



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:32 AM 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

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) : 2.36.2

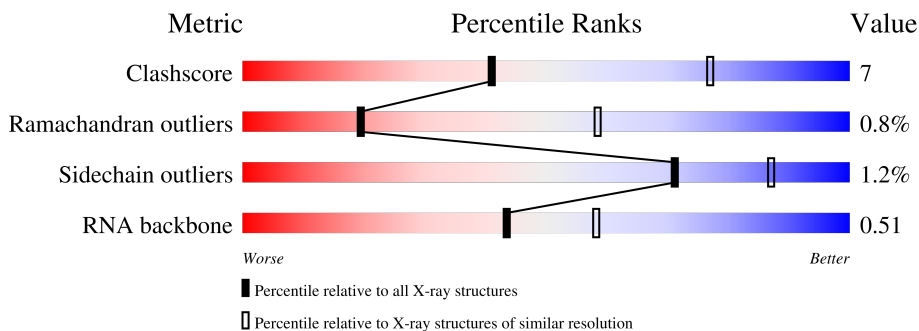
1 Overall quality at a glance

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 ≥ 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	

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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%

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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%

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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% . .

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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% ..

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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			

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

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

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

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

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

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

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

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

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

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

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

- 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			

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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			

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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
48	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
48	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

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

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

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

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

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

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

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

- 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: Fe₄S₄).



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).

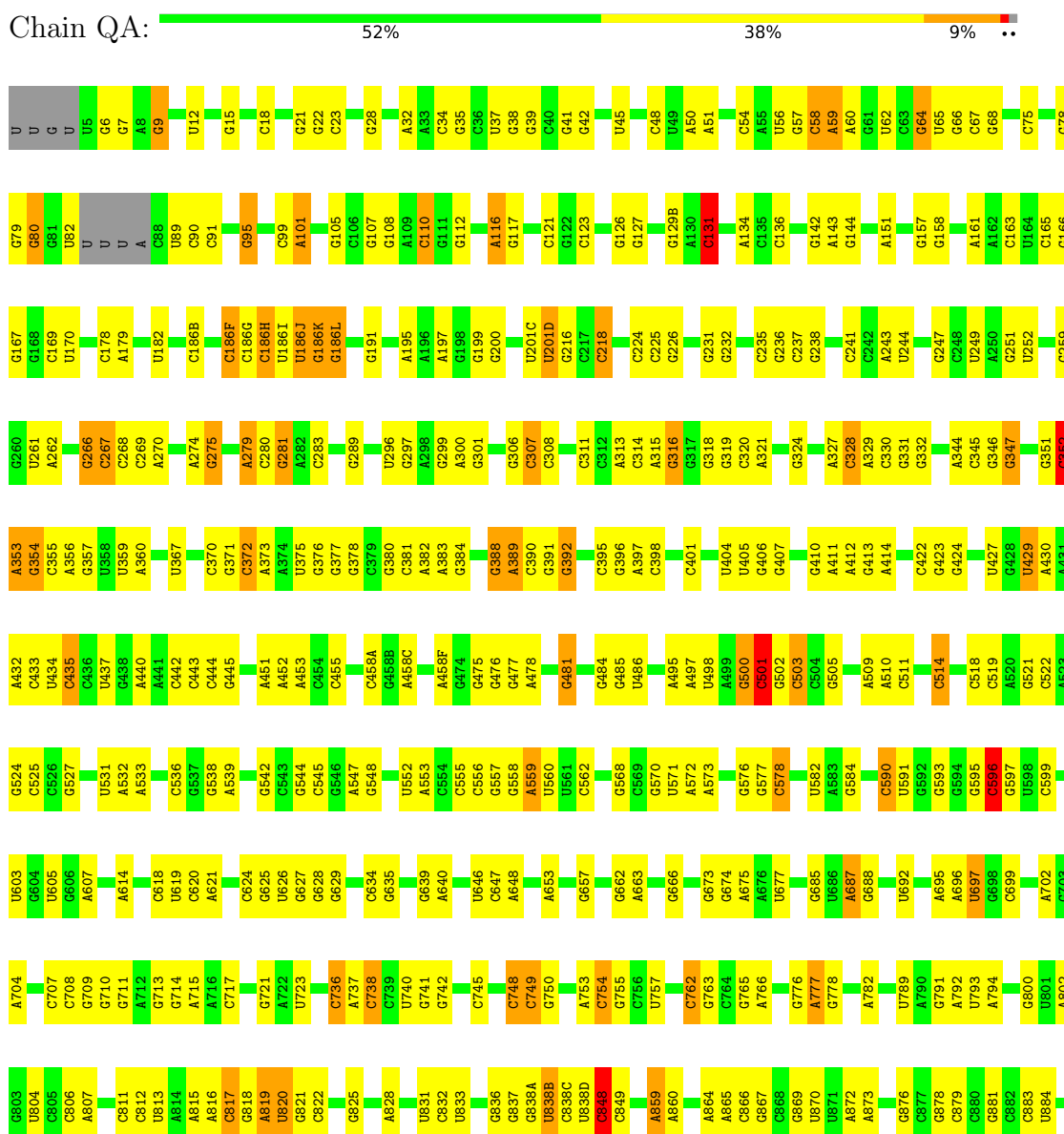
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	Y9	1	Total	Zn	0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

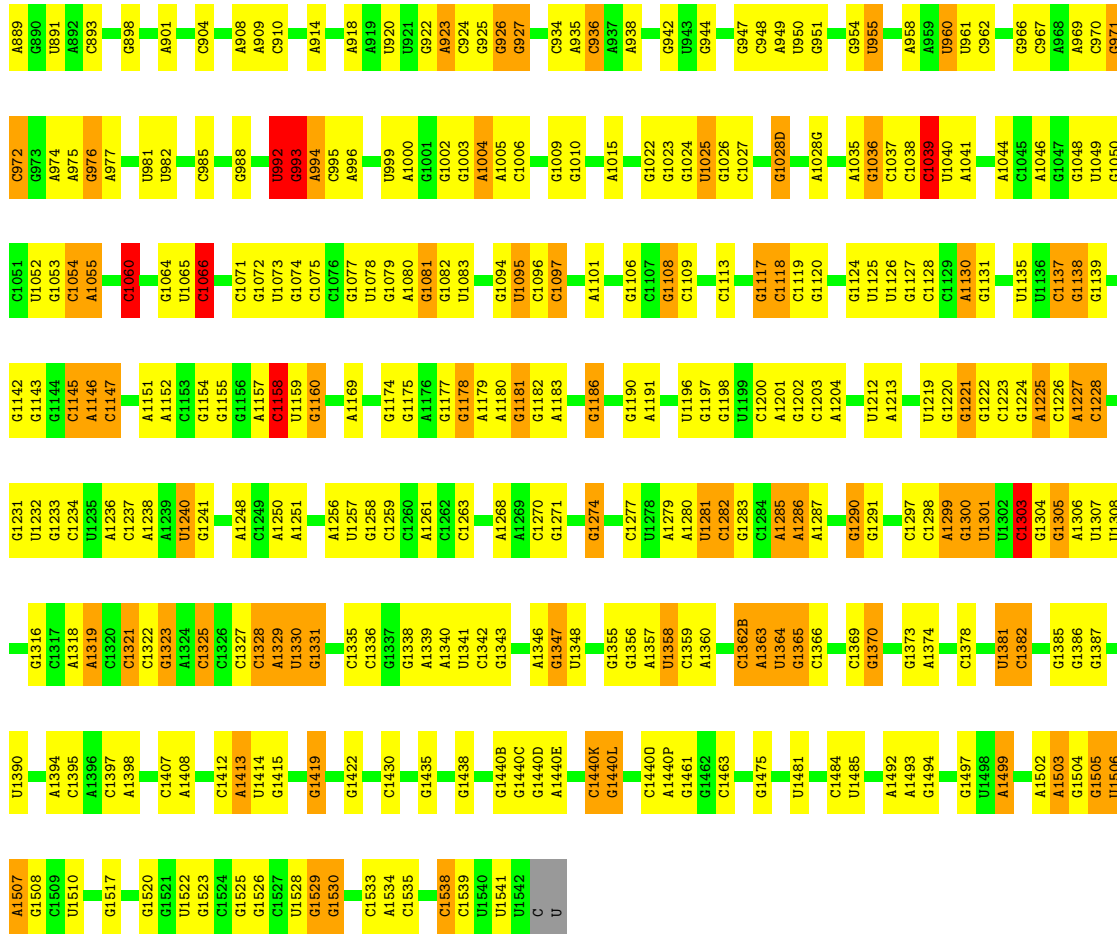
3 Residue-property plots [i](#)

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.

