



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 12:21 AM EDT

PDB ID : 6BZ7
Title : Thermus thermophilus 70S containing 16S G299A point mutation and near-cognate ASL Leucine in A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.68 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)
Xtriage (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

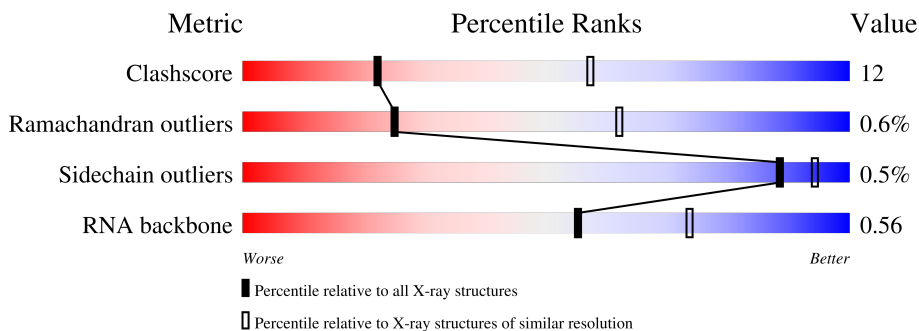
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RNA backbone	3102	1024 (4.30-3.00)

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	1508	45% 44% 10% ..
1	XA	1508	44% 45% 10% .
2	QB	256	61% 30% . 8%
2	XB	256	63% 28% . 8%
3	QC	239	65% 21% 14%
3	XC	239	66% 20% 14%

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Mol	Chain	Length	Quality of chain	
4	QD	209	68%	31%
4	XD	209	70%	29%
5	QE	162	71%	22% 7%
5	XE	162	77%	17% 7%
6	QF	101	74%	24%
6	XF	101	68%	32%
7	QG	156	81%	18%
7	XG	156	83%	16%
8	QH	138	74%	25%
8	XH	138	80%	20%
9	QI	128	65%	33%
9	XI	128	62%	36%
10	QJ	105	60%	33% 6%
10	XJ	105	69%	23% 9%
11	QK	129	65%	27% 8%
11	XK	129	66%	24% 10%
12	QL	132	72%	23% 5%
12	XL	132	70%	20% 8%
13	QM	126	59%	36% 5%
13	XM	126	61%	33% 6%
14	QN	61	72%	25%
14	XN	61	72%	25%
15	QO	89	80%	19%
15	XO	89	72%	26%
16	QP	88	66%	30% 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain	
28	RE	206	61%	37%
28	YE	206	59%	40%
29	RF	210	66%	30%
29	YF	210	63%	32%
30	RG	182	59%	40%
30	YG	182	54%	44%
31	RH	180	68%	26%
31	YH	180	64%	29%
32	RI	148	68%	30%
32	YI	148	70%	27%
33	RN	140	65%	33%
33	YN	140	71%	26%
34	RO	122	71%	28%
34	YO	122	78%	21%
35	RP	150	69%	31%
35	YP	150	61%	37%
36	RQ	141	62%	38%
36	YQ	141	60%	40%
37	RR	118	66%	33%
37	YR	118	65%	34%
38	RS	112	72%	26%
38	YS	112	71%	28%
39	RT	146	56%	37%
39	YT	146	55%	38%
40	RU	118	70%	27%





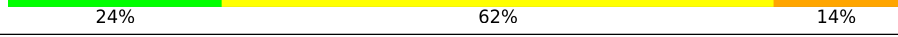
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Mol	Chain	Length	Quality of chain
40	YU	118	70% 27% ..
41	RV	101	64% 35% .
41	YV	101	71% 29%
42	RW	113	74% 24% .
42	YW	113	75% 23% .
43	RX	96	71% 25% .
43	YX	96	63% 33% .
44	RY	110	78% 19% .
44	YY	110	76% 21% .
45	RZ	206	56% 32% . 11%
45	YZ	206	59% 29% . 11%
46	R0	85	66% 29% 5%
46	Y0	85	59% 28% . 12%
47	R1	98	73% 26% .
47	Y1	98	61% 34% 5%
48	R2	72	71% 25% .
48	Y2	72	67% 29% .
49	R3	60	67% 32% .
49	Y3	60	63% 35% .
50	R4	71	69% 25% . .
50	Y4	71	66% 27% . .
51	R5	60	90% 8% .
51	Y5	60	85% 13% .
52	R6	54	81% 17% .
52	Y6	54	89% 9% .

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Mol	Chain	Length	Quality of chain
53	R7	49	 63% 33% .
53	Y7	49	 71% 27% .
54	R8	65	 65% 31% . .
54	Y8	65	 69% 26% . .
55	R9	37	 38% 62%
55	Y9	37	 24% 62% 14%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295575 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	1500	Total 32246	C 14353	N 5981	O 10413	P 1499	0	0	0
1	XA	1500	Total 32248	C 14354	N 5984	O 10411	P 1499	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	299	A	G	engineered mutation	GB 55771382
XA	299	A	G	engineered mutation	GB 55771382

- 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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
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			
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	119	Total	C	N	O	S	0	0	0
			946	585	195	164	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
23	XX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			
24	XY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	RA	2882	Total 62071	C 27627	N 11611	O 19952	P 2881	0	0	0
25	YA	2883	Total 62091	C 27636	N 11613	O 19960	P 2882	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
50	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	68	Total	Mg	0	0
			68	68		
56	QC	1	Total	Mg	0	0
			1	1		
56	QE	1	Total	Mg	0	0
			1	1		
56	QF	1	Total	Mg	0	0
			1	1		

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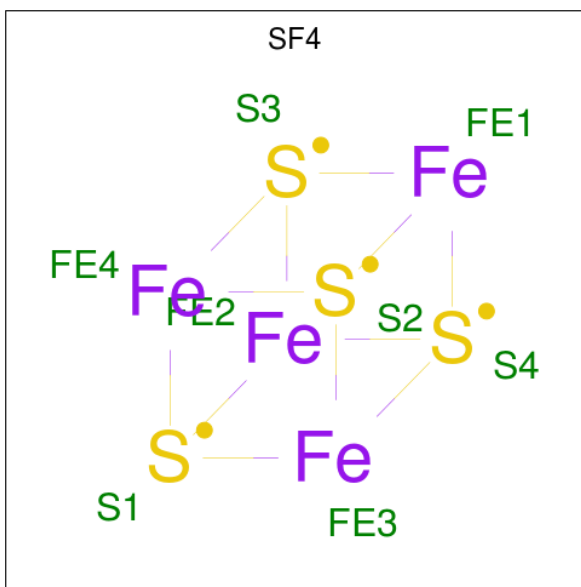
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QH	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	QV	6	Total 6	Mg 6	0	0
56	QY	1	Total 1	Mg 1	0	0
56	RA	508	Total 508	Mg 508	0	0
56	RB	7	Total 7	Mg 7	0	0
56	RE	2	Total 2	Mg 2	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RN	1	Total 1	Mg 1	0	0
56	RO	2	Total 2	Mg 2	0	0
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56	RR	1	Total 1	Mg 1	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	4	Total 4	Mg 4	0	0
56	R1	2	Total 2	Mg 2	0	0
56	R4	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XA	82	Total 82	Mg 82	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0
56	XS	1	Total 1	Mg 1	0	0
56	XV	6	Total 6	Mg 6	0	0
56	YA	546	Total 546	Mg 546	0	0
56	YB	12	Total 12	Mg 12	0	0
56	YD	2	Total 2	Mg 2	0	0
56	YE	2	Total 2	Mg 2	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	3	Total 3	Mg 3	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YX	2	Total 2	Mg 2	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QN	1	Total	Zn	0	0
			1	1		
58	RY	1	Total	Zn	0	0
			1	1		
58	R4	1	Total	Zn	0	0
			1	1		
58	R5	1	Total	Zn	0	0
			1	1		
58	R6	1	Total	Zn	0	0
			1	1		
58	R9	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	YY	1	Total	Zn	0	0
			1	1		
58	Y4	1	Total	Zn	0	0
			1	1		
58	Y5	1	Total	Zn	0	0
			1	1		

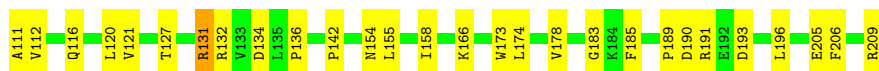
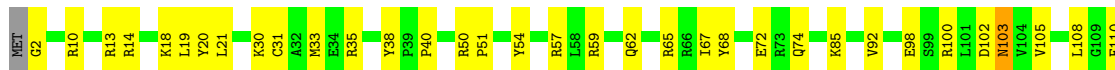
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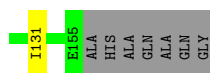
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y6	1	Total 1	Zn 1	0	0
58	Y9	1	Total 1	Zn 1	0	0



