



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 01:36 PM EDT

PDB ID : 6NWY  
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (near-cognate)  
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2019-02-07  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

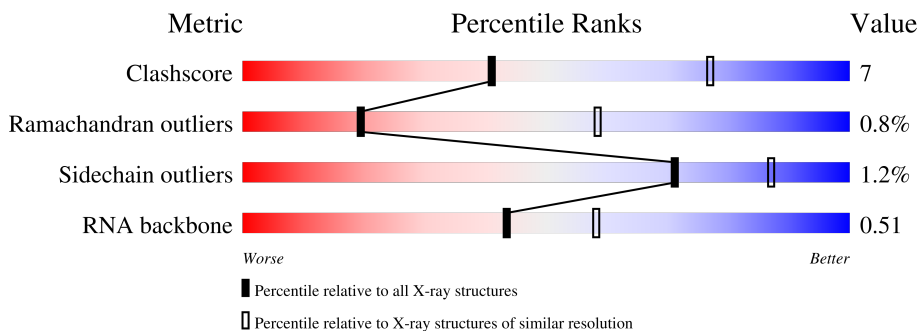
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	
1	XA	1521	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	QD	209	76% 22%
4	XD	209	70% 27%
5	QE	162	75% 18% 7%
5	XE	162	72% 21% 7%
6	QF	101	84% 16%
6	XF	101	82% 18%
7	QG	156	81% 18%
7	XG	156	79% 20%
8	QH	138	80% 20%
8	XH	138	78% 22%
9	QI	128	75% 23%
9	XI	128	77% 20%
10	QJ	105	63% 31% 6%
10	XJ	105	75% 16% 9%
11	QK	129	83% 9% 8%
11	XK	129	78% 12% 10%
12	QL	132	72% 21% 5%
12	XL	132	73% 17% 8%
13	QM	126	68% 27% 5%
13	XM	126	66% 24% 10%
14	QN	61	70% 25%
14	XN	61	62% 31% 5%
15	QO	89	89% 10%
15	XO	89	83% 15%
16	QP	88	74% 22% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	XP	88	76% 19% 5%
17	QQ	105	83% 12% 5%
17	XQ	105	76% 19% 5%
18	QR	88	70% 9% 20%
18	XR	88	67% 13% 20%
19	QS	93	73% 15% 11%
19	XS	93	68% 23% 10%
20	QT	106	70% 22% 7%
20	XT	106	69% 21% 7%
21	QU	27	59% 33% 7%
21	XU	27	74% 19% 7%
22	QV	77	52% 36% 10%
22	XV	77	51% 40% 8%
23	QX	19	32% 42% 16%
23	XX	19	42% 47% 11%
24	R0	85	85% 11% 5%
24	Y0	85	80% 16% 4%
25	R1	98	80% 17% 3%
25	Y1	98	83% 12% 5%
26	R2	72	82% 14% 4%
26	Y2	72	82% 12% 6%
27	R3	60	85% 13% 2%
27	Y3	60	77% 22% 1%
28	R4	71	52% 11% 37%
28	Y4	71	39% 21% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	R5	60	68% 25% 5% .
29	Y5	60	67% 27% . . . .
30	R6	54	72% 22% . . . .
30	Y6	54	65% 26% 6% . .
31	R7	49	67% 29% .
31	Y7	49	86% 12% .
32	R8	65	69% 23% 6% .
32	Y8	65	72% 26% .
33	R9	37	70% 24% 5%
33	Y9	37	68% 27% 5%
34	RA	2915	53% 36% 9% . .
34	YA	2915	53% 35% 10% . .
35	RB	122	57% 37% . . . .
35	YB	122	53% 36% 7% . .
36	RD	276	76% 21% . .
36	YD	276	80% 18% . .
37	RE	206	72% 25% .
37	YE	206	75% 24%
38	RF	210	75% 20% . .
38	YF	210	73% 23% .
39	RG	182	76% 23% . .
39	YG	182	78% 21% .
40	RH	180	64% 27% 6% .
40	YH	180	77% 18% . . . .
41	RI	148	72% 23% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
41	YI	148	68%	30% ..
42	RN	140	82%	16% ..
42	YN	140	79%	20% .
43	RO	122	75%	25%
43	YO	122	84%	16%
44	RP	150	77%	21% .
44	YP	150	75%	23% .
45	RQ	141	75%	25%
45	YQ	141	74%	26% .
46	RR	118	69%	28% ..
46	YR	118	75%	24% .
47	RS	112	75%	24% .
47	YS	112	79%	18% ...
48	RT	146	75%	19% 6%
48	YT	146	66%	27% 6%
49	RU	118	77%	19% ..
49	YU	118	79%	19% ..
50	RV	101	78%	22%
50	YV	101	79%	21%
51	RW	113	79%	21%
51	YW	113	81%	19%
52	RX	96	80%	16% .
52	YX	96	76%	20% .
53	RY	110	72%	22% . .
53	YY	110	75%	22% . .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
54	RZ	206	
54	YZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	QD	301	-	-	X	-

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 292039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1511	Total 32469	C 14453	N 6011	O 10495	P 1510	0	0	0
1	XA	1515	Total 32551	C 14490	N 6022	O 10525	P 1514	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	235	Total 1907	C 1217	N 342	O 343	S 5	0	0	0
2	XB	236	Total 1915	C 1223	N 343	O 344	S 5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	XC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0
4	XD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	XI	126	Total	C	N	O	0	0	0
			998	633	193	172			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			
23	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
27	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
29	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
31	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	R8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0
32	Y8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	R9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0
33	Y9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	RA	2882	Total 62070	C 27627	N 11611	O 19951	P 2881	0	0	0
34	YA	2883	Total 62091	C 27636	N 11613	O 19960	P 2882	0	0	0

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	RB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0
35	YB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	RD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
36	YD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
38	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 39 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
39	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
41	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 42 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	YN	138	1104	712	206	182	4	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	RO	122	933	588	171	170	4	0	0	0
43	YO	122	933	588	171	170	4	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RP	150	1145	712	232	198	3	0	0	0
44	YP	147	1122	698	229	192	3	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	RQ	141	1122	715	212	188	7	0	0	0
45	YQ	141	1122	715	212	188	7	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
46	RR	117	960	599	202	159	0	0	0
46	YR	117	960	599	202	159	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
47	RS	111	882	556	176	150	0	0	0
47	YS	111	882	556	176	150	0	0	0



- Molecule 48 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	RT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0
48	YT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	RU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
49	YU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	RV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0
50	YV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	RW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0
51	YW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	RX	92	Total 725	C 471	N 131	O 123	0	0	0
52	YX	92	Total 725	C 471	N 131	O 123	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
53	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	193	Total	C	N	O	S	0	0	0
			1529	973	270	283	3			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	87	Total	Mg	0	0
			87	87		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	2	Total	Mg	0	0
			2	2		
55	QL	1	Total	Mg	0	0
			1	1		
55	R0	2	Total	Mg	0	0
			2	2		
55	R1	1	Total	Mg	0	0
			1	1		
55	R3	1	Total	Mg	0	0
			1	1		
55	R8	1	Total	Mg	0	0
			1	1		
55	RA	429	Total	Mg	0	0
			429	429		
55	RB	11	Total	Mg	0	0
			11	11		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	4	Total	Mg	0	0
			4	4		
55	RF	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	RO	1	Total Mg 1 1	0	0
55	RP	1	Total Mg 1 1	0	0
55	RQ	1	Total Mg 1 1	0	0
55	XA	89	Total Mg 89 89	0	0
55	XE	1	Total Mg 1 1	0	0
55	Y1	1	Total Mg 1 1	0	0
55	Y2	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	1	Total Mg 1 1	0	0
55	Y8	1	Total Mg 1 1	0	0
55	YA	439	Total Mg 439 439	0	0
55	YB	8	Total Mg 8 8	0	0
55	YD	1	Total Mg 1 1	0	0
55	YE	2	Total Mg 2 2	0	0
55	YF	1	Total Mg 1 1	0	0
55	YQ	1	Total Mg 1 1	0	0
55	YR	2	Total Mg 2 2	0	0
55	YU	1	Total Mg 1 1	0	0
55	YX	1	Total Mg 1 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QD	1	Total	Fe S	0	0
			8	4 4		
56	XD	1	Total	Fe S	0	0
			8	4 4		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

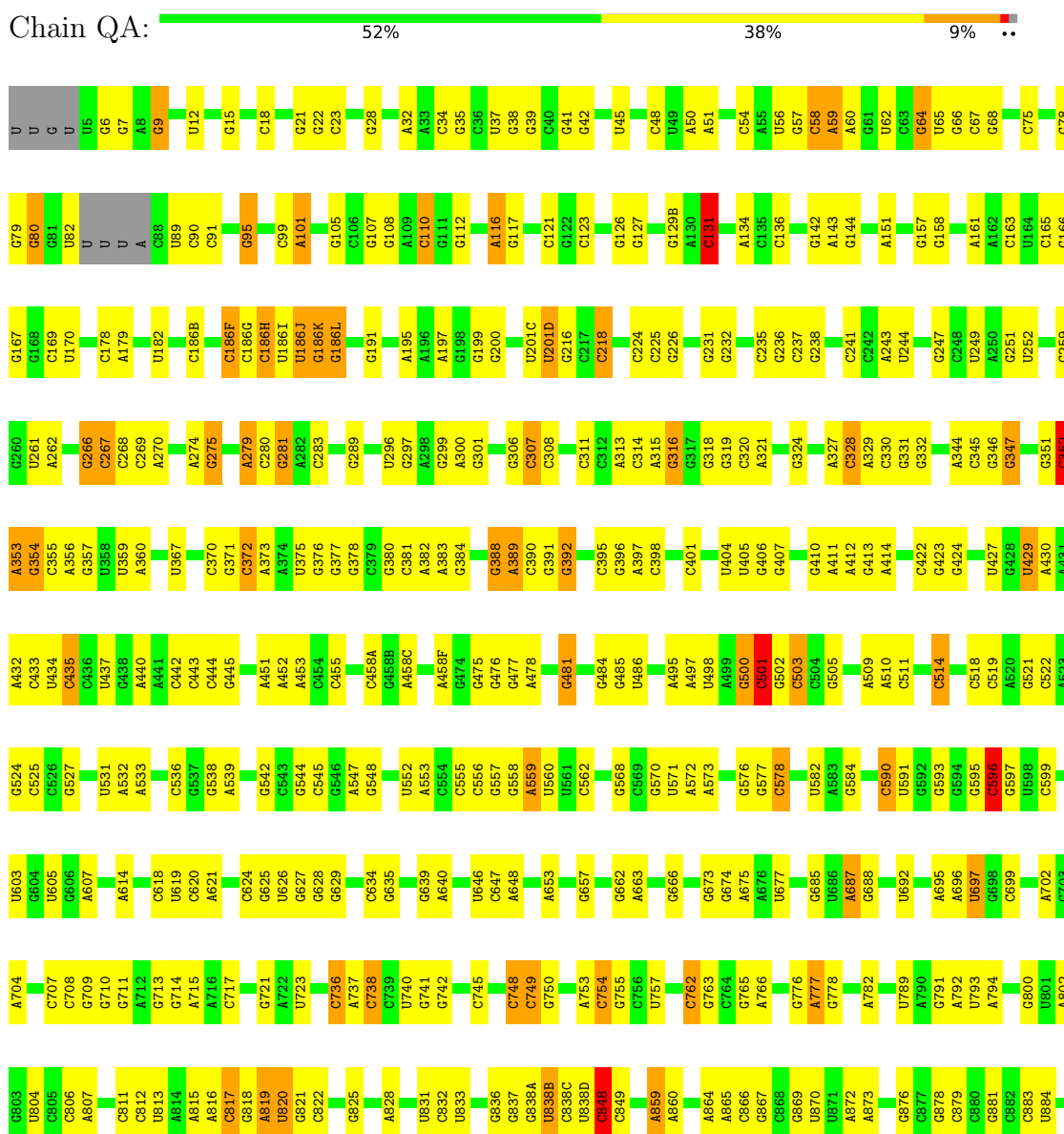
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	Y9	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		

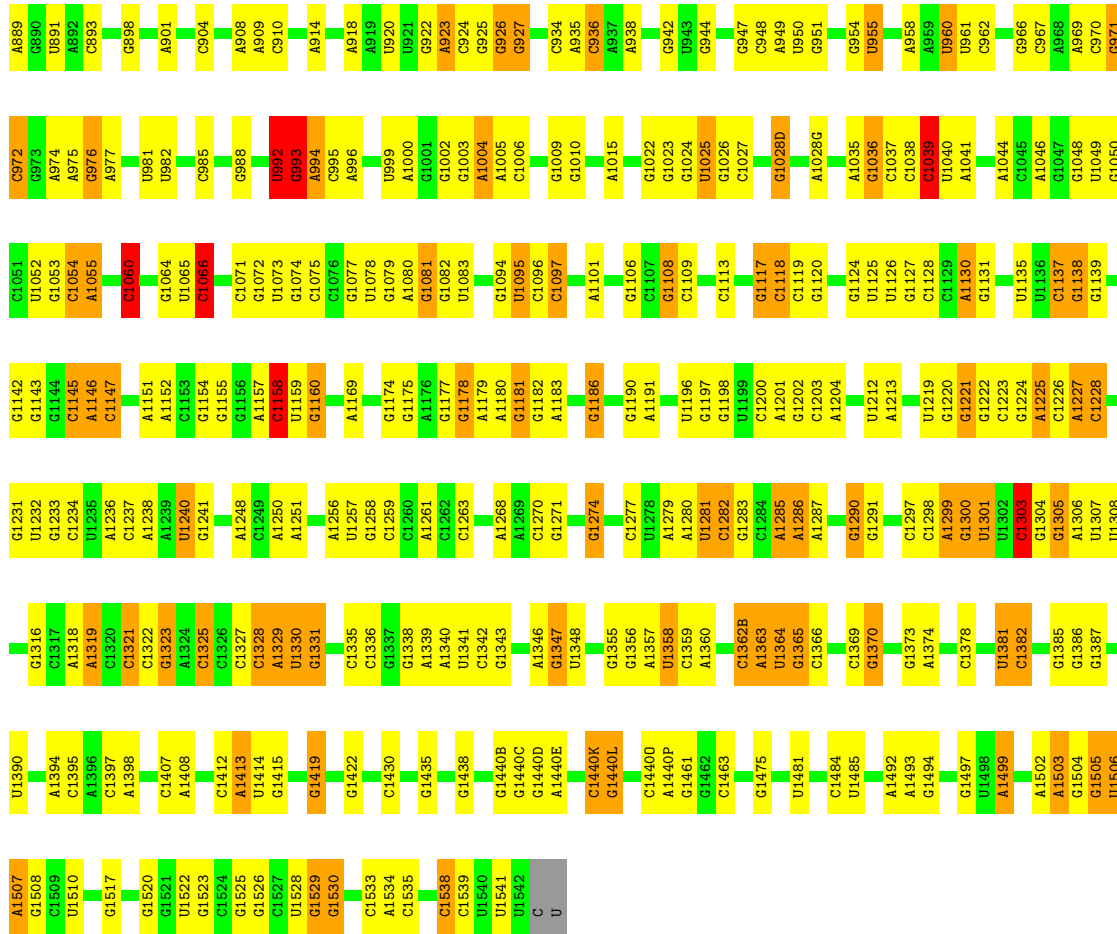
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