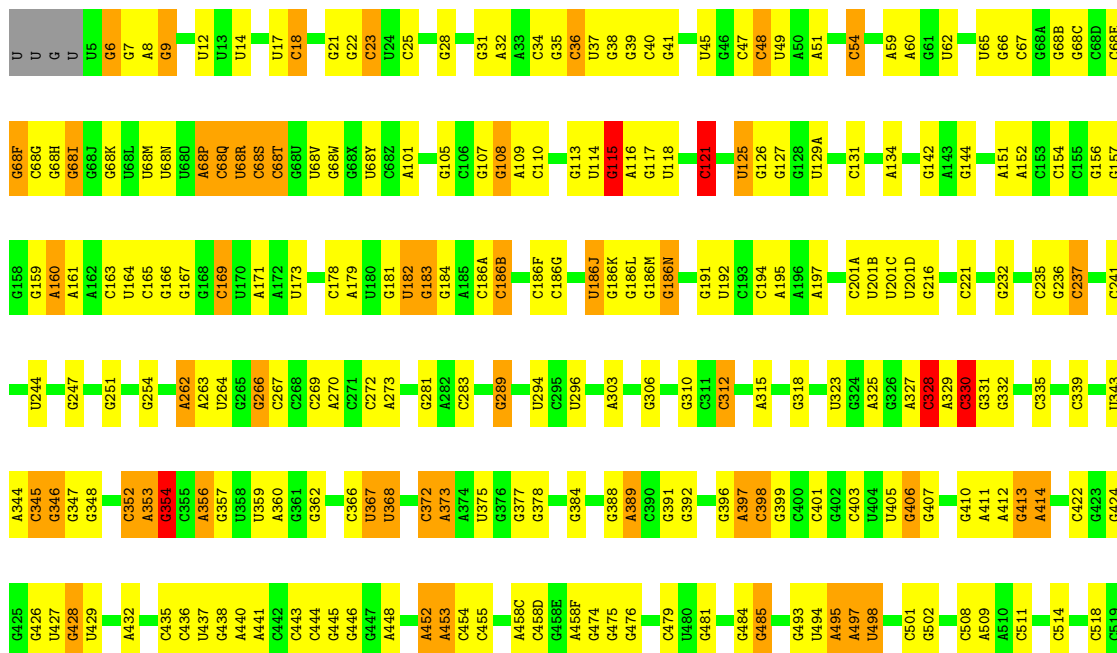
Note EDS failed to run properly.