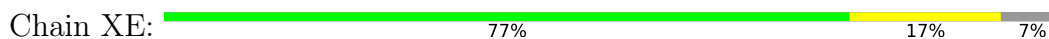
- Molecule 4: 30S ribosomal protein S4



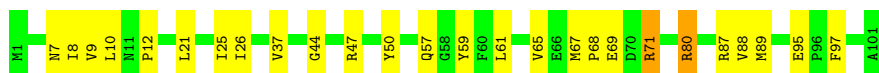
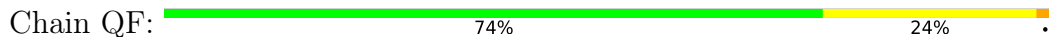
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5




- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6




- Molecule 7: 30S ribosomal protein S7

Chain QG:  81% 18%




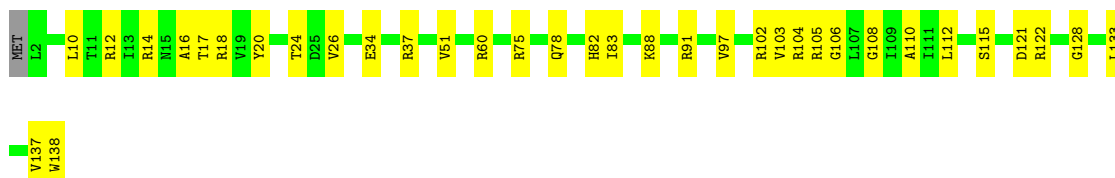
- Molecule 7: 30S ribosomal protein S7

Chain XG:  83% 16%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  74% 25%



- Molecule 8: 30S ribosomal protein S8

Chain XH:  80% 20%



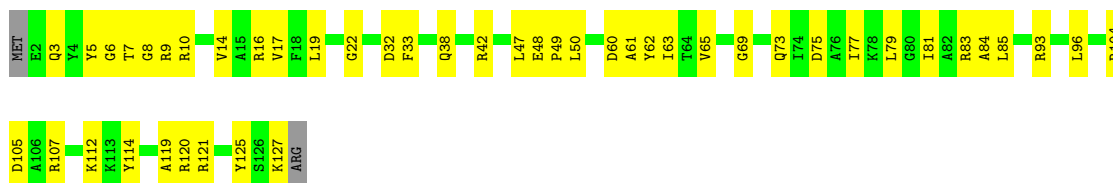
- Molecule 9: 30S ribosomal protein S9

Chain QI:  65% 33%



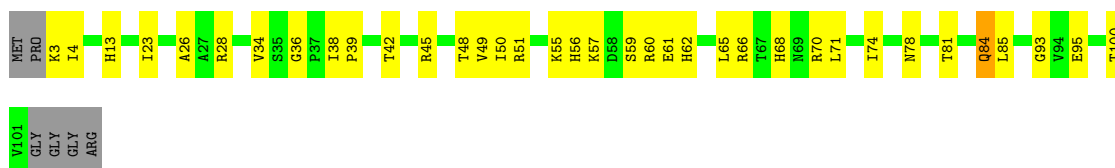
- Molecule 9: 30S ribosomal protein S9

Chain XI:  62% 36%



- Molecule 10: 30S ribosomal protein S10

Chain QJ:  60% 33% 6%



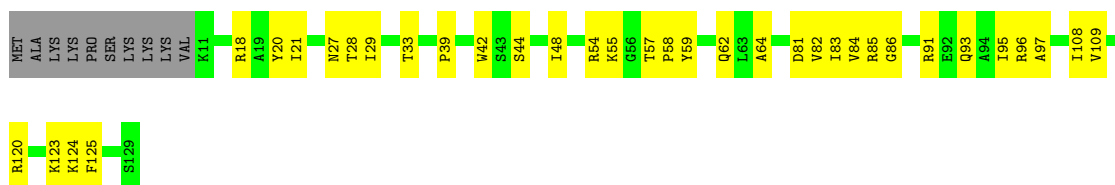
- Molecule 10: 30S ribosomal protein S10

Chain XJ:  69% 23% 9%



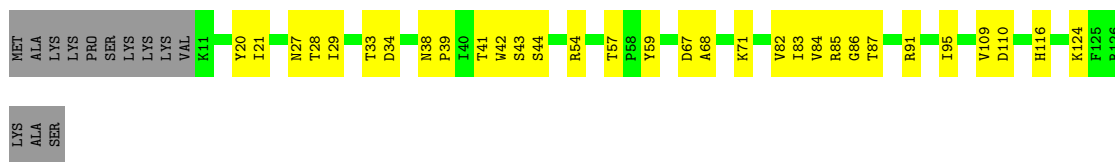
- Molecule 11: 30S ribosomal protein S11

Chain QK:  65% 27% 8%



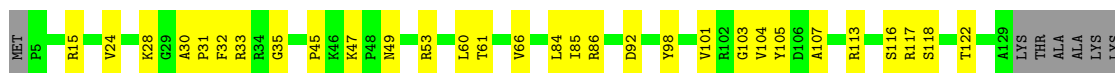
- Molecule 11: 30S ribosomal protein S11

Chain XK:  66% 24% 10%



- Molecule 12: 30S ribosomal protein S12

Chain QL:  72% 23% 5%



- Molecule 12: 30S ribosomal protein S12

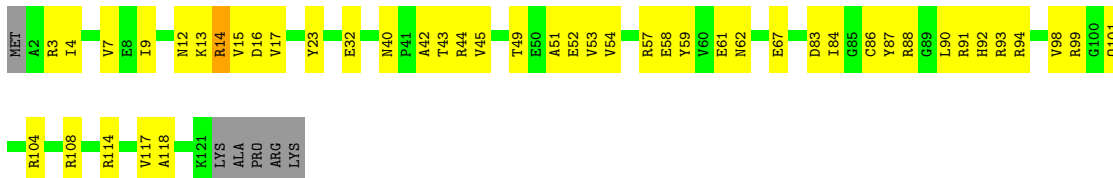
Chain XL:  70% 20% 8%



LYS
LYS

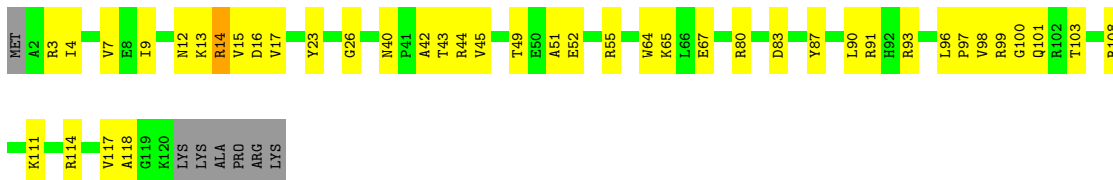
- Molecule 13: 30S ribosomal protein S13

Chain QM:  59% 36% • 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  61% 33% • 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  72% 25% ••




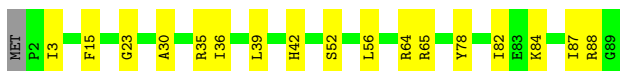
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  72% 25% ••



- Molecule 15: 30S ribosomal protein S15

Chain QO:  80% 19% •

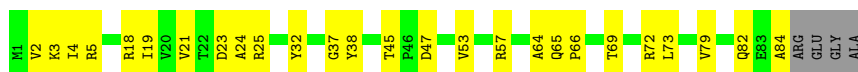


- Molecule 15: 30S ribosomal protein S15

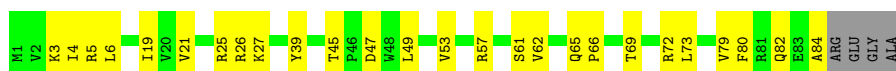
Chain XO:  72% 26% •



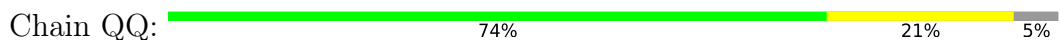
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

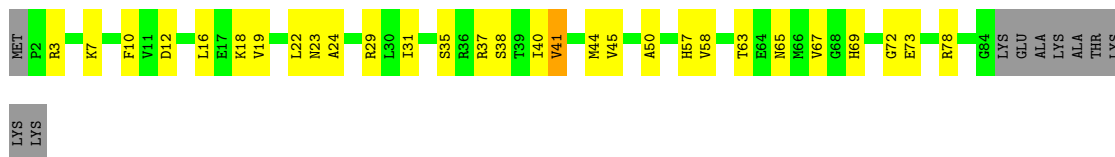


- Molecule 18: 30S ribosomal protein S18



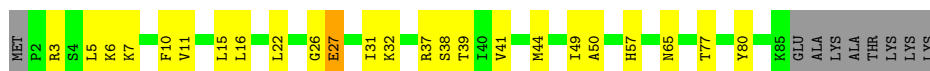
- Molecule 19: 30S ribosomal protein S19





