



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 10:13 PM BST

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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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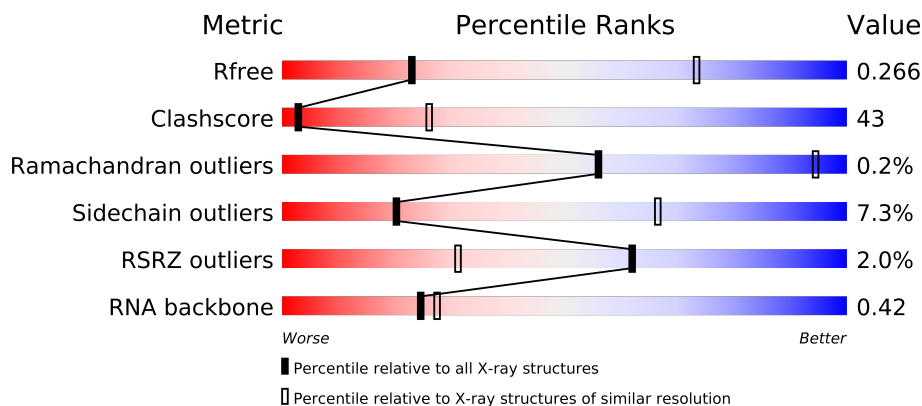
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 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))
$R_{free}$	66092	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)
RNA backbone	1838	1008 (4.26-2.76)

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

Mol	Chain	Length	Quality of chain
1	A1	3354	
1	D1	3354	
1	F1	3354	
1	H1	3354	
2	AA	94	
2	DA	94	
2	FA	94	
2	HA	94	
3	AB	52	
3	DB	52	
3	FB	52	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
14	DO	134	
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	
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	

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Mol	Chain	Length	Quality of chain
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	
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	
33	CL	204	
33	EL	204	
33	GL	204	
34	BM	301	
34	CM	301	
34	EM	301	
34	GM	301	
35	BN	181	

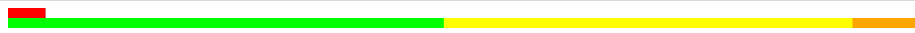
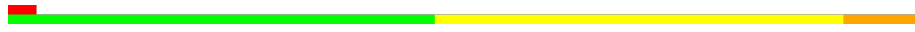


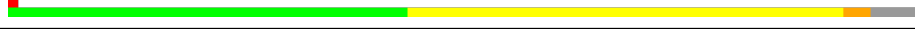
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Mol	Chain	Length	Quality of chain
35	CN	181	
35	EN	181	
35	GN	181	
36	BO	185	
36	EO	185	
36	GO	185	
37	BP	157	
37	CP	157	
37	EP	157	
37	GP	157	
38	BQ	183	
38	CQ	183	
38	EQ	183	
38	GQ	183	
39	BR	150	
39	CR	150	
39	ER	150	
39	GR	150	
40	BS	135	
40	CS	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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
48	MG	A1	3408	-	X
48	MG	A1	3412	-	X
48	MG	A1	3420	-	X
48	MG	A1	3422	-	X
48	MG	A1	3423	-	X
48	MG	A1	3428	-	X
48	MG	A1	3430	-	X
48	MG	A1	3435	-	X
48	MG	A1	3437	-	X
48	MG	A1	3438	-	X
48	MG	A1	3441	-	X
48	MG	A1	3453	-	X
48	MG	A1	3457	-	X
48	MG	A1	3459	-	X
48	MG	A1	3470	-	X
48	MG	A1	3471	-	X
48	MG	A1	3472	-	X
48	MG	A1	3479	-	X
48	MG	A1	3480	-	X
48	MG	A1	3487	-	X
48	MG	A1	3491	-	X
48	MG	A1	3492	-	X
48	MG	A1	3500	-	X
48	MG	A1	3504	-	X
48	MG	A1	3507	-	X
48	MG	A1	3513	-	X
48	MG	A1	3515	-	X
48	MG	A1	3516	-	X
48	MG	A1	3522	-	X
48	MG	A1	3527	-	X
48	MG	A1	3528	-	X
48	MG	A1	3530	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	A1	3531	-	X
48	MG	A1	3533	-	X
48	MG	A1	3541	-	X
48	MG	A1	3544	-	X
48	MG	A1	3545	-	X
48	MG	A1	3555	-	X
48	MG	A1	3560	-	X
48	MG	A1	3562	-	X
48	MG	A1	3567	-	X
48	MG	A1	3568	-	X
48	MG	A1	3571	-	X
48	MG	A1	3573	-	X
48	MG	A1	3575	-	X
48	MG	A1	3576	-	X
48	MG	A1	3578	-	X
48	MG	A1	3579	-	X
48	MG	A1	3581	-	X
48	MG	A1	3583	-	X
48	MG	A1	3584	-	X
48	MG	A1	3585	-	X
48	MG	A1	3586	-	X
48	MG	A1	3592	-	X
48	MG	A1	3594	-	X
48	MG	A1	3595	-	X
48	MG	A1	3596	-	X
48	MG	A1	3597	-	X
48	MG	AK	202	-	X
48	MG	B2	206	-	X
48	MG	B2	207	-	X
48	MG	B2	208	-	X
48	MG	B3	201	-	X
48	MG	C2	206	-	X
48	MG	C3	205	-	X
48	MG	D1	3401	-	X
48	MG	D1	3408	-	X
48	MG	D1	3412	-	X
48	MG	D1	3416	-	X
48	MG	D1	3417	-	X
48	MG	D1	3421	-	X
48	MG	D1	3424	-	X
48	MG	D1	3425	-	X
48	MG	D1	3429	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	D1	3434	-	X
48	MG	D1	3437	-	X
48	MG	D1	3439	-	X
48	MG	D1	3442	-	X
48	MG	D1	3443	-	X
48	MG	D1	3444	-	X
48	MG	D1	3446	-	X
48	MG	D1	3448	-	X
48	MG	D1	3451	-	X
48	MG	D1	3462	-	X
48	MG	D1	3470	-	X
48	MG	D1	3475	-	X
48	MG	D1	3481	-	X
48	MG	D1	3484	-	X
48	MG	D1	3488	-	X
48	MG	D1	3492	-	X
48	MG	D1	3493	-	X
48	MG	D1	3497	-	X
48	MG	D1	3498	-	X
48	MG	D1	3504	-	X
48	MG	D1	3506	-	X
48	MG	D1	3511	-	X
48	MG	D1	3512	-	X
48	MG	D1	3516	-	X
48	MG	D1	3517	-	X
48	MG	D1	3521	-	X
48	MG	D1	3522	-	X
48	MG	D1	3525	-	X
48	MG	D1	3527	-	X
48	MG	D1	3528	-	X
48	MG	D1	3537	-	X
48	MG	D1	3541	-	X
48	MG	D1	3543	-	X
48	MG	D1	3547	-	X
48	MG	D1	3550	-	X
48	MG	D1	3555	-	X
48	MG	D1	3565	-	X
48	MG	D1	3567	-	X
48	MG	D1	3568	-	X
48	MG	D1	3571	-	X
48	MG	D1	3576	-	X
48	MG	D1	3583	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	D1	3588	-	X
48	MG	D1	3589	-	X
48	MG	D1	3592	-	X
48	MG	D1	3593	-	X
48	MG	D1	3594	-	X
48	MG	D1	3597	-	X
48	MG	D1	3599	-	X
48	MG	D1	3600	-	X
48	MG	D1	3602	-	X
48	MG	D1	3603	-	X
48	MG	D1	3604	-	X
48	MG	D1	3606	-	X
48	MG	D1	3607	-	X
48	MG	D1	3608	-	X
48	MG	D1	3609	-	X
48	MG	D1	3611	-	X
48	MG	D1	3612	-	X
48	MG	D1	3613	-	X
48	MG	D1	3617	-	X
48	MG	D1	3622	-	X
48	MG	D1	3623	-	X
48	MG	D1	3624	-	X
48	MG	DA	102	-	X
48	MG	DK	201	-	X
48	MG	E2	201	-	X
48	MG	E2	205	-	X
48	MG	E2	207	-	X
48	MG	E3	202	-	X
48	MG	E3	204	-	X
48	MG	E3	206	-	X
48	MG	EN	202	-	X
48	MG	F1	3401	-	X
48	MG	F1	3411	-	X
48	MG	F1	3413	-	X
48	MG	F1	3414	-	X
48	MG	F1	3416	-	X
48	MG	F1	3422	-	X
48	MG	F1	3424	-	X
48	MG	F1	3425	-	X
48	MG	F1	3428	-	X
48	MG	F1	3433	-	X
48	MG	F1	3442	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	F1	3444	-	X
48	MG	F1	3446	-	X
48	MG	F1	3451	-	X
48	MG	F1	3457	-	X
48	MG	F1	3461	-	X
48	MG	F1	3463	-	X
48	MG	F1	3466	-	X
48	MG	F1	3473	-	X
48	MG	F1	3477	-	X
48	MG	F1	3479	-	X
48	MG	F1	3482	-	X
48	MG	F1	3483	-	X
48	MG	F1	3488	-	X
48	MG	F1	3493	-	X
48	MG	F1	3496	-	X
48	MG	F1	3498	-	X
48	MG	F1	3502	-	X
48	MG	F1	3503	-	X
48	MG	F1	3506	-	X
48	MG	F1	3508	-	X
48	MG	F1	3511	-	X
48	MG	F1	3516	-	X
48	MG	F1	3527	-	X
48	MG	F1	3529	-	X
48	MG	F1	3532	-	X
48	MG	F1	3538	-	X
48	MG	F1	3540	-	X
48	MG	F1	3544	-	X
48	MG	F1	3545	-	X
48	MG	F1	3550	-	X
48	MG	F1	3551	-	X
48	MG	F1	3555	-	X
48	MG	F1	3560	-	X
48	MG	F1	3562	-	X
48	MG	F1	3563	-	X
48	MG	F1	3564	-	X
48	MG	F1	3565	-	X
48	MG	F1	3566	-	X
48	MG	F1	3567	-	X
48	MG	F1	3569	-	X
48	MG	F1	3572	-	X
48	MG	F1	3574	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	F1	3577	-	X
48	MG	F1	3578	-	X
48	MG	F1	3581	-	X
48	MG	F1	3582	-	X
48	MG	FK	201	-	X
48	MG	G2	202	-	X
48	MG	G2	204	-	X
48	MG	G2	206	-	X
48	MG	G3	202	-	X
48	MG	G3	204	-	X
48	MG	G3	205	-	X
48	MG	GN	201	-	X
48	MG	GO	201	-	X
48	MG	GP	201	-	X
48	MG	GW	201	-	X
48	MG	H1	3405	-	X
48	MG	H1	3408	-	X
48	MG	H1	3409	-	X
48	MG	H1	3410	-	X
48	MG	H1	3412	-	X
48	MG	H1	3414	-	X
48	MG	H1	3420	-	X
48	MG	H1	3422	-	X
48	MG	H1	3425	-	X
48	MG	H1	3436	-	X
48	MG	H1	3438	-	X
48	MG	H1	3441	-	X
48	MG	H1	3443	-	X
48	MG	H1	3446	-	X
48	MG	H1	3447	-	X
48	MG	H1	3449	-	X
48	MG	H1	3450	-	X
48	MG	H1	3456	-	X
48	MG	H1	3457	-	X
48	MG	H1	3462	-	X
48	MG	H1	3465	-	X
48	MG	H1	3469	-	X
48	MG	H1	3472	-	X
48	MG	H1	3477	-	X
48	MG	H1	3481	-	X
48	MG	H1	3482	-	X
48	MG	H1	3484	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
48	MG	H1	3489	-	X
48	MG	H1	3490	-	X
48	MG	H1	3496	-	X
48	MG	H1	3501	-	X
48	MG	H1	3511	-	X
48	MG	H1	3519	-	X
48	MG	H1	3521	-	X
48	MG	H1	3524	-	X
48	MG	H1	3525	-	X
48	MG	H1	3529	-	X
48	MG	H1	3530	-	X
48	MG	H1	3531	-	X
48	MG	H1	3532	-	X
48	MG	H1	3533	-	X
48	MG	H1	3534	-	X
48	MG	H1	3535	-	X
48	MG	H1	3536	-	X
48	MG	H1	3537	-	X
48	MG	H1	3538	-	X
48	MG	H1	3539	-	X
48	MG	H1	3540	-	X
48	MG	H1	3541	-	X
48	MG	H1	3542	-	X
48	MG	H1	3547	-	X
48	MG	H1	3549	-	X
48	MG	H1	3550	-	X
48	MG	H1	3551	-	X
48	MG	H1	3553	-	X
48	MG	H1	3554	-	X

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 511395 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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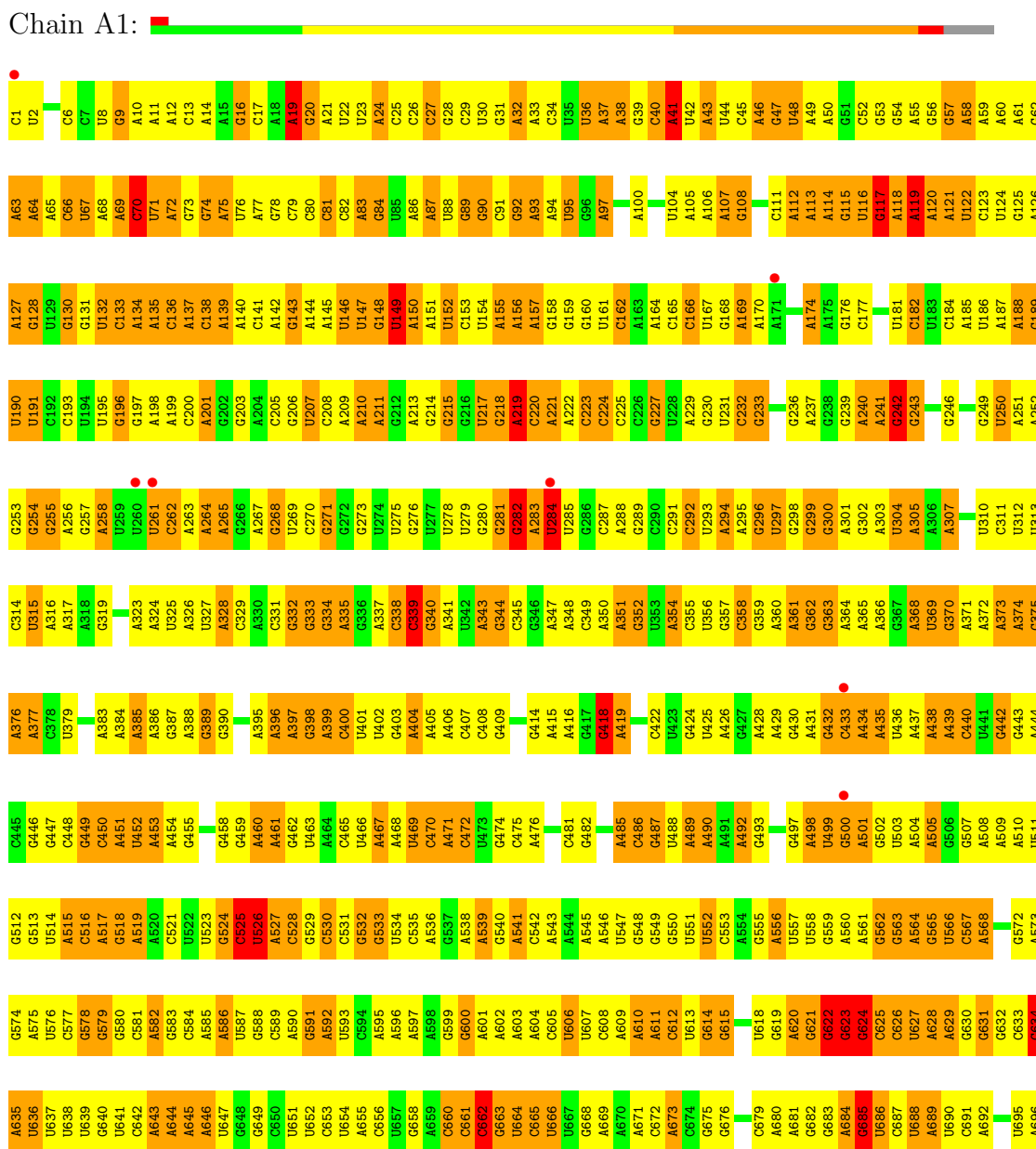
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
50	GY	1	Total 1	O 1	0	0
50	H1	924	Total 924	O 924	0	0
50	HA	4	Total 4	O 4	0	0
50	HB	4	Total 4	O 4	0	0
50	HJ	2	Total 2	O 2	0	0
50	HK	2	Total 2	O 2	0	0
50	HP	1	Total 1	O 1	0	0
50	HT	5	Total 5	O 5	0	0
50	HU	2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

### 3 Residue-property plots

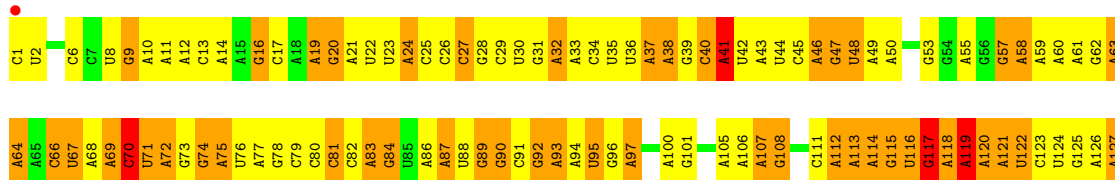
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 26S rRNA





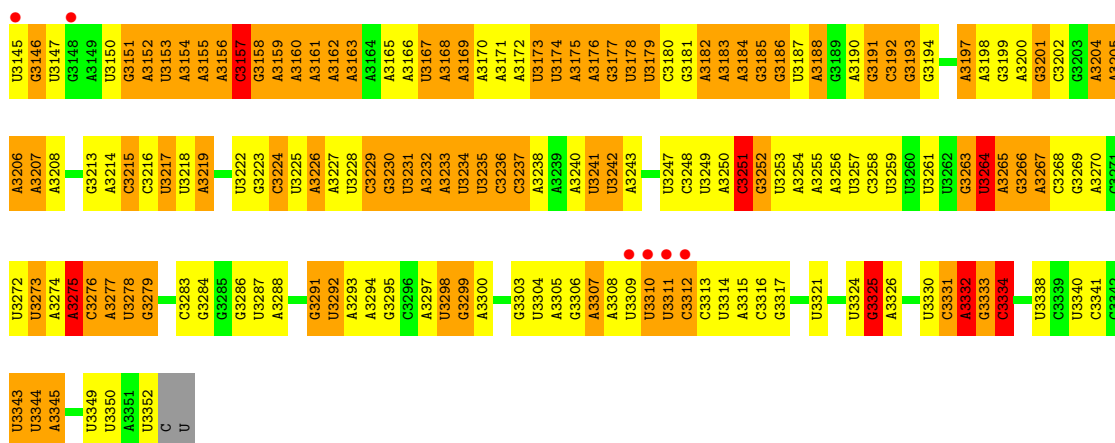




U1076	U1077	U1078	A1079	U1083	G1084	G1085	U1086	A1087	A1088	G1089	A1090	G1091	C1092	C1093	G1094	C1095	G1096	G1097	A1098	G1099	U1100	U1101	U1102	A1103	C1104	U1105	A1106	A1107	A1108	A1109	U1110	G1111	A1112	A1113	C1114	U1115	C1116	U1117	G1121	A1122	A1123	G1124	A1125	A1126	U1127	G1128	C1129	A1130	U1131	U1132	G1133	C1134	U1135	C1136	U1137	U1138	A1139									
U1011	U1012	U1013	U1016	U1017	A1018	G1019	G1020	U1021	U1022	A1023	A1024	G1025	C1026	U1027	G1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075				
C948	G949	A950	A951	C952	C953	U957	A958	G959	U960	A961	G962	C963	U964	U965	U966	U967	U968	C969	C970	U971	U972	U973	C974	C975	A976	A977	U978	U979	U980	U981	U982	U983	C984	U985	U986	A987	U988	U989	U990	U991	U992	C993	A994	A995	A996	C997	A998	G999	U1002	G1003	U1004	A1005	C1006	G1007	C1008	A1009	G1010									
G879	U880	G881	G882	A883	A884	C885	C886	G889	G890	A891	U892	C893	C894	U895	U896	U897	U898	G899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947
A816	A817	U818	U819	G820	U821	U822	A823	A824	U825	U826	U827	U828	U829	U830	A831	A832	A833	G834	A835	U836	G837	U838	U839	U840	A841	A842	C846	G847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	C864	C865	C866	C867	U868	C869	U870	A871	A872	A873	A874	A875	U876	U877	U878							
C751	C752	A753	A754	C755	C756	C757	A761	G762	G763	U764	A765	G766	C767	U768	U769	U770	U771	U772	C773	A774	C775	C776	C777	C778	A779	C780	U784	U785	G786	U787	C788	U789	C790	C791	C792	U793	C794	U795	U796	U797	U798	U799	U800	U801	U802	C803	G804	A805	G806	U807	A808	A809	G810	A811	G812	C813	U814	U815								
A629	G630	G631	G632	G633	G634	A635	U636	U637	U638	U639	G640	U641	C642	A643	A644	A645	A646	U647	G648	G649	C650	U651	U652	C653	U654	A655	A656	U657	U658	A659	C660	C661	G662	G663	U664	C665	U666	U667	C668	A669	A670	A671	C672	A673	C674	G675	G676	A677	C678	C679	A680	A681	G682	G683	A684	G685	U686	C687	U688							
C567	A568	U572	A573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	A602	A603	A604	C605	U606	U607	C608	A609	A610	A611	C612	U613	U614	U615	A616	U617	U618	U619	A620	G621	G622	A623	A624	G625	U626	U627	A628								
A689	U690	C691	A692	U695	A696	A697	U698	C699	U700	A701	G702	U703	U704	A705	U706	A707	G708	G709	U710	U711	U712	U713	U714	A715	A716	U717	U718	U719	C720	U723	C724	C725	U726	C727	U728	A729	A730	U731	A732	U733	A734	A735	U736	U737	U738	U739	U740	G741	U742	A743	C744	A745	G746	U747	U748	U749	G750									
C751	C752	A753	A754	C755	C756	C757	A761	G762	G763	U764	A765	G766	C767	U768	U769	U770	U771	U772	C773	A774	C775	C776	C777	C778	A779	C780	U784	U785	G786	U787	C788	U789	C790	C791	C792	U793	C794	U795	U796	U797	U798	U799	U800	U801	U802	C803	G804	A805	G806	U807	A808	A809	G810	A811	G812	C813	U814	U815								
A816	A817	U818	U819	G820	U821	U822	A823	A824	U825	U826	U827	U828	U829	U830	A831	A832	A833	G834	A835	U836	G837	U838	U839	U840	A841	A842	C846	G847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	C864	C865	C866	C867	U868	C869	U870	A871	A872	A873	A874	A875	U876	U877	U878							
G879	U880	G881	G882	A883	A884	C885	C886	G889	G890	A891	U892	C893	C894	U895	U896	U897	U898	G899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947
C948	G949	A950	A951	C952	C953	U957	A958	G959	U960	A961	G962	C963	U964	U965	U966	U967	U968	C969	C970	U971	U972	U973	C974	C975	A976	A977	U978	U979	U980	U981	U982	U983	C984	U985	U986	A987	U988	U989	U990	U991	U992	C993	A994	A995	A996	C997	A998	G999	U1002	G1003	U1004	A1005	C1006	G1007	C1008	A1009	G1010									
U1011	U1012	U1013	U1016	U1017	A1018	G1019	G1020	U1021	U1022	A1023	A1024	G1025	C1026	U1027	G1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075				
U1076	U1077	U1078	A1079	U1083	G1084	G1085	U1086	A1087	A1088	G1089	A1090	G1091	C1092	C1093	G1094	C1095	G1096	G1097	A1098	G1099	U1100	U1101	U1102	A1103	C1104	U1105	A1106	A1107	A1108	A1109	U1110	G1111	A1112	A1113	C1114	U1115	C1116	U1117	G1121	A1122	A1123	G1124	A1125	A1126	U1127	G1128	C1129	A1130	U1131	U1132	G1133	C1134	U1135	C1136	U1137	U1138	A1139									
G128	U129	G130	G131	U132	U133	U134	A135	C136	A137	C138	A139	A140	C141	A142	G143	A144	A145	U146	U147	G148	U149	A150	A151	A152	C153	U154	A155	A156	A157	G158	G159	A160	C161	A162	A163	A164	C165	C166	U167	G168	A169	A170	G171	G172	G173	G174	G175	G176	G177	G178	U179	U180	U181	C182	U183	U184	U185	U186	A187	U188	A189	G190				
U191	C192	C193	U194	U195	U196	A197	A198	A199	C200	A201	G202	A203	A204	C205	G206	U207	C208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	C220	A221	A222	C223	C224	C225	C226	C227	U228	A229	U230	U231	C232	C233	G234	G235	G236	A237	G238	G239	A240	A241	A242	A243	A244	G245	G246	U247	U248	U249	U250	A251	A252	G253				
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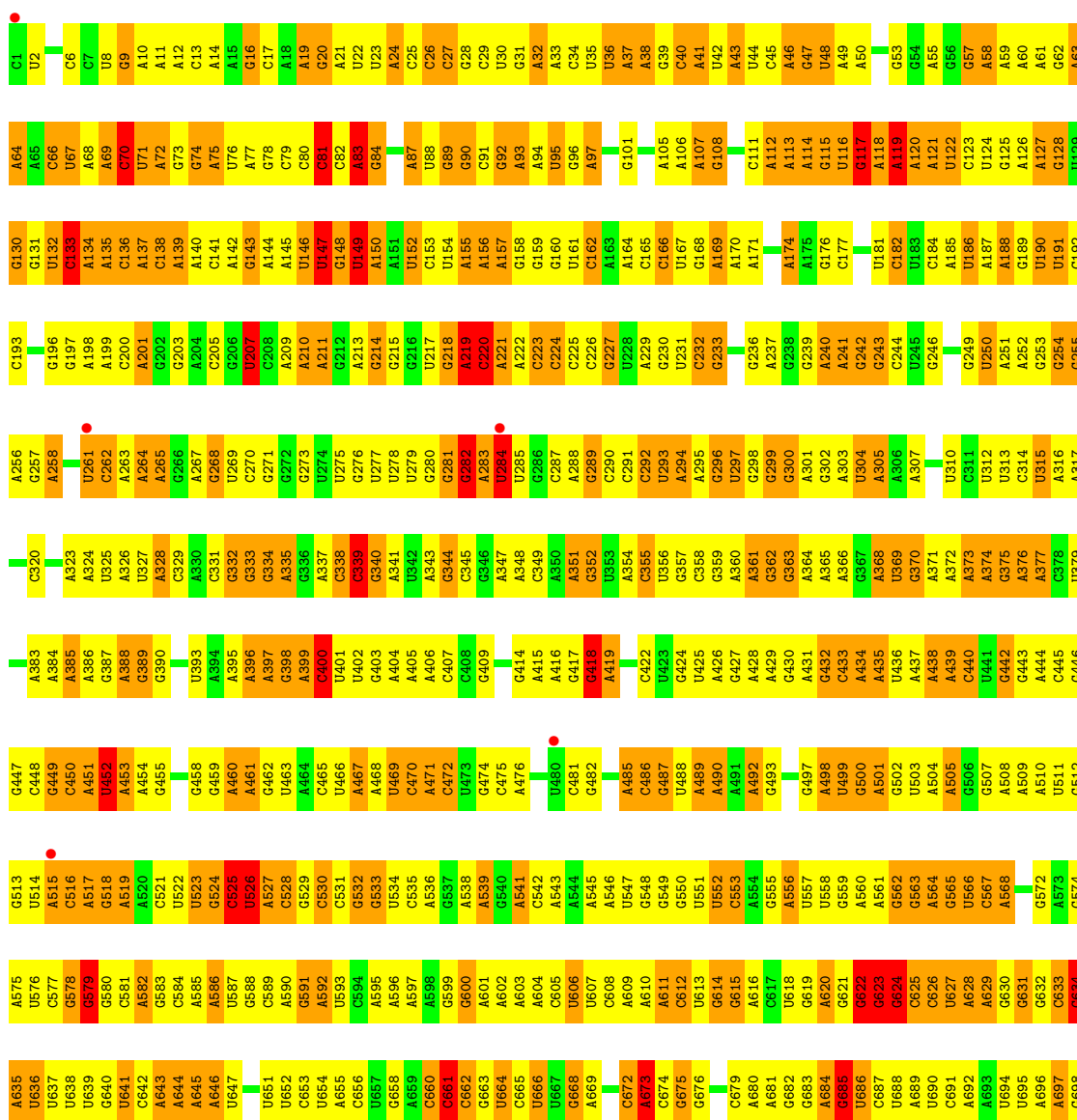
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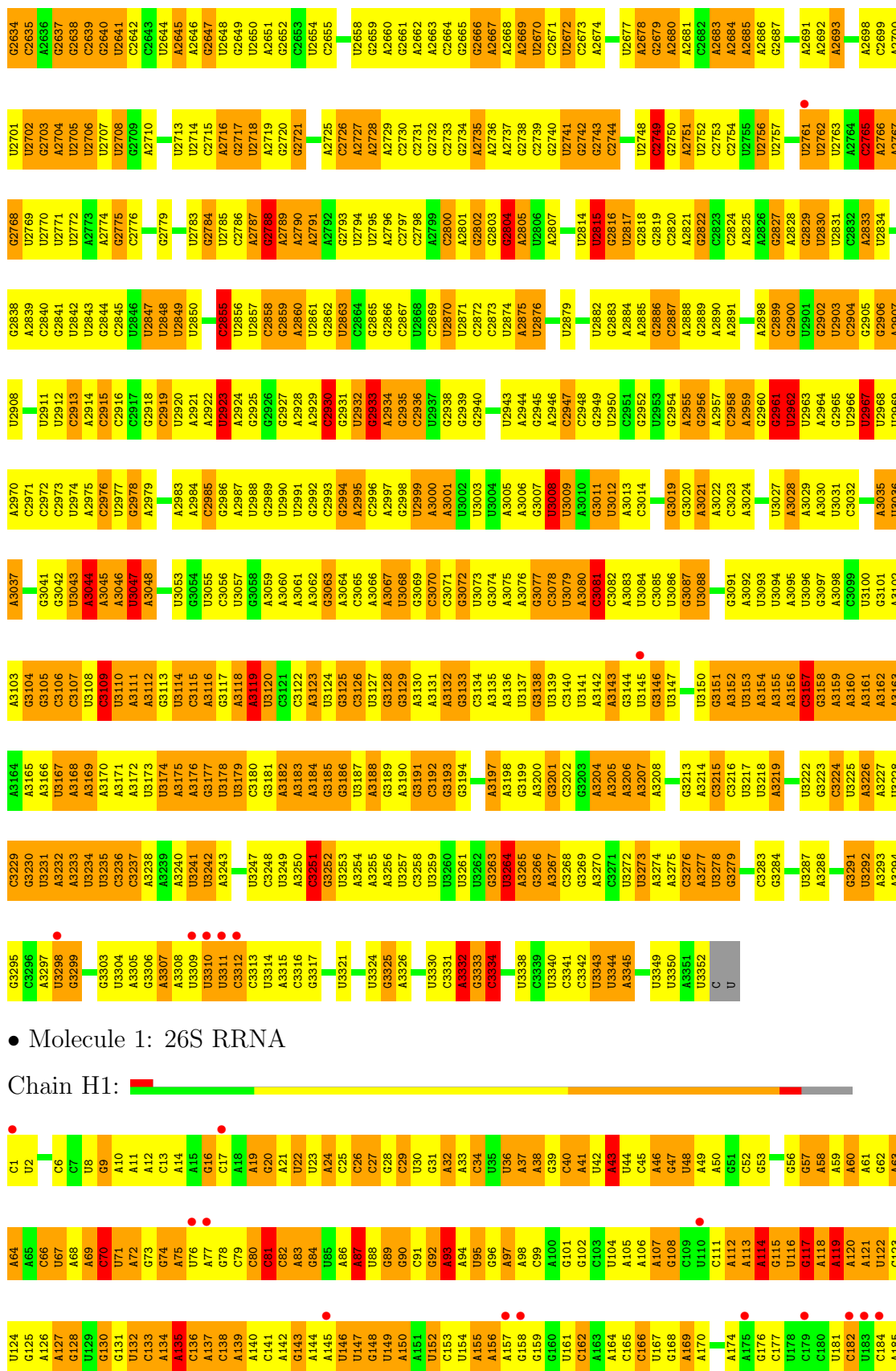
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Chain F1:



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U1601	C1534	U1471	G1404	G1343	A1220	G1160	G1097	U1035	U972	U904	G830	G762	G701
U1602	U1472	A1473	U1405	A1344	G1221	G1161	A1098	G1036	C973	U905	G830	G765	G702
U1603	U1537	G1474	G1406	A1345	A1222	G1162	G1099	G1037	C974	C906	A832	G766	G703
C1604	U1638	G1475	A1407	U1345	U1223	A1163	U1100	G1038	G975	A907	A833	G767	G704
G1605	G1539	A1476	U1408	G1348	A1224	C1164	U1101	G1039	A976	A908	G834	A768	A705
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G1608	C1542	A1478	U1411	U1351	A1227	G1167	C1104	U1042	U979	C911	G837	U773	G708
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C1610	U1544	G1480	G1413	G1353	A1231	G1169	U1106	G1044	U981	U913	U839	A774	G710
A1613	U1545	U1481	C1414	C1354	U1232	U1170	U1107	G1045	C982	U914	U840	C775	U711
G1614	G1546	A1482	C1415	C1355	A1232	U1171	A1108	G1046	U983	C915	A841	C776	G712
G1615	U1547	U1483	U1416	G1356	G1233	G1172	A1109	U1047	U984	U916	U842	C777	G713
G1616	U1548	U1484	A1417	A1357	G1234	A1173	U1173	U1048	U985	G917	U843	G778	A714
G1617	U1549	A1485	G1418	U1358	U1235	G1174	U1174	U1049	C986	A919	C946	A715	A716
A1618	A1486	U1486	U1359	U1359	G1236	G1175	A1112	C1050	A987	A919	C947	A785	A717
A1619	A1487	G1487	C1360	C1360	U1237	A1176	A1113	C1051	G988	A920	C948	A786	A718
A1620	U1552	U1488	U1361	U1361	U1238	A1177	C1114	A1052	G989	A921	U849	G787	C719
G1621	U1553	U1489	C1362	C1362	U1239	U1178	U1115	A1053	U990	U922	U850	U788	C720
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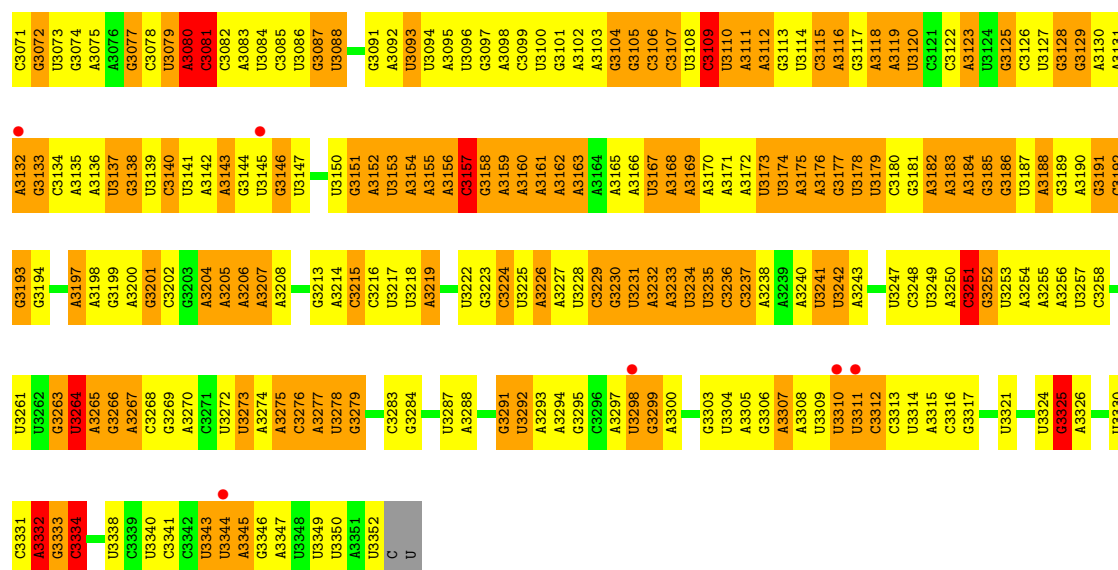




