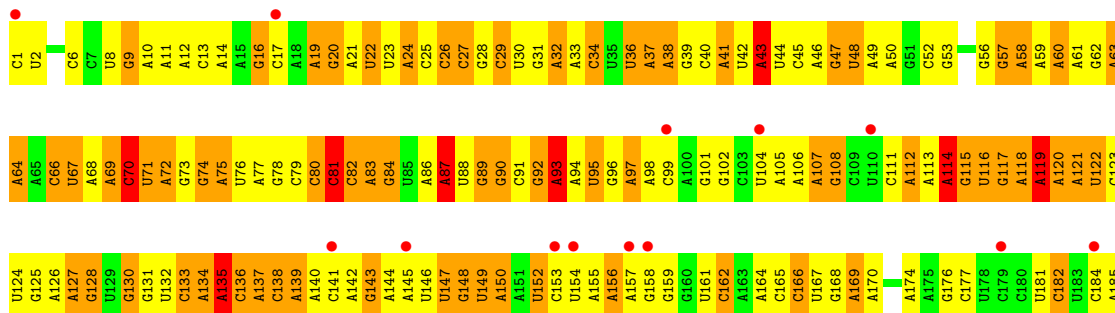
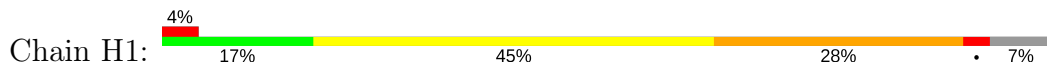


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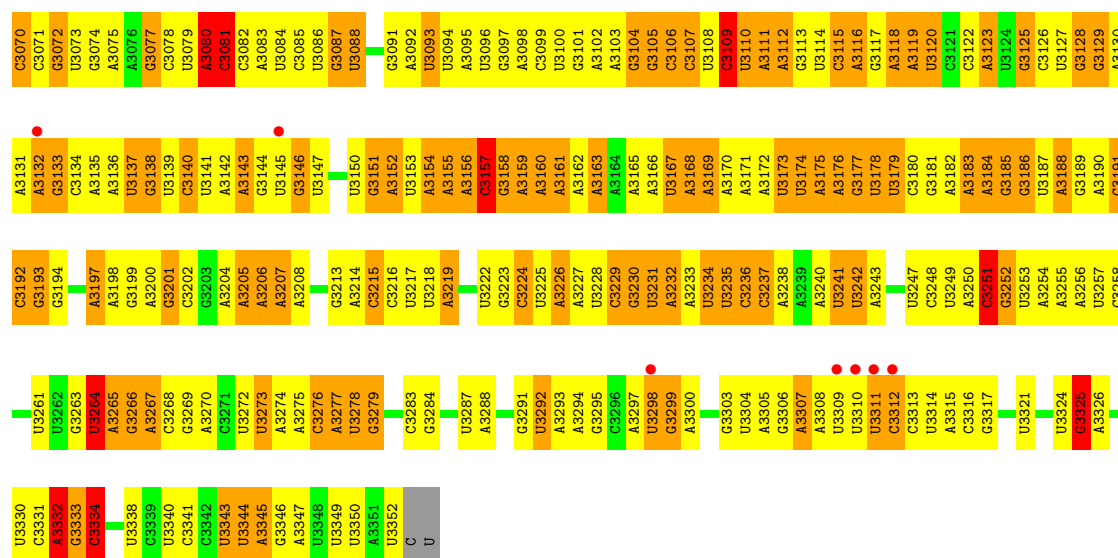
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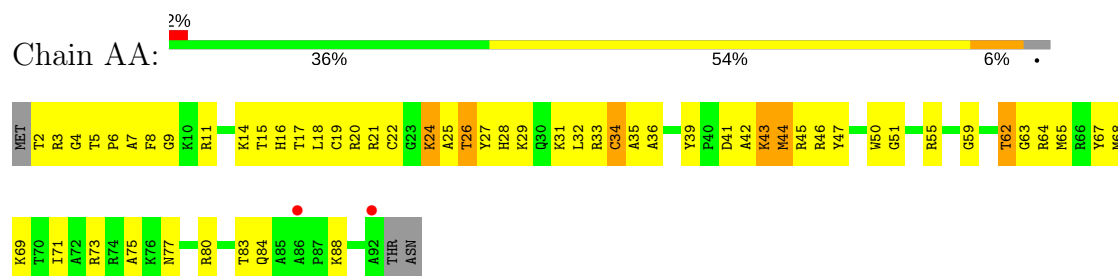
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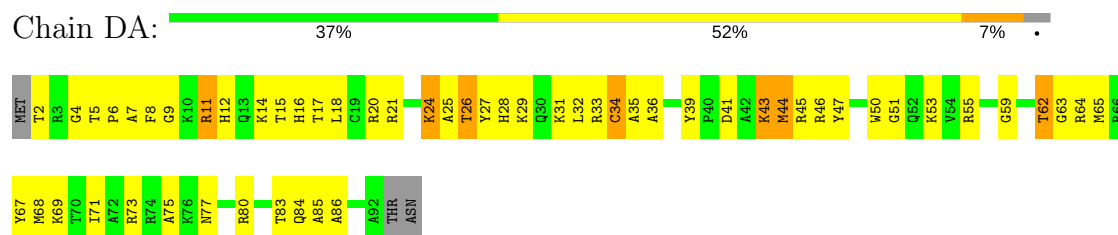
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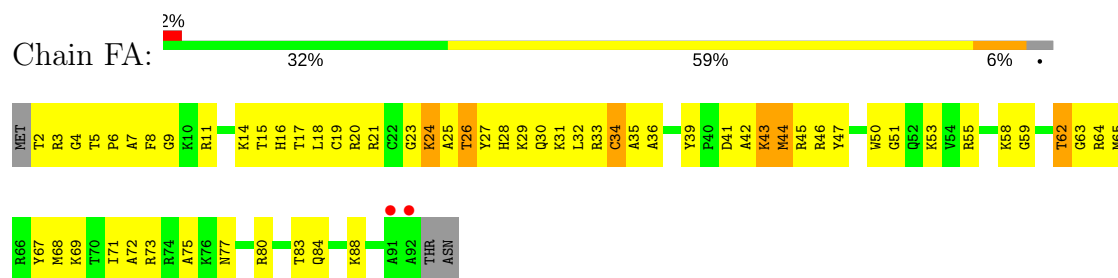
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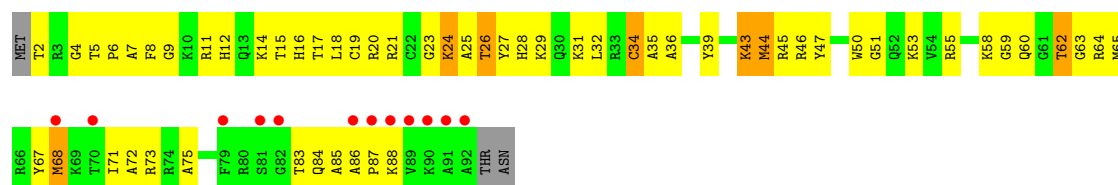


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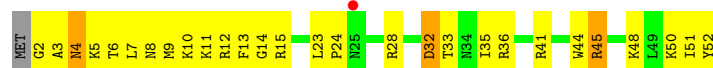


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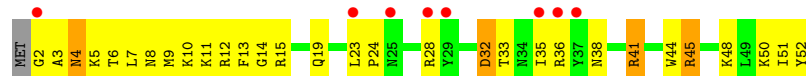
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• Molecule 3: RPL39



• Molecule 3: RPL39



• Molecule 4: 60S RIBOSOMAL PROTEIN L36A

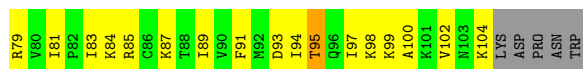
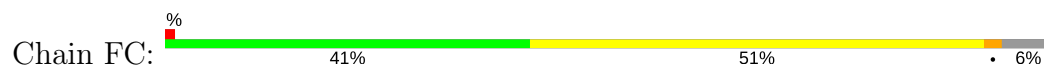


• Molecule 4: 60S RIBOSOMAL PROTEIN L36A





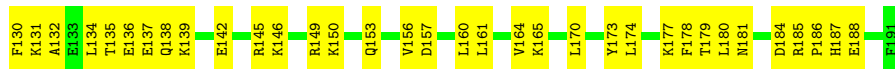
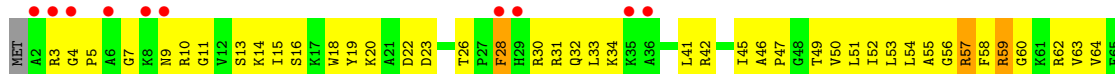
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



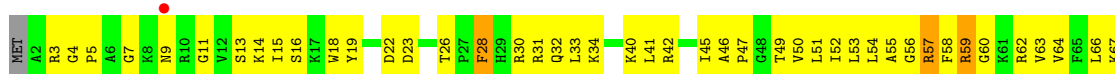
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



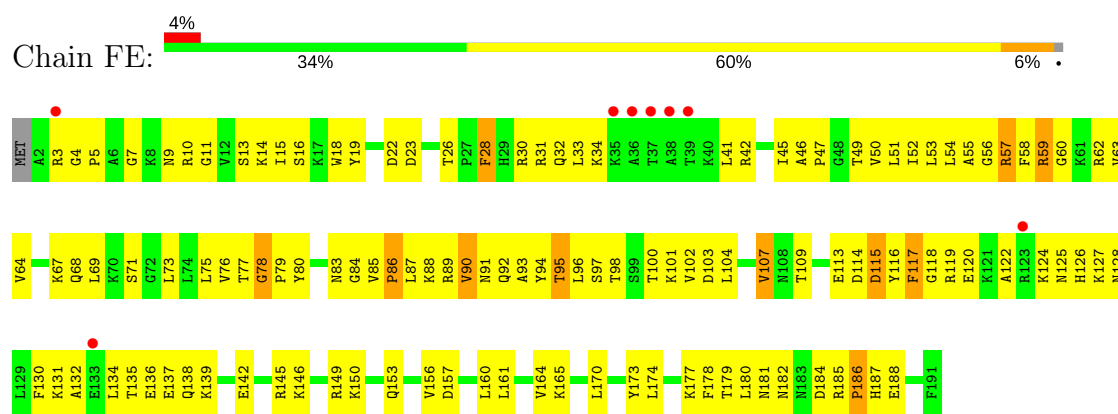
• Molecule 5: RPL6



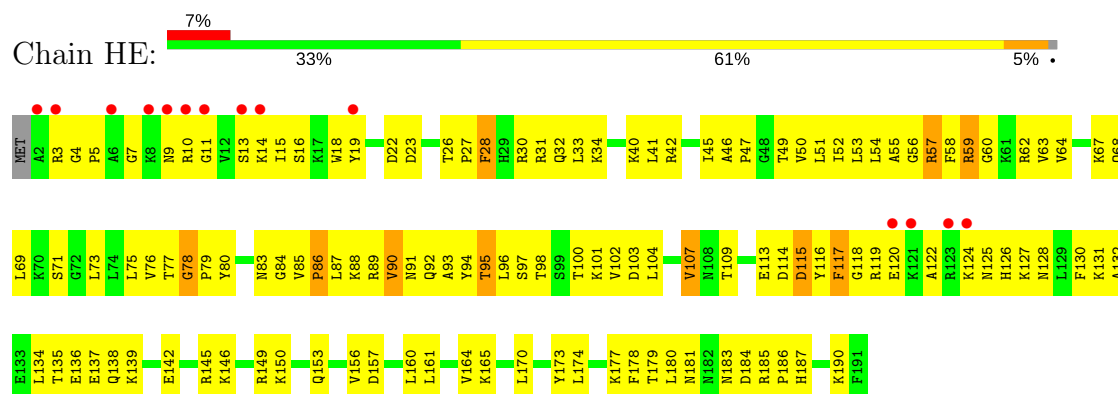
• Molecule 5: RPL6



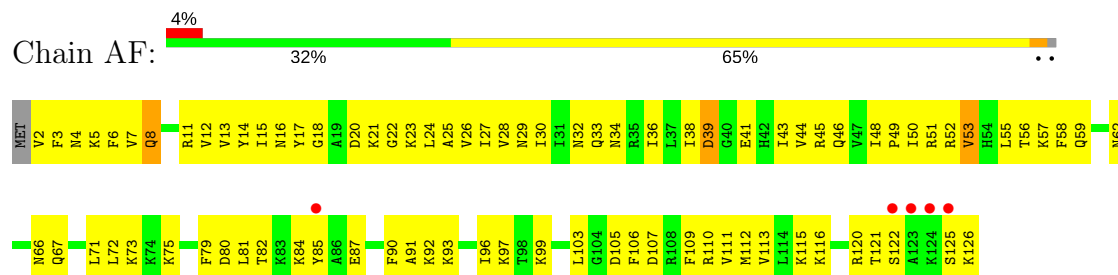
• Molecule 5: RPL6



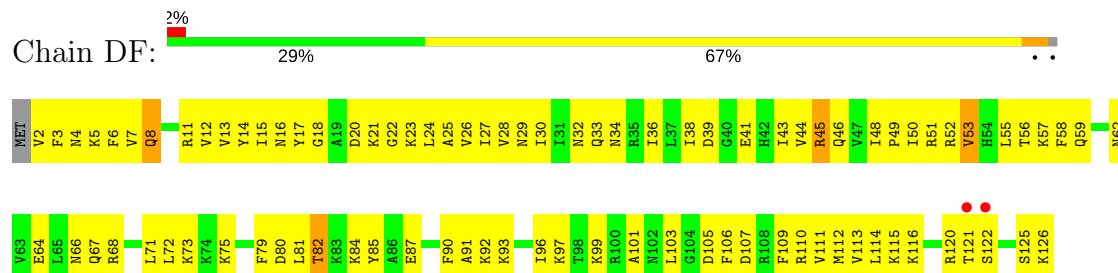
• Molecule 5: RPL6



• Molecule 6: RPL14

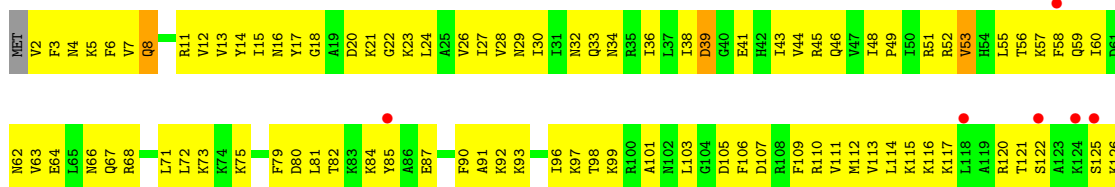


• Molecule 6: RPL14

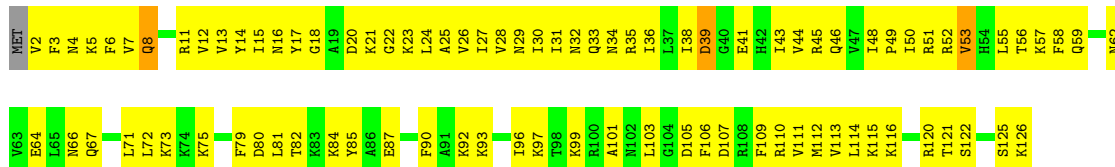
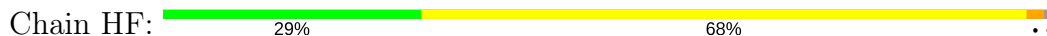


• Molecule 6: RPL14

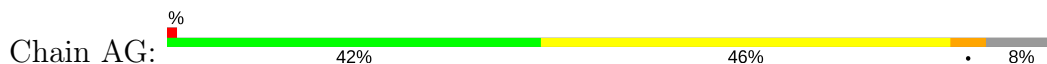




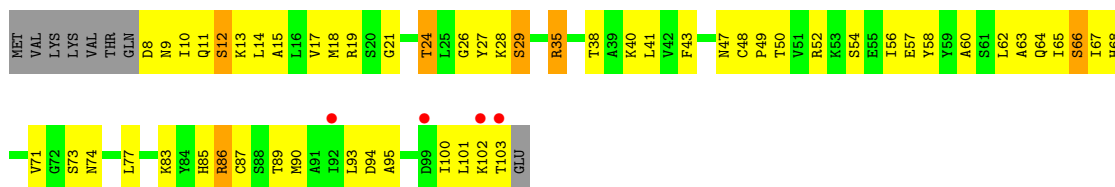
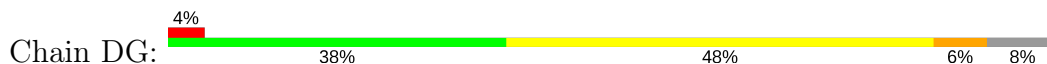
• Molecule 6: RPL14



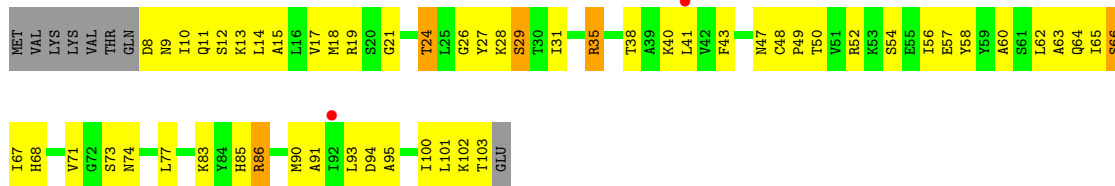
• Molecule 7: RPL30



• Molecule 7: RPL30

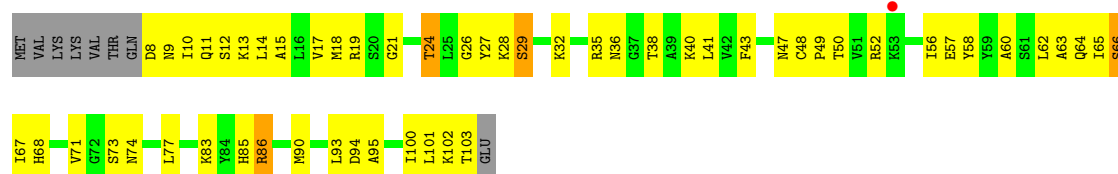


• Molecule 7: RPL30

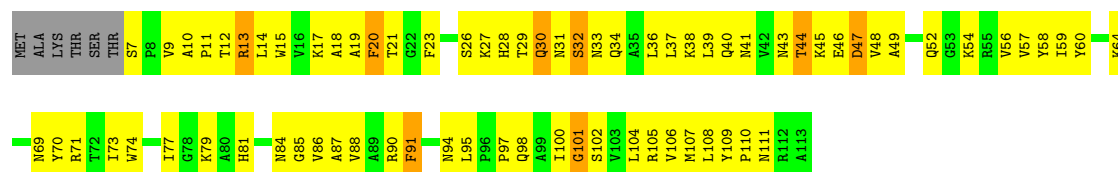


• Molecule 7: RPL30

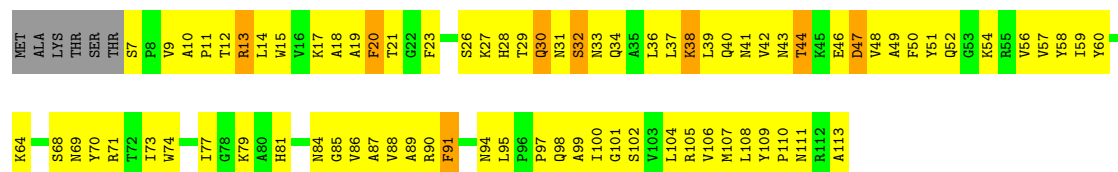
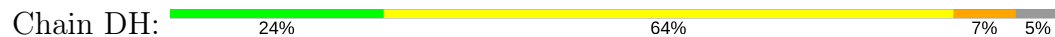




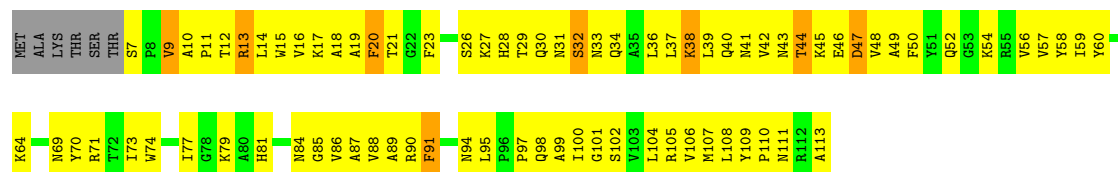
• Molecule 8: RPL35A



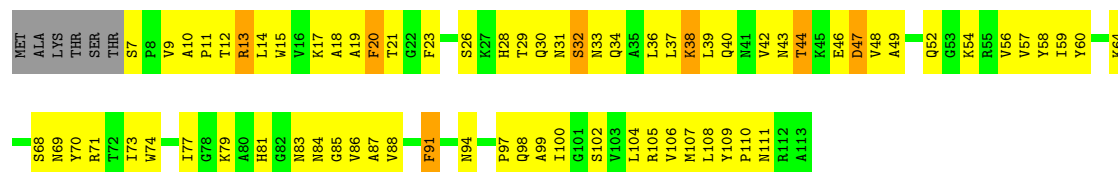
• Molecule 8: RPL35A



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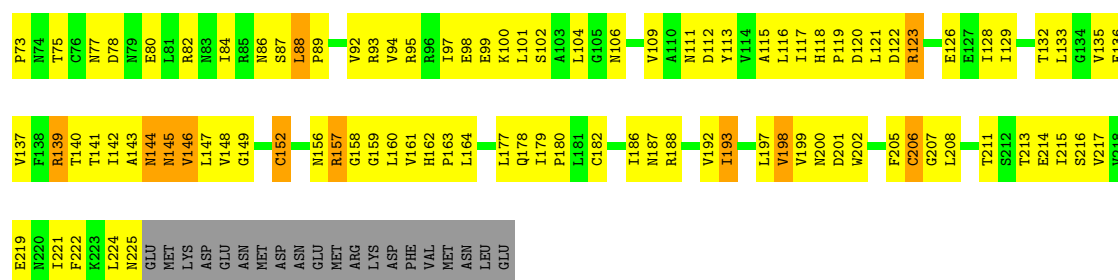


• Molecule 8: RPL35A



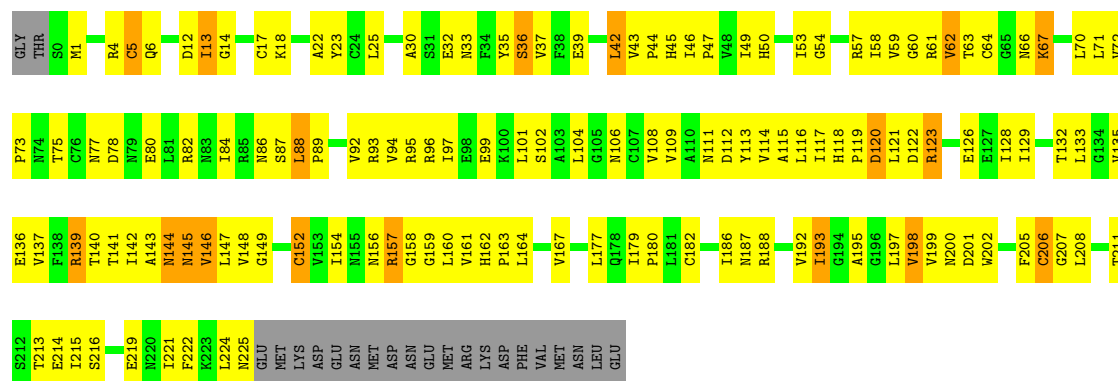
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN





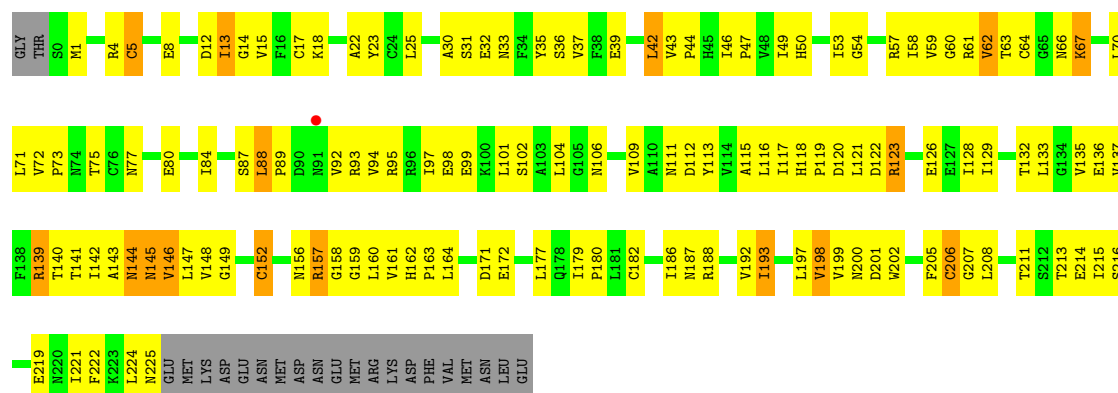
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain DJ: 35% 49% 7% 9%



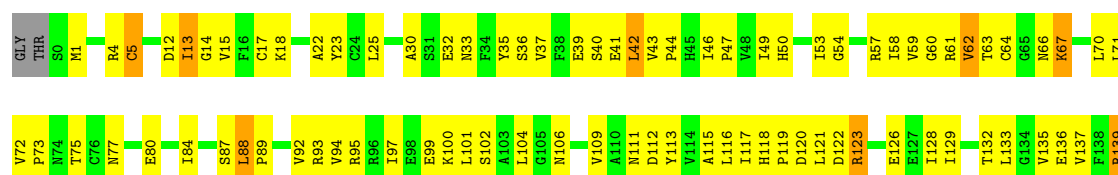
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

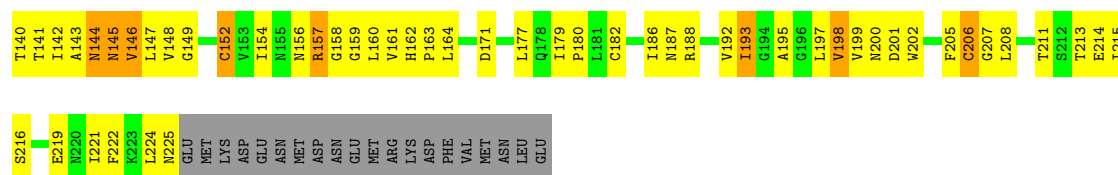
Chain FJ: 37% 48% 6% 9%



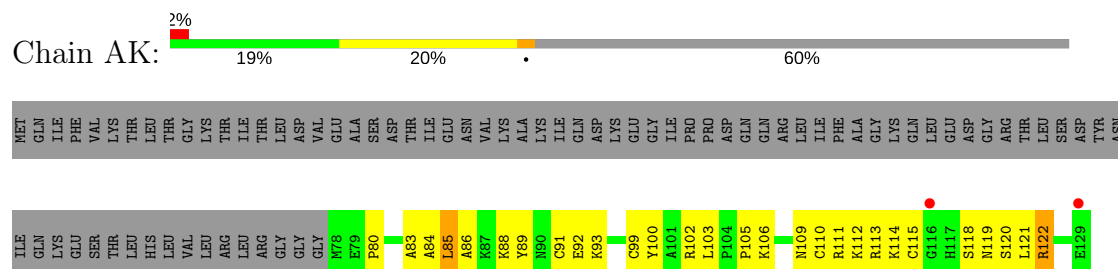
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain HJ: 36% 48% 6% 9%

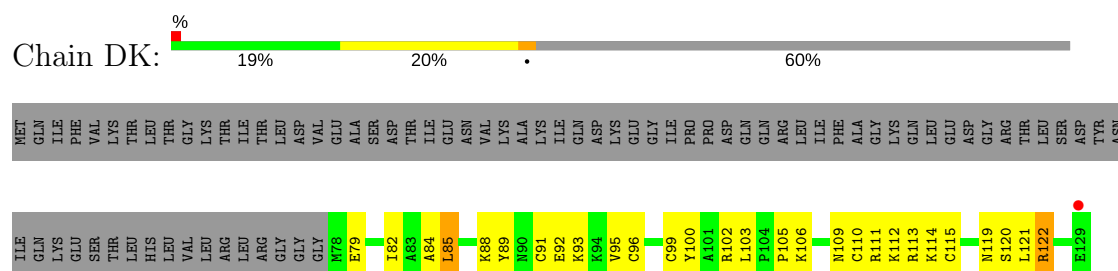




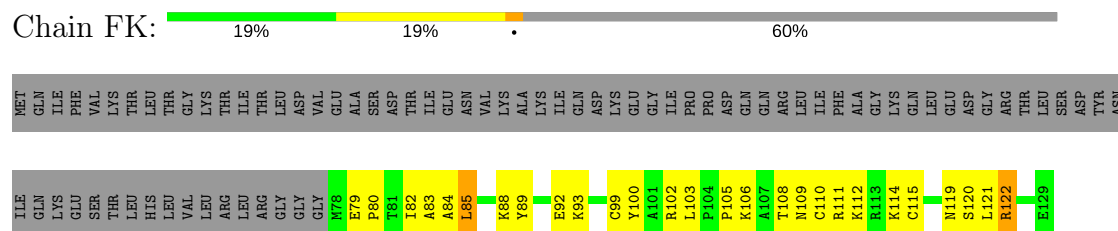
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



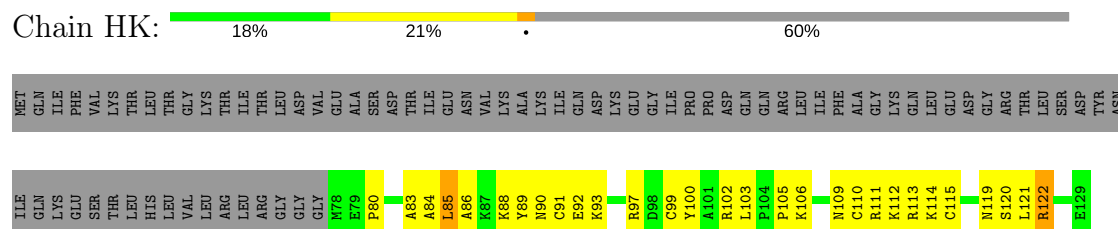
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



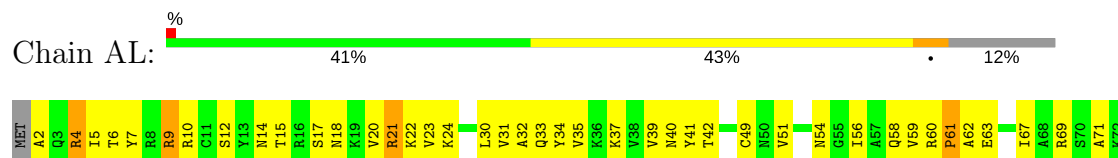
- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