- Molecule 19: 30S ribosomal protein S19

Chain XS: 65% 25% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 69% 25% 7%



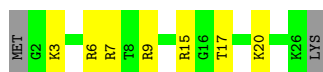
- Molecule 20: 30S ribosomal protein S20

Chain XT: 72% 22% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 67% 26% 7%



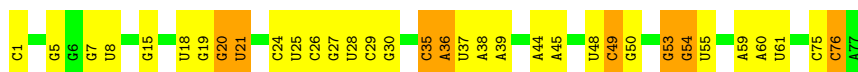
- Molecule 21: 30S ribosomal protein Thx

Chain XU: 52% 41% 7%

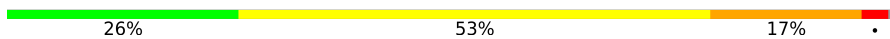


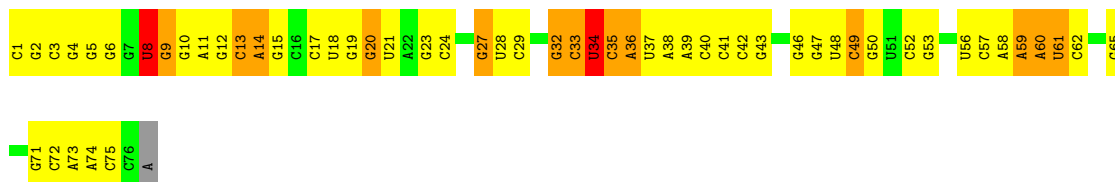
- Molecule 22: tRNA fMet

Chain QV: 56% 34% 10%



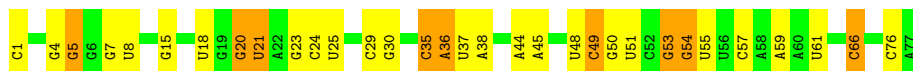
- Molecule 22: tRNA fMet

Chain QW:  26% 53% 17%



- Molecule 22: tRNA fMet

Chain XV:  58% 30% 12%



- Molecule 22: tRNA fMet

Chain XW:  26% 48% 22%



- Molecule 23: messenger RNA

Chain QX:  32% 68%



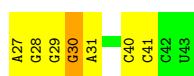
- Molecule 23: messenger RNA

Chain XX:  28% 8% 60%



- Molecule 24: ASL Leu

Chain QY:  59% 35% 6%

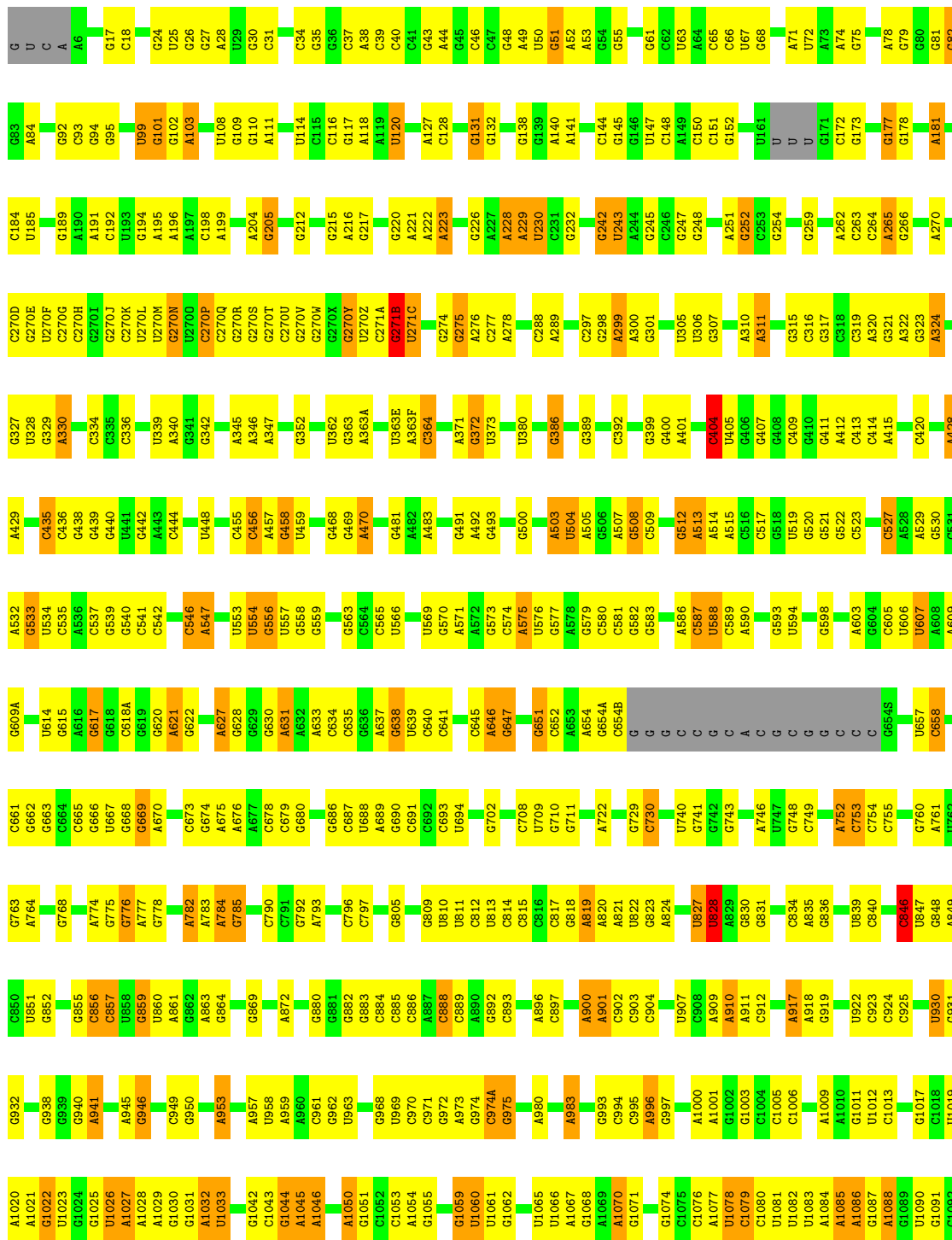


- Molecule 24: ASL Leu

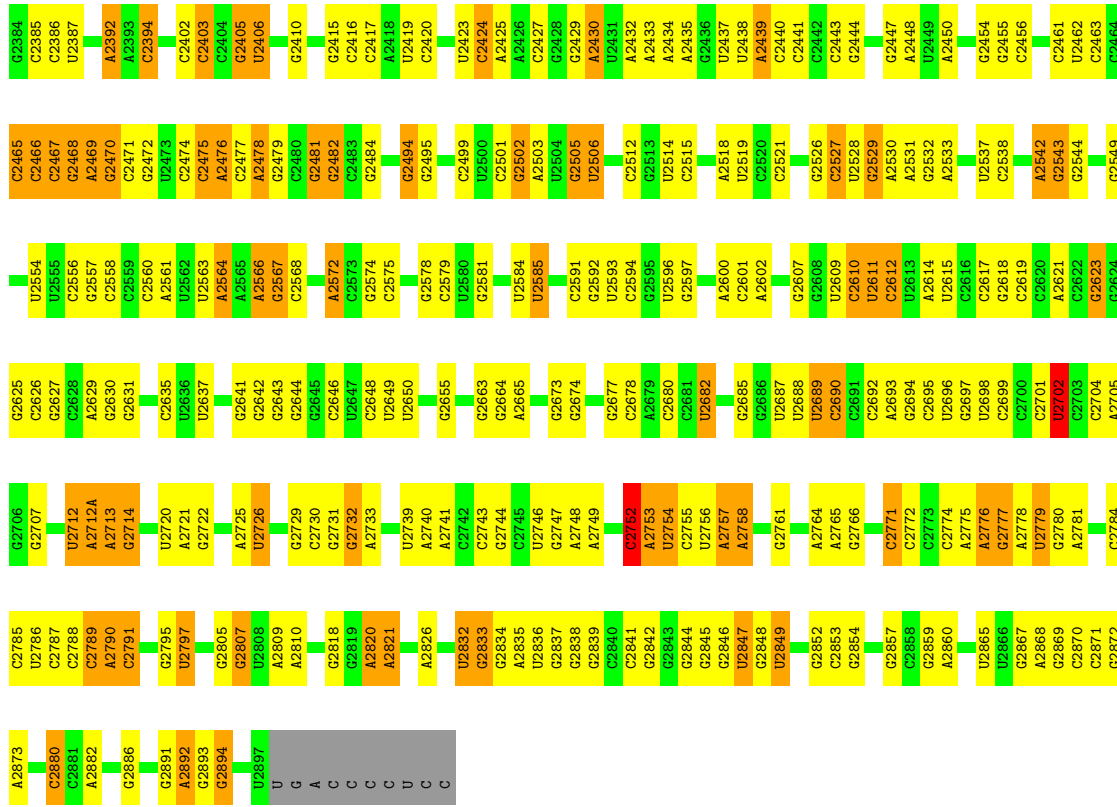
Chain XY:  41% 53% 6%



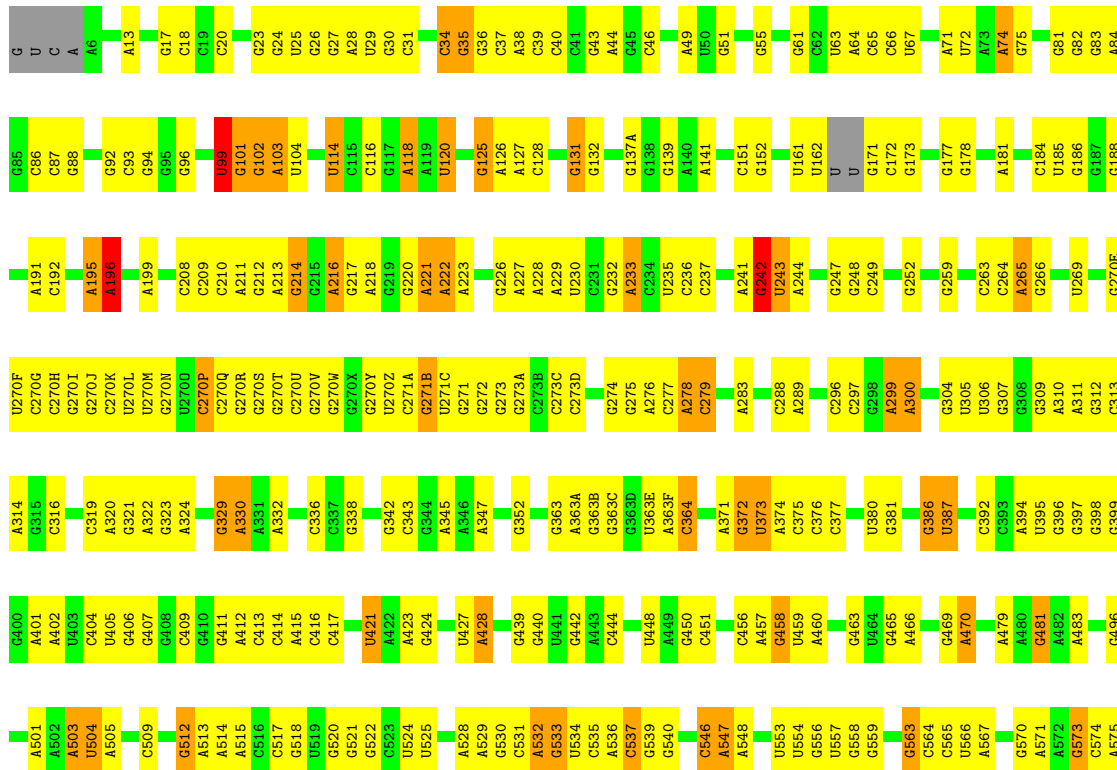
● Molecule 25: 23S rRNA

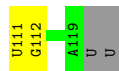


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A1095	A1177	G1258	G1338	A1419	A1494	G1568	U1659	G1764	U1851	U1955	C2043	C2128	G2220	A2309