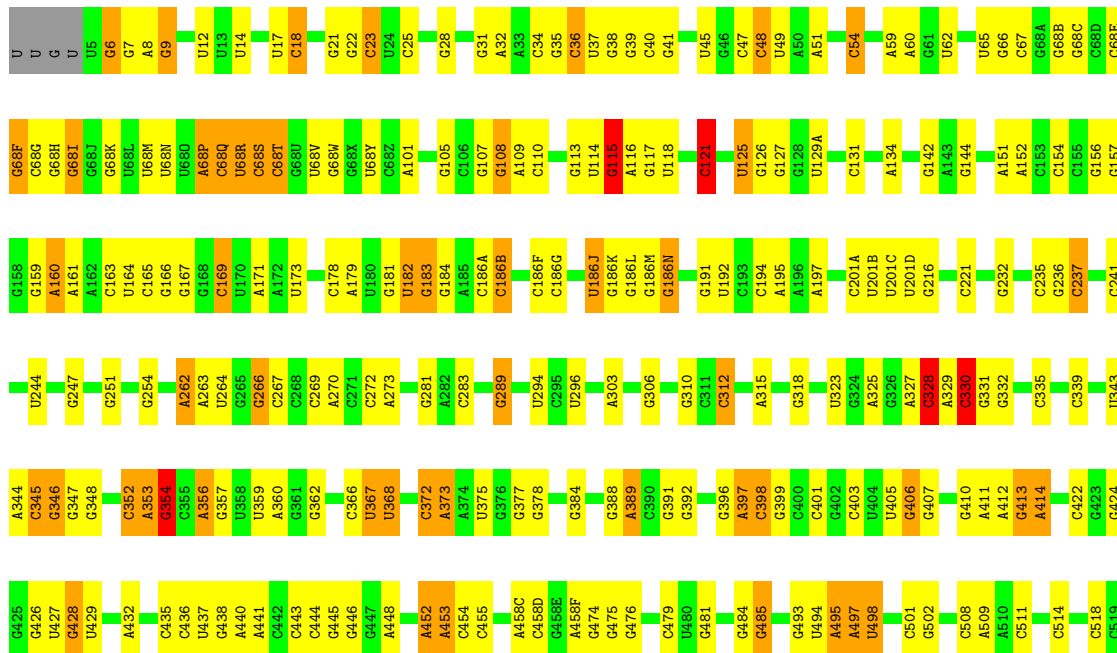
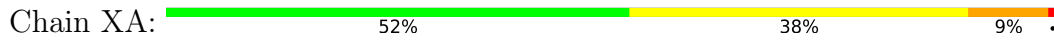
Note EDS failed to run properly.