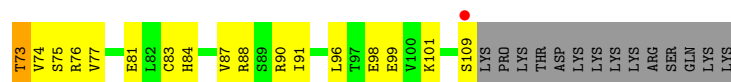


- Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



- Molecule 11: RPL34

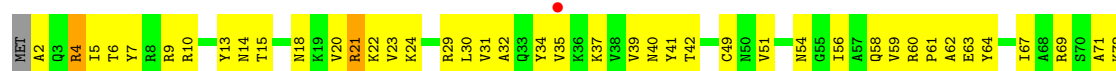




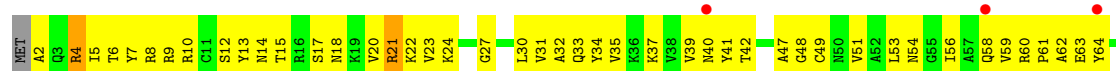
• Molecule 11: RPL34



• Molecule 11: RPL34



• Molecule 11: RPL34

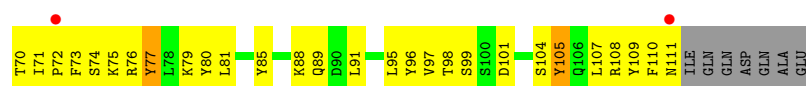


• Molecule 12: RIBOSOMAL PROTEIN L22



• Molecule 12: RIBOSOMAL PROTEIN L22





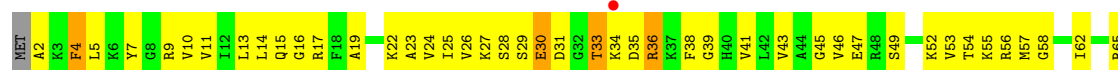
• Molecule 12: RIBOSOMAL PROTEIN L22



• Molecule 12: RIBOSOMAL PROTEIN L22



• Molecule 13: RPL27



• Molecule 13: RPL27



• Molecule 13: RPL27

- Molecule 13: RPL27

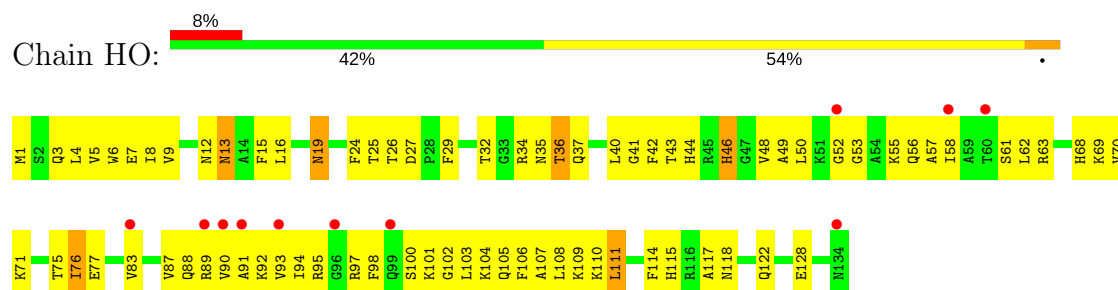
- Molecule 14: RPL28

- Molecule 14: RPL28

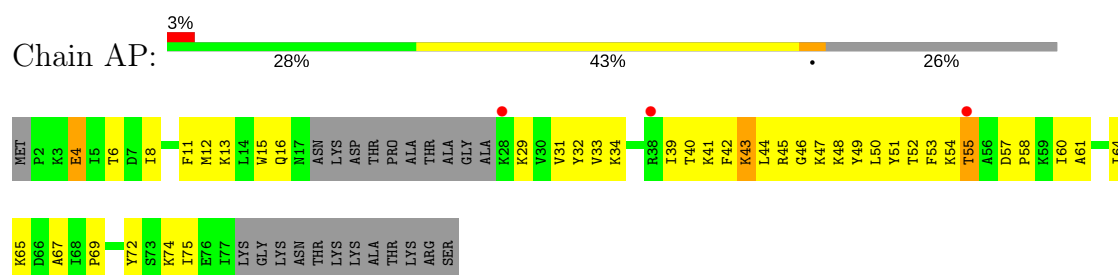
- Molecule 14: RPL28



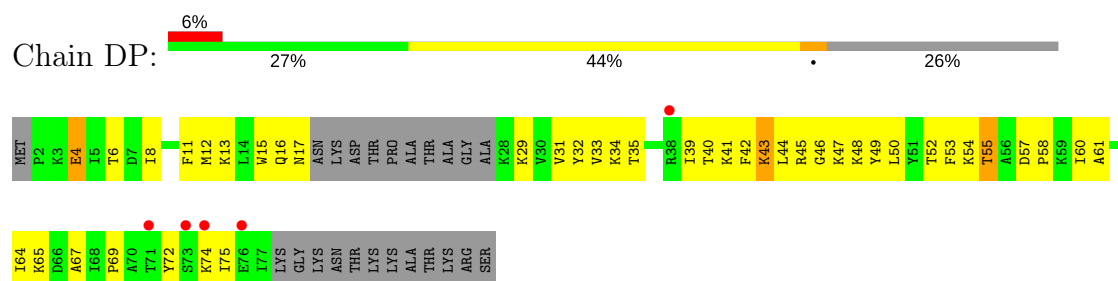
- Molecule 14: RPL28



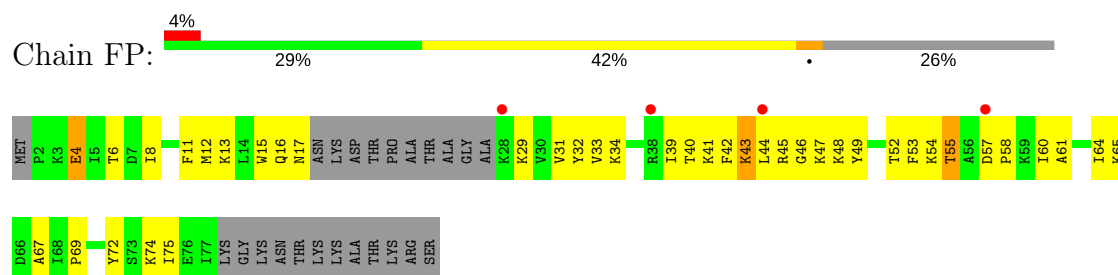
- Molecule 15: RPL38



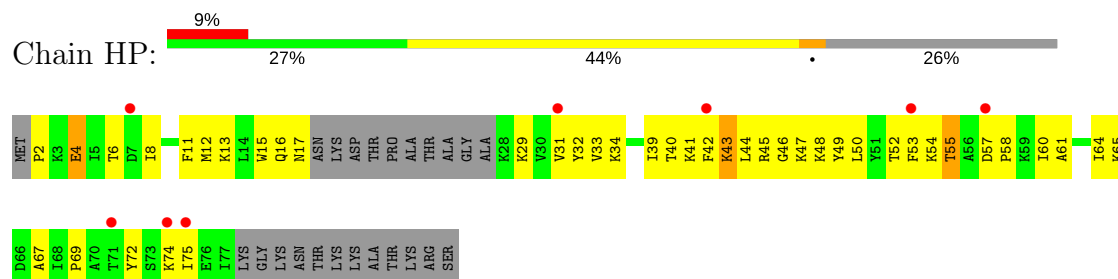
- Molecule 15: RPL38



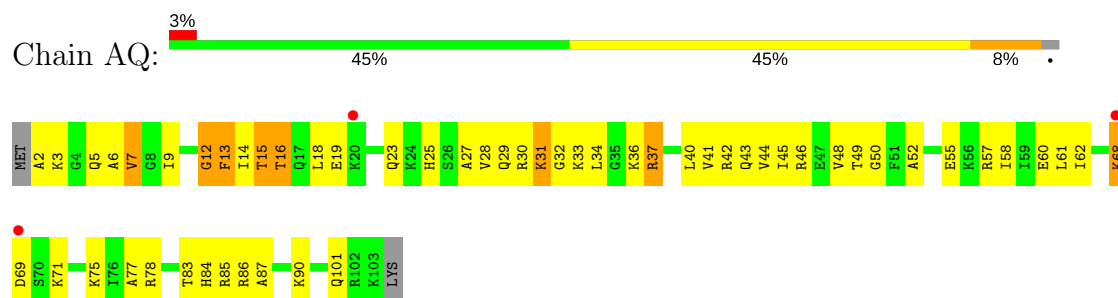
- Molecule 15: RPL38



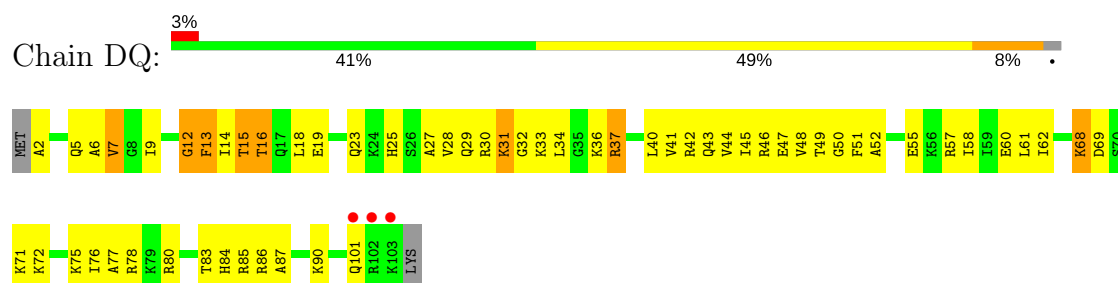
- Molecule 15: RPL38



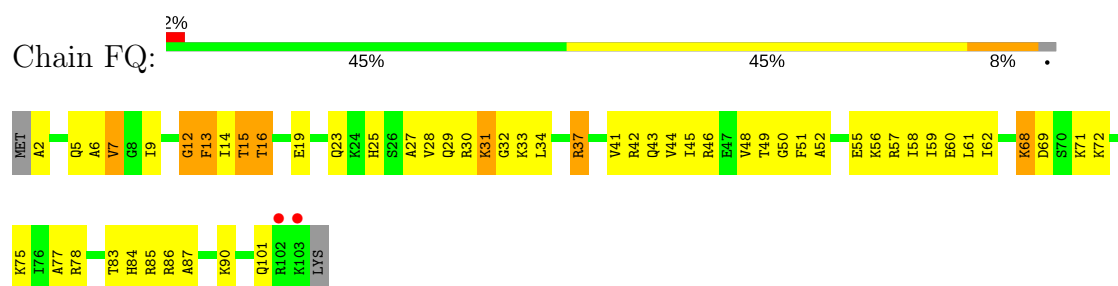
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



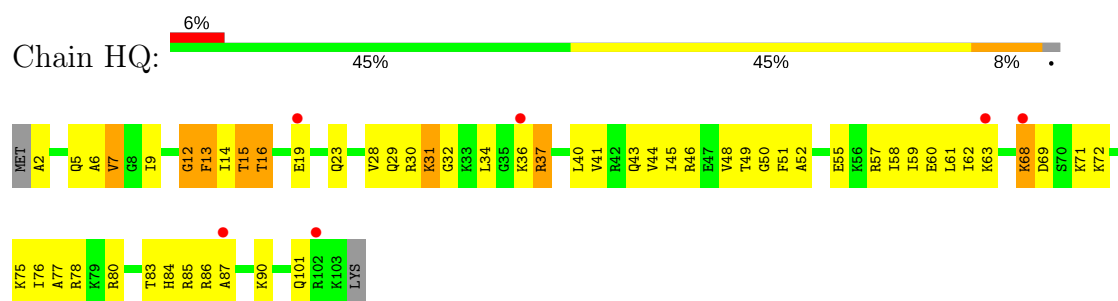
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



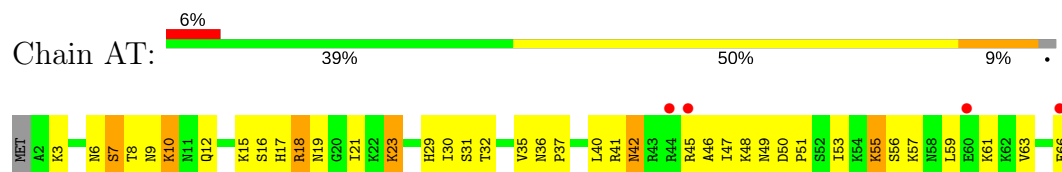
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



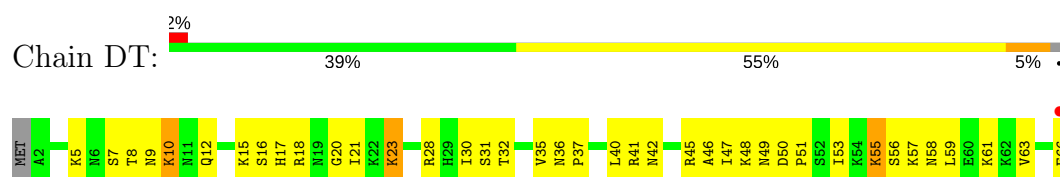
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



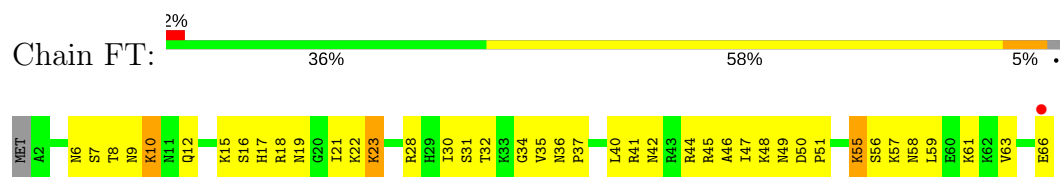
- Molecule 17: RPL29



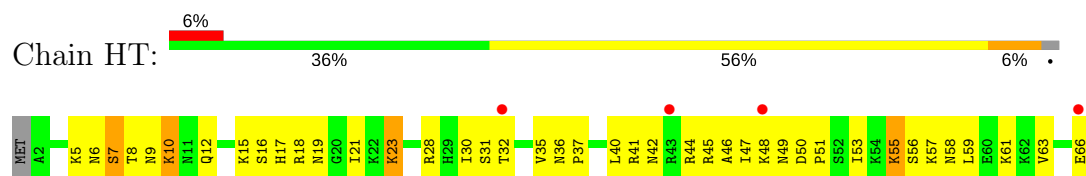
- Molecule 17: RPL29



- Molecule 17: RPL29



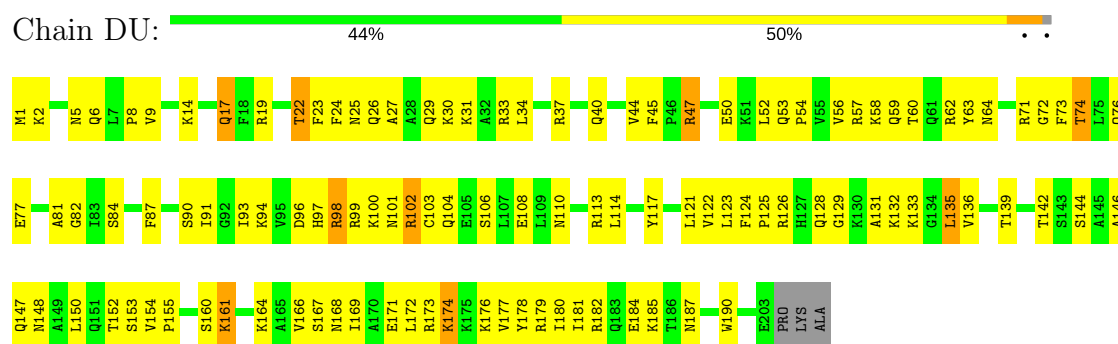
- Molecule 17: RPL29



- Molecule 18: RPL13

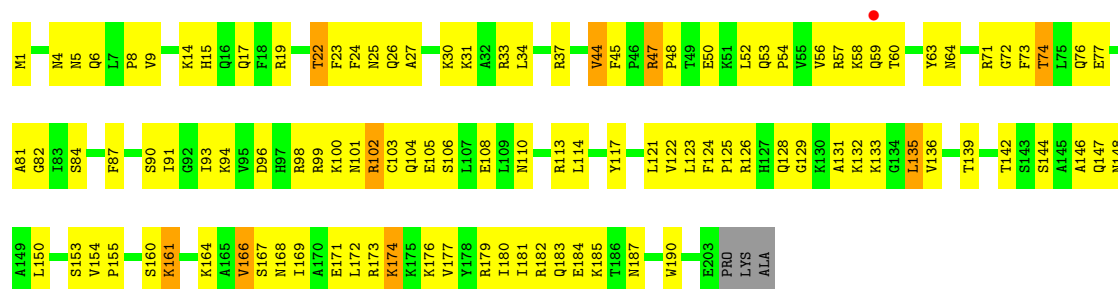


- Molecule 18: RPL13

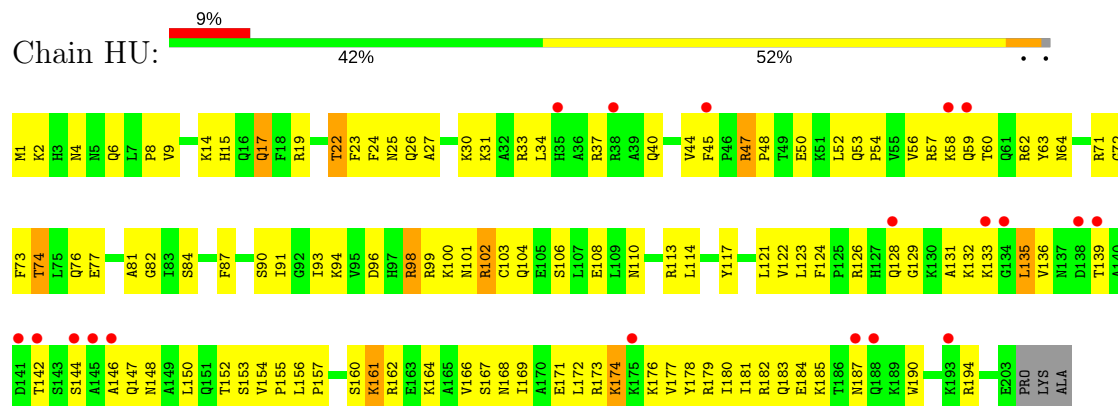


- Molecule 18: RPL13

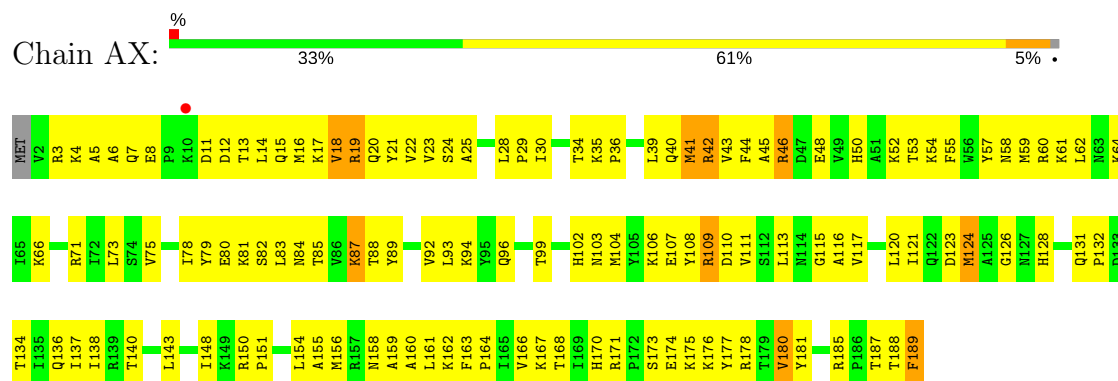




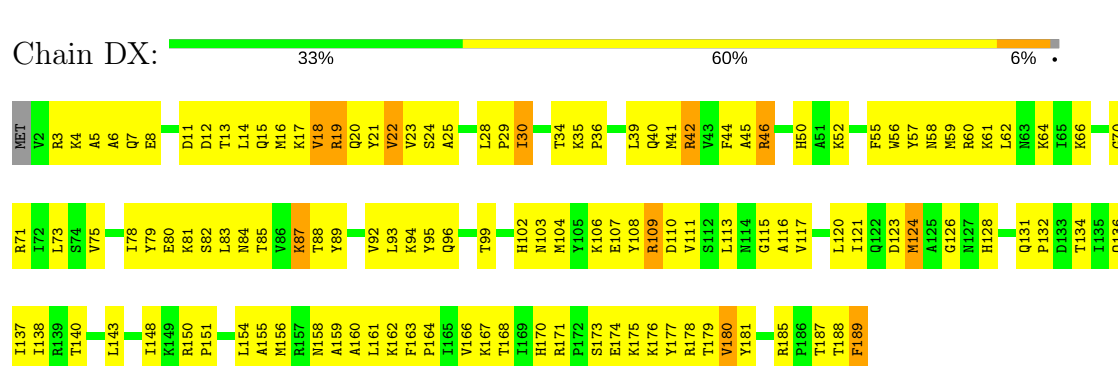
• Molecule 18: RPL13



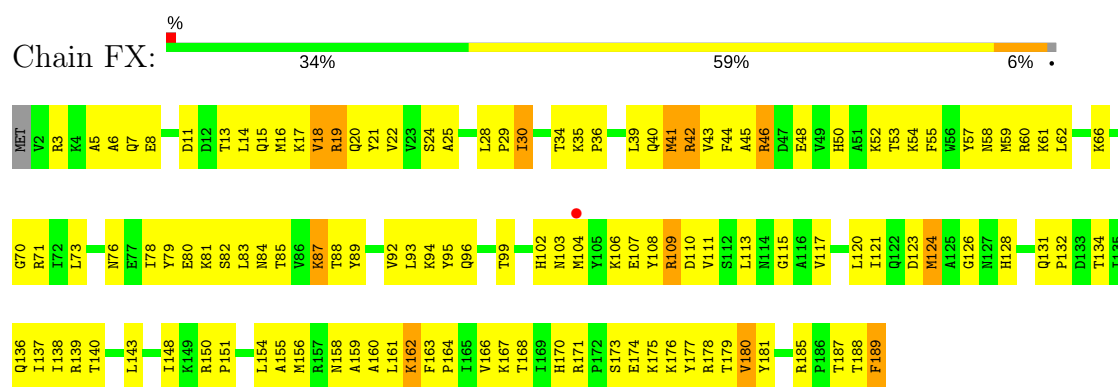
• Molecule 19: RPL18A



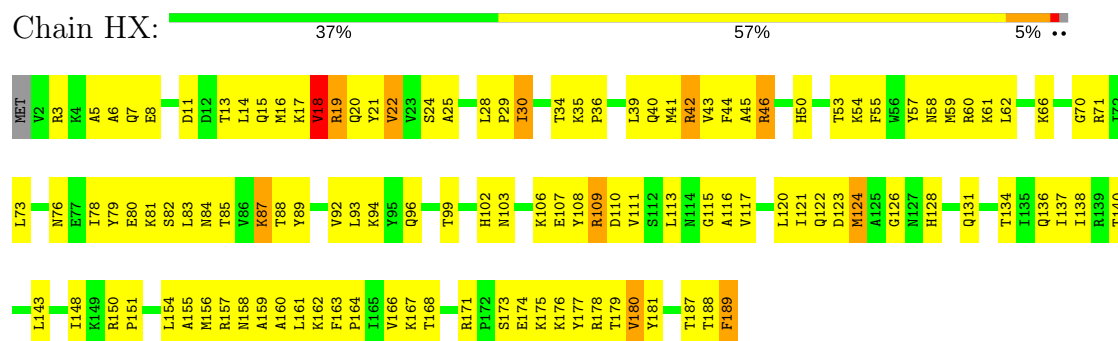
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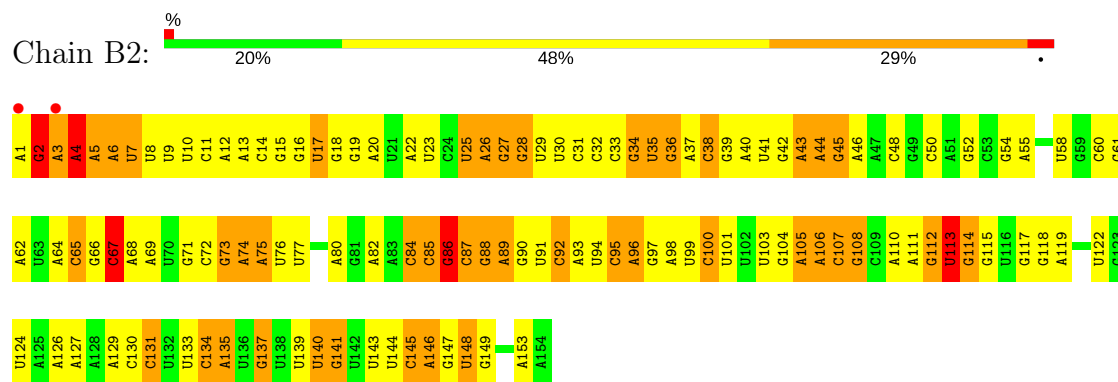
• Molecule 19: RPL18A



• Molecule 19: RPL18A



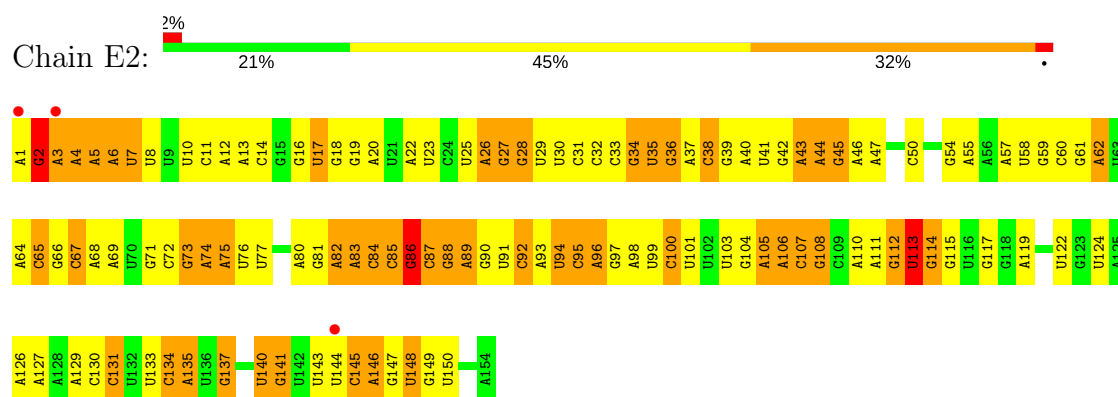
• Molecule 20: 5.8S RRNA



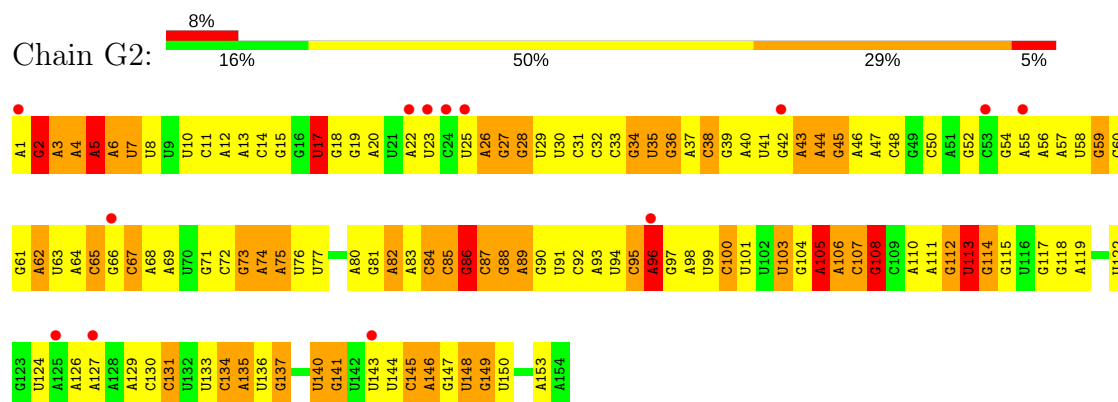
• Molecule 20: 5.8S RRNA



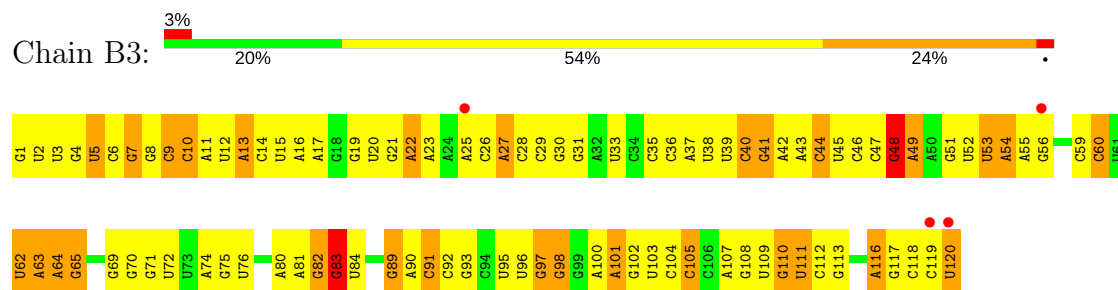
• Molecule 20: 5.8S RRNA



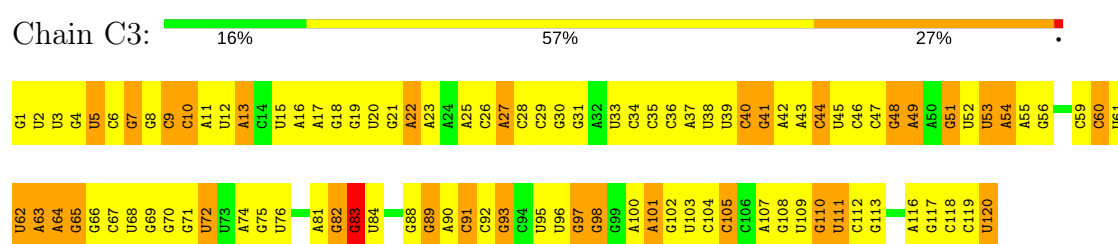
• Molecule 20: 5.8S RRNA



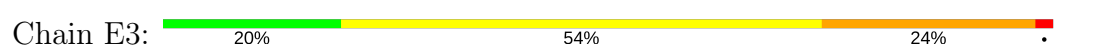
• Molecule 21: 5S RRNA

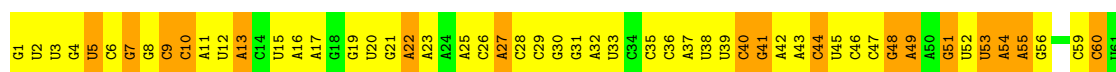


• Molecule 21: 5S RRNA

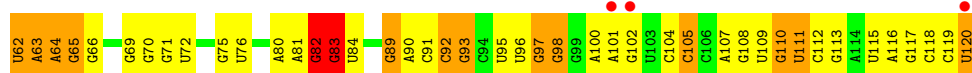
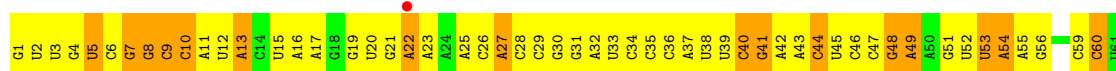


• Molecule 21: 5S RRNA

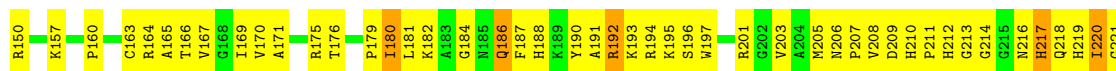
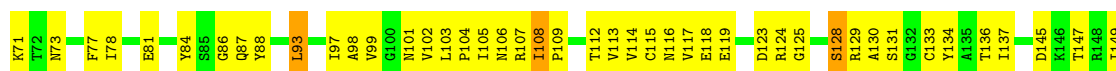