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G1151			G1309	G1466	U1540	C1630A	C1710	U1818	C1924	G2024	G2104			
C1152	U1234		G1310	C1467	U1541		G1725	U1820	A1927	C2025	C2108			
G1153	G1235		G1311	C1468	G1542		G1726	A1825	A1928	C2026	U2109			
G1154	G1236		U1312	C1469	U1543		G1727	G1826	G1929	G2027	G2110			
A1155	A1237		C1313	A1469	A1544		G1728	G1827	U1930	G2028	C2111			
A1156	G1238		C1314	C1470	C1545		U1729	C1828	U1931	G2029	C2112			
G1157	G1239		U1316	A1471	A1545		G1730	G1829	G1932	A2030	U2113			
	U1240		A1317	A1472	C1550		G1731	A1830	G1935	A2031	U2114			
G1164	A1246		A1321	C1476	C1551		G1732	A1831	G1936	G2032	A2115			
U1165	A1247		A1322	U1477	C1552		G1733	A1832	A1937	A2033	G2116			
C1166	G1248		A1323	G1478	C1553		G1734	A1833	U1938	A2034	U2117			
U1167			G1410	A1479	C1554		G1735	A1834	U1939	G2035	A2118			
G1168			C1327	G1480	A1555		G1736	A1835	U1940	C2036	U2119			
G1169	G1252		A1412	U1482	C1556		A1754	G1839	C1941	G2037	A2120			
	A1253		G1413	U1483	C1557		A1755	G1840	U1942	G2038	G2123			
G1173	U1254		C1329	G1483	A1558		C1754	U1841	U1943	G2039	G2216			
A1174	A1255		U1330	G1483	C1559		A1756	G1842	U1944	C2040	G2217			
	U1255		C1330	A1490	A1562		G1756							

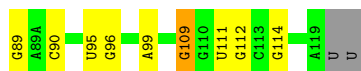
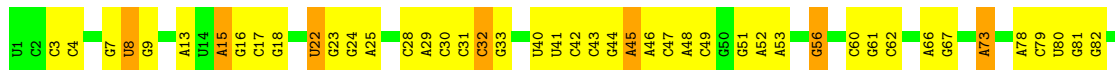


• Molecule 25: 23S rRNA

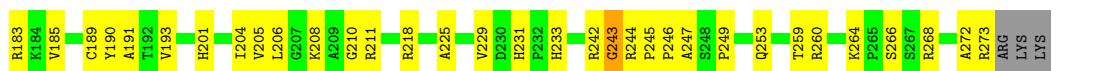
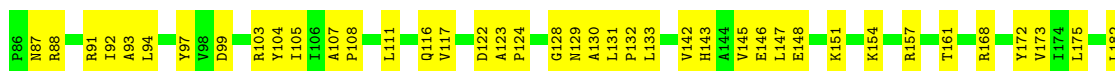