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C757	A761	G762	C763	U764	A765	G766	C767	G768	G769	U772	C773	A774	C775	C776	C777	G778	A779	C780	G784	U785	G786	U787	C788	U789	U790	C791	G792	A793	C794	A795	U796	A797	G798	G799	U800	U801	U802	C803	G804	A805	G806	A807	A808	A809	U810	A811	G812	U813	U814	U815	A816	A817	U818	U819	A820	U821											
A696	A697	G698	C699	U700	A701	G702	U703	G704	A705	U706	A707	G708	G709	U710	C711	G712	C713	A714	A715	G716	A717	U718	C719	G720	C721	U722	G723	C724	G725	G726	C727	G728	A729	A730	A731	C732	G733	A734	A735	A736	G737	U738	G739	A740	U741	U742	U743	A744	A745	U746	U747	U750	C751	G752	A753	U754	G755	C756									
G631	G632	C633	G634	U635	U636	U637	U638	U639	U640	U641	C642	A643	A644	A645	U646	U651	C652	U653	A654	A655	C656	C660	C661	C662	U663	U664	C665	U666	U667	G668	A669	C672	A673	C674	G675	U676	A677	C678	C679	A680	G681	U682	A683	G684	A685	U686	C687	U688	A689	G690	C691	U692	A693	U694	U695												
A508	A509	U510	U511	G512	U513	U514	A515	C516	A517	G518	A519	A520	C521	U522	G523	U524	A525	U526	A527	G528	C529	C530	C531	A532	G533	U534	C535	A536	G537	A538	A539	G540	A541	C542	A543	A546	U547	G548	G549	U550	U551	U552	C553	A554	U555	A556	U557	U558	G559	A560	A561	G562	G563	U564	G565	U566	A568										
G442	G443	A444	C445	U446	C447	C448	G449	C450	A451	U452	A453	A454	G455	C458	A459	A460	A461	G462	U463	A464	C465	U466	A467	A468	U469	C470	C471	C472	U473	C474	C475	A476	C481	G482	A483	U484	A485	C486	U487	U488	U489	A490	A491	A492	C493	C497	A498	U499	G500	A501	G502	U503	A504	U505	G506	G507											
G375	A376	C377	U378	A383	A384	A385	A386	G387	A388	G389	G390	A396	A397	G398	A399	C400	U401	U402	G403	A404	A405	A406	C407	C408	G409	G412	A413	G414	A415	A416	G417	A418	A419	A420	G421	C422	U423	U424	U425	A426	G427	A428	A429	G430	A431	G432	C433	A434	A435	U436	U437	A438	A439	C440	U441												
C314	U315	A316	A317	A318	G319	C320	A323	A324	U325	A326	U327	A328	C329	A330	G331	C332	G333	C334	A335	G336	A337	C338	G339	G340	A341	U342	G343	G344	C345	A346	A347	A348	A350	A351	G352	U353	C354	C355	U356	G357	C358	U359	A360	G361	G362	C363	A364	A365	U366	G367	A368	U369	G370	A371	A372	U373											
A252	G253	G254	G255	A256	G257	A258	U261	A262	G263	A264	A265	G266	A267	G268	G269	G270	G271	G272	G273	U274	G275	G276	U277	U278	U279	G280	G281	G282	A283	U284	U285	G286	A287	G288	G289	C290	C291	U292	U293	A294	A295	U296	U297	G298	G299	C300	A301	G302	U303	A305	A306	A307	U310	G311	U312	U313											
U186	A187	A188	G189	U190	U191	C192	C193	G196	A197	A198	A199	C200	A201	G202	A203	A204	C205	G206	U207	C208	A209	A210	A211	G212	G213	G214	G215	G216	U217	G218	A219	C220	A221	A222	C223	C224	C225	U226	U227	U228	A229	G230	U231	C232	G233	G236	A237	G238	G239	A240	A241	G242	G243	G249	U250	A251											







### • Molecule 2: RIBOSOMAL PROTEIN L37

Chain AA:

### • Molecule 2: RIBOSOMAL PROTEIN L37

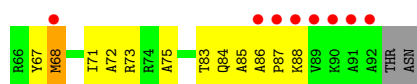
Chain DA:

### • Molecule 2: RIBOSOMAL PROTEIN L37

Chain FA:

### • Molecule 2: RIBOSOMAL PROTEIN L37

Chain HA:



- Molecule 3: RPL39

Chain AB:



- Molecule 3: RPL39

Chain DB:



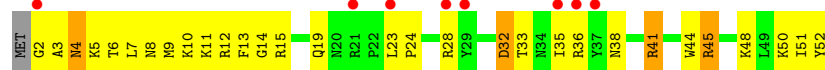
- Molecule 3: RPL39

Chain FB:



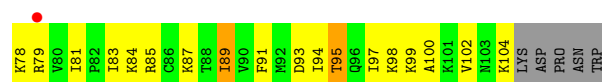
- Molecule 3: RPL39

Chain HB:



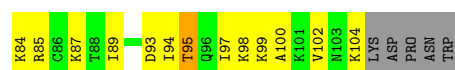
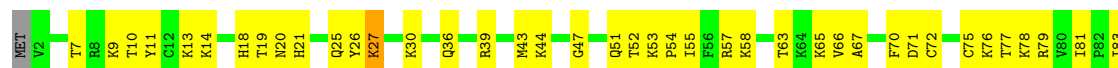
- Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain AC:



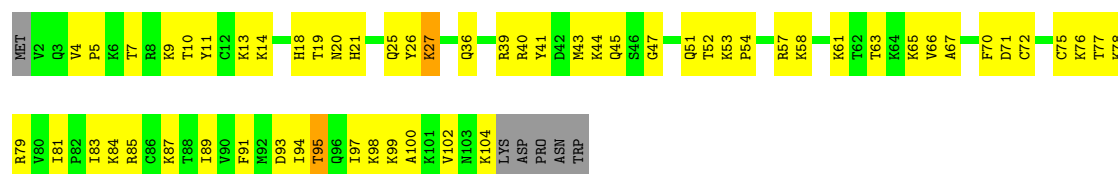
- Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain DC:



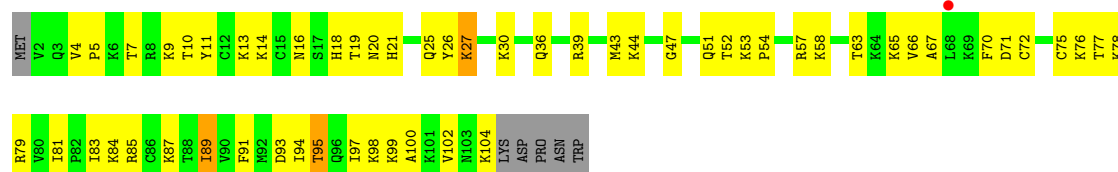
- Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain FC:



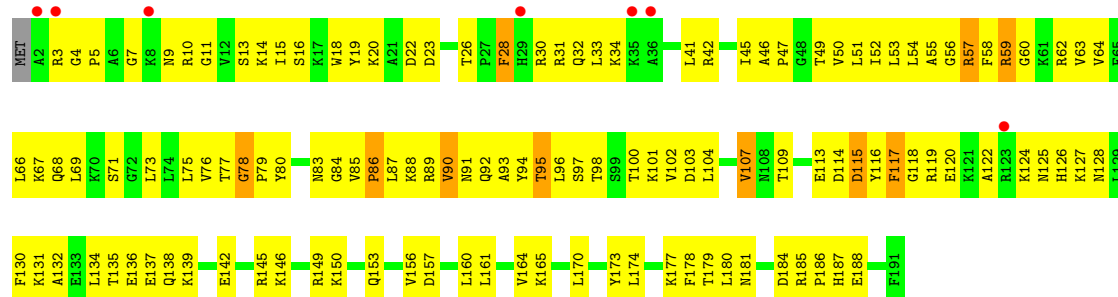
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain HC:



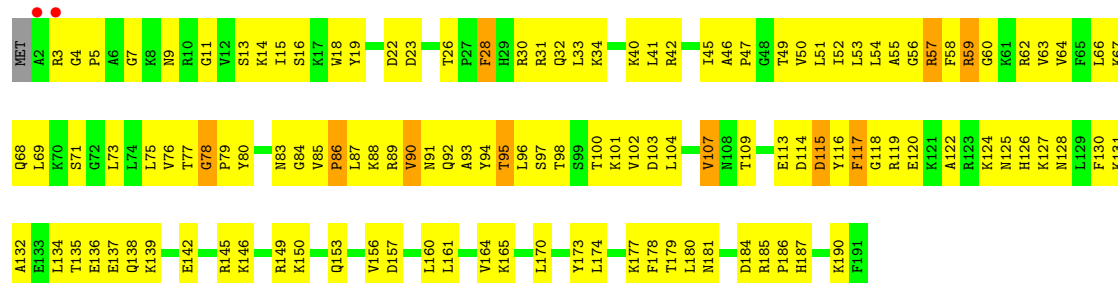
• Molecule 5: RPL6

Chain AE:



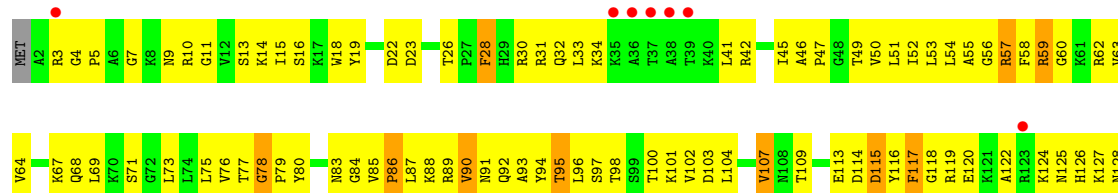
• Molecule 5: RPL6

Chain DE:



• Molecule 5: RPL6

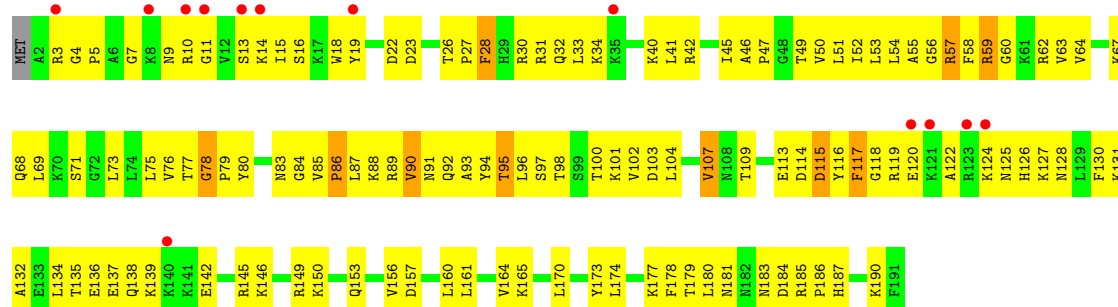
Chain FE:





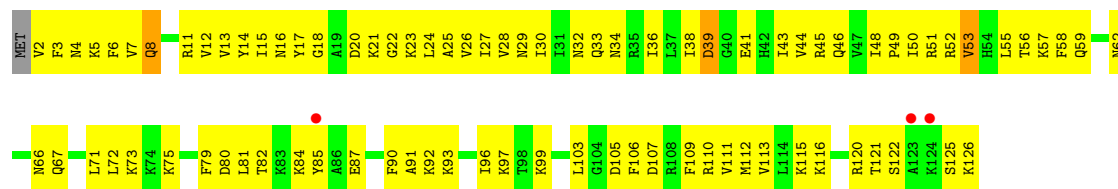
• Molecule 5: RPL6

Chain HE:



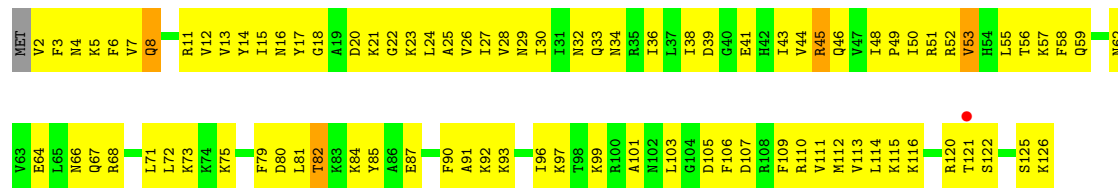
• Molecule 6: RPL14

Chain AF:



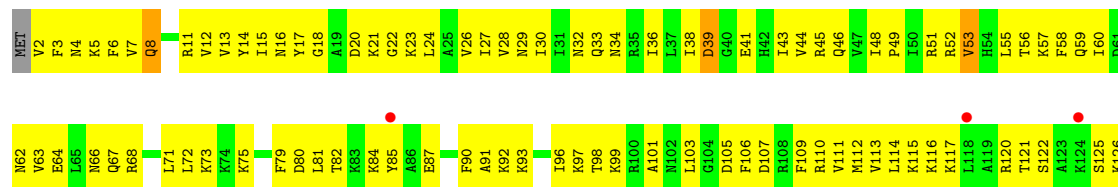
• Molecule 6: RPL14

Chain DF:



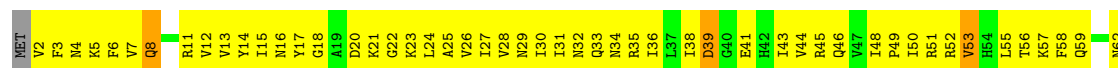
• Molecule 6: RPL14

Chain FF:



• Molecule 6: RPL14

Chain HF:





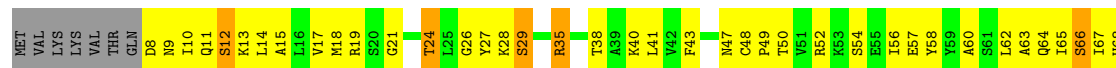
• Molecule 7: RPL30

Chain AG:



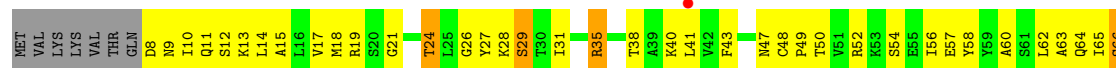
• Molecule 7: RPL30

Chain DG:



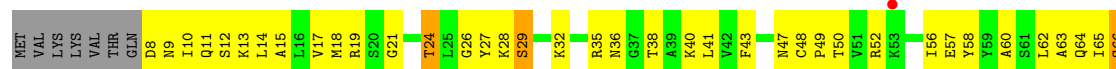
• Molecule 7: RPL30

Chain FG:



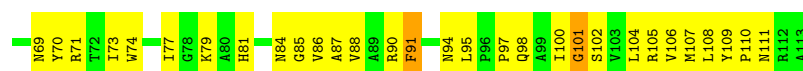
• Molecule 7: RPL30

Chain HG:



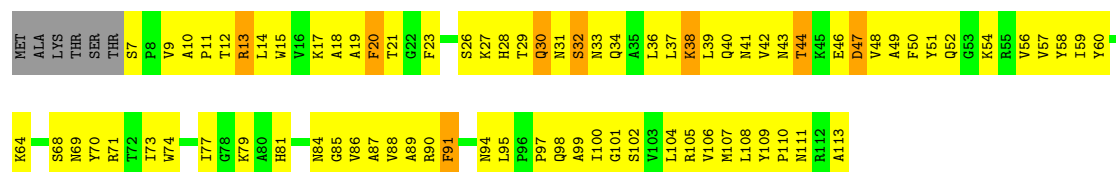
• Molecule 8: RPL35A

Chain AH:



- Molecule 8: RPL35A

Chain DH:



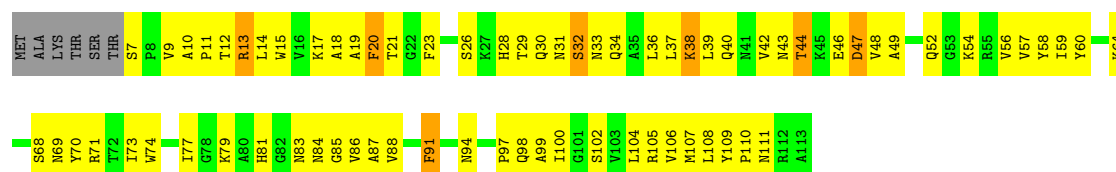
- Molecule 8: RPL35A

Chain FH:



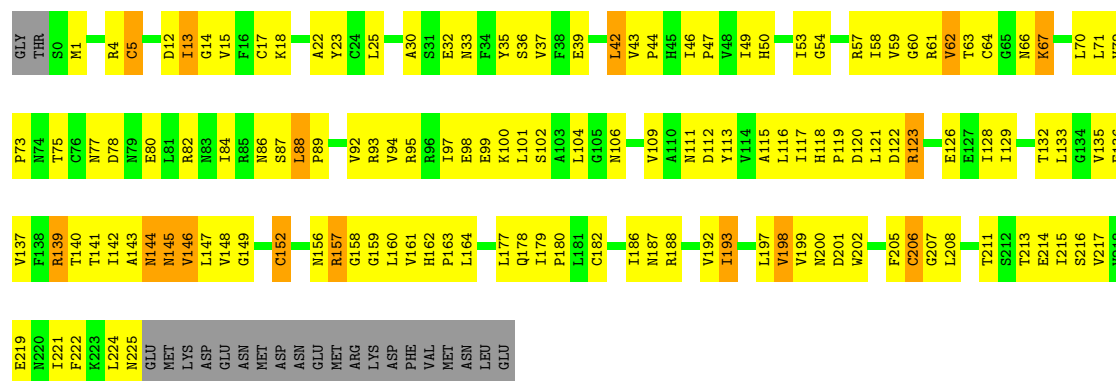
- Molecule 8: RPL35A

Chain HH:



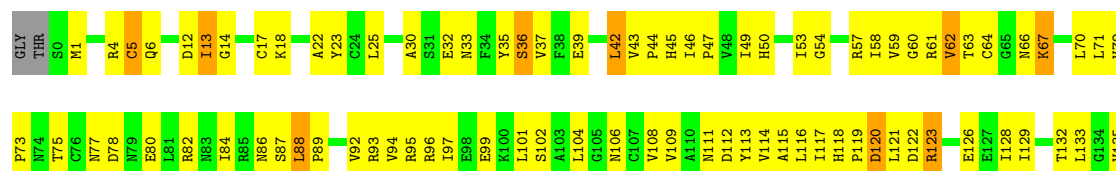
- Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

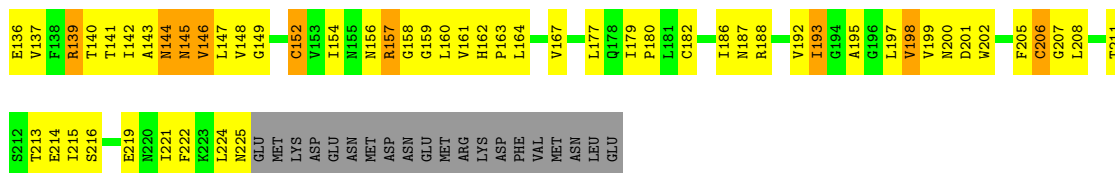
Chain AJ:



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

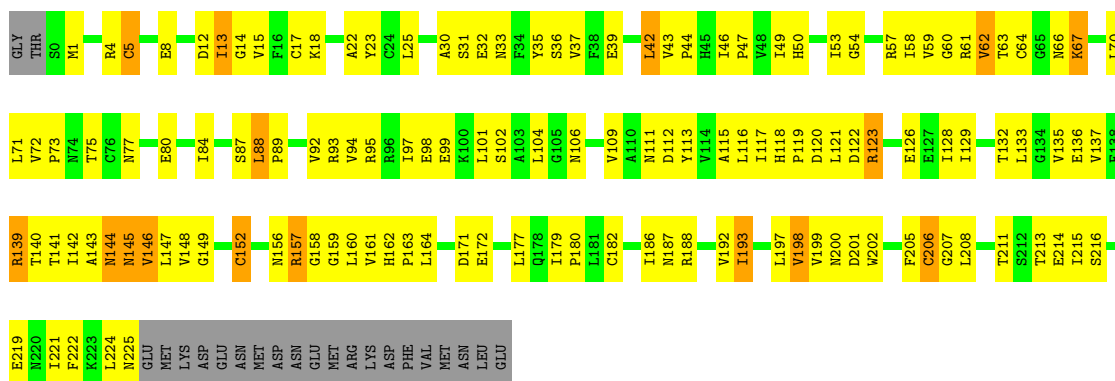
Chain DJ:





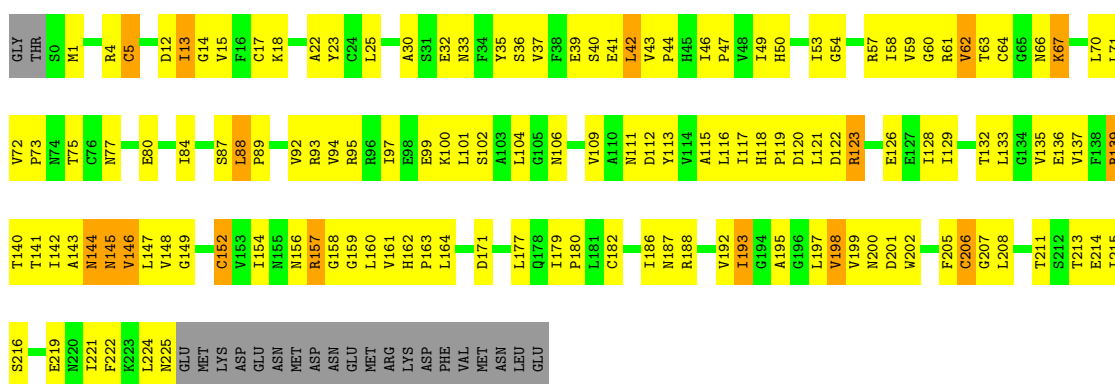
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain FJ:



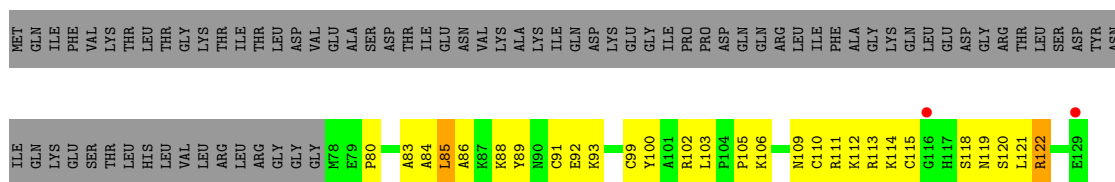
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN

Chain HJ:



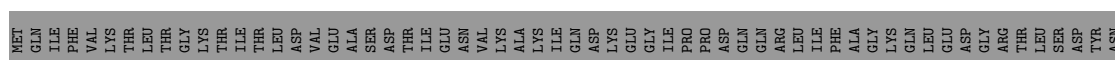
• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

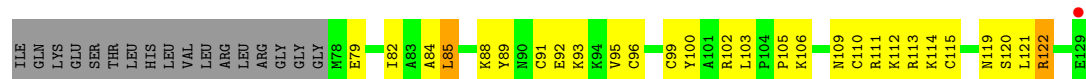
Chain AK:



• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

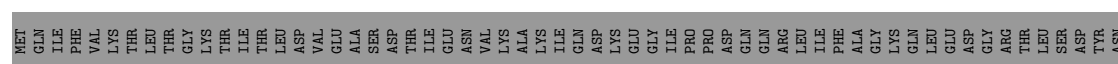
Chain DK:





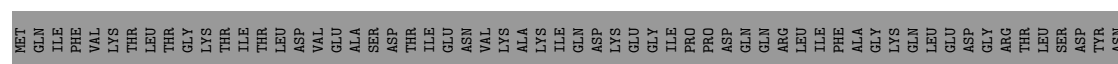
• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain FK:



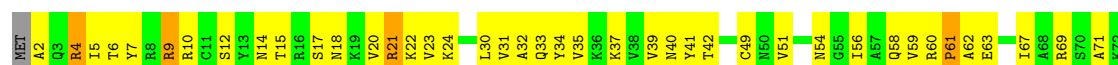
• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain HK:



• Molecule 11: RPL34

Chain AL:



• Molecule 11: RPL34

Chain DL:



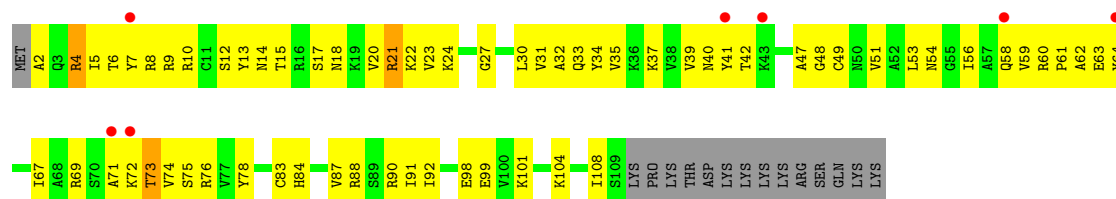
• Molecule 11: RPL34

Chain FL:



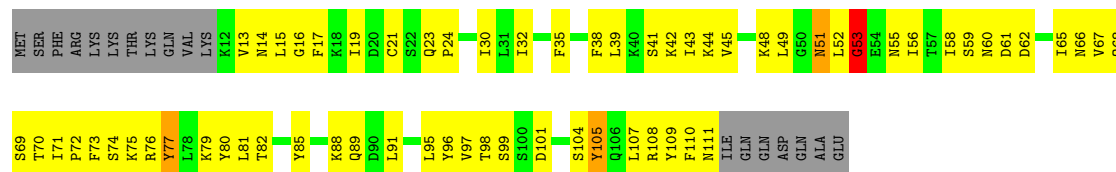
• Molecule 11: RPL34

Chain HL: 



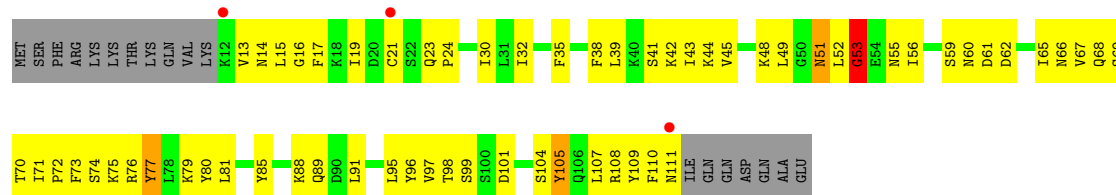
• Molecule 12: RIBOSOMAL PROTEIN L22

Chain AM: 



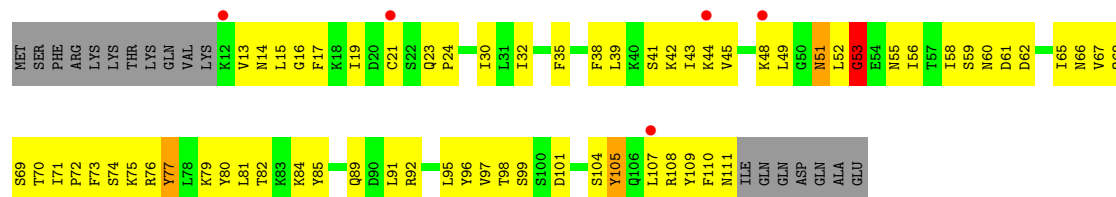
• Molecule 12: RIBOSOMAL PROTEIN L22

Chain DM: 



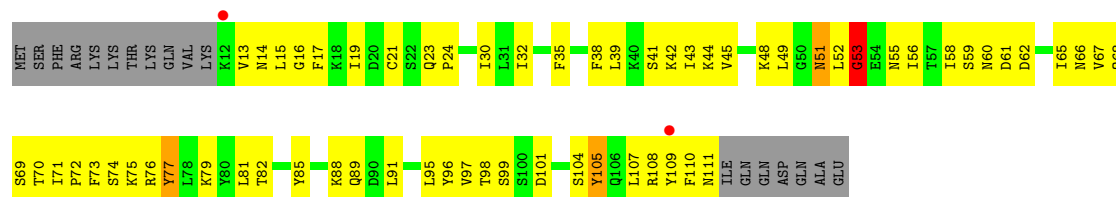
• Molecule 12: RIBOSOMAL PROTEIN L22

Chain FM: 



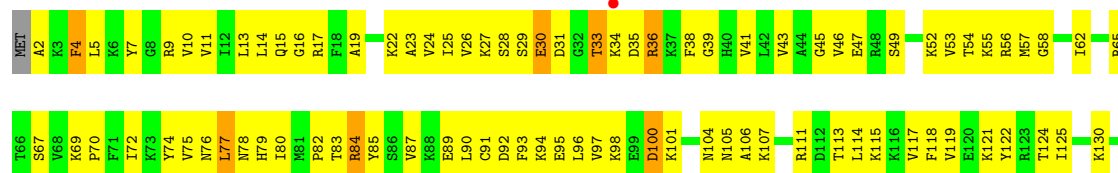
• Molecule 12: RIBOSOMAL PROTEIN L22

Chain HM: 



• Molecule 13: RPL27

Chain AN: 



F138  
F139  
K141  
L142  
R143  
F144

• Molecule 13: RPL27

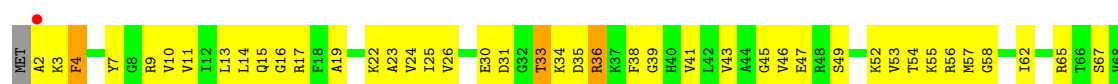
Chain DN:



R143  
F144

• Molecule 13: RPL27

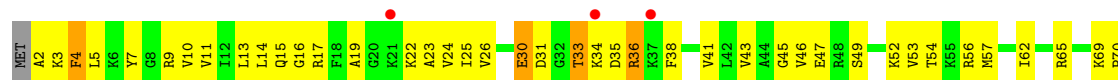
Chain FN:



K141  
L142  
R143  
F144

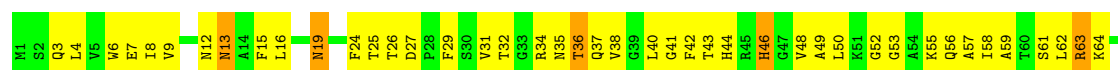
• Molecule 13: RPL27

Chain HN:



• Molecule 14: RPL28

Chain AO:

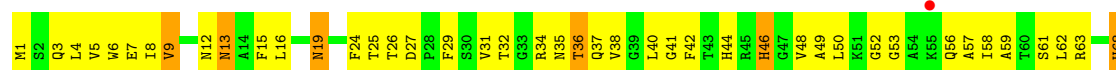




• Molecule 14: RPL28



• Molecule 14: RPL28



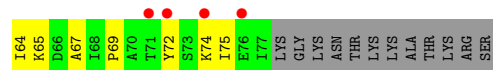
• Molecule 14: RPL28



• Molecule 15: RPL38

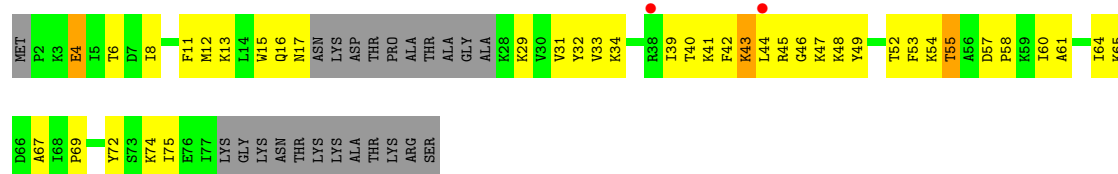


• Molecule 15: RPL38



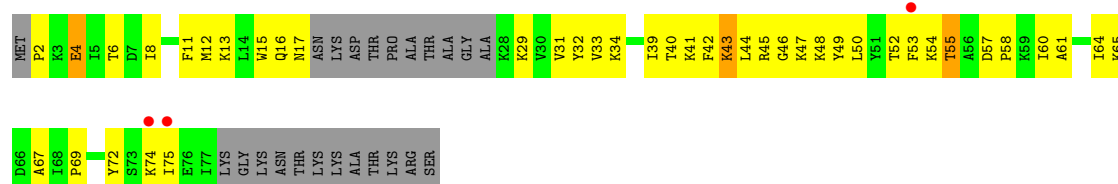
- Molecule 15: RPL38

Chain FP:



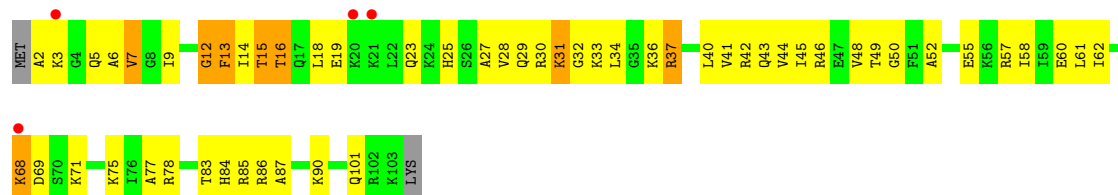
- Molecule 15: RPL38

Chain HP:



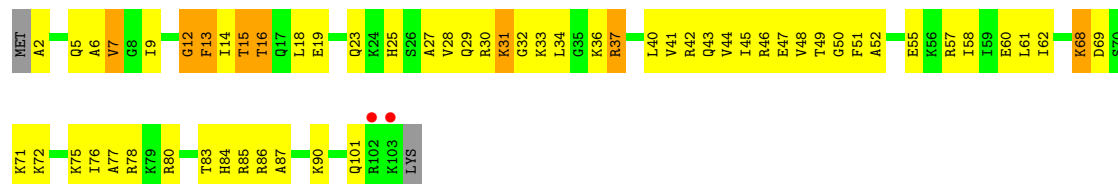
- Molecule 16: 60S RIBOSOMAL PROTEIN L36

Chain AQ:



- Molecule 16: 60S RIBOSOMAL PROTEIN L36

Chain DQ:



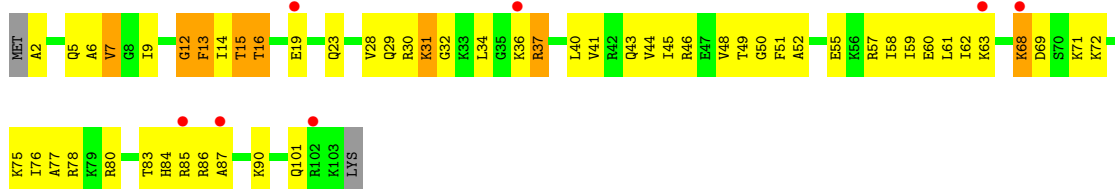
- Molecule 16: 60S RIBOSOMAL PROTEIN L36

Chain FQ:



- Molecule 16: 60S RIBOSOMAL PROTEIN L36

Chain HQ: 



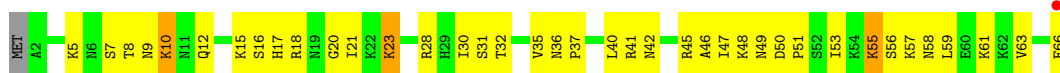
• Molecule 17: RPL29

Chain AT: 



• Molecule 17: RPL29

Chain DT: 



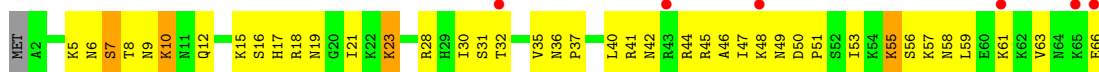
• Molecule 17: RPL29

Chain FT: 



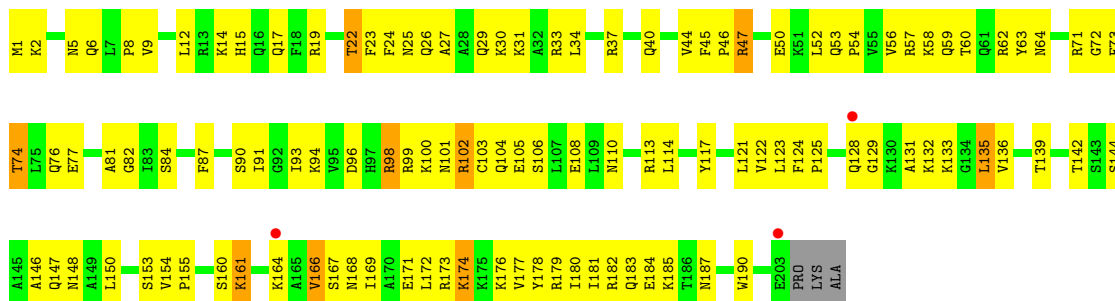
• Molecule 17: RPL29

Chain HT: 



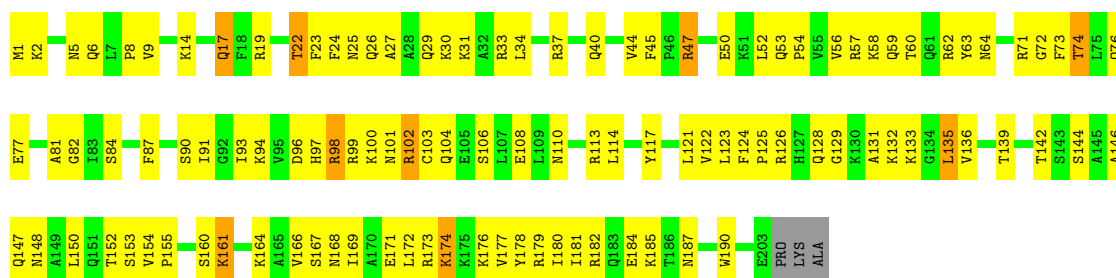
• Molecule 18: RPL13

Chain AU: 



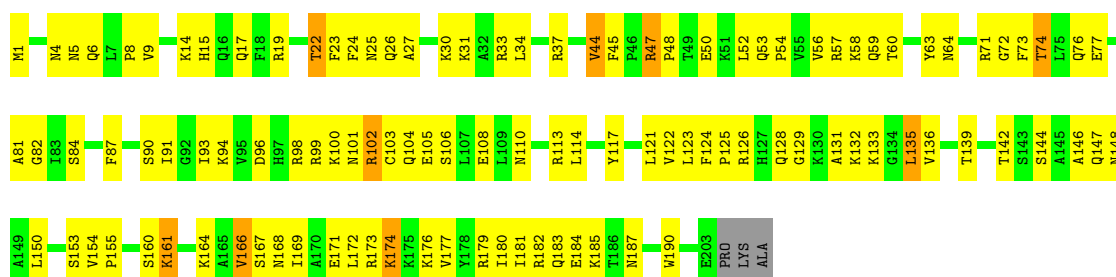
• Molecule 18: RPL13

Chain DU: 



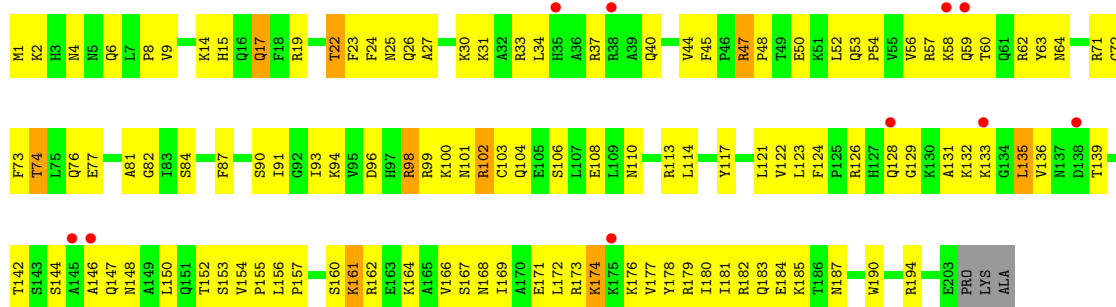
• Molecule 18: RPL13

Chain FU:



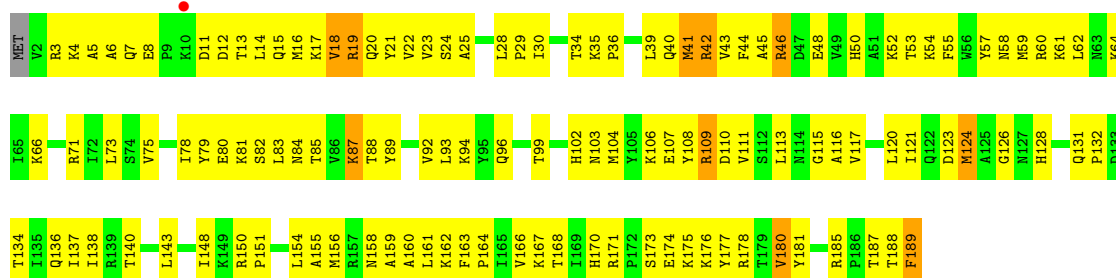
• Molecule 18: RPL13

Chain HU:



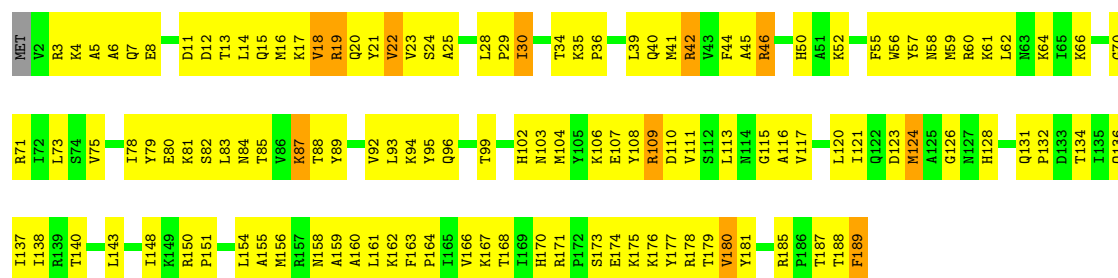
• Molecule 19: RPL18A

Chain AX:



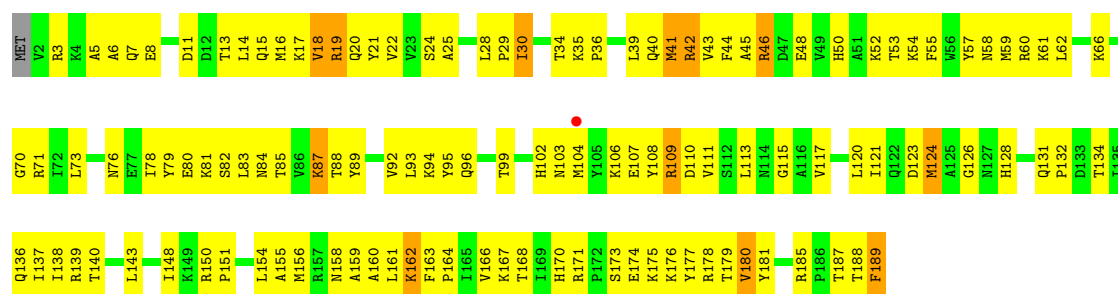
• Molecule 19: RPL18A

Chain DX:



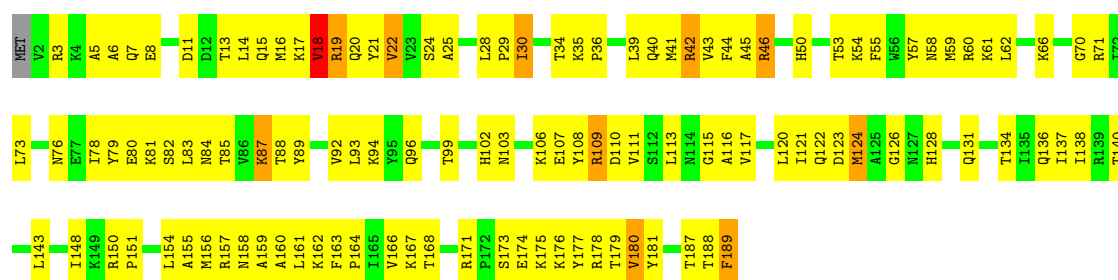
• Molecule 19: RPL18A

Chain FX:



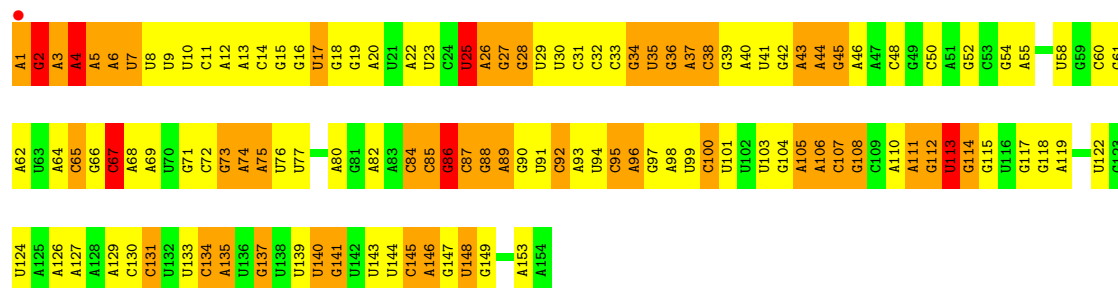
• Molecule 19: RPL18A

Chain HX:



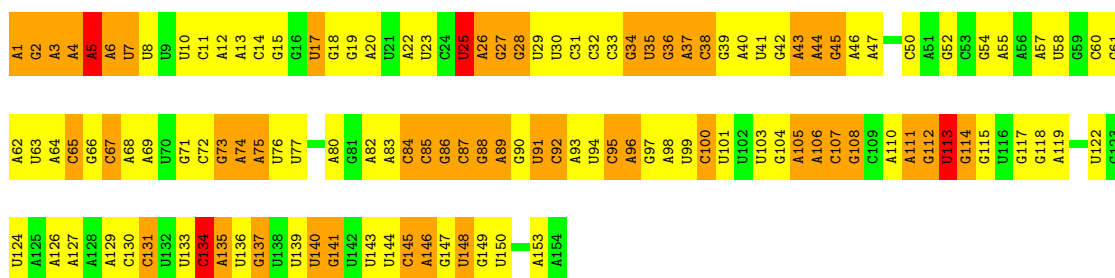
• Molecule 20: 5.8S RRNA

Chain B2:



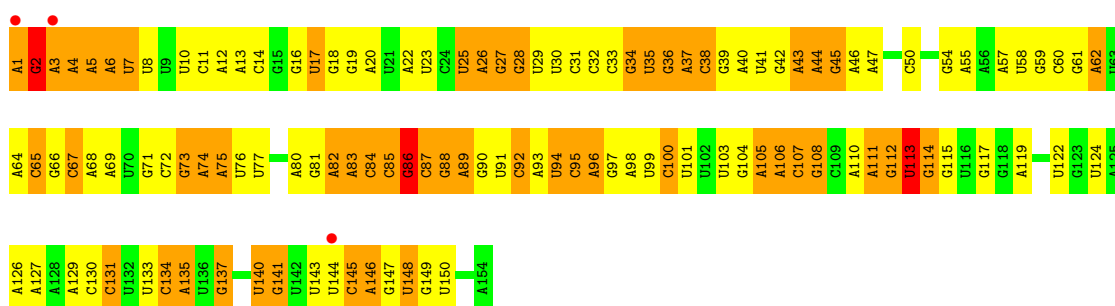
• Molecule 20: 5.8S RRNA

Chain C2:



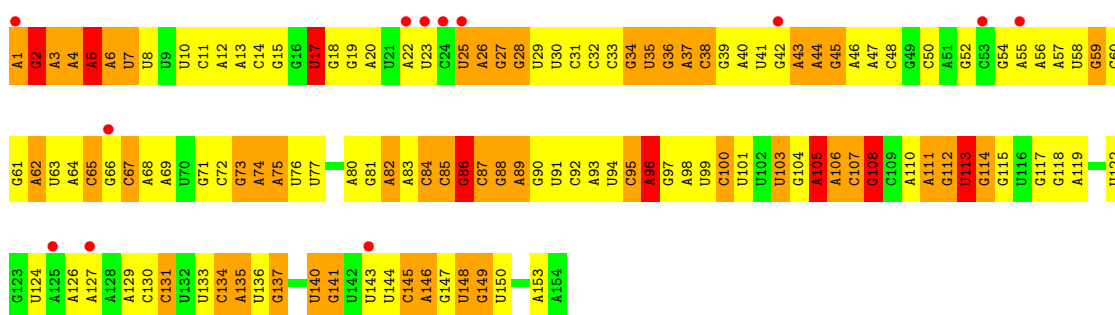
• Molecule 20: 5.8S rRNA

Chain E2:



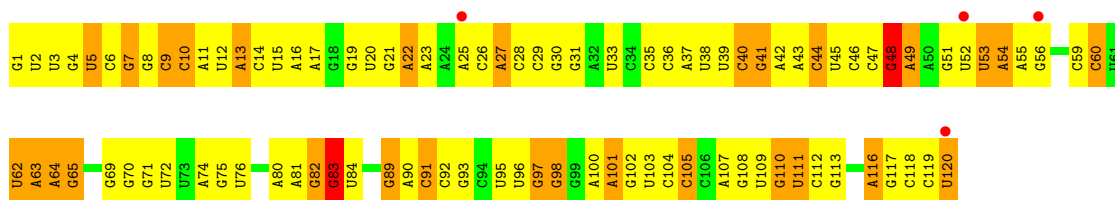
• Molecule 20: 5.8S rRNA

Chain G2:



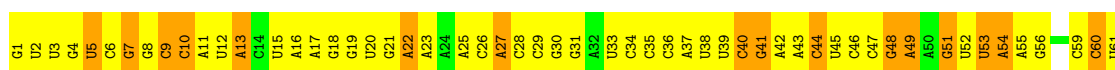
• Molecule 21: 5S rRNA

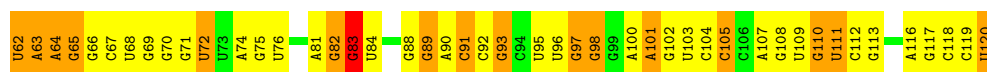
Chain B3:



• Molecule 21: 5S rRNA

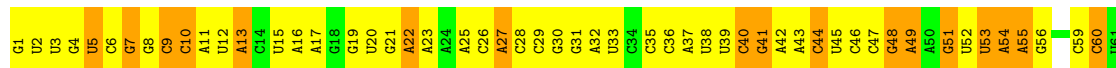
Chain C3:





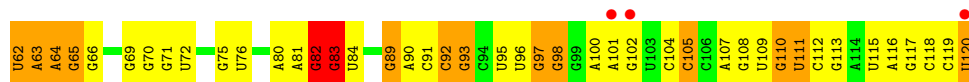
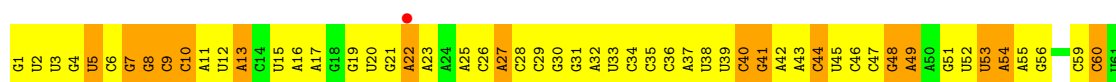
• Molecule 21: 5S rRNA

Chain E3:



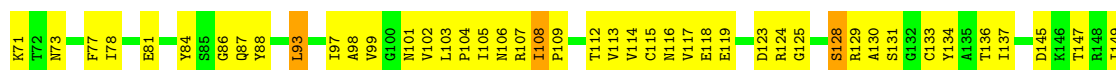
• Molecule 21: 5S rRNA

Chain G3:



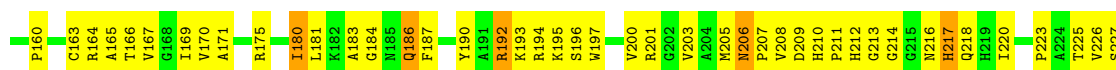
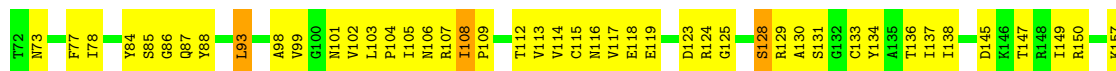
• Molecule 22: RPL8

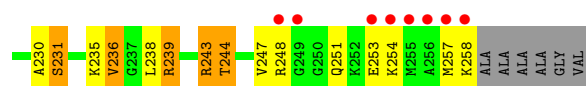
Chain BA:



• Molecule 22: RPL8

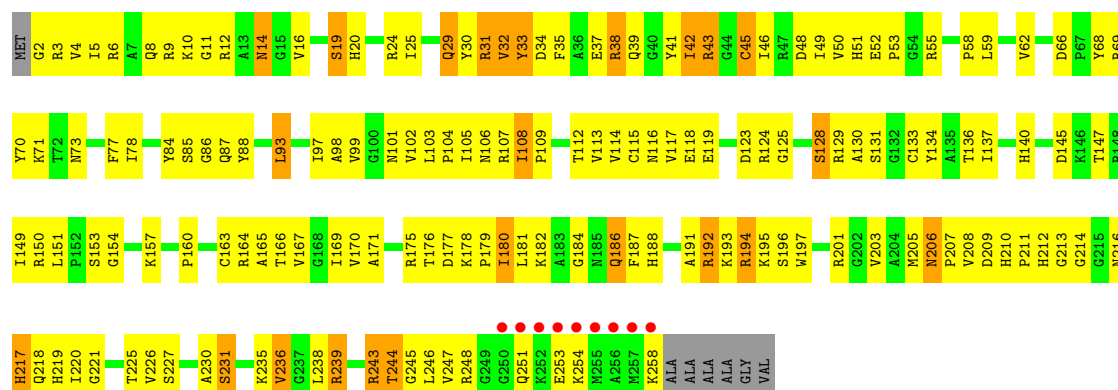
Chain CA:





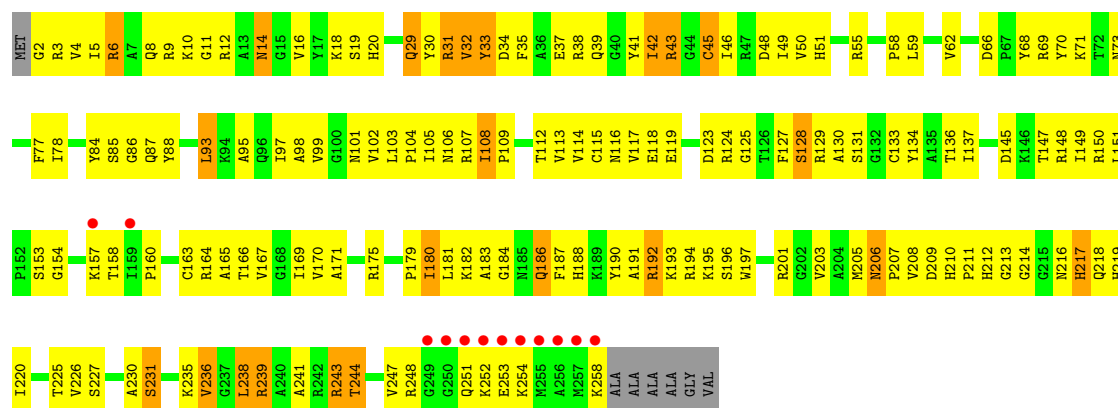
• Molecule 22: RPL8

Chain EA:



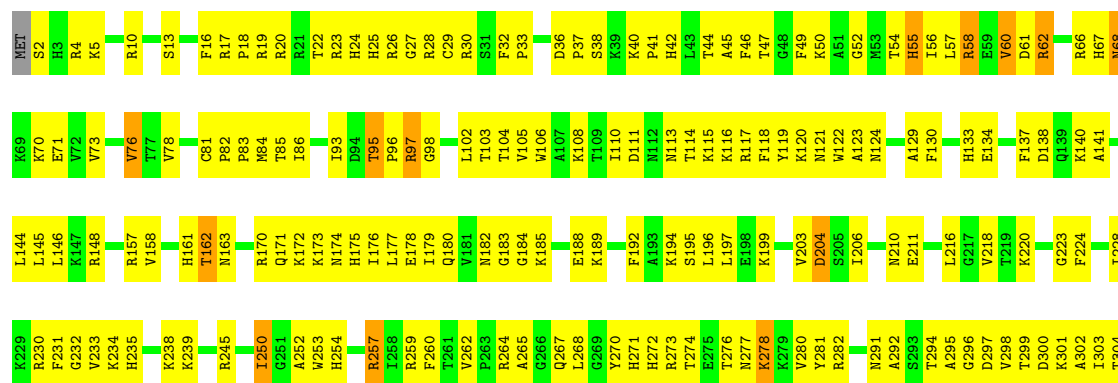
• Molecule 22: RPL8

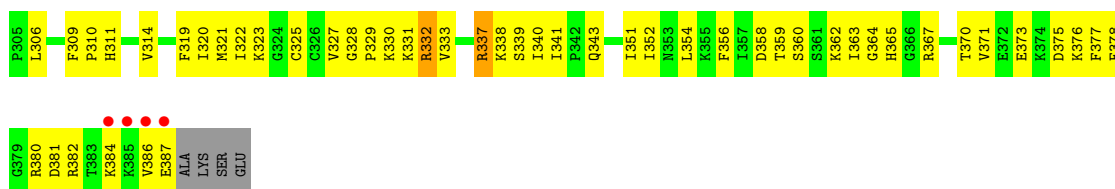
Chain GA:



• Molecule 23: RIBOSOMAL PROTEIN L3

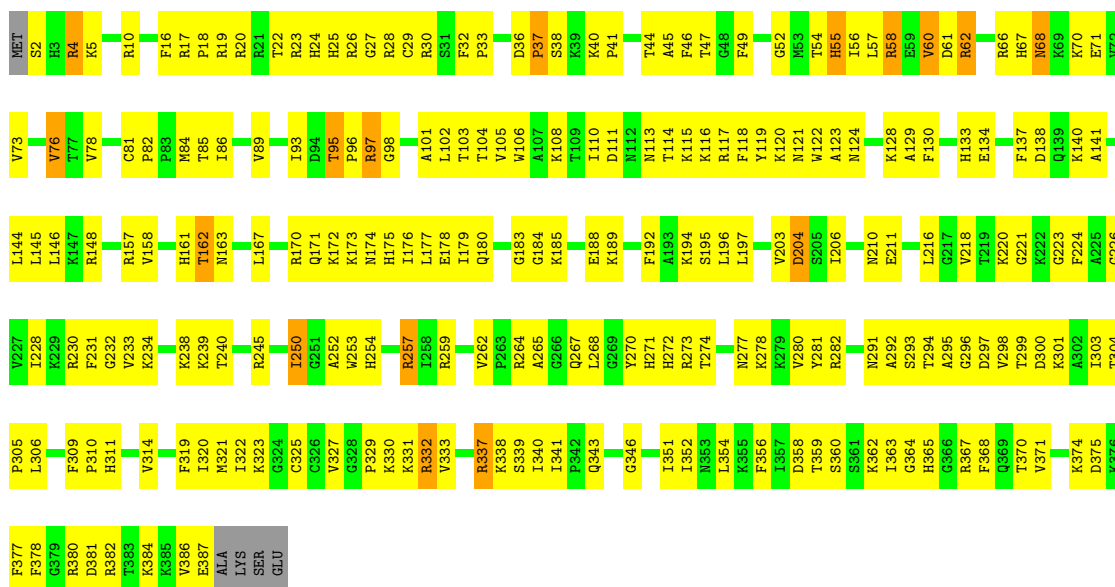
Chain BB:





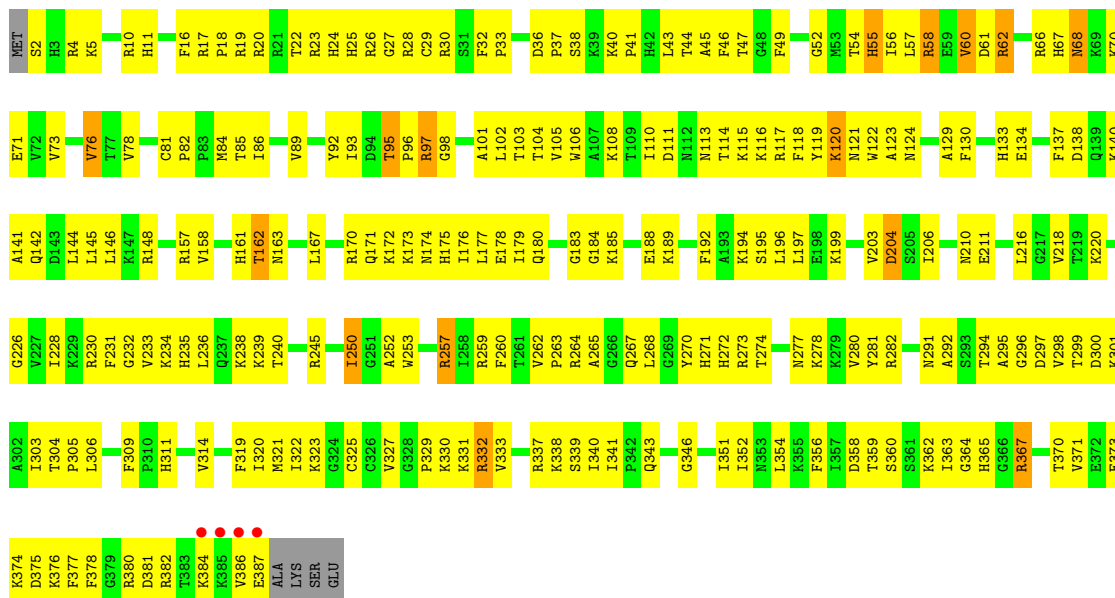
• Molecule 23: RIBOSOMAL PROTEIN L3

Chain CB:



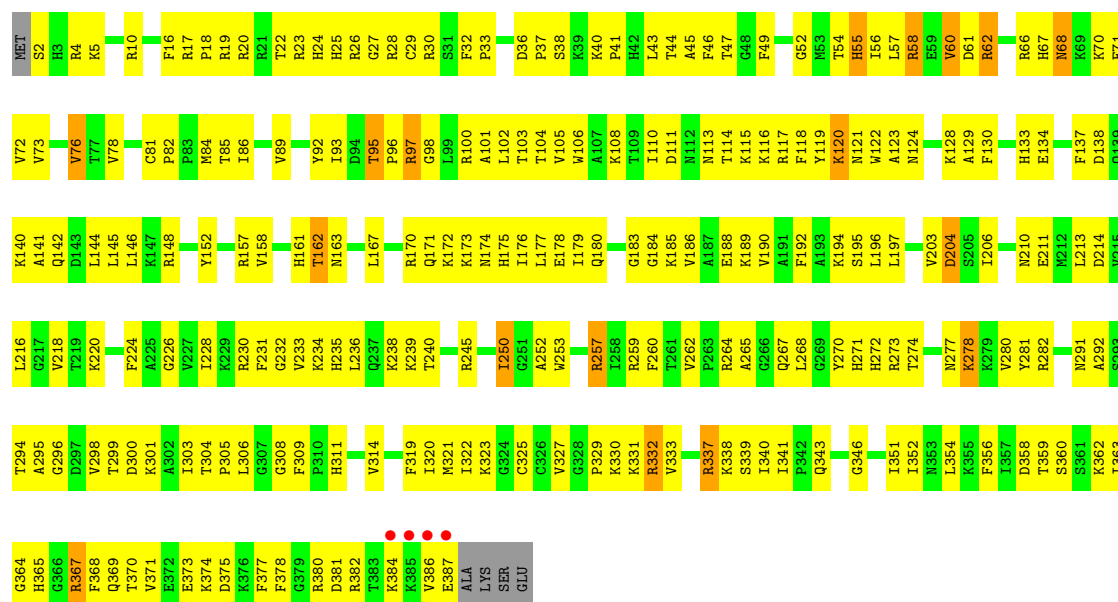
• Molecule 23: RIBOSOMAL PROTEIN L3

Chain EB:



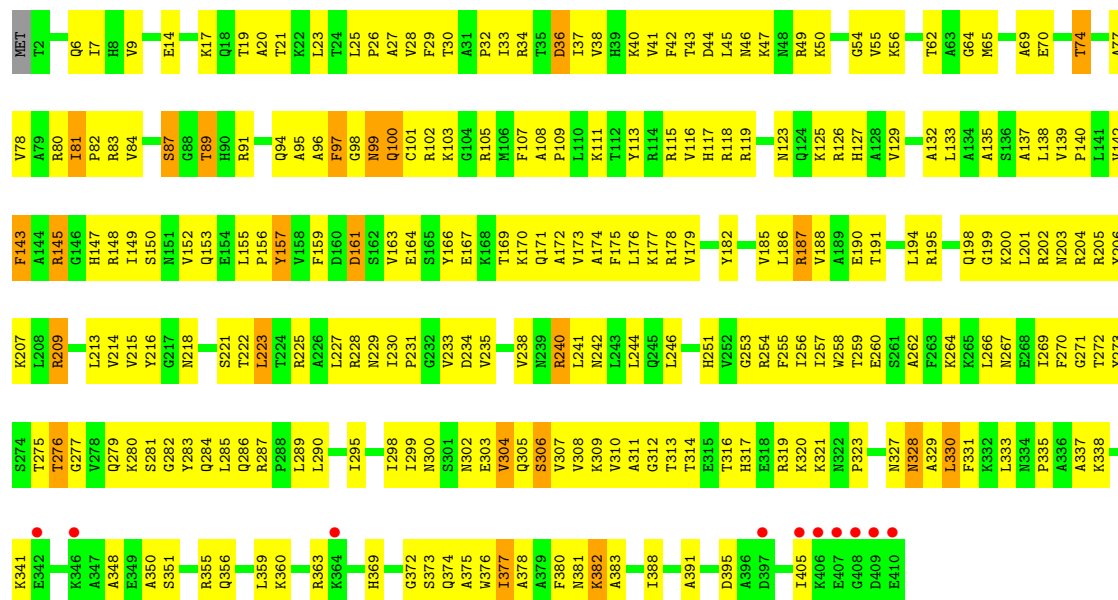
• Molecule 23: RIBOSOMAL PROTEIN L3

Chain GB:



• Molecule 24: RPL4

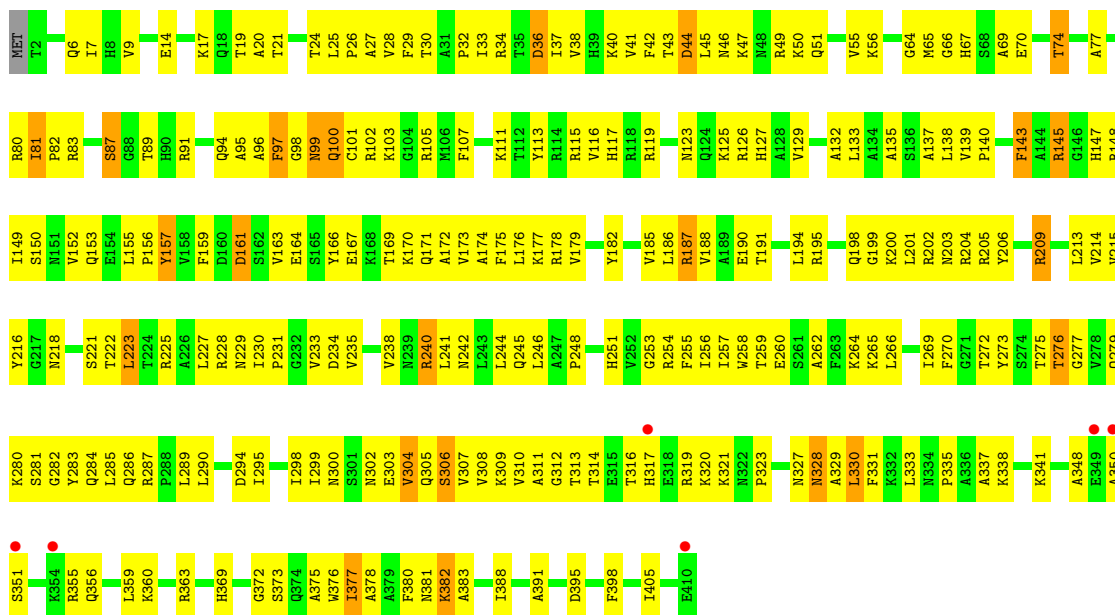
Chain BC:





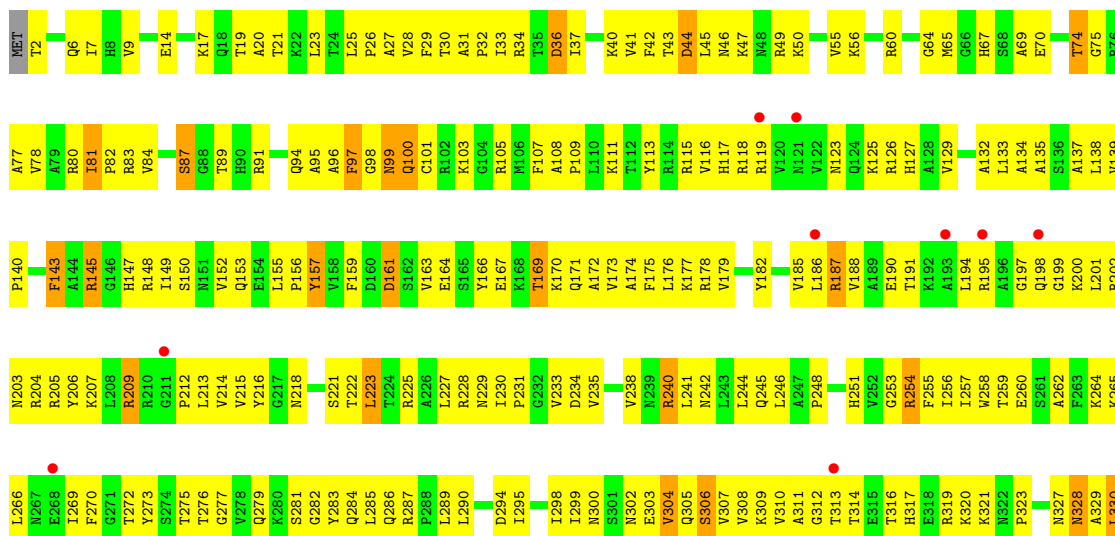
• Molecule 24: RPL4

Chain EC:



• Molecule 24: RPL4

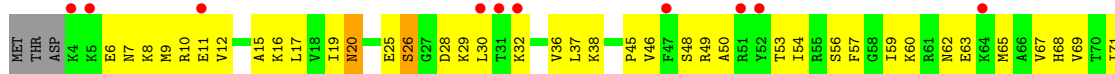
Chain GC:





• Molecule 25: 60S RIBOSOMAL PROTEIN L11

Chain BD:



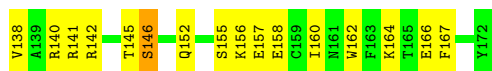
• Molecule 25: 60S RIBOSOMAL PROTEIN L11

Chain CD:



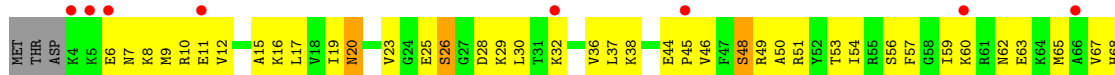
• Molecule 25: 60S RIBOSOMAL PROTEIN L11

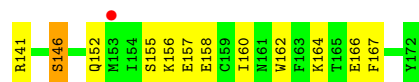
Chain ED:



• Molecule 25: 60S RIBOSOMAL PROTEIN L11

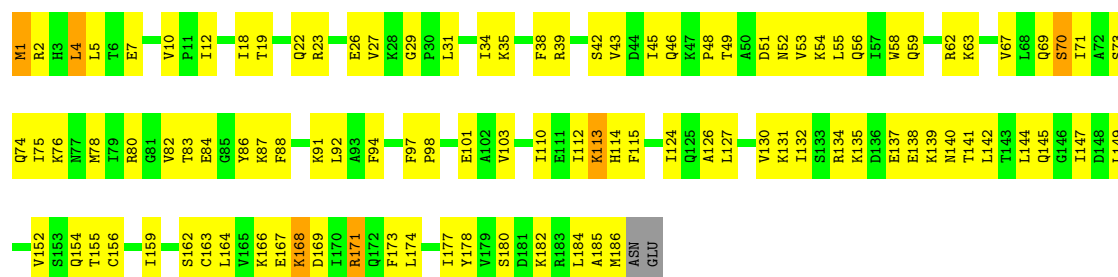
Chain GD:





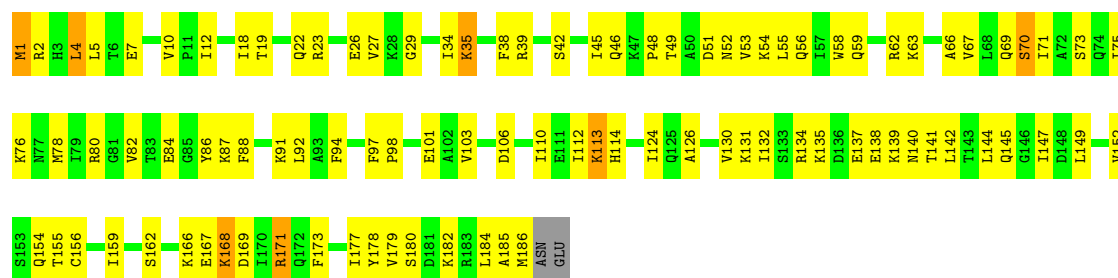
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

Chain BE:



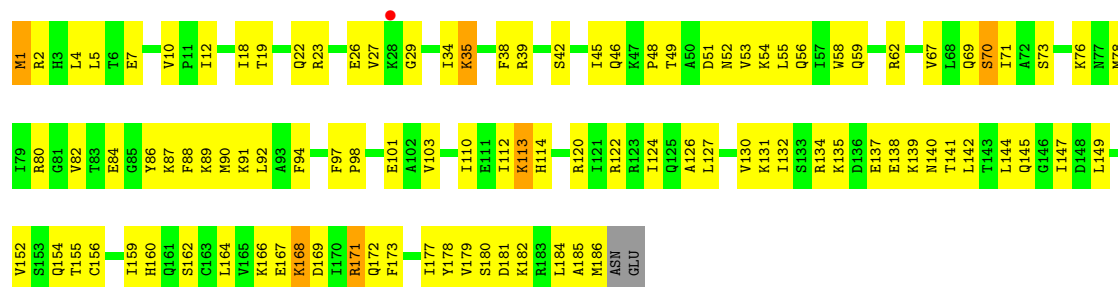
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

Chain CE:



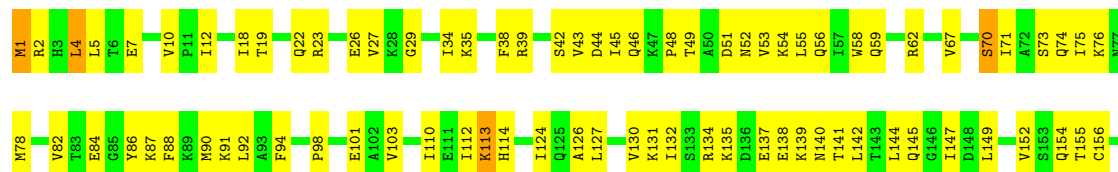
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

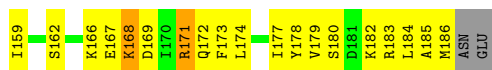
Chain EE:



• Molecule 26: 60S RIBOSOMAL PROTEIN L9

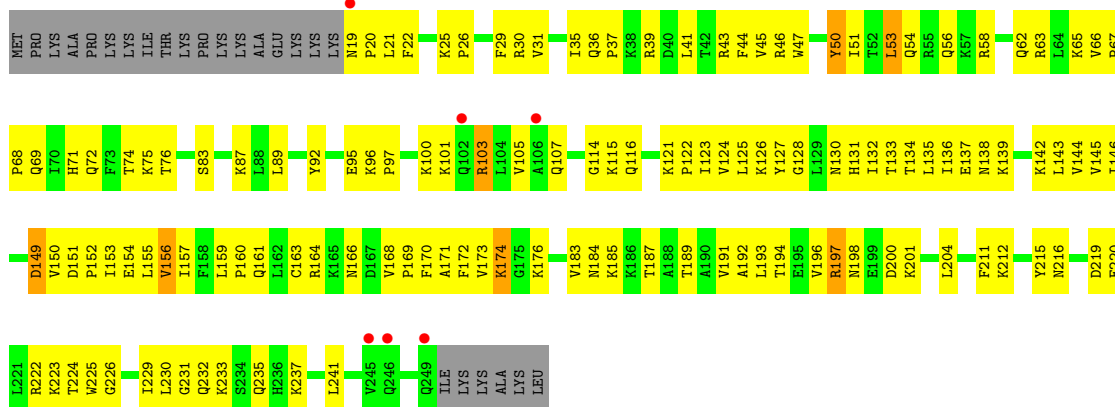
Chain GE:





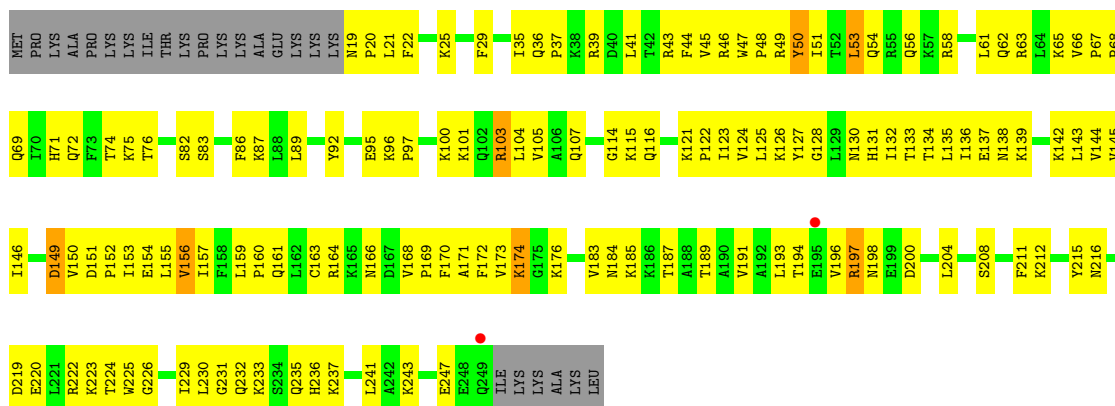
• Molecule 27: RPL7A

Chain BF:



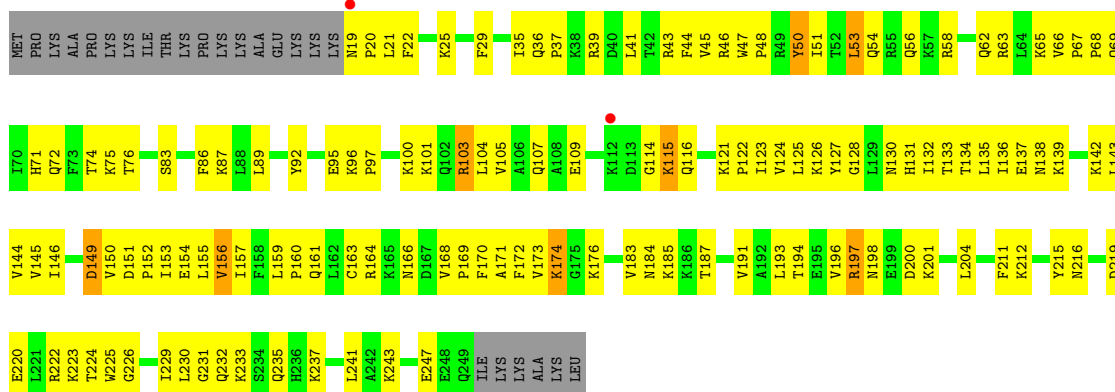
• Molecule 27: RPL7A

Chain CF:



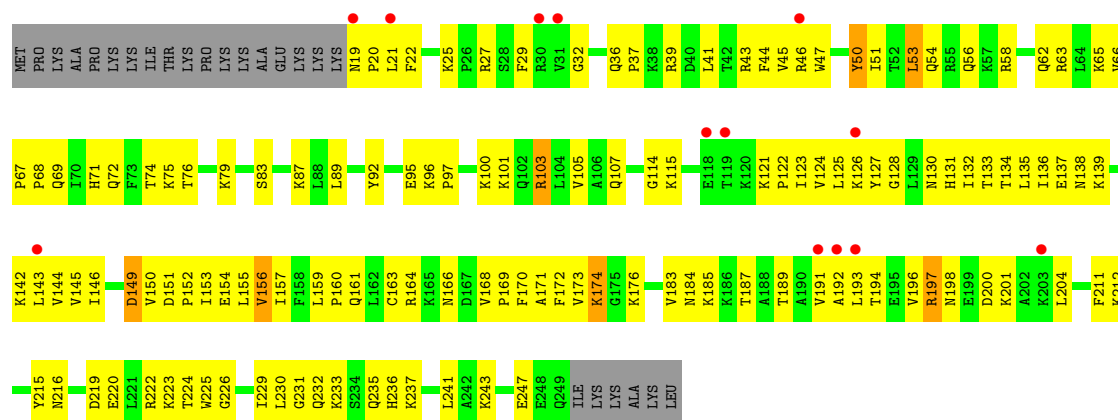
• Molecule 27: RPL7A

Chain EF:



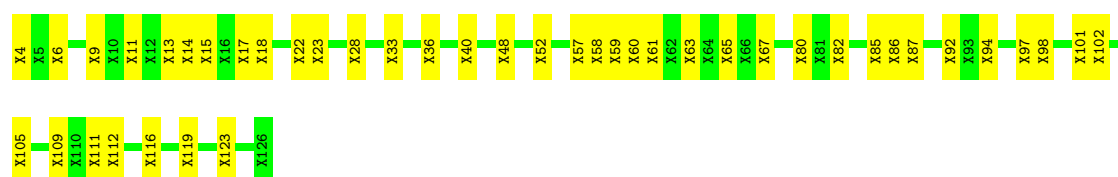
- Molecule 27: RPL7A

Chain GF:



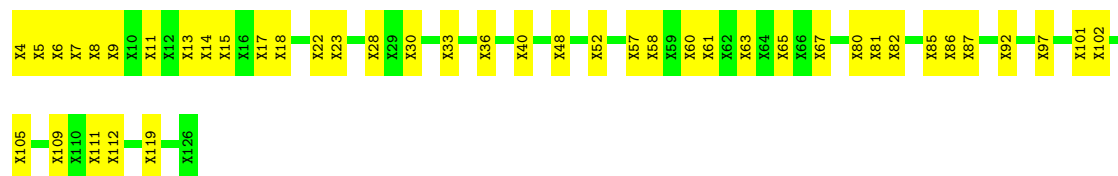
- Molecule 28: RPLP0

Chain BG:



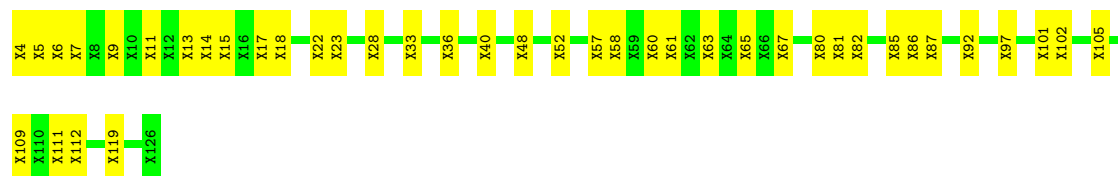
- Molecule 28: RPLP0

Chain CG:



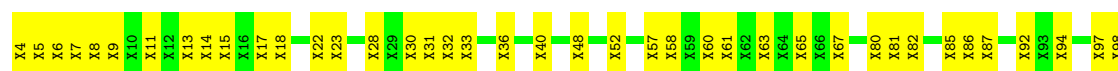
- Molecule 28: RPLP0

Chain EG:



- Molecule 28: RPLP0

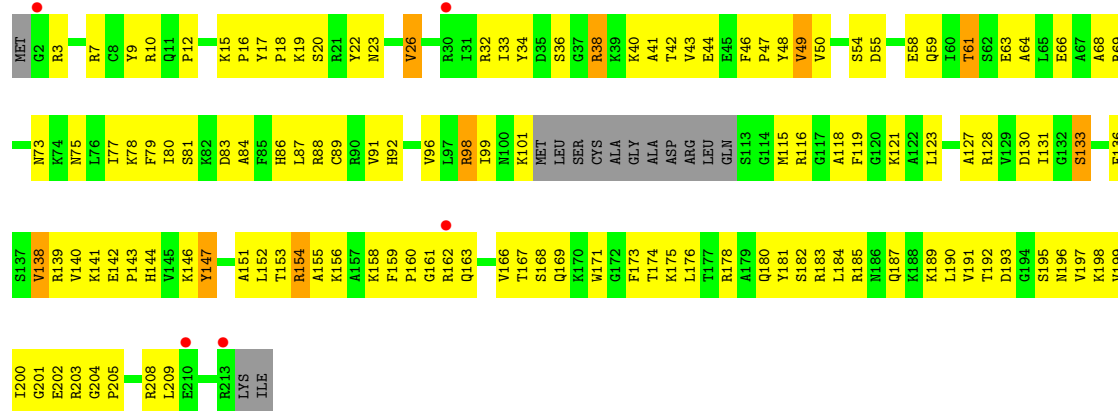
Chain GG:





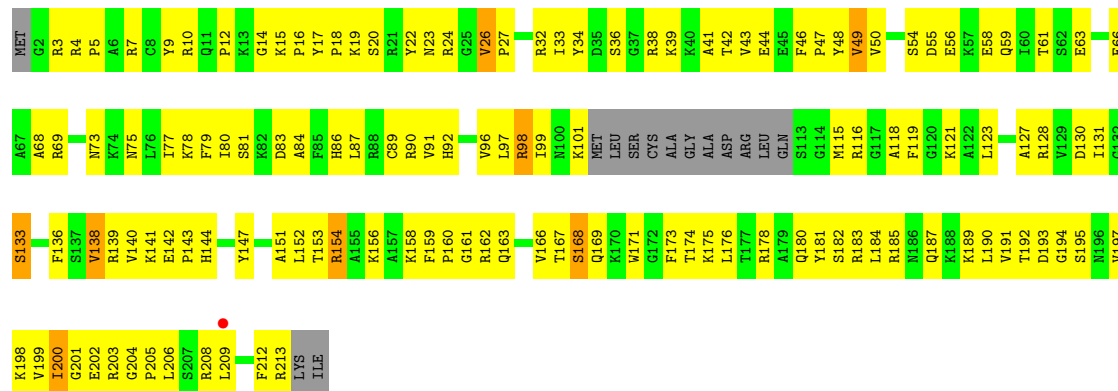
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain BH:



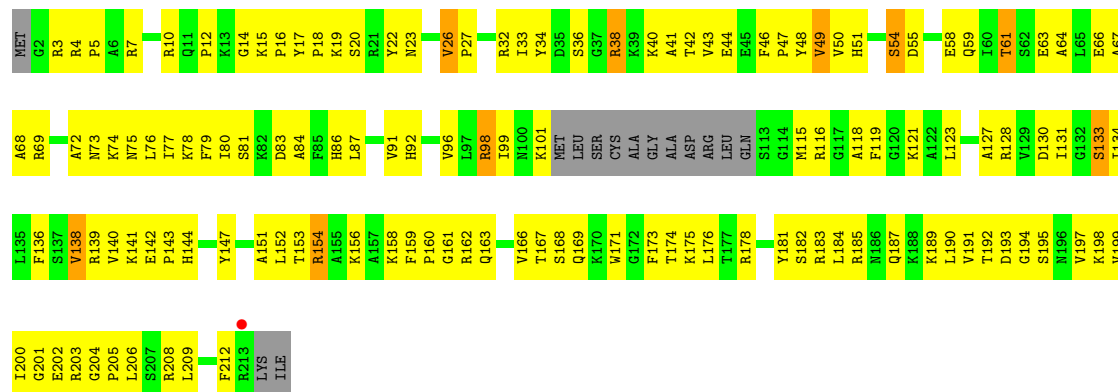
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain CH:



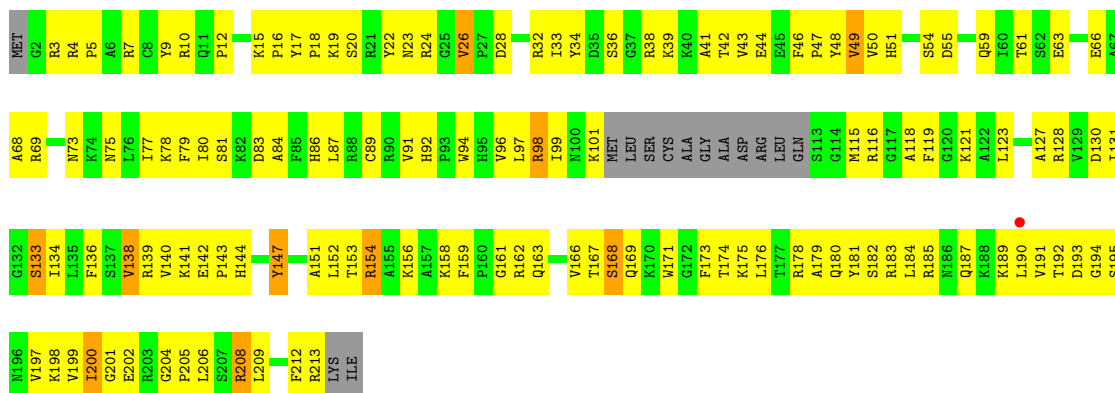
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain EH:



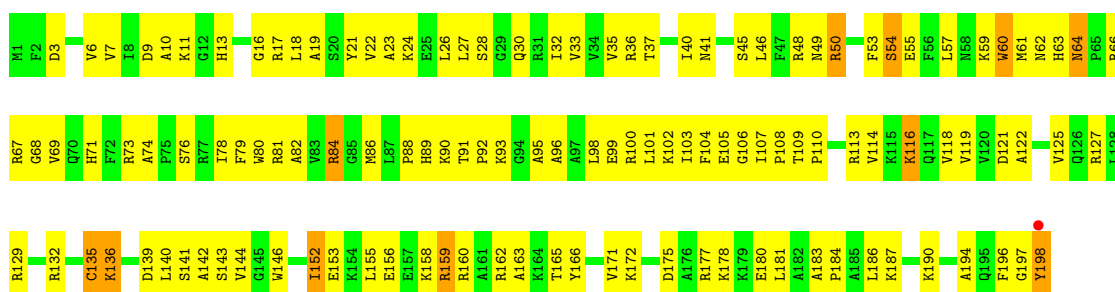
• Molecule 29: 60S RIBOSOMAL PROTEIN L10

Chain GH:



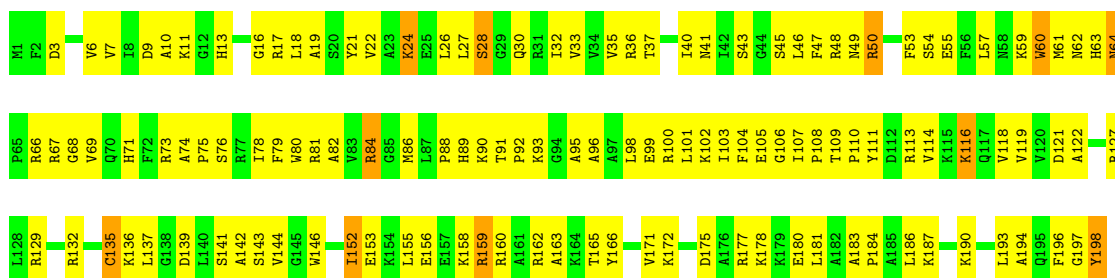
- Molecule 30: 60S RIBOSOMAL PROTEIN L13A

Chain BI:



- Molecule 30: 60S RIBOSOMAL PROTEIN L13A

Chain CI:



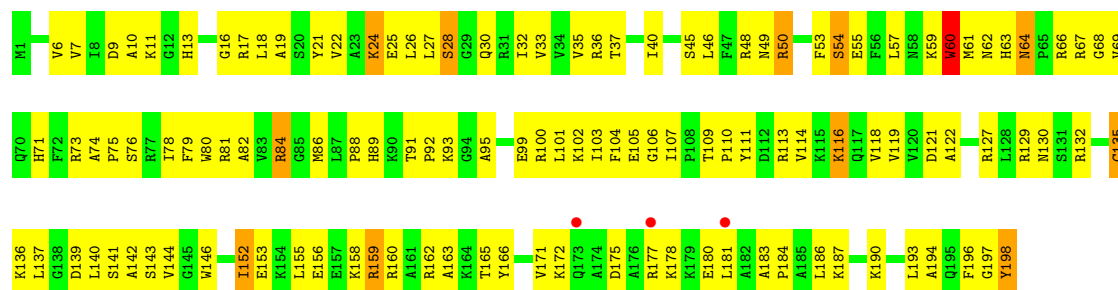
- Molecule 30: 60S RIBOSOMAL PROTEIN L13A

Chain EI:



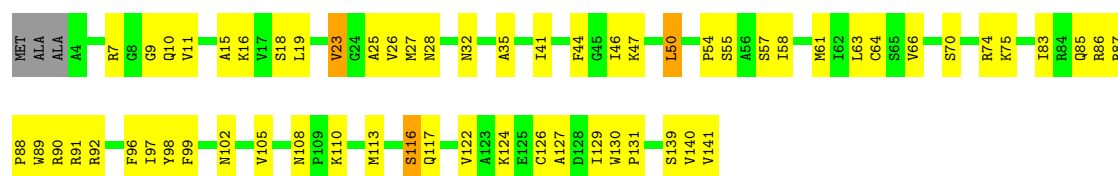
- Molecule 30: 60S RIBOSOMAL PROTEIN L13A

Chain GI:



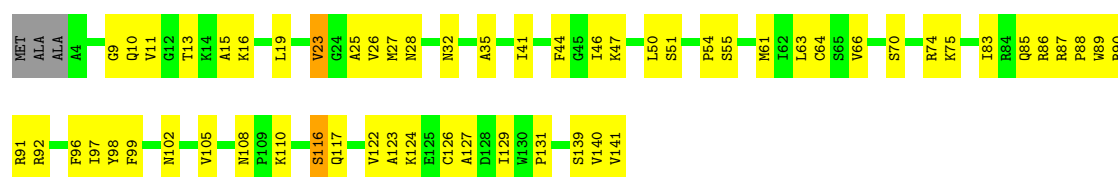
- Molecule 31: RPL23

Chain BJ:



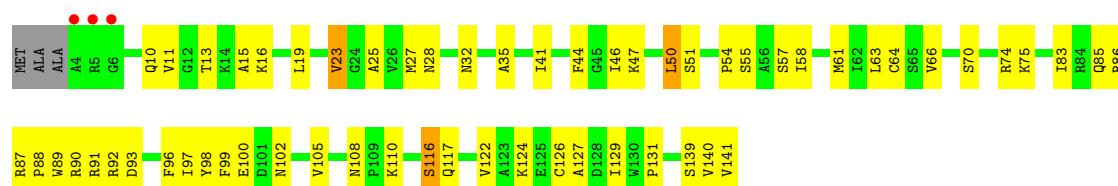
- Molecule 31: RPL23

Chain CJ:



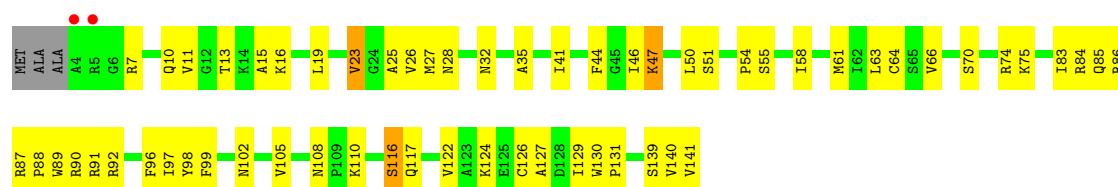
- Molecule 31: RPL23

Chain EJ:



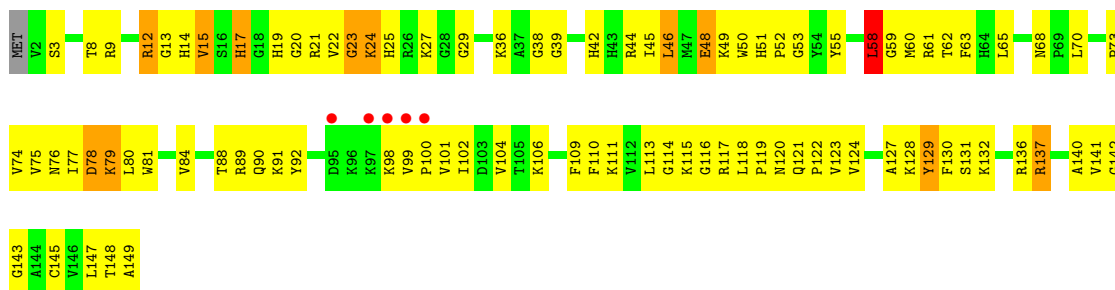
- Molecule 31: RPL23

Chain GJ:



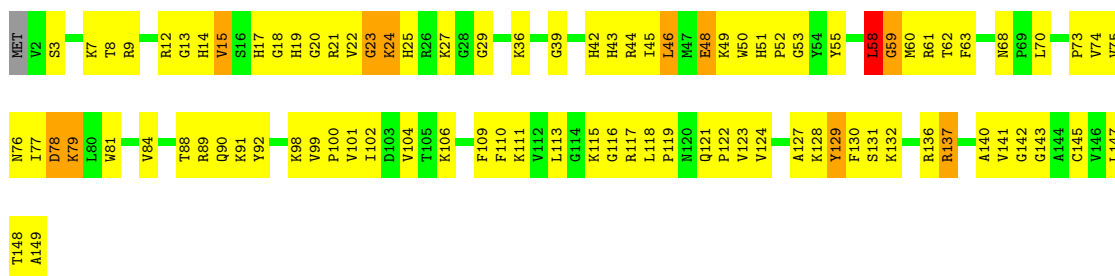
- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

Chain BK:



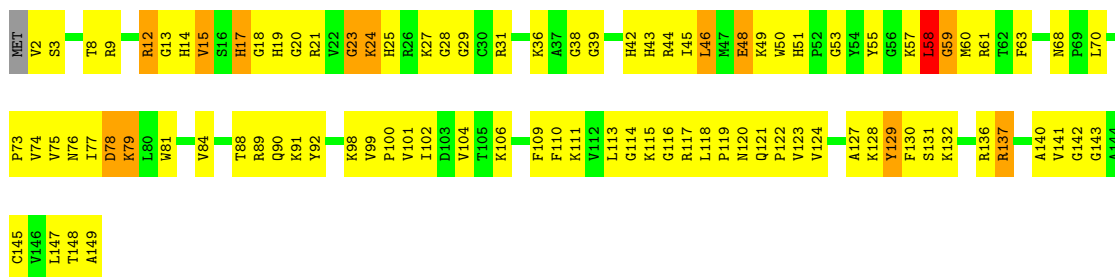
- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

Chain CK:



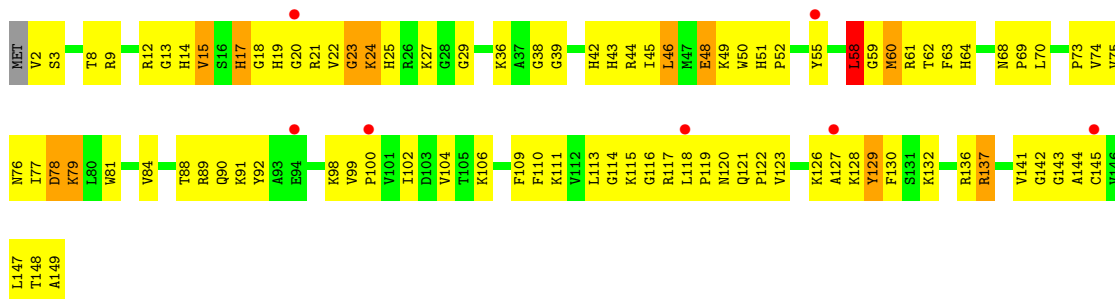
- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

Chain EK:



- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

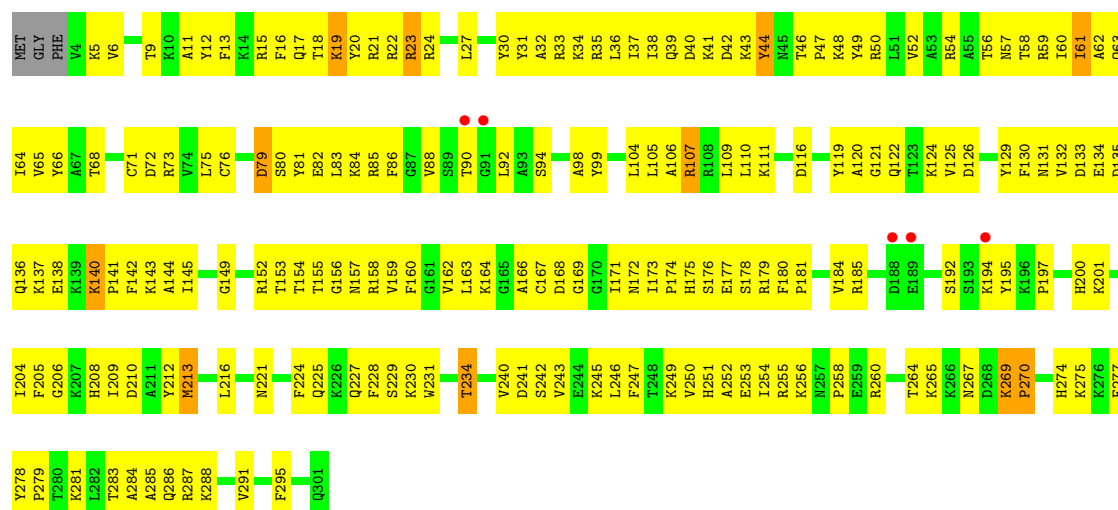
Chain GK:



- Molecule 33: RIBOSOMAL PROTEIN L15

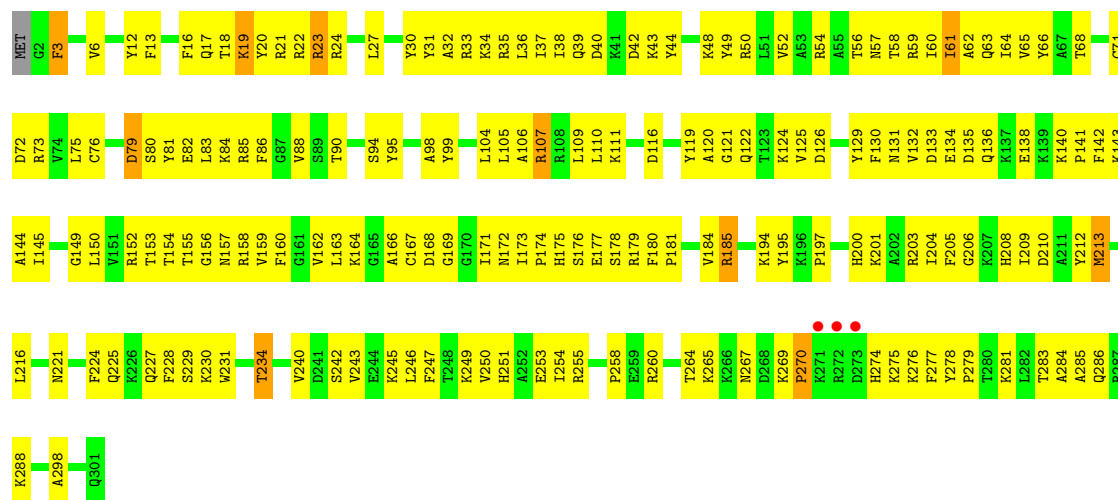
Chain BL:





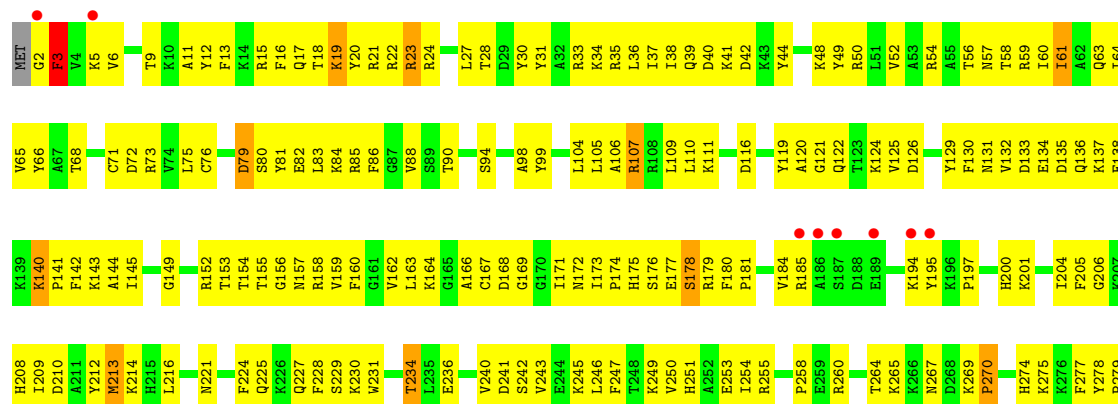
### • Molecule 34: 60S RIBOSOMAL PROTEIN L5

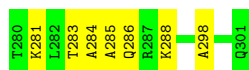
Chain CM:



### • Molecule 34: 60S RIBOSOMAL PROTEIN L5

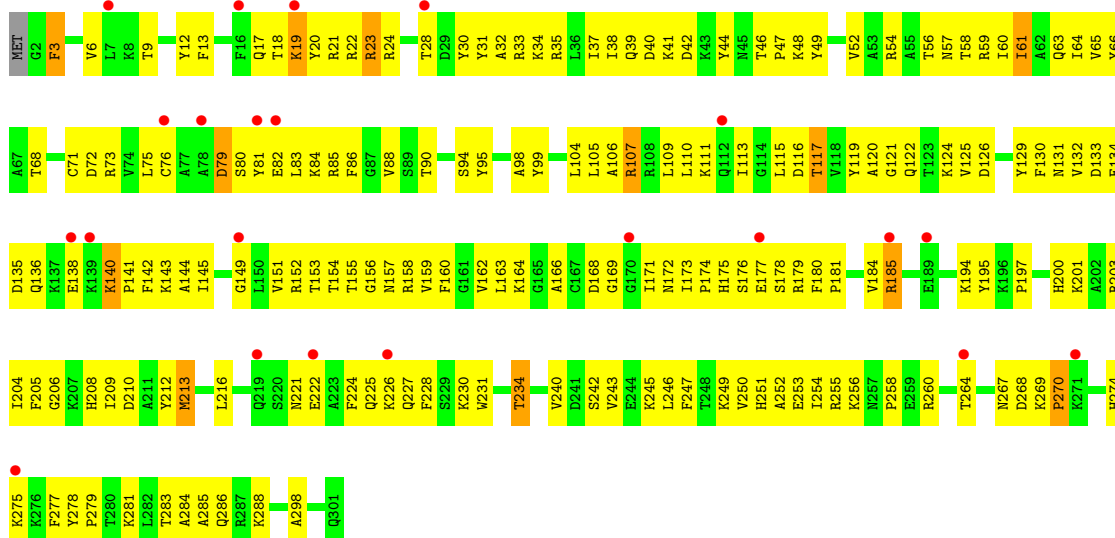
Chain EM:





• Molecule 34: 60S RIBOSOMAL PROTEIN L5

Chain GM:



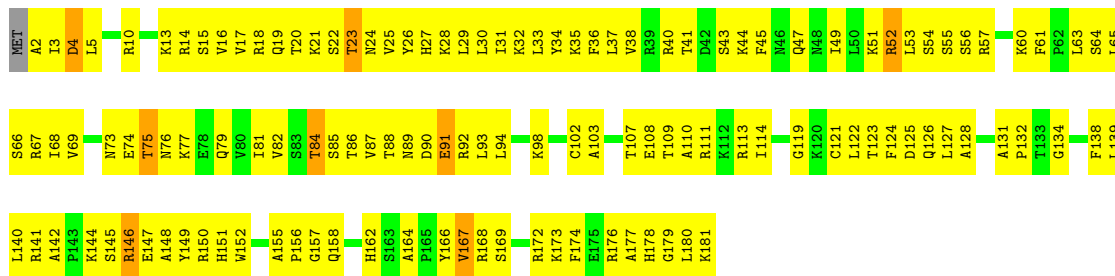
• Molecule 35: RPL18

Chain BN:



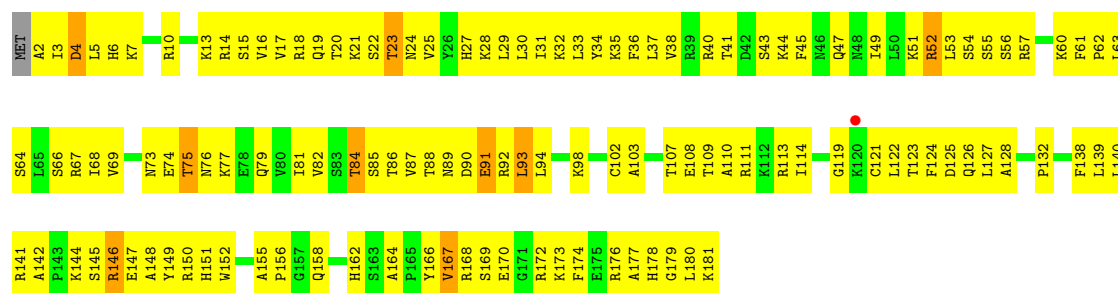
• Molecule 35: RPL18

Chain CN:



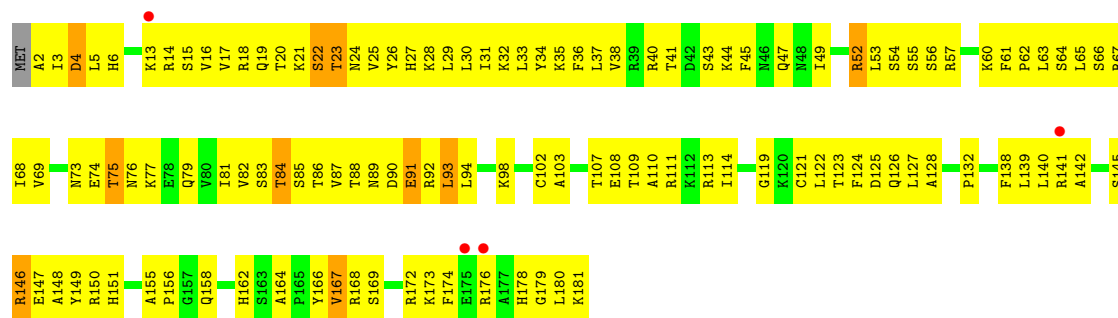
• Molecule 35: RPL18

Chain EN:



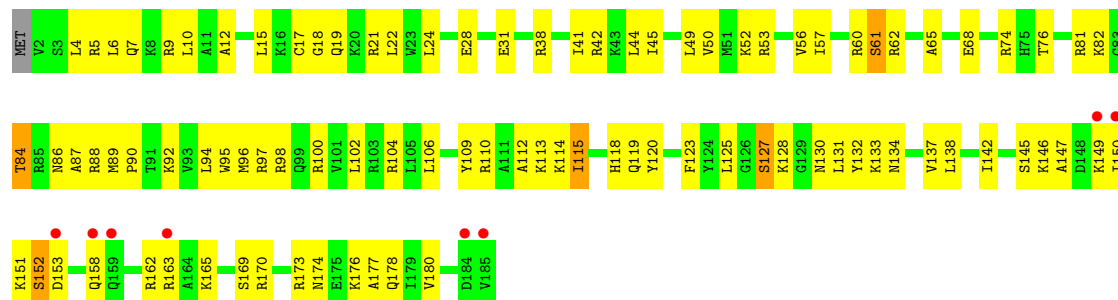
• Molecule 35: RPL18

Chain GN:



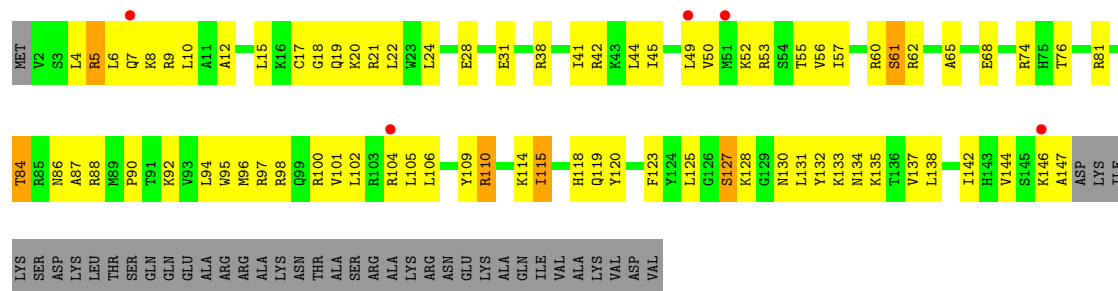
• Molecule 36: RPL19

Chain BO:



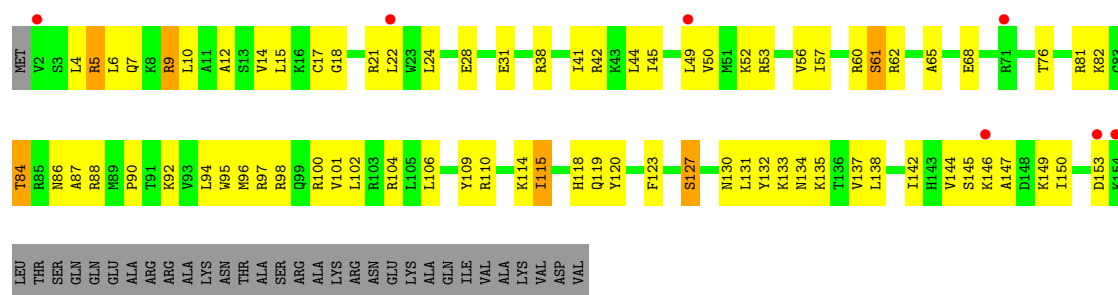
• Molecule 36: RPL19

Chain EO:



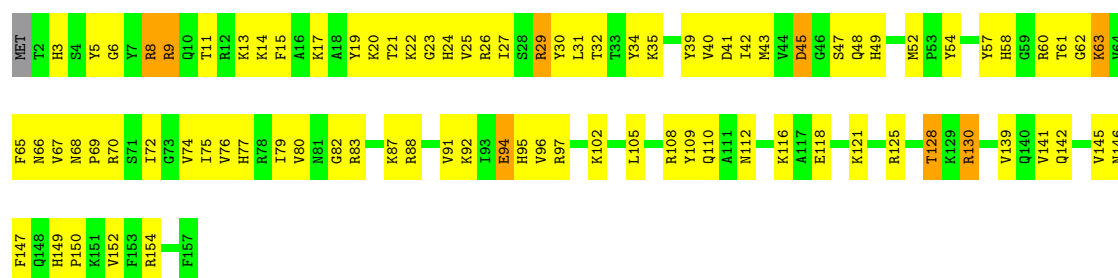
• Molecule 36: RPL19

Chain GO:



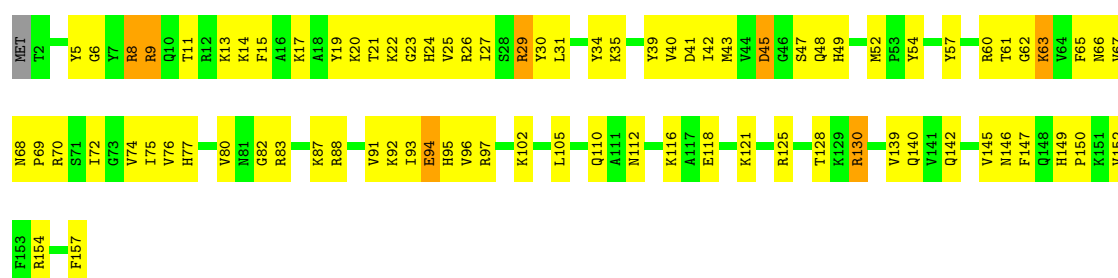
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

Chain BP:



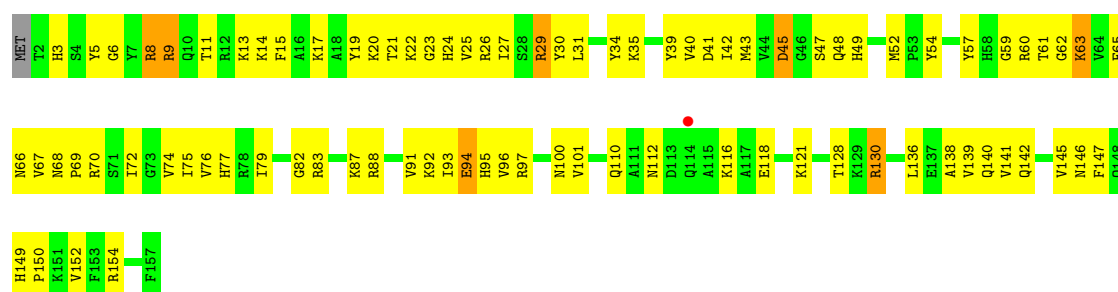
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

Chain CP:



• Molecule 37: 60S RIBOSOMAL PROTEIN L21

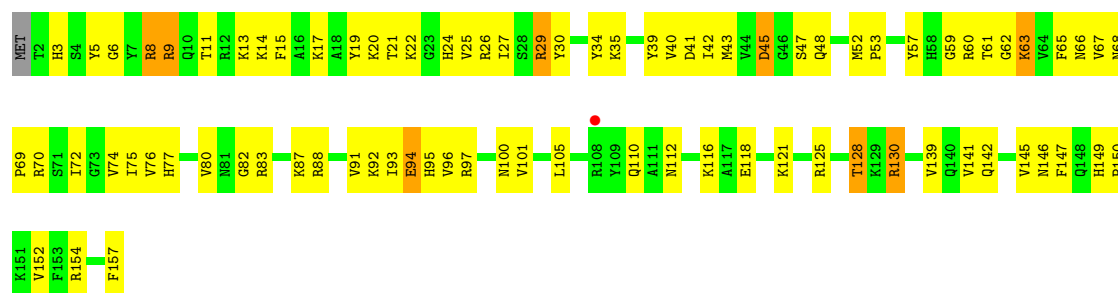
Chain EP:



• Molecule 37: 60S RIBOSOMAL PROTEIN L21

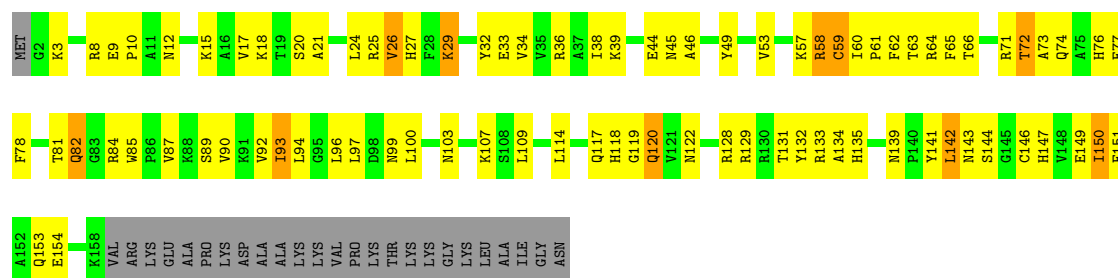
Chain GP:





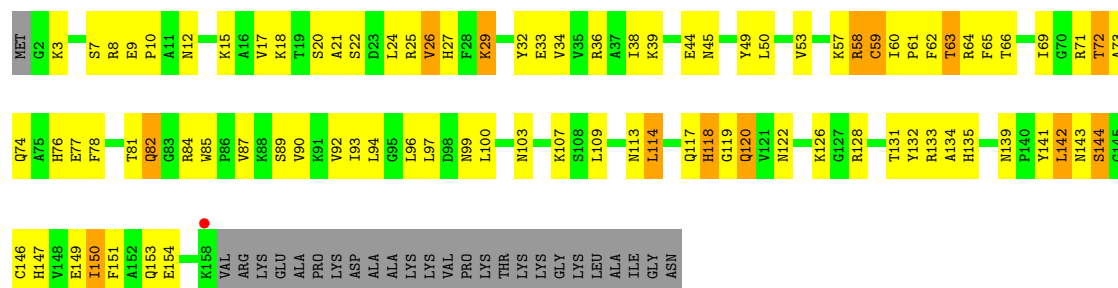
- Molecule 38: RPL17

Chain BQ:



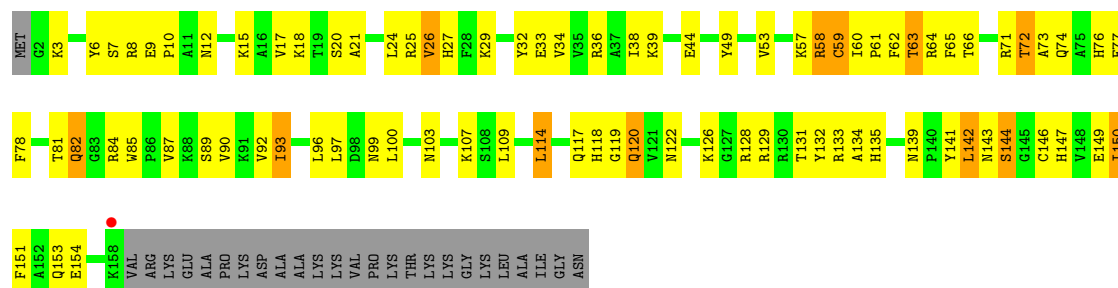
- Molecule 38: RPL17

Chain CQ:



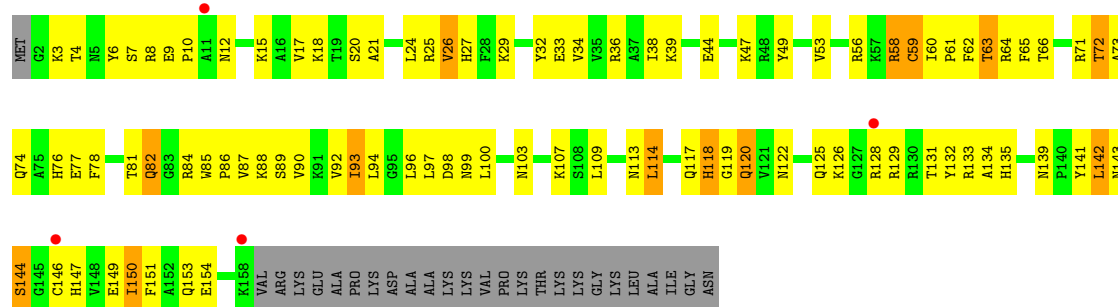
- Molecule 38: RPL17

Chain EQ:



- Molecule 38: RPL17

Chain GQ:



• Molecule 39: RPL23A

Chain BR:

• Molecule 39: RPL23A

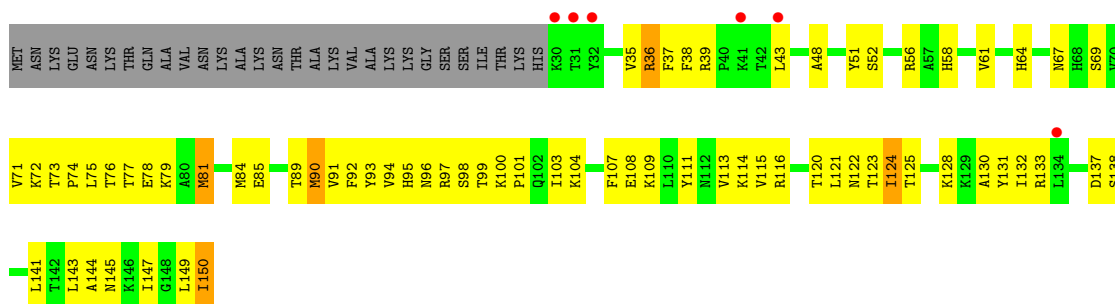
Chain CR:

• Molecule 39: RPL23A

Chain ER:

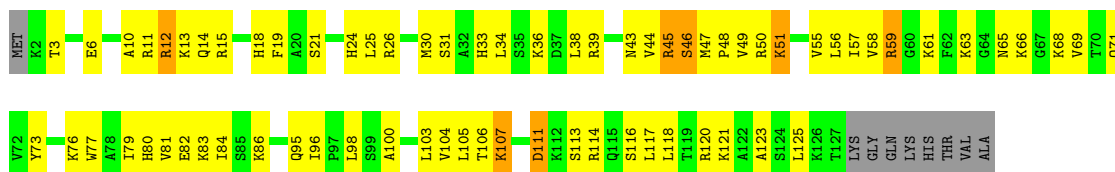
• Molecule 39: RPL23A

Chain GR:



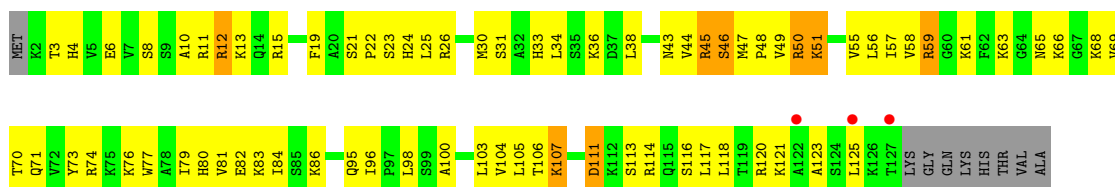
- Molecule 40: RPL26

Chain BS:



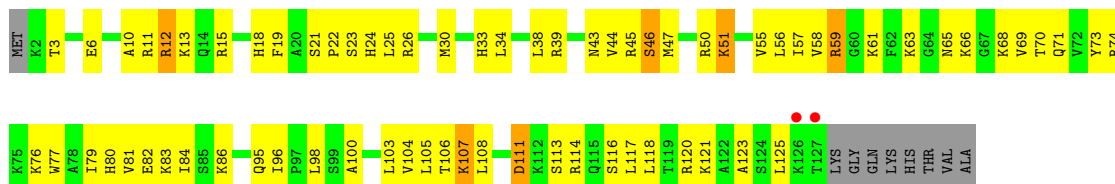
- Molecule 40: RPL26

Chain CS:



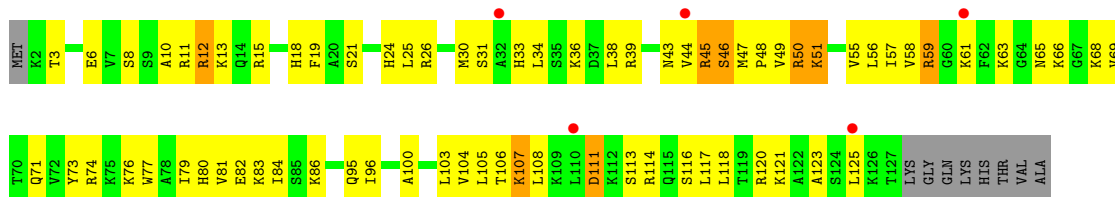
- Molecule 40: RPL26

Chain ES:



- Molecule 40: RPL26

Chain GS:



- Molecule 41: RPL24

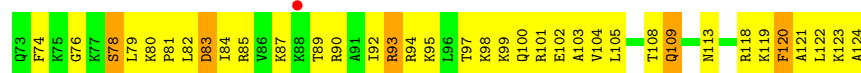
Chain BT:





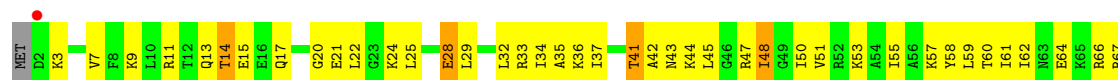
- Molecule 42: RPL35

Chain CU:



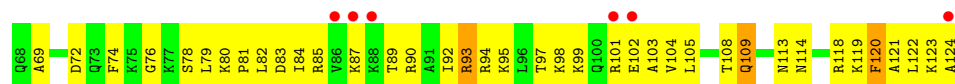
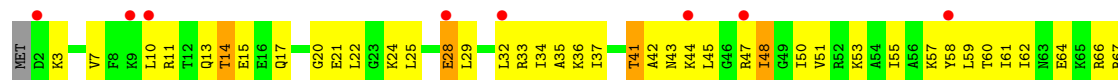
- Molecule 42: RPL35

Chain EU:



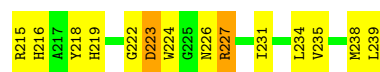
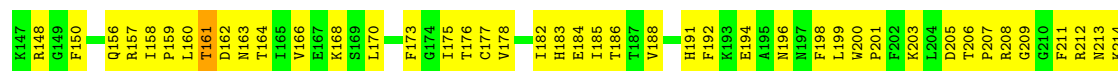
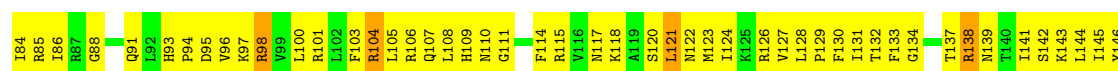
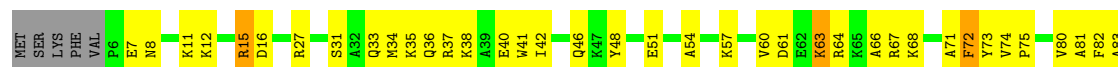
- Molecule 42: RPL35

Chain GU:



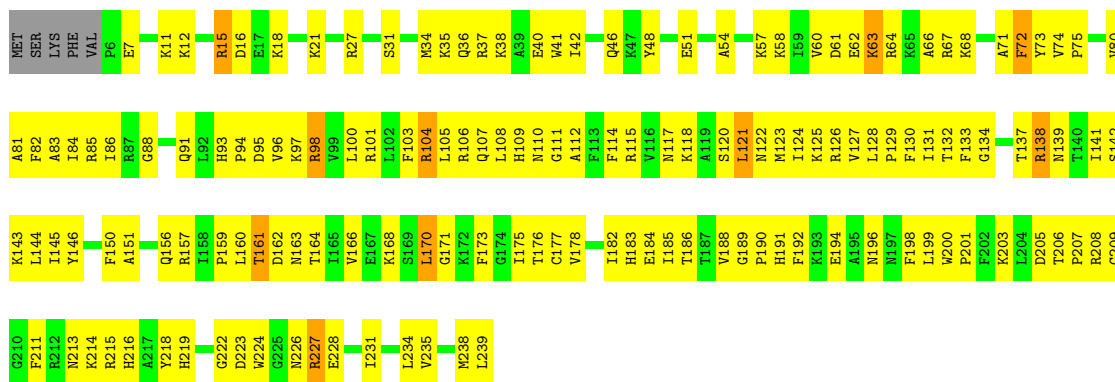
- Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain BV:



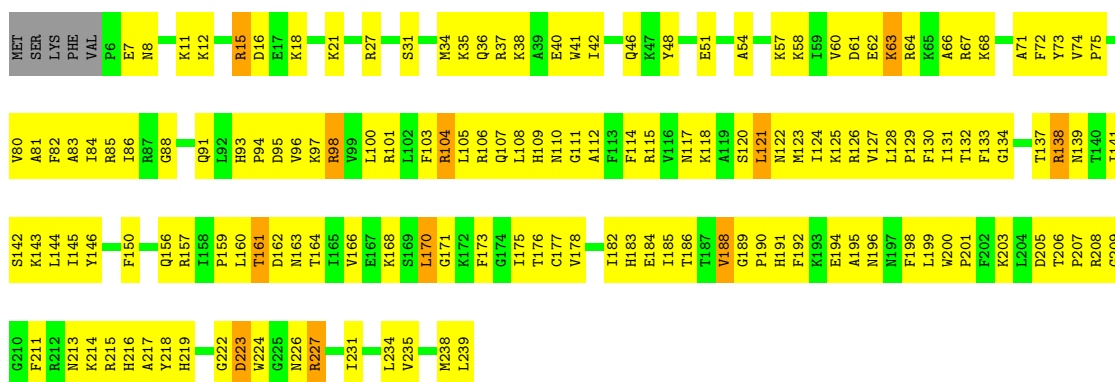
- Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain CV:



• Molecule 43: 60S RIBOSOMAL PROTEIN L7

Chain EV:



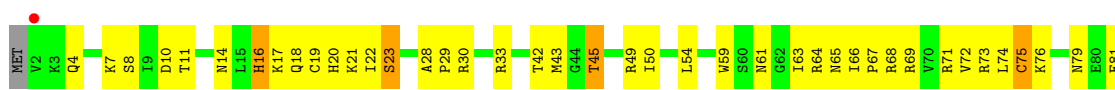
• Molecule 43: 60S RIBOSOMAL PROTEIN L7

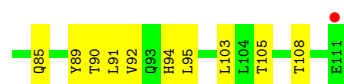
Chain GV:



• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain BW:





• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain CW:



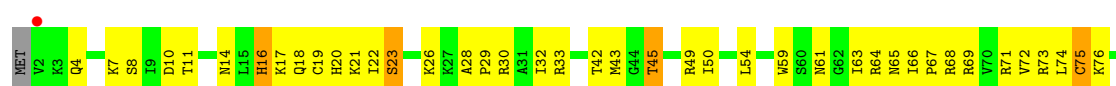
• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain EW:



• Molecule 44: 60S RIBOSOMAL PROTEIN L31

Chain GW:



• Molecule 45: 60S RIBOSOMAL PROTEIN L32

Chain BX:



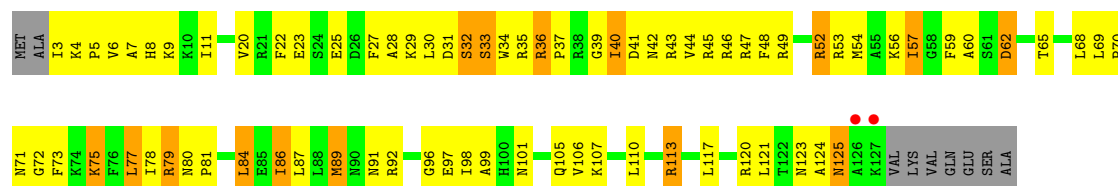
• Molecule 45: 60S RIBOSOMAL PROTEIN L32

Chain CX:



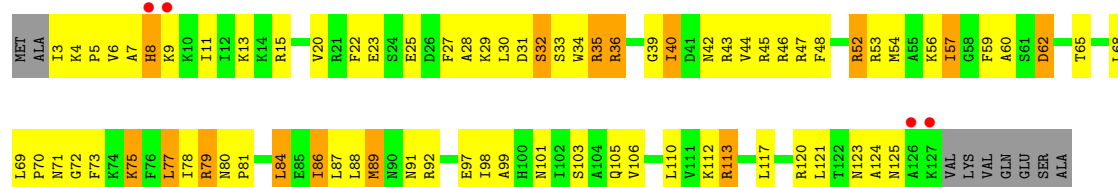
- Molecule 45: 60S RIBOSOMAL PROTEIN L32

Chain EX:



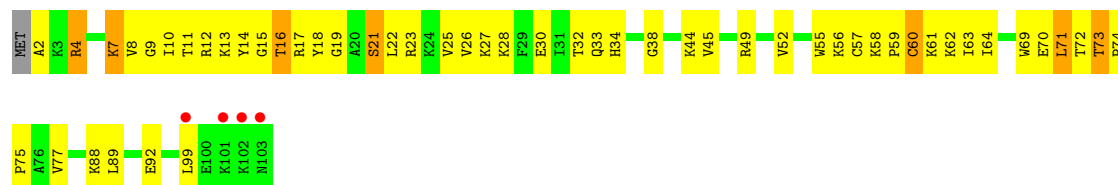
- Molecule 45: 60S RIBOSOMAL PROTEIN L32

Chain GX:



- Molecule 46: RPL37A

Chain BY:



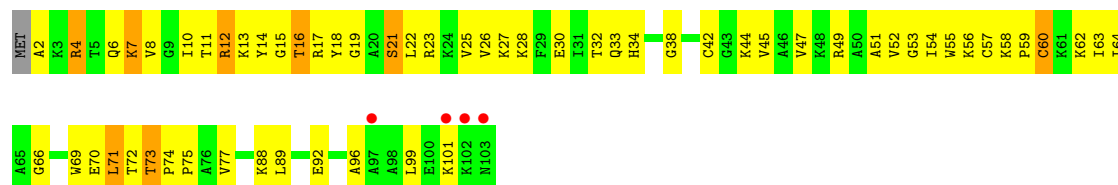
- Molecule 46: RPL37A

Chain CY:



- Molecule 46: RPL37A

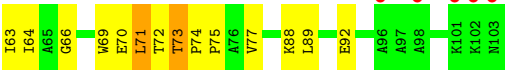
Chain EY:



- Molecule 46: RPL37A

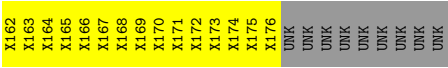
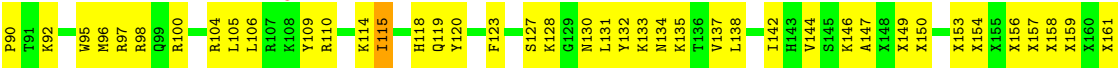
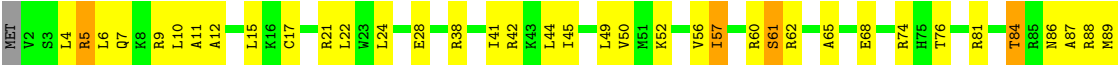
Chain GY:





● Molecule 47: RPL19

Chain CO:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	320.19Å 289.25Å 535.04Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 39.96 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.52) 99.4 (39.96-3.52)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.216 , 0.244 0.240 , 0.266	Depositor DCC
$R_{free}$ test set	10000 reflections (0.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.1	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1192534 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	511395	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AA	51	GLY	Peptide
8	AH	101	GLY	Peptide
12	AM	53	GLY	Peptide
16	AQ	12	GLY	Peptide
27	BF	174	LYS	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	HJ	1716	0	1712	176	0
10	AK	415	0	446	42	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C2	3300	0	1657	225	0
20	E2	3300	0	1657	227	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	GI	1594	0	1701	179	0
31	BJ	1022	0	1078	65	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	ET	510	0	546	59	0
41	GT	510	0	546	52	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	CY	1	0	0	0	0
48	D1	232	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	FK	1	0	0	0	0
49	FL	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	CE	2	0	0	1	0
50	CI	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	EY	5	0	0	0	0
50	F1	1076	0	0	268	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 37509 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	38	87
5	DE	188/191 (98%)	176 (94%)	11 (6%)	1 (0%)	38	87
5	FE	188/191 (98%)	178 (95%)	9 (5%)	1 (0%)	38	87
5	HE	188/191 (98%)	177 (94%)	10 (5%)	1 (0%)	38	87
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%)	22	78
8	HH	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
9	AJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	25	80
9	DJ	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	25	80
9	FJ	224/248 (90%)	212 (95%)	10 (4%)	2 (1%)	25	80
9	HJ	224/248 (90%)	213 (95%)	9 (4%)	2 (1%)	25	80
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%)	22	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	DM	98/118 (83%)	94 (96%)	3 (3%)	1 (1%)	22	78
12	FM	98/118 (83%)	93 (95%)	4 (4%)	1 (1%)	22	78
12	HM	98/118 (83%)	92 (94%)	5 (5%)	1 (1%)	22	78
13	AN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	30	83
13	DN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	30	83
13	FN	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
13	HN	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	30	83
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%)	11	63
16	DQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	11	63
16	FQ	100/104 (96%)	88 (88%)	10 (10%)	2 (2%)	11	63
16	HQ	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	11	63
17	AT	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	14	68
17	DT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	14	68
17	FT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	14	68
17	HT	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	14	68
18	AU	201/206 (98%)	188 (94%)	12 (6%)	1 (0%)	38	87
18	DU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	38	87
18	FU	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	38	87
18	HU	201/206 (98%)	189 (94%)	11 (6%)	1 (0%)	38	87
19	AX	186/189 (98%)	177 (95%)	8 (4%)	1 (0%)	38	87
19	DX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	21	77
19	FX	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	21	77
19	HX	186/189 (98%)	177 (95%)	7 (4%)	2 (1%)	21	77

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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%)	43	90
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%)	16	70
32	CK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	11	62
32	EK	146/149 (98%)	137 (94%)	7 (5%)	2 (1%)	16	70
32	GK	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	11	62
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%)	38	87
34	BM	296/301 (98%)	282 (95%)	13 (4%)	1 (0%)	50	92
34	CM	298/301 (99%)	282 (95%)	15 (5%)	1 (0%)	50	92
34	EM	298/301 (99%)	283 (95%)	14 (5%)	1 (0%)	50	92
34	GM	298/301 (99%)	285 (96%)	12 (4%)	1 (0%)	50	92
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%)	38	87
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%)	43	90
43	GV	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	43	90
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%)	56	94

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%)	4	22
2	DA	69/72 (96%)	58 (84%)	11 (16%)	4	22
2	FA	69/72 (96%)	59 (86%)	10 (14%)	5	27
2	HA	69/72 (96%)	58 (84%)	11 (16%)	4	22
3	AB	48/49 (98%)	44 (92%)	4 (8%)	16	59
3	DB	48/49 (98%)	44 (92%)	4 (8%)	16	59
3	FB	48/49 (98%)	44 (92%)	4 (8%)	16	59
3	HB	48/49 (98%)	44 (92%)	4 (8%)	16	59
4	AC	95/101 (94%)	92 (97%)	3 (3%)	51	89
4	DC	95/101 (94%)	92 (97%)	3 (3%)	51	89
4	FC	95/101 (94%)	92 (97%)	3 (3%)	51	89
4	HC	95/101 (94%)	92 (97%)	3 (3%)	51	89
5	AE	162/163 (99%)	152 (94%)	10 (6%)	26	73
5	DE	162/163 (99%)	152 (94%)	10 (6%)	26	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	FE	162/163 (99%)	151 (93%)	11 (7%)	22	70
5	HE	162/163 (99%)	151 (93%)	11 (7%)	22	70
6	AF	111/112 (99%)	107 (96%)	4 (4%)	47	87
6	DF	111/112 (99%)	106 (96%)	5 (4%)	38	83
6	FF	111/112 (99%)	107 (96%)	4 (4%)	47	87
6	HF	111/112 (99%)	107 (96%)	4 (4%)	47	87
7	AG	80/88 (91%)	76 (95%)	4 (5%)	34	80
7	DG	80/88 (91%)	74 (92%)	6 (8%)	19	65
7	FG	80/88 (91%)	75 (94%)	5 (6%)	25	73
7	HG	80/88 (91%)	76 (95%)	4 (5%)	34	80
8	AH	87/92 (95%)	78 (90%)	9 (10%)	10	47
8	DH	87/92 (95%)	78 (90%)	9 (10%)	10	47
8	FH	87/92 (95%)	78 (90%)	9 (10%)	10	47
8	HH	87/92 (95%)	78 (90%)	9 (10%)	10	47
9	AJ	195/216 (90%)	177 (91%)	18 (9%)	13	54
9	DJ	195/216 (90%)	176 (90%)	19 (10%)	12	50
9	FJ	195/216 (90%)	177 (91%)	18 (9%)	13	54
9	HJ	195/216 (90%)	177 (91%)	18 (9%)	13	54
10	AK	46/113 (41%)	43 (94%)	3 (6%)	24	72
10	DK	46/113 (41%)	43 (94%)	3 (6%)	24	72
10	FK	46/113 (41%)	43 (94%)	3 (6%)	24	72
10	HK	46/113 (41%)	43 (94%)	3 (6%)	24	72
11	AL	92/107 (86%)	87 (95%)	5 (5%)	31	78
11	DL	92/107 (86%)	87 (95%)	5 (5%)	31	78
11	FL	92/107 (86%)	88 (96%)	4 (4%)	40	84
11	HL	92/107 (86%)	87 (95%)	5 (5%)	31	78
12	AM	93/110 (84%)	90 (97%)	3 (3%)	51	89
12	DM	93/110 (84%)	90 (97%)	3 (3%)	51	89
12	FM	93/110 (84%)	90 (97%)	3 (3%)	51	89
12	HM	93/110 (84%)	90 (97%)	3 (3%)	51	89
13	AN	130/131 (99%)	123 (95%)	7 (5%)	31	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	DN	130/131 (99%)	122 (94%)	8 (6%)	26	73
13	FN	130/131 (99%)	123 (95%)	7 (5%)	31	78
13	HN	130/131 (99%)	123 (95%)	7 (5%)	31	78
14	AO	108/108 (100%)	102 (94%)	6 (6%)	30	77
14	DO	108/108 (100%)	102 (94%)	6 (6%)	30	77
14	FO	108/108 (100%)	100 (93%)	8 (7%)	20	66
14	HO	108/108 (100%)	102 (94%)	6 (6%)	30	77
15	AP	60/77 (78%)	56 (93%)	4 (7%)	23	70
15	DP	60/77 (78%)	56 (93%)	4 (7%)	23	70
15	FP	60/77 (78%)	56 (93%)	4 (7%)	23	70
15	HP	60/77 (78%)	56 (93%)	4 (7%)	23	70
16	AQ	81/83 (98%)	75 (93%)	6 (7%)	20	66
16	DQ	81/83 (98%)	75 (93%)	6 (7%)	20	66
16	FQ	81/83 (98%)	75 (93%)	6 (7%)	20	66
16	HQ	81/83 (98%)	75 (93%)	6 (7%)	20	66
17	AT	61/62 (98%)	55 (90%)	6 (10%)	12	49
17	DT	61/62 (98%)	57 (93%)	4 (7%)	24	71
17	FT	61/62 (98%)	57 (93%)	4 (7%)	24	71
17	HT	61/62 (98%)	57 (93%)	4 (7%)	24	71
18	AU	169/171 (99%)	159 (94%)	10 (6%)	28	75
18	DU	169/171 (99%)	161 (95%)	8 (5%)	36	82
18	FU	169/171 (99%)	160 (95%)	9 (5%)	32	78
18	HU	169/171 (99%)	161 (95%)	8 (5%)	36	82
19	AX	167/168 (99%)	153 (92%)	14 (8%)	16	59
19	DX	167/168 (99%)	152 (91%)	15 (9%)	14	55
19	FX	167/168 (99%)	151 (90%)	16 (10%)	12	51
19	HX	167/168 (99%)	154 (92%)	13 (8%)	18	63
22	BA	196/198 (99%)	165 (84%)	31 (16%)	4	23
22	CA	196/198 (99%)	164 (84%)	32 (16%)	3	21
22	EA	196/198 (99%)	164 (84%)	32 (16%)	3	21
22	GA	196/198 (99%)	165 (84%)	31 (16%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	BB	330/334 (99%)	306 (93%)	24 (7%)	20	66
23	CB	330/334 (99%)	307 (93%)	23 (7%)	21	68
23	EB	330/334 (99%)	308 (93%)	22 (7%)	23	70
23	GB	330/334 (99%)	306 (93%)	24 (7%)	20	66
24	BC	325/326 (100%)	302 (93%)	23 (7%)	21	67
24	CC	325/326 (100%)	302 (93%)	23 (7%)	21	67
24	EC	325/326 (100%)	300 (92%)	25 (8%)	18	64
24	GC	325/326 (100%)	300 (92%)	25 (8%)	18	64
25	BD	146/149 (98%)	136 (93%)	10 (7%)	22	70
25	CD	146/149 (98%)	136 (93%)	10 (7%)	22	70
25	ED	146/149 (98%)	135 (92%)	11 (8%)	19	65
25	GD	146/149 (98%)	136 (93%)	10 (7%)	22	70
26	BE	163/165 (99%)	157 (96%)	6 (4%)	45	86
26	CE	163/165 (99%)	157 (96%)	6 (4%)	45	86
26	EE	163/165 (99%)	157 (96%)	6 (4%)	45	86
26	GE	163/165 (99%)	157 (96%)	6 (4%)	45	86
27	BF	201/222 (90%)	194 (96%)	7 (4%)	48	88
27	CF	201/222 (90%)	194 (96%)	7 (4%)	48	88
27	EF	201/222 (90%)	194 (96%)	7 (4%)	48	88
27	GF	201/222 (90%)	194 (96%)	7 (4%)	48	88
29	BH	169/180 (94%)	155 (92%)	14 (8%)	16	59
29	CH	169/180 (94%)	155 (92%)	14 (8%)	16	59
29	EH	169/180 (94%)	156 (92%)	13 (8%)	18	64
29	GH	169/180 (94%)	153 (90%)	16 (10%)	12	51
30	BI	166/166 (100%)	150 (90%)	16 (10%)	12	51
30	CI	166/166 (100%)	149 (90%)	17 (10%)	11	47
30	EI	166/166 (100%)	150 (90%)	16 (10%)	12	51
30	GI	166/166 (100%)	150 (90%)	16 (10%)	12	51
31	BJ	107/108 (99%)	98 (92%)	9 (8%)	16	59
31	CJ	107/108 (99%)	99 (92%)	8 (8%)	19	65
31	EJ	107/108 (99%)	99 (92%)	8 (8%)	19	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	GJ	107/108 (99%)	99 (92%)	8 (8%)	19	65
32	BK	120/121 (99%)	110 (92%)	10 (8%)	16	59
32	CK	120/121 (99%)	111 (92%)	9 (8%)	19	65
32	EK	120/121 (99%)	110 (92%)	10 (8%)	16	59
32	GK	120/121 (99%)	110 (92%)	10 (8%)	16	59
33	BL	174/175 (99%)	165 (95%)	9 (5%)	32	79
33	CL	174/175 (99%)	165 (95%)	9 (5%)	32	79
33	EL	174/175 (99%)	165 (95%)	9 (5%)	32	79
33	GL	174/175 (99%)	166 (95%)	8 (5%)	37	82
34	BM	252/254 (99%)	239 (95%)	13 (5%)	32	79
34	CM	253/254 (100%)	242 (96%)	11 (4%)	40	84
34	EM	253/254 (100%)	242 (96%)	11 (4%)	40	84
34	GM	253/254 (100%)	240 (95%)	13 (5%)	33	80
35	BN	159/160 (99%)	145 (91%)	14 (9%)	14	57
35	CN	159/160 (99%)	146 (92%)	13 (8%)	17	60
35	EN	159/160 (99%)	145 (91%)	14 (9%)	14	57
35	GN	159/160 (99%)	146 (92%)	13 (8%)	17	60
36	BO	158/159 (99%)	148 (94%)	10 (6%)	25	73
36	EO	126/159 (79%)	116 (92%)	10 (8%)	18	62
36	GO	127/159 (80%)	117 (92%)	10 (8%)	18	62
37	BP	134/135 (99%)	124 (92%)	10 (8%)	19	65
37	CP	134/135 (99%)	126 (94%)	8 (6%)	27	74
37	EP	134/135 (99%)	125 (93%)	9 (7%)	23	70
37	GP	134/135 (99%)	125 (93%)	9 (7%)	23	70
38	BQ	128/148 (86%)	115 (90%)	13 (10%)	11	47
38	CQ	128/148 (86%)	115 (90%)	13 (10%)	11	47
38	EQ	128/148 (86%)	115 (90%)	13 (10%)	11	47
38	GQ	128/148 (86%)	115 (90%)	13 (10%)	11	47
39	BR	108/132 (82%)	101 (94%)	7 (6%)	24	72
39	CR	108/132 (82%)	101 (94%)	7 (6%)	24	72
39	ER	108/132 (82%)	102 (94%)	6 (6%)	30	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	GR	108/132 (82%)	103 (95%)	5 (5%)	37	82
40	BS	113/120 (94%)	105 (93%)	8 (7%)	21	67
40	CS	113/120 (94%)	104 (92%)	9 (8%)	17	62
40	ES	113/120 (94%)	105 (93%)	8 (7%)	21	67
40	GS	113/120 (94%)	104 (92%)	9 (8%)	17	62
41	BT	52/130 (40%)	46 (88%)	6 (12%)	8	39
41	CT	52/130 (40%)	46 (88%)	6 (12%)	8	39
41	ET	52/130 (40%)	46 (88%)	6 (12%)	8	39
41	GT	52/130 (40%)	46 (88%)	6 (12%)	8	39
42	BU	105/106 (99%)	96 (91%)	9 (9%)	15	58
42	CU	105/106 (99%)	96 (91%)	9 (9%)	15	58
42	EU	105/106 (99%)	96 (91%)	9 (9%)	15	58
42	GU	105/106 (99%)	96 (91%)	9 (9%)	15	58
43	BV	197/202 (98%)	186 (94%)	11 (6%)	30	77
43	CV	197/202 (98%)	187 (95%)	10 (5%)	33	80
43	EV	197/202 (98%)	188 (95%)	9 (5%)	37	82
43	GV	197/202 (98%)	187 (95%)	10 (5%)	33	80
44	BW	100/101 (99%)	96 (96%)	4 (4%)	42	85
44	CW	100/101 (99%)	95 (95%)	5 (5%)	34	80
44	EW	100/101 (99%)	95 (95%)	5 (5%)	34	80
44	GW	100/101 (99%)	96 (96%)	4 (4%)	42	85
45	BX	104/111 (94%)	88 (85%)	16 (15%)	4	24
45	CX	104/111 (94%)	87 (84%)	17 (16%)	3	21
45	EX	104/111 (94%)	88 (85%)	16 (15%)	4	24
45	GX	104/111 (94%)	88 (85%)	16 (15%)	4	24
46	BY	79/80 (99%)	72 (91%)	7 (9%)	14	56
46	CY	79/80 (99%)	71 (90%)	8 (10%)	11	48
46	EY	79/80 (99%)	71 (90%)	8 (10%)	11	48
46	GY	79/80 (99%)	73 (92%)	6 (8%)	19	65
47	CO	126/127 (99%)	116 (92%)	10 (8%)	18	62
All	All	22468/23988 (94%)	20823 (93%)	1645 (7%)	20	66

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 4848 RNA backbone outliers are listed below:

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

5 of 901 RNA pucker outliers are listed below:

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

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F1	1

All chain breaks are listed below:

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

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A1	3119/3354 (92%)	0.09	81 (2%) 53 25	42, 91, 187, 390	0
1	D1	3119/3354 (92%)	0.02	29 (0%) 81 51	40, 79, 164, 330	0
1	F1	3119/3354 (92%)	0.13	53 (1%) 67 35	51, 94, 176, 357	0
1	H1	3119/3354 (92%)	0.44	110 (3%) 42 20	54, 121, 213, 367	0
2	AA	91/94 (96%)	0.10	1 (1%) 77 45	29, 65, 120, 243	0
2	DA	91/94 (96%)	0.11	0 100 100	34, 66, 123, 226	0
2	FA	91/94 (96%)	0.35	2 (2%) 59 29	47, 83, 132, 204	0
2	HA	91/94 (96%)	0.89	8 (8%) 10 6	74, 119, 186, 243	0
3	AB	51/52 (98%)	0.14	0 100 100	44, 63, 110, 148	0
3	DB	51/52 (98%)	0.10	1 (1%) 62 31	49, 69, 111, 146	0
3	FB	51/52 (98%)	0.37	1 (1%) 62 31	59, 86, 118, 167	0
3	HB	51/52 (98%)	0.85	8 (15%) 3 3	90, 114, 144, 197	0
4	AC	103/109 (94%)	0.50	2 (1%) 64 32	73, 117, 154, 228	0
4	DC	103/109 (94%)	0.22	0 100 100	46, 84, 135, 194	0
4	FC	103/109 (94%)	0.25	0 100 100	58, 96, 156, 192	0
4	HC	103/109 (94%)	0.48	1 (0%) 79 48	81, 130, 176, 199	0
5	AE	190/191 (99%)	0.37	7 (3%) 39 18	69, 122, 171, 214	0
5	DE	190/191 (99%)	0.28	2 (1%) 77 45	74, 124, 169, 226	0
5	FE	190/191 (99%)	0.39	7 (3%) 39 18	60, 123, 176, 227	0
5	HE	190/191 (99%)	0.50	13 (6%) 17 8	76, 141, 194, 227	0
6	AF	125/126 (99%)	0.18	3 (2%) 56 27	71, 111, 156, 213	0
6	DF	125/126 (99%)	0.07	1 (0%) 83 53	70, 106, 157, 190	0
6	FF	125/126 (99%)	0.21	3 (2%) 56 27	63, 109, 166, 245	0
6	HF	125/126 (99%)	0.26	0 100 100	74, 113, 163, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AG	96/104 (92%)	0.20	2 (2%) 60 30	62, 103, 188, 218	0
7	DG	96/104 (92%)	0.21	2 (2%) 60 30	57, 114, 179, 222	0
7	FG	96/104 (92%)	0.34	2 (2%) 60 30	81, 112, 176, 199	0
7	HG	96/104 (92%)	0.32	1 (1%) 79 48	94, 134, 183, 218	0
8	AH	107/113 (94%)	0.13	0 100 100	61, 91, 127, 159	0
8	DH	107/113 (94%)	0.14	0 100 100	54, 89, 127, 138	0
8	FH	107/113 (94%)	0.18	0 100 100	57, 89, 122, 164	0
8	HH	107/113 (94%)	0.30	0 100 100	68, 109, 141, 181	0
9	AJ	226/248 (91%)	-0.11	0 100 100	52, 90, 138, 190	0
9	DJ	226/248 (91%)	-0.08	0 100 100	51, 89, 136, 206	0
9	FJ	226/248 (91%)	-0.13	0 100 100	38, 82, 130, 183	0
9	HJ	226/248 (91%)	-0.16	0 100 100	40, 78, 123, 155	0
10	AK	52/129 (40%)	0.37	2 (3%) 38 18	73, 101, 146, 182	0
10	DK	52/129 (40%)	-0.06	1 (1%) 64 32	53, 79, 134, 151	0
10	FK	52/129 (40%)	0.03	1 (1%) 64 32	56, 81, 139, 189	0
10	HK	52/129 (40%)	0.01	0 100 100	61, 77, 118, 158	0
11	AL	108/123 (87%)	0.16	1 (0%) 81 51	38, 73, 130, 165	0
11	DL	108/123 (87%)	0.13	0 100 100	47, 85, 144, 217	0
11	FL	108/123 (87%)	0.30	1 (0%) 81 51	66, 98, 135, 174	0
11	HL	108/123 (87%)	0.70	7 (6%) 18 9	90, 117, 156, 183	0
12	AM	100/118 (84%)	0.33	0 100 100	72, 121, 155, 185	0
12	DM	100/118 (84%)	0.36	3 (3%) 48 23	73, 126, 179, 199	0
12	FM	100/118 (84%)	0.51	5 (5%) 28 12	93, 144, 196, 208	0
12	HM	100/118 (84%)	0.31	2 (2%) 62 31	98, 151, 195, 214	0
13	AN	143/144 (99%)	0.08	1 (0%) 84 56	59, 97, 163, 189	0
13	DN	143/144 (99%)	0.14	1 (0%) 84 56	73, 121, 179, 214	0
13	FN	143/144 (99%)	0.17	1 (0%) 84 56	72, 122, 175, 208	0
13	HN	143/144 (99%)	0.44	3 (2%) 60 30	92, 148, 189, 217	0
14	AO	134/134 (100%)	0.07	0 100 100	66, 116, 162, 202	0
14	DO	134/134 (100%)	0.12	2 (1%) 70 37	52, 99, 151, 209	0
14	FO	134/134 (100%)	0.22	1 (0%) 84 56	65, 118, 167, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
14	HO	134/134 (100%)	0.59	8 (5%)	21 10	96, 143, 197, 227	0
15	AP	66/89 (74%)	0.56	3 (4%)	32 14	55, 128, 209, 241	0
15	DP	66/89 (74%)	0.52	6 (9%)	9 6	73, 116, 176, 245	0
15	FP	66/89 (74%)	0.61	2 (3%)	48 23	99, 143, 202, 214	0
15	HP	66/89 (74%)	0.99	3 (4%)	32 14	99, 149, 219, 247	0
16	AQ	102/104 (98%)	0.33	4 (3%)	37 17	72, 122, 172, 208	0
16	DQ	102/104 (98%)	0.23	2 (1%)	62 31	63, 105, 151, 186	0
16	FQ	102/104 (98%)	0.29	3 (2%)	49 24	72, 114, 166, 190	0
16	HQ	102/104 (98%)	0.73	7 (6%)	17 8	110, 154, 195, 203	0
17	AT	65/66 (98%)	0.56	5 (7%)	13 7	76, 121, 156, 193	0
17	DT	65/66 (98%)	0.32	1 (1%)	70 37	51, 87, 122, 211	0
17	FT	65/66 (98%)	0.42	2 (3%)	47 22	51, 107, 144, 201	0
17	HT	65/66 (98%)	0.82	6 (9%)	9 6	69, 136, 171, 222	0
18	AU	203/206 (98%)	0.28	3 (1%)	70 37	74, 122, 179, 233	0
18	DU	203/206 (98%)	0.13	0	100 100	48, 98, 158, 198	0
18	FU	203/206 (98%)	0.15	0	100 100	67, 116, 174, 203	0
18	HU	203/206 (98%)	0.63	10 (4%)	28 13	102, 155, 206, 240	0
19	AX	188/189 (99%)	0.09	1 (0%)	88 65	72, 105, 145, 201	0
19	DX	188/189 (99%)	-0.03	0	100 100	54, 89, 128, 170	0
19	FX	188/189 (99%)	0.14	1 (0%)	88 65	62, 98, 141, 179	0
19	HX	188/189 (99%)	0.16	0	100 100	74, 106, 135, 193	0
20	B2	154/154 (100%)	-0.14	1 (0%)	86 60	61, 80, 118, 192	0
20	C2	154/154 (100%)	-0.04	0	100 100	54, 80, 120, 186	0
20	E2	154/154 (100%)	0.11	3 (1%)	64 32	74, 105, 142, 189	0
20	G2	154/154 (100%)	0.68	12 (7%)	13 7	98, 146, 182, 210	0
21	B3	120/120 (100%)	0.38	4 (3%)	44 21	90, 150, 184, 217	0
21	C3	120/120 (100%)	-0.11	0	100 100	64, 98, 116, 161	0
21	E3	120/120 (100%)	0.02	0	100 100	72, 120, 147, 172	0
21	G3	120/120 (100%)	0.39	4 (3%)	44 21	95, 138, 175, 235	0
22	BA	257/264 (97%)	0.20	10 (3%)	37 17	30, 70, 134, 233	0
22	CA	257/264 (97%)	0.07	8 (3%)	47 22	31, 75, 139, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
22	EA	257/264 (97%)	0.08	9 (3%)	42	20	40, 79, 136, 217	0
22	GA	257/264 (97%)	0.41	12 (4%)	30	14	60, 106, 157, 242	0
23	BB	386/391 (98%)	-0.03	4 (1%)	79	48	33, 69, 120, 227	0
23	CB	386/391 (98%)	-0.13	0	100	100	34, 75, 123, 222	0
23	EB	386/391 (98%)	-0.06	4 (1%)	79	48	38, 75, 123, 230	0
23	GB	386/391 (98%)	-0.06	4 (1%)	79	48	51, 82, 132, 217	0
24	BC	409/410 (99%)	0.22	10 (2%)	56	27	37, 107, 173, 241	0
24	CC	409/410 (99%)	0.06	1 (0%)	93	80	40, 91, 151, 206	0
24	EC	409/410 (99%)	0.19	6 (1%)	70	37	54, 107, 162, 237	0
24	GC	409/410 (99%)	0.48	12 (2%)	49	24	77, 143, 195, 252	0
25	BD	169/172 (98%)	0.98	20 (11%)	5	4	116, 159, 200, 225	0
25	CD	169/172 (98%)	0.29	3 (1%)	65	34	70, 110, 151, 188	0
25	ED	169/172 (98%)	0.52	6 (3%)	41	19	89, 133, 179, 209	0
25	GD	169/172 (98%)	0.67	11 (6%)	18	9	96, 139, 182, 216	0
26	BE	186/188 (98%)	0.11	0	100	100	65, 109, 150, 194	0
26	CE	186/188 (98%)	0.02	0	100	100	59, 94, 131, 171	0
26	EE	186/188 (98%)	0.15	1 (0%)	88	65	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%)	0.33	6 (2%)	53	25	70, 122, 176, 252	0
27	CF	231/255 (90%)	0.12	2 (0%)	81	51	71, 115, 175, 233	0
27	EF	231/255 (90%)	0.24	2 (0%)	81	51	76, 120, 187, 241	0
27	GF	231/255 (90%)	0.69	13 (5%)	24	10	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%)	0.39	5 (2%)	54	26	79, 133, 181, 221	0
29	CH	201/215 (93%)	0.02	1 (0%)	88	65	42, 93, 139, 153	0
29	EH	201/215 (93%)	0.08	1 (0%)	88	65	50, 105, 158, 202	0
29	GH	201/215 (93%)	0.30	1 (0%)	88	65	71, 118, 171, 203	0
30	BI	198/198 (100%)	0.09	1 (0%)	88	65	51, 85, 152, 185	0
30	CI	198/198 (100%)	-0.05	0	100	100	48, 78, 149, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	EI	198/198 (100%)	0.07	1 (0%) 88 65	47, 79, 152, 174	0
30	GI	198/198 (100%)	0.08	3 (1%) 70 37	53, 91, 151, 195	0
31	BJ	138/141 (97%)	-0.11	0 100 100	42, 68, 112, 160	0
31	CJ	138/141 (97%)	-0.15	0 100 100	40, 65, 108, 150	0
31	EJ	138/141 (97%)	-0.13	3 (2%) 59 29	40, 65, 108, 202	0
31	GJ	138/141 (97%)	-0.11	2 (1%) 72 39	30, 60, 98, 186	0
32	BK	148/149 (99%)	0.27	5 (3%) 43 20	50, 105, 158, 221	0
32	CK	148/149 (99%)	0.04	0 100 100	36, 74, 124, 184	0
32	EK	148/149 (99%)	0.14	0 100 100	50, 95, 140, 228	0
32	GK	148/149 (99%)	0.67	7 (4%) 30 14	78, 129, 181, 208	0
33	BL	203/204 (99%)	0.03	0 100 100	57, 83, 120, 153	0
33	CL	203/204 (99%)	-0.06	0 100 100	37, 74, 106, 180	0
33	EL	203/204 (99%)	0.13	0 100 100	51, 89, 121, 160	0
33	GL	203/204 (99%)	0.57	7 (3%) 43 20	89, 133, 165, 205	0
34	BM	298/301 (99%)	0.45	5 (1%) 67 35	87, 152, 201, 240	0
34	CM	300/301 (99%)	0.12	3 (1%) 79 48	61, 110, 166, 208	0
34	EM	300/301 (99%)	0.38	8 (2%) 52 25	76, 127, 183, 233	0
34	GM	300/301 (99%)	0.77	22 (7%) 15 7	98, 157, 204, 233	0
35	BN	180/181 (99%)	0.29	1 (0%) 86 60	68, 110, 150, 224	0
35	CN	180/181 (99%)	-0.03	0 100 100	47, 82, 125, 185	0
35	EN	180/181 (99%)	0.15	1 (0%) 86 60	63, 101, 142, 187	0
35	GN	180/181 (99%)	0.47	4 (2%) 59 29	94, 139, 188, 248	0
36	BO	184/185 (99%)	0.46	8 (4%) 34 15	29, 78, 184, 207	0
36	EO	146/185 (78%)	0.42	5 (3%) 43 20	57, 95, 128, 194	0
36	GO	153/185 (82%)	0.53	7 (4%) 31 14	67, 109, 153, 262	0
37	BP	156/157 (99%)	0.35	0 100 100	70, 116, 169, 203	0
37	CP	156/157 (99%)	-0.00	0 100 100	42, 79, 136, 152	0
37	EP	156/157 (99%)	0.17	1 (0%) 86 60	56, 100, 148, 183	0
37	GP	156/157 (99%)	0.50	1 (0%) 86 60	69, 122, 163, 222	0
38	BQ	157/183 (85%)	-0.06	0 100 100	31, 68, 121, 173	0
38	CQ	157/183 (85%)	-0.05	1 (0%) 86 60	26, 70, 124, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
38	EQ	157/183 (85%)	0.06	1 (0%)	86 60	48, 86, 141, 177	0
38	GQ	157/183 (85%)	0.33	4 (2%)	54 26	60, 106, 157, 200	0
39	BR	121/150 (80%)	0.09	1 (0%)	83 53	42, 78, 129, 185	0
39	CR	121/150 (80%)	0.24	2 (1%)	67 35	54, 88, 129, 172	0
39	ER	121/150 (80%)	0.40	3 (2%)	54 26	65, 112, 146, 172	0
39	GR	121/150 (80%)	0.62	6 (4%)	28 12	97, 138, 175, 191	0
40	BS	126/135 (93%)	0.11	0	100 100	62, 98, 133, 177	0
40	CS	126/135 (93%)	0.27	3 (2%)	56 27	46, 89, 127, 152	0
40	ES	126/135 (93%)	0.38	2 (1%)	68 36	74, 112, 151, 184	0
40	GS	126/135 (93%)	0.64	5 (3%)	36 17	101, 143, 186, 218	0
41	BT	61/158 (38%)	-0.07	0	100 100	39, 73, 127, 158	0
41	CT	61/158 (38%)	0.00	0	100 100	37, 73, 105, 137	0
41	ET	61/158 (38%)	-0.02	0	100 100	45, 78, 113, 147	0
41	GT	61/158 (38%)	-0.04	0	100 100	42, 76, 115, 138	0
42	BU	123/124 (99%)	0.18	1 (0%)	83 53	59, 101, 139, 204	0
42	CU	123/124 (99%)	0.09	1 (0%)	83 53	49, 92, 143, 163	0
42	EU	123/124 (99%)	0.24	1 (0%)	83 53	79, 114, 157, 220	0
42	GU	123/124 (99%)	0.92	14 (11%)	6 4	113, 157, 193, 233	0
43	BV	234/239 (97%)	-0.03	0	100 100	61, 107, 160, 213	0
43	CV	234/239 (97%)	-0.14	0	100 100	47, 87, 145, 213	0
43	EV	234/239 (97%)	-0.06	0	100 100	53, 102, 159, 232	0
43	GV	234/239 (97%)	0.14	1 (0%)	90 71	75, 121, 173, 239	0
44	BW	110/111 (99%)	0.06	2 (1%)	65 34	36, 64, 155, 204	0
44	CW	110/111 (99%)	0.09	0	100 100	43, 76, 138, 178	0
44	EW	110/111 (99%)	0.18	1 (0%)	81 51	56, 88, 170, 227	0
44	GW	110/111 (99%)	0.23	1 (0%)	81 51	63, 102, 183, 216	0
45	BX	125/134 (93%)	0.20	2 (1%)	68 36	53, 89, 128, 202	0
45	CX	125/134 (93%)	0.03	1 (0%)	83 53	40, 78, 116, 196	0
45	EX	125/134 (93%)	0.15	2 (1%)	68 36	49, 88, 129, 233	0
45	GX	125/134 (93%)	0.50	4 (3%)	45 21	73, 117, 162, 215	0
46	BY	102/103 (99%)	0.17	4 (3%)	37 17	40, 74, 164, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
46	CY	102/103 (99%)	0.08	3 (2%)	49	24	41, 83, 173, 196	0
46	EY	102/103 (99%)	0.19	4 (3%)	37	17	45, 84, 156, 193	0
46	GY	102/103 (99%)	0.30	5 (4%)	28	13	53, 102, 189, 222	0
47	CO	146/185 (78%)	0.21	1 (0%)	84	56	45, 79, 115, 148	0
All	All	40083/43352 (92%)	0.20	786 (1%)	62	31	26, 101, 177, 390	0

The worst 5 of 786 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HA	92	ALA	10.9
1	A1	2500	C	10.2
1	H1	1597	U	9.8
1	A1	1597	U	9.2
23	BB	387	GLU	9.2