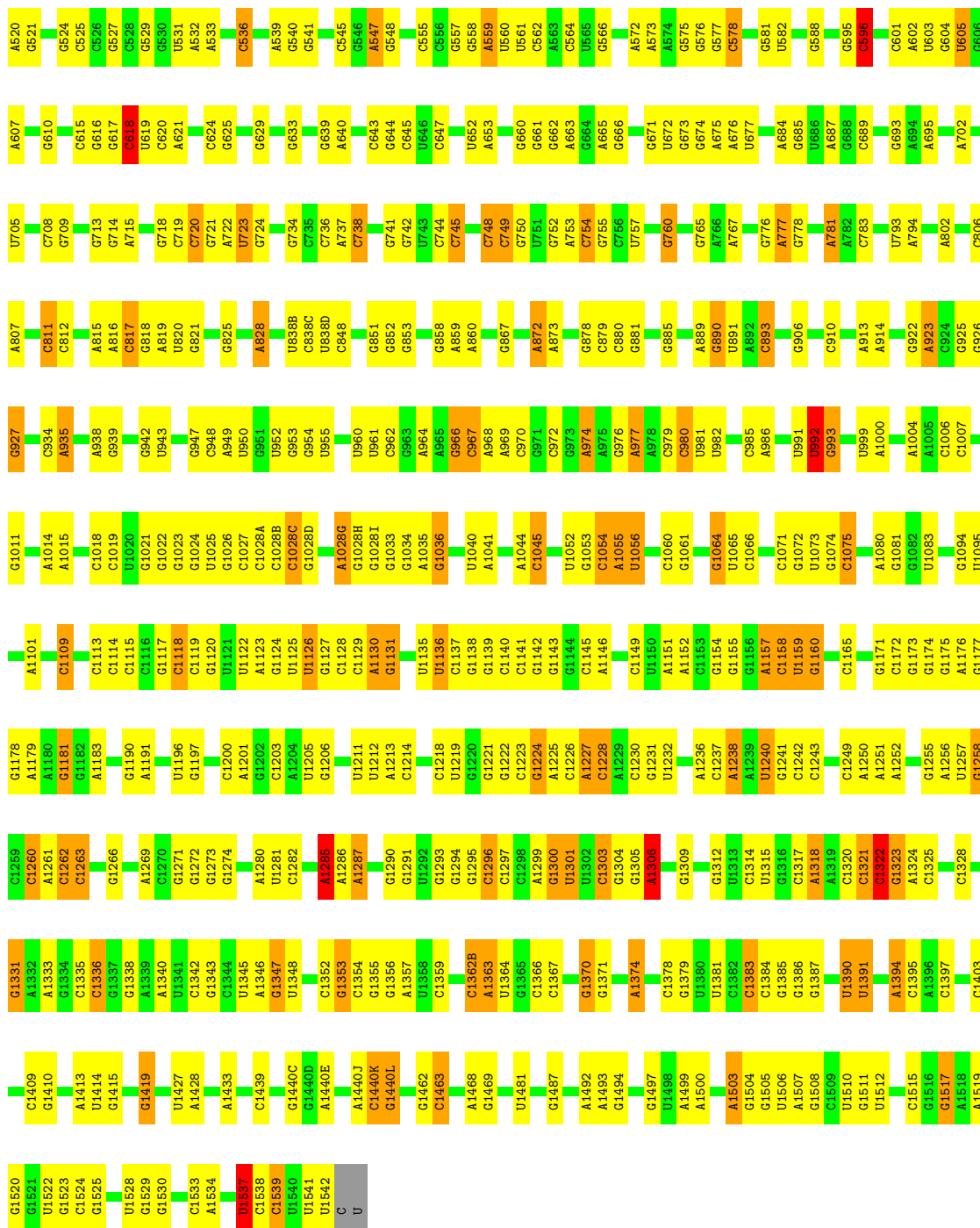
- Molecule 1: 16S rRNA



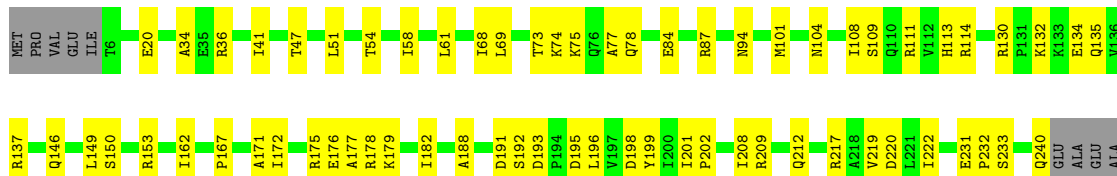


• Molecule 1: 16S rRNA





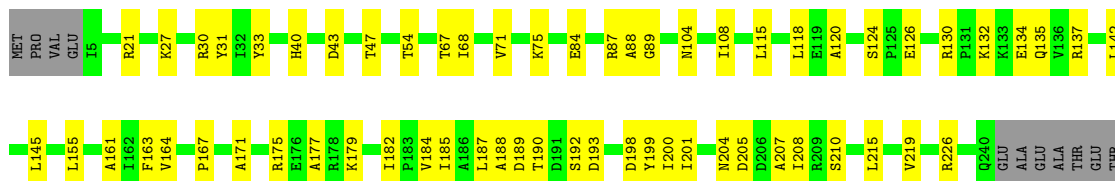
• Molecule 2: 30S ribosomal protein S2



THR  
GLU  
THR  
PRO  
GLU  
GLY  
GLU  
SER  
VAL  
GLU  
ALA

• Molecule 2: 30S ribosomal protein S2

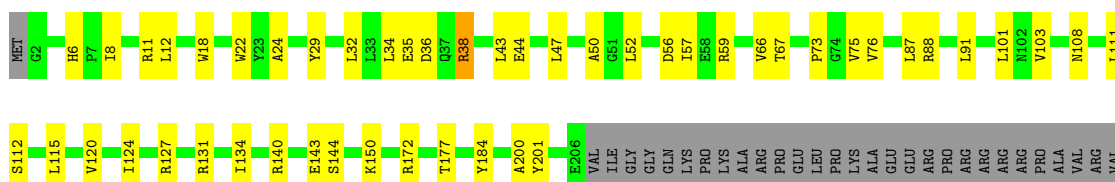
Chain XB:    68% 24% 8%



PRO  
GLU  
GLY  
GLU  
SER  
VAL  
GLU  
ALA

• Molecule 3: 30S ribosomal protein S3

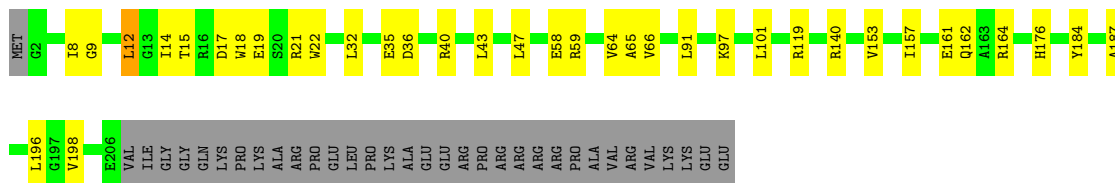
Chain QC:    65% 20% 14%



LYS  
LYS  
GLU  
GLU

• Molecule 3: 30S ribosomal protein S3

Chain XC:    71% 15% 14%



• Molecule 4: 30S ribosomal protein S4

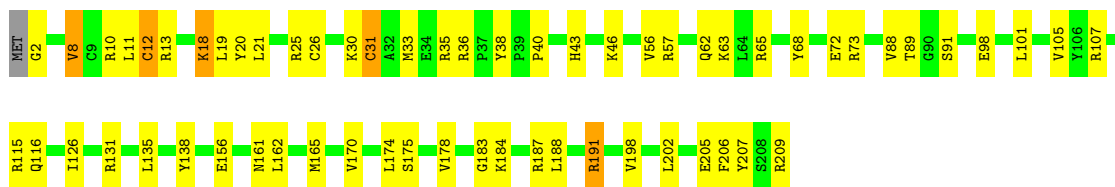
Chain QD:    76% 22% 2%




• Molecule 4: 30S ribosomal protein S4



Chain XD:  70% 27%



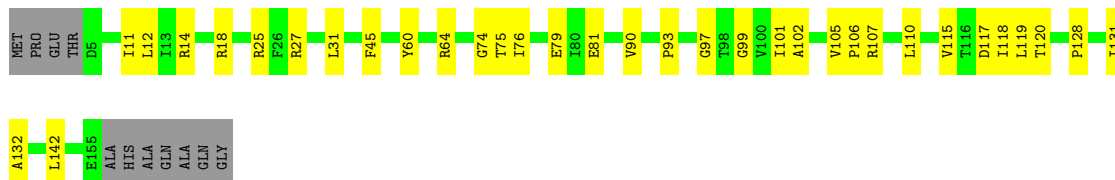
- Molecule 5: 30S ribosomal protein S5

Chain QE:  75% 18% 7%




- Molecule 5: 30S ribosomal protein S5

Chain XE:  72% 21% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  84% 16%




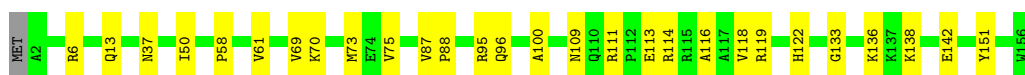
- Molecule 6: 30S ribosomal protein S6

Chain XF:  82% 18%

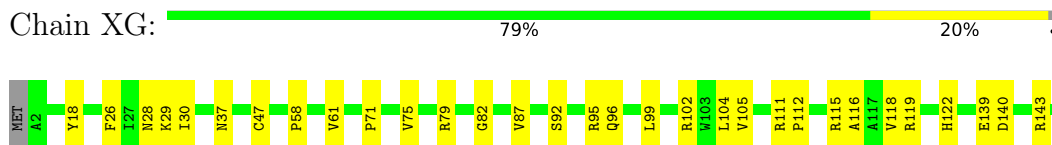


- Molecule 7: 30S ribosomal protein S7

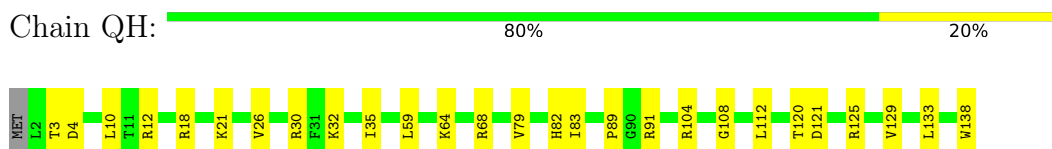
Chain QG:  81% 18%



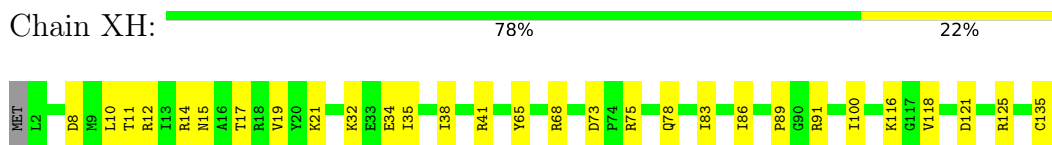
- Molecule 7: 30S ribosomal protein S7



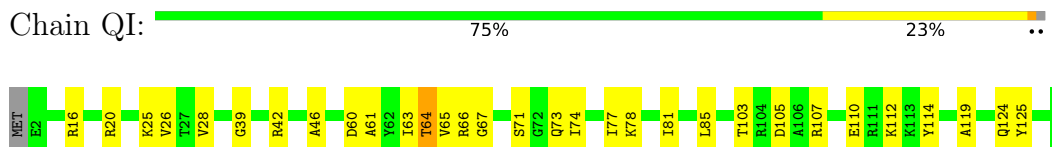
- Molecule 8: 30S ribosomal protein S8



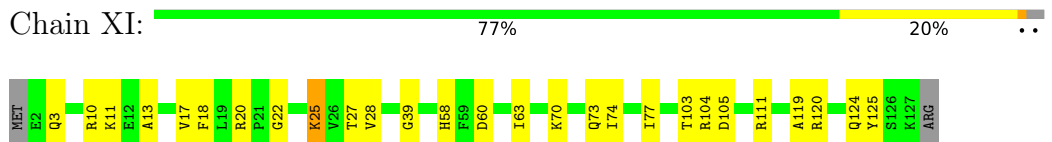
- Molecule 8: 30S ribosomal protein S8



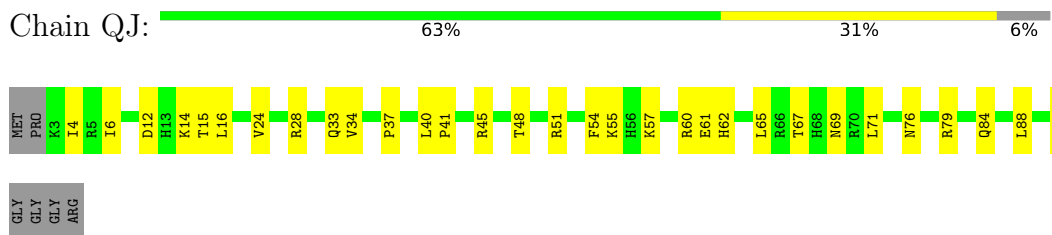
- Molecule 9: 30S ribosomal protein S9



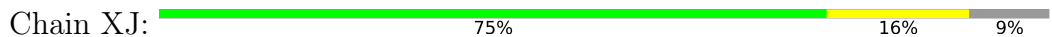
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

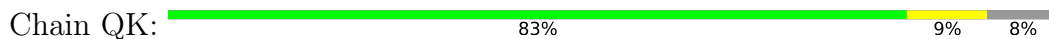


- Molecule 10: 30S ribosomal protein S10

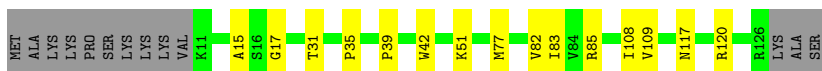
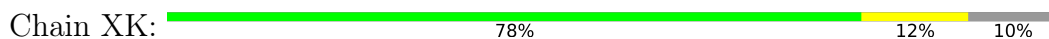




• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



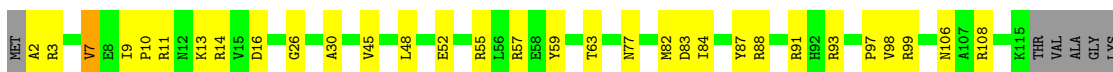
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



LYS  
LYS  
ALA  
PRD  
ARG  
LYS

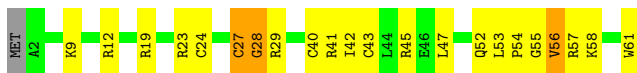
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  70% 25% 5%



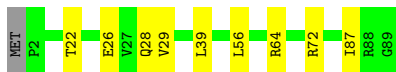
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  62% 31% 5%




- Molecule 15: 30S ribosomal protein S15

Chain QO:  89% 10% 1%



- Molecule 15: 30S ribosomal protein S15

Chain XO:  83% 15% 2%




- Molecule 16: 30S ribosomal protein S16

Chain QP:  74% 22% 5%




- Molecule 16: 30S ribosomal protein S16

Chain XP:  76% 19% 5%

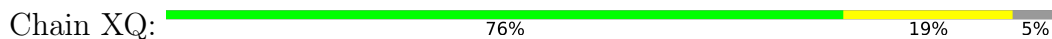


- Molecule 17: 30S ribosomal protein S17

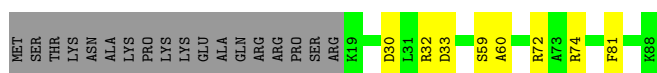
Chain QQ:  83% 12% 5%



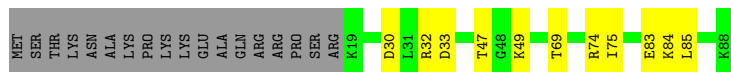
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

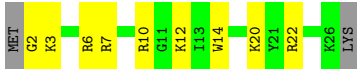


- Molecule 20: 30S ribosomal protein S20

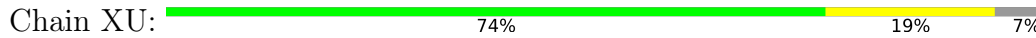




- Molecule 21: 30S ribosomal protein Thx



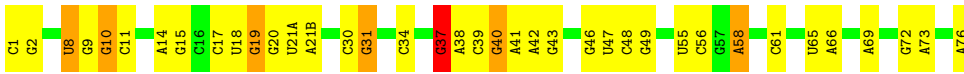
- Molecule 21: 30S ribosomal protein Thx



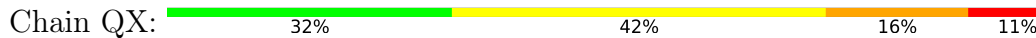
- Molecule 22: E-site tRNA-Pro



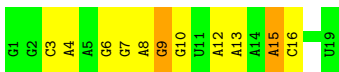
- Molecule 22: E-site tRNA-Pro



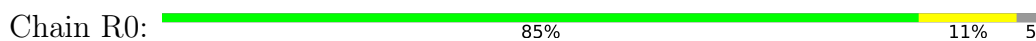
- Molecule 23: mRNA



- Molecule 23: mRNA

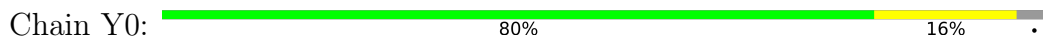


- Molecule 24: 50S ribosomal protein L27

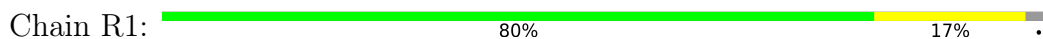




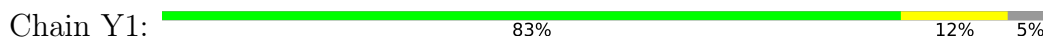
- Molecule 24: 50S ribosomal protein L27



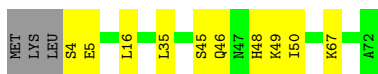
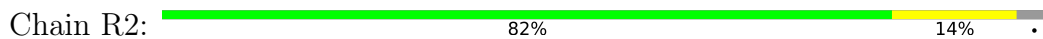
- Molecule 25: 50S ribosomal protein L28



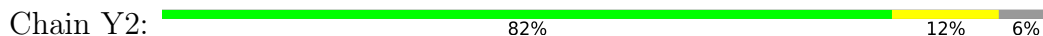
- Molecule 25: 50S ribosomal protein L28



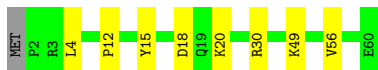
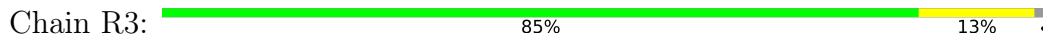
- Molecule 26: 50S ribosomal protein L29



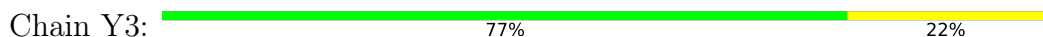
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

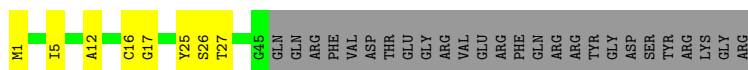


- Molecule 27: 50S ribosomal protein L30

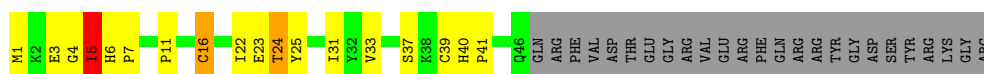




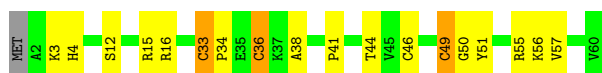
- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33



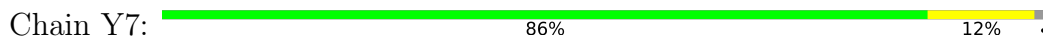
- Molecule 31: 50S ribosomal protein L34







- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



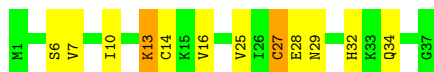
- Molecule 32: 50S ribosomal protein L35



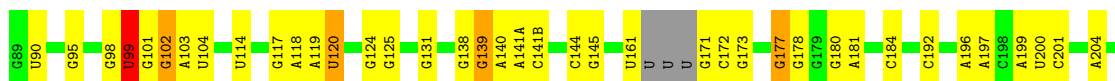
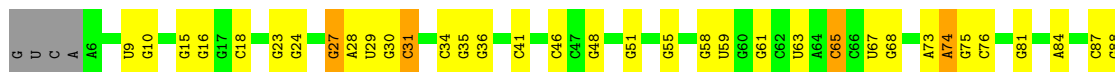
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36