• Molecule 26: 5S rRNA



• Molecule 27: 50S ribosomal protein L2

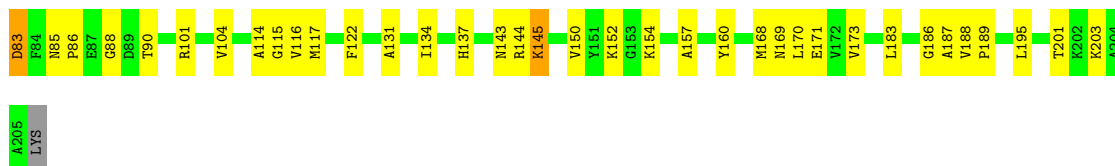


• Molecule 27: 50S ribosomal protein L2



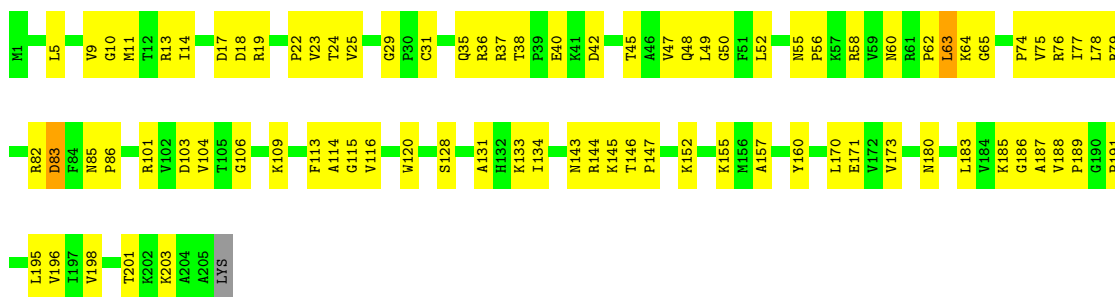
• Molecule 28: 50S ribosomal protein L3





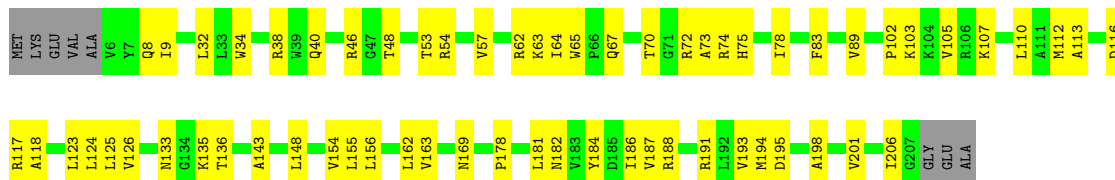
- Molecule 28: 50S ribosomal protein L3

Chain YE: 59% 40%



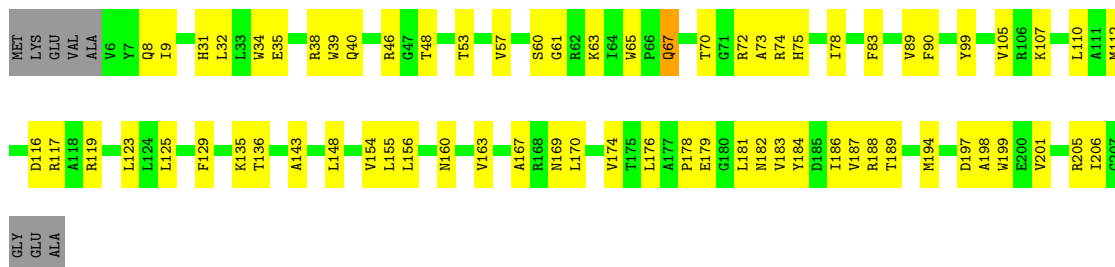
- Molecule 29: 50S ribosomal protein L4

Chain RF: 66% 30%



- Molecule 29: 50S ribosomal protein L4

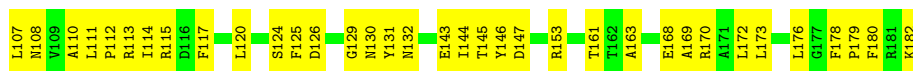
Chain YF: 63% 32%



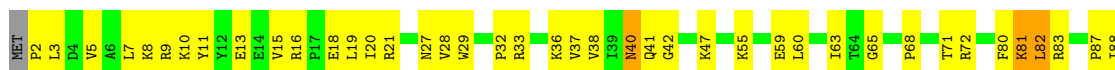
- Molecule 30: 50S ribosomal protein L5

Chain RG: 59% 40%

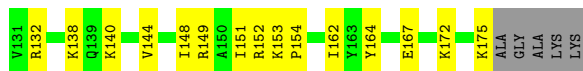
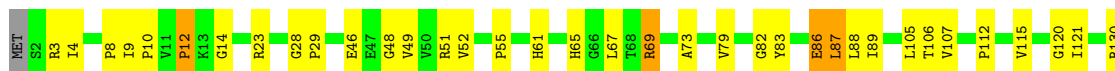




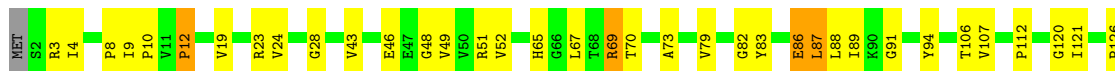
- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9



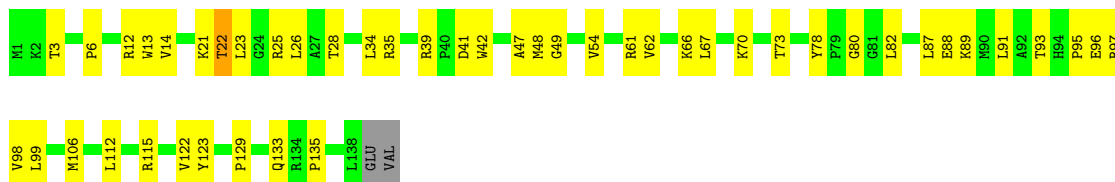
- Molecule 32: 50S ribosomal protein L9





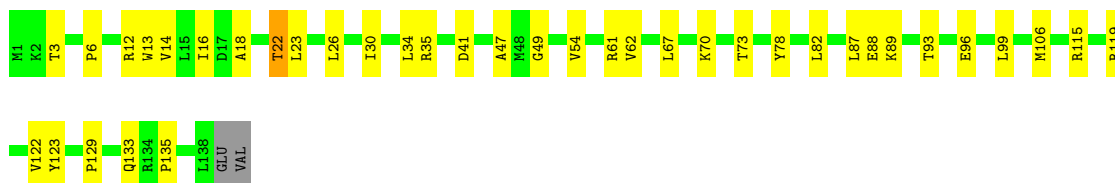
- Molecule 33: 50S ribosomal protein L13

Chain RN: 65% 33%



- Molecule 33: 50S ribosomal protein L13

Chain YN: 71% 26%



- Molecule 34: 50S ribosomal protein L14

Chain RO: 71% 28%



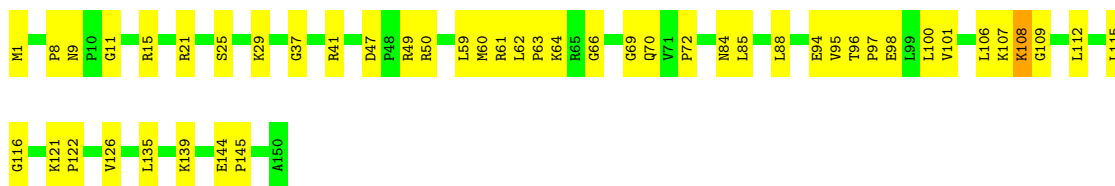
- Molecule 34: 50S ribosomal protein L14

Chain YO: 78% 21%



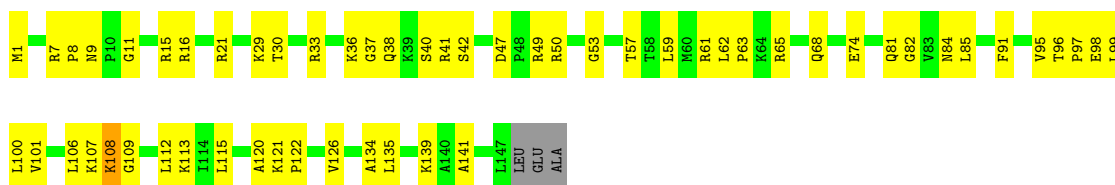
- Molecule 35: 50S ribosomal protein L15

Chain RP: 69% 31%



- Molecule 35: 50S ribosomal protein L15

Chain YP:  61% 37% ..



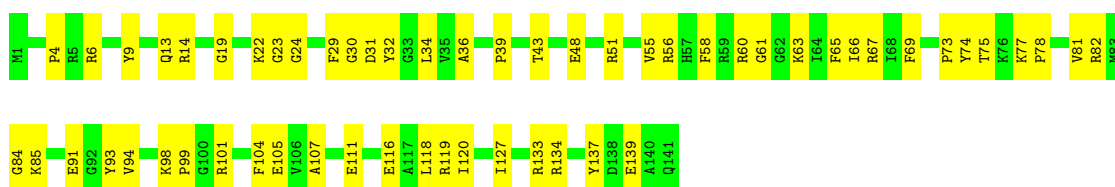
- Molecule 36: 50S ribosomal protein L16

Chain RQ:  62% 38%



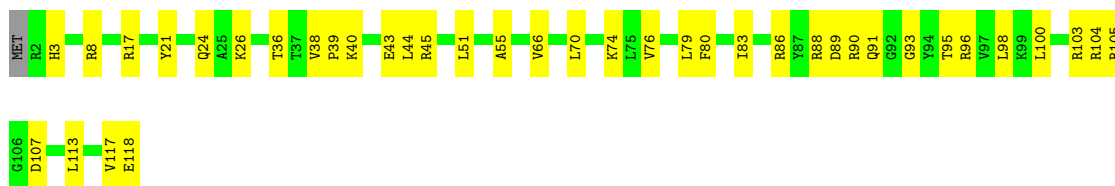
- Molecule 36: 50S ribosomal protein L16

Chain YQ:  60% 40%



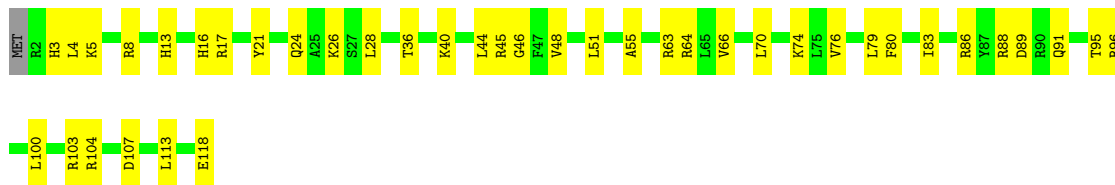
- Molecule 37: 50S ribosomal protein L17

Chain RR:  66% 33%



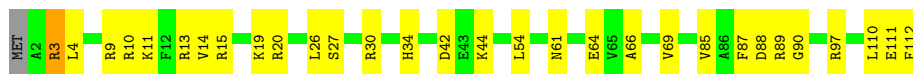
- Molecule 37: 50S ribosomal protein L17

Chain YR:  65% 34%



- Molecule 38: 50S ribosomal protein L18

Chain RS:  72% 26% ..