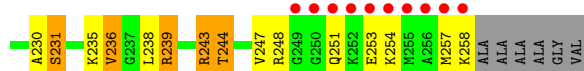
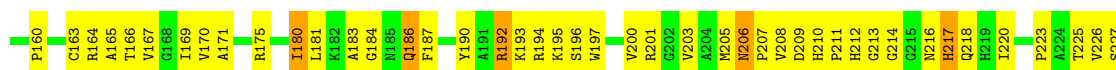
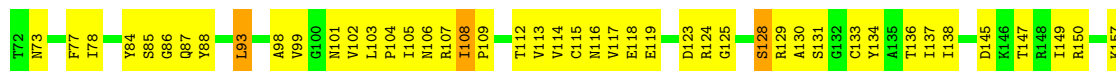
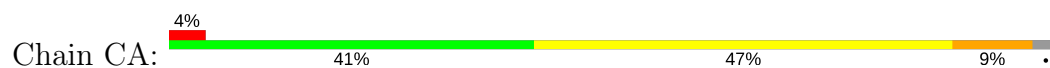
• Molecule 21: 5S RRNA



• Molecule 22: RPL8

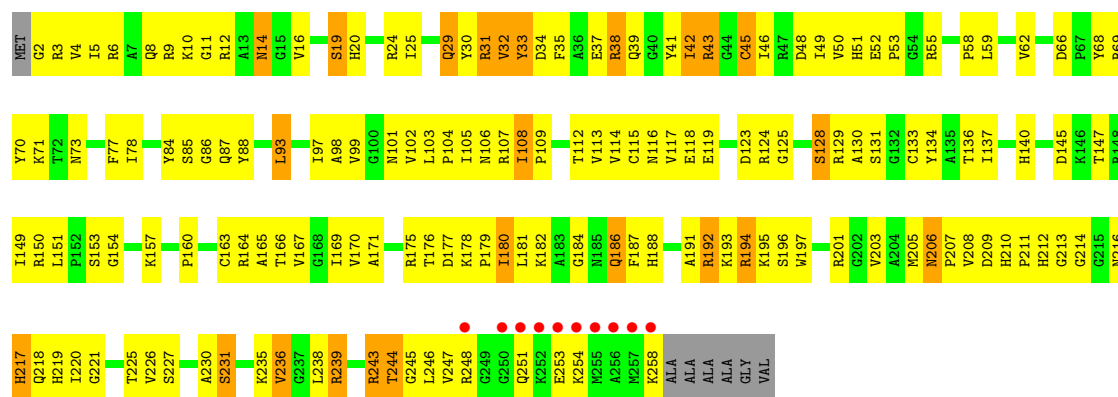


• Molecule 22: RPL8

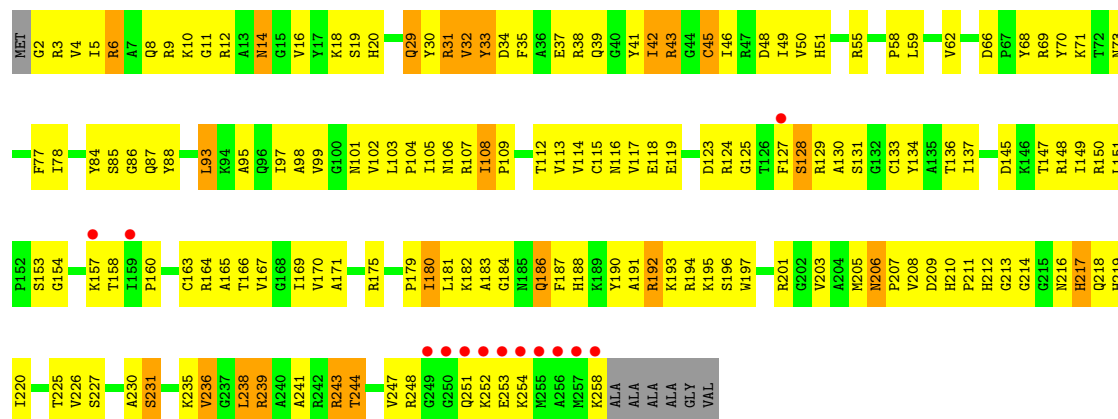
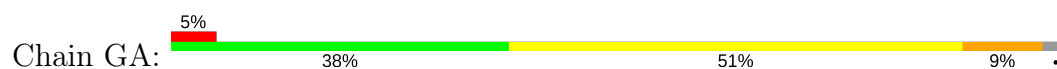


• Molecule 22: RPL8

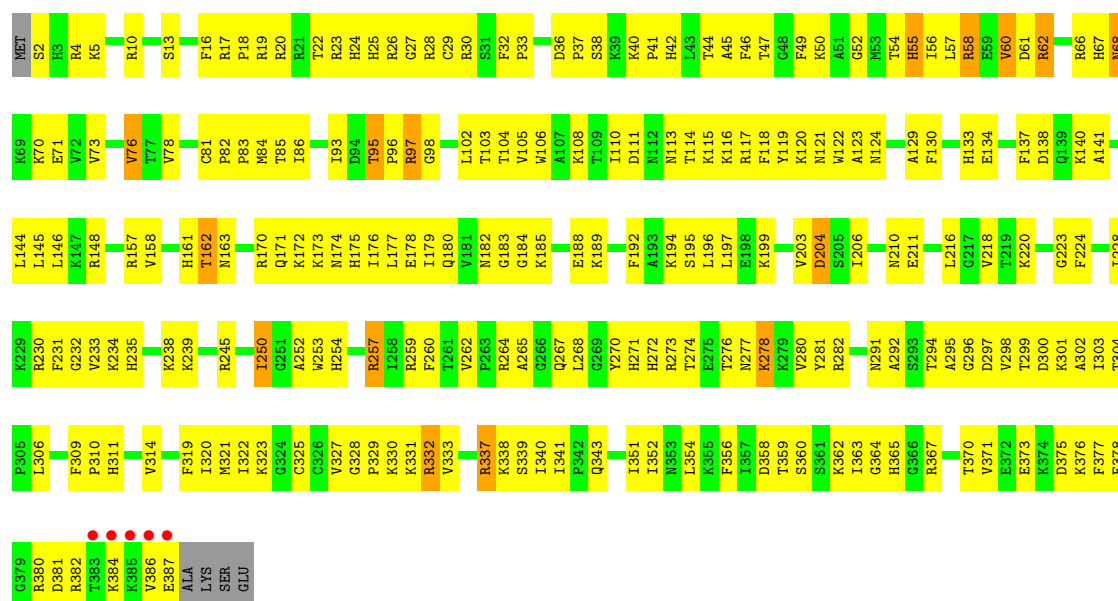
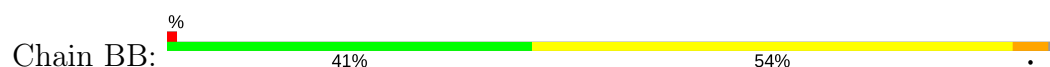




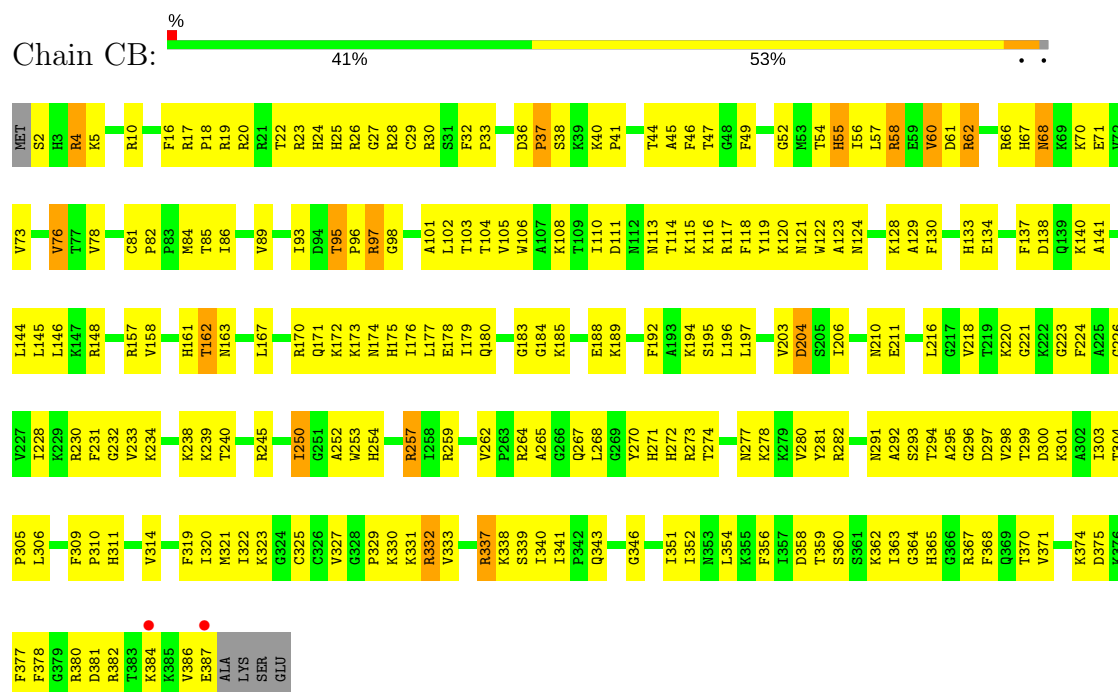
• Molecule 22: RPL8



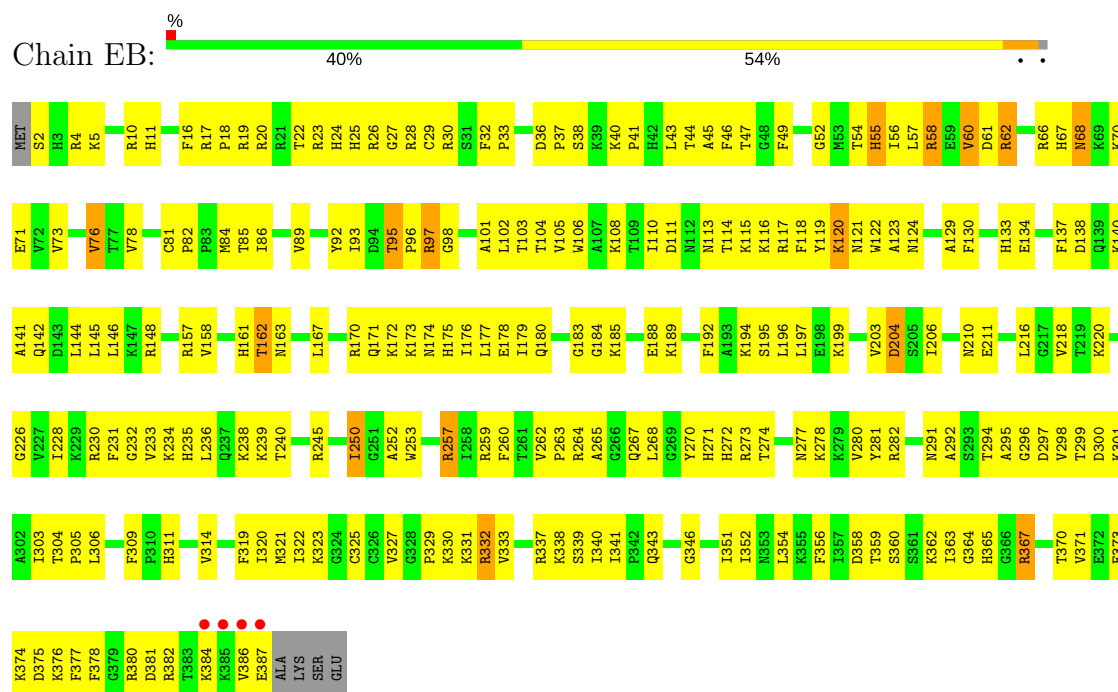
• Molecule 23: RIBOSOMAL PROTEIN L3



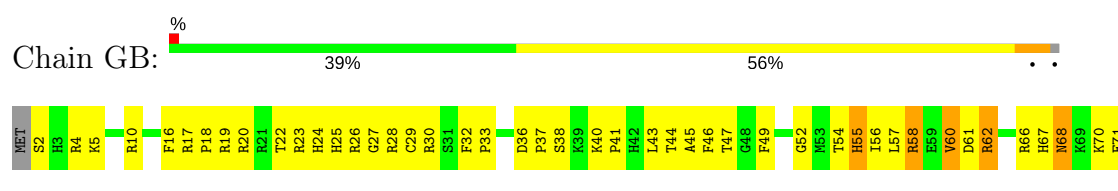
● Molecule 23: RIBOSOMAL PROTEIN L3

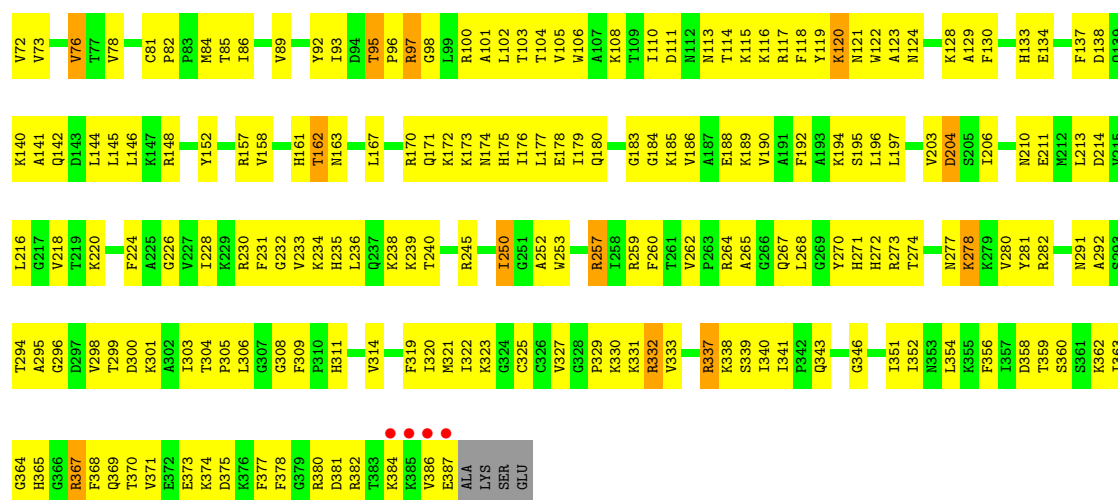


● Molecule 23: RIBOSOMAL PROTEIN L3



● Molecule 23: RIBOSOMAL PROTEIN L3

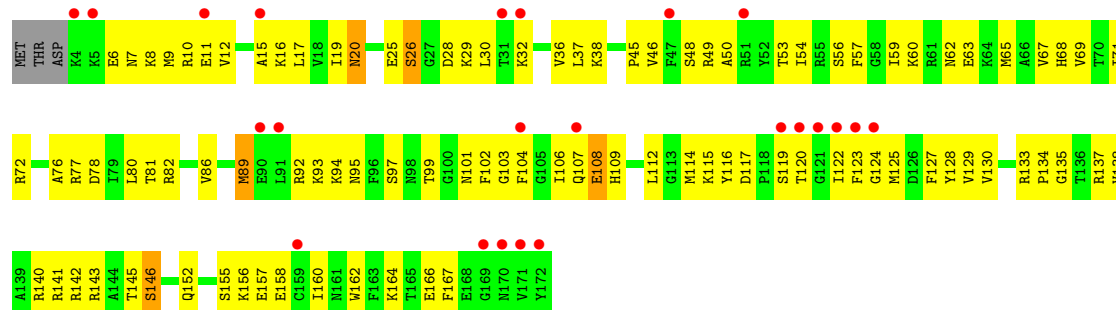
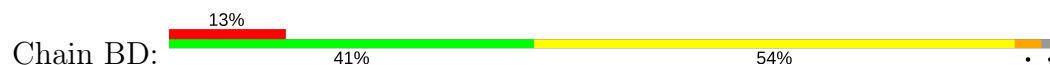




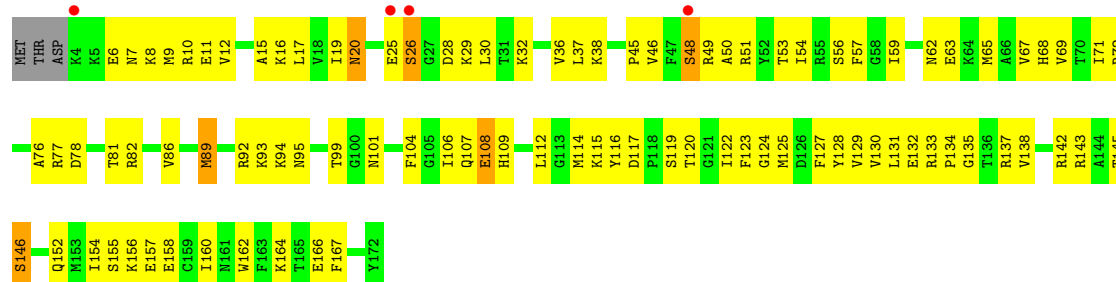
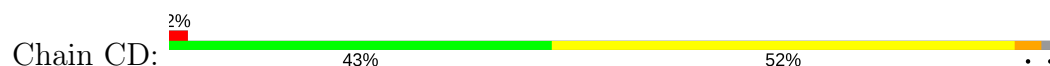




• Molecule 25: 60S RIBOSOMAL PROTEIN L11



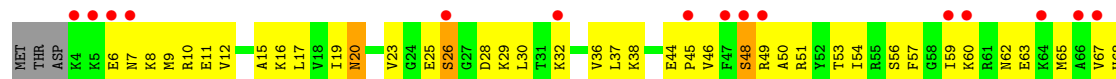
• Molecule 25: 60S RIBOSOMAL PROTEIN L11

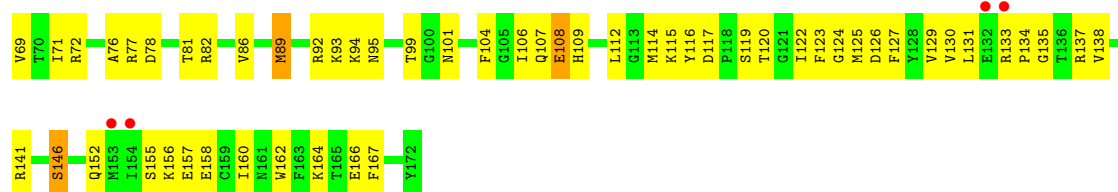


• Molecule 25: 60S RIBOSOMAL PROTEIN L11



• Molecule 25: 60S RIBOSOMAL PROTEIN L11

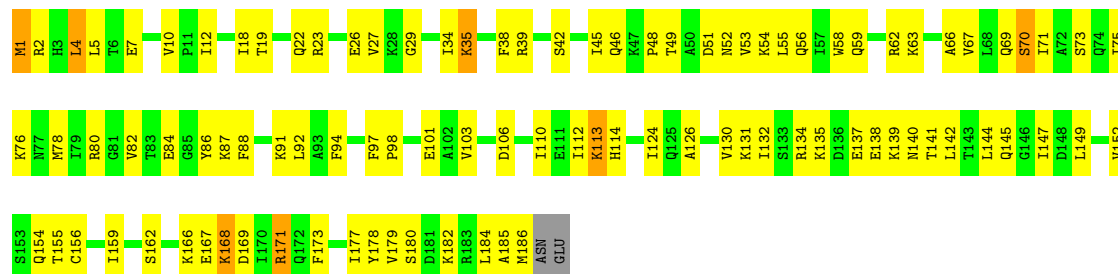




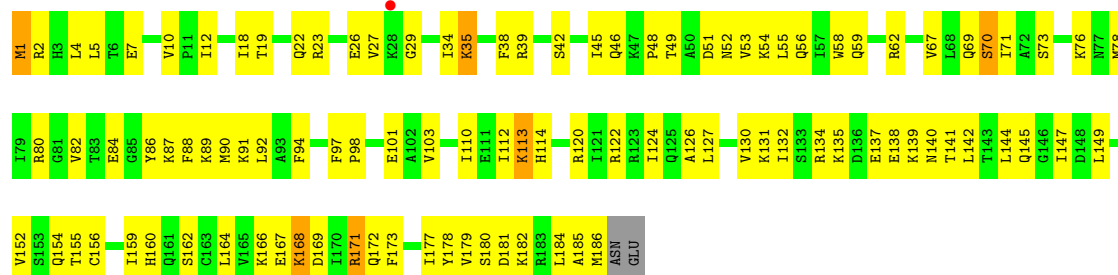
• Molecule 26: 60S RIBOSOMAL PROTEIN L9



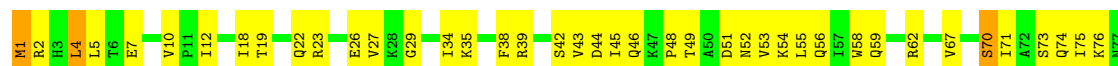
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

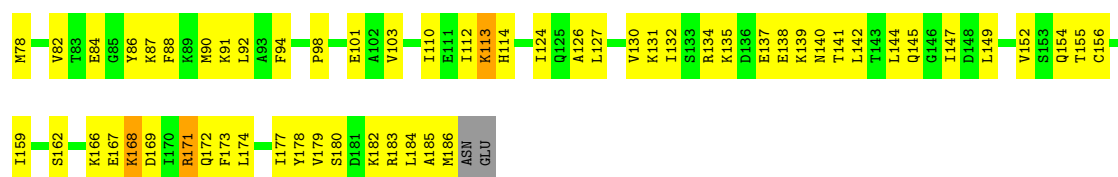


• Molecule 26: 60S RIBOSOMAL PROTEIN L9

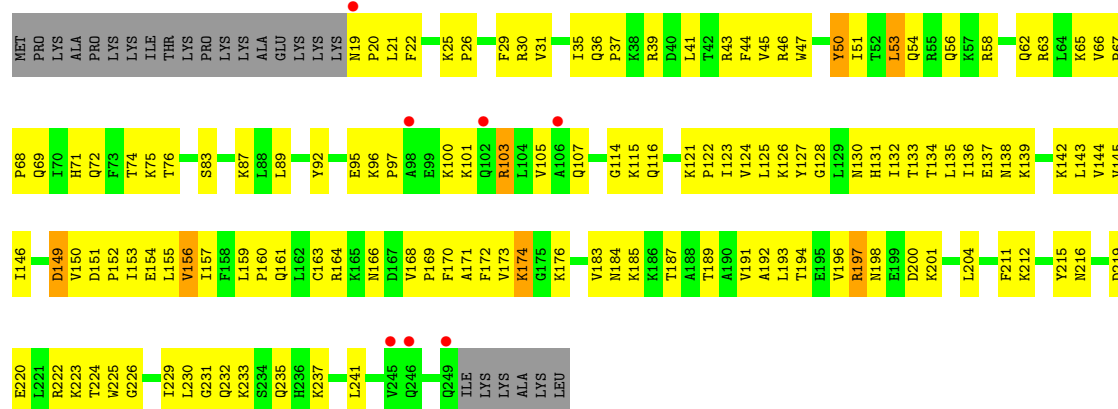
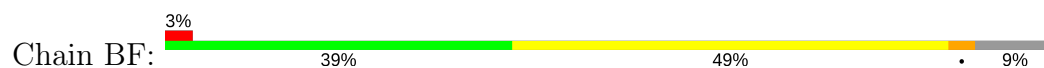


• Molecule 26: 60S RIBOSOMAL PROTEIN L9

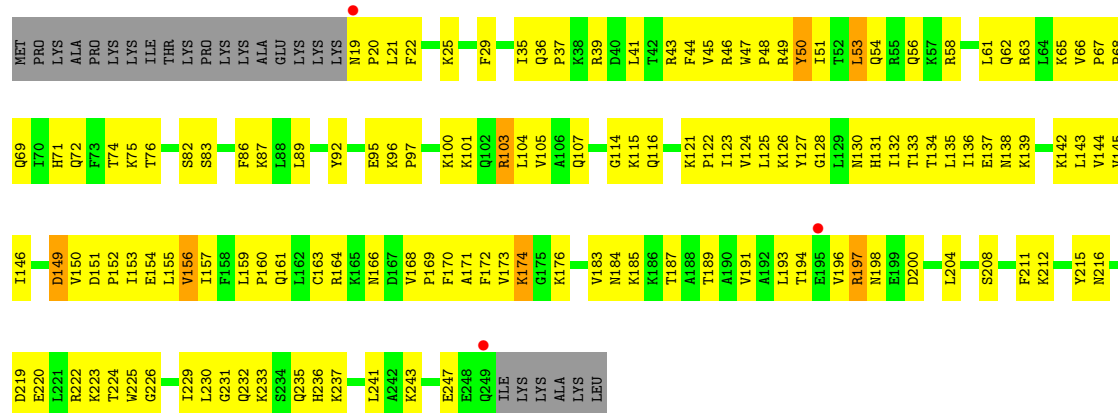




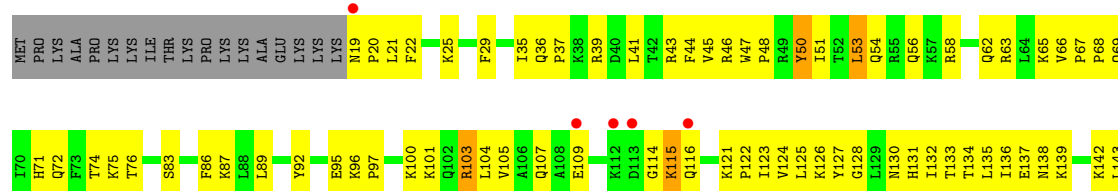
• Molecule 27: RPL7A

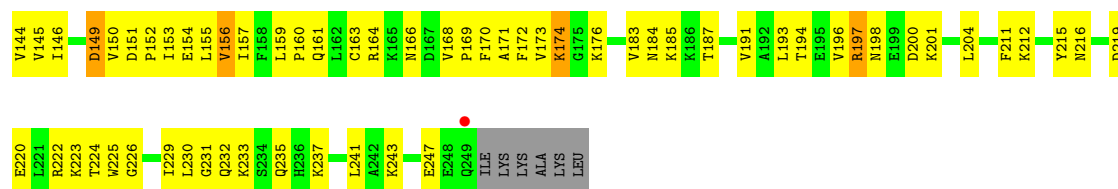


• Molecule 27: RPL7A

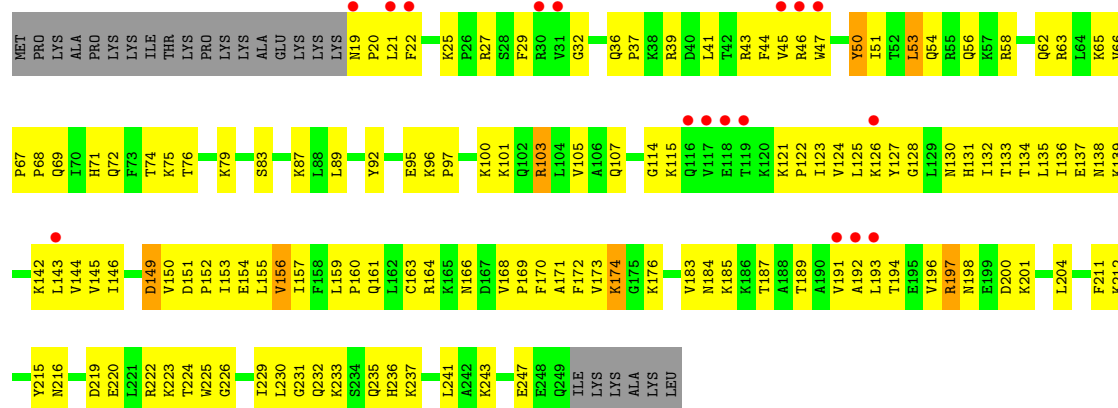


• Molecule 27: RPL7A

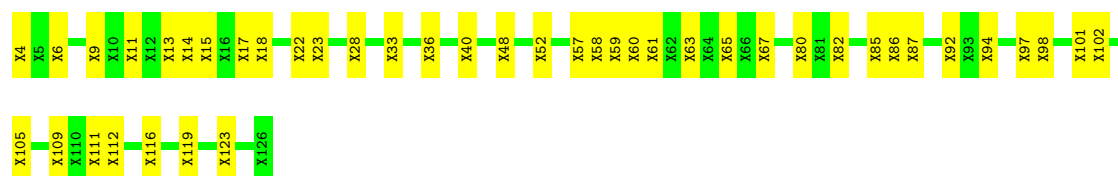




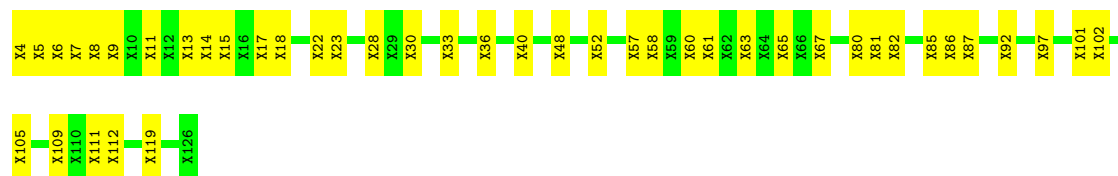
• Molecule 27: RPL7A



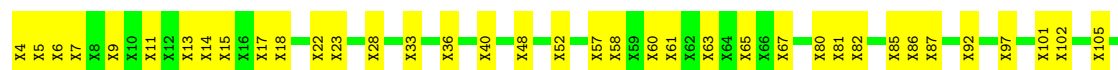
• Molecule 28: RPLP0



• Molecule 28: RPLP0



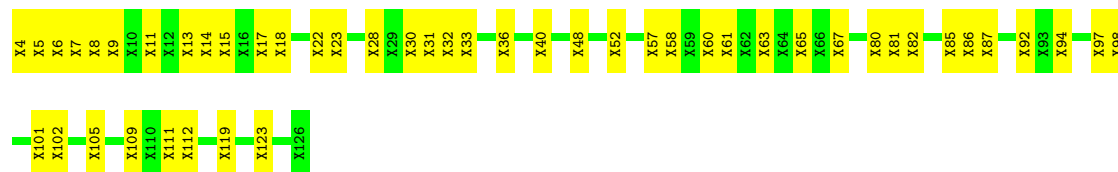
• Molecule 28: RPLP0





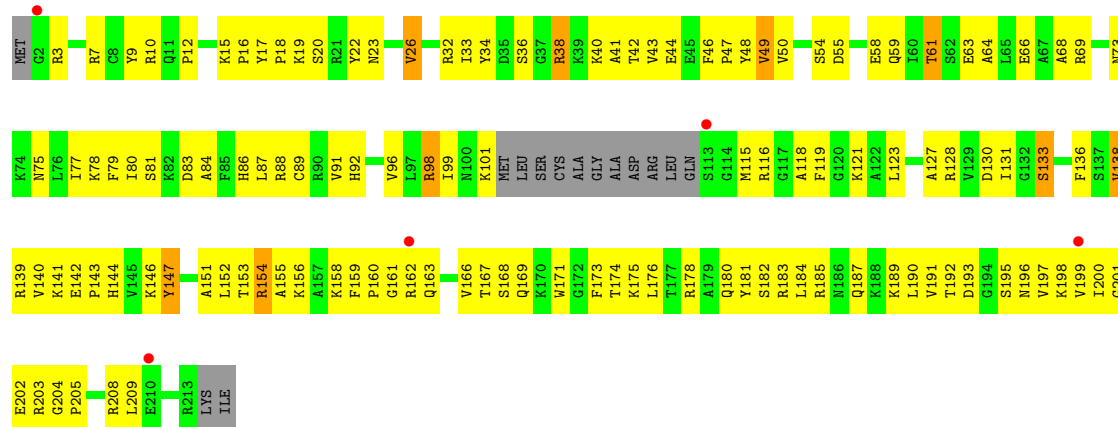
• Molecule 28: RPLP0

Chain GG: 61% 39%



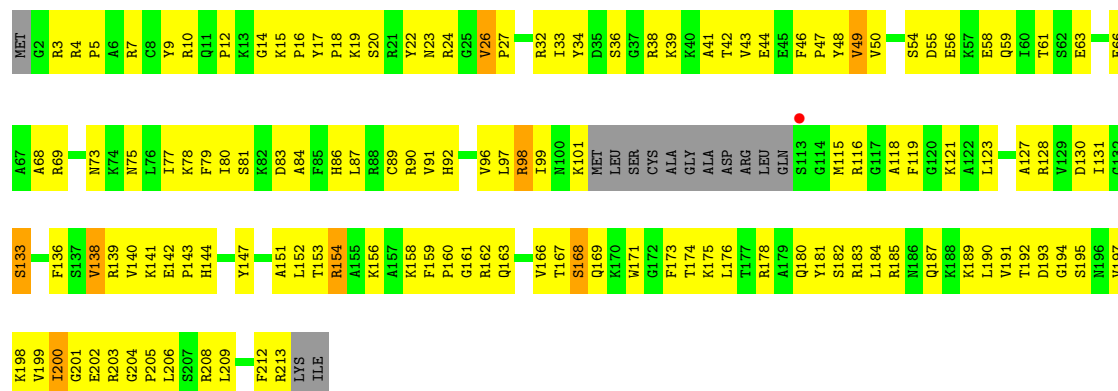
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain BH: 2% 35% 54% 7%