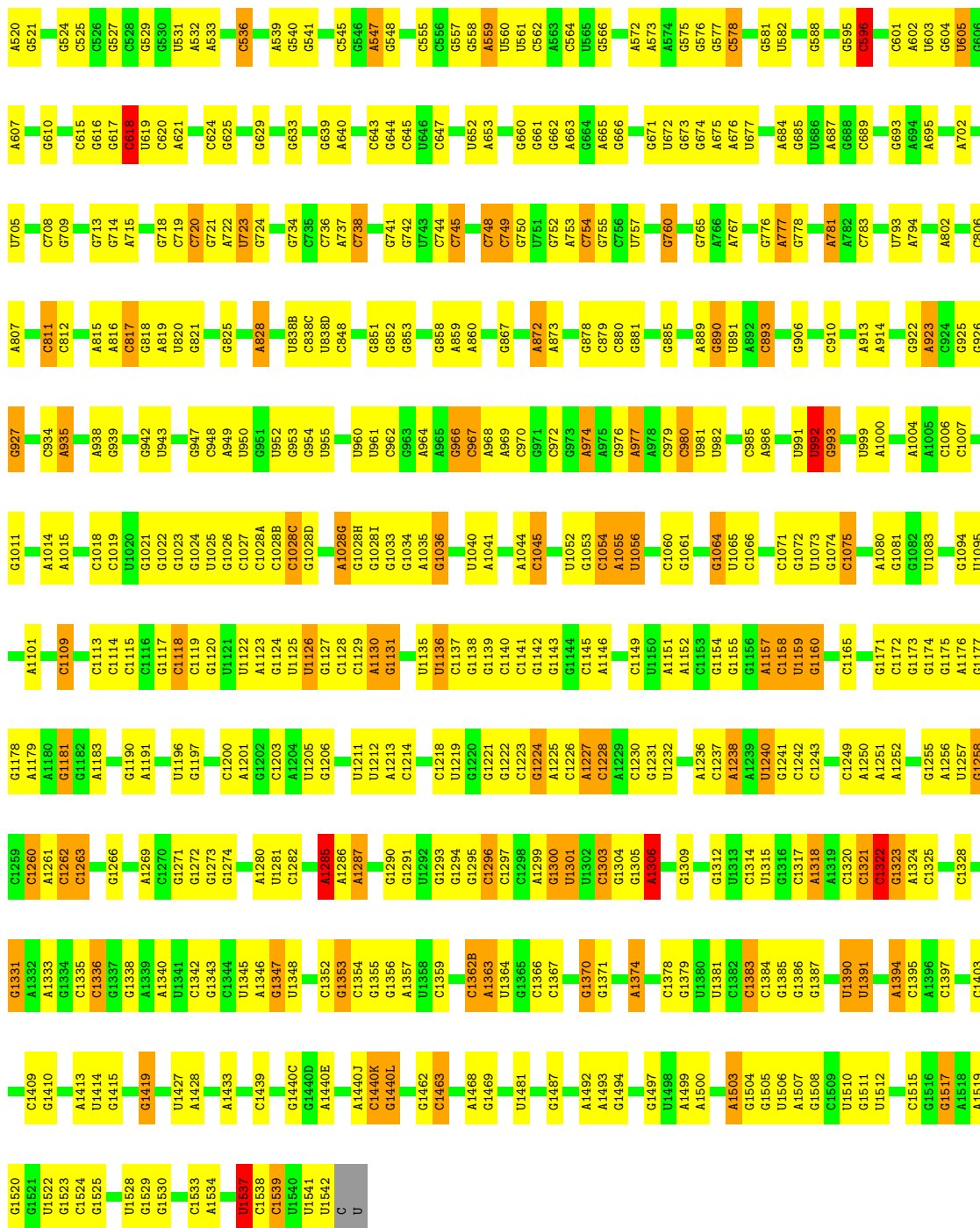
- Molecule 1: 16S rRNA



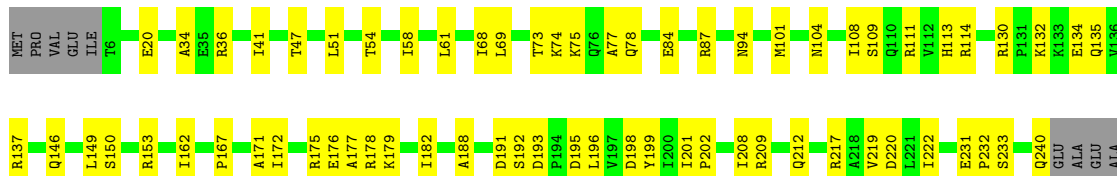


• Molecule 1: 16S rRNA





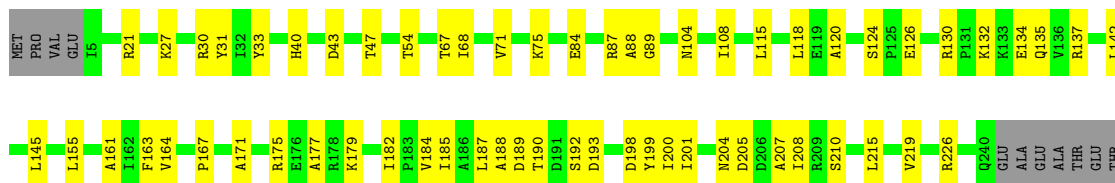
• Molecule 2: 30S ribosomal protein S2



THR
GLU
THR
PRO
GLU
GLY
GLU
SER
VAL
GLU
ALA

• Molecule 2: 30S ribosomal protein S2

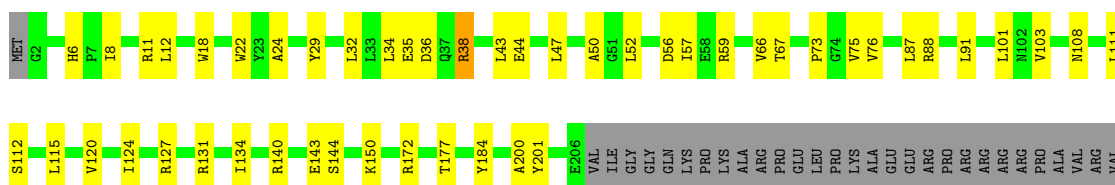
Chain XB: 68% 24% 8%



PRO
GLU
GLY
GLU
SER
GLU
VAL
GLU
ALA

• Molecule 3: 30S ribosomal protein S3

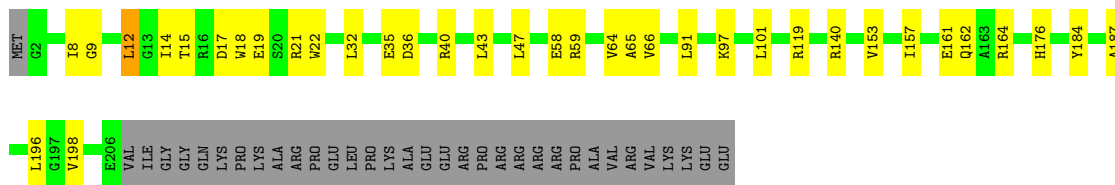
Chain QC: 65% 20% 14%



LYS
LYS
GLU
GLU

• Molecule 3: 30S ribosomal protein S3

Chain XC: 71% 15% 14%



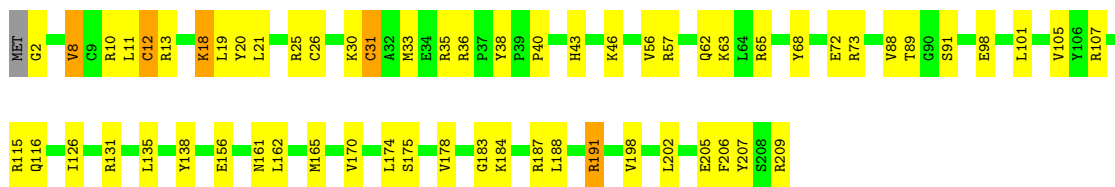
• Molecule 4: 30S ribosomal protein S4

Chain QD: 76% 22% 2%




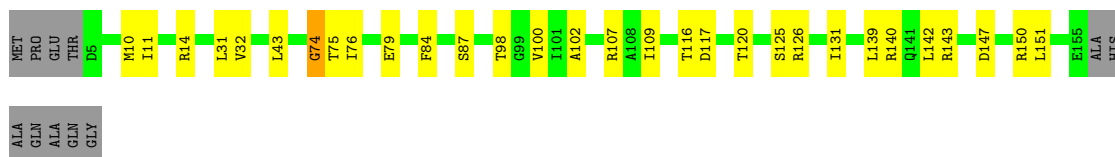
• Molecule 4: 30S ribosomal protein S4

Chain XD:  70% 27%



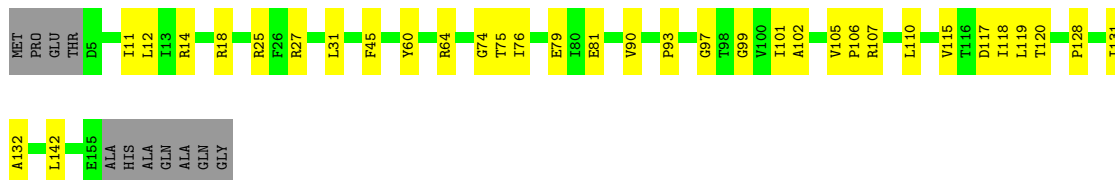
- Molecule 5: 30S ribosomal protein S5

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%




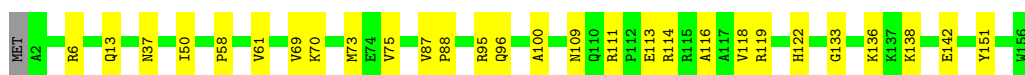
- Molecule 6: 30S ribosomal protein S6

Chain XF:  82% 18%

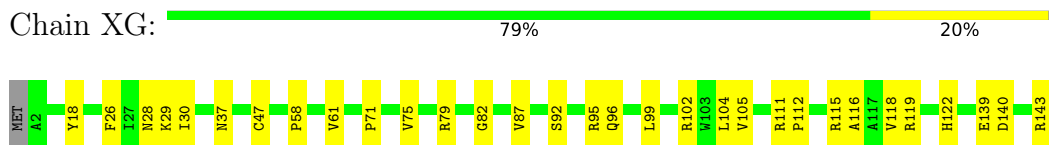


- Molecule 7: 30S ribosomal protein S7

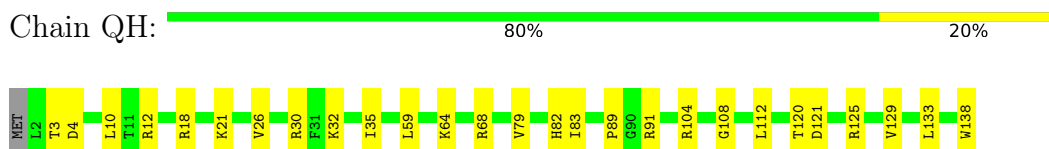
Chain QG:  81% 18%



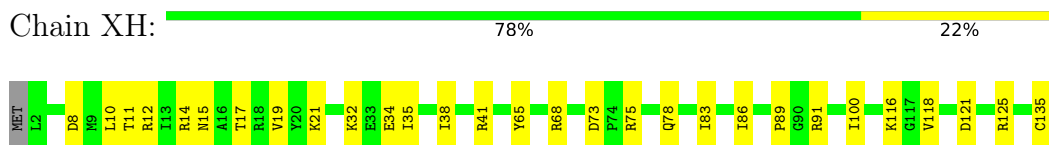
- Molecule 7: 30S ribosomal protein S7



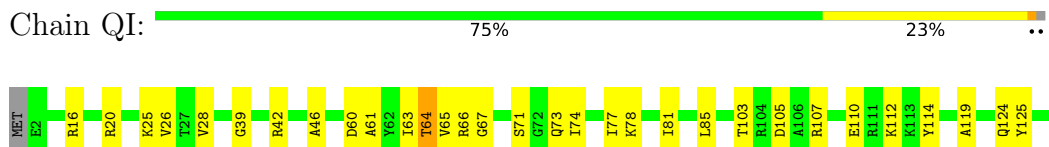
- Molecule 8: 30S ribosomal protein S8



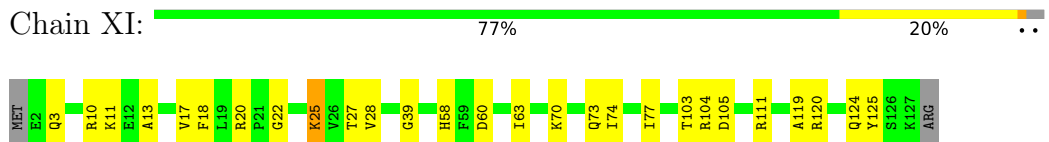
- Molecule 8: 30S ribosomal protein S8



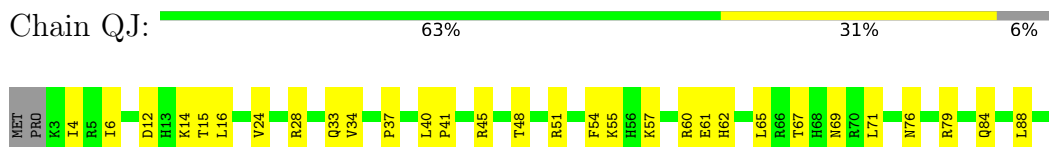
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9

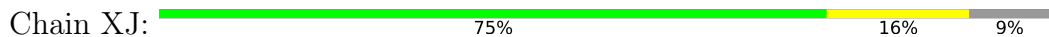


- Molecule 10: 30S ribosomal protein S10



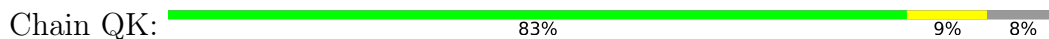
GLY
GLY
GLY
ARG

- Molecule 10: 30S ribosomal protein S10

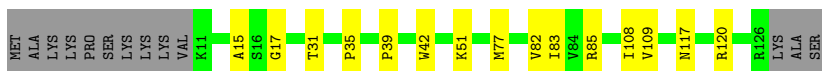
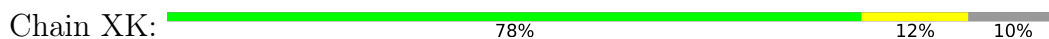




• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



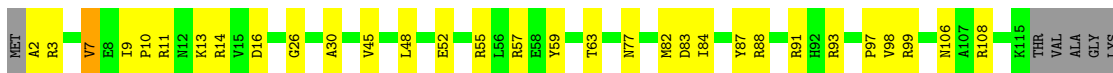
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



LYS
LYS
ALA
PRD
ARG
LYS

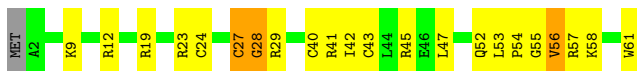
- Molecule 14: 30S ribosomal protein S14 type Z

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%




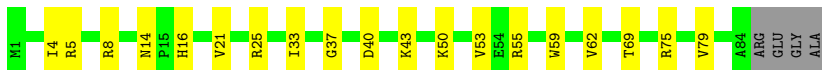
- Molecule 15: 30S ribosomal protein S15