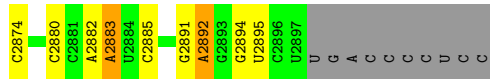


- Molecule 34: 23S rRNA

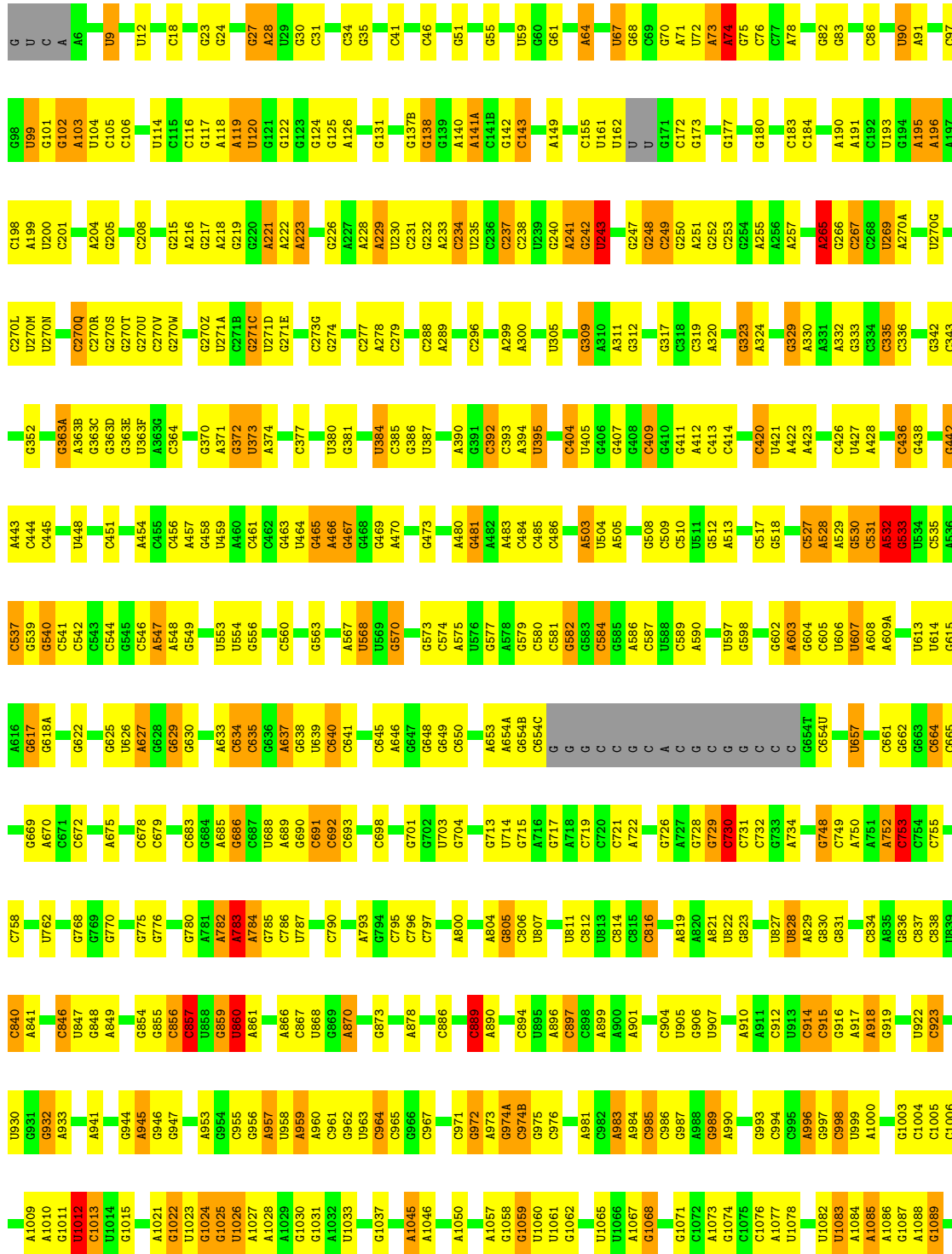


G1400	G1401	C1304	G1216	A1127	G977	G892	A800	G690	C641	G566	G481	C208
G1407	G1408	C1305	C1217	A1128	G978	C893	A805	C691	G642	U567	A482	C209
G1409	G1410	C1306	A1220	U1130	A980	U895	G806	C645	C646	A567	A483	G214
G1411	G1412	C1307	G1224	A1131	A981	A896	U807	G702	A646	U568	C484	G215
G1413	G1414	C1308	G1225	C1155	A982	C904	G808	G707	C650	A571	C487	A221
G1415	G1416	C1309	C1226	G1136	A984	U907	G809	G715	G651	A572	A278	A222
G1417	G1418	C1310	A1227	G1137	C985	A910	U810	A716	G652	C574	G494	A223
G1419	G1420	C1311	G1230	G1138	C986	A911	U811	G717	A653	A575	G495	A228
G1421	G1422	C1312	C1231	U1140	C987	A912	C812	G721	A654A	U576	A501	A229
G1423	G1424	C1313	G1232	U1141	A990	C911	C815	A722	G654B	G577	A502	U230
G1425	G1426	C1314	U1142A	U1066	C991	U913	G816	G723	G	A578	A503	C231
G1427	G1428	C1315	A1143	U1067	C994	C914	C817	G724	G	C581	A504	C232
G1429	G1430	C1316	A1144	A1068	C995	G916	G818	U725	G	C582	A505	A233
G1431	G1432	C1317	G1144	A1069	A996	A917	A819	G726	C	G582	G508	C234
G1433	G1434	C1318	C1147	A1070	C997	A918	A820	G729	C	G585	C509	G240
G1435	G1436	C1319	A1148	G1071	C998	A919	C825	C730	C	A586	C510	A241
G1437	G1438	C1320	U1149	C1072	U999	U922	U826	U747	A	U588	U511	U243
G1439	G1440	C1321	G1074	A1073	A1000	C923	U827	C748	C	G603	G512	G247
G1441	G1442	C1322	C1075	C1075	C924	C924	U828	G749	C	G604	G513	G248
G1443	G1444	C1323	A1076	A1076	C925	C925	U829	C758	C	G605	A514	C249
G1445	G1446	C1324	A1077	A1077	A926	A926	G830	C759	C	U607	A515	G257
G1447	G1448	C1325	U1078	G1003	G932	G932	C834	A752	C	U607	A516	G258
G1449	G1450	C1326	U1079	G1005	A933	A933	A835	C753	C	G603	C517	G259
G1451	G1452	C1327	U1080	C1008	A934	A934	U836	C754	C	G604	G521	A265
G1453	G1454	C1328	U1081	G1011	G939	G939	U837	C755	C	G604	G522	C266
G1455	G1456	C1329	U1082	U1012	G940	G940	U838	C756	C	G605	U525	C267
G1457	G1458	C1330	U1083	U1013	A941	A941	U839	C757	C	U607	U526	C268
G1459	G1460	C1331	U1084	U1014	G942	G942	C840	C758	C	U607	A527	U269
G1461	G1462	C1332	U1085	U1015	A943	A943	U841	C759	C	U607	A528	A270A
G1463	G1464	C1333	U1086	U1016	A944	A944	U842	G776	C	U607	A529	G270F
G1465	G1466	C1334	U1087	U1017	A945	A945	U843	G780	C	U607	A530	C270L
G1467	G1468	C1335	U1088	U1018	A946	A946	U844	A781	C	U607	A531	U270M
G1469	G1470	C1336	U1089	U1019	A947	A947	U845	A782	C	U607	A532	U270N
G1471	G1472	C1337	U1090	U1020	A948	A948	U846	A783	C	U607	A533	G270O
G1473	G1474	C1338	U1091	U1021	A949	A949	U847	A784	C	U607	A534	G270P
G1475	G1476	C1339	U1092	U1022	A950	A950	U848	A785	C	U607	A535	C270Q
G1477	G1478	C1340	U1093	U1023	A951	A951	U849	C786	C	U607	A536	C270R
G1479	G1480	C1341	U1094	U1024	A952	A952	U850	U787	C	U607	A537	G270S
G1481	G1482	C1342	U1095	U1025	A953	A953	U851	C664	C	U607	A538	G270T
G1483	G1484	C1343	U1096	U1026	A954	A954	U852	C665	C	U607	A539	G270U
G1485	G1486	C1344	U1097	U1027	A955	A955	U853	U667	C	U607	A540	C270V
G1487	G1488	C1345	U1098	U1028	A956	A956	U854	C668	C	U607	A541	G270W
G1489	G1490	C1346	U1099	U1029	A957	A957	U855	C669	C	U607	A542	C270X
G1491	G1492	C1347	U1100	U1030	A958	A958	U856	C670	C	U607	A543	G270Y
G1493	G1494	C1348	G1110	U1031	A959	A959	U857	C671	C	U607	A544	C270Z
G1495	G1496	C1349	A1111	U1032	A960	A960	U858	A675	C	U607	A545	G270A
G1497	G1498	C1350	A1112	U1033	A961	A961	U859	A676	C	U607	A546	G270B
G1499	G1500	C1351	G1112	U1034	A962	A962	U860	C672	C	U607	A547	G270C
G1501	G1502	C1352	G1113	U1035	A963	A963	U861	C673	C	U607	A548	G270D
G1503	G1504	C1353	A1114	U1036	A964	A964	U862	G674	C	U607	A549	G270E
G1505	G1506	C1354	A1115	U1037	A965	A965	U863	A675	C	U607	A550	G270F
G1507	G1508	C1355	A1116	U1038	A966	A966	U864	A676	C	U607	A551	G270G
G1509	G1510	C1356	C1116	U1039	A967	A967	U865	C675	C	U607	A552	G270H
G1511	G1512	C1357	C1117	U1040	A968	A968	U866	C676	C	U607	A553	G270I
G1513	G1514	C1358	G1118	U1041	A969	A969	U867	C677	C	U607	A554	G270J
G1515	G1516	C1359	C1119	U1042	A970	A970	U868	C678	C	U607	A555	G270K
G1517	G1518	C1360	C1120	U1043	A971	A971	U869	C679	C	U607	A556	G270L
G1519	G1520	C1361	C1121	U1044	A972	A972	U870	C680	C	U607	A557	G270M
G1521	G1522	C1362	G1120	U1045	A973	A973	U871	C681	C	U607	A558	G270N
G1523	G1524	C1363	G1121	U1046	A974	A974	U872	C682	C	U607	A559	G270O
G1525	G1526	C1364	G1122	U1047	A975	A975	U873	C683	C	U607	A560	G270P
G1527	G1528	C1365	G1123	U1048	A976	A976	U874	C684	C	U607	A561	G270Q
G1529	G1530	C1366	G1124	U1049	A977	A977	U875	C685	C	U607	A562	C270R
G1531	G1532	C1367	G1125	U1050	A978	A978	U876	C686	C	U607	A563	G270S
G1533	G1534	C1368	G1126	U1051	A979	A979	U877	C687	C	U607	A564	G270T
G1535	G1536	C1369	G1127	U1052	A980	A980	U878	C688	C	U607	A565	G270U
G1537	G1538	C1370	G1128	U1053	A981	A981	U879	C689	C	U607	A566	G270V
G1539	G1540	C1371	G1129	U1054	A982	A982	U880	C690	C	U607	A567	G270W
G1541	G1542	C1372	G1130	U1055	A983	A983	U881	C691	C	U607	A568	G270X
G1543	G1544	C1373	G1131	U1056	A984	A984	U882	C692	C	U607	A569	G270Y
G1545	G1546	C1374	G1132	U1057	A985	A985	U883	C693	C	U607	A570	G270Z
G1547	G1548	C1375	G1133	U1058	A986	A986	U884	C694	C	U607	A571	G270A
G1549	G1550	C1376	G1134	U1059	A987	A987	U885	C695	C	U607	A572	G270B
G1551	G1552	C1377	G1135	U1060	A988	A988	U886	C696	C	U607	A573	G270C
G1553	G1554	C1378	G1136	U1061	A989	A989	U887	C697	C	U607	A574	G270D
G1555	G1556	C1379	G1137	U1062	A990	A990	U888	C698	C	U607	A575	G270E
G1557	G1558	C1380	G1138	U1063	A991	A991	U889	C699	C	U607	A576	G270F
G1559	G1560	C1381	G1139	U1064	A992	A992	U890	C700	C	U607	A577	G270G
G1561	G1562	C1382	G1140	U1065	A993	A993	U891	C701	C	U607	A578	G270H
G1563	G1564	C1383	G1141	U1066	A994	A994	U892	C702	C	U607	A579	G270I
G1565	G1566	C1384	G1142	U1067	A995	A995	U893	C703	C	U607	A580	G270J
G1567	G1568	C1385	G1143	U1068	A996	A996	U894	C704	C	U607	A581	G270K
G1569	G1570	C1386	G1144	U1069	A997	A997	U895	C705	C	U607	A582	G270L
G1571	G1572	C1387	G1145	U1070	A998	A998	U896	C706	C	U607	A583	G270M
G1573	G1574	C1388	G1146	U1071	A999	A999	U897	C707	C	U607	A584	G270N
G1575	G1576	C1389	G1147	U1072	A1000	A1000	U898	C708	C	U607	A585	G270O
G1577	G1578	C1390	G1148	U1073	A1001	A1001	U899	C709	C	U607	A586	G270P
G1579	G1580	C1391	G1149	U1074	A1002	A1002	U900	C710	C	U607	A587	G270Q
G1581	G1582	C1392	G1150	U1075	A1003	A1003	U901	C711	C	U607	A588	G270R
G1583	G1584	C1393	G1151	U1076	A1004	A1004	U902	C712	C	U607	A589	G270S
G1585	G1586	C1394	G1152	U1077	A1005	A1005	U903	C713	C	U607	A590	G270T
G1587	G1588	C1395	G1153	U1078	A1006	A1006	U904	C714	C	U607	A591	G270U
G1589	G1590	C1396	G1154	U1079	A1007	A1007	U905	C715	C	U607	A592	G270V
G1591	G1592	C1397	G1155	U1080	A1008	A1008	U906	C716	C	U607	A593	G270W
G1593	G1594	C1398	G1156	U1081	A1009	A1009	U907	C717	C	U607	A594	G270X
G1595	G1596	C1399	G1157	U1082	A1010	A1010	U908	C718	C	U607	A595	G270Y
G1597	G1598	C1400	G1158	U1083	A1011	A1011	U909	C719	C	U607	A596	G270Z
G1599	G1600	C1401	G1159	U1084	A1012	A1012	U910	C720	C	U607	A597	G270A
G1601	G1602	C1402	G1160	U1085	A1013	A1013	U911	C721	C	U607	A598	G270B
G1603	G1604	C1403	G1161	U1086	A1014	A1014	U912	C722	C	U607	A599	G270C
G1605	G1606	C1404	G1162	U1087	A1015	A1015	U913	C723	C	U607	A600	G270D
G1607	G1608	C1405	G1163	U1088	A1016	A1016	U914	C724	C	U607	A601	G270E
G1609	G1610	C1406	G1164	U1089	A1017	A1017	U915	C725	C	U607	A602	G270F
G1611	G1612	C1407	G1165	U1090	A1018	A1018	U916	C726	C	U607	A603	G270G
G1613	G1614	C1408	G1166	U1091	A1019	A1019	U917	C727	C	U607	A604	G270H
G1615	G1616	C1409	G1167	U1092	A1020	A1020	U918	C728	C	U607	A605	G270I
G1617	G1618	C1410	G1168	U1093	A1021	A1021	U919	C729	C	U607	A606	G270J
G												