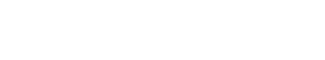
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

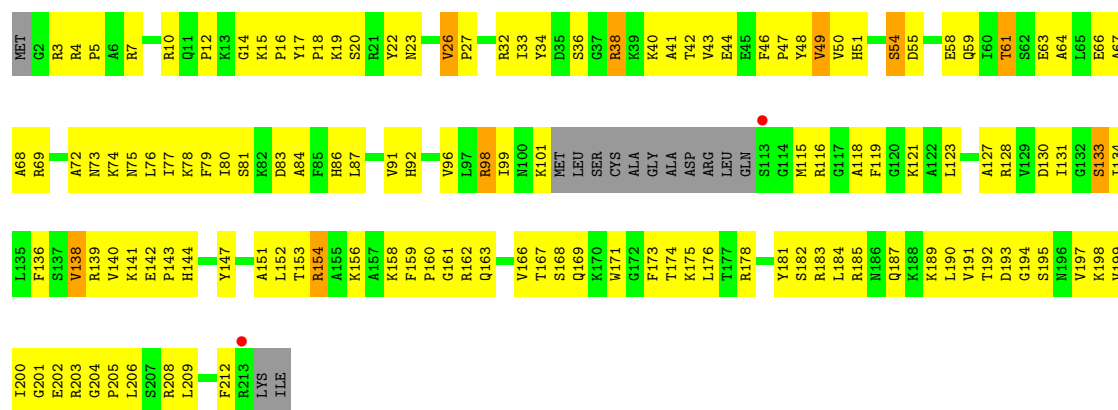
Chain CH: 32% 58% 7%



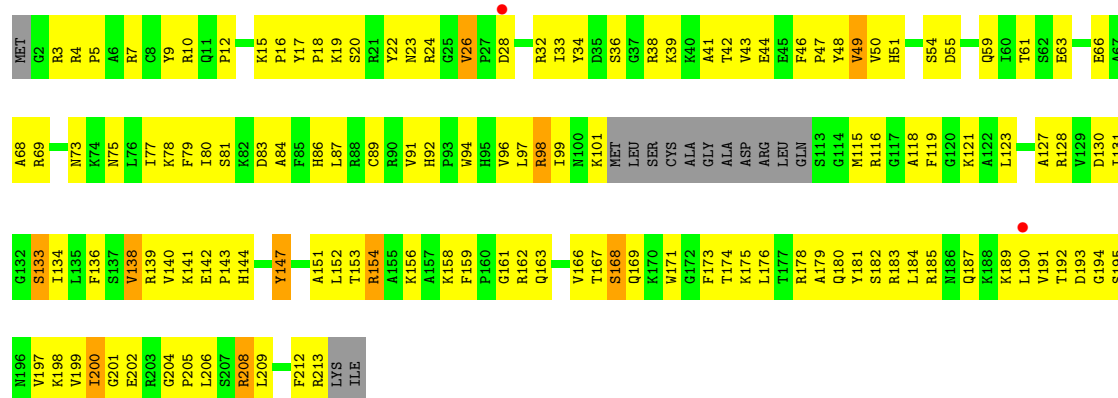
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain EH: % 32% 57% 7%

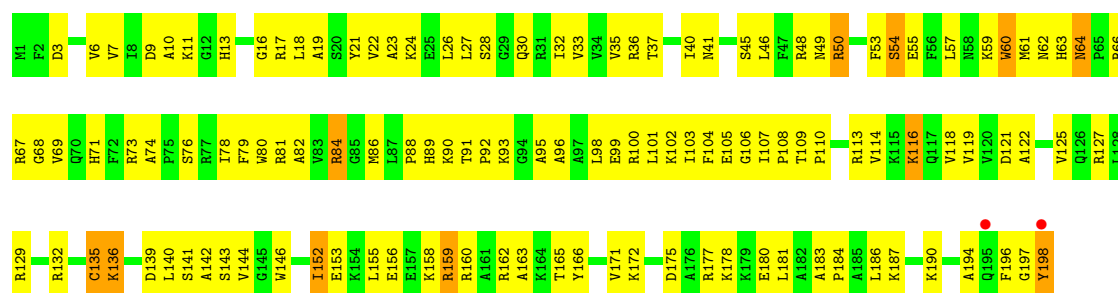




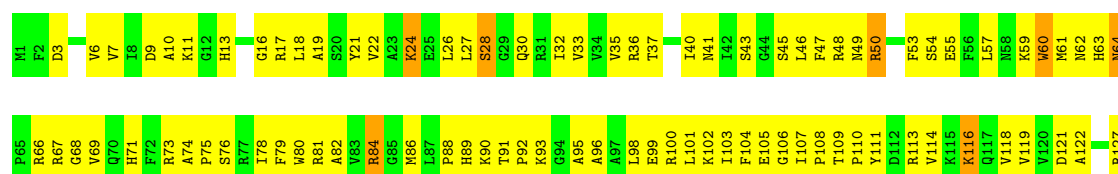
• Molecule 29: 60S RIBOSOMAL PROTEIN L10



• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



• Molecule 30: 60S RIBOSOMAL PROTEIN L13A

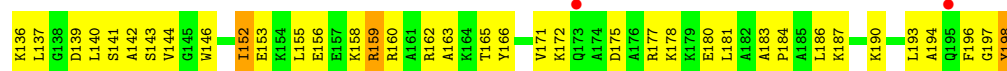
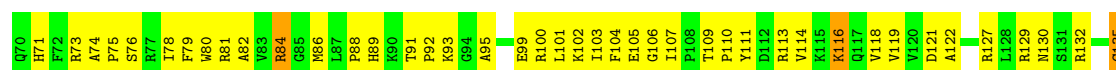




• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



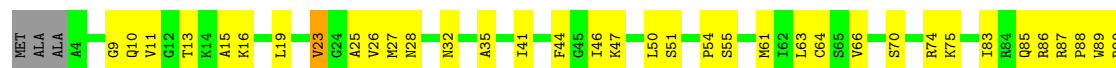
• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



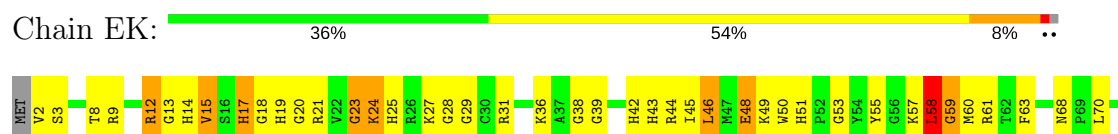
• Molecule 31: RPL23

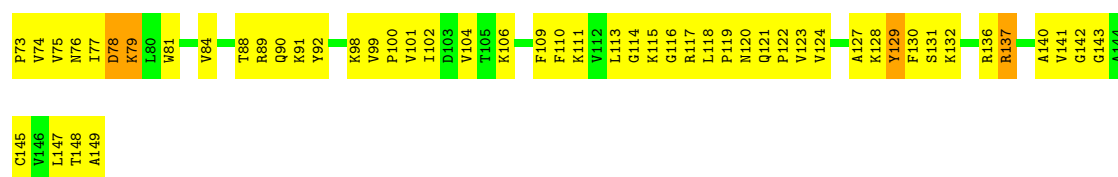


• Molecule 31: RPL23

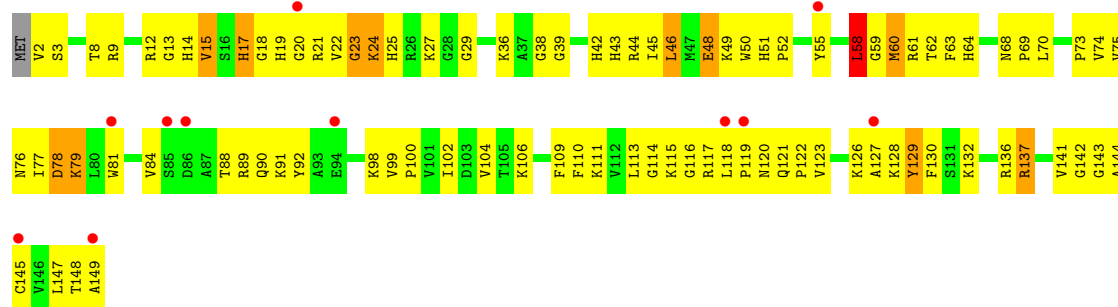


• Molecule 31: RPL23

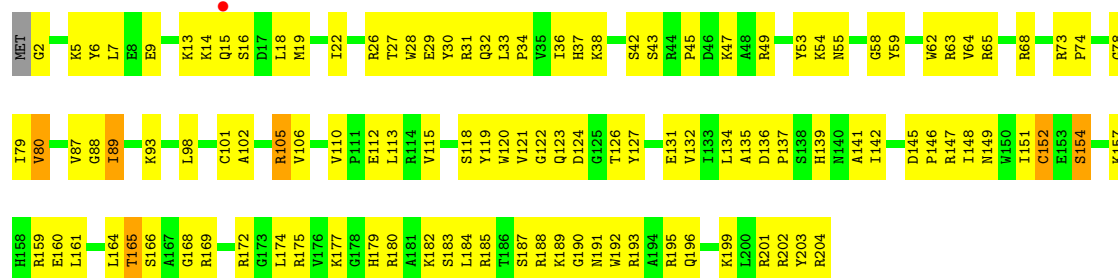




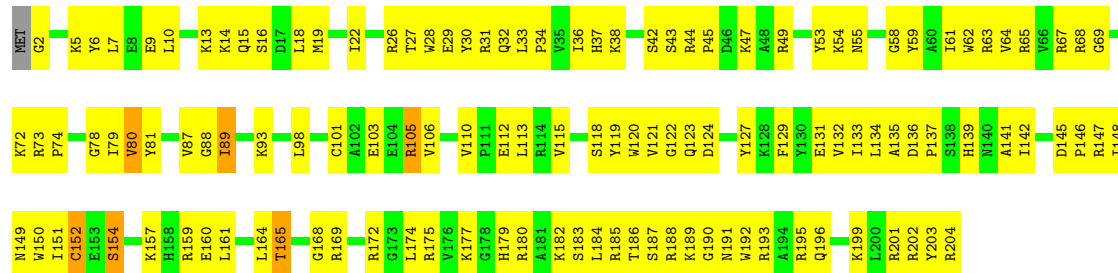
• Molecule 32: 60S RIBOSOMAL PROTEIN L27A



• Molecule 33: RIBOSOMAL PROTEIN L15

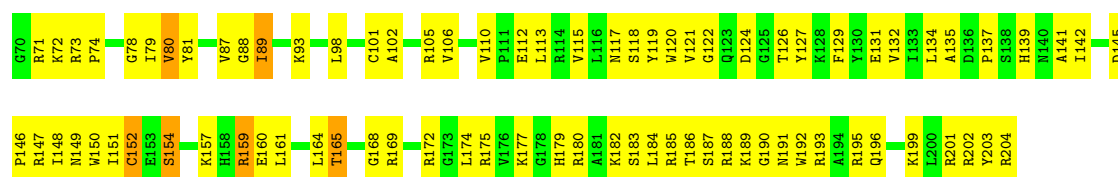


• Molecule 33: RIBOSOMAL PROTEIN L15

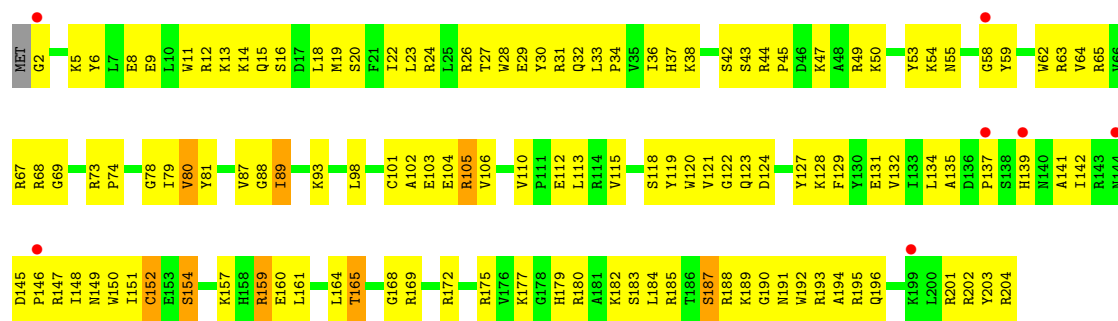
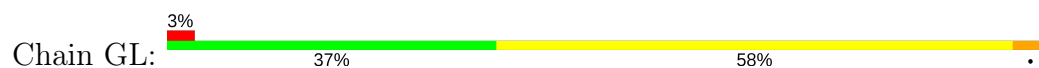


• Molecule 33: RIBOSOMAL PROTEIN L15

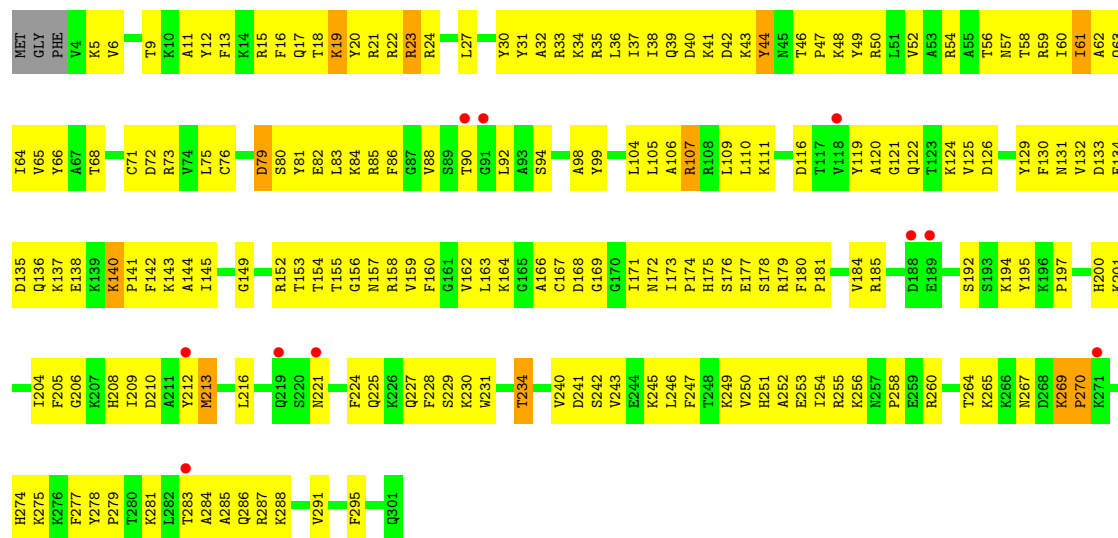




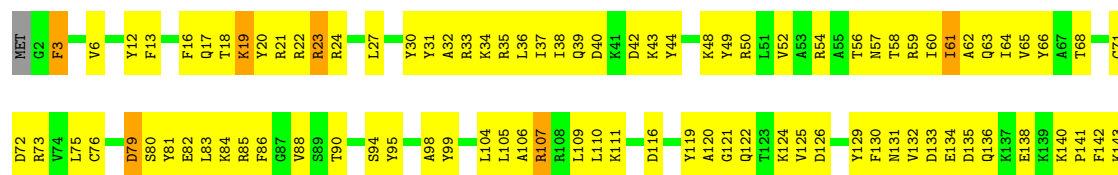
• Molecule 33: RIBOSOMAL PROTEIN L15



• Molecule 34: 60S RIBOSOMAL PROTEIN L5

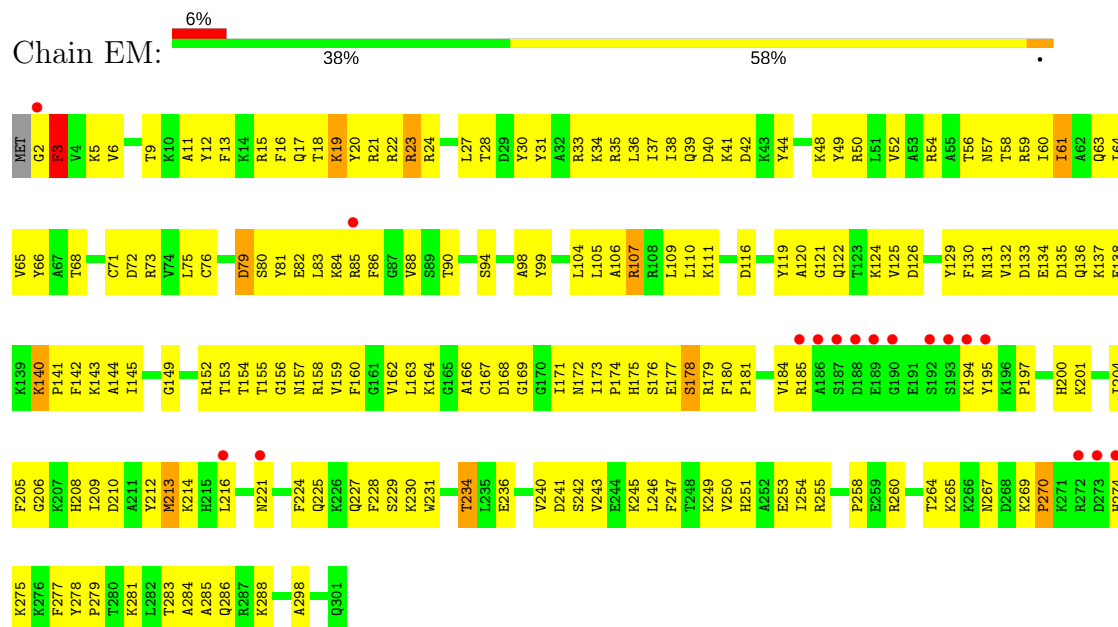


• Molecule 34: 60S RIBOSOMAL PROTEIN L5

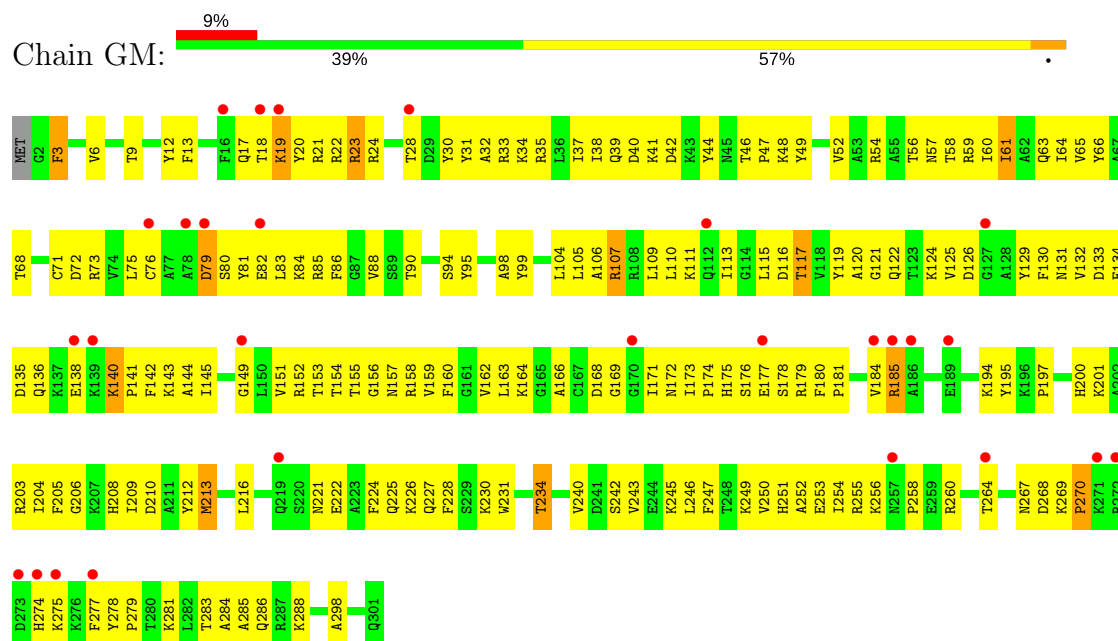




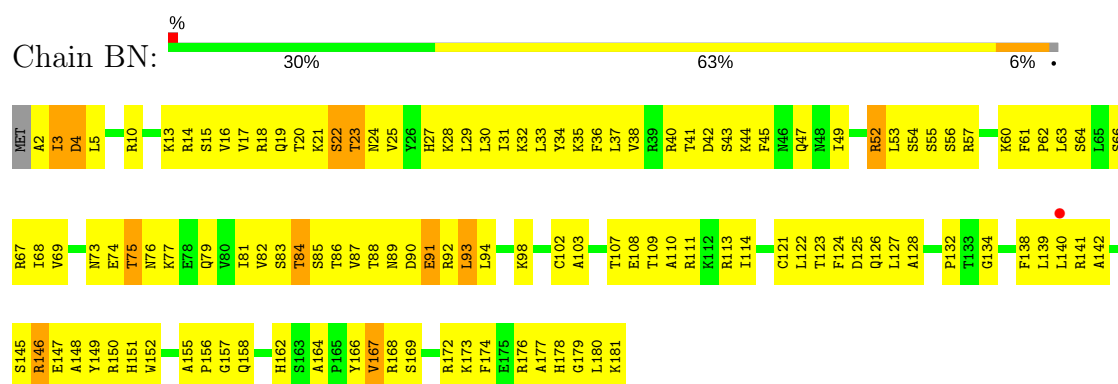
• Molecule 34: 60S RIBOSOMAL PROTEIN L5



• Molecule 34: 60S RIBOSOMAL PROTEIN L5



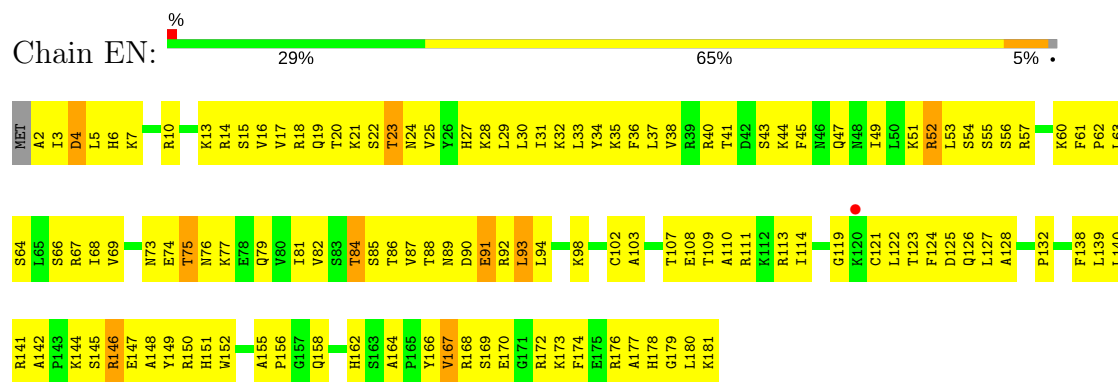
• Molecule 35: RPL18



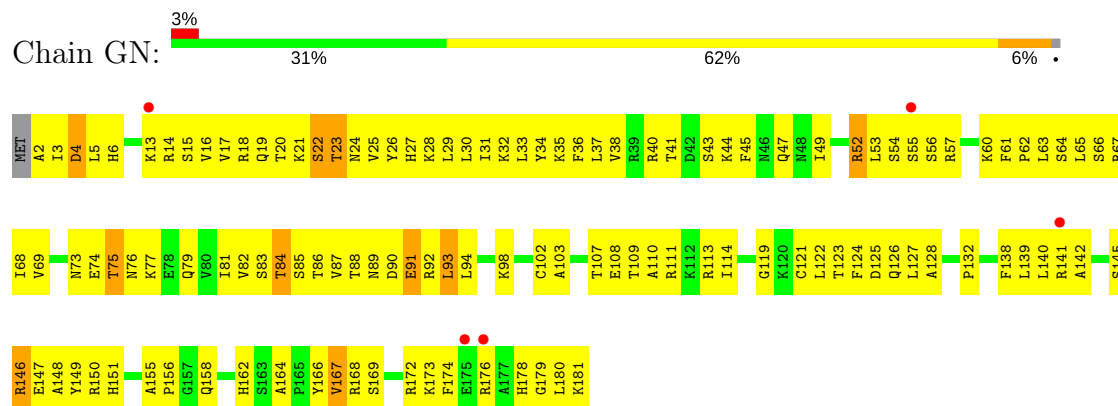
• Molecule 35: RPL18



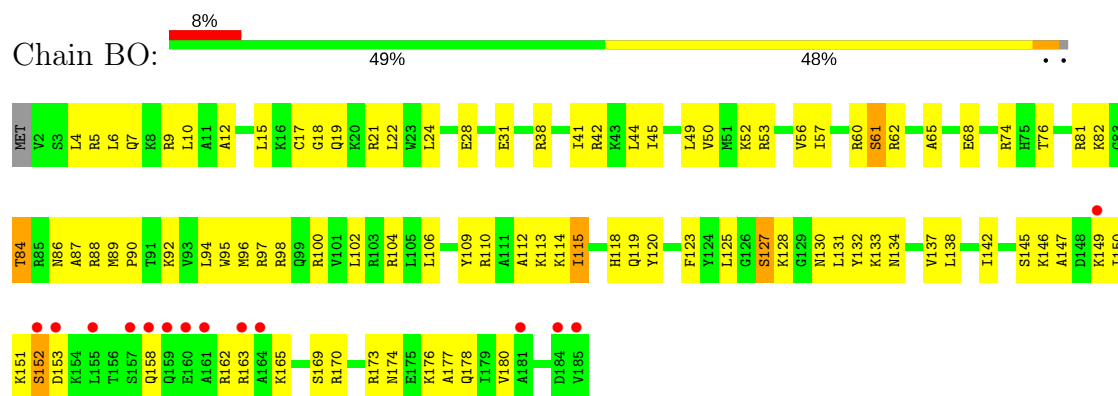
• Molecule 35: RPL18



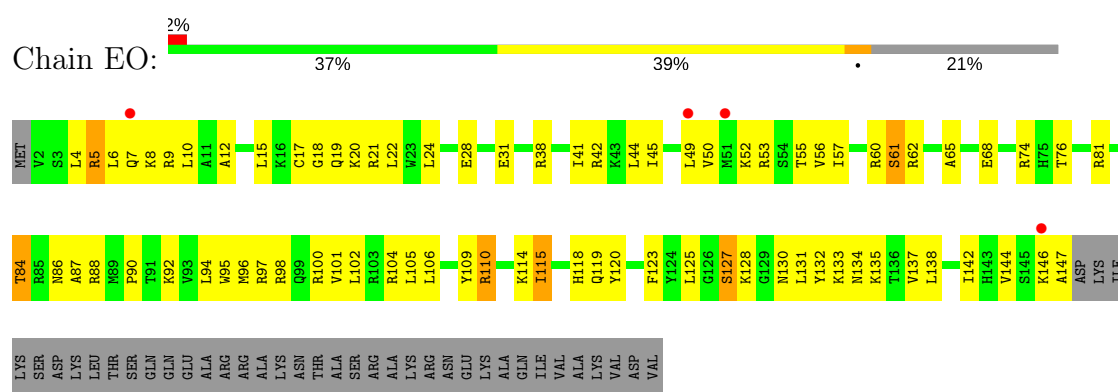
• Molecule 35: RPL18



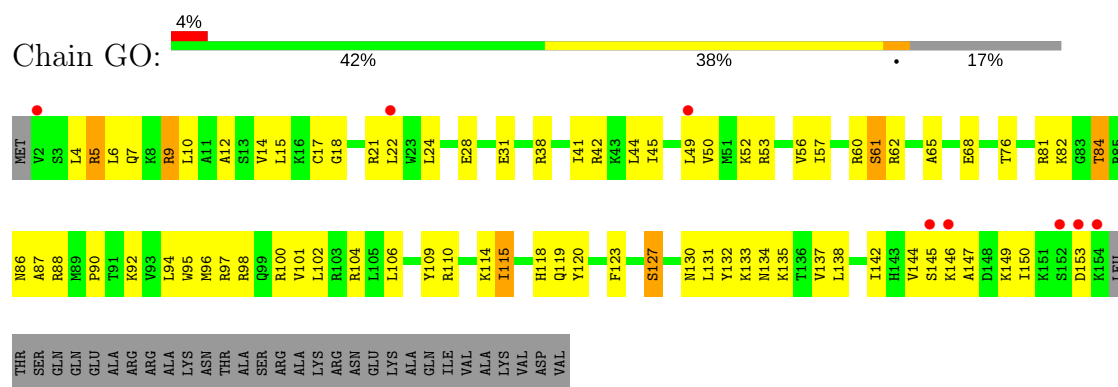
- Molecule 36: RPL19



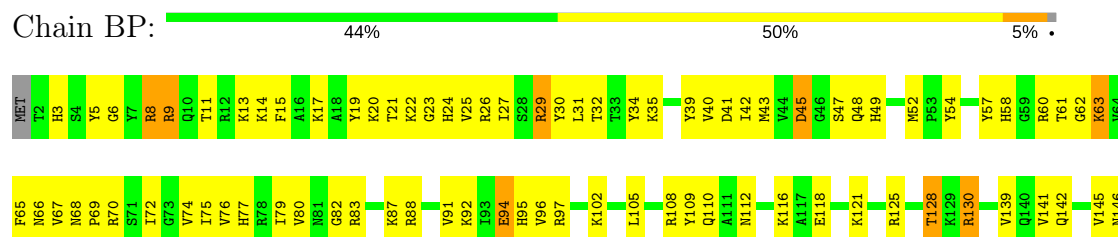
- Molecule 36: RPL19



- Molecule 36: RPL19



- Molecule 37: 60S RIBOSOMAL PROTEIN L21





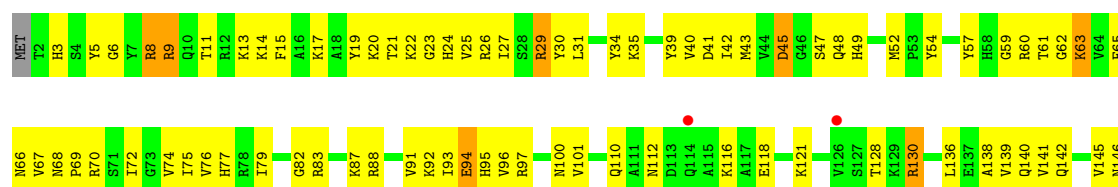
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