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%

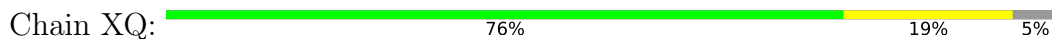


- Molecule 17: 30S ribosomal protein S17

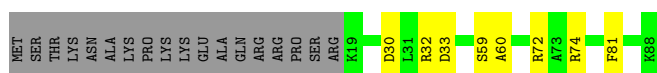
Chain QQ:  83% 12% 5%



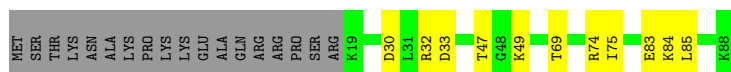
- Molecule 17: 30S ribosomal protein S17



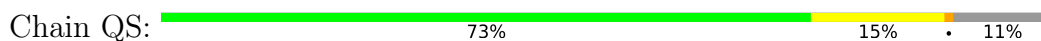
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

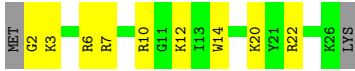


- Molecule 20: 30S ribosomal protein S20

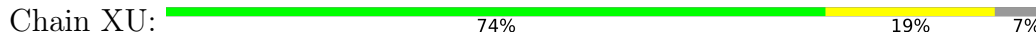




- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



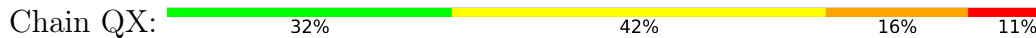
- Molecule 22: E-site tRNA-Pro



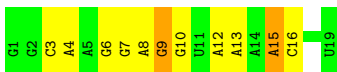
- Molecule 22: E-site tRNA-Pro



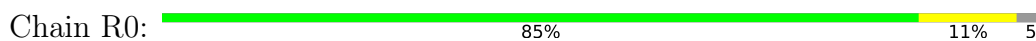
- Molecule 23: mRNA



- Molecule 23: mRNA

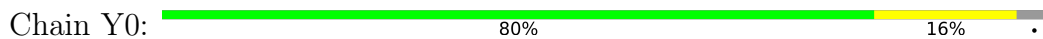


- Molecule 24: 50S ribosomal protein L27

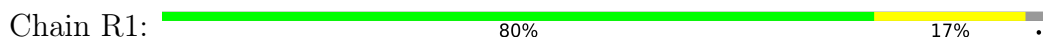




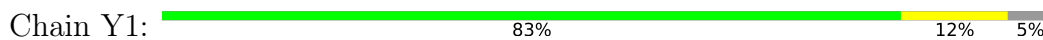
- Molecule 24: 50S ribosomal protein L27



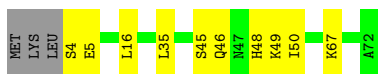
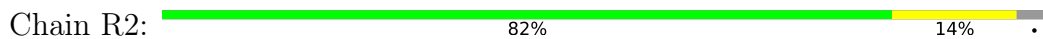
- Molecule 25: 50S ribosomal protein L28



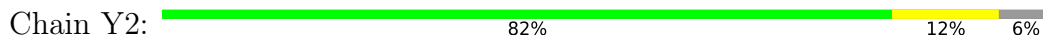
- Molecule 25: 50S ribosomal protein L28



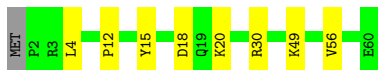
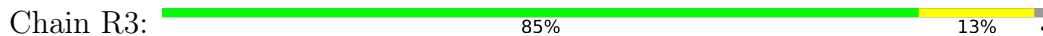
- Molecule 26: 50S ribosomal protein L29



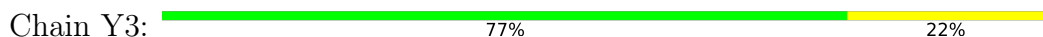
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

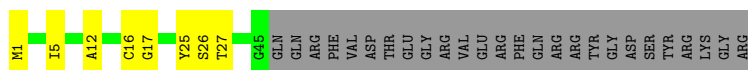


- Molecule 27: 50S ribosomal protein L30





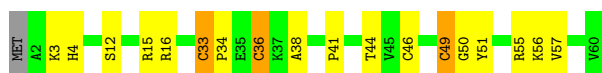
- Molecule 28: 50S ribosomal protein L31



- 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

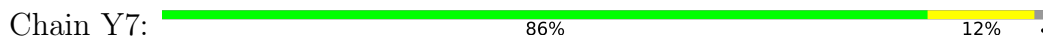


- Molecule 31: 50S ribosomal protein L34





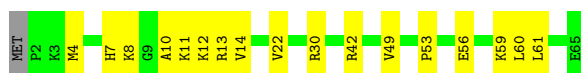
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



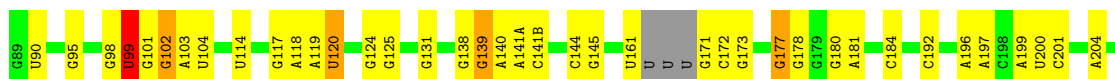
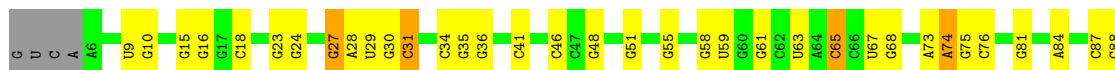
- Molecule 33: 50S ribosomal protein L36

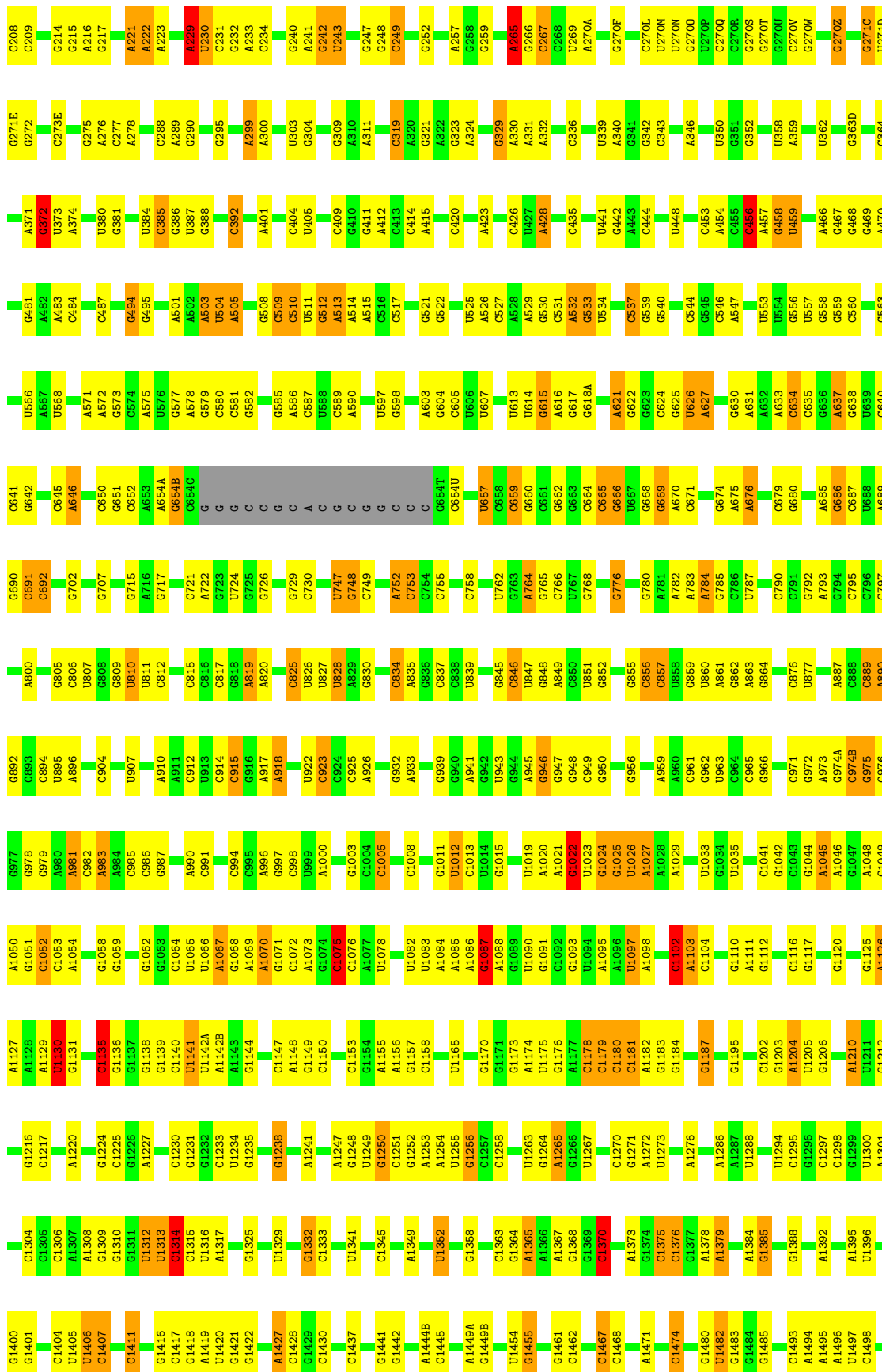


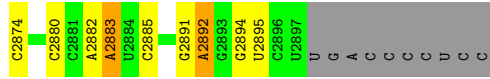
- Molecule 33: 50S ribosomal protein L36