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	F1	3451	1/1	0.53	657.00	122,122,122,122	0
48	MG	A1	3575	1/1	0.73	548.00	143,143,143,143	0
48	MG	A1	3567	1/1	0.32	301.00	144,144,144,144	0
48	MG	E3	204	1/1	1.64	271.73	199,199,199,199	0
48	MG	D1	3606	1/1	0.91	165.26	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	G2	206	1/1	1.13	115.63	174,174,174,174	0
48	MG	F1	3572	1/1	0.35	111.00	155,155,155,155	0
48	MG	F1	3498	1/1	0.29	107.71	141,141,141,141	0
48	MG	A1	3555	1/1	0.59	107.00	128,128,128,128	0
48	MG	D1	3550	1/1	0.57	92.66	136,136,136,136	0
48	MG	A1	3576	1/1	0.29	90.00	122,122,122,122	0
48	MG	D1	3624	1/1	0.68	70.88	162,162,162,162	0
48	MG	A1	3513	1/1	0.30	69.44	133,133,133,133	0
48	MG	H1	3533	1/1	1.09	67.54	153,153,153,153	0
48	MG	F1	3562	1/1	0.48	65.60	140,140,140,140	0
48	MG	D1	3522	1/1	0.72	65.29	162,162,162,162	0
48	MG	D1	3592	1/1	1.00	64.78	159,159,159,159	0
48	MG	H1	3551	1/1	2.92	63.53	202,202,202,202	0
48	MG	H1	3535	1/1	0.77	56.99	150,150,150,150	0
48	MG	A1	3522	1/1	1.08	54.15	146,146,146,146	0
48	MG	D1	3617	1/1	0.39	53.75	113,113,113,113	0
48	MG	F1	3566	1/1	1.27	52.29	146,146,146,146	0
48	MG	B2	208	1/1	0.39	51.22	138,138,138,138	0
48	MG	D1	3434	1/1	0.50	49.36	144,144,144,144	0
48	MG	F1	3428	1/1	0.36	47.00	111,111,111,111	0
48	MG	A1	3583	1/1	0.45	45.78	112,112,112,112	0
48	MG	H1	3441	1/1	0.18	39.00	102,102,102,102	0
48	MG	D1	3425	1/1	0.68	37.32	123,123,123,123	0
48	MG	A1	3441	1/1	0.49	35.95	127,127,127,127	0
48	MG	C3	205	1/1	1.21	35.95	175,175,175,175	0
48	MG	F1	3473	1/1	0.56	35.57	156,156,156,156	0
48	MG	A1	3430	1/1	0.53	33.38	146,146,146,146	0
48	MG	H1	3524	1/1	0.73	32.65	139,139,139,139	0
48	MG	A1	3428	1/1	0.64	31.25	159,159,159,159	0
48	MG	F1	3477	1/1	0.54	30.12	146,146,146,146	0
48	MG	F1	3569	1/1	0.34	30.11	130,130,130,130	0
48	MG	F1	3577	1/1	0.28	29.93	152,152,152,152	0
48	MG	F1	3433	1/1	0.64	29.50	95,95,95,95	0
48	MG	D1	3604	1/1	0.46	29.09	141,141,141,141	0
48	MG	D1	3446	1/1	0.80	28.90	176,176,176,176	0
48	MG	H1	3532	1/1	0.35	28.43	162,162,162,162	0
48	MG	G3	205	1/1	0.80	27.99	171,171,171,171	0
48	MG	D1	3475	1/1	0.56	27.23	120,120,120,120	0
48	MG	D1	3609	1/1	0.60	27.12	120,120,120,120	0
48	MG	D1	3611	1/1	0.55	26.85	205,205,205,205	0
48	MG	G2	204	1/1	1.02	26.44	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3550	1/1	0.46	25.64	152,152,152,152	0
48	MG	F1	3527	1/1	0.27	24.60	105,105,105,105	0
48	MG	F1	3578	1/1	1.00	24.48	161,161,161,161	0
48	MG	H1	3539	1/1	0.34	24.22	128,128,128,128	0
48	MG	F1	3564	1/1	0.50	24.13	143,143,143,143	0
48	MG	H1	3450	1/1	0.79	23.76	156,156,156,156	0
48	MG	D1	3576	1/1	0.53	23.53	150,150,150,150	0
48	MG	H1	3553	1/1	0.46	22.37	146,146,146,146	0
48	MG	D1	3597	1/1	0.62	22.24	158,158,158,158	0
48	MG	H1	3531	1/1	0.65	21.97	157,157,157,157	0
48	MG	D1	3525	1/1	0.34	21.81	113,113,113,113	0
48	MG	H1	3482	1/1	0.73	21.53	162,162,162,162	0
48	MG	H1	3436	1/1	0.42	21.45	146,146,146,146	0
48	MG	D1	3448	1/1	0.25	20.71	125,125,125,125	0
48	MG	F1	3544	1/1	0.20	20.00	97,97,97,97	0
48	MG	H1	3534	1/1	1.54	19.61	221,221,221,221	0
48	MG	D1	3451	1/1	0.48	19.49	115,115,115,115	0
48	MG	D1	3543	1/1	0.35	19.45	127,127,127,127	0
48	MG	F1	3574	1/1	0.52	18.89	161,161,161,161	0
48	MG	H1	3410	1/1	0.36	18.50	192,192,192,192	0
48	MG	A1	3422	1/1	0.50	17.97	144,144,144,144	0
48	MG	F1	3511	1/1	0.72	17.23	154,154,154,154	0
48	MG	H1	3457	1/1	0.61	17.03	147,147,147,147	0
48	MG	G3	202	1/1	0.61	16.96	136,136,136,136	0
48	MG	F1	3506	1/1	0.28	16.76	114,114,114,114	0
48	MG	A1	3545	1/1	0.29	16.60	71,71,71,71	0
48	MG	H1	3412	1/1	0.80	16.14	173,173,173,173	0
48	MG	F1	3401	1/1	0.37	15.74	101,101,101,101	0
48	MG	A1	3596	1/1	0.36	15.73	163,163,163,163	0
48	MG	D1	3600	1/1	0.38	15.58	123,123,123,123	0
48	MG	D1	3599	1/1	0.22	15.41	126,126,126,126	0
48	MG	D1	3470	1/1	0.39	15.34	134,134,134,134	0
48	MG	E2	201	1/1	0.41	15.30	156,156,156,156	0
48	MG	H1	3521	1/1	0.26	15.29	123,123,123,123	0
48	MG	D1	3622	1/1	0.33	15.13	133,133,133,133	0
48	MG	F1	3545	1/1	0.22	14.74	137,137,137,137	0
48	MG	H1	3449	1/1	0.59	14.64	118,118,118,118	0
48	MG	F1	3529	1/1	0.67	14.42	140,140,140,140	0
48	MG	H1	3537	1/1	0.19	14.20	152,152,152,152	0
48	MG	A1	3470	1/1	0.46	14.16	164,164,164,164	0
48	MG	H1	3490	1/1	0.53	14.12	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	A1	3586	1/1	0.82	14.12	177,177,177,177	0
48	MG	G3	204	1/1	0.41	14.06	143,143,143,143	0
48	MG	B2	206	1/1	0.43	13.91	139,139,139,139	0
48	MG	D1	3417	1/1	0.26	13.86	132,132,132,132	0
48	MG	A1	3472	1/1	0.57	13.28	149,149,149,149	0
48	MG	A1	3571	1/1	0.25	13.20	100,100,100,100	0
48	MG	E3	206	1/1	0.30	12.96	132,132,132,132	0
48	MG	A1	3435	1/1	0.54	12.67	151,151,151,151	0
48	MG	H1	3456	1/1	0.65	12.65	145,145,145,145	0
48	MG	B2	207	1/1	0.29	12.63	149,149,149,149	0
48	MG	F1	3413	1/1	0.32	12.56	110,110,110,110	0
48	MG	H1	3405	1/1	0.27	12.56	101,101,101,101	0
48	MG	A1	3457	1/1	0.35	12.55	94,94,94,94	0
48	MG	A1	3507	1/1	0.24	12.53	129,129,129,129	0
48	MG	H1	3477	1/1	0.29	12.17	103,103,103,103	0
48	MG	F1	3411	1/1	0.65	12.17	142,142,142,142	0
48	MG	H1	3536	1/1	0.66	11.66	168,168,168,168	0
48	MG	AK	202	1/1	0.94	11.48	179,179,179,179	0
48	MG	F1	3581	1/1	0.36	11.42	144,144,144,144	0
48	MG	H1	3554	1/1	0.65	11.41	128,128,128,128	0
48	MG	F1	3442	1/1	0.29	11.16	109,109,109,109	0
48	MG	F1	3516	1/1	0.26	10.94	121,121,121,121	0
48	MG	A1	3597	1/1	0.37	10.90	133,133,133,133	0
48	MG	A1	3592	1/1	0.34	10.86	134,134,134,134	0
48	MG	A1	3595	1/1	0.94	10.27	151,151,151,151	0
48	MG	D1	3516	1/1	0.31	10.08	82,82,82,82	0
48	MG	A1	3453	1/1	0.77	9.98	184,184,184,184	0
48	MG	A1	3516	1/1	0.22	9.91	88,88,88,88	0
48	MG	H1	3547	1/1	0.32	9.90	175,175,175,175	0
48	MG	A1	3480	1/1	0.45	9.88	120,120,120,120	0
48	MG	A1	3471	1/1	0.32	9.73	88,88,88,88	0
48	MG	EN	202	1/1	0.90	9.68	238,238,238,238	0
48	MG	F1	3414	1/1	0.23	9.49	123,123,123,123	0
48	MG	D1	3488	1/1	0.31	9.32	97,97,97,97	0
48	MG	FK	201	1/1	0.53	9.31	168,168,168,168	0
48	MG	H1	3465	1/1	0.31	9.23	143,143,143,143	0
48	MG	H1	3525	1/1	0.35	9.05	157,157,157,157	0
48	MG	A1	3515	1/1	0.25	8.90	111,111,111,111	0
48	MG	D1	3424	1/1	0.38	8.78	150,150,150,150	0
48	MG	A1	3579	1/1	0.57	8.56	94,94,94,94	0
48	MG	F1	3466	1/1	0.33	8.52	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	A1	3504	1/1	0.53	8.51	138,138,138,138	0
48	MG	A1	3568	1/1	0.39	8.37	173,173,173,173	0
48	MG	D1	3527	1/1	0.28	8.34	106,106,106,106	0
48	MG	A1	3408	1/1	0.27	8.31	122,122,122,122	0
48	MG	A1	3437	1/1	0.44	8.25	141,141,141,141	0
48	MG	H1	3530	1/1	0.35	8.06	154,154,154,154	0
48	MG	F1	3503	1/1	0.17	8.04	129,129,129,129	0
48	MG	H1	3489	1/1	0.48	8.03	206,206,206,206	0
48	MG	H1	3409	1/1	0.50	8.02	193,193,193,193	0
48	MG	A1	3544	1/1	0.49	7.70	135,135,135,135	0
48	MG	A1	3412	1/1	0.36	7.65	117,117,117,117	0
48	MG	D1	3437	1/1	0.30	7.64	148,148,148,148	0
48	MG	F1	3444	1/1	0.43	7.50	155,155,155,155	0
48	MG	F1	3493	1/1	0.52	7.35	145,145,145,145	0
48	MG	H1	3501	1/1	0.30	7.25	110,110,110,110	0
48	MG	F1	3496	1/1	0.23	7.13	122,122,122,122	0
48	MG	A1	3530	1/1	0.35	7.13	149,149,149,149	0
48	MG	D1	3593	1/1	0.38	7.08	180,180,180,180	0
48	MG	D1	3416	1/1	0.29	7.06	110,110,110,110	0
48	MG	F1	3555	1/1	0.25	7.06	168,168,168,168	0
48	MG	D1	3588	1/1	0.22	7.00	156,156,156,156	0
48	MG	H1	3462	1/1	0.37	6.92	131,131,131,131	0
48	MG	D1	3565	1/1	0.31	6.86	114,114,114,114	0
48	MG	F1	3416	1/1	0.50	6.81	116,116,116,116	0
48	MG	D1	3498	1/1	0.44	6.76	99,99,99,99	0
48	MG	D1	3408	1/1	0.32	6.76	106,106,106,106	0
48	MG	D1	3541	1/1	0.34	6.72	114,114,114,114	0
48	MG	D1	3444	1/1	0.24	6.67	139,139,139,139	0
48	MG	D1	3443	1/1	0.49	6.59	112,112,112,112	0
48	MG	A1	3420	1/1	0.27	6.56	155,155,155,155	0
48	MG	A1	3541	1/1	0.32	6.34	86,86,86,86	0
48	MG	A1	3528	1/1	0.41	6.28	120,120,120,120	0
48	MG	H1	3511	1/1	0.33	6.19	140,140,140,140	0
48	MG	D1	3608	1/1	0.24	6.15	115,115,115,115	0
48	MG	D1	3462	1/1	0.22	6.13	116,116,116,116	0
48	MG	A1	3527	1/1	0.27	6.07	119,119,119,119	0
48	MG	DK	201	1/1	0.40	6.04	101,101,101,101	0
48	MG	H1	3425	1/1	0.33	6.03	108,108,108,108	0
48	MG	D1	3439	1/1	0.26	5.98	146,146,146,146	0
48	MG	D1	3492	1/1	0.35	5.93	125,125,125,125	0
48	MG	F1	3502	1/1	0.28	5.89	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3567	1/1	0.25	5.83	60,60,60,60	0
48	MG	A1	3594	1/1	0.27	5.76	150,150,150,150	0
48	MG	E2	205	1/1	0.67	5.72	140,140,140,140	0
48	MG	GP	201	1/1	0.52	5.65	109,109,109,109	0
48	MG	D1	3412	1/1	0.32	5.63	95,95,95,95	0
48	MG	F1	3461	1/1	0.51	5.62	106,106,106,106	0
48	MG	D1	3603	1/1	0.48	5.48	125,125,125,125	0
48	MG	F1	3550	1/1	0.25	5.46	154,154,154,154	0
48	MG	D1	3607	1/1	0.32	5.44	89,89,89,89	0
48	MG	H1	3446	1/1	0.33	5.40	120,120,120,120	0
48	MG	D1	3481	1/1	0.43	5.31	114,114,114,114	0
48	MG	F1	3488	1/1	0.41	5.12	110,110,110,110	0
48	MG	A1	3581	1/1	0.27	4.95	126,126,126,126	0
48	MG	F1	3567	1/1	0.27	4.93	128,128,128,128	0
48	MG	F1	3425	1/1	0.32	4.88	115,115,115,115	0
48	MG	F1	3565	1/1	0.83	4.83	168,168,168,168	0
48	MG	D1	3583	1/1	0.29	4.79	139,139,139,139	0
48	MG	E2	207	1/1	0.33	4.74	147,147,147,147	0
48	MG	A1	3459	1/1	0.23	4.71	90,90,90,90	0
48	MG	H1	3519	1/1	0.34	4.70	151,151,151,151	0
48	MG	H1	3496	1/1	0.39	4.55	141,141,141,141	0
48	MG	F1	3463	1/1	0.20	4.52	100,100,100,100	0
48	MG	D1	3493	1/1	0.32	4.51	128,128,128,128	0
48	MG	F1	3424	1/1	0.32	4.49	114,114,114,114	0
48	MG	D1	3497	1/1	0.49	4.41	151,151,151,151	0
48	MG	F1	3582	1/1	0.20	4.40	77,77,77,77	0
48	MG	F1	3422	1/1	0.27	4.39	149,149,149,149	0
48	MG	F1	3479	1/1	0.39	4.36	81,81,81,81	0
48	MG	D1	3547	1/1	0.26	4.28	109,109,109,109	0
48	MG	GO	201	1/1	0.46	4.24	141,141,141,141	0
48	MG	D1	3484	1/1	0.27	4.21	96,96,96,96	0
48	MG	D1	3623	1/1	0.26	4.16	151,151,151,151	0
48	MG	DA	102	1/1	0.29	4.13	115,115,115,115	0
48	MG	D1	3421	1/1	0.25	4.10	126,126,126,126	0
48	MG	H1	3542	1/1	0.36	4.09	137,137,137,137	0
48	MG	D1	3571	1/1	0.40	4.08	130,130,130,130	0
48	MG	A1	3423	1/1	0.24	3.98	115,115,115,115	0
48	MG	H1	3549	1/1	0.41	3.92	124,124,124,124	0
48	MG	B3	201	1/1	0.24	3.91	129,129,129,129	0
48	MG	A1	3531	1/1	0.26	3.90	128,128,128,128	0
48	MG	D1	3537	1/1	0.38	3.87	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	D1	3442	1/1	0.32	3.83	126,126,126,126	0
48	MG	A1	3560	1/1	0.32	3.81	138,138,138,138	0
48	MG	A1	3500	1/1	0.33	3.79	89,89,89,89	0
48	MG	D1	3613	1/1	0.24	3.71	120,120,120,120	0
48	MG	F1	3538	1/1	0.32	3.69	113,113,113,113	0
48	MG	F1	3560	1/1	0.41	3.68	169,169,169,169	0
48	MG	D1	3506	1/1	0.21	3.63	132,132,132,132	0
48	MG	D1	3555	1/1	0.36	3.58	119,119,119,119	0
48	MG	F1	3483	1/1	0.32	3.49	129,129,129,129	0
48	MG	F1	3508	1/1	0.29	3.49	127,127,127,127	0
48	MG	GN	201	1/1	0.52	3.48	212,212,212,212	0
48	MG	A1	3533	1/1	0.24	3.46	73,73,73,73	0
48	MG	H1	3540	1/1	0.23	3.39	136,136,136,136	0
48	MG	A1	3573	1/1	0.36	3.37	186,186,186,186	0
48	MG	D1	3589	1/1	0.26	3.36	107,107,107,107	0
48	MG	D1	3429	1/1	0.27	3.31	113,113,113,113	0
48	MG	H1	3469	1/1	0.38	3.29	119,119,119,119	0
48	MG	A1	3438	1/1	0.23	3.27	148,148,148,148	0
48	MG	H1	3408	1/1	0.33	3.23	111,111,111,111	0
48	MG	A1	3491	1/1	0.27	3.22	125,125,125,125	0
48	MG	H1	3538	1/1	0.31	3.19	140,140,140,140	0
48	MG	H1	3422	1/1	0.43	3.16	151,151,151,151	0
48	MG	D1	3517	1/1	0.31	3.15	127,127,127,127	0
48	MG	D1	3504	1/1	0.28	3.14	98,98,98,98	0
48	MG	D1	3568	1/1	0.22	3.01	105,105,105,105	0
48	MG	G2	202	1/1	0.39	2.99	122,122,122,122	0
48	MG	H1	3443	1/1	0.37	2.94	157,157,157,157	0
48	MG	D1	3521	1/1	0.27	2.93	129,129,129,129	0
48	MG	A1	3584	1/1	0.18	2.85	125,125,125,125	0
48	MG	A1	3492	1/1	0.26	2.73	127,127,127,127	0
48	MG	H1	3484	1/1	0.24	2.70	166,166,166,166	0
48	MG	A1	3487	1/1	0.29	2.69	121,121,121,121	0
48	MG	F1	3540	1/1	0.24	2.68	111,111,111,111	0
48	MG	F1	3446	1/1	0.21	2.62	130,130,130,130	0
48	MG	F1	3482	1/1	0.23	2.60	130,130,130,130	0
48	MG	A1	3479	1/1	0.21	2.54	120,120,120,120	0
48	MG	H1	3529	1/1	0.29	2.49	214,214,214,214	0
48	MG	A1	3585	1/1	0.45	2.49	152,152,152,152	0
48	MG	D1	3511	1/1	0.21	2.49	118,118,118,118	0
48	MG	D1	3612	1/1	0.22	2.47	123,123,123,123	0
48	MG	H1	3481	1/1	0.29	2.41	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	D1	3594	1/1	0.22	2.34	106,106,106,106	0
48	MG	H1	3420	1/1	0.24	2.27	113,113,113,113	0
48	MG	D1	3512	1/1	0.19	2.25	101,101,101,101	0
48	MG	H1	3472	1/1	0.31	2.20	104,104,104,104	0
48	MG	A1	3578	1/1	0.19	2.20	117,117,117,117	0
48	MG	E3	202	1/1	0.20	2.19	122,122,122,122	0
48	MG	H1	3541	1/1	0.26	2.17	154,154,154,154	0
48	MG	D1	3602	1/1	0.26	2.17	118,118,118,118	0
48	MG	C2	206	1/1	0.24	2.16	123,123,123,123	0
48	MG	F1	3457	1/1	0.28	2.16	91,91,91,91	0
48	MG	F1	3551	1/1	0.25	2.16	91,91,91,91	0
48	MG	A1	3562	1/1	0.19	2.15	91,91,91,91	0
48	MG	D1	3528	1/1	0.24	2.14	123,123,123,123	0
48	MG	H1	3447	1/1	0.23	2.09	110,110,110,110	0
48	MG	F1	3532	1/1	0.20	2.08	87,87,87,87	0
48	MG	F1	3563	1/1	0.20	2.08	124,124,124,124	0
48	MG	H1	3438	1/1	0.27	2.07	120,120,120,120	0
48	MG	D1	3401	1/1	0.22	2.04	109,109,109,109	0
48	MG	GW	201	1/1	0.28	2.04	114,114,114,114	0
48	MG	H1	3414	1/1	0.54	2.02	169,169,169,169	0
48	MG	B3	203	1/1	0.23	2.00	160,160,160,160	0
48	MG	F1	3571	1/1	0.22	1.98	132,132,132,132	0
48	MG	C2	202	1/1	0.23	1.97	112,112,112,112	0
48	MG	A1	3449	1/1	0.22	1.95	115,115,115,115	0
48	MG	E2	206	1/1	0.32	1.92	151,151,151,151	0
48	MG	D1	3615	1/1	0.23	1.86	132,132,132,132	0
48	MG	D1	3445	1/1	0.20	1.85	126,126,126,126	0
48	MG	A1	3590	1/1	0.18	1.72	142,142,142,142	0
48	MG	A1	3450	1/1	0.24	1.68	133,133,133,133	0
48	MG	D1	3534	1/1	0.19	1.65	98,98,98,98	0
48	MG	A1	3551	1/1	0.35	1.64	123,123,123,123	0
48	MG	D1	3447	1/1	0.24	1.56	101,101,101,101	0
48	MG	H1	3548	1/1	0.28	1.55	188,188,188,188	0
48	MG	F1	3570	1/1	0.26	1.52	113,113,113,113	0
48	MG	D1	3431	1/1	0.20	1.46	95,95,95,95	0
48	MG	F1	3464	1/1	0.23	1.46	120,120,120,120	0
48	MG	D1	3577	1/1	0.23	1.40	121,121,121,121	0
48	MG	D1	3471	1/1	0.21	1.39	40,40,40,40	0
48	MG	H1	3411	1/1	0.30	1.35	120,120,120,120	0
48	MG	A1	3424	1/1	0.41	1.31	150,150,150,150	0
48	MG	CQ	201	1/1	0.17	1.29	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	D1	3540	1/1	0.21	1.27	139,139,139,139	0
48	MG	F1	3453	1/1	0.22	1.25	131,131,131,131	0
48	MG	A1	3410	1/1	0.22	1.23	62,62,62,62	0
48	MG	F1	3537	1/1	0.20	1.23	136,136,136,136	0
48	MG	A1	3436	1/1	0.24	1.21	110,110,110,110	0
48	MG	A1	3402	1/1	0.32	1.18	143,143,143,143	0
48	MG	A1	3475	1/1	0.21	1.17	80,80,80,80	0
48	MG	D1	3595	1/1	0.23	1.17	94,94,94,94	0
48	MG	EW	201	1/1	0.34	1.16	172,172,172,172	0
48	MG	A1	3591	1/1	0.29	1.14	121,121,121,121	0
48	MG	D1	3432	1/1	0.15	1.12	118,118,118,118	0
48	MG	D1	3426	1/1	0.41	1.10	143,143,143,143	0
48	MG	F1	3417	1/1	0.20	1.10	110,110,110,110	0
48	MG	H1	3518	1/1	0.16	1.09	110,110,110,110	0
48	MG	F1	3492	1/1	0.25	1.07	78,78,78,78	0
48	MG	DJ	301	1/1	0.32	1.07	150,150,150,150	0
48	MG	D1	3467	1/1	0.17	1.05	123,123,123,123	0
48	MG	A1	3496	1/1	0.25	1.05	137,137,137,137	0
48	MG	F1	3576	1/1	0.34	1.04	142,142,142,142	0
48	MG	F1	3558	1/1	0.21	0.97	144,144,144,144	0
48	MG	H1	3516	1/1	0.26	0.97	129,129,129,129	0
48	MG	H1	3413	1/1	0.27	0.96	117,117,117,117	0
48	MG	D1	3551	1/1	0.18	0.95	142,142,142,142	0
48	MG	A1	3588	1/1	0.19	0.95	144,144,144,144	0
48	MG	E3	205	1/1	0.18	0.95	127,127,127,127	0
48	MG	F1	3421	1/1	0.42	0.93	174,174,174,174	0
48	MG	H1	3512	1/1	0.32	0.92	121,121,121,121	0
48	MG	F1	3465	1/1	0.21	0.89	101,101,101,101	0
48	MG	D1	3598	1/1	0.17	0.88	159,159,159,159	0
48	MG	A1	3427	1/1	0.24	0.86	152,152,152,152	0
48	MG	H1	3431	1/1	0.23	0.86	94,94,94,94	0
48	MG	F1	3541	1/1	0.26	0.81	112,112,112,112	0
48	MG	CN	201	1/1	0.27	0.78	175,175,175,175	0
48	MG	F1	3522	1/1	0.18	0.72	111,111,111,111	0
48	MG	A1	3518	1/1	0.23	0.66	109,109,109,109	0
48	MG	A1	3493	1/1	0.20	0.66	113,113,113,113	0
48	MG	A1	3415	1/1	0.18	0.59	120,120,120,120	0
48	MG	CY	201	1/1	0.21	0.58	99,99,99,99	0
48	MG	BN	201	1/1	0.34	0.57	147,147,147,147	0
48	MG	A1	3490	1/1	0.19	0.56	105,105,105,105	0
48	MG	F1	3486	1/1	0.14	0.54	90,90,90,90	0
48	MG	F1	3507	1/1	0.17	0.54	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	D1	3601	1/1	0.14	0.53	124,124,124,124	0
48	MG	D1	3427	1/1	0.22	0.52	153,153,153,153	0
48	MG	H1	3528	1/1	0.18	0.46	119,119,119,119	0
48	MG	A1	3542	1/1	0.22	0.44	96,96,96,96	0
48	MG	H1	3546	1/1	0.23	0.44	120,120,120,120	0
48	MG	D1	3466	1/1	0.29	0.43	132,132,132,132	0
48	MG	F1	3447	1/1	0.27	0.40	156,156,156,156	0
48	MG	H1	3510	1/1	0.21	0.40	120,120,120,120	0
48	MG	F1	3490	1/1	0.19	0.38	139,139,139,139	0
48	MG	A1	3451	1/1	0.16	0.38	146,146,146,146	0
48	MG	D1	3610	1/1	0.21	0.37	66,66,66,66	0
48	MG	H1	3468	1/1	0.23	0.35	121,121,121,121	0
48	MG	A1	3468	1/1	0.20	0.31	109,109,109,109	0
48	MG	HT	101	1/1	0.35	0.31	174,174,174,174	0
48	MG	D1	3570	1/1	0.20	0.28	54,54,54,54	0
48	MG	F1	3445	1/1	0.18	0.16	78,78,78,78	0
48	MG	F1	3469	1/1	0.18	0.15	112,112,112,112	0
48	MG	A1	3556	1/1	0.17	0.14	124,124,124,124	0
48	MG	F1	3500	1/1	0.18	0.13	105,105,105,105	0
48	MG	GQ	201	1/1	0.30	0.11	102,102,102,102	0
48	MG	D1	3564	1/1	0.19	0.10	92,92,92,92	0
48	MG	A1	3582	1/1	0.21	0.09	110,110,110,110	0
48	MG	A1	3499	1/1	0.21	0.06	117,117,117,117	0
48	MG	A1	3414	1/1	0.21	0.03	142,142,142,142	0
48	MG	D1	3510	1/1	0.19	0.02	81,81,81,81	0
48	MG	H1	3526	1/1	0.20	0.02	94,94,94,94	0
48	MG	D1	3590	1/1	0.17	-0.01	89,89,89,89	0
48	MG	A1	3417	1/1	0.25	-0.07	150,150,150,150	0
48	MG	A1	3501	1/1	0.22	-0.15	102,102,102,102	0
48	MG	H1	3471	1/1	0.23	-0.18	124,124,124,124	0
48	MG	D1	3614	1/1	0.23	-0.24	129,129,129,129	0
48	MG	CD	201	1/1	0.24	-0.25	93,93,93,93	0
48	MG	H1	3418	1/1	0.19	-0.25	141,141,141,141	0
48	MG	E3	203	1/1	0.17	-0.25	104,104,104,104	0
48	MG	A1	3510	1/1	0.20	-0.27	109,109,109,109	0
48	MG	A1	3546	1/1	0.17	-0.30	51,51,51,51	0
48	MG	A1	3445	1/1	0.18	-0.31	88,88,88,88	0
48	MG	BQ	201	1/1	0.20	-0.32	122,122,122,122	0
48	MG	H1	3508	1/1	0.19	-0.33	80,80,80,80	0
48	MG	H1	3503	1/1	0.21	-0.36	91,91,91,91	0
48	MG	GP	202	1/1	0.24	-0.36	137,137,137,137	0
48	MG	F1	3561	1/1	0.19	-0.38	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	A1	3548	1/1	0.15	-0.43	124,124,124,124	0
48	MG	D1	3514	1/1	0.19	-0.43	128,128,128,128	0
48	MG	DQ	201	1/1	0.29	-0.44	118,118,118,118	0
48	MG	A1	3523	1/1	0.13	-0.45	91,91,91,91	0
48	MG	H1	3488	1/1	0.24	-0.47	108,108,108,108	0
48	MG	D1	3515	1/1	0.20	-0.47	106,106,106,106	0
48	MG	D1	3620	1/1	0.14	-0.51	106,106,106,106	0
48	MG	CW	201	1/1	0.25	-0.51	90,90,90,90	0
48	MG	F1	3580	1/1	0.16	-0.53	147,147,147,147	0
48	MG	D1	3496	1/1	0.16	-0.53	78,78,78,78	0
48	MG	A1	3413	1/1	0.19	-0.54	136,136,136,136	0
48	MG	A1	3565	1/1	0.15	-0.55	132,132,132,132	0
48	MG	H1	3455	1/1	0.18	-0.57	113,113,113,113	0
48	MG	BJ	201	1/1	0.17	-0.60	66,66,66,66	0
48	MG	H1	3473	1/1	0.20	-0.63	123,123,123,123	0
48	MG	F1	3468	1/1	0.17	-0.66	103,103,103,103	0
48	MG	D1	3530	1/1	0.18	-0.67	94,94,94,94	0
48	MG	F1	3484	1/1	0.15	-0.71	78,78,78,78	0
48	MG	F1	3549	1/1	0.20	-0.73	125,125,125,125	0
48	MG	B2	201	1/1	0.17	-0.75	119,119,119,119	0
48	MG	D1	3418	1/1	0.18	-0.76	114,114,114,114	0
48	MG	A1	3572	1/1	0.18	-0.77	121,121,121,121	0
48	MG	A1	3409	1/1	0.14	-0.77	87,87,87,87	0
48	MG	A1	3481	1/1	0.15	-0.79	88,88,88,88	0
48	MG	A1	3467	1/1	0.17	-0.80	106,106,106,106	0
48	MG	F1	3430	1/1	0.14	-0.80	128,128,128,128	0
48	MG	D1	3436	1/1	0.17	-0.81	78,78,78,78	0
48	MG	D1	3518	1/1	0.17	-0.81	92,92,92,92	0
48	MG	A1	3536	1/1	0.15	-0.82	104,104,104,104	0
48	MG	FT	101	1/1	0.14	-0.83	124,124,124,124	0
48	MG	A1	3461	1/1	0.15	-0.86	67,67,67,67	0
48	MG	EN	201	1/1	0.18	-0.86	111,111,111,111	0
49	ZN	DA	103	1/1	0.14	-0.86	69,69,69,69	0
48	MG	GA	301	1/1	0.26	-0.86	142,142,142,142	0
48	MG	F1	3475	1/1	0.17	-0.89	93,93,93,93	0
48	MG	A1	3557	1/1	0.16	-0.91	104,104,104,104	0
48	MG	H1	3497	1/1	0.14	-0.92	50,50,50,50	0
48	MG	F1	3533	1/1	0.14	-0.92	101,101,101,101	0
48	MG	B3	202	1/1	0.17	-0.92	113,113,113,113	0
48	MG	A1	3549	1/1	0.12	-0.94	54,54,54,54	0
48	MG	H1	3434	1/1	0.19	-0.94	93,93,93,93	0
48	MG	A1	3434	1/1	0.15	-0.96	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
48	MG	A1	3419	1/1	0.13	-0.96	100,100,100,100	0
48	MG	H1	3464	1/1	0.19	-0.99	108,108,108,108	0
48	MG	F1	3472	1/1	0.15	-1.00	111,111,111,111	0
48	MG	D1	3626	1/1	0.15	-1.02	137,137,137,137	0
48	MG	H1	3433	1/1	0.21	-1.03	132,132,132,132	0
48	MG	A1	3446	1/1	0.17	-1.04	64,64,64,64	0
49	ZN	EY	201	1/1	0.09	-1.06	77,77,77,77	0
48	MG	D1	3482	1/1	0.16	-1.07	106,106,106,106	0
48	MG	D1	3569	1/1	0.11	-1.07	48,48,48,48	0
48	MG	CL	302	1/1	0.12	-1.13	68,68,68,68	0
48	MG	A1	3520	1/1	0.16	-1.14	70,70,70,70	0
48	MG	F1	3534	1/1	0.08	-1.15	79,79,79,79	0
48	MG	A1	3547	1/1	0.15	-1.15	81,81,81,81	0
48	MG	D1	3505	1/1	0.15	-1.15	84,84,84,84	0
48	MG	A1	3401	1/1	0.12	-1.16	108,108,108,108	0
49	ZN	HA	101	1/1	0.13	-1.17	112,112,112,112	0