Chain CP: 46% 48%



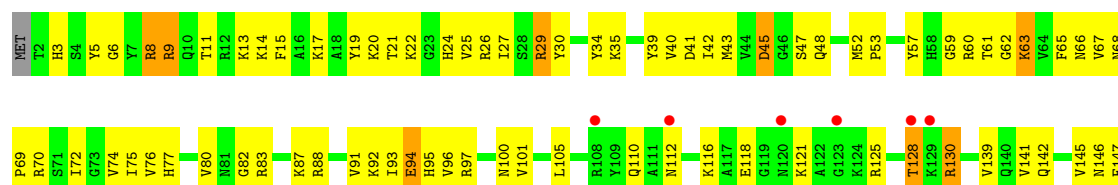
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

Chain EP: 45% 50%



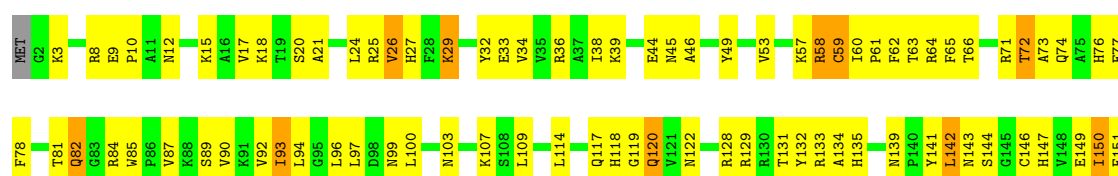
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

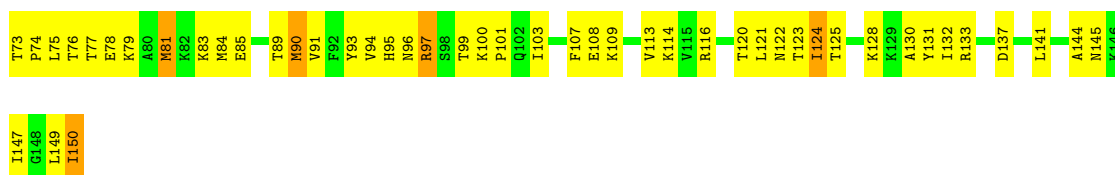
Chain GP: 4% 46% 48% 5%



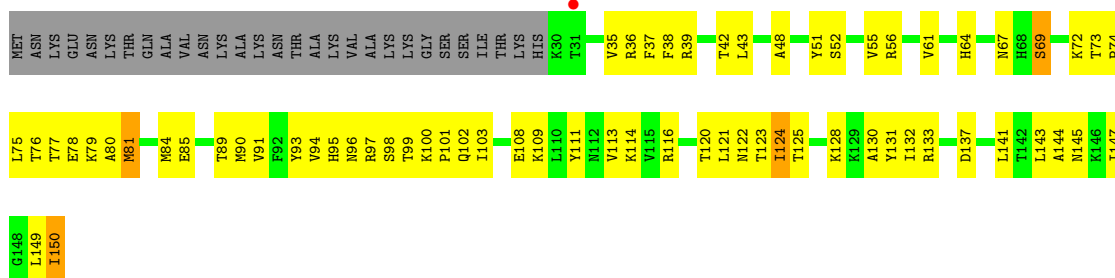
• Molecule 38: RPL17

Chain BQ: 39% 41% 5% 14%

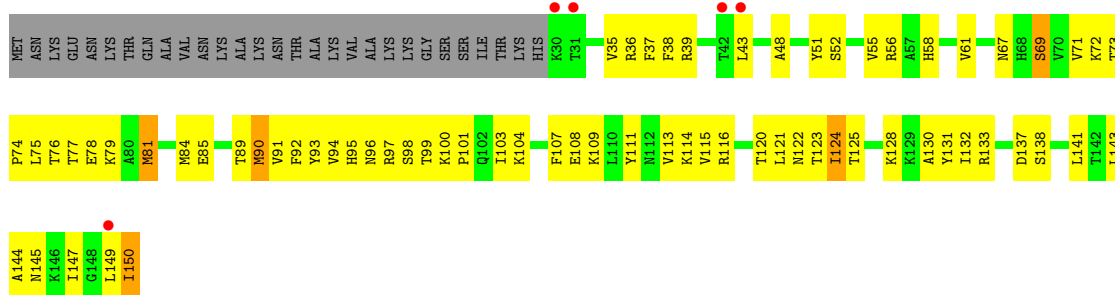




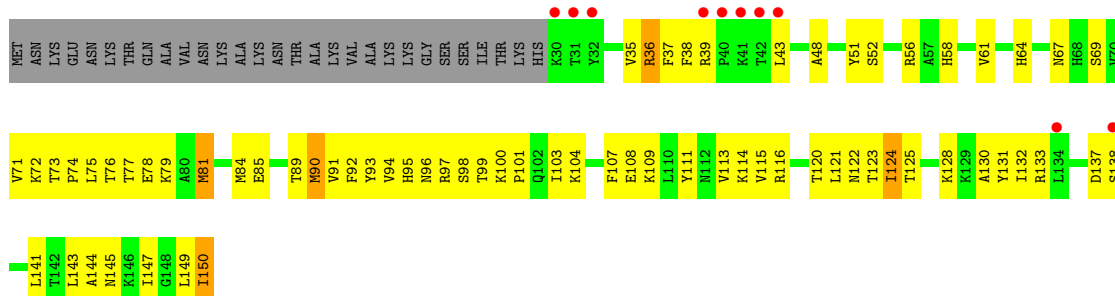
• Molecule 39: RPL23A



• Molecule 39: RPL23A

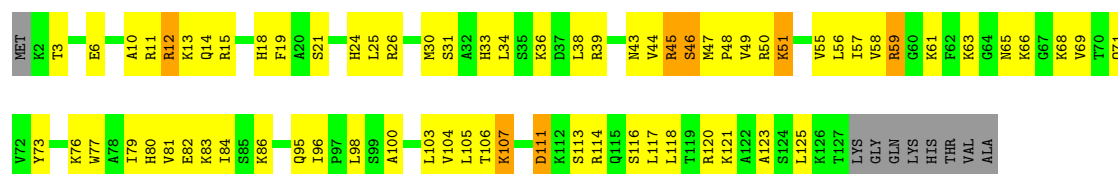


• Molecule 39: RPL23A

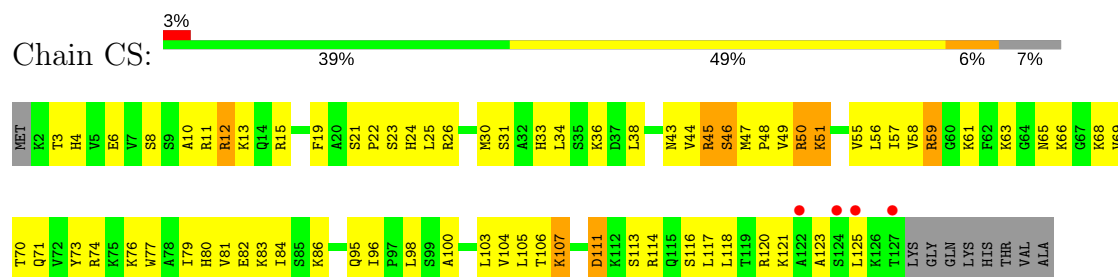


• Molecule 40: RPL26

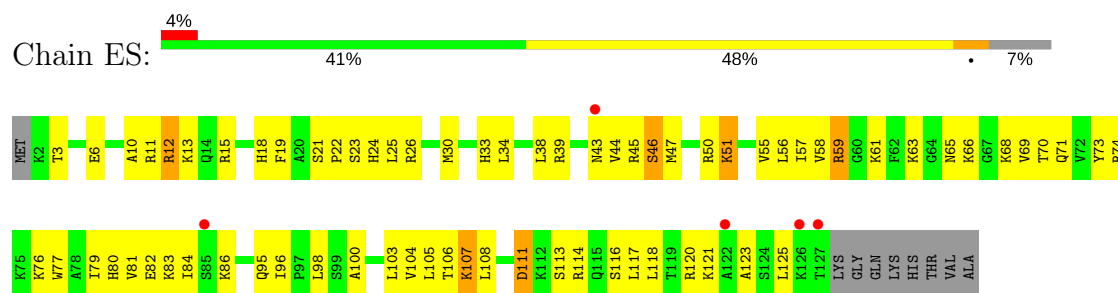




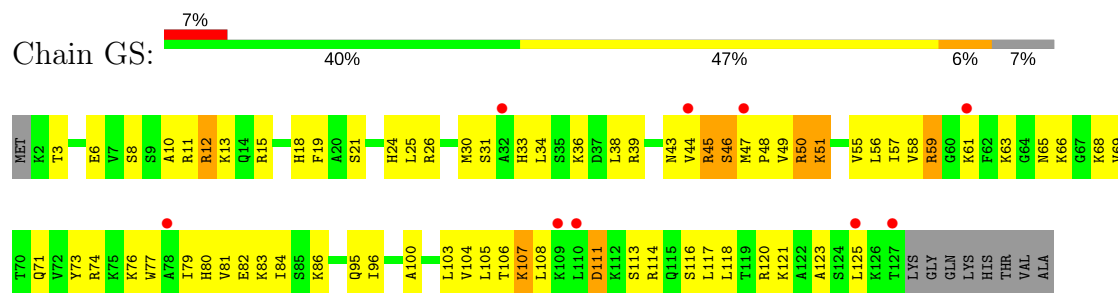
• Molecule 40: RPL26



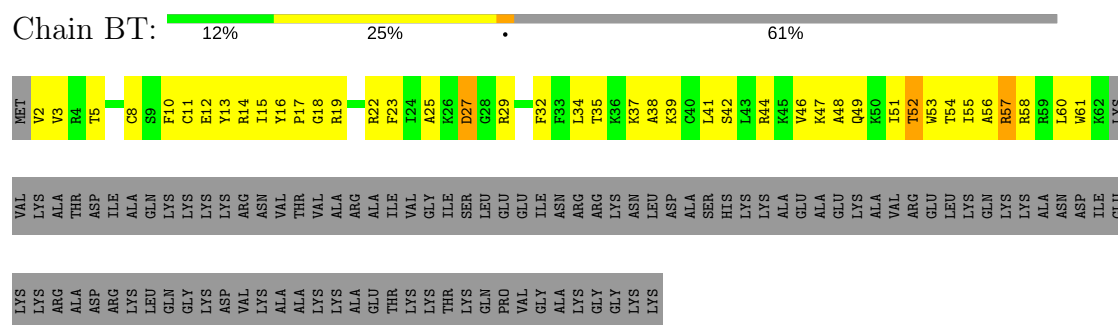
• Molecule 40: RPL26



• Molecule 40: RPL26

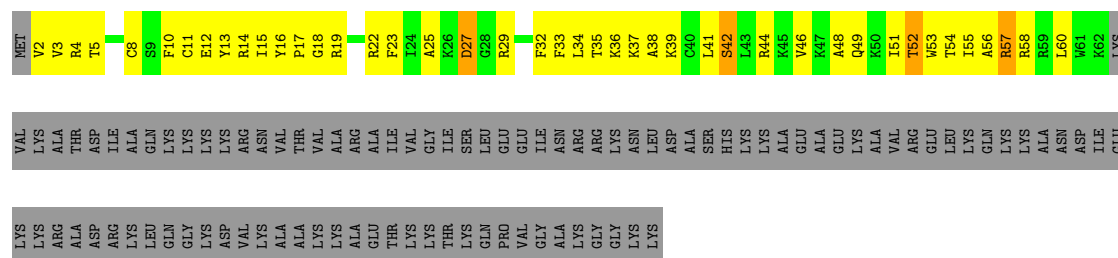


• Molecule 41: RPL24



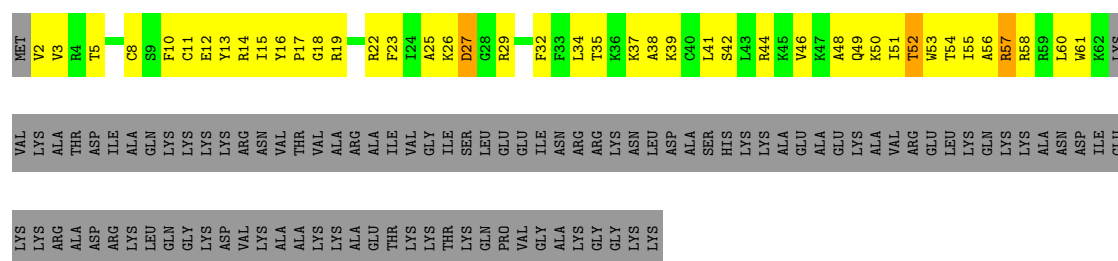
• Molecule 41: RPL24

Chain CT: 



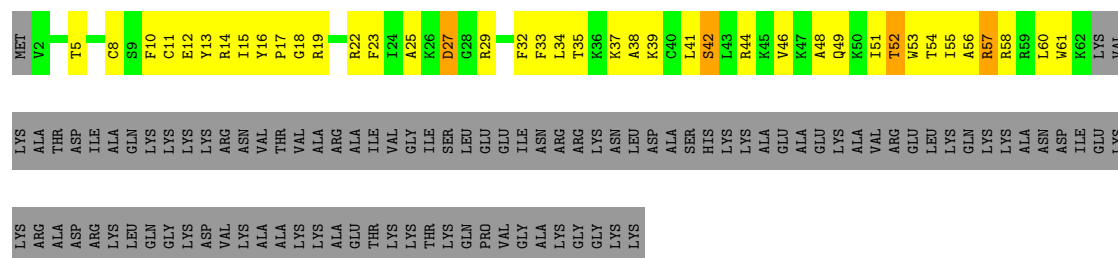
• Molecule 41: RPL24

Chain ET: 



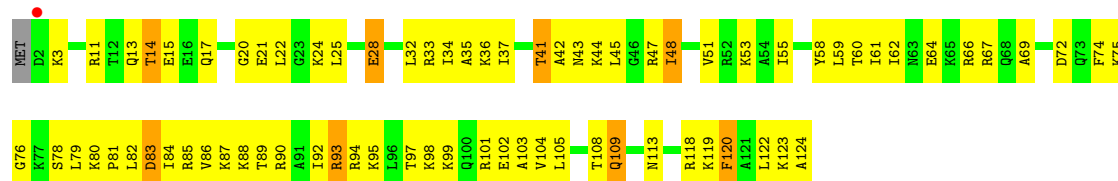
• Molecule 41: RPL24

Chain GT: 



• Molecule 42: RPL35

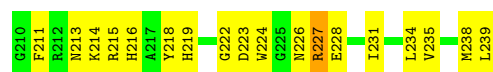
Chain BU: 



• Molecule 42: RPL35

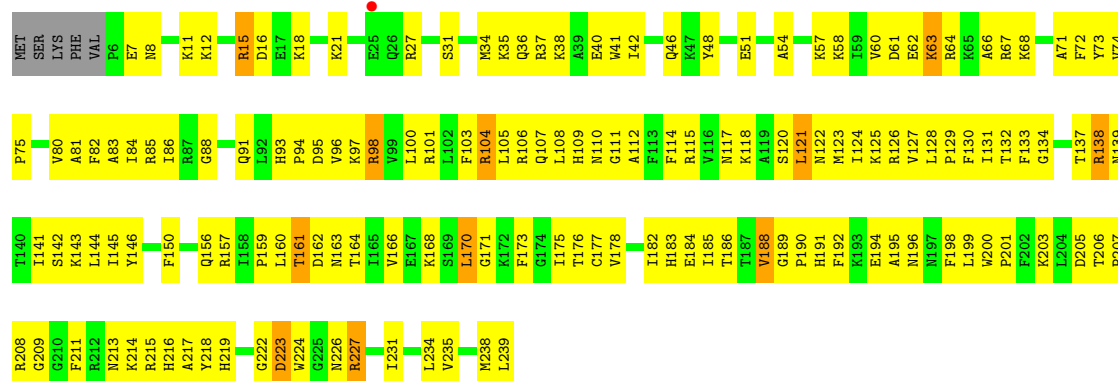
Chain CU: 





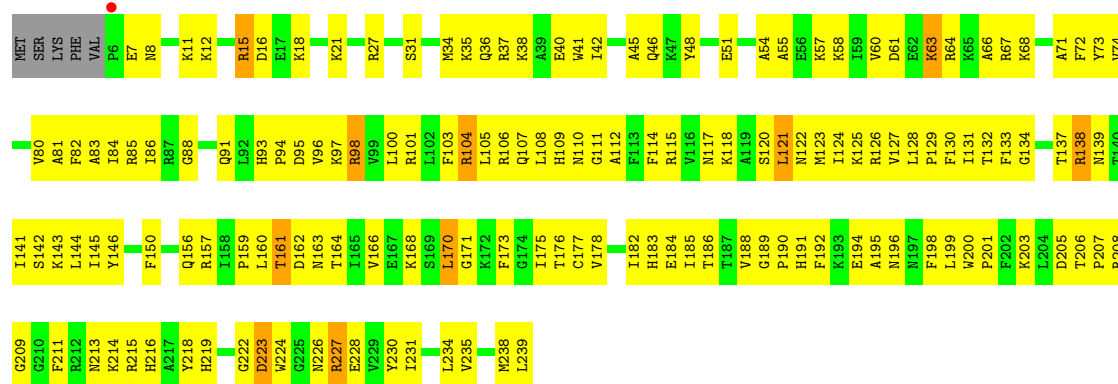
• Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain EV: 35% 59% 5%



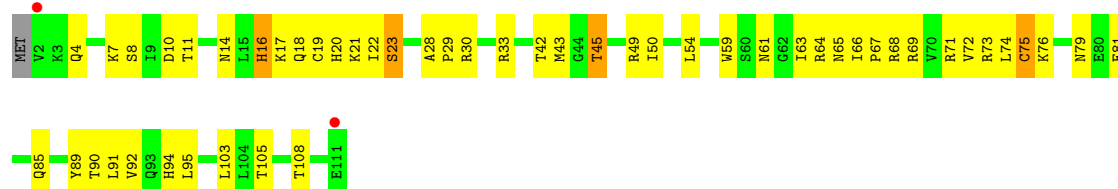
• Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain GV: 34% 59% 7%



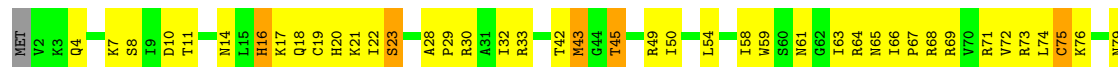
• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain BW: 2% 53% 42%



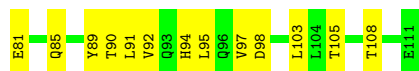
• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain CW: 50% 45% 5%

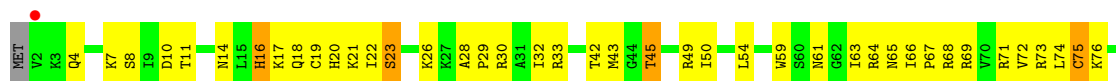




• Molecule 44: 60S RIBOSOMAL PROTEIN L31



• Molecule 44: 60S RIBOSOMAL PROTEIN L31



• Molecule 45: 60S RIBOSOMAL PROTEIN L32



• Molecule 45: 60S RIBOSOMAL PROTEIN L32



• Molecule 45: 60S RIBOSOMAL PROTEIN L32





• Molecule 45: 60S RIBOSOMAL PROTEIN L32



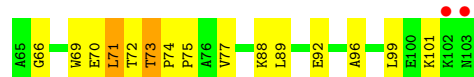
• Molecule 46: RPL37A



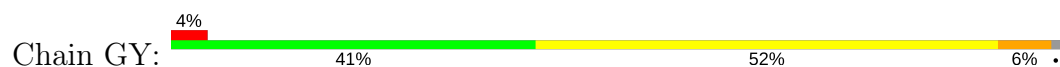
• Molecule 46: RPL37A

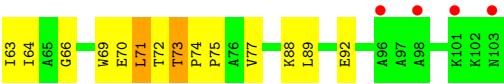


• Molecule 46: RPL37A

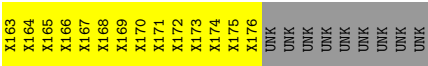
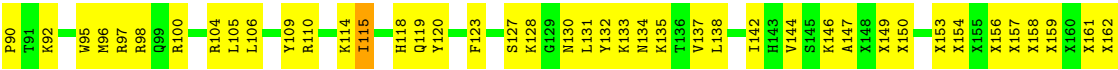
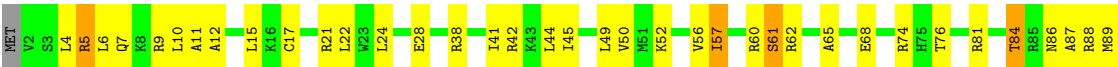


• Molecule 46: RPL37A





● Molecule 47: RPL19



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.216 , 0.244 0.240 , 0.266	Depositor DCC
R_{free} test set	10000 reflections (0.85%)	DCC
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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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	4647	2
1	D1	66769	0	33568	4657	1
1	F1	66769	0	33568	4661	3
1	H1	66769	0	33570	4686	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	37509	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 37509 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%)	32	73
5	DE	188/191 (98%)	176 (94%)	11 (6%)	1 (0%)	32	73
5	FE	188/191 (98%)	178 (95%)	9 (5%)	1 (0%)	32	73
5	HE	188/191 (98%)	177 (94%)	10 (5%)	1 (0%)	32	73
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%)	18	60
8	HH	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
9	AJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	20	63
9	DJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	20	63
9	FJ	224/248 (90%)	212 (95%)	10 (4%)	2 (1%)	20	63
9	HJ	224/248 (90%)	213 (95%)	9 (4%)	2 (1%)	20	63
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%)	18	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	DM	98/118 (83%)	94 (96%)	3 (3%)	1 (1%)	18	60
12	FM	98/118 (83%)	93 (95%)	4 (4%)	1 (1%)	18	60
12	HM	98/118 (83%)	92 (94%)	5 (5%)	1 (1%)	18	60
13	AN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	25	67
13	DN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	25	67
13	FN	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
13	HN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	25	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%)	9	46
16	DQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	9	46
16	FQ	100/104 (96%)	88 (88%)	10 (10%)	2 (2%)	9	46
16	HQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	9	46
17	AT	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	11	50
17	DT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	50
17	FT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	50
17	HT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	11	50
18	AU	201/206 (98%)	188 (94%)	12 (6%)	1 (0%)	32	73
18	DU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	32	73
18	FU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	32	73
18	HU	201/206 (98%)	189 (94%)	11 (6%)	1 (0%)	32	73
19	AX	186/189 (98%)	177 (95%)	8 (4%)	1 (0%)	32	73
19	DX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	17	58
19	FX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	17	58
19	HX	186/189 (98%)	177 (95%)	7 (4%)	2 (1%)	17	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%)	38	77
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%)	13	53
32	CK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	8	45
32	EK	146/149 (98%)	137 (94%)	7 (5%)	2 (1%)	13	53
32	GK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	8	45
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%)	32	73
34	BM	296/301 (98%)	282 (95%)	13 (4%)	1 (0%)	44	80
34	CM	298/301 (99%)	282 (95%)	15 (5%)	1 (0%)	44	80
34	EM	298/301 (99%)	283 (95%)	14 (5%)	1 (0%)	44	80
34	GM	298/301 (99%)	285 (96%)	12 (4%)	1 (0%)	44	80
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%)	32	73
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%)	38	77
43	GV	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	38	77
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%)	51	85

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%)	4	21
2	HA	69/72 (96%)	58 (84%)	11 (16%)	3	17
3	AB	48/49 (98%)	44 (92%)	4 (8%)	13	46
3	DB	48/49 (98%)	44 (92%)	4 (8%)	13	46
3	FB	48/49 (98%)	44 (92%)	4 (8%)	13	46
3	HB	48/49 (98%)	44 (92%)	4 (8%)	13	46
4	AC	95/101 (94%)	92 (97%)	3 (3%)	44	76
4	DC	95/101 (94%)	92 (97%)	3 (3%)	44	76
4	FC	95/101 (94%)	92 (97%)	3 (3%)	44	76
4	HC	95/101 (94%)	92 (97%)	3 (3%)	44	76
5	AE	162/163 (99%)	152 (94%)	10 (6%)	21	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	DE	162/163 (99%)	152 (94%)	10 (6%)	21	59
5	FE	162/163 (99%)	151 (93%)	11 (7%)	18	56
5	HE	162/163 (99%)	151 (93%)	11 (7%)	18	56
6	AF	111/112 (99%)	107 (96%)	4 (4%)	40	74
6	DF	111/112 (99%)	106 (96%)	5 (4%)	32	69
6	FF	111/112 (99%)	107 (96%)	4 (4%)	40	74
6	HF	111/112 (99%)	107 (96%)	4 (4%)	40	74
7	AG	80/88 (91%)	76 (95%)	4 (5%)	28	65
7	DG	80/88 (91%)	74 (92%)	6 (8%)	16	51
7	FG	80/88 (91%)	75 (94%)	5 (6%)	21	59
7	HG	80/88 (91%)	76 (95%)	4 (5%)	28	65
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%)	11	41
9	DJ	195/216 (90%)	176 (90%)	19 (10%)	9	38
9	FJ	195/216 (90%)	177 (91%)	18 (9%)	11	41
9	HJ	195/216 (90%)	177 (91%)	18 (9%)	11	41
10	AK	46/113 (41%)	43 (94%)	3 (6%)	20	58
10	DK	46/113 (41%)	43 (94%)	3 (6%)	20	58
10	FK	46/113 (41%)	43 (94%)	3 (6%)	20	58
10	HK	46/113 (41%)	43 (94%)	3 (6%)	20	58
11	AL	92/107 (86%)	87 (95%)	5 (5%)	26	63
11	DL	92/107 (86%)	87 (95%)	5 (5%)	26	63
11	FL	92/107 (86%)	88 (96%)	4 (4%)	33	70
11	HL	92/107 (86%)	87 (95%)	5 (5%)	26	63
12	AM	93/110 (84%)	90 (97%)	3 (3%)	44	76
12	DM	93/110 (84%)	90 (97%)	3 (3%)	44	76
12	FM	93/110 (84%)	90 (97%)	3 (3%)	44	76
12	HM	93/110 (84%)	90 (97%)	3 (3%)	44	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AN	130/131 (99%)	123 (95%)	7 (5%)	26	63
13	DN	130/131 (99%)	122 (94%)	8 (6%)	21	59
13	FN	130/131 (99%)	123 (95%)	7 (5%)	26	63
13	HN	130/131 (99%)	123 (95%)	7 (5%)	26	63
14	AO	108/108 (100%)	102 (94%)	6 (6%)	25	62
14	DO	108/108 (100%)	102 (94%)	6 (6%)	25	62
14	FO	108/108 (100%)	100 (93%)	8 (7%)	16	52
14	HO	108/108 (100%)	102 (94%)	6 (6%)	25	62
15	AP	60/77 (78%)	56 (93%)	4 (7%)	19	57
15	DP	60/77 (78%)	56 (93%)	4 (7%)	19	57
15	FP	60/77 (78%)	56 (93%)	4 (7%)	19	57
15	HP	60/77 (78%)	56 (93%)	4 (7%)	19	57
16	AQ	81/83 (98%)	75 (93%)	6 (7%)	16	52
16	DQ	81/83 (98%)	75 (93%)	6 (7%)	16	52
16	FQ	81/83 (98%)	75 (93%)	6 (7%)	16	52
16	HQ	81/83 (98%)	75 (93%)	6 (7%)	16	52
17	AT	61/62 (98%)	55 (90%)	6 (10%)	9	38
17	DT	61/62 (98%)	57 (93%)	4 (7%)	19	57
17	FT	61/62 (98%)	57 (93%)	4 (7%)	19	57
17	HT	61/62 (98%)	57 (93%)	4 (7%)	19	57
18	AU	169/171 (99%)	159 (94%)	10 (6%)	23	61
18	DU	169/171 (99%)	161 (95%)	8 (5%)	30	67
18	FU	169/171 (99%)	160 (95%)	9 (5%)	26	63
18	HU	169/171 (99%)	161 (95%)	8 (5%)	30	67
19	AX	167/168 (99%)	153 (92%)	14 (8%)	13	46
19	DX	167/168 (99%)	152 (91%)	15 (9%)	11	42
19	FX	167/168 (99%)	151 (90%)	16 (10%)	10	39
19	HX	167/168 (99%)	154 (92%)	13 (8%)	15	49
22	BA	196/198 (99%)	165 (84%)	31 (16%)	3	17
22	CA	196/198 (99%)	164 (84%)	32 (16%)	3	16
22	EA	196/198 (99%)	164 (84%)	32 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	GA	196/198 (99%)	165 (84%)	31 (16%)	3	17
23	BB	330/334 (99%)	306 (93%)	24 (7%)	16	53
23	CB	330/334 (99%)	307 (93%)	23 (7%)	18	55
23	EB	330/334 (99%)	308 (93%)	22 (7%)	19	57
23	GB	330/334 (99%)	306 (93%)	24 (7%)	16	53
24	BC	325/326 (100%)	302 (93%)	23 (7%)	17	54
24	CC	325/326 (100%)	302 (93%)	23 (7%)	17	54
24	EC	325/326 (100%)	300 (92%)	25 (8%)	15	50
24	GC	325/326 (100%)	300 (92%)	25 (8%)	15	50
25	BD	146/149 (98%)	136 (93%)	10 (7%)	18	56
25	CD	146/149 (98%)	136 (93%)	10 (7%)	18	56
25	ED	146/149 (98%)	135 (92%)	11 (8%)	16	51
25	GD	146/149 (98%)	136 (93%)	10 (7%)	18	56
26	BE	163/165 (99%)	157 (96%)	6 (4%)	39	73
26	CE	163/165 (99%)	157 (96%)	6 (4%)	39	73
26	EE	163/165 (99%)	157 (96%)	6 (4%)	39	73
26	GE	163/165 (99%)	157 (96%)	6 (4%)	39	73
27	BF	201/222 (90%)	194 (96%)	7 (4%)	41	75
27	CF	201/222 (90%)	194 (96%)	7 (4%)	41	75
27	EF	201/222 (90%)	194 (96%)	7 (4%)	41	75
27	GF	201/222 (90%)	194 (96%)	7 (4%)	41	75
29	BH	169/180 (94%)	155 (92%)	14 (8%)	13	46
29	CH	169/180 (94%)	155 (92%)	14 (8%)	13	46
29	EH	169/180 (94%)	156 (92%)	13 (8%)	15	50
29	GH	169/180 (94%)	153 (90%)	16 (10%)	10	40
30	BI	166/166 (100%)	150 (90%)	16 (10%)	10	39
30	CI	166/166 (100%)	149 (90%)	17 (10%)	8	36
30	EI	166/166 (100%)	150 (90%)	16 (10%)	10	39
30	GI	166/166 (100%)	150 (90%)	16 (10%)	10	39
31	BJ	107/108 (99%)	98 (92%)	9 (8%)	13	46
31	CJ	107/108 (99%)	99 (92%)	8 (8%)	16	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	EJ	107/108 (99%)	99 (92%)	8 (8%)	16	51
31	GJ	107/108 (99%)	99 (92%)	8 (8%)	16	51
32	BK	120/121 (99%)	110 (92%)	10 (8%)	13	46
32	CK	120/121 (99%)	111 (92%)	9 (8%)	16	51
32	EK	120/121 (99%)	110 (92%)	10 (8%)	13	46
32	GK	120/121 (99%)	110 (92%)	10 (8%)	13	46
33	BL	174/175 (99%)	165 (95%)	9 (5%)	27	64
33	CL	174/175 (99%)	165 (95%)	9 (5%)	27	64
33	EL	174/175 (99%)	165 (95%)	9 (5%)	27	64
33	GL	174/175 (99%)	166 (95%)	8 (5%)	31	68
34	BM	252/254 (99%)	239 (95%)	13 (5%)	27	64
34	CM	253/254 (100%)	242 (96%)	11 (4%)	33	70
34	EM	253/254 (100%)	242 (96%)	11 (4%)	33	70
34	GM	253/254 (100%)	240 (95%)	13 (5%)	28	64
35	BN	159/160 (99%)	145 (91%)	14 (9%)	12	44
35	CN	159/160 (99%)	146 (92%)	13 (8%)	13	47
35	EN	159/160 (99%)	145 (91%)	14 (9%)	12	44
35	GN	159/160 (99%)	146 (92%)	13 (8%)	13	47
36	BO	158/159 (99%)	148 (94%)	10 (6%)	21	59
36	EO	126/159 (79%)	116 (92%)	10 (8%)	14	49
36	GO	127/159 (80%)	117 (92%)	10 (8%)	14	49
37	BP	134/135 (99%)	124 (92%)	10 (8%)	16	51
37	CP	134/135 (99%)	126 (94%)	8 (6%)	22	60
37	EP	134/135 (99%)	125 (93%)	9 (7%)	19	57
37	GP	134/135 (99%)	125 (93%)	9 (7%)	19	57
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%)	20	58
39	CR	108/132 (82%)	101 (94%)	7 (6%)	20	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	ER	108/132 (82%)	102 (94%)	6 (6%)	25	62
39	GR	108/132 (82%)	103 (95%)	5 (5%)	31	68
40	BS	113/120 (94%)	105 (93%)	8 (7%)	17	54
40	CS	113/120 (94%)	104 (92%)	9 (8%)	14	48
40	ES	113/120 (94%)	105 (93%)	8 (7%)	17	54
40	GS	113/120 (94%)	104 (92%)	9 (8%)	14	48
41	BT	52/130 (40%)	46 (88%)	6 (12%)	6	30
41	CT	52/130 (40%)	46 (88%)	6 (12%)	6	30
41	ET	52/130 (40%)	46 (88%)	6 (12%)	6	30
41	GT	52/130 (40%)	46 (88%)	6 (12%)	6	30
42	BU	105/106 (99%)	96 (91%)	9 (9%)	12	45
42	CU	105/106 (99%)	96 (91%)	9 (9%)	12	45
42	EU	105/106 (99%)	96 (91%)	9 (9%)	12	45
42	GU	105/106 (99%)	96 (91%)	9 (9%)	12	45
43	BV	197/202 (98%)	186 (94%)	11 (6%)	25	62
43	CV	197/202 (98%)	187 (95%)	10 (5%)	28	64
43	EV	197/202 (98%)	188 (95%)	9 (5%)	31	68
43	GV	197/202 (98%)	187 (95%)	10 (5%)	28	64
44	BW	100/101 (99%)	96 (96%)	4 (4%)	36	71
44	CW	100/101 (99%)	95 (95%)	5 (5%)	28	65
44	EW	100/101 (99%)	95 (95%)	5 (5%)	28	65
44	GW	100/101 (99%)	96 (96%)	4 (4%)	36	71
45	BX	104/111 (94%)	88 (85%)	16 (15%)	3	18
45	CX	104/111 (94%)	87 (84%)	17 (16%)	3	16
45	EX	104/111 (94%)	88 (85%)	16 (15%)	3	18
45	GX	104/111 (94%)	88 (85%)	16 (15%)	3	18
46	BY	79/80 (99%)	72 (91%)	7 (9%)	11	43
46	CY	79/80 (99%)	71 (90%)	8 (10%)	9	37
46	EY	79/80 (99%)	71 (90%)	8 (10%)	9	37
46	GY	79/80 (99%)	73 (92%)	6 (8%)	15	51
47	CO	126/127 (99%)	116 (92%)	10 (8%)	14	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	22468/23988 (94%)	20823 (93%)	1645 (7%)	16 53