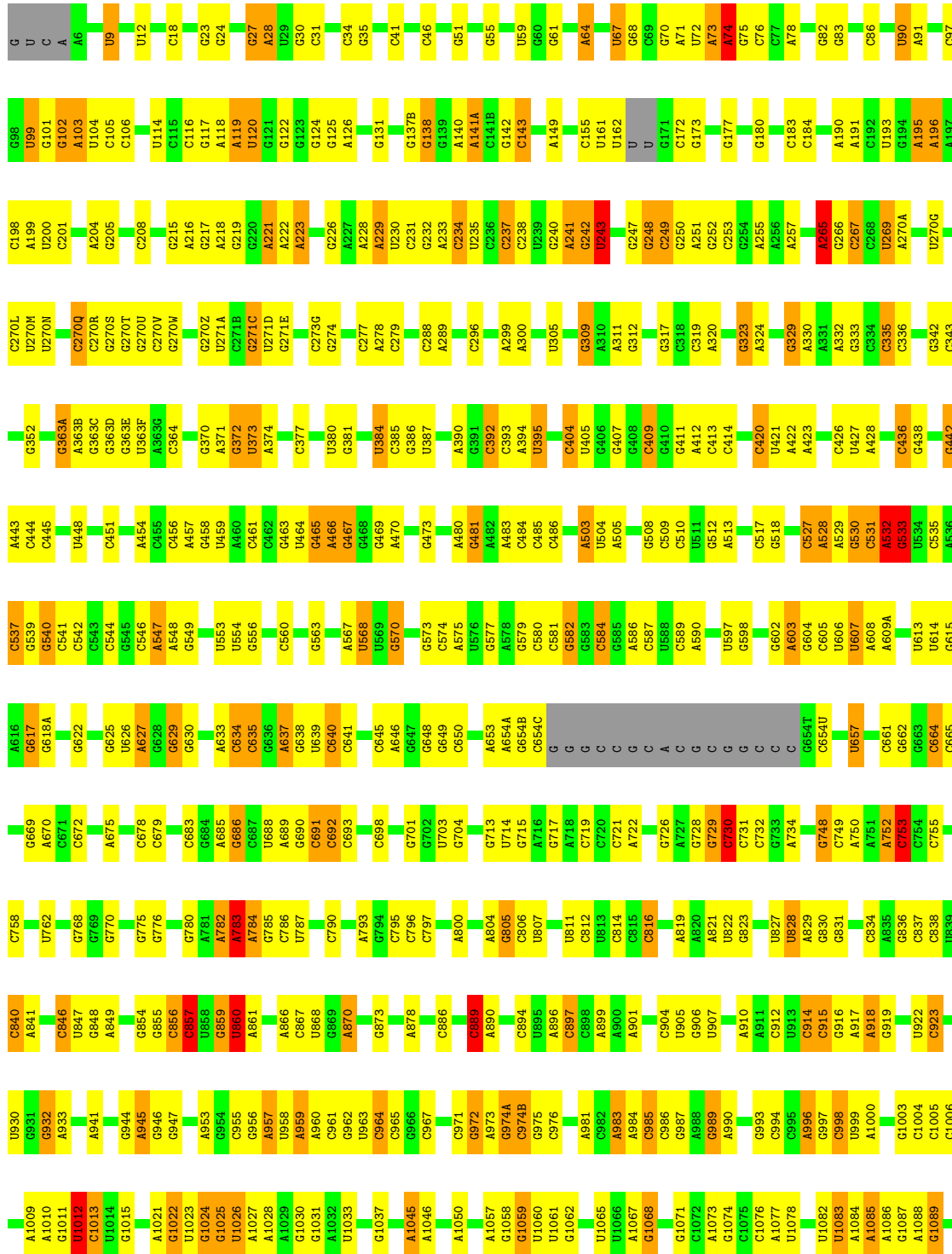
- Molecule 34: 23S rRNA



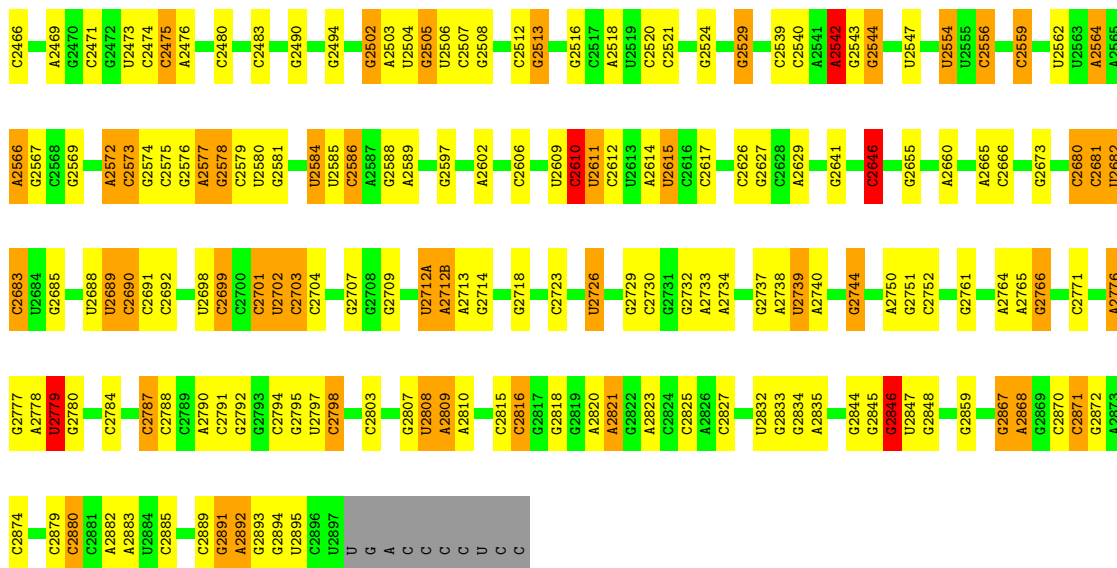




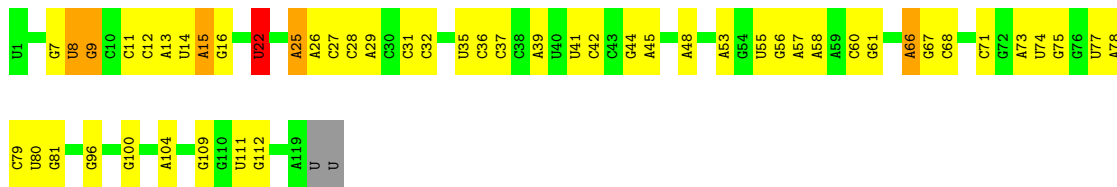
● Molecule 34: 23S rRNA



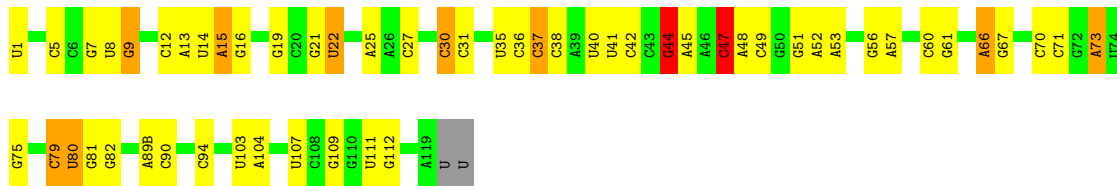
G1093	U1094	A1095	U1096	A1097	G1098	U1100	A1101	C1102	U1103	A1104	U1105	G1110	A1111	U1112	U1113	C1121	G1122	A1126	G1131	C1135	G1136	G1139	C1140	U1141	A1142A	A1142B	C1145	U1146	C1147	G1151	C1152	C1153	G1154	G1157	C1158	U1165	A1174	U1175	G1176	A1177	C1178	U1179	C1180	G1184																																																																					
C1185	G1186	A1187	U1188	G1193	A1194	C1195	U1196	G1203	A1204	U1205	G1206	A1210	U1211	G1212	G1215	C1217	U1218	G1219	A1220	G1224	C1225	G1226	U1227	G1228	C1233	U1240	U1242	C1235	G1236	A1237	G1238	G1244	G1245	A1246	G1250	C1251	G1252	A1253	U1254	U1255	G1256	C1257	G1264	A1265	G1266	U1267	C1270	A1272																																																																	
U1273	A1274	A1275	A1286	C1289	C1290	C1293	U1294	A1295	U1296	C1297	G1298	U1299	A1300	A1301	C1306	A1307	U1308	C1309	U1313	C1314	C1318	G1325	U1326	C1327	C1328	U1329	C1330	A1331	G1332	C1333	G1338	U1339	U1340	U1341	A1342	G1343	A1349	U1352	A1353	C1362	C1363	G1364	A1365	G1368	U1369	C1370	A1375	A1378	A1379	C1383	A1384	G1385	A1392	A1393	U1394	A1395	C1398	C1399	C1402	C1403	C1404	U1405	U1406	C1407	C1408	C1410	C1411	G1416	U1417	U1418	A1419	U1420	U1421	A1427	C1428	C1429	U1431	U1432	U1433	A1434	G1435	G1436	C1437	A1444B	C1445	U1448A	G1449B	G1455	G1461	C1462	C1463	C1467																					
C1468	A1471	A1472	G1473	C1474	A1477	G1478	G1479	U1480	U1482	G1483	G1484	G1485	A1490	C1493	U1497	C1498	C1499	G1500	C1506	A1507	A1508	C1509	A1510	A1511	G1512	U1516	G1519	U1520	G1526	C1533	G1534	U1535	A1536	C1537	G1538	A1543	C1544	A1545A	C1549	A1554	A1558	G1559	G1560	A1566	A1567	A1569	C1575	U1578	C1585	A1586	G1595	C1598	C1607	A1608	A1610	C1611	C1612	G1613	A1616	C1617	A1618	G1619	A1620	U1621	G1622	C1636	A1637	C1640	C1644	G1645	G1646	G1647	C1648	G1651	A1652	G1653	A1654	A1655	C1656	C1657	C1658	A1664	A1665	G1666	G1667	A1668	A1669	C1670																									
U1671	C1672	U1673	G1674	C1675	U1679	G1682	C1683	C1684	U1685	C1686	A1689	C1690	C1694	G1695	A1698	G1699	A1700	C1701	G1709	A1725	G1728	A1729	U1730	U1731	A1732	G1733	C1741	U1742	G1743	G1750	G1753	C1754	A1755	G1756	U1757	G1758	G1763	G1764	C1765	U1766	C1767	U1768	G1769	A1773	U1775	A1776	G1776	U1779	C1781	A1782	A1783	A1784	A1785	G1786	C1787	A1788	A1789	C1790	A1791	C1792	C1793	G1799	C1800	G1801	A1802	A1803	C1804	U1805	C1806	A1809	A1812	G1813	U1814	A1815	G1816	A1819	U1820	G1824	G1828	A1829	C1830	U1833	G1839	C1844	A1847	A1853	A1854	G1858	A1859	U1864	C1870																						