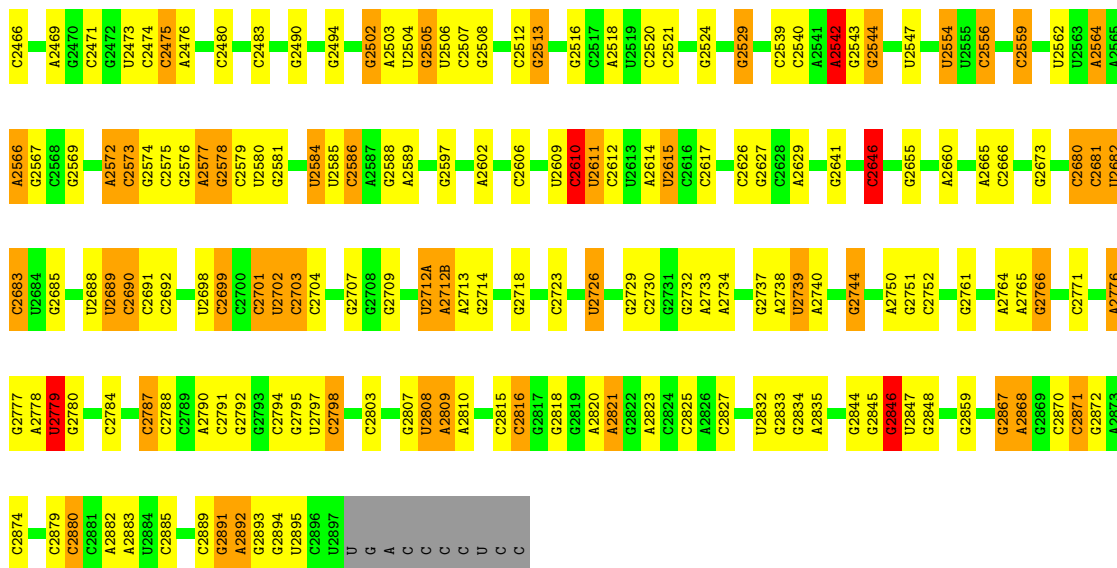
C1504	G1596	A1676	A1789	C1870	A1970	A2060	U2132	G2210	C2313	G2410	A2487	U2584	U2686	C2784	C2844	G2887	C2984	A3084	G3184	C3284	A3384	G3484	C3584	A3684	G3784	C3884	A3984	G4084	C4184	A4284	G4384	C4484	A4584	G4684	C4784	A4884	G4984	C5084	A5184	G5284	C5384	A5484	G5584	C5684	A5784	G5884	C5984	A6084	G6184	C6284	A6384	G6484	C6584	A6684	G6784	C6884	A6984	G7084	C7184	A7284	G7384	C7484	A7584	G7684	C7784	A7884	G7984	C8084	A8184	G8284	C8384	A8484	G8584	C8684	A8784	G8884	C8984	A9084	G9184	C9284	A9384	G9484	C9584	A9684	G9784	C9884	A9984	G10084	C10184	A10284	G10384	C10484	A10584	G10684	C10784	A10884	G10984	C11084	A11184	G11284	C11384	A11484	G11584	C11684	A11784	G11884	C11984	A12084	G12084	C12184	A12284	G12384	C12484	A12584	G12684	C12784	A12884	G12984	C12984	A13084	G13084	C13184	A13284	G13384	C13484	A13584	G13684	C13784	A13884	G13984	C14084	A14184	G14284	C14384	A14484	G14584	C14684	A14784	G14884	C14984	A15084	G15084	C15184	A15284	G15284	C15384	A15484	G15584	C15684	A15784	G15884	C15984	A16084	G16084	C16184	A16284	G16384	C16484	A16584	G16684	C16784	A16884	G16984	C17084	A17184	G17284	C17384	A17484	G17584	C17684	A17784	G17884	C17984	A18084	G18084	C18184	A18284	G18384	C18484	A18584	G18684	C18784	A18884	G18984	C19084	A19184	G19284	C19384	A19484	G19584	C19684	A19784	G19884	C19984	A20084	G20084	C20184	A20284	G20384	C20484	A20584	G20684	C20784	A20884	G20984	C21084	A21184	G21284	C21384	A21484	G21584	C21684	A21784	G21884	C21984	A22084	G22084	C22184	A22284	G22384	C22484	A22584	G22684	C22784	A22884	G22984	C23084	A23184	G23284	C23384	A23484	G23584	C23684	A23784	G23884	C23984	A24084	G24084	C24184	A24284	G24384	C24484	A24584	G24684	C24784	A24884	G24984	C25084	A25184	G25284	C25384	A25484	G25584	C25684	A25784	G25884	C25984	A26084	G26084	C26184	A26284	G26384	C26484	A26584	G26684	C26784	A26884	G26984	C27084	A27184	G27284	C27384	A27484	G27584	C27684	A27784	G27884	C27984	A28084	G28084	C28184	A28284	G28384	C28484	A28584	G28684	C28784	A28884	G28984	C29084	A29184	G29284	C29384	A29484	G29584	C29684	A29784	G29884	C29984	A30084	G30084	C30184	A30284	G30384	C30484	A30584	G30684	C30784	A30884	G30984	C31084	A31184	G31284	C31384	A31484	G31584	C31684	A31784	G31884	C31984	A32084	G32084	C32184	A32284	G32384	C32484	A32584	G32684	C32784	A32884	G32984	C33084	A33184	G33284	C33384	A33484	G33584	C33684	A33784	G33884	C33984	A34084	G34084	C34184	A34284	G34384	C34484	A34584	G34684	C34784	A34884	G34984	C35084	A35184	G35284	C35384	A35484	G35584	C35684	A35784	G35884	C35984	A36084	G36084	C36184	A36284	G36384	C36484	A36584	G36684	C36784	A36884	G36984	C37084	A37184	G37284	C37384	A37484	G37584	C37684	A37784	G37884	C37984	A38084	G38084	C38184	A38284	G38384	C38484	A38584	G38684	C38784	A38884	G38984	C39084	A39184	G39284	C39384	A39484	G39584	C39684	A39784	G39884	C39984	A40084	G40084	C40184	A40284	G40384	C40484	A40584	G40684	C40784	A40884	G40984	C41084	A41184	G41284	C41384	A41484	G41584	C41684	A41784	G41884	C41984	A42084	G42084	C42184	A42284	G42384	C42484	A42584	G42684	C42784	A42884	G42984	C43084	A43184	G43284	C43384	A43484	G43584	C43684	A43784	G43884	C43984	A44084	G44084	C44184	A44284	G44384	C44484	A44584	G44684	C44784	A44884	G44984	C45084	A45184	G45284	C45384	A45484	G45584	C45684	A45784	G45884	C45984	A46084	G46084	C46184	A46284	G46384	C46484	A46584	G46684	C46784	A46884	G46984	C47084	A47184	G47284	C47384	A47484	G47584	C47684	A47784	G47884	C47984	A48084	G48084	C48184	A48284	G48384	C48484	A48584	G48684	C48784	A48884	G48984	C49084	A49184	G49284	C49384	A49484	G49584	C49684	A49784	G49884	C49984	A50084	G50084	C50184	A50284	G50384	C50484	A50584	G50684	C50784	A50884	G50984	C51084	A51184	G51284	C51384	A51484	G51584	C51684	A51784	G51884	C51984	A52084	G52084	C52184	A52284	G52384	C52484	A52584	G52684	C52784	A52884	G52984	C53084	A53184	G53284	C53384	A53484	G53584	C53684	A53784	G53884	C53984	A54084	G54084	C54184	A54284	G54384	C54484	A54584	G54684	C54784	A54884	G54984	C55084	A55184	G55284	C55384	A55484	G55584	C55684	A55784	G55884	C55984	A56084	G56084	C56184	A56284	G56384	C56484	A56584	G56684	C56784	A56884	G56984	C57084	A57184	G57284	C57384	A57484	G57584	C57684	A57784	G57884	C57984	A58084	G58084	C58184	A58284	G58384	C58484	A58584	G58684	C58784	A58884	G58984	C59084	A59184	G59284	C59384	A59484	G59584	C59684	A59784	G59884	C59984	A60084	G60084	C60184	A60284	G60384	C60484	A60584	G60684	C60784	A60884	G60984	C61084	A61184	G61284	C61384	A61484	G61584	C61684	A61784	G61884	C61984	A62084	G62084	C62184	A62284	G62384	C62484	A62584	G62684	C62784	A62884	G62984	C63084	A63184	G63284	C63384	A63484	G63584	C63684	A63784	G63884	C63984	A64084	G64084	C64184	A64284	G64384	C64484	A64584	G64684	C64784	A64884	G64984	C65084	A65184	G65284	C65384	A65484	G65584	C65684	A65784	G65884	C65984	A66084	G66084	C66184	A66284	G66384	C66484	A66584	G66684	C66784	A66884	G66984	C67084	A67184	G67284	C67384	A67484	G67584	C67684	A67784	G67884	C67984	A68084	G68084	C68184	A68284	G68384	C68484	A68584	G68684	C68784	A68884	G68984	C69084	A69184	G69284	C69384	A69484	G69584	C69684	A69784	G69884	C69984	A70084	G70084	C70184	A70284	G70384	C70484	A70584	G70684	C70784	A70884	G70984	C71084	A71184	G71284	C71384	A71484	G71584	C71684	A71784	G71884	C71984	A72084	G72084	C72184	A72284	G72384	C72484	A72584	G72684	C72784	A72884	G72984	C73084	A73184	G73284	C73384	A73484	G73584	C73684	A73784	G73884	C73984	A74084	G74084	C74184	A74284	G74384	C74484	A74584	G74684	C74784	A74884	G74984	C75084	A75184	G75284	C75384	A75484	G75584	C75684	A75784	G75884	C75984	A76084	G76084	C76184	A76284	G76384	C76484	A76584	G76684	C76784	A76884	G76984	C77084	A77184	G77284	C77384	A77484	G77584	C77684	A77784	G77884	C77984	A78084	G78084	C78184	A78284	G78384	C78484	A78584	G78684	C78784	A78884	G78984	C79084	A79184	G79284	C79384	A79484	G79584	C79684	A79784	G79884	C79984	A80084	G80084	C80184	A80284	G80384	C80484	A80584	G80684	C80784	A80884	G80984	C81084	A81184	G81284	C81384	A81484	G81584	C81684	A81784	G81884	C81984	A82084	G82084	C82184	A82284	G82384	C82484	A82584	G82684	C82784	A82884	G82984	C83084	A83184	G83284	C83384	A83484	G83584	C83684	A83784	G83884	C83984	A84084	G84084	C84184	A84284	G84384	C84484	A84584	G84684	C84784	A84884	G84984	C85084	A85184	G85284	C85384	A85484	G85584	C85684	A85784	G85884	C85984	A86084	G86084	C86184	A86284	G86384	C86484	A86584	G86684	C86784	A86884	G86984	C87084	A87184	G87284	C87384	A87484	G87584	C87684	A87784	G87884	C87984	A88084	G88084	C88184	A88284	G88384	C88484	A88584	G88684	C88784	A88884	G88984	C89084	A89184	G89284	C89384	A89484	G89584	C89684	A89784	G89884	C89984	A90084	G90084	C90184	A90284	G90384	C90484	A90584	G90684	C90784	A90884	G90984	C91084	A91184	G91284	C91384	A91484	G91584	C91684	A91784	G91884	C91984	A92084	G92084	C92184	A92284	G92384	C92484	A92584	G92684	C92784	A92884	G92984	C93084	A93184	G93284	C93384	A93484	G93584	C93684	A93784	G93884	C93984	A94084	G94084	C94184	A94284	G94384	C94484	A94584	G94684	C94784	A94884	G94984	C95084	A95184	G95284	C95384	A95484	G95584	C95684	A95784	G95884	C95984	A96084	G96084	C96184	A96284	G96384	C96484	A96584	G96684	C96784	A96884	G96984	C97084	A97184	G97284	C97384	A97484	G97584	C97684	A97784	G97884	C97984	A98084	G98084	C98184	A98284	G98384	C98484	A98584	G98684	C98784	A98884	G98984	C99084	A99184	G99284	C99384	A99484	G99584	C99684	A99784	G99884	C99984	A100084	G100084	C100184	A100284	G100384	C100484	A100584	G100684	C100784	A100884	G100984	C101084	A101184	G101284	C101384	A101484	G101584	C101684	A101784	G101884	C101984	A102084	G102084	C102184	A102284	G102384	C102484	A102584	G102684	C102784	A102884	G102984	C103084	A103184	G103284	C103384	A103484	G103584	C103684	A103784	G103884	C103984	A104084	G104084	C104184	A104284	G104384	C104484	A104584	G104684	C104784	A104884	G104984	C105084	A105184	G105284	C105384	A105484	G105584	C105684	A105784	G105884	C105984	A106084	G106084	C106184	A106284	G106384	C106484	A106584	G106684	C106784	A106884	G106984	C107084	A107184	G107284	C107384	A107484	G107584	C107684	A107784	G107884	C107984	A108084	G108084	C108184	A108284	G108384	C108484	A108584	G108684	C108784	A108884	G108984	C109084	A109184	G109284	C109384	A109484	G109584	C109684	A109784	G109884	C109984	A110084	G110084	C110184	A110284	G110384	C110484	A110584	G110684	C110784	A110884	G110984	C111084	A111184	G111284	C111384	A111484	G111584	C111684	A111784	G111884	C111984	A112084	G112084	C112184	A112284	G112384	C112484	A112584	G112684	C112784	A112884	G112984	C113084	A113184	G113284	C113384	A113484	G113584	C113684	A113784	G113884	C113984	A114084	G114084	C114184	A114284	G114384	C114484	A114584	G114684	C114784	A114884	G114984	C115084	A115184	G115284	C115384	A115484	G115584	C115684	A115784	G115884	C115984	A116084	G116084	C116184	A116284	G116384	C116484	A116584	G116684	C116784	A116884	G11698
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	--------