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%)	0
1	D1	3114/3354 (92%)	1113 (35%)	0
1	F1	3114/3354 (92%)	1113 (35%)	0
1	H1	3114/3354 (92%)	1113 (35%)	0
20	B2	153/154 (99%)	58 (37%)	0
20	C2	153/154 (99%)	60 (39%)	0
20	E2	153/154 (99%)	60 (39%)	0
20	G2	153/154 (99%)	60 (39%)	0
21	B3	119/120 (99%)	38 (31%)	0
21	C3	119/120 (99%)	39 (32%)	0
21	E3	119/120 (99%)	38 (31%)	0
21	G3	119/120 (99%)	38 (31%)	0
All	All	13544/14512 (93%)	4848 (35%)	0

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

There are no RNA pucker outliers to report.

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 [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	3119/3354 (92%)	0.12	89 (2%) 52 43	42, 91, 187, 390	0
1	D1	3119/3354 (92%)	0.05	34 (1%) 80 73	40, 79, 164, 330	0
1	F1	3119/3354 (92%)	0.18	62 (1%) 65 57	51, 94, 176, 357	0
1	H1	3119/3354 (92%)	0.49	136 (4%) 35 28	54, 121, 213, 367	0
2	AA	91/94 (96%)	-0.16	2 (2%) 62 53	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%)	0.20	2 (2%) 62 53	47, 83, 132, 204	0
2	HA	91/94 (96%)	0.87	12 (13%) 4 5	74, 119, 186, 243	0
3	AB	51/52 (98%)	-0.20	1 (1%) 65 57	44, 63, 110, 148	0
3	DB	51/52 (98%)	-0.13	1 (1%) 65 57	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 3	90, 114, 144, 197	0
4	AC	103/109 (94%)	0.37	3 (2%) 52 43	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 75	58, 96, 156, 192	0
4	HC	103/109 (94%)	0.32	3 (2%) 52 43	81, 130, 176, 199	0
5	AE	190/191 (99%)	0.19	12 (6%) 21 17	69, 122, 171, 214	0
5	DE	190/191 (99%)	0.08	1 (0%) 90 87	74, 124, 169, 226	0
5	FE	190/191 (99%)	0.20	8 (4%) 37 30	60, 123, 176, 227	0
5	HE	190/191 (99%)	0.34	14 (7%) 15 14	76, 141, 194, 227	0
6	AF	125/126 (99%)	0.02	5 (4%) 39 32	71, 111, 156, 213	0
6	DF	125/126 (99%)	-0.22	2 (1%) 72 64	70, 106, 157, 190	0
6	FF	125/126 (99%)	0.01	6 (4%) 31 25	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 ²)	Q<0.9
7	AG	96/104 (92%)	0.08	1 (1%) 82 75	62, 103, 188, 218	0
7	DG	96/104 (92%)	0.06	4 (4%) 37 30	57, 114, 179, 222	0
7	FG	96/104 (92%)	0.18	2 (2%) 64 56	81, 112, 176, 199	0
7	HG	96/104 (92%)	0.21	1 (1%) 82 75	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 89	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%) 41 34	73, 101, 146, 182	0
10	DK	52/129 (40%)	-0.32	1 (1%) 67 59	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%)	-0.26	0 100 100	61, 77, 118, 158	0
11	AL	108/123 (87%)	-0.12	1 (0%) 84 77	38, 73, 130, 165	0
11	DL	108/123 (87%)	-0.10	1 (0%) 84 77	47, 85, 144, 217	0
11	FL	108/123 (87%)	0.13	2 (1%) 67 59	66, 98, 135, 174	0
11	HL	108/123 (87%)	0.52	5 (4%) 33 27	90, 117, 156, 183	0
12	AM	100/118 (84%)	0.20	2 (2%) 65 57	72, 121, 155, 185	0
12	DM	100/118 (84%)	0.16	4 (4%) 39 32	73, 126, 179, 199	0
12	FM	100/118 (84%)	0.29	2 (2%) 65 57	93, 144, 196, 208	0
12	HM	100/118 (84%)	0.06	2 (2%) 65 57	98, 151, 195, 214	0
13	AN	143/144 (99%)	-0.20	1 (0%) 87 82	59, 97, 163, 189	0
13	DN	143/144 (99%)	-0.06	1 (0%) 87 82	73, 121, 179, 214	0
13	FN	143/144 (99%)	-0.02	1 (0%) 87 82	72, 122, 175, 208	0
13	HN	143/144 (99%)	0.30	3 (2%) 64 56	92, 148, 189, 217	0
14	AO	134/134 (100%)	-0.20	1 (0%) 87 82	66, 116, 162, 202	0
14	DO	134/134 (100%)	-0.11	1 (0%) 87 82	52, 99, 151, 209	0
14	FO	134/134 (100%)	0.03	2 (1%) 74 66	65, 118, 167, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	HO	134/134 (100%)	0.48	11 (8%) 12 12	96, 143, 197, 227	0
15	AP	66/89 (74%)	0.39	3 (4%) 34 27	55, 128, 209, 241	0
15	DP	66/89 (74%)	0.32	5 (7%) 15 13	73, 116, 176, 245	0
15	FP	66/89 (74%)	0.56	4 (6%) 22 18	99, 143, 202, 214	0
15	HP	66/89 (74%)	1.03	8 (12%) 5 6	99, 149, 219, 247	0
16	AQ	102/104 (98%)	0.09	3 (2%) 52 43	72, 122, 172, 208	0
16	DQ	102/104 (98%)	-0.02	3 (2%) 52 43	63, 105, 151, 186	0
16	FQ	102/104 (98%)	0.01	2 (1%) 65 57	72, 114, 166, 190	0
16	HQ	102/104 (98%)	0.57	6 (5%) 23 19	110, 154, 195, 203	0
17	AT	65/66 (98%)	0.37	4 (6%) 21 17	76, 121, 156, 193	0
17	DT	65/66 (98%)	0.11	1 (1%) 74 66	51, 87, 122, 211	0
17	FT	65/66 (98%)	0.26	1 (1%) 74 66	51, 107, 144, 201	0
17	HT	65/66 (98%)	0.77	4 (6%) 21 17	69, 136, 171, 222	0
18	AU	203/206 (98%)	0.09	4 (1%) 65 57	74, 122, 179, 233	0
18	DU	203/206 (98%)	-0.14	0 100 100	48, 98, 158, 198	0
18	FU	203/206 (98%)	-0.07	1 (0%) 90 87	67, 116, 174, 203	0
18	HU	203/206 (98%)	0.54	19 (9%) 9 9	102, 155, 206, 240	0
19	AX	188/189 (99%)	-0.20	1 (0%) 90 87	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 87	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 69	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%)	0.15	3 (1%) 67 59	74, 105, 142, 189	0
20	G2	154/154 (100%)	0.73	13 (8%) 12 12	98, 146, 182, 210	0
21	B3	120/120 (100%)	0.45	4 (3%) 47 39	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%) 47 39	95, 138, 175, 235	0
22	BA	257/264 (97%)	-0.02	9 (3%) 44 37	30, 70, 134, 233	0
22	CA	257/264 (97%)	-0.18	10 (3%) 40 33	31, 75, 139, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
22	EA	257/264 (97%)	-0.16	10 (3%) 40 33	40, 79, 136, 217	0
22	GA	257/264 (97%)	0.22	13 (5%) 29 23	60, 106, 157, 242	0
23	BB	386/391 (98%)	-0.32	5 (1%) 77 69	33, 69, 120, 227	0
23	CB	386/391 (98%)	-0.44	2 (0%) 90 87	34, 75, 123, 222	0
23	EB	386/391 (98%)	-0.36	4 (1%) 82 75	38, 75, 123, 230	0
23	GB	386/391 (98%)	-0.35	4 (1%) 82 75	51, 82, 132, 217	0
24	BC	409/410 (99%)	-0.01	12 (2%) 52 43	37, 107, 173, 241	0
24	CC	409/410 (99%)	-0.20	2 (0%) 90 87	40, 91, 151, 206	0
24	EC	409/410 (99%)	-0.07	5 (1%) 79 71	54, 107, 162, 237	0
24	GC	409/410 (99%)	0.34	17 (4%) 37 30	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 50	70, 110, 151, 188	0
25	ED	169/172 (98%)	0.49	8 (4%) 32 26	89, 133, 179, 209	0
25	GD	169/172 (98%)	0.66	19 (11%) 6 7	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 87	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%) 51 42	70, 122, 176, 252	0
27	CF	231/255 (90%)	-0.15	3 (1%) 77 69	71, 115, 175, 233	0
27	EF	231/255 (90%)	0.00	6 (2%) 56 47	76, 120, 187, 241	0
27	GF	231/255 (90%)	0.60	17 (7%) 15 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	5 (2%) 58 48	79, 133, 181, 221	0
29	CH	201/215 (93%)	-0.24	1 (0%) 90 87	42, 93, 139, 153	0
29	EH	201/215 (93%)	-0.15	2 (0%) 82 75	50, 105, 158, 202	0
29	GH	201/215 (93%)	0.08	2 (0%) 82 75	71, 118, 171, 203	0
30	BI	198/198 (100%)	-0.21	2 (1%) 82 75	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 ²)	Q<0.9
30	EI	198/198 (100%)	-0.26	2 (1%) 82 75	47, 79, 152, 174	0
30	GI	198/198 (100%)	-0.20	2 (1%) 82 75	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 53	40, 65, 108, 202	0
31	GJ	138/141 (97%)	-0.41	1 (0%) 87 82	30, 60, 98, 186	0
32	BK	148/149 (99%)	0.01	4 (2%) 55 46	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%) 15 14	78, 129, 181, 208	0
33	BL	203/204 (99%)	-0.26	1 (0%) 90 87	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%) 46 38	89, 133, 165, 205	0
34	BM	298/301 (99%)	0.35	10 (3%) 46 38	87, 152, 201, 240	0
34	CM	300/301 (99%)	-0.12	3 (1%) 82 75	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%) 9 9	98, 157, 204, 233	0
35	BN	180/181 (99%)	0.04	1 (0%) 89 84	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 84	63, 101, 142, 187	0
35	GN	180/181 (99%)	0.28	5 (2%) 53 45	94, 139, 188, 248	0
36	BO	184/185 (99%)	0.27	14 (7%) 15 13	29, 78, 184, 207	0
36	EO	146/185 (78%)	0.19	4 (2%) 55 46	57, 95, 128, 194	0
36	GO	153/185 (82%)	0.39	8 (5%) 28 23	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 69	56, 100, 148, 183	0
37	GP	156/157 (99%)	0.46	6 (3%) 41 34	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 84	26, 70, 124, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
38	EQ	157/183 (85%)	-0.19	1 (0%) 89 84	48, 86, 141, 177	0
38	GQ	157/183 (85%)	0.16	2 (1%) 77 69	60, 106, 157, 200	0
39	BR	121/150 (80%)	-0.20	1 (0%) 86 79	42, 78, 129, 185	0
39	CR	121/150 (80%)	0.05	1 (0%) 86 79	54, 88, 129, 172	0
39	ER	121/150 (80%)	0.18	5 (4%) 38 31	65, 112, 146, 172	0
39	GR	121/150 (80%)	0.45	10 (8%) 12 12	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%) 48 40	46, 89, 127, 152	0
40	ES	126/135 (93%)	0.17	5 (3%) 39 32	74, 112, 151, 184	0
40	GS	126/135 (93%)	0.58	9 (7%) 17 14	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 79	59, 101, 139, 204	0
42	CU	123/124 (99%)	-0.21	1 (0%) 86 79	49, 92, 143, 163	0
42	EU	123/124 (99%)	-0.06	2 (1%) 72 64	79, 114, 157, 220	0
42	GU	123/124 (99%)	0.80	19 (15%) 2 3	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%)	-0.43	0 100 100	47, 87, 145, 213	0
43	EV	234/239 (97%)	-0.36	1 (0%) 92 89	53, 102, 159, 232	0
43	GV	234/239 (97%)	-0.15	1 (0%) 92 89	75, 121, 173, 239	0
44	BW	110/111 (99%)	-0.21	2 (1%) 69 60	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 77	56, 88, 170, 227	0
44	GW	110/111 (99%)	0.09	1 (0%) 84 77	63, 102, 183, 216	0
45	BX	125/134 (93%)	-0.01	2 (1%) 72 64	53, 89, 128, 202	0
45	CX	125/134 (93%)	-0.27	1 (0%) 86 79	40, 78, 116, 196	0
45	EX	125/134 (93%)	-0.13	2 (1%) 72 64	49, 88, 129, 233	0
45	GX	125/134 (93%)	0.35	4 (3%) 48 40	73, 117, 162, 215	0
46	BY	102/103 (99%)	-0.11	4 (3%) 40 33	40, 74, 164, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
46	CY	102/103 (99%)	-0.21	3 (2%)	52	43	41, 83, 173, 196	0
46	EY	102/103 (99%)	-0.08	3 (2%)	52	43	45, 84, 156, 193	0
46	GY	102/103 (99%)	0.05	4 (3%)	40	33	53, 102, 189, 222	0
47	CO	146/185 (78%)	-0.07	0	100	100	45, 79, 115, 148	0
All	All	40083/43352 (92%)	0.07	964 (2%)	59	50	26, 101, 177, 390	0