A1871	A1872	G1878	C1881	C1882	G1883	A1884	C1887	A1888	A1889	A1890	G1891	C1892	C1893	C1894	A1899	A1900	A1901	C1905	G1906	A1913	C1914	U1915	A1918	A1919	C1920	G1929	G1930	U1931	G1935	A1936	A1937	U1938	U1939	C1947	G1950	A1953	G1954	U1955	U1956	C1957	C1958	U1963	U1964	C1965	A1966	C1967	G1968	A1977	C1979	A1982	C1988	G1989	C1990	U1991	U1992	U1993	U1994	U1995	U1996	A2005	C2006	C2007	C2008	G2009	G2010	U2011	G2012	A2015	A2019	U2022	G2023	G2024	C2025	C2026	A2030	A2031	G2032	A2033	C2036	C2039	C2040	U2041	A2042	C2043	C2044	U2047	G2048	G2049	G2052	C2055																							
G2056	A2059	U2060	G2061	A2062	C2063	C2064	C2065	U2068	G2069	G2070	A2071	U2074	U2075	U2076	C2081	A2082	G2083	U2086	G2087	G2088	U2089	U2092	G2093	C2094	C2095	U2096	C2097	U2098	U2099	U2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	U2117	U2118	A2119	C2120	U2121	A2125	A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	C2136	C2137	C2140	G2141	C2145	G2148	C2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	C2159	G2160	C2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	U2172	A2173	C2176	A2177	C2175	A2178	G2179	G2180	C2181	G2182	C2183	G2184	C2185	C2186	G2187	G2188	C2189	G2191	G2192	G2193	A2197	U2197	A2198	C2199	A2202	C2194
G2210	G2211	A2212	G2234	G2235	G2236	G2237	G2238	G2239	U2243	U2244	U2245	G2246	U2249	G2250	G2253	C2254	C2260	C2261	A2266	A2267	A2268	A2269	A2273	A2274	C2275	A2278	G2279	G2280	C2281	G2282	C2283	G2284	C2285	A2286	A2287	A2288	U2291	C2292	C2293	C2294	G2299	C2300	C2301	A2311	U2312	C2313	C2314	G2315	C2316	G2317	G2318	U2319	A2320	G2321	G2325	C2326	A2327	A2328	G2329	G2330	G2334	A2335	U2341	U2342	U2343	G2344	A2345	A2346	C2347	U2348	C2349	C2350	G2351	A2352	G2353	C2354	C2355	G2356	U2357	C2358	C2359	C2368	G2369	C2371	C2374	G2375	A2376	C2382	C2383	C2384	G2385	A2386	U2387	A2388	U2391	G2392	C2393	C2394															
G2382	G2383	G2384	C2386	G2387	A2392	A2393	C2394	C2395	G2399	C2402	C2403	C2404	C2405	U2406	G2410	A2411	U2421	U2422	G2424	A2425	A2426	C2427	G2428	A2430	A2435	A2439	C2440	C2441	C2442	G2446	G2447	A2448	A2453	G2454	G2455	C2456	U2457	U2460	C2461	C2465	G2299	C2300	C2301	A2311	U2312	C2313	C2314	G2315	C2316	G2317	G2318	U2319	A2320	G2321	G2325	C2326	A2327	A2328	G2329	G2330	G2334	A2335	U2341	U2342	U2343	G2344	A2345	A2346	C2347	U2348	C2349	C2350	G2351	A2352	G2353	C2354	C2355	G2356	U2357	C2358	C2359	C2368	G2369	C2371	C2374	G2375	A2376	C2382	C2383	C2384	G2385	A2386	U2387	A2388	U2391	G2392	C2393	C2394															



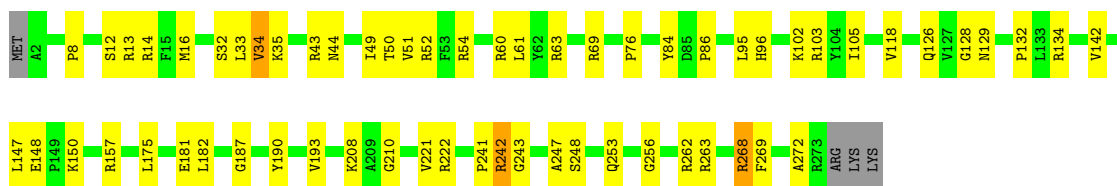
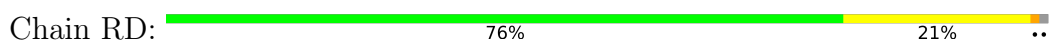
• Molecule 35: 5S rRNA



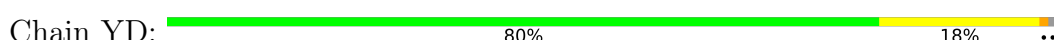
• Molecule 35: 5S rRNA

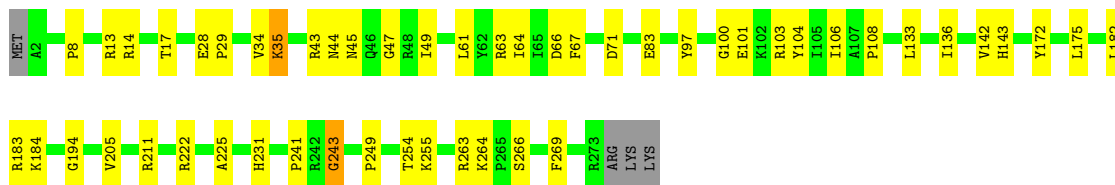


• Molecule 36: 50S ribosomal protein L2

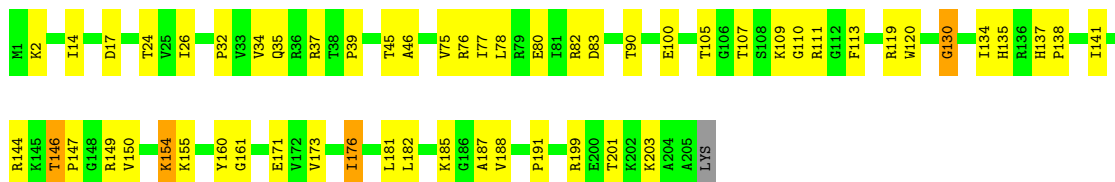


• Molecule 36: 50S ribosomal protein L2

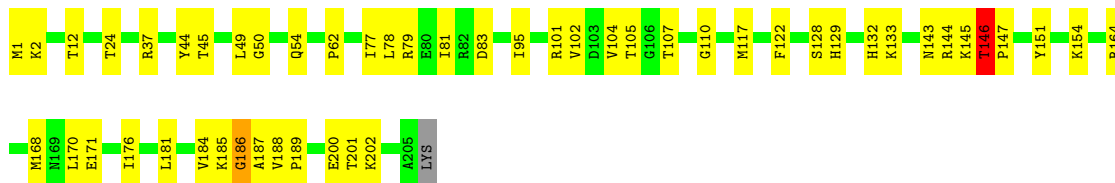
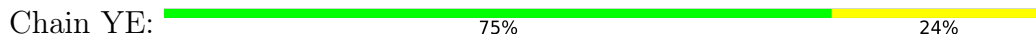