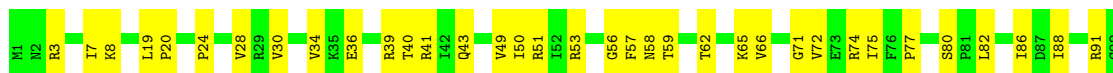
- Molecule 38: 50S ribosomal protein L18

Chain YS:  71% 28% ..



- Molecule 39: 50S ribosomal protein L19

Chain RT:  56% 37% 6% .



- Molecule 39: 50S ribosomal protein L19

Chain YT:  55% 38% 6% .



- Molecule 40: 50S ribosomal protein L20

Chain RU:  70% 27% ..



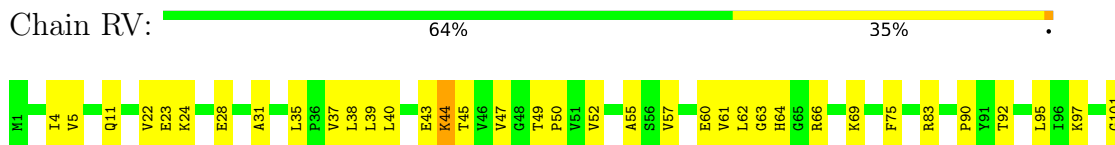
- Molecule 40: 50S ribosomal protein L20

Chain YU:  70% 27% ..

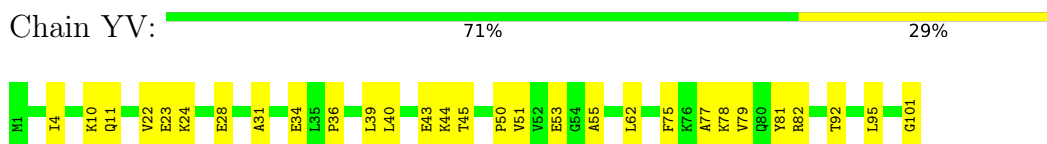


G118

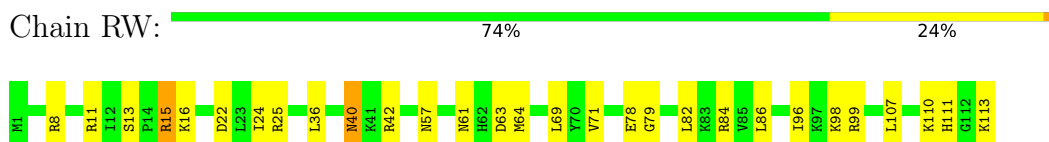
- Molecule 41: 50S ribosomal protein L21



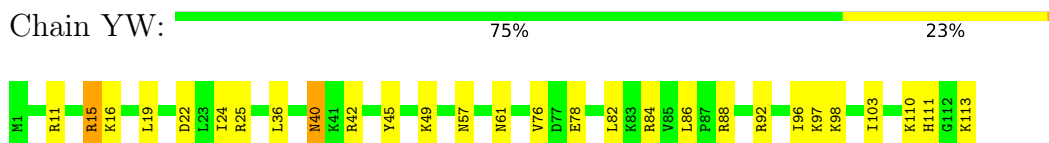
- Molecule 41: 50S ribosomal protein L21



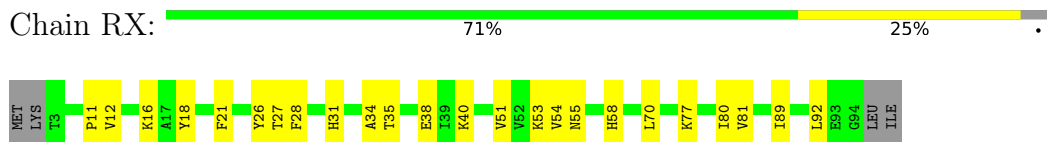
- Molecule 42: 50S ribosomal protein L22



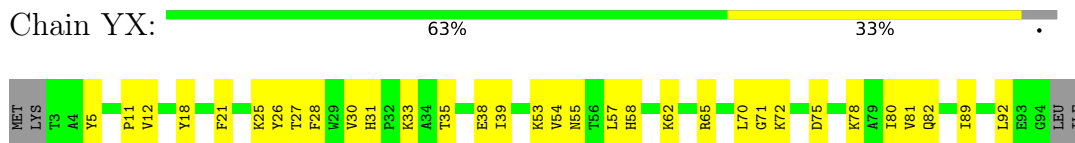
- Molecule 42: 50S ribosomal protein L22



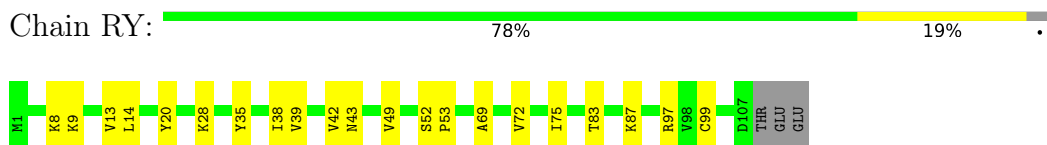
- Molecule 43: 50S ribosomal protein L23



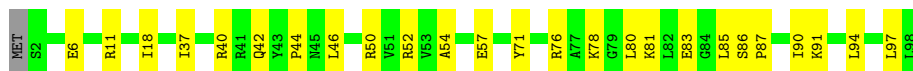
- Molecule 43: 50S ribosomal protein L23



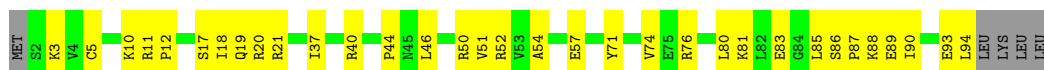
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24



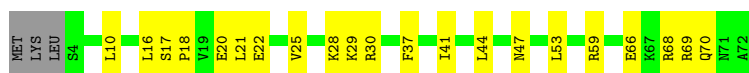
- Molecule 47: 50S ribosomal protein L28



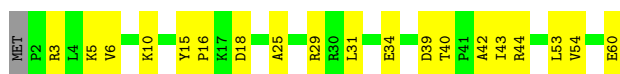
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31

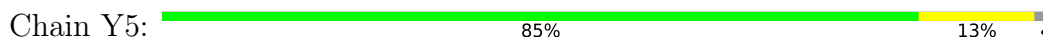




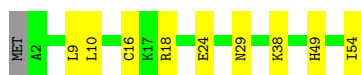
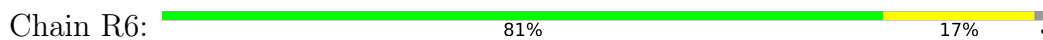
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