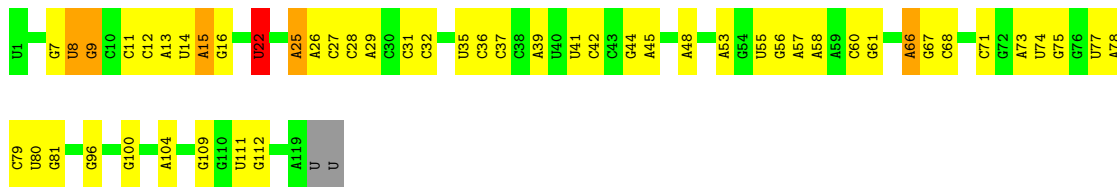
• Molecule 34: 23S rRNA



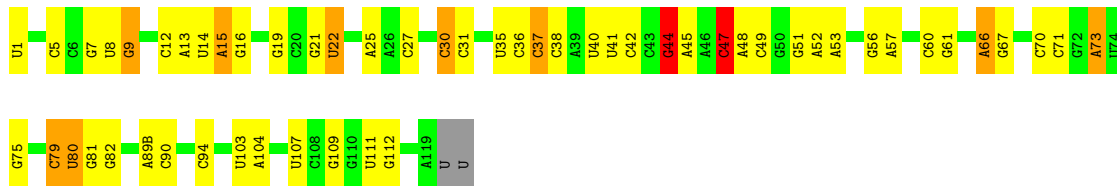
G1093	U1273	C1375	C1468	A1567	U1671	U1779	A1871	A1969	G2056	C2128	G2210	G2289	G2382
U1094	A1274	A1378	A1471	G1568	C1672	U1779	A1872	A1970	G2056	C2129	G2211	G2299	G2383
A1095	A1275	A1379	A1472	A1569	U1673	C1781	G1878	A2060	A2059	U2130	A2212	G2303	G2384
U1097	A1286	C1383	C1473	C1575	C1675	C1782	C1882	G2061	G2062	U2133	G2215	C2306	C2386
A1098	C1289	A1384	C1474	U1578	U1679	A1784	G1883	C1979	A2062	G2133	G2219	G2307	C2387
G1099	C1290	G1385	A1477	A1578	A1679	A1785	A1884	C1982	C2064	A2134	G2224	G2308	U2387
U1101	C1291	A1386	A1478	C1585	G1682	A1786	C1887	C1988	C2065	A2135	A2225	A2311	A2392
A1102	C1293	A1392	G1478	A1586	C1683	C1787	G1888	C1989	U2068	C2136	A2226	U2312	A2393
A1103	U1294	A1393	G1479	A1587	C1684	C1788	A1889	G1990	G2069	C2141	G2226	U2314	C2394
U1104	C1295	U1394	A1480	G1595	C1685	A1789	A1890	C1991	G2070	G2141	G2230	C2314	C2395
U1105	U1205	A1395	U1482	G1598	C1686	C1790	G1891	U1991	A2071	C2145	U2233	G2315	G2399
G1110	G1206	C1398	G1485	C1599	A1689	A1791	C1892	G1992	A2071	C2148	G2234	C2316	C2402
A1111	A1210	C1399	G1485	C1600	A1689	A1792	C1893	U1993	U2074	G2149	G2235	U2317	C2403
G1112	U1211	U1300	A1490	C1601	C1694	C1793	C1894	U1994	U2075	G2150	G2236	C2318	G2404
U1113	U1212	A1301	C1493	A1608	G1695	C1793	C1894	C1996	U2076	U2151	G2237	G2319	G2405
C1121	G1215	C1306	C1497	A1609	A1698	G1799	A1899	A1996	U2081	G2152	G2239	G2321	U2406
G1122	C1217	A1307	C1498	A1610	G1699	C1800	A1900	A2005	A2082	G2153	U2243	C2325	G2410
A1126	C1218	U1406	C1499	C1611	A1700	A1802	A1901	C2006	G2083	G2154	G2244	C2326	A2411
G1131	G1219	C1407	C1500	C1612	C1701	C1803	C1905	C2007	U2086	G2155	U2245	G2327	G2412
C1135	A1220	U1313	G1500	G1613	G1613	U1805	G1906	G2009	G2087	G2156	G2246	A2328	G2415
G1136	G1224	C1314	C1506	A1616	U1709	C1806	A1913	G2010	G2088	G2157	G2246	G2329	G2416
G1139	U1225	C1318	A1507	C1617	G1725	A1809	C1914	U2011	U2089	A2158	U2249	G2330	C2420
C1140	C1226	C1318	A1508	A1618	G1728	A1812	U1915	G2012	U2092	G2159	G2250	G2334	A2421
U1141	G1227	G1325	C1509	G1619	A1729	G1813	A1918	A2015	U2093	C2160	G2253	A2335	G2422
A1142A	U1228	U1326	A1511	U1621	G1730	C1814	A1919	C2019	G2094	G2162	C2254	C2336	U2423
A1142B	C1233	C1327	C1512	G1622	U1731	A1815	C1920	A2019	C2095	C2163	C2254	G2340	U2424
G1145	U1420	U1328	U1516	C1636	A1732	G1816	A1929	G2022	U2096	G2164	C2260	G2341	C2424
C1146	U1234	U1329	G1519	A1637	G1733	A1819	G1930	G2024	C2097	G2165	C2261	C2342	A2426
C1147	G1235	C1330	G1520	C1640	C1741	U1820	U1931	G2025	U2099	G2166	A2266	C2343	C2427
G1151	G1238	C1333	G1526	C1644	G1743	G1824	G1935	C2026	U2102	A2167	A2267	G2344	G2428
C1152	U1244	G1338	C1533	U1645	G1750	G1828	A1936	A2030	C2103	U2172	A2268	C2345	A2430
C1153	G1246	U1340	G1534	C1646	C1753	A1829	A1938	A2031	G2104	A2173	A2273	G2349	G2435
G1154	U1341	U1341	U1535	C1648	C1754	C1830	U1939	G2032	C2105	A2174	A2274	C2350	A2439
G1157	G1250	A1342	A1536	G1651	U1755	U1833	C1947	A2033	C2107	A2176	C2275	G2351	C2440
C1158	C1251	G1343	C1537	G1652	G1756	U1833	C1947	C2036	U2109	G2182	A2278	A2352	C2441
U1165	A1253	A1349	G1538	G1653	U1757	G1839	G1950	C2039	G2110	G2185	A2279	G2353	C2442
C1166	U1254	U1352	A1543	A1654	G1758	C1844	A1953	C2040	C2111	C2186	G2280	C2354	G2446
G1173	G1256	A1353	A1545A	A1655	G1763	A1845	G1954	U2041	G2112	G2187	C2281	C2355	G2447
A1174	C1257	C1362	C1549	C1657	U1766	A1853	U1955	A2042	A2114	G2188	C2282	U2357	A2448
U1175	G1264	C1363	G1554	C1658	U1767	A1854	U1956	C2043	G2115	G2190	C2284	G2358	A2453
G1176	A1265	G1364	A1554	A1664	C1767	A1854	C1958	C2044	G2116	G2191	C2285	C2359	G2454
A1177	G1266	A1365	A1554	A1665	U1768	A1854	C1958	U2047	U2117	G2192	A2286	C2368	G2455
C1179	U1267	A1365	A1558	G1666	G1769	G1858	U1963	G2048	U2118	G2193	A2287	U2371	C2456
U1180	C1270	G1368	G1559	G1667	U1773	A1859	U1964	G2049	A2119	G2196	A2288	G2371	U2457
G1184	A1272	C1370	G1560	A1668	U1775	U1864	G1964	G2049	A2120	C2196	U2291	C2374	U2460
			A1566	A1669	C1776	C1870	A1966	G2052	G2125	A2199	C2292	G2375	C2461
				C1670	G1776		G1967	C2055	G2127	A2378	C2294	A2378	C2465



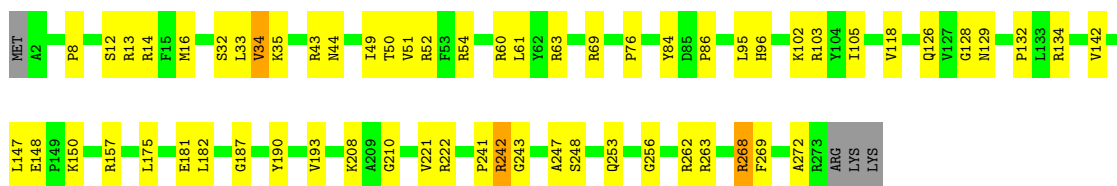
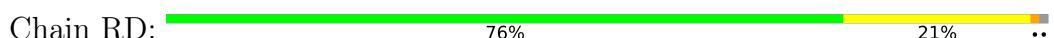
• Molecule 35: 5S rRNA



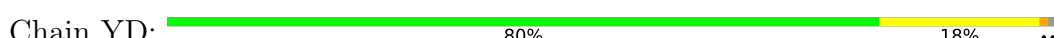
• Molecule 35: 5S rRNA

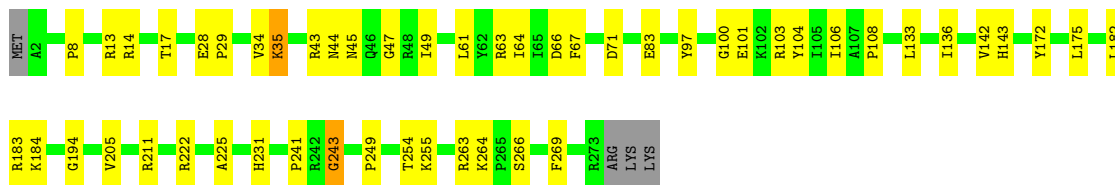


• Molecule 36: 50S ribosomal protein L2



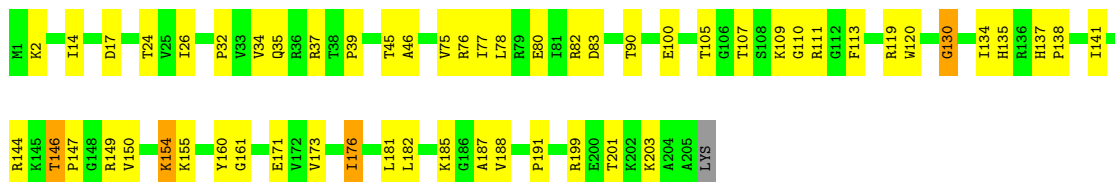
• Molecule 36: 50S ribosomal protein L2





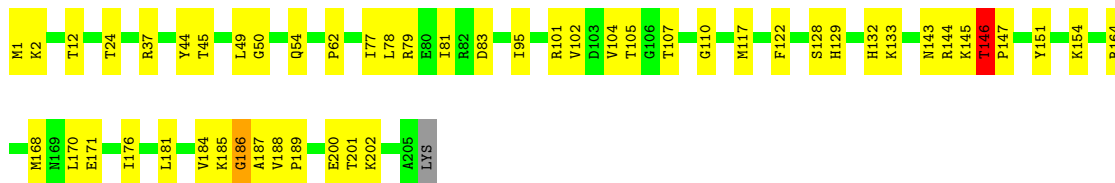
- Molecule 37: 50S ribosomal protein L3

Chain RE: 72% 25%



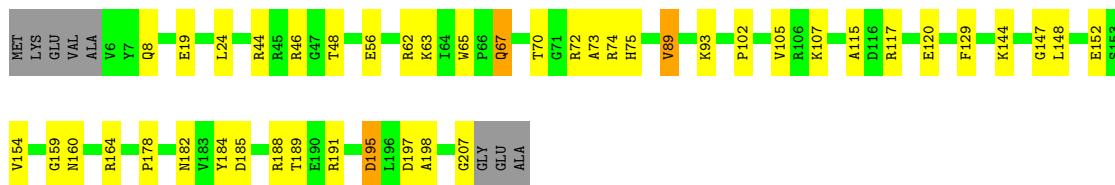
- Molecule 37: 50S ribosomal protein L3

Chain YE: 75% 24%



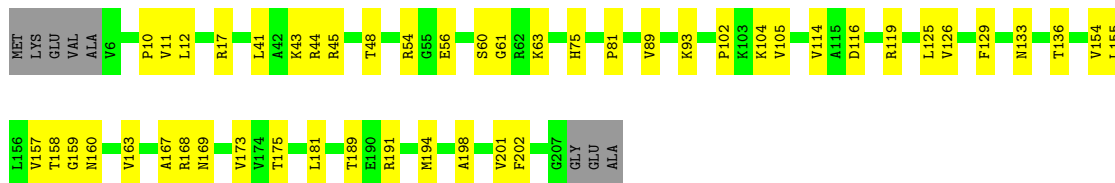
- Molecule 38: 50S ribosomal protein L4

Chain RF: 75% 20%



- Molecule 38: 50S ribosomal protein L4

Chain YF: 73% 23%



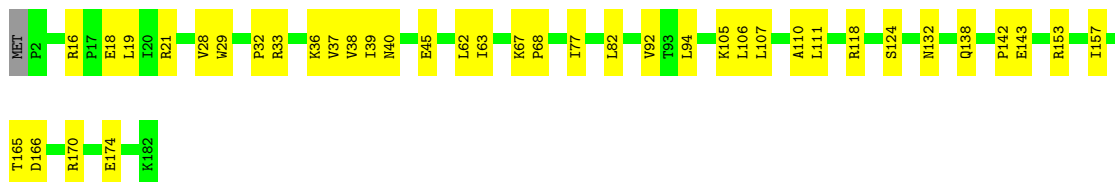
- Molecule 39: 50S ribosomal protein L5

Chain RG: 76% 23%



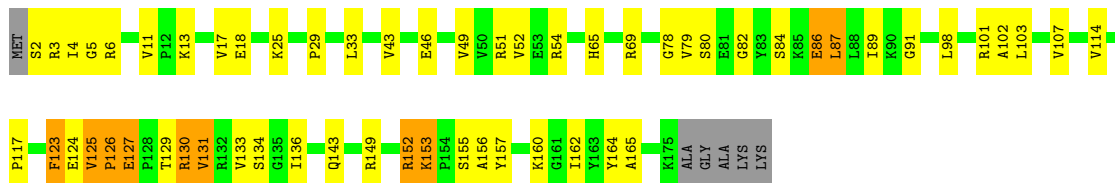
- Molecule 39: 50S ribosomal protein L5

Chain YG: 78% 21%



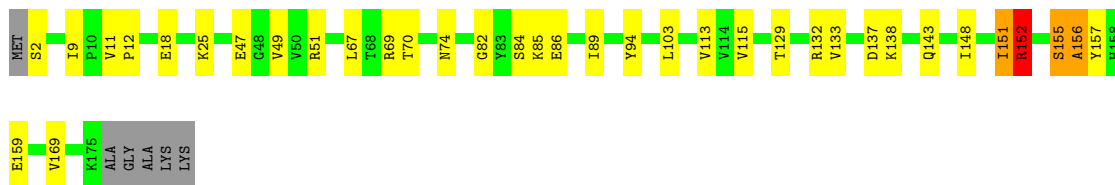
- Molecule 40: 50S ribosomal protein L6

Chain RH: 64% 27% 6%



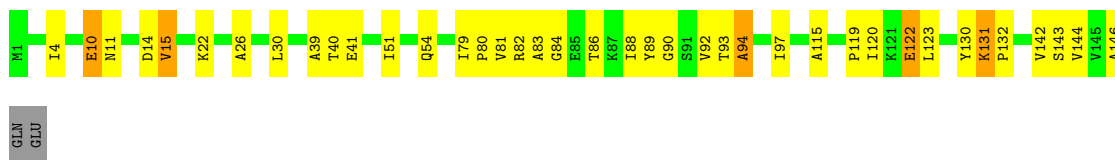
- Molecule 40: 50S ribosomal protein L6

Chain YH: 77% 18%



- Molecule 41: 50S ribosomal protein L9

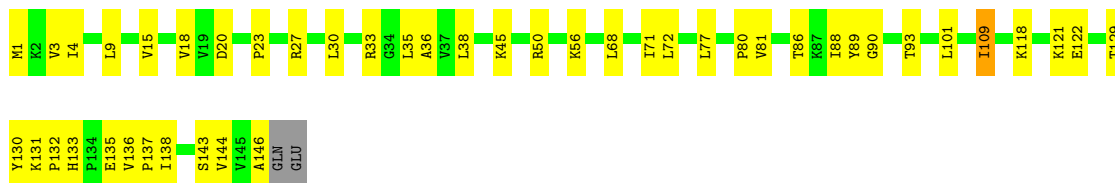
Chain RI: 72% 23%



- Molecule 41: 50S ribosomal protein L9

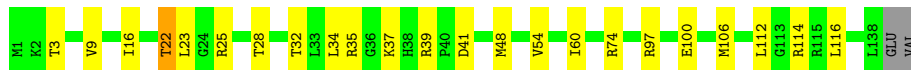
Chain YI: 68% 30%





- Molecule 42: 50S ribosomal protein L13

Chain RN: 82% 16% ..