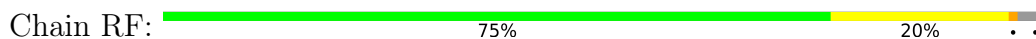
- Molecule 37: 50S ribosomal protein L3



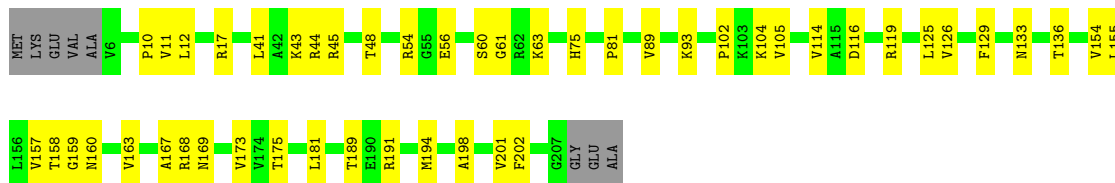
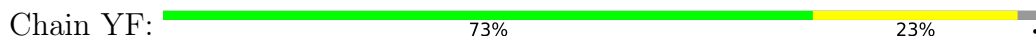
- Molecule 37: 50S ribosomal protein L3



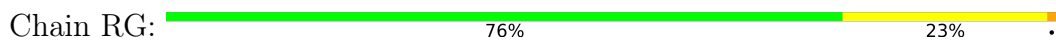
- Molecule 38: 50S ribosomal protein L4

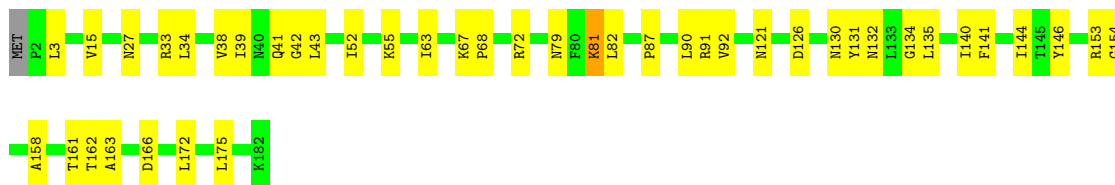


- Molecule 38: 50S ribosomal protein L4



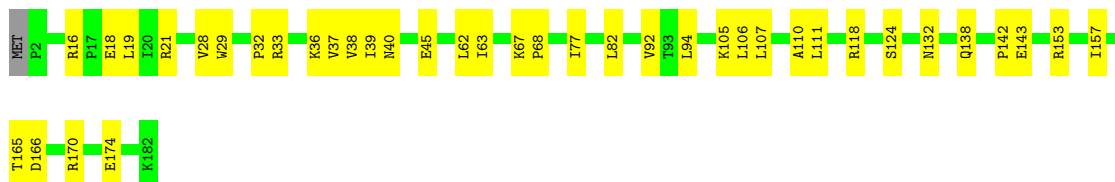
- Molecule 39: 50S ribosomal protein L5





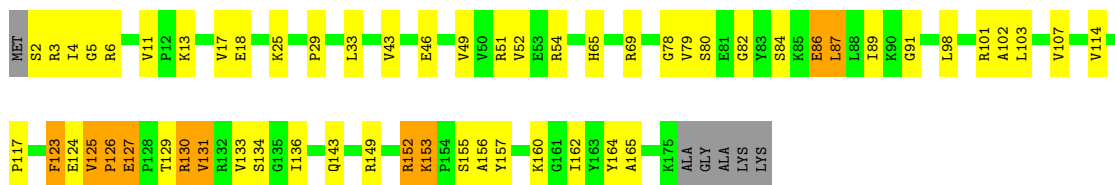
- Molecule 39: 50S ribosomal protein L5

Chain YG: 78% 21%



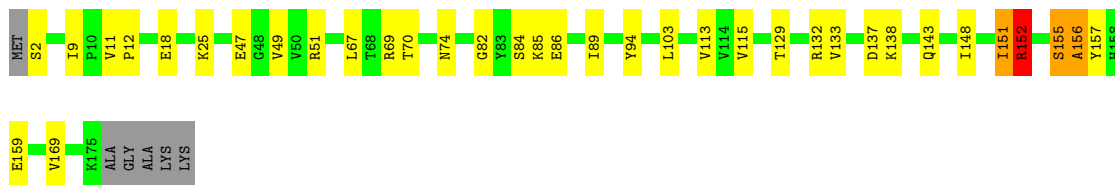
- Molecule 40: 50S ribosomal protein L6

Chain RH: 64% 27% 6%



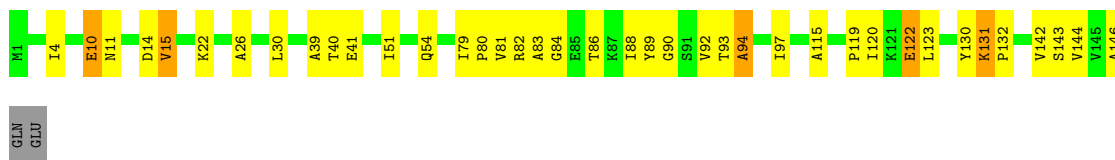
- Molecule 40: 50S ribosomal protein L6

Chain YH: 77% 18%



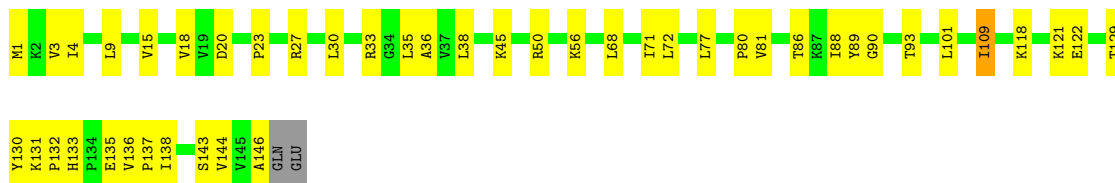
- Molecule 41: 50S ribosomal protein L9

Chain RI: 72% 23%



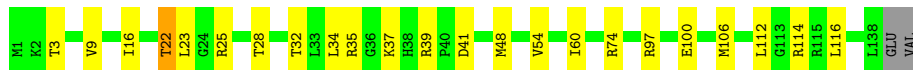
- Molecule 41: 50S ribosomal protein L9

Chain YI: 68% 30%



- Molecule 42: 50S ribosomal protein L13

Chain RN: 82% 16% ..



- Molecule 42: 50S ribosomal protein L13

Chain YN: 79% 20% .



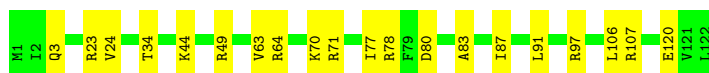
- Molecule 43: 50S ribosomal protein L14

Chain RO: 75% 25%



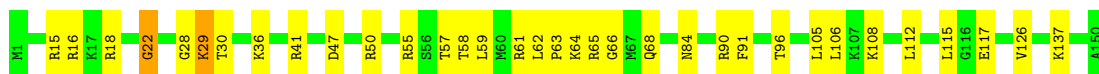
- Molecule 43: 50S ribosomal protein L14

Chain YO: 84% 16%



- Molecule 44: 50S ribosomal protein L15

Chain RP: 77% 21% .



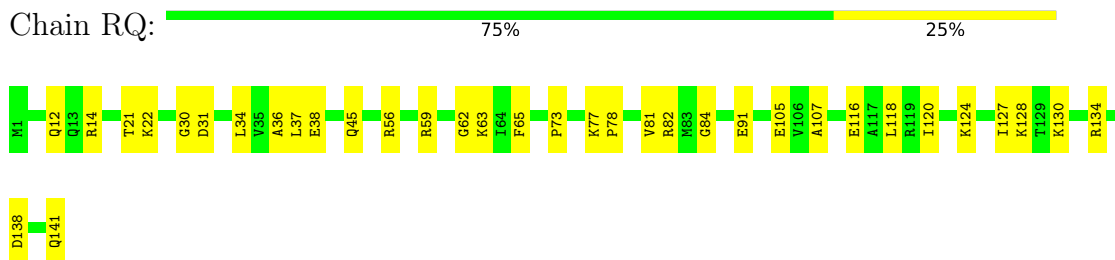
- Molecule 44: 50S ribosomal protein L15

Chain YP: 75% 23% .