The worst 5 of 964 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HA	92	ALA	14.9
1	H1	1597	U	11.1
1	A1	2500	C	11.1
1	A1	1597	U	10.4
23	BB	387	GLU	10.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
48	MG	F1	3566	1/1	0.68	1.27	45.32	146,146,146,146	0
48	MG	F1	3506	1/1	0.82	0.32	24.43	114,114,114,114	0
48	MG	G3	204	1/1	0.83	0.36	10.48	143,143,143,143	0
48	MG	D1	3516	1/1	0.80	0.36	10.12	82,82,82,82	0
48	MG	H1	3409	1/1	0.54	0.56	9.76	193,193,193,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3579	1/1	0.76	0.52	8.98	94,94,94,94	0
48	MG	F1	3493	1/1	0.67	0.50	8.45	145,145,145,145	0
48	MG	D1	3481	1/1	0.90	0.40	8.44	114,114,114,114	0
48	MG	D1	3484	1/1	0.83	0.32	7.02	96,96,96,96	0
48	MG	A1	3412	1/1	0.84	0.33	6.68	117,117,117,117	0
48	MG	D1	3412	1/1	0.93	0.35	6.60	95,95,95,95	0
48	MG	D1	3511	1/1	0.90	0.24	5.60	118,118,118,118	0
48	MG	D1	3603	1/1	0.72	0.44	5.05	125,125,125,125	0
48	MG	D1	3497	1/1	0.67	0.53	4.97	151,151,151,151	0
48	MG	F1	3538	1/1	0.87	0.36	4.39	113,113,113,113	0
48	MG	F1	3479	1/1	0.93	0.29	4.04	81,81,81,81	0
48	MG	D1	3607	1/1	0.84	0.29	3.97	89,89,89,89	0
48	MG	GO	201	1/1	0.84	0.44	3.78	141,141,141,141	0
48	MG	D1	3589	1/1	0.94	0.26	3.42	107,107,107,107	0
48	MG	F1	3483	1/1	0.79	0.32	3.26	129,129,129,129	0
48	MG	H1	3529	1/1	0.03	0.33	3.19	214,214,214,214	0
48	MG	A1	3500	1/1	0.89	0.30	3.10	89,89,89,89	0
48	MG	DJ	301	1/1	0.77	0.45	2.98	150,150,150,150	0
48	MG	D1	3517	1/1	0.92	0.30	2.87	127,127,127,127	0
48	MG	D1	3504	1/1	0.86	0.27	2.82	98,98,98,98	0
48	MG	H1	3519	1/1	0.21	0.31	2.62	151,151,151,151	0
48	MG	H1	3469	1/1	0.94	0.34	2.54	119,119,119,119	0
48	MG	G2	202	1/1	0.91	0.35	2.24	122,122,122,122	0
48	MG	H1	3408	1/1	0.75	0.30	1.94	111,111,111,111	0
48	MG	F1	3537	1/1	0.90	0.21	1.75	136,136,136,136	0
48	MG	A1	3490	1/1	0.92	0.21	1.70	105,105,105,105	0
48	MG	F1	3453	1/1	0.83	0.23	1.66	131,131,131,131	0
48	MG	F1	3482	1/1	0.83	0.21	1.63	130,130,130,130	0
48	MG	A1	3578	1/1	0.62	0.18	1.60	117,117,117,117	0
48	MG	F1	3551	1/1	0.93	0.24	1.47	91,91,91,91	0
48	MG	A1	3491	1/1	0.74	0.24	1.40	125,125,125,125	0
48	MG	A1	3496	1/1	0.91	0.24	1.20	137,137,137,137	0
48	MG	H1	3510	1/1	0.88	0.24	1.12	120,120,120,120	0
48	MG	A1	3487	1/1	0.95	0.23	1.12	121,121,121,121	0
48	MG	H1	3431	1/1	0.92	0.25	0.94	94,94,94,94	0
48	MG	D1	3471	1/1	0.99	0.20	0.71	40,40,40,40	0
48	MG	A1	3410	1/1	0.98	0.21	0.68	62,62,62,62	0
48	MG	D1	3610	1/1	0.92	0.22	0.61	66,66,66,66	0
48	MG	E3	205	1/1	0.76	0.17	0.46	127,127,127,127	0
48	MG	F1	3561	1/1	0.30	0.24	0.18	167,167,167,167	0
48	MG	HT	101	1/1	0.81	0.35	0.17	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3501	1/1	0.92	0.22	0.08	102,102,102,102	0
48	MG	GQ	201	1/1	0.86	0.29	-0.05	102,102,102,102	0
48	MG	D1	3510	1/1	0.95	0.19	-0.11	81,81,81,81	0
48	MG	D1	3466	1/1	0.96	0.22	-0.29	132,132,132,132	0
48	MG	A1	3445	1/1	0.95	0.18	-0.31	88,88,88,88	0
48	MG	BJ	201	1/1	0.94	0.17	-0.58	66,66,66,66	0
48	MG	A1	3413	1/1	0.99	0.18	-0.74	136,136,136,136	0
48	MG	H1	3488	1/1	0.90	0.19	-0.76	108,108,108,108	0
48	MG	A1	3446	1/1	0.97	0.19	-0.81	64,64,64,64	0
48	MG	F1	3492	1/1	0.87	0.20	-0.82	78,78,78,78	0
49	ZN	DL	201	1/1	0.98	0.17	-0.82	86,86,86,86	0
48	MG	A1	3488	1/1	0.93	0.17	-0.86	91,91,91,91	0
49	ZN	DA	103	1/1	0.99	0.14	-0.86	69,69,69,69	0
48	MG	A1	3549	1/1	0.93	0.13	-0.87	54,54,54,54	0
48	MG	F1	3445	1/1	0.96	0.16	-0.92	78,78,78,78	0
48	MG	D1	3505	1/1	0.88	0.16	-0.96	84,84,84,84	0
49	ZN	EY	201	1/1	0.98	0.10	-0.98	77,77,77,77	0
48	MG	C3	202	1/1	0.80	0.15	-1.03	135,135,135,135	0
49	ZN	HA	101	1/1	0.98	0.14	-1.07	112,112,112,112	0
48	MG	F1	3534	1/1	0.90	0.08	-1.13	79,79,79,79	0
49	ZN	AA	101	1/1	0.98	0.14	-1.16	64,64,64,64	0
48	MG	H1	3509	1/1	0.83	0.18	-1.17	143,143,143,143	0
48	MG	H1	3419	1/1	0.93	0.17	-1.19	62,62,62,62	0
48	MG	F1	3472	1/1	0.90	0.15	-1.20	111,111,111,111	0
48	MG	H1	3434	1/1	0.81	0.18	-1.25	93,93,93,93	0
48	MG	D1	3569	1/1	0.98	0.09	-1.26	48,48,48,48	0
48	MG	A1	3443	1/1	0.90	0.14	-1.26	90,90,90,90	0
49	ZN	DK	202	1/1	0.99	0.11	-1.35	68,68,68,68	0
48	MG	A1	3558	1/1	0.94	0.10	-1.35	91,91,91,91	0
48	MG	H1	3497	1/1	0.99	0.13	-1.36	50,50,50,50	0
48	MG	FT	101	1/1	0.79	0.11	-1.37	124,124,124,124	0
48	MG	D1	3581	1/1	0.92	0.08	-1.38	68,68,68,68	0
48	MG	A1	3524	1/1	0.98	0.12	-1.38	63,63,63,63	0
48	MG	D1	3587	1/1	0.97	0.14	-1.39	93,93,93,93	0
48	MG	F1	3501	1/1	0.81	0.16	-1.40	116,116,116,116	0
48	MG	H1	3507	1/1	0.95	0.07	-1.40	64,64,64,64	0
49	ZN	DC	201	1/1	0.98	0.07	-1.44	89,89,89,89	0
48	MG	H1	3476	1/1	0.95	0.08	-1.47	52,52,52,52	0
48	MG	H1	3486	1/1	0.80	0.15	-1.50	105,105,105,105	0
48	MG	D1	3496	1/1	0.89	0.16	-1.52	78,78,78,78	0
48	MG	F1	3514	1/1	0.95	0.13	-1.54	70,70,70,70	0
49	ZN	FA	103	1/1	0.99	0.12	-1.57	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
49	ZN	FK	202	1/1	0.99	0.12	-1.57	74,74,74,74	0
48	MG	A1	3564	1/1	0.93	0.07	-1.58	141,141,141,141	0
48	MG	EQ	201	1/1	0.96	0.18	-1.64	88,88,88,88	0
48	MG	A1	3497	1/1	0.87	0.12	-1.64	116,116,116,116	0
49	ZN	FL	201	1/1	0.96	0.09	-1.69	86,86,86,86	0
48	MG	F1	3513	1/1	0.90	0.17	-1.72	79,79,79,79	0
49	ZN	CY	202	1/1	0.99	0.08	-1.73	70,70,70,70	0
48	MG	C3	206	1/1	0.96	0.15	-1.73	120,120,120,120	0
48	MG	F1	3437	1/1	0.94	0.17	-1.76	100,100,100,100	0
48	MG	CL	301	1/1	0.90	0.15	-1.77	109,109,109,109	0
48	MG	E2	203	1/1	0.94	0.07	-1.80	77,77,77,77	0
48	MG	F1	3476	1/1	0.96	0.16	-1.80	99,99,99,99	0
48	MG	D1	3573	1/1	0.91	0.14	-1.82	126,126,126,126	0
49	ZN	AK	201	1/1	0.98	0.10	-1.84	89,89,89,89	0
48	MG	F1	3427	1/1	0.97	0.16	-1.85	51,51,51,51	0
48	MG	CJ	201	1/1	0.96	0.14	-1.85	64,64,64,64	0
48	MG	A1	3452	1/1	0.97	0.11	-1.88	90,90,90,90	0
49	ZN	HC	201	1/1	0.90	0.04	-1.88	168,168,168,168	0
48	MG	D1	3546	1/1	0.97	0.10	-1.88	49,49,49,49	0
49	ZN	AL	201	1/1	0.99	0.09	-1.91	70,70,70,70	0
48	MG	D1	3544	1/1	0.96	0.09	-1.91	50,50,50,50	0
48	MG	A1	3411	1/1	0.95	0.17	-1.91	83,83,83,83	0
48	MG	A1	3553	1/1	0.84	0.16	-1.92	108,108,108,108	0
48	MG	A1	3421	1/1	0.98	0.06	-1.92	71,71,71,71	0
48	MG	B2	204	1/1	0.92	0.08	-1.92	85,85,85,85	0
48	MG	G3	201	1/1	0.88	0.12	-1.95	119,119,119,119	0
48	MG	EL	301	1/1	0.92	0.12	-1.95	119,119,119,119	0
48	MG	F1	3543	1/1	0.92	0.09	-2.01	71,71,71,71	0
48	MG	H1	3514	1/1	0.96	0.07	-2.02	66,66,66,66	0
48	MG	F1	3552	1/1	0.95	0.15	-2.03	139,139,139,139	0
49	ZN	GY	201	1/1	0.98	0.10	-2.04	116,116,116,116	0
48	MG	EJ	201	1/1	0.94	0.12	-2.04	69,69,69,69	0
48	MG	D1	3494	1/1	0.93	0.13	-2.04	78,78,78,78	0
48	MG	D1	3605	1/1	0.65	0.13	-2.09	108,108,108,108	0
48	MG	D1	3452	1/1	0.92	0.15	-2.11	106,106,106,106	0
48	MG	A1	3484	1/1	0.95	0.13	-2.12	108,108,108,108	0
48	MG	A1	3554	1/1	0.88	0.14	-2.14	76,76,76,76	0
49	ZN	BY	201	1/1	0.98	0.09	-2.17	59,59,59,59	0
48	MG	D1	3438	1/1	0.96	0.09	-2.18	39,39,39,39	0
48	MG	A1	3432	1/1	0.98	0.07	-2.18	45,45,45,45	0
49	ZN	FC	201	1/1	0.98	0.04	-2.21	108,108,108,108	0
48	MG	H1	3430	1/1	0.90	0.20	-2.23	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3505	1/1	0.94	0.12	-2.23	137,137,137,137	0
48	MG	D1	3423	1/1	0.94	0.16	-2.25	67,67,67,67	0
48	MG	H1	3464	1/1	0.88	0.15	-2.25	108,108,108,108	0
48	MG	H1	3523	1/1	0.90	0.12	-2.32	167,167,167,167	0
48	MG	H1	3478	1/1	0.78	0.11	-2.32	114,114,114,114	0
48	MG	A1	3444	1/1	0.83	0.13	-2.39	126,126,126,126	0
48	MG	D1	3574	1/1	0.83	0.12	-2.46	80,80,80,80	0
48	MG	H1	3407	1/1	0.88	0.20	-2.48	105,105,105,105	0
49	ZN	HL	201	1/1	0.98	0.08	-2.48	118,118,118,118	0
48	MG	A1	3600	1/1	0.90	0.11	-2.50	111,111,111,111	0
48	MG	D1	3503	1/1	0.97	0.15	-2.53	82,82,82,82	0
48	MG	D1	3535	1/1	0.90	0.17	-2.53	86,86,86,86	0
48	MG	H1	3403	1/1	0.92	0.14	-2.58	111,111,111,111	0
48	MG	A1	3447	1/1	0.91	0.13	-2.61	58,58,58,58	0
48	MG	BQ	202	1/1	0.97	0.07	-2.73	53,53,53,53	0
48	MG	D1	3457	1/1	0.95	0.12	-2.76	34,34,34,34	0
48	MG	F1	3438	1/1	0.99	0.14	-2.80	58,58,58,58	0
48	MG	H1	3448	1/1	0.82	0.15	-2.81	98,98,98,98	0
48	MG	H1	3463	1/1	0.95	0.11	-2.85	78,78,78,78	0
48	MG	H1	3455	1/1	0.91	0.14	-2.92	113,113,113,113	0
48	MG	A1	3483	1/1	0.72	0.14	-2.95	83,83,83,83	0
48	MG	D1	3486	1/1	0.97	0.13	-2.97	47,47,47,47	0
48	MG	D1	3456	1/1	0.97	0.11	-3.00	70,70,70,70	0
48	MG	D1	3469	1/1	0.98	0.10	-3.01	64,64,64,64	0
48	MG	H1	3470	1/1	0.63	0.16	-3.04	140,140,140,140	0
48	MG	D1	3554	1/1	0.99	0.12	-3.04	59,59,59,59	0
48	MG	H1	3439	1/1	0.97	0.13	-3.08	75,75,75,75	0
48	MG	A1	3477	1/1	0.95	0.13	-3.09	62,62,62,62	0
49	ZN	AC	201	1/1	0.96	0.08	-3.13	143,143,143,143	0
48	MG	F1	3499	1/1	0.98	0.04	-3.15	57,57,57,57	0
48	MG	F1	3452	1/1	0.95	0.10	-3.15	50,50,50,50	0
48	MG	F1	3480	1/1	0.94	0.12	-3.16	59,59,59,59	0
48	MG	D1	3464	1/1	0.97	0.08	-3.16	44,44,44,44	0
48	MG	D1	3560	1/1	0.97	0.11	-3.20	64,64,64,64	0
48	MG	F1	3454	1/1	0.98	0.15	-3.26	56,56,56,56	0
48	MG	A1	3460	1/1	0.99	0.13	-3.27	61,61,61,61	0
48	MG	F1	3410	1/1	0.94	0.17	-3.28	42,42,42,42	0
48	MG	CQ	202	1/1	0.97	0.06	-3.35	62,62,62,62	0
48	MG	A1	3456	1/1	0.97	0.12	-3.38	49,49,49,49	0
49	ZN	HK	201	1/1	0.99	0.11	-3.42	70,70,70,70	0
48	MG	GJ	201	1/1	0.95	0.13	-3.52	69,69,69,69	0
48	MG	H1	3437	1/1	0.97	0.11	-3.53	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	D1	3473	1/1	0.96	0.11	-3.58	63,63,63,63	0
48	MG	H1	3451	1/1	0.93	0.12	-3.58	78,78,78,78	0
48	MG	A1	3537	1/1	0.96	0.12	-3.59	54,54,54,54	0
48	MG	H1	3444	1/1	0.97	0.06	-3.59	65,65,65,65	0
48	MG	D1	3545	1/1	0.91	0.15	-3.62	88,88,88,88	0
48	MG	D1	3403	1/1	0.92	0.08	-3.67	89,89,89,89	0
48	MG	H1	3445	1/1	0.96	0.14	-3.68	68,68,68,68	0
48	MG	F1	3481	1/1	0.95	0.13	-3.69	45,45,45,45	0
48	MG	A1	3442	1/1	0.96	0.10	-3.69	52,52,52,52	0
48	MG	F1	3584	1/1	0.95	0.16	-3.75	97,97,97,97	0
48	MG	A1	3489	1/1	0.99	0.07	-3.81	33,33,33,33	0
48	MG	A1	3526	1/1	0.97	0.10	-3.82	48,48,48,48	0
48	MG	D1	3455	1/1	0.94	0.09	-3.85	80,80,80,80	0
48	MG	H1	3461	1/1	0.93	0.15	-3.86	134,134,134,134	0
48	MG	F1	3409	1/1	0.96	0.16	-3.90	60,60,60,60	0
48	MG	H1	3427	1/1	0.94	0.14	-3.99	83,83,83,83	0
48	MG	H1	3454	1/1	0.94	0.12	-3.99	111,111,111,111	0
48	MG	D1	3453	1/1	0.97	0.11	-4.00	54,54,54,54	0
48	MG	H1	3428	1/1	0.94	0.12	-4.02	77,77,77,77	0
48	MG	F1	3460	1/1	0.98	0.14	-4.02	36,36,36,36	0
48	MG	C2	203	1/1	0.97	0.06	-4.10	63,63,63,63	0
48	MG	F1	3450	1/1	0.98	0.09	-4.12	59,59,59,59	0
48	MG	D1	3501	1/1	0.97	0.13	-4.34	51,51,51,51	0
48	MG	F1	3459	1/1	0.97	0.07	-4.44	79,79,79,79	0
48	MG	D1	3410	1/1	0.99	0.12	-4.46	39,39,39,39	0
48	MG	A1	3463	1/1	0.96	0.10	-4.72	59,59,59,59	0
48	MG	F1	3439	1/1	0.90	0.09	-4.83	62,62,62,62	0
48	MG	F1	3402	1/1	0.92	0.09	-4.87	83,83,83,83	0
48	MG	F1	3404	1/1	0.97	0.11	-5.16	75,75,75,75	0
48	MG	D1	3454	1/1	0.93	0.14	-5.19	64,64,64,64	0
48	MG	D1	3411	1/1	0.98	0.11	-5.39	44,44,44,44	0
48	MG	A1	3458	1/1	0.97	0.10	-5.39	59,59,59,59	0
48	MG	D1	3558	1/1	0.94	0.07	-5.55	56,56,56,56	0
48	MG	F1	3436	1/1	0.93	0.10	-6.06	70,70,70,70	0
48	MG	A1	3465	1/1	0.96	0.08	-6.21	54,54,54,54	0
48	MG	D1	3405	1/1	0.98	0.10	-6.21	59,59,59,59	0
48	MG	H1	3440	1/1	0.94	0.08	-6.43	73,73,73,73	0
48	MG	A1	3405	1/1	0.94	0.08	-6.62	65,65,65,65	0
48	MG	A1	3534	1/1	0.99	0.13	-6.91	62,62,62,62	0
48	MG	A1	3473	1/1	0.99	0.08	-7.28	55,55,55,55	0
48	MG	D1	3480	1/1	0.98	0.09	-8.02	32,32,32,32	0
48	MG	D1	3502	1/1	0.99	0.07	-8.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	F1	3523	1/1	0.98	0.09	-8.49	55,55,55,55	0
48	MG	F1	3467	1/1	0.99	0.10	-8.90	57,57,57,57	0
48	MG	D1	3472	1/1	0.90	0.10	-9.60	82,82,82,82	0
48	MG	D1	3428	1/1	0.98	0.06	-10.16	106,106,106,106	0
48	MG	D1	3458	1/1	0.93	0.06	-10.27	51,51,51,51	0
48	MG	F1	3435	1/1	0.99	0.11	-10.56	44,44,44,44	0
48	MG	D1	3479	1/1	0.97	0.04	-10.75	50,50,50,50	0
48	MG	A1	3466	1/1	0.97	0.12	-10.97	40,40,40,40	0
48	MG	H1	3429	1/1	0.91	0.14	-13.56	87,87,87,87	0
48	MG	H1	3528	1/1	0.83	0.22	-	119,119,119,119	0
48	MG	A1	3494	1/1	0.94	0.07	-	98,98,98,98	0
48	MG	BQ	201	1/1	0.66	0.21	-	122,122,122,122	0
48	MG	FA	102	1/1	0.93	0.10	-	84,84,84,84	0
48	MG	F1	3579	1/1	0.90	0.12	-	166,166,166,166	0
48	MG	F1	3431	1/1	0.89	0.17	-	103,103,103,103	0
48	MG	F1	3475	1/1	0.90	0.16	-	93,93,93,93	0
48	MG	H1	3543	1/1	0.52	0.46	-	183,183,183,183	0
48	MG	A1	3572	1/1	0.91	0.23	-	121,121,121,121	0
48	MG	F1	3416	1/1	0.95	0.45	-	116,116,116,116	0
48	MG	EN	201	1/1	0.67	0.17	-	111,111,111,111	0
48	MG	D1	3433	1/1	0.83	0.14	-	149,149,149,149	0
48	MG	H1	3467	1/1	0.92	0.11	-	95,95,95,95	0
48	MG	AA	102	1/1	0.94	0.08	-	98,98,98,98	0
48	MG	A1	3529	1/1	0.90	0.11	-	96,96,96,96	0
48	MG	H1	3496	1/1	0.89	0.44	-	141,141,141,141	0
48	MG	H1	3456	1/1	0.91	0.76	-	145,145,145,145	0
48	MG	F1	3553	1/1	0.90	0.09	-	68,68,68,68	0
48	MG	A1	3408	1/1	0.76	0.27	-	122,122,122,122	0
48	MG	F1	3516	1/1	0.88	0.29	-	121,121,121,121	0
48	MG	F1	3408	1/1	0.86	0.14	-	82,82,82,82	0
48	MG	A1	3470	1/1	0.89	0.32	-	164,164,164,164	0
48	MG	F1	3464	1/1	0.84	0.23	-	120,120,120,120	0
48	MG	H1	3474	1/1	0.92	0.09	-	123,123,123,123	0
48	MG	F1	3415	1/1	0.35	0.32	-	118,118,118,118	0
48	MG	A1	3423	1/1	0.89	0.21	-	115,115,115,115	0
48	MG	F1	3417	1/1	0.94	0.17	-	110,110,110,110	0
48	MG	H1	3487	1/1	0.85	0.19	-	122,122,122,122	0
48	MG	F1	3522	1/1	0.58	0.18	-	111,111,111,111	0
48	MG	H1	3492	1/1	0.78	0.13	-	96,96,96,96	0
48	MG	GN	201	1/1	0.66	0.51	-	212,212,212,212	0
48	MG	A1	3520	1/1	0.95	0.16	-	70,70,70,70	0
48	MG	H1	3503	1/1	0.81	0.26	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3424	1/1	0.88	0.37	-	150,150,150,150	0
48	MG	D1	3621	1/1	0.87	0.15	-	110,110,110,110	0
48	MG	A1	3580	1/1	0.68	0.21	-	130,130,130,130	0
48	MG	GL	301	1/1	0.95	0.11	-	113,113,113,113	0
48	MG	F1	3502	1/1	0.89	0.26	-	108,108,108,108	0
48	MG	H1	3471	1/1	0.94	0.22	-	124,124,124,124	0
48	MG	G2	203	1/1	0.96	0.10	-	112,112,112,112	0
48	MG	F1	3526	1/1	0.96	0.14	-	72,72,72,72	0
48	MG	A1	3535	1/1	0.95	0.09	-	99,99,99,99	0
48	MG	F1	3536	1/1	0.94	0.20	-	67,67,67,67	0
48	MG	F1	3508	1/1	0.96	0.24	-	127,127,127,127	0
48	MG	D1	3406	1/1	0.91	0.14	-	67,67,67,67	0
48	MG	D1	3562	1/1	0.92	0.22	-	93,93,93,93	0
48	MG	A1	3568	1/1	0.34	0.36	-	173,173,173,173	0
48	MG	H1	3542	1/1	0.69	0.37	-	137,137,137,137	0
48	MG	F1	3510	1/1	0.97	0.10	-	95,95,95,95	0
48	MG	F1	3447	1/1	0.82	0.30	-	156,156,156,156	0
48	MG	F1	3573	1/1	0.83	0.08	-	84,84,84,84	0
48	MG	D1	3575	1/1	0.87	0.13	-	124,124,124,124	0
48	MG	F1	3474	1/1	0.97	0.13	-	64,64,64,64	0
48	MG	F1	3446	1/1	0.89	0.20	-	130,130,130,130	0
48	MG	A1	3420	1/1	0.75	0.30	-	155,155,155,155	0
48	MG	CL	302	1/1	0.97	0.10	-	68,68,68,68	0
48	MG	A1	3592	1/1	0.68	0.30	-	134,134,134,134	0
48	MG	D1	3592	1/1	0.63	0.97	-	159,159,159,159	0
48	MG	A1	3481	1/1	0.94	0.16	-	88,88,88,88	0
48	MG	D1	3420	1/1	0.97	0.08	-	105,105,105,105	0
48	MG	C2	205	1/1	0.84	0.18	-	127,127,127,127	0
48	MG	E2	201	1/1	0.83	0.34	-	156,156,156,156	0
48	MG	B2	206	1/1	0.88	0.45	-	139,139,139,139	0
48	MG	H1	3401	1/1	0.65	0.12	-	146,146,146,146	0
48	MG	D1	3584	1/1	0.94	0.13	-	101,101,101,101	0
48	MG	D1	3518	1/1	0.96	0.21	-	92,92,92,92	0
48	MG	D1	3523	1/1	0.89	0.11	-	105,105,105,105	0
48	MG	H1	3499	1/1	0.89	0.11	-	75,75,75,75	0
48	MG	D1	3555	1/1	0.95	0.39	-	119,119,119,119	0
48	MG	H1	3449	1/1	0.89	0.62	-	118,118,118,118	0
48	MG	A1	3545	1/1	0.95	0.30	-	71,71,71,71	0
48	MG	F1	3458	1/1	0.93	0.09	-	95,95,95,95	0
48	MG	F1	3582	1/1	0.95	0.20	-	77,77,77,77	0
48	MG	D1	3414	1/1	0.93	0.15	-	96,96,96,96	0
48	MG	A1	3571	1/1	0.85	0.24	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	D1	3527	1/1	0.93	0.28	-	106,106,106,106	0
48	MG	G2	205	1/1	0.64	0.18	-	146,146,146,146	0
48	MG	D1	3602	1/1	0.88	0.19	-	118,118,118,118	0
48	MG	F1	3565	1/1	0.80	0.86	-	168,168,168,168	0
48	MG	F1	3540	1/1	0.53	0.21	-	111,111,111,111	0
48	MG	D1	3594	1/1	0.82	0.23	-	106,106,106,106	0
48	MG	H1	3450	1/1	0.53	0.73	-	156,156,156,156	0
48	MG	D1	3631	1/1	0.85	0.08	-	78,78,78,78	0
48	MG	F1	3546	1/1	0.98	0.07	-	59,59,59,59	0
48	MG	A1	3541	1/1	0.93	0.35	-	86,86,86,86	0
48	MG	D1	3426	1/1	0.85	0.38	-	143,143,143,143	0
48	MG	D1	3461	1/1	0.96	0.10	-	86,86,86,86	0
48	MG	A1	3561	1/1	0.98	0.14	-	60,60,60,60	0
48	MG	H1	3446	1/1	0.77	0.34	-	120,120,120,120	0
48	MG	A1	3504	1/1	0.94	0.49	-	138,138,138,138	0
48	MG	D1	3522	1/1	0.86	0.64	-	162,162,162,162	0
48	MG	F1	3559	1/1	0.89	0.10	-	133,133,133,133	0
48	MG	A1	3406	1/1	0.95	0.10	-	75,75,75,75	0
48	MG	A1	3453	1/1	0.83	0.72	-	184,184,184,184	0
48	MG	F1	3557	1/1	0.94	0.15	-	84,84,84,84	0
48	MG	GA	301	1/1	0.75	0.24	-	142,142,142,142	0
48	MG	AK	202	1/1	0.92	0.72	-	179,179,179,179	0
48	MG	D1	3608	1/1	0.53	0.23	-	115,115,115,115	0
48	MG	D1	3431	1/1	0.94	0.19	-	95,95,95,95	0
48	MG	A1	3499	1/1	0.82	0.16	-	117,117,117,117	0
48	MG	D1	3415	1/1	0.95	0.11	-	117,117,117,117	0
48	MG	GW	201	1/1	0.91	0.22	-	114,114,114,114	0
48	MG	F1	3463	1/1	0.86	0.19	-	100,100,100,100	0
48	MG	A1	3543	1/1	0.98	0.08	-	96,96,96,96	0
48	MG	H1	3426	1/1	0.85	0.15	-	105,105,105,105	0
48	MG	H1	3410	1/1	0.73	0.44	-	192,192,192,192	0
48	MG	D1	3564	1/1	0.94	0.21	-	92,92,92,92	0
48	MG	H1	3538	1/1	0.59	0.28	-	140,140,140,140	0
48	MG	D1	3616	1/1	0.62	0.20	-	150,150,150,150	0
48	MG	H1	3511	1/1	0.66	0.27	-	140,140,140,140	0
48	MG	D1	3507	1/1	0.91	0.10	-	75,75,75,75	0
48	MG	H1	3505	1/1	0.92	0.11	-	95,95,95,95	0
48	MG	F1	3484	1/1	0.89	0.17	-	78,78,78,78	0
48	MG	F1	3517	1/1	0.92	0.11	-	62,62,62,62	0
48	MG	F1	3574	1/1	0.71	0.70	-	161,161,161,161	0
48	MG	H1	3412	1/1	0.59	0.89	-	173,173,173,173	0
48	MG	F1	3412	1/1	0.95	0.11	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	F1	3520	1/1	0.91	0.19	-	85,85,85,85	0
48	MG	A1	3409	1/1	0.84	0.14	-	87,87,87,87	0
48	MG	H1	3489	1/1	0.10	0.45	-	206,206,206,206	0
48	MG	A1	3540	1/1	0.97	0.15	-	66,66,66,66	0
48	MG	F1	3442	1/1	0.92	0.27	-	109,109,109,109	0
48	MG	D1	3538	1/1	0.90	0.10	-	119,119,119,119	0
48	MG	BP	200	1/1	0.88	0.10	-	123,123,123,123	0
48	MG	A1	3563	1/1	0.89	0.13	-	100,100,100,100	0
48	MG	F1	3432	1/1	0.97	0.08	-	68,68,68,68	0
48	MG	B3	201	1/1	0.59	0.28	-	129,129,129,129	0
48	MG	A1	3512	1/1	0.88	0.10	-	90,90,90,90	0
48	MG	D1	3492	1/1	0.94	0.34	-	125,125,125,125	0
48	MG	F1	3485	1/1	0.88	0.16	-	117,117,117,117	0
48	MG	D1	3536	1/1	0.97	0.10	-	73,73,73,73	0
48	MG	A1	3449	1/1	0.75	0.23	-	115,115,115,115	0
48	MG	D1	3463	1/1	-0.16	1.03	-	176,176,176,176	0
48	MG	H1	3443	1/1	0.82	0.42	-	157,157,157,157	0
48	MG	EW	202	1/1	0.75	0.21	-	121,121,121,121	0
48	MG	D1	3601	1/1	0.94	0.22	-	124,124,124,124	0
48	MG	D1	3531	1/1	0.93	0.08	-	87,87,87,87	0
48	MG	A1	3434	1/1	0.95	0.16	-	74,74,74,74	0
48	MG	D1	3488	1/1	0.95	0.18	-	97,97,97,97	0
48	MG	A1	3575	1/1	0.90	0.62	-	143,143,143,143	0
48	MG	F1	3515	1/1	0.39	0.41	-	143,143,143,143	0
48	MG	AA	103	1/1	0.94	0.08	-	56,56,56,56	0
48	MG	D1	3498	1/1	0.88	0.47	-	99,99,99,99	0
48	MG	H1	3477	1/1	0.68	0.30	-	103,103,103,103	0
48	MG	D1	3440	1/1	0.89	0.12	-	99,99,99,99	0
48	MG	D1	3597	1/1	0.69	0.83	-	158,158,158,158	0
48	MG	D1	3534	1/1	0.85	0.20	-	98,98,98,98	0
48	MG	D1	3528	1/1	0.39	0.26	-	123,123,123,123	0
48	MG	D1	3459	1/1	0.96	0.07	-	63,63,63,63	0
48	MG	F1	3539	1/1	0.46	1.12	-	187,187,187,187	0
48	MG	C3	205	1/1	0.76	1.45	-	175,175,175,175	0
48	MG	A1	3498	1/1	0.91	0.11	-	116,116,116,116	0
48	MG	F1	3519	1/1	0.77	0.16	-	65,65,65,65	0
48	MG	H1	3548	1/1	0.40	0.38	-	188,188,188,188	0
48	MG	D1	3475	1/1	0.87	0.51	-	120,120,120,120	0
48	MG	H1	3541	1/1	0.46	0.35	-	154,154,154,154	0
48	MG	H1	3555	1/1	0.89	0.15	-	123,123,123,123	0
48	MG	F1	3576	1/1	0.77	0.45	-	142,142,142,142	0
48	MG	F1	3449	1/1	0.97	0.11	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	F1	3581	1/1	0.90	0.38	-	144,144,144,144	0
48	MG	D1	3430	1/1	0.98	0.08	-	59,59,59,59	0
48	MG	F1	3569	1/1	0.86	0.40	-	130,130,130,130	0
48	MG	H1	3432	1/1	0.91	0.09	-	91,91,91,91	0
48	MG	A1	3503	1/1	0.77	0.16	-	95,95,95,95	0
48	MG	F1	3542	1/1	0.86	0.13	-	107,107,107,107	0
48	MG	D1	3495	1/1	0.96	0.07	-	88,88,88,88	0
48	MG	F1	3505	1/1	0.98	0.09	-	83,83,83,83	0
48	MG	A1	3469	1/1	0.94	0.17	-	113,113,113,113	0
48	MG	H1	3524	1/1	0.74	0.57	-	139,139,139,139	0
48	MG	D1	3588	1/1	0.77	0.18	-	156,156,156,156	0
48	MG	C2	206	1/1	0.81	0.31	-	123,123,123,123	0
48	MG	H1	3525	1/1	0.42	0.39	-	157,157,157,157	0
48	MG	D1	3404	1/1	0.96	0.11	-	55,55,55,55	0
48	MG	H1	3411	1/1	0.82	0.32	-	120,120,120,120	0
48	MG	F1	3558	1/1	0.84	0.17	-	144,144,144,144	0
48	MG	D1	3450	1/1	0.95	0.07	-	49,49,49,49	0
48	MG	D1	3460	1/1	0.96	0.09	-	85,85,85,85	0
48	MG	A1	3577	1/1	0.77	0.15	-	104,104,104,104	0
48	MG	A1	3415	1/1	0.88	0.20	-	120,120,120,120	0
48	MG	A1	3570	1/1	0.93	0.08	-	70,70,70,70	0
48	MG	D1	3487	1/1	0.93	0.09	-	65,65,65,65	0
48	MG	H1	3465	1/1	0.84	0.42	-	143,143,143,143	0
48	MG	F1	3470	1/1	0.92	0.09	-	49,49,49,49	0
48	MG	D1	3557	1/1	0.82	0.13	-	116,116,116,116	0
48	MG	D1	3524	1/1	0.95	0.06	-	69,69,69,69	0
48	MG	D1	3566	1/1	0.95	0.14	-	80,80,80,80	0
48	MG	CY	201	1/1	0.92	0.20	-	99,99,99,99	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
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	3555	1/1	0.70	0.27	-	168,168,168,168	0
48	MG	A1	3457	1/1	0.97	0.35	-	94,94,94,94	0
48	MG	H1	3404	1/1	0.89	0.11	-	132,132,132,132	0
48	MG	D1	3416	1/1	0.91	0.24	-	110,110,110,110	0
48	MG	D1	3409	1/1	0.91	0.13	-	57,57,57,57	0
48	MG	EW	201	1/1	-0.02	0.33	-	172,172,172,172	0
48	MG	E3	204	1/1	0.36	1.60	-	199,199,199,199	0
48	MG	F1	3504	1/1	0.95	0.13	-	84,84,84,84	0
48	MG	D1	3580	1/1	0.85	0.11	-	95,95,95,95	0
48	MG	A1	3599	1/1	0.93	0.12	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	H1	3516	1/1	0.66	0.28	-	129,129,129,129	0
48	MG	B3	202	1/1	0.80	0.15	-	113,113,113,113	0
48	MG	D1	3425	1/1	0.83	0.59	-	123,123,123,123	0
48	MG	A1	3517	1/1	0.97	0.08	-	74,74,74,74	0
48	MG	A1	3521	1/1	0.92	0.12	-	105,105,105,105	0
48	MG	A1	3492	1/1	0.89	0.28	-	127,127,127,127	0
48	MG	F1	3568	1/1	0.91	0.13	-	98,98,98,98	0
48	MG	G3	202	1/1	0.20	0.61	-	136,136,136,136	0
48	MG	D1	3493	1/1	0.96	0.33	-	128,128,128,128	0
48	MG	G3	203	1/1	0.92	0.13	-	86,86,86,86	0
48	MG	A1	3515	1/1	0.66	0.25	-	111,111,111,111	0