- Molecule 42: 50S ribosomal protein L13

Chain YN: 79% 20% .



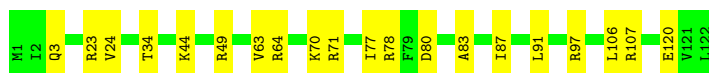
- Molecule 43: 50S ribosomal protein L14

Chain RO: 75% 25%



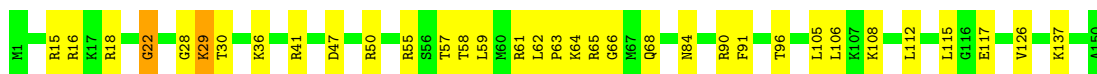
- Molecule 43: 50S ribosomal protein L14

Chain YO: 84% 16%



- Molecule 44: 50S ribosomal protein L15

Chain RP: 77% 21% .



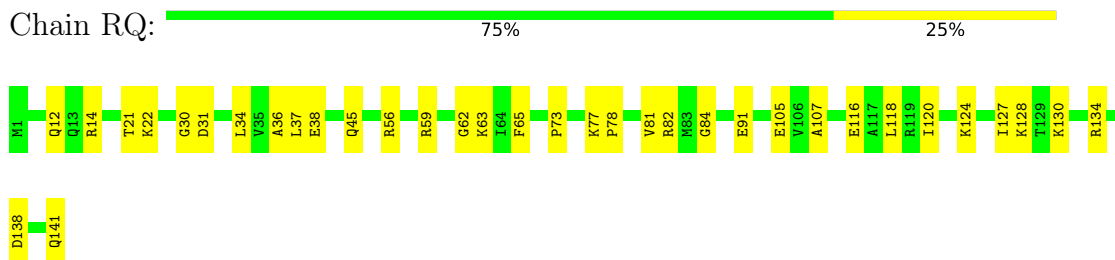
- Molecule 44: 50S ribosomal protein L15

Chain YP: 75% 23% .

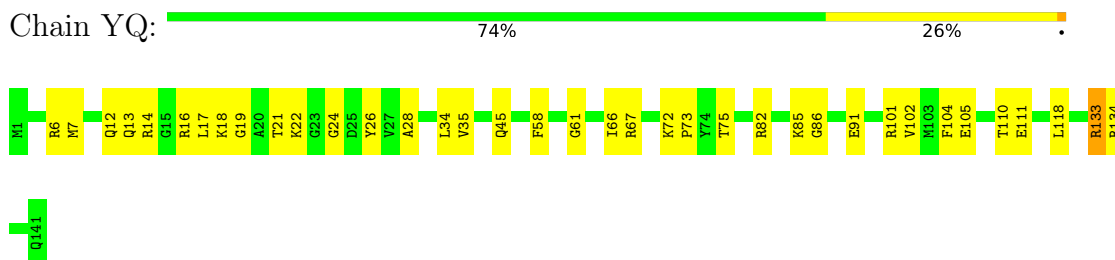


GLU  
ALA

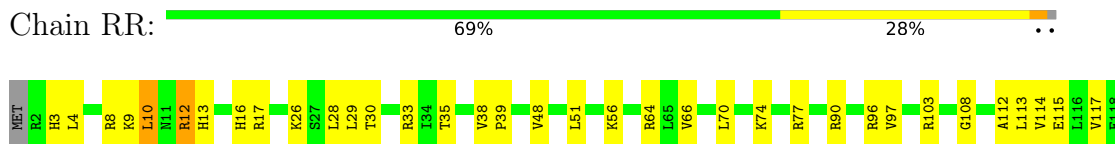
- Molecule 45: 50S ribosomal protein L16



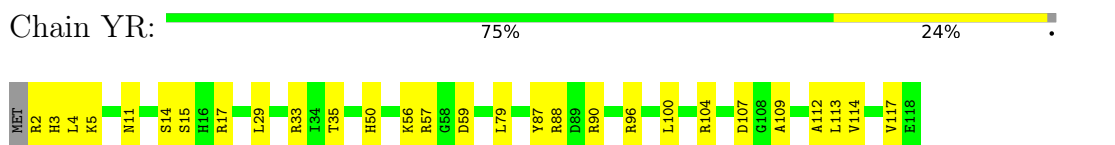
- Molecule 45: 50S ribosomal protein L16



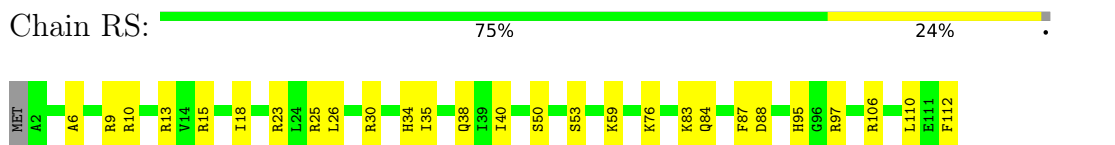
- Molecule 46: 50S ribosomal protein L17



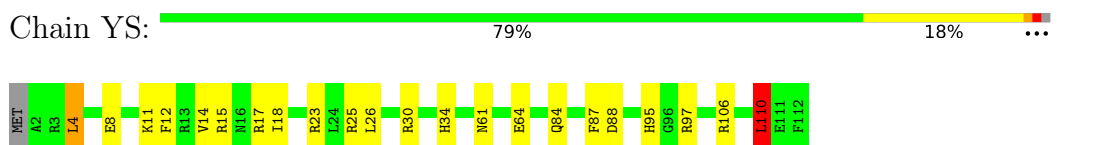
- Molecule 46: 50S ribosomal protein L17




- Molecule 47: 50S ribosomal protein L18

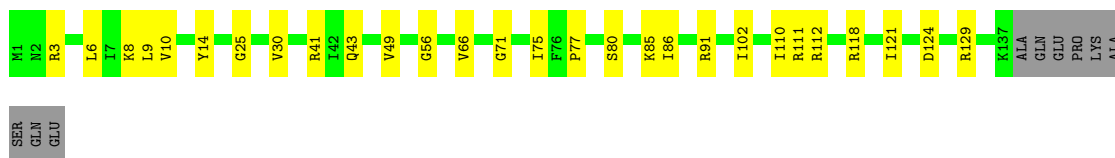


- Molecule 47: 50S ribosomal protein L18



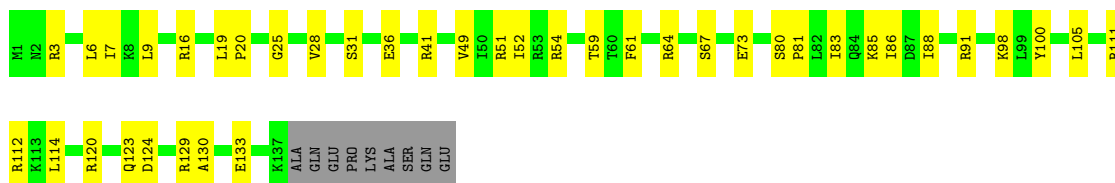
- Molecule 48: 50S ribosomal protein L19

Chain RT:  75% 19% 6%




- Molecule 48: 50S ribosomal protein L19

Chain YT:  66% 27% 6%




- Molecule 49: 50S ribosomal protein L20

Chain RU:  77% 19% ..




- Molecule 49: 50S ribosomal protein L20

Chain YU:  79% 19% ..




- Molecule 50: 50S ribosomal protein L21

Chain RV:  78% 22%




- Molecule 50: 50S ribosomal protein L21

Chain YV:  79% 21%

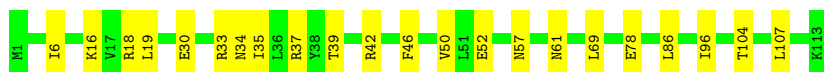
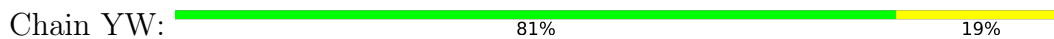


- Molecule 51: 50S ribosomal protein L22

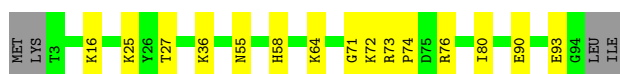
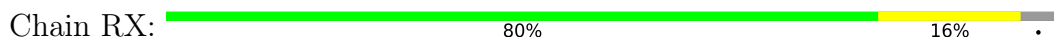
Chain RW:  79% 21%



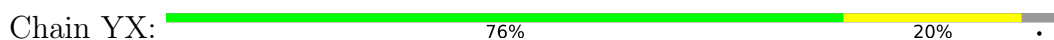
- Molecule 51: 50S ribosomal protein L22



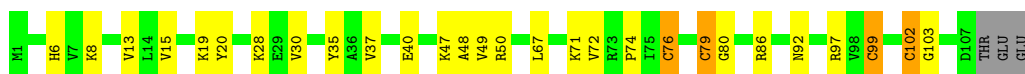
- Molecule 52: 50S ribosomal protein L23



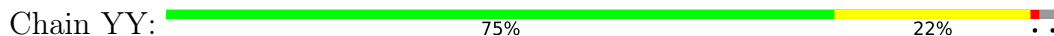
- Molecule 52: 50S ribosomal protein L23