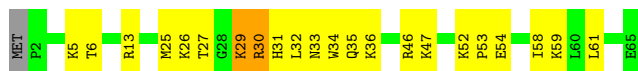


- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

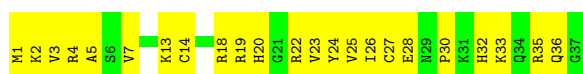




- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



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	210.70Å 446.14Å 616.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.57 – 3.68	Depositor
% Data completeness (in resolution range)	99.3 (145.57-3.68)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.196	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295575	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: ZN, SF4, 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	0.22	0/36097	0.80	21/56339 (0.0%)
1	XA	0.22	0/36100	0.82	27/56344 (0.0%)
2	QB	0.26	0/1942	0.50	0/2619
2	XB	0.25	0/1950	0.49	0/2630
3	QC	0.25	0/1629	0.47	0/2195
3	XC	0.24	0/1629	0.46	0/2195
4	QD	0.35	1/1733 (0.1%)	0.49	1/2318 (0.0%)
4	XD	0.26	0/1733	0.47	0/2318
5	QE	0.24	0/1171	0.48	0/1576
5	XE	0.25	0/1171	0.49	0/1576
6	QF	0.24	0/856	0.49	0/1154
6	XF	0.24	0/856	0.48	0/1154
7	QG	0.24	0/1276	0.43	0/1709
7	XG	0.24	0/1276	0.42	0/1709
8	QH	0.24	0/1128	0.45	0/1517
8	XH	0.24	0/1128	0.46	0/1517
9	QI	0.26	0/1029	0.50	0/1379
9	XI	0.27	0/1017	0.52	0/1365
10	QJ	0.45	1/814 (0.1%)	0.63	3/1095 (0.3%)
10	XJ	0.24	0/790	0.49	0/1063
11	QK	0.25	0/900	0.46	0/1213
11	XK	0.24	0/879	0.47	0/1187
12	QL	0.26	0/991	0.59	0/1327
12	XL	0.26	0/972	0.63	1/1301 (0.1%)
13	QM	0.25	0/965	0.53	0/1292
13	XM	0.24	0/956	0.53	0/1281
14	QN	0.26	0/501	0.46	0/664
14	XN	0.25	0/501	0.46	0/664
15	QO	0.24	0/745	0.43	0/992
15	XO	0.23	0/740	0.40	0/987
16	QP	0.24	0/721	0.49	0/970
16	XP	0.24	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.24	0/847	0.46	0/1131
17	XQ	0.24	0/847	0.45	0/1131
18	QR	0.24	0/579	0.48	0/768
18	XR	0.24	0/579	0.49	0/768
19	QS	0.25	0/680	0.57	0/915
19	XS	0.26	0/689	0.57	0/926
20	QT	0.25	0/765	0.52	0/1007
20	XT	0.25	0/765	0.50	0/1007
21	QU	0.22	0/221	0.45	0/288
21	XU	0.23	0/221	0.46	0/288
22	QV	0.33	1/1836 (0.1%)	0.83	0/2859
22	QW	0.26	0/1807	0.92	2/2816 (0.1%)
22	XV	0.33	1/1836 (0.1%)	0.84	1/2859 (0.0%)
22	XW	0.26	0/1807	0.91	2/2816 (0.1%)
23	QX	0.19	0/188	0.73	0/290
23	XX	0.19	0/235	0.73	0/364
24	QY	0.19	0/400	0.80	0/621
24	XY	0.20	0/400	0.79	0/621
25	RA	0.24	0/69521	0.83	34/108529 (0.0%)
25	YA	0.27	6/69543 (0.0%)	0.85	91/108563 (0.1%)
26	RB	0.22	0/2878	0.81	1/4490 (0.0%)
26	YB	0.23	0/2878	0.82	0/4490
27	RD	0.28	0/2165	0.56	0/2919
27	YD	0.28	0/2165	0.56	0/2919
28	RE	0.26	0/1601	0.60	1/2160 (0.0%)
28	YE	0.26	0/1601	0.60	0/2160
29	RF	0.26	0/1620	0.50	0/2194
29	YF	0.27	0/1620	0.51	0/2194
30	RG	0.26	0/1499	0.55	0/2016
30	YG	0.26	0/1499	0.54	0/2016
31	RH	0.26	0/1362	0.57	1/1841 (0.1%)
31	YH	0.29	0/1362	0.62	1/1841 (0.1%)
32	RI	0.25	0/1151	0.56	0/1558
32	YI	0.25	0/1151	0.56	0/1558
33	RN	0.26	0/1131	0.58	0/1525
33	YN	0.26	0/1131	0.56	0/1525
34	RO	0.26	0/943	0.48	0/1269
34	YO	0.26	0/943	0.50	0/1269
35	RP	0.27	0/1162	0.61	0/1544
35	YP	0.27	0/1139	0.62	0/1514
36	RQ	0.26	0/1143	0.55	0/1527
36	YQ	0.26	0/1143	0.57	0/1527
37	RR	0.26	0/974	0.52	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.25	0/974	0.49	0/1302
38	RS	0.25	0/892	0.54	0/1187
38	YS	0.25	0/892	0.54	0/1187
39	RT	0.25	0/1155	0.53	0/1542
39	YT	0.25	0/1155	0.54	0/1542
40	RU	0.26	0/982	0.51	0/1306
40	YU	0.26	0/982	0.51	0/1306
41	RV	0.26	0/790	0.58	0/1057
41	YV	0.26	0/790	0.58	0/1057
42	RW	0.25	0/911	0.50	0/1220
42	YW	0.25	0/911	0.50	0/1220
43	RX	0.26	0/739	0.48	0/993
43	YX	0.26	0/739	0.48	0/993
44	RY	0.26	0/831	0.48	0/1108
44	YY	0.26	0/831	0.51	0/1108
45	RZ	0.25	0/1493	0.63	0/2026
45	YZ	0.26	0/1493	0.64	0/2026
46	R0	0.24	0/652	0.47	0/867
46	Y0	0.25	0/607	0.48	0/809
47	R1	0.27	0/770	0.55	0/1022
47	Y1	0.29	0/736	0.53	0/978
48	R2	0.24	0/583	0.49	0/771
48	Y2	0.24	0/583	0.51	0/771
49	R3	0.24	0/474	0.48	0/635
49	Y3	0.25	0/474	0.48	0/635
50	R4	0.25	0/578	0.53	0/776
50	Y4	0.27	0/578	0.54	0/776
51	R5	0.26	0/473	0.48	0/639
51	Y5	0.25	0/473	0.46	0/639
52	R6	0.22	0/460	0.47	0/613
52	Y6	0.22	0/460	0.47	0/613
53	R7	0.24	0/417	0.48	0/550
53	Y7	0.24	0/426	0.49	0/561
54	R8	0.33	0/525	0.67	0/691
54	Y8	0.33	0/525	0.67	0/691
55	R9	0.27	0/310	0.64	0/407
55	Y9	0.63	0/310	1.20	2/407 (0.5%)
All	All	0.25	10/319918 (0.0%)	0.76	189/478576 (0.0%)

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	YE	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.62	1.48	1.61
22	QV	1	C	OP3-P	-10.59	1.48	1.61
10	QJ	84	GLN	CD-NE2	9.70	1.57	1.32
4	QD	119	GLN	CB-CG	9.68	1.78	1.52
25	YA	2743	C	P-O5'	7.27	1.67	1.59

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2743	C	O4'-C1'-N1	17.82	122.46	108.20
25	YA	2755	C	OP1-P-OP2	12.48	138.32	119.60
25	YA	2754	U	OP1-P-O3'	-11.78	79.29	105.20
25	YA	2525	G	O4'-C1'-N9	11.27	117.22	108.20
25	YA	2754	U	OP2-P-O3'	-11.23	80.50	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	YE	146	THR	Peptide,Mainchain

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	32246	0	16278	644	0
1	XA	32248	0	16279	617	0
2	QB	1907	0	1958	51	0
2	XB	1915	0	1969	47	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	33	0
4	QD	1703	0	1766	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1767	46	0
5	QE	1155	0	1213	23	0
5	XE	1155	0	1213	18	0
6	QF	843	0	857	18	0
6	XF	843	0	857	22	0
7	QG	1257	0	1296	20	0
7	XG	1257	0	1296	18	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	35	0
9	XI	998	0	1024	39	0
10	QJ	801	0	849	39	0
10	XJ	777	0	816	24	0
11	QK	885	0	904	33	0
11	XK	864	0	881	25	0
12	QL	975	0	1062	26	0
12	XL	956	0	1046	28	0
13	QM	955	0	1021	46	0
13	XM	946	0	1007	36	0
14	QN	492	0	529	15	0
14	XN	492	0	529	12	0
15	QO	734	0	771	13	0
15	XO	729	0	768	17	0
16	QP	705	0	725	19	0
16	XP	705	0	725	22	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	21	0
18	QR	574	0	644	19	0
18	XR	574	0	644	22	0
19	QS	665	0	686	26	0
19	XS	674	0	699	21	0
20	QT	763	0	861	17	0
20	XT	763	0	861	19	0
21	QU	217	0	234	6	0
21	XU	217	0	234	10	0
22	QV	1644	0	836	21	0
22	QW	1618	0	826	45	0
22	XV	1644	0	836	19	0
22	XW	1618	0	826	44	0
23	QX	169	0	86	0	0
23	XX	210	0	109	3	0
24	QY	358	0	183	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	XY	358	0	184	5	0
25	RA	62071	0	31291	1006	0
25	YA	62091	0	31297	1166	0
26	RB	2573	0	1306	29	0
26	YB	2573	0	1306	42	0
27	RD	2115	0	2195	101	0
27	YD	2115	0	2195	102	0
28	RE	1568	0	1634	67	0
28	YE	1568	0	1634	64	0
29	RF	1585	0	1632	53	0
29	YF	1585	0	1632	55	0
30	RG	1474	0	1535	58	0
30	YG	1474	0	1535	69	0
31	RH	1336	0	1418	37	0
31	YH	1336	0	1418	72	0
32	RI	1136	0	1223	28	0
32	YI	1136	0	1223	27	0
33	RN	1104	0	1180	30	0
33	YN	1104	0	1180	25	0
34	RO	933	0	996	32	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	48	0
35	YP	1122	0	1206	50	0
36	RQ	1122	0	1179	49	0
36	YQ	1122	0	1179	47	0
37	RR	960	0	1021	30	0
37	YR	960	0	1021	27	0
38	RS	882	0	943	23	0
38	YS	882	0	943	27	0
39	RT	1141	0	1202	46	0
39	YT	1141	0	1202	49	0
40	RU	964	0	1022	47	0
40	YU	964	0	1022	45	0
41	RV	779	0	852	31	0
41	YV	779	0	852	24	0
42	RW	900	0	964	21	1
42	YW	900	0	964	21	0
43	RX	725	0	778	17	0
43	YX	725	0	778	25	0
44	RY	818	0	910	13	0
44	YY	818	0	912	14	1
45	RZ	1461	0	1493	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	YZ	1461	0	1493	46	0
46	R0	643	0	667	20	0
46	Y0	599	0	617	23	0
47	R1	763	0	848	18	0
47	Y1	729	0	802	22	0
48	R2	581	0	629	12	0
48	Y2	581	0	629	14	0
49	R3	469	0	518	14	0
49	Y3	469	0	518	16	0
50	R4	565	0	557	18	0
50	Y4	565	0	558	25	0
51	R5	459	0	477	5	0
51	Y5	459	0	480	10	0
52	R6	453	0	474	7	0
52	Y6	453	0	473	3	0
53	R7	409	0	454	12	0
53	Y7	418	0	467	9	0
54	R8	517	0	582	22	0
54	Y8	517	0	582	21	0
55	R9	307	0	338	22	0
55	Y9	307	0	338	141	0
56	QA	68	0	0	0	0
56	QC	1	0	0	0	0
56	QE	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QV	6	0	0	0	0
56	QY	1	0	0	0	0
56	R0	4	0	0	0	0
56	R1	2	0	0	0	0
56	R4	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	508	0	0	0	0
56	RB	7	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RN	1	0	0	0	0
56	RO	2	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0
56	RU	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	82	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	6	0	0	0	0
56	Y0	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	546	0	0	0	0
56	YB	12	0	0	0	0
56	YD	2	0	0	0	0
56	YE	2	0	0	0	0
56	YO	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295575	0	199664	5705	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 12.