49	ZN	DL	201	1/1	0.15	-1.17	86,86,86,86	0
48	MG	EJ	201	1/1	0.13	-1.18	69,69,69,69	0
49	ZN	AA	101	1/1	0.14	-1.19	64,64,64,64	0
48	MG	F1	3462	1/1	0.14	-1.19	118,118,118,118	0
48	MG	F1	3491	1/1	0.20	-1.19	96,96,96,96	0
49	ZN	DK	202	1/1	0.11	-1.22	68,68,68,68	0
48	MG	A1	3564	1/1	0.09	-1.23	141,141,141,141	0
48	MG	F1	3485	1/1	0.17	-1.23	117,117,117,117	0
48	MG	D1	3490	1/1	0.15	-1.25	92,92,92,92	0
48	MG	A1	3407	1/1	0.13	-1.26	83,83,83,83	0
48	MG	H1	3419	1/1	0.16	-1.27	62,62,62,62	0
48	MG	F1	3501	1/1	0.16	-1.30	116,116,116,116	0
48	MG	H1	3509	1/1	0.17	-1.31	143,143,143,143	0
48	MG	EW	202	1/1	0.17	-1.32	121,121,121,121	0
48	MG	F1	3434	1/1	0.16	-1.32	83,83,83,83	0
48	MG	D1	3561	1/1	0.19	-1.33	57,57,57,57	0
48	MG	D1	3572	1/1	0.20	-1.33	69,69,69,69	0
48	MG	A1	3524	1/1	0.12	-1.34	63,63,63,63	0
49	ZN	DC	201	1/1	0.07	-1.35	89,89,89,89	0
48	MG	F1	3513	1/1	0.17	-1.37	79,79,79,79	0
48	MG	F1	3517	1/1	0.11	-1.38	62,62,62,62	0
48	MG	D1	3441	1/1	0.14	-1.38	75,75,75,75	0
48	MG	H1	3507	1/1	0.07	-1.39	64,64,64,64	0
48	MG	H1	3491	1/1	0.13	-1.41	111,111,111,111	0
48	MG	A1	3566	1/1	0.12	-1.42	75,75,75,75	0
48	MG	H1	3402	1/1	0.19	-1.43	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3581	1/1	0.07	-1.44	68,68,68,68	0
48	MG	FA	101	1/1	0.13	-1.44	97,97,97,97	0
48	MG	A1	3558	1/1	0.10	-1.45	91,91,91,91	0
48	MG	D1	3485	1/1	0.14	-1.46	120,120,120,120	0
48	MG	H1	3476	1/1	0.08	-1.47	52,52,52,52	0
48	MG	D1	3586	1/1	0.14	-1.50	109,109,109,109	0
48	MG	A1	3569	1/1	0.09	-1.51	91,91,91,91	0
48	MG	CL	301	1/1	0.17	-1.51	109,109,109,109	0
48	MG	F1	3514	1/1	0.13	-1.53	70,70,70,70	0
48	MG	E2	202	1/1	0.16	-1.55	89,89,89,89	0
48	MG	G2	203	1/1	0.12	-1.57	112,112,112,112	0
48	MG	F1	3431	1/1	0.17	-1.57	103,103,103,103	0
48	MG	G3	203	1/1	0.12	-1.59	86,86,86,86	0
49	ZN	FA	103	1/1	0.12	-1.60	80,80,80,80	0
48	MG	A1	3484	1/1	0.15	-1.61	108,108,108,108	0
48	MG	G3	201	1/1	0.13	-1.61	119,119,119,119	0
48	MG	A1	3443	1/1	0.13	-1.62	90,90,90,90	0
48	MG	H1	3520	1/1	0.17	-1.62	114,114,114,114	0
48	MG	C3	202	1/1	0.12	-1.62	135,135,135,135	0
48	MG	A1	3552	1/1	0.11	-1.63	97,97,97,97	0
48	MG	F1	3448	1/1	0.15	-1.64	126,126,126,126	0
48	MG	GL	301	1/1	0.10	-1.66	113,113,113,113	0
48	MG	H1	3492	1/1	0.13	-1.66	96,96,96,96	0
48	MG	H1	3514	1/1	0.09	-1.70	66,66,66,66	0
48	MG	D1	3587	1/1	0.13	-1.70	93,93,93,93	0
48	MG	H1	3487	1/1	0.21	-1.71	122,122,122,122	0
48	MG	EQ	201	1/1	0.17	-1.71	88,88,88,88	0
48	MG	H1	3426	1/1	0.16	-1.72	105,105,105,105	0
48	MG	F1	3408	1/1	0.15	-1.72	82,82,82,82	0
48	MG	D1	3440	1/1	0.12	-1.73	99,99,99,99	0
48	MG	D1	3523	1/1	0.13	-1.73	105,105,105,105	0
48	MG	G2	205	1/1	0.17	-1.77	146,146,146,146	0
48	MG	D1	3491	1/1	0.16	-1.77	97,97,97,97	0
49	ZN	FL	201	1/1	0.09	-1.79	86,86,86,86	0
48	MG	D1	3554	1/1	0.15	-1.79	59,59,59,59	0
48	MG	A1	3497	1/1	0.11	-1.80	116,116,116,116	0
48	MG	F1	3556	1/1	0.08	-1.81	90,90,90,90	0
48	MG	A1	3505	1/1	0.14	-1.82	137,137,137,137	0
48	MG	EL	301	1/1	0.14	-1.83	119,119,119,119	0
48	MG	A1	3554	1/1	0.14	-1.83	76,76,76,76	0
48	MG	H1	3493	1/1	0.13	-1.83	79,79,79,79	0
48	MG	D1	3539	1/1	0.14	-1.83	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3430	1/1	0.21	-1.84	82,82,82,82	0
48	MG	D1	3562	1/1	0.19	-1.84	93,93,93,93	0
48	MG	E2	203	1/1	0.07	-1.85	77,77,77,77	0
48	MG	F1	3543	1/1	0.09	-1.86	71,71,71,71	0
48	MG	D1	3499	1/1	0.14	-1.89	118,118,118,118	0
49	ZN	FK	202	1/1	0.12	-1.90	74,74,74,74	0
49	ZN	CY	202	1/1	0.07	-1.91	70,70,70,70	0
49	ZN	HC	201	1/1	0.05	-1.92	168,168,168,168	0
48	MG	A1	3421	1/1	0.06	-1.92	71,71,71,71	0
48	MG	D1	3507	1/1	0.13	-1.92	75,75,75,75	0
48	MG	D1	3494	1/1	0.13	-1.93	78,78,78,78	0
48	MG	AA	103	1/1	0.07	-1.94	56,56,56,56	0
48	MG	H1	3407	1/1	0.20	-1.94	105,105,105,105	0
48	MG	D1	3552	1/1	0.06	-1.97	55,55,55,55	0
49	ZN	FC	201	1/1	0.03	-1.97	108,108,108,108	0
48	MG	F1	3429	1/1	0.18	-1.98	73,73,73,73	0
48	MG	D1	3423	1/1	0.17	-1.98	67,67,67,67	0
48	MG	A1	3444	1/1	0.13	-1.99	126,126,126,126	0
48	MG	D1	3546	1/1	0.09	-2.00	49,49,49,49	0
48	MG	H1	3523	1/1	0.13	-2.01	167,167,167,167	0
48	MG	D1	3621	1/1	0.15	-2.01	110,110,110,110	0
49	ZN	BY	201	1/1	0.09	-2.01	59,59,59,59	0
49	ZN	AK	201	1/1	0.09	-2.03	89,89,89,89	0
48	MG	B2	204	1/1	0.08	-2.03	85,85,85,85	0
49	ZN	AL	201	1/1	0.08	-2.03	70,70,70,70	0
48	MG	F1	3552	1/1	0.14	-2.07	139,139,139,139	0
48	MG	A1	3452	1/1	0.10	-2.07	90,90,90,90	0
48	MG	F1	3542	1/1	0.13	-2.07	107,107,107,107	0
48	MG	D1	3544	1/1	0.09	-2.08	50,50,50,50	0
48	MG	BP	200	1/1	0.12	-2.08	123,123,123,123	0
48	MG	A1	3494	1/1	0.07	-2.11	98,98,98,98	0
48	MG	H1	3478	1/1	0.12	-2.12	114,114,114,114	0
48	MG	F1	3427	1/1	0.13	-2.13	51,51,51,51	0
48	MG	A1	3488	1/1	0.15	-2.14	91,91,91,91	0
48	MG	A1	3512	1/1	0.11	-2.15	90,90,90,90	0
48	MG	F1	3583	1/1	0.17	-2.15	104,104,104,104	0
48	MG	D1	3438	1/1	0.08	-2.17	39,39,39,39	0
48	MG	A1	3432	1/1	0.06	-2.18	45,45,45,45	0
49	ZN	HL	201	1/1	0.07	-2.18	118,118,118,118	0
48	MG	H1	3486	1/1	0.12	-2.19	105,105,105,105	0
48	MG	CJ	201	1/1	0.12	-2.19	64,64,64,64	0
48	MG	H1	3460	1/1	0.16	-2.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3518	1/1	0.11	-2.20	77,77,77,77	0
48	MG	C2	201	1/1	0.13	-2.21	121,121,121,121	0
48	MG	A1	3474	1/1	0.12	-2.24	88,88,88,88	0
48	MG	F1	3535	1/1	0.12	-2.25	58,58,58,58	0
48	MG	A1	3485	1/1	0.16	-2.25	137,137,137,137	0
48	MG	CQ	202	1/1	0.08	-2.26	62,62,62,62	0
48	MG	D1	3452	1/1	0.13	-2.26	106,106,106,106	0
48	MG	C3	206	1/1	0.14	-2.26	120,120,120,120	0
48	MG	D1	3414	1/1	0.14	-2.27	96,96,96,96	0
48	MG	H1	3448	1/1	0.16	-2.27	98,98,98,98	0
48	MG	D1	3464	1/1	0.09	-2.29	44,44,44,44	0
48	MG	D1	3409	1/1	0.14	-2.29	57,57,57,57	0
48	MG	H1	3442	1/1	0.12	-2.29	79,79,79,79	0
48	MG	F1	3548	1/1	0.12	-2.31	106,106,106,106	0
48	MG	H1	3494	1/1	0.14	-2.31	56,56,56,56	0
48	MG	G2	201	1/1	0.13	-2.31	141,141,141,141	0
48	MG	A1	3495	1/1	0.07	-2.31	70,70,70,70	0
48	MG	F1	3480	1/1	0.12	-2.32	59,59,59,59	0
48	MG	A1	3517	1/1	0.06	-2.33	74,74,74,74	0
48	MG	D1	3557	1/1	0.13	-2.34	116,116,116,116	0
48	MG	H1	3421	1/1	0.16	-2.35	97,97,97,97	0
48	MG	D1	3404	1/1	0.10	-2.36	55,55,55,55	0
48	MG	D1	3413	1/1	0.09	-2.36	51,51,51,51	0
48	MG	D1	3605	1/1	0.13	-2.36	108,108,108,108	0
48	MG	C2	205	1/1	0.15	-2.37	127,127,127,127	0
48	MG	H1	3545	1/1	0.15	-2.38	156,156,156,156	0
48	MG	F1	3418	1/1	0.11	-2.39	126,126,126,126	0
48	MG	F1	3536	1/1	0.19	-2.40	67,67,67,67	0
48	MG	D1	3477	1/1	0.09	-2.40	60,60,60,60	0
48	MG	F1	3487	1/1	0.09	-2.41	60,60,60,60	0
48	MG	A1	3511	1/1	0.09	-2.41	90,90,90,90	0
48	MG	F1	3497	1/1	0.14	-2.41	93,93,93,93	0
48	MG	D1	3553	1/1	0.06	-2.42	90,90,90,90	0
48	MG	F1	3460	1/1	0.15	-2.42	36,36,36,36	0
48	MG	F1	3510	1/1	0.10	-2.42	95,95,95,95	0
48	MG	A1	3411	1/1	0.16	-2.43	83,83,83,83	0
48	MG	F1	3407	1/1	0.07	-2.44	111,111,111,111	0
48	MG	D1	3469	1/1	0.11	-2.44	64,64,64,64	0
48	MG	H1	3517	1/1	0.14	-2.46	79,79,79,79	0
48	MG	F1	3471	1/1	0.16	-2.46	90,90,90,90	0
48	MG	A1	3561	1/1	0.14	-2.48	60,60,60,60	0
49	ZN	GY	201	1/1	0.10	-2.50	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	A1	3439	1/1	0.10	-2.50	106,106,106,106	0
48	MG	A1	3532	1/1	0.07	-2.52	74,74,74,74	0
48	MG	H1	3439	1/1	0.13	-2.52	75,75,75,75	0
48	MG	F1	3452	1/1	0.12	-2.53	50,50,50,50	0
48	MG	H1	3483	1/1	0.17	-2.53	108,108,108,108	0
48	MG	H1	3474	1/1	0.12	-2.53	123,123,123,123	0
48	MG	A1	3537	1/1	0.13	-2.54	54,54,54,54	0
48	MG	F1	3524	1/1	0.14	-2.55	56,56,56,56	0
48	MG	A1	3600	1/1	0.09	-2.55	111,111,111,111	0
48	MG	A1	3483	1/1	0.13	-2.56	83,83,83,83	0
48	MG	H1	3527	1/1	0.10	-2.57	99,99,99,99	0
48	MG	F1	3476	1/1	0.14	-2.58	99,99,99,99	0
48	MG	D1	3503	1/1	0.14	-2.58	82,82,82,82	0
48	MG	F1	3438	1/1	0.15	-2.60	58,58,58,58	0
48	MG	H1	3461	1/1	0.18	-2.60	134,134,134,134	0
48	MG	H1	3463	1/1	0.12	-2.61	78,78,78,78	0
48	MG	D1	3422	1/1	0.14	-2.61	150,150,150,150	0
48	MG	D1	3406	1/1	0.14	-2.63	67,67,67,67	0
48	MG	H1	3424	1/1	0.08	-2.63	96,96,96,96	0
48	MG	D1	3579	1/1	0.09	-2.64	97,97,97,97	0
48	MG	F1	3579	1/1	0.12	-2.65	166,166,166,166	0
48	MG	A1	3599	1/1	0.12	-2.66	103,103,103,103	0
48	MG	H1	3403	1/1	0.15	-2.69	111,111,111,111	0
48	MG	FA	102	1/1	0.10	-2.69	84,84,84,84	0
48	MG	D1	3618	1/1	0.09	-2.71	95,95,95,95	0
48	MG	A1	3404	1/1	0.11	-2.71	94,94,94,94	0
48	MG	A1	3529	1/1	0.11	-2.72	96,96,96,96	0
48	MG	D1	3433	1/1	0.16	-2.74	149,149,149,149	0
48	MG	F1	3499	1/1	0.04	-2.75	57,57,57,57	0
48	MG	H1	3500	1/1	0.16	-2.75	82,82,82,82	0
48	MG	D1	3449	1/1	0.09	-2.76	68,68,68,68	0
49	ZN	AC	201	1/1	0.08	-2.78	143,143,143,143	0
48	MG	H1	3470	1/1	0.16	-2.78	140,140,140,140	0
48	MG	BQ	202	1/1	0.07	-2.78	53,53,53,53	0
48	MG	H1	3467	1/1	0.12	-2.78	95,95,95,95	0
48	MG	H1	3504	1/1	0.10	-2.80	111,111,111,111	0
48	MG	D1	3486	1/1	0.12	-2.80	47,47,47,47	0
48	MG	D1	3573	1/1	0.10	-2.80	126,126,126,126	0
48	MG	A1	3440	1/1	0.05	-2.83	78,78,78,78	0
48	MG	EL	302	1/1	0.09	-2.84	68,68,68,68	0
48	MG	F1	3437	1/1	0.15	-2.85	100,100,100,100	0
48	MG	D1	3545	1/1	0.13	-2.85	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3409	1/1	0.17	-2.86	60,60,60,60	0
48	MG	H1	3427	1/1	0.17	-2.86	83,83,83,83	0
48	MG	A1	3525	1/1	0.10	-2.87	51,51,51,51	0
48	MG	F1	3530	1/1	0.12	-2.88	107,107,107,107	0
48	MG	A1	3563	1/1	0.12	-2.89	100,100,100,100	0
48	MG	F1	3494	1/1	0.12	-2.91	97,97,97,97	0
48	MG	A1	3426	1/1	0.11	-2.93	73,73,73,73	0
48	MG	GJ	201	1/1	0.12	-2.96	69,69,69,69	0
48	MG	H1	3423	1/1	0.11	-3.00	98,98,98,98	0
48	MG	D1	3535	1/1	0.15	-3.00	86,86,86,86	0
48	MG	H1	3445	1/1	0.14	-3.02	68,68,68,68	0
48	MG	F1	3573	1/1	0.08	-3.02	84,84,84,84	0
48	MG	D1	3513	1/1	0.14	-3.02	89,89,89,89	0
48	MG	D1	3520	1/1	0.12	-3.04	93,93,93,93	0
48	MG	F1	3459	1/1	0.07	-3.05	79,79,79,79	0
48	MG	AA	102	1/1	0.07	-3.06	98,98,98,98	0
48	MG	D1	3560	1/1	0.11	-3.08	64,64,64,64	0
48	MG	D1	3407	1/1	0.08	-3.09	70,70,70,70	0
48	MG	A1	3502	1/1	0.10	-3.11	80,80,80,80	0
48	MG	F1	3531	1/1	0.09	-3.13	95,95,95,95	0
48	MG	A1	3553	1/1	0.14	-3.13	108,108,108,108	0
48	MG	F1	3481	1/1	0.12	-3.13	45,45,45,45	0
48	MG	A1	3447	1/1	0.12	-3.16	58,58,58,58	0
48	MG	F1	3454	1/1	0.14	-3.18	56,56,56,56	0
48	MG	D1	3457	1/1	0.10	-3.19	34,34,34,34	0
48	MG	D1	3526	1/1	0.05	-3.20	54,54,54,54	0
48	MG	D1	3616	1/1	0.14	-3.21	150,150,150,150	0
49	ZN	HK	201	1/1	0.10	-3.22	70,70,70,70	0
48	MG	A1	3503	1/1	0.14	-3.25	95,95,95,95	0
48	MG	A1	3456	1/1	0.12	-3.27	49,49,49,49	0
48	MG	H1	3522	1/1	0.16	-3.32	107,107,107,107	0
48	MG	D1	3410	1/1	0.14	-3.32	39,39,39,39	0
48	MG	F1	3495	1/1	0.13	-3.32	83,83,83,83	0
48	MG	D1	3473	1/1	0.11	-3.33	63,63,63,63	0
48	MG	D1	3578	1/1	0.06	-3.34	88,88,88,88	0
48	MG	H1	3452	1/1	0.13	-3.34	108,108,108,108	0
48	MG	A1	3477	1/1	0.12	-3.35	62,62,62,62	0
48	MG	D1	3476	1/1	0.08	-3.35	43,43,43,43	0
48	MG	D1	3455	1/1	0.09	-3.37	80,80,80,80	0
48	MG	B2	203	1/1	0.07	-3.37	81,81,81,81	0
48	MG	B2	205	1/1	0.08	-3.38	81,81,81,81	0
48	MG	DA	101	1/1	0.07	-3.39	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3412	1/1	0.11	-3.41	60,60,60,60	0
48	MG	A1	3514	1/1	0.12	-3.44	59,59,59,59	0
48	MG	D1	3574	1/1	0.12	-3.45	80,80,80,80	0
48	MG	D1	3420	1/1	0.07	-3.46	105,105,105,105	0
48	MG	A1	3489	1/1	0.07	-3.54	33,33,33,33	0
48	MG	F1	3450	1/1	0.09	-3.54	59,59,59,59	0
48	MG	A1	3442	1/1	0.10	-3.55	52,52,52,52	0
48	MG	E3	201	1/1	0.10	-3.55	90,90,90,90	0
48	MG	D1	3575	1/1	0.13	-3.56	124,124,124,124	0
48	MG	D1	3419	1/1	0.10	-3.57	92,92,92,92	0
48	MG	A1	3460	1/1	0.12	-3.60	61,61,61,61	0
48	MG	F1	3526	1/1	0.13	-3.61	72,72,72,72	0
48	MG	A1	3403	1/1	0.12	-3.62	96,96,96,96	0
48	MG	D1	3460	1/1	0.09	-3.67	85,85,85,85	0
48	MG	A1	3539	1/1	0.07	-3.69	46,46,46,46	0
48	MG	D1	3631	1/1	0.08	-3.70	78,78,78,78	0
48	MG	D1	3501	1/1	0.14	-3.70	51,51,51,51	0
48	MG	D1	3533	1/1	0.07	-3.71	41,41,41,41	0
48	MG	D1	3508	1/1	0.06	-3.72	86,86,86,86	0
48	MG	F1	3410	1/1	0.16	-3.75	42,42,42,42	0
48	MG	F1	3568	1/1	0.12	-3.75	98,98,98,98	0
48	MG	H1	3401	1/1	0.10	-3.76	146,146,146,146	0
48	MG	A1	3526	1/1	0.10	-3.76	48,48,48,48	0
48	MG	A1	3425	1/1	0.12	-3.77	107,107,107,107	0
48	MG	A1	3418	1/1	0.09	-3.77	117,117,117,117	0
48	MG	F1	3519	1/1	0.16	-3.78	65,65,65,65	0
48	MG	A1	3508	1/1	0.07	-3.79	89,89,89,89	0
48	MG	A1	3431	1/1	0.12	-3.79	90,90,90,90	0
48	MG	A1	3521	1/1	0.12	-3.82	105,105,105,105	0
48	MG	F1	3520	1/1	0.17	-3.84	85,85,85,85	0
48	MG	D1	3403	1/1	0.07	-3.85	89,89,89,89	0
48	MG	A1	3465	1/1	0.08	-3.86	54,54,54,54	0
48	MG	D1	3456	1/1	0.10	-3.87	70,70,70,70	0
48	MG	H1	3513	1/1	0.10	-3.87	87,87,87,87	0
48	MG	C2	203	1/1	0.06	-3.87	63,63,63,63	0
48	MG	H1	3444	1/1	0.06	-3.89	65,65,65,65	0
48	MG	A1	3509	1/1	0.08	-3.90	128,128,128,128	0
48	MG	D1	3632	1/1	0.11	-3.92	83,83,83,83	0
48	MG	H1	3454	1/1	0.11	-3.92	111,111,111,111	0
48	MG	D1	3519	1/1	0.07	-3.97	72,72,72,72	0
48	MG	D1	3459	1/1	0.07	-3.99	63,63,63,63	0
48	MG	A1	3540	1/1	0.15	-4.00	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3480	1/1	0.12	-4.00	81,81,81,81	0
48	MG	C2	204	1/1	0.11	-4.01	75,75,75,75	0
48	MG	C3	204	1/1	0.12	-4.02	85,85,85,85	0
48	MG	A1	3574	1/1	0.13	-4.05	119,119,119,119	0
48	MG	A1	3462	1/1	0.12	-4.05	46,46,46,46	0
48	MG	F1	3406	1/1	0.10	-4.05	83,83,83,83	0
48	MG	F1	3584	1/1	0.13	-4.09	97,97,97,97	0
48	MG	H1	3417	1/1	0.10	-4.18	114,114,114,114	0
48	MG	F1	3458	1/1	0.09	-4.19	95,95,95,95	0
48	MG	F1	3423	1/1	0.08	-4.22	56,56,56,56	0
48	MG	D1	3483	1/1	0.08	-4.23	88,88,88,88	0
48	MG	A1	3543	1/1	0.07	-4.31	96,96,96,96	0
48	MG	H1	3428	1/1	0.12	-4.36	77,77,77,77	0
48	MG	H1	3502	1/1	0.06	-4.37	82,82,82,82	0
48	MG	D1	3627	1/1	0.07	-4.37	119,119,119,119	0
48	MG	F1	3521	1/1	0.08	-4.38	65,65,65,65	0
48	MG	F1	3432	1/1	0.06	-4.44	68,68,68,68	0
48	MG	C3	203	1/1	0.10	-4.46	69,69,69,69	0
48	MG	H1	3406	1/1	0.15	-4.47	143,143,143,143	0
48	MG	A1	3506	1/1	0.11	-4.48	77,77,77,77	0
48	MG	H1	3437	1/1	0.11	-4.50	93,93,93,93	0
48	MG	A1	3498	1/1	0.14	-4.53	116,116,116,116	0
48	MG	D1	3542	1/1	0.12	-4.55	71,71,71,71	0
48	MG	D1	3453	1/1	0.10	-4.56	54,54,54,54	0
48	MG	A1	3406	1/1	0.09	-4.61	75,75,75,75	0
48	MG	D1	3478	1/1	0.12	-4.61	81,81,81,81	0
48	MG	E2	204	1/1	0.08	-4.64	75,75,75,75	0
48	MG	D1	3461	1/1	0.10	-4.64	86,86,86,86	0
48	MG	H1	3451	1/1	0.12	-4.68	78,78,78,78	0
48	MG	H1	3475	1/1	0.10	-4.73	70,70,70,70	0
48	MG	F1	3440	1/1	0.12	-4.79	82,82,82,82	0
48	MG	F1	3553	1/1	0.09	-4.80	68,68,68,68	0
48	MG	A1	3482	1/1	0.06	-4.80	62,62,62,62	0
48	MG	H1	3485	1/1	0.12	-4.87	104,104,104,104	0
48	MG	F1	3402	1/1	0.09	-4.90	83,83,83,83	0
48	MG	F1	3443	1/1	0.09	-4.96	104,104,104,104	0
48	MG	H1	3495	1/1	0.06	-5.07	65,65,65,65	0
48	MG	A1	3458	1/1	0.09	-5.09	59,59,59,59	0
48	MG	D1	3411	1/1	0.11	-5.09	44,44,44,44	0
48	MG	D1	3558	1/1	0.07	-5.12	56,56,56,56	0
48	MG	F1	3456	1/1	0.07	-5.13	62,62,62,62	0
48	MG	D1	3435	1/1	0.13	-5.17	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	F1	3436	1/1	0.10	-5.25	70,70,70,70	0
48	MG	H1	3404	1/1	0.11	-5.25	132,132,132,132	0
48	MG	D1	3556	1/1	0.07	-5.26	76,76,76,76	0
48	MG	F1	3489	1/1	0.09	-5.29	85,85,85,85	0
48	MG	F1	3546	1/1	0.09	-5.32	59,59,59,59	0
48	MG	F1	3474	1/1	0.12	-5.34	64,64,64,64	0
48	MG	A1	3463	1/1	0.11	-5.40	59,59,59,59	0
48	MG	F1	3405	1/1	0.12	-5.42	79,79,79,79	0
48	MG	A1	3589	1/1	0.10	-5.46	113,113,113,113	0
48	MG	H1	3466	1/1	0.08	-5.55	107,107,107,107	0
48	MG	D1	3549	1/1	0.12	-5.57	99,99,99,99	0
48	MG	F1	3420	1/1	0.09	-5.57	88,88,88,88	0
48	MG	BW	201	1/1	0.11	-5.62	67,67,67,67	0
48	MG	B2	202	1/1	0.12	-5.65	103,103,103,103	0
48	MG	D1	3402	1/1	0.08	-5.72	52,52,52,52	0
48	MG	H1	3515	1/1	0.15	-5.86	73,73,73,73	0
48	MG	D1	3405	1/1	0.10	-5.86	59,59,59,59	0
48	MG	H1	3440	1/1	0.08	-5.87	73,73,73,73	0
48	MG	D1	3500	1/1	0.09	-5.89	44,44,44,44	0
48	MG	A1	3466	1/1	0.13	-5.90	40,40,40,40	0
48	MG	F1	3439	1/1	0.07	-5.96	62,62,62,62	0
48	MG	A1	3429	1/1	0.12	-5.98	122,122,122,122	0
48	MG	D1	3580	1/1	0.10	-6.07	95,95,95,95	0
48	MG	F1	3426	1/1	0.14	-6.07	110,110,110,110	0
48	MG	F1	3467	1/1	0.11	-6.11	57,57,57,57	0
48	MG	D1	3415	1/1	0.10	-6.13	117,117,117,117	0
48	MG	H1	3459	1/1	0.13	-6.17	97,97,97,97	0
48	MG	A1	3455	1/1	0.14	-6.17	111,111,111,111	0
48	MG	F1	3523	1/1	0.10	-6.20	55,55,55,55	0
48	MG	D1	3480	1/1	0.10	-6.22	32,32,32,32	0
48	MG	F1	3528	1/1	0.07	-6.26	75,75,75,75	0
48	MG	D1	3529	1/1	0.09	-6.28	80,80,80,80	0
48	MG	F1	3557	1/1	0.13	-6.38	84,84,84,84	0
48	MG	H1	3506	1/1	0.14	-6.43	75,75,75,75	0
48	MG	F1	3404	1/1	0.11	-6.45	75,75,75,75	0
48	MG	H1	3498	1/1	0.07	-6.52	60,60,60,60	0
48	MG	A1	3486	1/1	0.14	-6.55	93,93,93,93	0
48	MG	A1	3478	1/1	0.09	-6.69	79,79,79,79	0
48	MG	A1	3473	1/1	0.08	-6.69	55,55,55,55	0
48	MG	A1	3433	1/1	0.11	-6.70	84,84,84,84	0
48	MG	D1	3489	1/1	0.07	-6.76	44,44,44,44	0
48	MG	D1	3563	1/1	0.11	-6.78	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3499	1/1	0.10	-6.79	75,75,75,75	0
48	MG	A1	3534	1/1	0.14	-6.80	62,62,62,62	0
48	MG	D1	3628	1/1	0.07	-6.90	107,107,107,107	0
48	MG	D1	3454	1/1	0.12	-6.92	64,64,64,64	0
48	MG	BL	301	1/1	0.09	-7.42	71,71,71,71	0
48	MG	H1	3432	1/1	0.09	-7.45	91,91,91,91	0
48	MG	D1	3487	1/1	0.09	-7.48	65,65,65,65	0
48	MG	D1	3509	1/1	0.08	-7.59	41,41,41,41	0
48	MG	D1	3591	1/1	0.09	-7.73	55,55,55,55	0
48	MG	F1	3525	1/1	0.08	-7.88	73,73,73,73	0
48	MG	F1	3559	1/1	0.09	-8.04	133,133,133,133	0
48	MG	A1	3448	1/1	0.12	-8.08	78,78,78,78	0
48	MG	D1	3495	1/1	0.07	-8.13	88,88,88,88	0
48	MG	F1	3478	1/1	0.08	-8.19	73,73,73,73	0
48	MG	F1	3441	1/1	0.15	-8.35	111,111,111,111	0
48	MG	H1	3458	1/1	0.06	-8.41	90,90,90,90	0
48	MG	D1	3502	1/1	0.06	-8.42	38,38,38,38	0
48	MG	A1	3577	1/1	0.15	-8.45	104,104,104,104	0
48	MG	F1	3547	1/1	0.09	-8.61	112,112,112,112	0
48	MG	D1	3472	1/1	0.09	-8.80	82,82,82,82	0
48	MG	D1	3531	1/1	0.07	-8.96	87,87,87,87	0
48	MG	D1	3619	1/1	0.05	-9.00	101,101,101,101	0
48	MG	D1	3584	1/1	0.10	-9.02	101,101,101,101	0
48	MG	D1	3524	1/1	0.06	-9.16	69,69,69,69	0
48	MG	D1	3428	1/1	0.06	-9.42	106,106,106,106	0
48	MG	A1	3405	1/1	0.08	-9.57	65,65,65,65	0
48	MG	F1	3512	1/1	0.12	-9.62	94,94,94,94	0
48	MG	A1	3550	1/1	0.05	-9.82	69,69,69,69	0
48	MG	F1	3470	1/1	0.08	-9.90	49,49,49,49	0
48	MG	A1	3464	1/1	0.07	-10.02	64,64,64,64	0
48	MG	D1	3458	1/1	0.06	-10.06	51,51,51,51	0
48	MG	D1	3465	1/1	0.07	-10.10	65,65,65,65	0
48	MG	D1	3566	1/1	0.10	-10.14	80,80,80,80	0
48	MG	D1	3450	1/1	0.07	-10.32	49,49,49,49	0
48	MG	D1	3468	1/1	0.11	-10.62	75,75,75,75	0
48	MG	D1	3629	1/1	0.09	-10.63	121,121,121,121	0
48	MG	H1	3505	1/1	0.08	-10.67	95,95,95,95	0
48	MG	F1	3435	1/1	0.09	-10.69	44,44,44,44	0
48	MG	D1	3559	1/1	0.08	-11.09	55,55,55,55	0
48	MG	F1	3419	1/1	0.13	-11.13	124,124,124,124	0
48	MG	H1	3435	1/1	0.14	-11.53	116,116,116,116	0
48	MG	D1	3532	1/1	0.13	-11.58	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	H1	3415	1/1	0.15	-11.72	133,133,133,133	0
48	MG	F1	3505	1/1	0.10	-12.08	83,83,83,83	0
48	MG	A1	3476	1/1	0.07	-12.16	59,59,59,59	0
48	MG	D1	3582	1/1	0.16	-13.00	93,93,93,93	0
48	MG	F1	3504	1/1	0.11	-14.20	84,84,84,84	0
48	MG	H1	3429	1/1	0.13	-14.23	87,87,87,87	0
48	MG	A1	3559	1/1	0.08	-14.50	89,89,89,89	0
48	MG	D1	3430	1/1	0.07	-14.78	59,59,59,59	0
48	MG	D1	3479	1/1	0.04	-15.49	50,50,50,50	0
48	MG	H1	3453	1/1	0.10	-17.88	66,66,66,66	0
48	MG	A1	3538	1/1	0.08	-18.00	49,49,49,49	0
48	MG	F1	3403	1/1	0.08	-18.21	96,96,96,96	0
48	MG	F1	3455	1/1	0.11	-18.33	65,65,65,65	0
48	MG	A1	3469	1/1	0.09	-22.14	113,113,113,113	0
48	MG	D1	3585	1/1	0.09	-27.80	108,108,108,108	0
48	MG	D1	3536	1/1	0.09	-29.53	73,73,73,73	0
48	MG	A1	3535	1/1	0.09	-30.30	99,99,99,99	0
48	MG	A1	3570	1/1	0.08	-32.60	70,70,70,70	0
48	MG	A1	3454	1/1	0.15	-33.00	101,101,101,101	0
48	MG	H1	3552	1/1	0.22	-35.80	131,131,131,131	0
48	MG	D1	3474	1/1	0.10	-39.67	58,58,58,58	0
48	MG	D1	3630	1/1	0.11	-53.00	71,71,71,71	0
48	MG	F1	3449	1/1	0.11	-71.00	90,90,90,90	0
48	MG	A1	3587	1/1	0.84	-	182,182,182,182	0
48	MG	H1	3543	1/1	0.47	-	183,183,183,183	0
48	MG	A1	3580	1/1	0.21	-	130,130,130,130	0
48	MG	F1	3509	1/1	0.27	-	144,144,144,144	0
48	MG	H1	3555	1/1	0.21	-	123,123,123,123	0
48	MG	F1	3515	1/1	0.36	-	143,143,143,143	0
48	MG	F1	3554	1/1	0.18	-	131,131,131,131	0
48	MG	F1	3415	1/1	0.30	-	118,118,118,118	0
48	MG	A1	3593	1/1	0.75	-	158,158,158,158	0
48	MG	D1	3538	1/1	0.10	-	119,119,119,119	0
48	MG	F1	3539	1/1	1.08	-	187,187,187,187	0
48	MG	F1	3575	1/1	0.29	-	130,130,130,130	0
48	MG	A1	3416	1/1	0.23	-	140,140,140,140	0
48	MG	H1	3416	1/1	0.65	-	113,113,113,113	0
48	MG	H1	3544	1/1	0.94	-	146,146,146,146	0
48	MG	H1	3479	1/1	0.44	-	132,132,132,132	0
48	MG	A1	3519	1/1	0.11	-	113,113,113,113	0
48	MG	D1	3548	1/1	0.96	-	183,183,183,183	0
48	MG	D1	3625	1/1	0.33	-	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
48	MG	D1	3596	1/1	0.53	-	165,165,165,165	0
48	MG	D1	3463	1/1	1.15	-	176,176,176,176	0
48	MG	C3	207	1/1	0.64	-	160,160,160,160	0
48	MG	A1	3598	1/1	0.24	-	111,111,111,111	0
48	MG	C3	201	1/1	0.36	-	123,123,123,123	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.