- Molecule 53: 50S ribosomal protein L24



- Molecule 53: 50S ribosomal protein L24

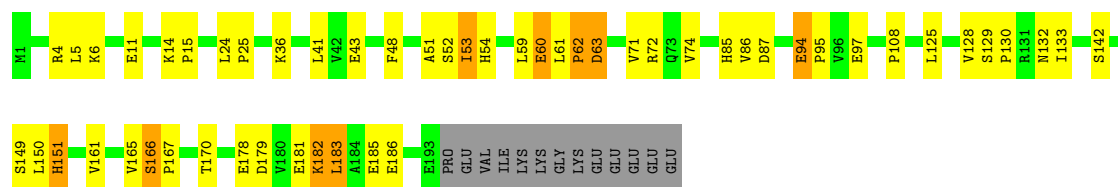


- Molecule 54: 50S ribosomal protein L25



- Molecule 54: 50S ribosomal protein L25

Chain YZ:  68% 21% 6%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.74Å 450.26Å 626.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.50	Depositor
% Data completeness (in resolution range)	97.6 (49.94-3.50)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.240 , 0.258	Depositor
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.423	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 1MG, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	QA	0.69	1/36343 (0.0%)	1.14	198/56720 (0.3%)
1	XA	0.77	0/36435	1.15	194/56865 (0.3%)
2	QB	0.35	0/1942	0.67	0/2619
2	XB	0.37	0/1950	0.64	1/2630 (0.0%)
3	QC	0.36	0/1629	0.66	0/2195
3	XC	0.37	0/1629	0.61	0/2195
4	QD	0.45	1/1733 (0.1%)	0.65	0/2318
4	XD	0.52	2/1733 (0.1%)	0.70	2/2318 (0.1%)
5	QE	0.37	0/1171	0.67	0/1576
5	XE	0.43	0/1171	0.62	0/1576
6	QF	0.39	0/856	0.68	0/1154
6	XF	0.41	0/856	0.62	0/1154
7	QG	0.35	0/1276	0.63	1/1709 (0.1%)
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1128	0.62	0/1517
8	XH	0.42	0/1128	0.66	0/1517
9	QI	0.42	0/1029	0.74	0/1379
9	XI	0.36	0/1017	0.70	0/1365
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.34	0/790	0.59	0/1063
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/879	0.59	0/1187
12	QL	0.41	0/991	0.70	1/1327 (0.1%)
12	XL	0.45	0/972	0.77	2/1301 (0.2%)
13	QM	0.35	0/965	0.78	0/1292
13	XM	0.37	0/924	0.66	0/1238
14	QN	0.67	1/501 (0.2%)	0.84	3/664 (0.5%)
14	XN	0.68	1/501 (0.2%)	0.88	2/664 (0.3%)
15	QO	0.38	0/745	0.57	0/992
15	XO	0.40	0/740	0.56	0/987
16	QP	0.40	0/721	0.64	0/970
16	XP	0.38	0/721	0.66	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.39	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.37	0/579	0.56	0/768
18	XR	0.39	0/579	0.58	0/768
19	QS	0.35	0/680	0.72	1/915 (0.1%)
19	XS	0.36	0/689	0.70	0/926
20	QT	0.77	2/765 (0.3%)	1.14	8/1007 (0.8%)
20	XT	0.37	0/765	0.75	2/1007 (0.2%)
21	QU	0.34	0/221	0.58	0/288
21	XU	0.32	0/221	0.54	0/288
22	QV	0.70	2/1813 (0.1%)	1.39	32/2825 (1.1%)
22	XV	0.66	0/1813	1.20	13/2825 (0.5%)
23	QX	0.99	1/459 (0.2%)	2.11	25/715 (3.5%)
23	XX	0.63	0/459	1.26	1/715 (0.1%)
24	R0	0.40	0/652	0.63	0/867
24	Y0	0.59	0/657	0.60	0/874
25	R1	0.54	0/753	0.68	0/1000
25	Y1	0.59	0/736	0.73	0/978
26	R2	0.37	0/583	0.62	0/771
26	Y2	0.47	0/577	0.62	0/764
27	R3	0.39	0/474	0.59	0/635
27	Y3	0.62	0/474	0.59	0/635
28	R4	0.33	0/357	0.60	0/483
28	Y4	1.56	2/366 (0.5%)	1.47	8/495 (1.6%)
29	R5	0.88	3/473 (0.6%)	0.79	2/639 (0.3%)
29	Y5	0.94	2/473 (0.4%)	0.77	1/639 (0.2%)
30	R6	0.96	3/460 (0.7%)	0.78	2/613 (0.3%)
30	Y6	1.33	6/460 (1.3%)	1.01	3/613 (0.5%)
31	R7	0.53	0/417	0.62	0/550
31	Y7	0.63	0/426	0.66	0/561
32	R8	0.43	0/525	0.88	3/691 (0.4%)
32	Y8	0.59	0/525	0.84	0/691
33	R9	0.62	1/310 (0.3%)	0.72	1/407 (0.2%)
33	Y9	0.63	0/310	0.73	0/407
34	RA	0.91	2/69520 (0.0%)	1.22	576/108527 (0.5%)
34	YA	1.27	23/69543 (0.0%)	1.33	807/108563 (0.7%)
35	RB	0.71	0/2878	1.14	18/4490 (0.4%)
35	YB	1.08	0/2878	1.32	38/4490 (0.8%)
36	RD	0.52	0/2165	0.71	3/2919 (0.1%)
36	YD	0.64	0/2165	0.74	4/2919 (0.1%)
37	RE	0.50	0/1601	0.83	3/2160 (0.1%)
37	YE	0.66	0/1601	0.84	3/2160 (0.1%)
38	RF	0.49	0/1620	0.70	1/2194 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YF	0.67	0/1620	0.65	1/2194 (0.0%)
39	RG	0.40	0/1499	0.69	0/2016
39	YG	0.43	0/1499	0.68	0/2016
40	RH	0.39	0/1362	0.83	5/1841 (0.3%)
40	YH	0.58	0/1362	0.82	4/1841 (0.2%)
41	RI	0.48	2/1151 (0.2%)	0.86	6/1558 (0.4%)
41	YI	0.45	1/1151 (0.1%)	0.79	0/1558
42	RN	0.45	0/1131	0.68	1/1525 (0.1%)
42	YN	0.63	0/1131	0.70	2/1525 (0.1%)
43	RO	0.51	0/943	0.65	0/1269
43	YO	0.60	0/943	0.63	0/1269
44	RP	0.44	0/1162	0.76	1/1544 (0.1%)
44	YP	0.54	0/1139	0.83	1/1514 (0.1%)
45	RQ	0.45	0/1143	0.73	0/1527
45	YQ	0.61	0/1143	0.77	2/1527 (0.1%)
46	RR	0.48	0/974	0.68	0/1302
46	YR	0.57	0/974	0.70	0/1302
47	RS	0.39	0/892	0.66	0/1187
47	YS	0.52	0/892	0.67	0/1187
48	RT	0.43	0/1155	0.69	0/1542
48	YT	0.54	0/1155	0.72	1/1542 (0.1%)
49	RU	0.49	0/982	0.62	0/1306
49	YU	0.70	0/982	0.61	0/1306
50	RV	0.47	0/790	0.74	1/1057 (0.1%)
50	YV	0.63	0/790	0.76	1/1057 (0.1%)
51	RW	0.52	0/911	0.63	0/1220
51	YW	0.68	0/911	0.64	0/1220
52	RX	0.52	0/739	0.60	0/993
52	YX	0.66	0/739	0.68	0/993
53	RY	0.72	4/831 (0.5%)	0.66	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	2/1108 (0.2%)
54	RZ	0.43	0/1493	0.89	6/2026 (0.3%)
54	YZ	0.51	0/1561	0.85	5/2119 (0.2%)
All	All	0.87	61/316163 (0.0%)	1.12	2000/472822 (0.4%)

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
28	Y4	1	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	1	7

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.70	1.04	1.54
28	Y4	4	GLY	N-CA	-18.70	1.18	1.46
30	R6	16	CYS	CB-SG	14.24	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82
20	QT	74	LYS	CA-CB	-13.71	1.23	1.53

The worst 5 of 2000 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	74	LYS	N-CA-CB	21.28	148.91	110.60
23	QX	17	C	C6-N1-C2	-19.01	112.70	120.30
22	QV	35	G	C8-N9-C4	-16.76	99.70	106.40
28	Y4	5	ILE	CB-CA-C	16.14	143.88	111.60
34	YA	2453	A	N1-C2-N3	-15.63	121.48	129.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	Y4	5	ILE	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
28	Y4	5	ILE	Mainchain
37	YE	146	THR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32469	0	16393	389	0
1	XA	32551	0	16433	382	1
2	QB	1907	0	1958	40	0
2	XB	1915	0	1968	37	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	22	0
4	QD	1703	0	1763	55	0
4	XD	1703	0	1763	47	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	9	0
6	XF	843	0	857	11	0
7	QG	1257	0	1296	21	0
7	XG	1257	0	1296	23	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	23	0
9	QI	1010	0	1037	22	0
9	XI	998	0	1024	21	0
10	QJ	801	0	849	22	0
10	XJ	777	0	816	13	0
11	QK	885	0	904	7	0
11	XK	864	0	881	11	0
12	QL	975	0	1062	23	0
12	XL	956	0	1046	14	0
13	QM	955	0	1021	27	0
13	XM	914	0	971	23	0
14	QN	492	0	532	18	0
14	XN	492	0	531	16	0
15	QO	734	0	771	5	0
15	XO	729	0	768	10	0
16	QP	705	0	725	13	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	5	0
18	XR	574	0	644	11	0
19	QS	665	0	686	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	16	0
20	QT	763	0	861	17	0
20	XT	763	0	861	17	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1647	0	834	23	0
22	XV	1647	0	834	18	0
23	QX	409	0	209	13	0
23	XX	409	0	209	6	0
24	R0	643	0	667	6	0
24	Y0	648	0	672	14	0
25	R1	746	0	826	21	0
25	Y1	729	0	802	7	0
26	R2	581	0	629	7	0
26	Y2	575	0	624	5	0
27	R3	469	0	518	6	0
27	Y3	469	0	518	10	0
28	R4	348	0	354	6	0
28	Y4	357	0	362	12	0
29	R5	459	0	477	23	0
29	Y5	459	0	476	17	0
30	R6	453	0	474	7	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	9	0
31	Y7	418	0	467	7	0
32	R8	517	0	582	19	0
32	Y8	517	0	582	16	0
33	R9	307	0	335	9	0
33	Y9	307	0	336	17	0
34	RA	62070	0	31284	607	0
34	YA	62091	0	31294	489	0
35	RB	2573	0	1306	26	0
35	YB	2573	0	1306	24	0
36	RD	2115	0	2195	50	0
36	YD	2115	0	2195	39	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	34	0
38	RF	1585	0	1632	30	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	32	0
39	YG	1474	0	1535	24	0
40	RH	1336	0	1418	57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	21	0
41	RI	1136	0	1223	32	1
41	YI	1136	0	1223	25	0
42	RN	1104	0	1180	14	0
42	YN	1104	0	1180	15	0
43	RO	933	0	996	21	0
43	YO	933	0	996	14	0
44	RP	1145	0	1228	27	0
44	YP	1122	0	1206	28	0
45	RQ	1122	0	1179	23	0
45	YQ	1122	0	1179	25	0
46	RR	960	0	1021	31	0
46	YR	960	0	1021	19	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	17	0
48	YT	1141	0	1202	27	0
49	RU	964	0	1022	25	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	14	0
50	YV	779	0	852	12	0
51	RW	900	0	964	17	0
51	YW	900	0	964	16	0
52	RX	725	0	778	9	0
52	YX	725	0	778	14	0
53	RY	818	0	911	24	0
53	YY	818	0	910	21	0
54	RZ	1461	0	1493	32	0
54	YZ	1529	0	1551	29	0
55	QA	87	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	1	0	0	0	0
55	R0	2	0	0	0	0
55	R1	1	0	0	0	0
55	R3	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	429	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	89	0	0	0	0
55	XE	1	0	0	0	0
55	Y1	1	0	0	0	0
55	Y2	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	439	0	0	0	0
55	YB	8	0	0	0	0
55	YD	1	0	0	0	0
55	YE	2	0	0	0	0
55	YF	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	1	0
All	All	292039	0	197760	3309	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3309 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:98:LEU:CD2	40:RH:125:VAL:HG11	1.44	1.45
29:Y5:32:PRO:N	29:Y5:32:PRO:CA	1.69	1.44
30:R6:16:CYS:SG	30:R6:16:CYS:CB	2.06	1.44
14:QN:24:CYS:SG	14:QN:40:CYS:CB	2.14	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.70	0.50

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	72
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	68
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	68
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	22	61
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	61
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	13 (10%)	1 (1%)	19	58
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	54
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	19	58
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	9	42
13	XM	112/126 (89%)	101 (90%)	10 (9%)	1 (1%)	17	56
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
14	XN	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	28
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	30
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	4	30
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	14	52

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	13 (30%)	3 (7%)	1	13
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	4	29
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	22	61
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	34	72
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	34
37	YE	203/206 (98%)	163 (80%)	38 (19%)	2 (1%)	15	54
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	54
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	68
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	64
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	9	42
40	YH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	4	31
41	RI	144/148 (97%)	115 (80%)	23 (16%)	6 (4%)	3	23
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	5	32
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	61
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	22	61
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	7	39
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	22	61
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	61
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	61
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	17	56
47	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	17	56
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	5	33
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	54
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	6	37
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	3	26
All	All	11414/12128 (94%)	10111 (89%)	1217 (11%)	86 (1%)	19	58

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR

### 5.3.2 Protein sidechains [i](#)

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	QB	203/220 (92%)	200 (98%)	3 (2%)	65	84
2	XB	204/220 (93%)	203 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	86
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	86
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	94
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	88
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	91
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	79
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	79
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	88
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	99 (96%)	4 (4%)	32	64
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	46 (94%)	3 (6%)	18	51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	86
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	58
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	47	75
25	Y1	78/83 (94%)	77 (99%)	1 (1%)	69	86
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	83
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	39 (95%)	2 (5%)	25	59
29	R5	51/52 (98%)	50 (98%)	1 (2%)	55	79
29	Y5	51/52 (98%)	47 (92%)	4 (8%)	12	42
30	R6	51/52 (98%)	48 (94%)	3 (6%)	19	53
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	53
36	RD	214/218 (98%)	212 (99%)	2 (1%)	78	90
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49	76
37	YE	165/166 (99%)	162 (98%)	3 (2%)	59	81
38	RF	161/166 (97%)	158 (98%)	3 (2%)	57	80
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	155 (100%)	0	100	100
39	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21	54
40	YH	145/148 (98%)	142 (98%)	3 (2%)	53	79
41	RI	122/124 (98%)	122 (100%)	0	100	100
41	YI	122/124 (98%)	118 (97%)	4 (3%)	38	68
42	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
42	YN	117/119 (98%)	115 (98%)	2 (2%)	60	82
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	97 (97%)	3 (3%)	41	71
44	RP	116/116 (100%)	115 (99%)	1 (1%)	78	90
44	YP	114/116 (98%)	114 (100%)	0	100	100
45	RQ	111/111 (100%)	111 (100%)	0	100	100
45	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	90
46	RR	100/101 (99%)	98 (98%)	2 (2%)	55	79
46	YR	100/101 (99%)	99 (99%)	1 (1%)	76	88
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47	75
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60	82
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52	78

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	30	63
52	YX	74/78 (95%)	72 (97%)	2 (3%)	44	73
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	71	87
All	All	9648/10066 (96%)	9536 (99%)	112 (1%)	71	87

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	XI	25	LYS
54	YZ	63	ASP
28	Y4	5	ILE
53	YY	79	CYS
47	YS	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
47	RS	38	GLN
50	RV	11	GLN
50	YV	11	GLN
37	YE	132	HIS
39	YG	132	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	309 (20%)	9 (0%)
1	XA	1514/1521 (99%)	322 (21%)	10 (0%)
22	QV	76/77 (98%)	17 (22%)	2 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QX	18/19 (94%)	4 (22%)	1 (5%)
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2915 (98%)	617 (21%)	40 (1%)
34	YA	2880/2915 (98%)	634 (22%)	44 (1%)
35	RB	119/122 (97%)	21 (17%)	1 (0%)
35	YB	119/122 (97%)	25 (21%)	1 (0%)
All	All	9207/9308 (98%)	1975 (21%)	109 (1%)

5 of 1975 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	38	G
1	QA	39	G

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	748	C
34	YA	278	A
34	YA	2402	C
1	XA	1064	G
34	YA	102	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	1MG	QV	37	22	18,26,27	1.43	3 (16%)	19,39,42	1.39	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	1MG	XV	37	22	18,26,27	0.72	0	19,39,42	1.43	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	QV	37	22	-	2/3/25/26	0/3/3/3
22	1MG	XV	37	22	-	2/3/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C5-C4	3.28	1.51	1.43
22	QV	37	1MG	C2-N3	2.48	1.38	1.34
22	QV	37	1MG	O6-C6	2.34	1.27	1.22

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	CM1-N1-C6	3.15	121.87	117.55
22	QV	37	1MG	C5-C6-N1	2.74	118.02	113.90
22	XV	37	1MG	C5-C6-N1	2.53	117.71	113.90
22	QV	37	1MG	CM1-N1-C2	2.44	123.25	120.72
22	QV	37	1MG	C2-N1-C6	-2.41	118.99	120.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	37	1MG	O4'-C4'-C5'-O5'
22	XV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	1MG	6	0
22	XV	37	1MG	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1110 ligands modelled in this entry, 1108 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	SF4	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	XD	301	4	-	-	0/6/5/5
56	SF4	QD	301	4	-	-	0/6/5/5

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	RI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RI	82:ARG	C	83:ALA	N	1.18

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

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

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

### 6.3 Carbohydrates

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

### 6.4 Ligands

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

### 6.5 Other polymers

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