The worst 5 of 5705 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)
4:QD:119:GLN:CG	4:QD:119:GLN:CB	1.78	1.55
25:YA:2755:C:H42	55:Y9:1:MET:HG2	1.08	1.16
25:RA:2747:G:N2	25:RA:2757:A:H62	1.43	1.15
25:YA:2742:C:H1 ⁷	55:Y9:26:ILE:HA	1.33	1.10
25:RA:2747:G:H21	25:RA:2757:A:N6	1.52	1.05

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)
42:RW:63:ASP:OD1	44:YY:92:ASN:ND2[3_555]	2.18	0.02

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%)	202 (87%)	29 (12%)	2 (1%)	17	54
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	69
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
4	QD	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	22	59
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	59
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
12	QL	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
12	XL	120/132 (91%)	97 (81%)	22 (18%)	1 (1%)	19	56
13	QM	118/126 (94%)	96 (81%)	21 (18%)	1 (1%)	19	56
13	XM	117/126 (93%)	94 (80%)	22 (19%)	1 (1%)	17	54
14	QN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	XS	82/93 (88%)	70 (85%)	11 (13%)	1 (1%)	13	49
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
27	RD	270/276 (98%)	235 (87%)	33 (12%)	2 (1%)	22	59
27	YD	270/276 (98%)	239 (88%)	29 (11%)	2 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	163 (80%)	37 (18%)	3 (2%)	10	44
28	YE	203/206 (98%)	158 (78%)	42 (21%)	3 (2%)	10	44
29	RF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
29	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	51
30	RG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	25	62
30	YG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	14	50
31	RH	172/180 (96%)	141 (82%)	28 (16%)	3 (2%)	9	42
31	YH	172/180 (96%)	137 (80%)	32 (19%)	3 (2%)	9	42
32	RI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	7	38
32	YI	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	7	38
33	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10	44
33	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	59
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	RP	148/150 (99%)	114 (77%)	33 (22%)	1 (1%)	22	59
35	YP	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	22	59
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
36	YQ	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	11	45
37	RR	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
37	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	54
38	RS	109/112 (97%)	86 (79%)	23 (21%)	0	100	100
38	YS	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
39	RT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
39	YT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
40	RU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
40	YU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
41	RV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	51
41	YV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
42	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
42	YW	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	RZ	181/206 (88%)	144 (80%)	33 (18%)	4 (2%)	6	37
45	YZ	181/206 (88%)	142 (78%)	36 (20%)	3 (2%)	9	42
46	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
46	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
47	R1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	14	50
47	Y1	91/98 (93%)	77 (85%)	13 (14%)	1 (1%)	14	50
48	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
48	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	44
49	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
49	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
50	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	Y6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	R8	62/65 (95%)	46 (74%)	14 (23%)	2 (3%)	4	31
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	31
55	R9	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
55	Y9	35/37 (95%)	18 (51%)	15 (43%)	2 (6%)	1	19
All	All	11452/12128 (94%)	10130 (88%)	1249 (11%)	73 (1%)	25	62

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	RE	18	ASP
31	RH	87	LEU
32	RI	15	VAL

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Mol	Chain	Res	Type
35	RP	108	LYS
39	RT	124	ASP

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%)	202 (100%)	1 (0%)	88	94
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	81
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	85
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	85
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	72
6	XF	90/90 (100%)	90 (100%)	0	100	100
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	89
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	89
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	74
9	XI	97/99 (98%)	97 (100%)	0	100	100
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%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	74
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	74
15	QO	79/80 (99%)	79 (100%)	0	100	100
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%)	94 (99%)	1 (1%)	73	85
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	85
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%)	71 (99%)	1 (1%)	67	82
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	83
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	83
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
27	YD	214/218 (98%)	213 (100%)	1 (0%)	88	94
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	160 (99%)	1 (1%)	86	93
29	YF	161/166 (97%)	160 (99%)	1 (1%)	86	93
30	RG	155/156 (99%)	154 (99%)	1 (1%)	86	93
30	YG	155/156 (99%)	154 (99%)	1 (1%)	86	93
31	RH	145/148 (98%)	142 (98%)	3 (2%)	53	73
31	YH	145/148 (98%)	142 (98%)	3 (2%)	53	73
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	YN	117/119 (98%)	116 (99%)	1 (1%)	78	88
34	RO	100/100 (100%)	99 (99%)	1 (1%)	76	86
34	YO	100/100 (100%)	99 (99%)	1 (1%)	76	86
35	RP	116/116 (100%)	116 (100%)	0	100	100
35	YP	114/116 (98%)	114 (100%)	0	100	100
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	85
38	YS	87/88 (99%)	86 (99%)	1 (1%)	73	85
39	RT	120/127 (94%)	120 (100%)	0	100	100
39	YT	120/127 (94%)	120 (100%)	0	100	100
40	RU	93/94 (99%)	92 (99%)	1 (1%)	73	85
40	YU	93/94 (99%)	92 (99%)	1 (1%)	73	85
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	52	72
42	YW	92/92 (100%)	90 (98%)	2 (2%)	52	72
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
46	R0	65/67 (97%)	65 (100%)	0	100	100
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	79
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	R3	51/52 (98%)	51 (100%)	0	100	100
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
50	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	64
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	66
All	All	9687/10066 (96%)	9635 (100%)	52 (0%)	88	94

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	XB	144	ARG
27	YD	273	ARG
50	Y4	56	VAL
4	XD	103	ASN
14	XN	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
31	YH	74	ASN
44	YY	6	HIS
37	RR	71	GLN
39	RT	58	ASN
42	RW	111	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	252 (16%)	34 (2%)
1	XA	1499/1508 (99%)	272 (18%)	37 (2%)
22	QV	76/77 (98%)	17 (22%)	3 (3%)
22	QW	75/77 (97%)	31 (41%)	2 (2%)
22	XV	76/77 (98%)	18 (23%)	3 (3%)
22	XW	75/77 (97%)	32 (42%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	16/17 (94%)	2 (12%)	0
24	XY	16/17 (94%)	2 (12%)	0
25	RA	2879/2915 (98%)	599 (20%)	47 (1%)
25	YA	2880/2915 (98%)	570 (19%)	48 (1%)
26	RB	119/122 (97%)	17 (14%)	1 (0%)
26	YB	119/122 (97%)	19 (15%)	1 (0%)
All	All	9344/9482 (98%)	1834 (19%)	178 (1%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	1027	C
25	YA	752	A
1	XA	1297	C
25	YA	195	A
25	YA	1026	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1301 ligands modelled in this entry, 1299 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
57	SF4	XD	301	4	0,12,12	-	-	-		
57	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
57	SF4	XD	301	4	-	-	0/6/5/5
57	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QD	301	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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