48	MG	H1	3485	1/1	0.88	0.12	-	104,104,104,104	0
48	MG	A1	3594	1/1	0.85	0.28	-	150,150,150,150	0
48	MG	A1	3495	1/1	0.97	0.06	-	70,70,70,70	0
48	MG	H1	3468	1/1	0.89	0.23	-	121,121,121,121	0
48	MG	H1	3453	1/1	0.96	0.11	-	66,66,66,66	0
48	MG	H1	3544	1/1	0.44	0.98	-	146,146,146,146	0
48	MG	D1	3513	1/1	0.85	0.16	-	89,89,89,89	0
48	MG	F1	3503	1/1	0.78	0.17	-	129,129,129,129	0
48	MG	H1	3502	1/1	0.96	0.07	-	82,82,82,82	0
48	MG	D1	3561	1/1	0.86	0.19	-	57,57,57,57	0
48	MG	F1	3548	1/1	0.81	0.12	-	106,106,106,106	0
48	MG	H1	3554	1/1	0.62	0.68	-	128,128,128,128	0
48	MG	A1	3448	1/1	0.94	0.14	-	78,78,78,78	0
48	MG	A1	3557	1/1	0.96	0.20	-	104,104,104,104	0
48	MG	H1	3422	1/1	0.83	0.45	-	151,151,151,151	0
48	MG	D1	3618	1/1	0.87	0.09	-	95,95,95,95	0
48	MG	H1	3405	1/1	0.93	0.25	-	101,101,101,101	0
48	MG	D1	3448	1/1	0.79	0.22	-	125,125,125,125	0
48	MG	A1	3480	1/1	0.95	0.32	-	120,120,120,120	0
48	MG	BN	201	1/1	0.84	0.22	-	147,147,147,147	0
48	MG	A1	3531	1/1	0.87	0.28	-	128,128,128,128	0
48	MG	F1	3424	1/1	0.84	0.31	-	114,114,114,114	0
48	MG	FK	201	1/1	0.91	0.50	-	168,168,168,168	0
48	MG	F1	3495	1/1	0.86	0.12	-	83,83,83,83	0
48	MG	F1	3507	1/1	0.94	0.17	-	87,87,87,87	0
48	MG	D1	3476	1/1	0.91	0.08	-	43,43,43,43	0
48	MG	F1	3440	1/1	0.90	0.11	-	82,82,82,82	0
48	MG	H1	3539	1/1	0.76	0.34	-	128,128,128,128	0
48	MG	H1	3540	1/1	0.63	0.20	-	136,136,136,136	0
48	MG	B2	208	1/1	0.84	0.42	-	138,138,138,138	0
48	MG	D1	3596	1/1	0.73	0.66	-	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	D1	3627	1/1	0.81	0.08	-	119,119,119,119	0
48	MG	D1	3413	1/1	0.94	0.09	-	51,51,51,51	0
48	MG	F1	3406	1/1	0.93	0.08	-	83,83,83,83	0
48	MG	D1	3586	1/1	0.80	0.16	-	109,109,109,109	0
48	MG	A1	3417	1/1	0.66	0.28	-	150,150,150,150	0
48	MG	A1	3476	1/1	0.98	0.06	-	59,59,59,59	0
48	MG	A1	3576	1/1	0.76	0.40	-	122,122,122,122	0
48	MG	D1	3490	1/1	0.97	0.16	-	92,92,92,92	0
48	MG	A1	3478	1/1	0.95	0.08	-	79,79,79,79	0
48	MG	H1	3459	1/1	0.87	0.10	-	97,97,97,97	0
48	MG	D1	3568	1/1	0.91	0.17	-	105,105,105,105	0
48	MG	A1	3582	1/1	0.75	0.19	-	110,110,110,110	0
48	MG	F1	3497	1/1	0.91	0.12	-	93,93,93,93	0
48	MG	BW	201	1/1	0.97	0.09	-	67,67,67,67	0
48	MG	D1	3604	1/1	0.81	0.44	-	141,141,141,141	0
48	MG	A1	3523	1/1	0.96	0.12	-	91,91,91,91	0
48	MG	D1	3489	1/1	0.98	0.07	-	44,44,44,44	0
48	MG	A1	3428	1/1	0.53	0.60	-	159,159,159,159	0
48	MG	B2	201	1/1	0.73	0.20	-	119,119,119,119	0
48	MG	H1	3547	1/1	0.44	0.32	-	175,175,175,175	0
48	MG	FA	101	1/1	0.91	0.11	-	97,97,97,97	0
48	MG	F1	3423	1/1	0.87	0.08	-	56,56,56,56	0
48	MG	D1	3441	1/1	0.91	0.15	-	75,75,75,75	0
48	MG	D1	3446	1/1	0.66	0.83	-	176,176,176,176	0
48	MG	A1	3595	1/1	0.73	1.09	-	151,151,151,151	0
48	MG	F1	3478	1/1	0.94	0.12	-	73,73,73,73	0
48	MG	A1	3555	1/1	0.79	0.58	-	128,128,128,128	0
48	MG	A1	3436	1/1	0.66	0.23	-	110,110,110,110	0
48	MG	F1	3511	1/1	0.77	0.71	-	154,154,154,154	0
48	MG	H1	3537	1/1	0.76	0.18	-	152,152,152,152	0
48	MG	D1	3419	1/1	0.95	0.10	-	92,92,92,92	0
48	MG	F1	3403	1/1	0.85	0.11	-	96,96,96,96	0
48	MG	H1	3458	1/1	0.98	0.06	-	90,90,90,90	0
48	MG	F1	3554	1/1	0.76	0.18	-	131,131,131,131	0
48	MG	A1	3461	1/1	0.82	0.14	-	67,67,67,67	0
48	MG	A1	3433	1/1	0.79	0.10	-	84,84,84,84	0
48	MG	A1	3513	1/1	0.84	0.33	-	133,133,133,133	0
48	MG	D1	3462	1/1	0.97	0.19	-	116,116,116,116	0
48	MG	D1	3515	1/1	0.86	0.15	-	106,106,106,106	0
48	MG	H1	3522	1/1	0.93	0.16	-	107,107,107,107	0
48	MG	H1	3500	1/1	0.95	0.17	-	82,82,82,82	0
48	MG	C3	207	1/1	0.69	0.62	-	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	F1	3444	1/1	0.92	0.42	-	155,155,155,155	0
48	MG	F1	3457	1/1	0.90	0.27	-	91,91,91,91	0
48	MG	F1	3580	1/1	0.75	0.21	-	147,147,147,147	0
48	MG	F1	3545	1/1	0.85	0.21	-	137,137,137,137	0
48	MG	A1	3514	1/1	0.96	0.14	-	59,59,59,59	0
48	MG	E2	207	1/1	0.90	0.41	-	147,147,147,147	0
48	MG	CW	201	1/1	0.87	0.30	-	90,90,90,90	0
48	MG	A1	3567	1/1	0.76	0.31	-	144,144,144,144	0
48	MG	F1	3535	1/1	0.90	0.11	-	58,58,58,58	0
48	MG	H1	3433	1/1	0.81	0.19	-	132,132,132,132	0
48	MG	A1	3574	1/1	0.87	0.15	-	119,119,119,119	0
48	MG	H1	3501	1/1	0.89	0.30	-	110,110,110,110	0
48	MG	D1	3482	1/1	0.85	0.15	-	106,106,106,106	0
48	MG	D1	3449	1/1	0.95	0.09	-	68,68,68,68	0
48	MG	F1	3433	1/1	0.84	0.64	-	95,95,95,95	0
48	MG	D1	3483	1/1	0.96	0.09	-	88,88,88,88	0
48	MG	D1	3477	1/1	0.95	0.09	-	60,60,60,60	0
48	MG	D1	3600	1/1	0.73	0.40	-	123,123,123,123	0
48	MG	D1	3508	1/1	0.94	0.05	-	86,86,86,86	0
48	MG	A1	3467	1/1	0.91	0.19	-	106,106,106,106	0
48	MG	H1	3518	1/1	0.90	0.14	-	110,110,110,110	0
48	MG	A1	3454	1/1	0.73	0.18	-	101,101,101,101	0
48	MG	F1	3489	1/1	0.72	0.10	-	85,85,85,85	0
48	MG	D1	3424	1/1	0.74	0.43	-	150,150,150,150	0
48	MG	F1	3429	1/1	0.91	0.17	-	73,73,73,73	0
48	MG	F1	3448	1/1	0.79	0.16	-	126,126,126,126	0
48	MG	H1	3416	1/1	0.91	0.66	-	113,113,113,113	0
48	MG	H1	3490	1/1	0.84	0.55	-	122,122,122,122	0
48	MG	D1	3532	1/1	0.87	0.14	-	119,119,119,119	0
48	MG	F1	3407	1/1	0.92	0.10	-	111,111,111,111	0
48	MG	H1	3483	1/1	0.94	0.14	-	108,108,108,108	0
48	MG	A1	3598	1/1	0.97	0.21	-	111,111,111,111	0
48	MG	D1	3590	1/1	0.95	0.20	-	89,89,89,89	0
48	MG	H1	3553	1/1	0.81	0.39	-	146,146,146,146	0
48	MG	A1	3525	1/1	0.98	0.08	-	51,51,51,51	0
48	MG	D1	3563	1/1	0.87	0.12	-	93,93,93,93	0
48	MG	D1	3478	1/1	0.94	0.12	-	81,81,81,81	0
48	MG	A1	3565	1/1	0.83	0.13	-	132,132,132,132	0
48	MG	H1	3533	1/1	0.63	1.06	-	153,153,153,153	0
48	MG	A1	3559	1/1	0.93	0.06	-	89,89,89,89	0
48	MG	D1	3565	1/1	0.82	0.33	-	114,114,114,114	0
48	MG	A1	3502	1/1	0.99	0.10	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3583	1/1	0.64	0.44	-	112,112,112,112	0
48	MG	E3	202	1/1	0.91	0.20	-	122,122,122,122	0
48	MG	H1	3495	1/1	0.93	0.06	-	65,65,65,65	0
48	MG	D1	3614	1/1	0.84	0.19	-	129,129,129,129	0
48	MG	H1	3447	1/1	0.92	0.25	-	110,110,110,110	0
48	MG	A1	3569	1/1	0.85	0.09	-	91,91,91,91	0
48	MG	H1	3536	1/1	0.60	0.86	-	168,168,168,168	0
48	MG	G2	206	1/1	0.67	0.90	-	174,174,174,174	0
48	MG	A1	3441	1/1	0.93	0.50	-	127,127,127,127	0
48	MG	F1	3529	1/1	0.86	0.71	-	140,140,140,140	0
48	MG	F1	3530	1/1	0.94	0.15	-	107,107,107,107	0
48	MG	D1	3576	1/1	0.72	0.54	-	150,150,150,150	0
48	MG	D1	3623	1/1	0.87	0.26	-	151,151,151,151	0
48	MG	D1	3442	1/1	0.79	0.35	-	126,126,126,126	0
48	MG	H1	3420	1/1	0.69	0.26	-	113,113,113,113	0
48	MG	E2	202	1/1	0.69	0.18	-	89,89,89,89	0
48	MG	A1	3482	1/1	0.95	0.06	-	62,62,62,62	0
48	MG	E2	204	1/1	0.97	0.06	-	75,75,75,75	0
48	MG	H1	3414	1/1	0.60	0.54	-	169,169,169,169	0
48	MG	A1	3532	1/1	0.89	0.07	-	74,74,74,74	0
48	MG	D1	3556	1/1	0.98	0.07	-	76,76,76,76	0
48	MG	EN	202	1/1	0.84	1.13	-	238,238,238,238	0
48	MG	F1	3564	1/1	0.76	0.38	-	143,143,143,143	0
48	MG	A1	3429	1/1	0.92	0.11	-	122,122,122,122	0
48	MG	A1	3522	1/1	0.63	1.27	-	146,146,146,146	0
48	MG	A1	3506	1/1	0.95	0.12	-	77,77,77,77	0
48	MG	F1	3521	1/1	0.96	0.09	-	65,65,65,65	0
48	MG	A1	3468	1/1	0.92	0.18	-	109,109,109,109	0
48	MG	D1	3533	1/1	0.99	0.07	-	41,41,41,41	0
48	MG	D1	3474	1/1	0.95	0.10	-	58,58,58,58	0
48	MG	BL	301	1/1	0.93	0.09	-	71,71,71,71	0
48	MG	A1	3590	1/1	0.89	0.26	-	142,142,142,142	0
48	MG	F1	3494	1/1	0.93	0.12	-	97,97,97,97	0
48	MG	H1	3484	1/1	0.86	0.24	-	166,166,166,166	0
48	MG	A1	3414	1/1	0.76	0.19	-	142,142,142,142	0
48	MG	H1	3493	1/1	0.97	0.12	-	79,79,79,79	0
48	MG	F1	3533	1/1	0.94	0.17	-	101,101,101,101	0
48	MG	H1	3479	1/1	0.53	0.43	-	132,132,132,132	0
48	MG	F1	3487	1/1	0.96	0.09	-	60,60,60,60	0
48	MG	H1	3491	1/1	0.95	0.13	-	111,111,111,111	0
48	MG	F1	3413	1/1	0.85	0.38	-	110,110,110,110	0
48	MG	D1	3447	1/1	0.91	0.23	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	F1	3456	1/1	0.89	0.07	-	62,62,62,62	0
48	MG	H1	3531	1/1	0.70	0.60	-	157,157,157,157	0
48	MG	A1	3596	1/1	0.90	0.30	-	163,163,163,163	0
48	MG	E3	201	1/1	0.95	0.09	-	90,90,90,90	0
48	MG	F1	3418	1/1	0.94	0.12	-	126,126,126,126	0
48	MG	A1	3464	1/1	0.92	0.06	-	64,64,64,64	0
48	MG	A1	3407	1/1	0.94	0.11	-	83,83,83,83	0
48	MG	A1	3587	1/1	0.75	1.10	-	182,182,182,182	0
48	MG	F1	3428	1/1	0.82	0.30	-	111,111,111,111	0
48	MG	D1	3583	1/1	0.75	0.32	-	139,139,139,139	0
48	MG	D1	3408	1/1	0.95	0.30	-	106,106,106,106	0
48	MG	D1	3577	1/1	0.89	0.22	-	121,121,121,121	0
48	MG	F1	3560	1/1	0.75	0.47	-	169,169,169,169	0
48	MG	A1	3586	1/1	0.81	0.72	-	177,177,177,177	0
48	MG	A1	3439	1/1	0.92	0.08	-	106,106,106,106	0
48	MG	H1	3418	1/1	0.74	0.21	-	141,141,141,141	0
48	MG	D1	3552	1/1	0.92	0.06	-	55,55,55,55	0
48	MG	D1	3585	1/1	0.93	0.08	-	108,108,108,108	0
48	MG	F1	3401	1/1	0.87	0.35	-	101,101,101,101	0
48	MG	C2	204	1/1	0.97	0.07	-	75,75,75,75	0
48	MG	A1	3573	1/1	0.54	0.47	-	186,186,186,186	0
48	MG	F1	3575	1/1	0.44	0.25	-	130,130,130,130	0
48	MG	D1	3525	1/1	0.87	0.33	-	113,113,113,113	0
48	MG	D1	3470	1/1	0.58	0.38	-	134,134,134,134	0
48	MG	H1	3438	1/1	0.83	0.29	-	120,120,120,120	0
48	MG	G3	205	1/1	0.64	0.94	-	171,171,171,171	0
48	MG	H1	3551	1/1	0.12	3.29	-	202,202,202,202	0
48	MG	D1	3591	1/1	0.95	0.10	-	55,55,55,55	0
48	MG	D1	3526	1/1	0.96	0.05	-	54,54,54,54	0
48	MG	A1	3548	1/1	0.92	0.16	-	124,124,124,124	0
48	MG	A1	3539	1/1	0.96	0.08	-	46,46,46,46	0
48	MG	D1	3571	1/1	0.77	0.43	-	130,130,130,130	0
48	MG	H1	3527	1/1	0.93	0.14	-	99,99,99,99	0
48	MG	D1	3539	1/1	0.97	0.14	-	57,57,57,57	0
48	MG	D1	3436	1/1	0.96	0.16	-	78,78,78,78	0
48	MG	D1	3444	1/1	0.86	0.22	-	139,139,139,139	0
48	MG	F1	3578	1/1	0.60	0.79	-	161,161,161,161	0
48	MG	H1	3520	1/1	0.93	0.17	-	114,114,114,114	0
48	MG	H1	3526	1/1	0.74	0.23	-	94,94,94,94	0
48	MG	A1	3450	1/1	0.85	0.20	-	133,133,133,133	0
48	MG	H1	3462	1/1	0.84	0.36	-	131,131,131,131	0
48	MG	A1	3508	1/1	0.95	0.12	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	G2	201	1/1	0.85	0.14	-	141,141,141,141	0
48	MG	A1	3585	1/1	0.47	0.45	-	152,152,152,152	0
48	MG	A1	3593	1/1	0.66	0.72	-	158,158,158,158	0
48	MG	F1	3421	1/1	0.59	0.35	-	174,174,174,174	0
48	MG	H1	3512	1/1	0.86	0.31	-	121,121,121,121	0
48	MG	D1	3439	1/1	0.87	0.38	-	146,146,146,146	0
48	MG	A1	3516	1/1	0.88	0.23	-	88,88,88,88	0
48	MG	A1	3560	1/1	0.93	0.45	-	138,138,138,138	0
48	MG	F1	3549	1/1	0.83	0.20	-	125,125,125,125	0
48	MG	A1	3588	1/1	0.62	0.26	-	144,144,144,144	0
48	MG	F1	3532	1/1	0.87	0.19	-	87,87,87,87	0
48	MG	F1	3430	1/1	0.61	0.15	-	128,128,128,128	0
48	MG	D1	3530	1/1	0.84	0.16	-	94,94,94,94	0
48	MG	H1	3425	1/1	0.88	0.31	-	108,108,108,108	0
48	MG	C2	202	1/1	0.91	0.23	-	112,112,112,112	0
48	MG	D1	3630	1/1	0.97	0.14	-	71,71,71,71	0
48	MG	A1	3552	1/1	0.86	0.11	-	97,97,97,97	0
48	MG	A1	3544	1/1	0.95	0.48	-	135,135,135,135	0
48	MG	D1	3613	1/1	0.83	0.23	-	120,120,120,120	0
48	MG	D1	3521	1/1	0.65	0.28	-	129,129,129,129	0
48	MG	D1	3622	1/1	0.86	0.30	-	133,133,133,133	0
48	MG	H1	3515	1/1	0.97	0.09	-	73,73,73,73	0
48	MG	A1	3455	1/1	0.87	0.13	-	111,111,111,111	0
48	MG	F1	3567	1/1	0.82	0.42	-	128,128,128,128	0
48	MG	D1	3578	1/1	0.96	0.07	-	88,88,88,88	0
48	MG	F1	3490	1/1	0.55	0.22	-	139,139,139,139	0
48	MG	F1	3556	1/1	0.88	0.08	-	90,90,90,90	0
48	MG	D1	3506	1/1	0.91	0.30	-	132,132,132,132	0
48	MG	D1	3548	1/1	0.68	0.95	-	183,183,183,183	0
48	MG	C3	201	1/1	0.94	0.34	-	123,123,123,123	0
48	MG	D1	3465	1/1	0.96	0.09	-	65,65,65,65	0
48	MG	F1	3443	1/1	0.94	0.05	-	104,104,104,104	0
48	MG	D1	3572	1/1	0.92	0.23	-	69,69,69,69	0
48	MG	A1	3419	1/1	0.80	0.14	-	100,100,100,100	0
48	MG	F1	3527	1/1	0.87	0.30	-	105,105,105,105	0
48	MG	H1	3481	1/1	0.44	0.29	-	134,134,134,134	0
48	MG	A1	3486	1/1	0.94	0.15	-	93,93,93,93	0
48	MG	A1	3485	1/1	0.95	0.15	-	137,137,137,137	0
48	MG	F1	3500	1/1	0.88	0.16	-	105,105,105,105	0
48	MG	A1	3597	1/1	0.97	0.38	-	133,133,133,133	0
48	MG	D1	3553	1/1	0.94	0.07	-	90,90,90,90	0
48	MG	H1	3508	1/1	0.92	0.16	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3438	1/1	0.88	0.23	-	148,148,148,148	0
48	MG	F1	3524	1/1	0.95	0.14	-	56,56,56,56	0
48	MG	F1	3473	1/1	0.87	0.42	-	156,156,156,156	0
48	MG	D1	3579	1/1	0.72	0.10	-	97,97,97,97	0
48	MG	H1	3480	1/1	0.92	0.14	-	81,81,81,81	0
48	MG	D1	3549	1/1	0.90	0.13	-	99,99,99,99	0
48	MG	H1	3413	1/1	0.78	0.21	-	117,117,117,117	0
48	MG	F1	3550	1/1	0.79	0.21	-	154,154,154,154	0
48	MG	H1	3517	1/1	0.93	0.16	-	79,79,79,79	0
48	MG	D1	3624	1/1	0.57	0.61	-	162,162,162,162	0
48	MG	F1	3528	1/1	0.98	0.06	-	75,75,75,75	0
48	MG	D1	3435	1/1	0.83	0.14	-	108,108,108,108	0
48	MG	D1	3520	1/1	0.93	0.11	-	93,93,93,93	0
48	MG	F1	3471	1/1	0.94	0.17	-	90,90,90,90	0
48	MG	D1	3615	1/1	0.83	0.24	-	132,132,132,132	0
48	MG	A1	3542	1/1	0.88	0.22	-	96,96,96,96	0
48	MG	H1	3494	1/1	0.96	0.14	-	56,56,56,56	0
48	MG	F1	3419	1/1	0.56	0.11	-	124,124,124,124	0
48	MG	F1	3518	1/1	0.96	0.13	-	77,77,77,77	0
48	MG	H1	3498	1/1	0.96	0.07	-	60,60,60,60	0
48	MG	D1	3626	1/1	0.81	0.20	-	137,137,137,137	0
48	MG	H1	3550	1/1	0.68	0.44	-	152,152,152,152	0
48	MG	F1	3434	1/1	0.87	0.13	-	83,83,83,83	0
48	MG	A1	3427	1/1	0.61	0.26	-	152,152,152,152	0
48	MG	D1	3540	1/1	0.83	0.20	-	139,139,139,139	0
48	MG	D1	3529	1/1	0.96	0.10	-	80,80,80,80	0
48	MG	F1	3562	1/1	0.91	0.41	-	140,140,140,140	0
48	MG	D1	3451	1/1	0.92	0.42	-	115,115,115,115	0
48	MG	F1	3512	1/1	0.96	0.11	-	94,94,94,94	0
48	MG	A1	3562	1/1	0.93	0.20	-	91,91,91,91	0
48	MG	CQ	201	1/1	0.86	0.18	-	127,127,127,127	0
48	MG	D1	3593	1/1	0.76	0.36	-	180,180,180,180	0
48	MG	F1	3498	1/1	0.82	0.22	-	141,141,141,141	0
48	MG	D1	3443	1/1	0.92	0.48	-	112,112,112,112	0
48	MG	D1	3402	1/1	0.95	0.08	-	52,52,52,52	0
48	MG	B2	202	1/1	0.78	0.12	-	103,103,103,103	0
48	MG	C3	203	1/1	0.90	0.08	-	69,69,69,69	0
48	MG	F1	3462	1/1	0.74	0.15	-	118,118,118,118	0
48	MG	A1	3547	1/1	0.76	0.16	-	81,81,81,81	0
48	MG	G2	204	1/1	-0.14	0.93	-	181,181,181,181	0
48	MG	GP	201	1/1	0.78	0.46	-	109,109,109,109	0
48	MG	H1	3406	1/1	0.41	0.16	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	H1	3452	1/1	0.88	0.10	-	108,108,108,108	0
48	MG	D1	3500	1/1	0.96	0.09	-	44,44,44,44	0
48	MG	F1	3425	1/1	0.82	0.33	-	115,115,115,115	0
48	MG	A1	3475	1/1	0.93	0.22	-	80,80,80,80	0
48	MG	A1	3440	1/1	0.98	0.04	-	78,78,78,78	0
48	MG	A1	3566	1/1	0.87	0.11	-	75,75,75,75	0
48	MG	H1	3504	1/1	0.88	0.11	-	111,111,111,111	0
48	MG	A1	3584	1/1	0.86	0.23	-	125,125,125,125	0
48	MG	A1	3527	1/1	0.28	0.30	-	119,119,119,119	0
48	MG	F1	3571	1/1	0.91	0.29	-	132,132,132,132	0
48	MG	B3	203	1/1	0.68	0.23	-	160,160,160,160	0
48	MG	B2	205	1/1	0.94	0.09	-	81,81,81,81	0
48	MG	D1	3547	1/1	0.71	0.27	-	109,109,109,109	0
48	MG	F1	3455	1/1	0.93	0.09	-	65,65,65,65	0
48	MG	A1	3509	1/1	0.92	0.12	-	128,128,128,128	0
48	MG	A1	3474	1/1	0.87	0.13	-	88,88,88,88	0
48	MG	D1	3401	1/1	0.53	0.25	-	109,109,109,109	0
48	MG	D1	3598	1/1	0.60	0.24	-	159,159,159,159	0
48	MG	A1	3591	1/1	0.80	0.27	-	121,121,121,121	0
48	MG	A1	3589	1/1	0.81	0.12	-	113,113,113,113	0
48	MG	H1	3402	1/1	0.66	0.23	-	118,118,118,118	0
48	MG	A1	3416	1/1	0.74	0.22	-	140,140,140,140	0
48	MG	H1	3535	1/1	0.64	0.98	-	150,150,150,150	0
48	MG	H1	3442	1/1	0.90	0.09	-	79,79,79,79	0
48	MG	D1	3606	1/1	0.56	1.18	-	157,157,157,157	0
48	MG	A1	3556	1/1	0.59	0.18	-	124,124,124,124	0
48	MG	A1	3451	1/1	0.71	0.16	-	146,146,146,146	0
48	MG	D1	3432	1/1	0.92	0.17	-	118,118,118,118	0
48	MG	A1	3422	1/1	0.44	0.58	-	144,144,144,144	0
48	MG	F1	3572	1/1	0.79	0.36	-	155,155,155,155	0
48	MG	D1	3543	1/1	0.91	0.27	-	127,127,127,127	0
48	MG	F1	3583	1/1	0.69	0.18	-	104,104,104,104	0
48	MG	A1	3435	1/1	0.71	0.54	-	151,151,151,151	0
48	MG	D1	3468	1/1	0.89	0.13	-	75,75,75,75	0
48	MG	F1	3509	1/1	0.65	0.34	-	144,144,144,144	0
48	MG	H1	3473	1/1	0.78	0.19	-	123,123,123,123	0
48	MG	D1	3620	1/1	0.88	0.15	-	106,106,106,106	0
48	MG	A1	3471	1/1	0.90	0.31	-	88,88,88,88	0
48	MG	C2	201	1/1	0.89	0.15	-	121,121,121,121	0
48	MG	D1	3611	1/1	0.41	0.63	-	205,205,205,205	0
48	MG	A1	3533	1/1	0.94	0.22	-	73,73,73,73	0
48	MG	E3	206	1/1	0.74	0.34	-	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	A1	3459	1/1	0.95	0.20	-	90,90,90,90	0
48	MG	D1	3582	1/1	0.84	0.19	-	93,93,93,93	0
48	MG	F1	3531	1/1	0.94	0.09	-	95,95,95,95	0
48	MG	A1	3493	1/1	0.93	0.21	-	113,113,113,113	0
48	MG	A1	3426	1/1	0.97	0.09	-	73,73,73,73	0
48	MG	D1	3491	1/1	0.92	0.15	-	97,97,97,97	0
48	MG	H1	3421	1/1	0.98	0.13	-	97,97,97,97	0
48	MG	D1	3512	1/1	0.91	0.14	-	101,101,101,101	0
48	MG	A1	3401	1/1	0.72	0.12	-	108,108,108,108	0
48	MG	A1	3550	1/1	0.95	0.04	-	69,69,69,69	0
48	MG	D1	3519	1/1	0.96	0.08	-	72,72,72,72	0
48	MG	D1	3429	1/1	0.74	0.23	-	113,113,113,113	0
48	MG	H1	3415	1/1	0.66	0.13	-	133,133,133,133	0
48	MG	F1	3570	1/1	0.67	0.27	-	113,113,113,113	0
48	MG	H1	3482	1/1	0.83	0.62	-	162,162,162,162	0
48	MG	D1	3437	1/1	0.50	0.32	-	148,148,148,148	0
48	MG	H1	3441	1/1	0.84	0.15	-	102,102,102,102	0
48	MG	F1	3441	1/1	0.97	0.19	-	111,111,111,111	0
48	MG	F1	3488	1/1	0.73	0.38	-	110,110,110,110	0
48	MG	F1	3420	1/1	0.93	0.09	-	88,88,88,88	0
48	MG	F1	3544	1/1	0.86	0.13	-	97,97,97,97	0
48	MG	CD	201	1/1	0.81	0.16	-	93,93,93,93	0
48	MG	F1	3477	1/1	0.86	0.68	-	146,146,146,146	0
48	MG	A1	3479	1/1	0.89	0.22	-	120,120,120,120	0
48	MG	DA	101	1/1	0.94	0.07	-	82,82,82,82	0
48	MG	D1	3632	1/1	0.97	0.12	-	83,83,83,83	0
48	MG	A1	3430	1/1	0.58	0.50	-	146,146,146,146	0
48	MG	D1	3567	1/1	0.95	0.26	-	60,60,60,60	0
48	MG	D1	3551	1/1	0.76	0.18	-	142,142,142,142	0
48	MG	D1	3609	1/1	0.83	0.67	-	120,120,120,120	0
48	MG	D1	3407	1/1	0.91	0.09	-	70,70,70,70	0
48	MG	H1	3424	1/1	0.92	0.08	-	96,96,96,96	0
48	MG	D1	3421	1/1	0.86	0.22	-	126,126,126,126	0
48	MG	F1	3563	1/1	0.73	0.18	-	124,124,124,124	0
48	MG	A1	3431	1/1	0.78	0.12	-	90,90,90,90	0
48	MG	H1	3457	1/1	0.90	0.56	-	147,147,147,147	0
48	MG	A1	3536	1/1	0.88	0.14	-	104,104,104,104	0
48	MG	D1	3427	1/1	0.79	0.26	-	153,153,153,153	0
48	MG	A1	3551	1/1	0.80	0.34	-	123,123,123,123	0
48	MG	EL	302	1/1	0.90	0.09	-	68,68,68,68	0
48	MG	DK	201	1/1	0.95	0.29	-	101,101,101,101	0
48	MG	A1	3546	1/1	0.96	0.23	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	H1	3549	1/1	0.80	0.47	-	124,124,124,124	0
48	MG	B2	203	1/1	0.96	0.06	-	81,81,81,81	0
48	MG	A1	3425	1/1	0.81	0.16	-	107,107,107,107	0
48	MG	A1	3472	1/1	0.80	0.63	-	149,149,149,149	0
48	MG	A1	3511	1/1	0.92	0.08	-	90,90,90,90	0
48	MG	C3	204	1/1	0.93	0.11	-	85,85,85,85	0
48	MG	D1	3417	1/1	0.80	0.20	-	132,132,132,132	0
48	MG	D1	3485	1/1	0.83	0.17	-	120,120,120,120	0
48	MG	F1	3465	1/1	0.96	0.26	-	101,101,101,101	0
48	MG	F1	3547	1/1	0.96	0.09	-	112,112,112,112	0
48	MG	A1	3581	1/1	0.92	0.31	-	126,126,126,126	0
48	MG	H1	3472	1/1	0.88	0.32	-	104,104,104,104	0
48	MG	H1	3546	1/1	0.85	0.27	-	120,120,120,120	0
48	MG	B2	207	1/1	0.66	0.38	-	149,149,149,149	0
48	MG	DQ	201	1/1	0.86	0.32	-	118,118,118,118	0
48	MG	D1	3619	1/1	0.96	0.07	-	101,101,101,101	0
48	MG	A1	3404	1/1	0.88	0.12	-	94,94,94,94	0
48	MG	F1	3541	1/1	0.90	0.23	-	112,112,112,112	0
48	MG	H1	3552	1/1	0.83	0.18	-	131,131,131,131	0
48	MG	CN	201	1/1	0.95	0.29	-	175,175,175,175	0
48	MG	D1	3537	1/1	0.92	0.28	-	121,121,121,121	0
48	MG	A1	3507	1/1	0.70	0.20	-	129,129,129,129	0
48	MG	F1	3468	1/1	0.77	0.16	-	103,103,103,103	0
48	MG	D1	3550	1/1	0.71	0.59	-	136,136,136,136	0
48	MG	F1	3469	1/1	0.66	0.16	-	112,112,112,112	0
48	MG	H1	3513	1/1	0.93	0.11	-	87,87,87,87	0
48	MG	H1	3435	1/1	0.90	0.17	-	116,116,116,116	0
48	MG	F1	3405	1/1	0.93	0.13	-	79,79,79,79	0
48	MG	D1	3514	1/1	0.78	0.20	-	128,128,128,128	0
48	MG	A1	3519	1/1	0.91	0.10	-	113,113,113,113	0
48	MG	DA	102	1/1	0.87	0.20	-	115,115,115,115	0
48	MG	F1	3422	1/1	0.81	0.29	-	149,149,149,149	0
48	MG	D1	3422	1/1	0.87	0.22	-	150,150,150,150	0
48	MG	F1	3525	1/1	0.97	0.09	-	73,73,73,73	0
48	MG	A1	3402	1/1	0.62	0.31	-	143,143,143,143	0
48	MG	F1	3491	1/1	0.87	0.18	-	96,96,96,96	0
48	MG	A1	3403	1/1	0.91	0.13	-	96,96,96,96	0
48	MG	A1	3538	1/1	0.97	0.08	-	49,49,49,49	0
48	MG	D1	3599	1/1	0.88	0.28	-	126,126,126,126	0
48	MG	D1	3509	1/1	0.97	0.09	-	41,41,41,41	0
48	MG	A1	3418	1/1	0.95	0.10	-	117,117,117,117	0
48	MG	A1	3462	1/1	0.96	0.10	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
48	MG	E3	203	1/1	0.84	0.17	-	104,104,104,104	0
48	MG	H1	3545	1/1	0.87	0.19	-	156,156,156,156	0
48	MG	F1	3451	1/1	0.76	0.49	-	122,122,122,122	0
48	MG	D1	3542	1/1	0.85	0.13	-	71,71,71,71	0
48	MG	GP	202	1/1	0.79	0.24	-	137,137,137,137	0
48	MG	D1	3570	1/1	0.97	0.20	-	54,54,54,54	0
48	MG	H1	3534	1/1	0.16	1.53	-	221,221,221,221	0
48	MG	F1	3414	1/1	0.65	0.20	-	123,123,123,123	0
48	MG	D1	3541	1/1	0.73	0.34	-	114,114,114,114	0
48	MG	D1	3559	1/1	0.97	0.08	-	55,55,55,55	0
48	MG	H1	3423	1/1	0.95	0.11	-	98,98,98,98	0
48	MG	E2	205	1/1	0.52	0.60	-	140,140,140,140	0
48	MG	H1	3530	1/1	0.82	0.34	-	154,154,154,154	0
48	MG	H1	3436	1/1	0.82	0.42	-	146,146,146,146	0
48	MG	F1	3496	1/1	0.61	0.24	-	122,122,122,122	0
48	MG	A1	3518	1/1	0.92	0.24	-	109,109,109,109	0
48	MG	F1	3466	1/1	0.91	0.34	-	140,140,140,140	0
48	MG	H1	3532	1/1	0.68	0.39	-	162,162,162,162	0
48	MG	D1	3418	1/1	0.72	0.16	-	114,114,114,114	0
48	MG	D1	3467	1/1	0.72	0.18	-	123,123,123,123	0
48	MG	H1	3460	1/1	0.95	0.13	-	69,69,69,69	0
48	MG	H1	3521	1/1	0.74	0.29	-	123,123,123,123	0
48	MG	D1	3595	1/1	0.87	0.23	-	94,94,94,94	0
48	MG	F1	3461	1/1	0.83	0.49	-	106,106,106,106	0
48	MG	H1	3417	1/1	0.84	0.11	-	114,114,114,114	0
48	MG	F1	3411	1/1	0.09	0.64	-	142,142,142,142	0
48	MG	F1	3426	1/1	0.97	0.24	-	110,110,110,110	0
48	MG	A1	3437	1/1	0.75	0.48	-	141,141,141,141	0
48	MG	H1	3506	1/1	0.97	0.12	-	75,75,75,75	0
48	MG	F1	3577	1/1	0.68	0.26	-	152,152,152,152	0
48	MG	A1	3530	1/1	0.78	0.48	-	149,149,149,149	0
48	MG	F1	3486	1/1	0.96	0.11	-	90,90,90,90	0
48	MG	D1	3612	1/1	0.94	0.23	-	123,123,123,123	0
48	MG	D1	3445	1/1	0.87	0.19	-	126,126,126,126	0
48	MG	H1	3466	1/1	0.95	0.08	-	107,107,107,107	0
48	MG	D1	3625	1/1	0.75	0.40	-	164,164,164,164	0
48	MG	H1	3475	1/1	0.94	0.10	-	70,70,70,70	0
48	MG	E2	206	1/1	0.51	0.32	-	151,151,151,151	0
48	MG	D1	3629	1/1	0.95	0.10	-	121,121,121,121	0
48	MG	D1	3617	1/1	0.94	0.35	-	113,113,113,113	0
48	MG	D1	3434	1/1	0.75	0.63	-	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.