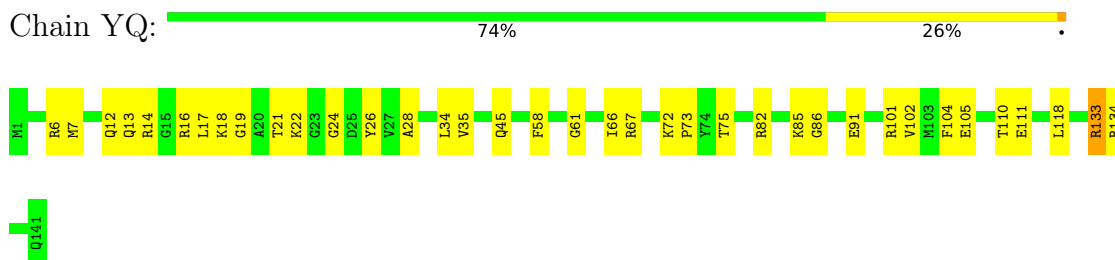


GLU
ALA

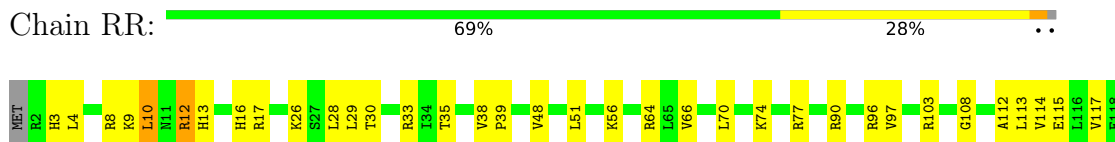
- Molecule 45: 50S ribosomal protein L16



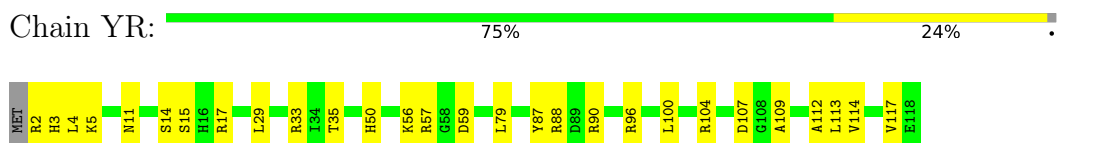
- Molecule 45: 50S ribosomal protein L16



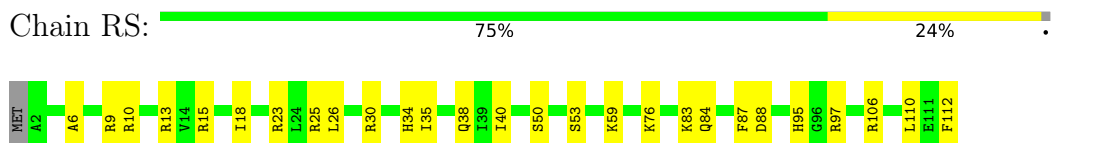
- Molecule 46: 50S ribosomal protein L17



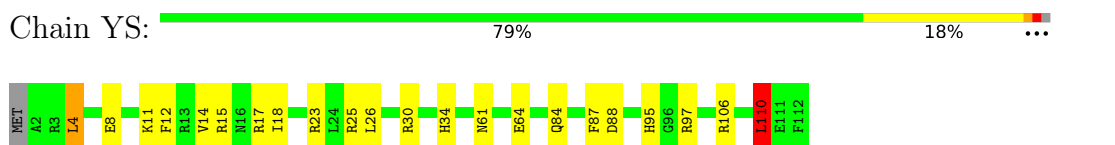
- Molecule 46: 50S ribosomal protein L17




- Molecule 47: 50S ribosomal protein L18

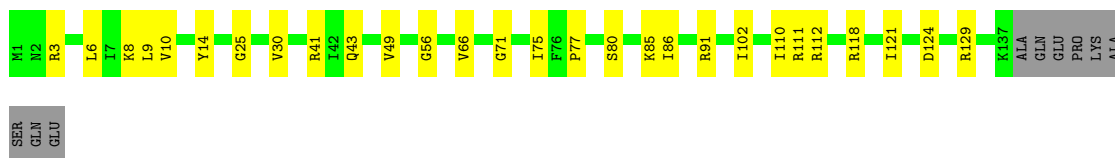


- Molecule 47: 50S ribosomal protein L18



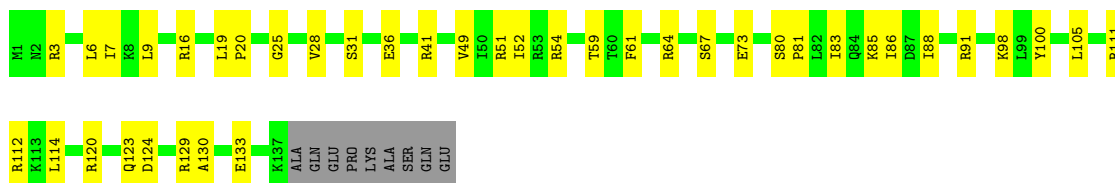
- Molecule 48: 50S ribosomal protein L19

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%

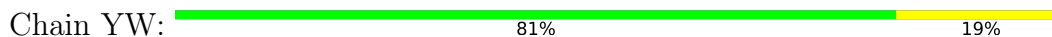


- Molecule 51: 50S ribosomal protein L22

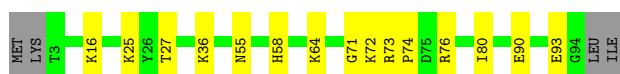
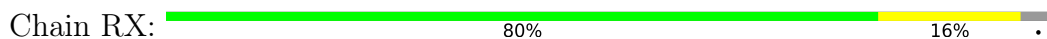
Chain RW:  79% 21%



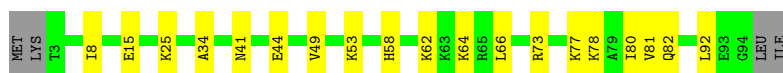
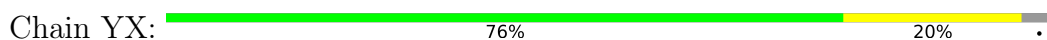
- Molecule 51: 50S ribosomal protein L22



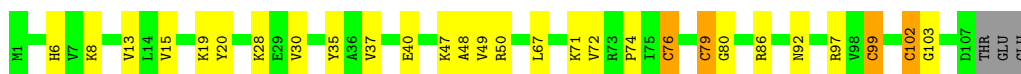
- Molecule 52: 50S ribosomal protein L23



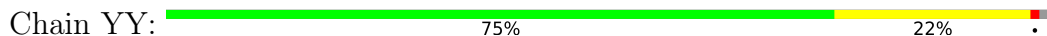
- Molecule 52: 50S ribosomal protein L23



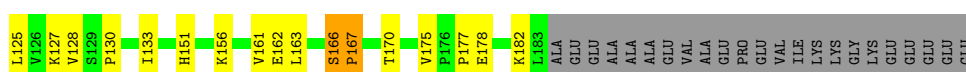
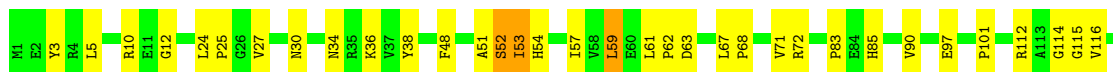
- Molecule 53: 50S ribosomal protein L24



- Molecule 53: 50S ribosomal protein L24

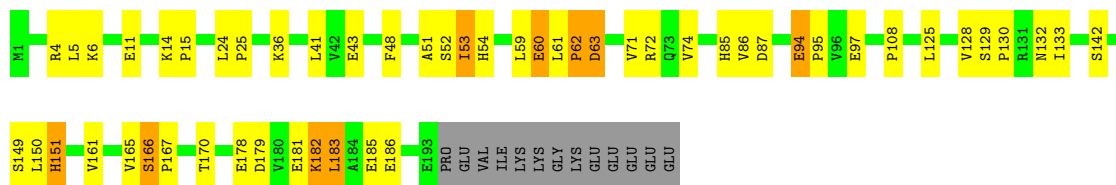


- Molecule 54: 50S ribosomal protein L25



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	75.0	Xtriage
Anisotropy	0.423	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	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

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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	Peptide,Mainchain
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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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%)

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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.