



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2020 – 03:07 AM EDT

PDB ID : 6NUO
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-01
Resolution : 3.20 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 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) : 2.14.6

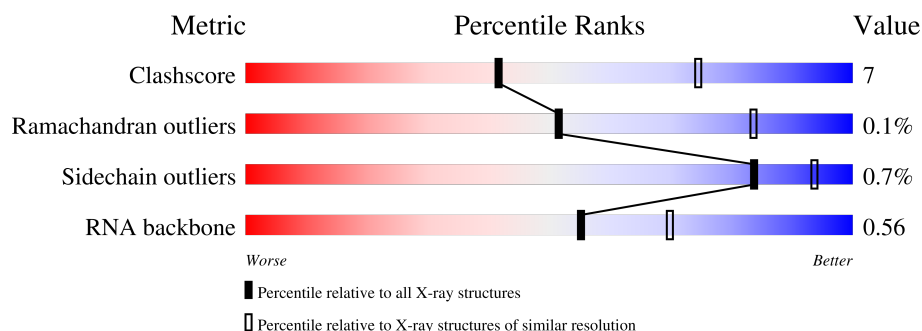
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	












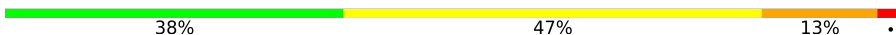
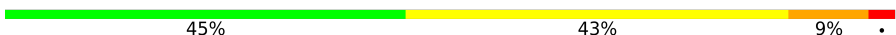
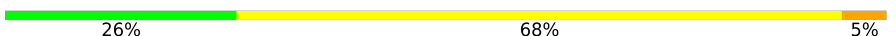











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Mol	Chain	Length	Quality of chain
4	QD	209	 77% 22% .
4	XD	209	 66% 30% .
5	QE	162	 67% 25% . 7%
5	XE	162	 76% 17% . 7%
6	QF	101	 74% 25% .
6	XF	101	 80% 18% .
7	QG	156	 79% 19% ..
7	XG	156	 72% 25% ..
8	QH	138	 78% 22% .
8	XH	138	 76% 22% ..
9	QI	128	 68% 27% . .
9	XI	128	 60% 32% 6% .
10	QJ	105	 56% 34% . 6%
10	XJ	105	 68% 21% . 9%
11	QK	129	 64% 25% . 8%
11	XK	129	 71% 18% . 10%
12	QL	132	 78% 15% . 5%
12	XL	132	 67% 20% 5% 8%
13	QM	126	 63% 28% . 5%
13	XM	126	 53% 37% . 6%
14	QN	61	 51% 43% 5% .
14	XN	61	 75% 18% 5% .
15	QO	89	 88% 10% ..
15	XO	89	 82% 16% .
16	QP	88	 68% 26% . 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	XV	77	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	
28	RF	210	
28	YF	210	


























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Mol	Chain	Length	Quality of chain
29	RG	182	
29	YG	182	
30	RH	180	
30	YH	180	
31	RI	148	
31	YI	148	
32	RN	140	
32	YN	140	
33	RO	122	
33	YO	122	
34	RP	150	
34	YP	150	
35	RQ	141	
35	YQ	141	
36	RR	118	
36	YR	118	
37	RS	112	
37	YS	112	
38	RT	146	
38	YT	146	
39	RU	118	
39	YU	118	
40	RV	101	
40	YV	101	
41	RW	113	



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Mol	Chain	Length	Quality of chain
41	YW	113	 82% 17% .
42	RX	96	 82% 14% .
42	YX	96	 86% 11% .
43	RY	110	 78% 18% . .
43	YY	110	 81% 15% . .
44	RZ	206	 54% 32% . 11%
44	YZ	206	 67% 21% 11%
45	R0	85	 71% 24% . 5%
45	Y0	85	 75% 13% 12%
46	R1	98	 79% 16% . .
46	Y1	98	 72% 20% . 5%
47	R2	72	 72% 24% .
47	Y2	72	 69% 22% 8%
48	R3	60	 72% 27% .
48	Y3	60	 78% 20% .
49	R4	71	 58% 37% . .
49	Y4	71	 56% 35% 6% .
50	R5	60	 83% 15% .
50	Y5	60	 83% 15% .
51	R6	54	 81% 15% . .
51	Y6	54	 78% 19% . .
52	R7	49	 80% 16% .
52	Y7	49	 90% 8% .
53	R8	65	 60% 38% .
53	Y8	65	 62% 34% . . .

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Mol	Chain	Length	Quality of chain
54	R9	37	 78%22%
54	Y9	37	 70%30%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291964 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
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
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
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
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			
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 P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1648	734	295	542	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1648	734	295	542	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
			418	186	86	127	19			
23	XX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
24	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
30	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
34	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	YS	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
47	Y2	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	64	Total	Mg	0	0
			64	64		
55	YA	510	Total	Mg	0	0
			510	510		
55	Y5	1	Total	Mg	0	0
			1	1		
55	YR	1	Total	Mg	0	0
			1	1		
55	RT	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	1	Total	Mg	0	0
			1	1		
55	Y1	2	Total	Mg	0	0
			2	2		
55	YD	2	Total	Mg	0	0
			2	2		
55	QV	1	Total	Mg	0	0
			1	1		
55	RX	1	Total	Mg	0	0
			1	1		
55	Y8	1	Total	Mg	0	0
			1	1		
55	XA	78	Total	Mg	0	0
			78	78		
55	RQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	R0	2	Total 2	Mg 2	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	YQ	3	Total 3	Mg 3	0	0
55	R8	2	Total 2	Mg 2	0	0
55	RR	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	RA	444	Total 444	Mg 444	0	0
55	Y3	1	Total 1	Mg 1	0	0
55	YP	3	Total 3	Mg 3	0	0
55	RE	5	Total 5	Mg 5	0	0
55	YB	7	Total 7	Mg 7	0	0
55	XV	1	Total 1	Mg 1	0	0
55	RB	7	Total 7	Mg 7	0	0
55	RF	1	Total 1	Mg 1	0	0
55	XM	2	Total 2	Mg 2	0	0
55	YE	5	Total 5	Mg 5	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).

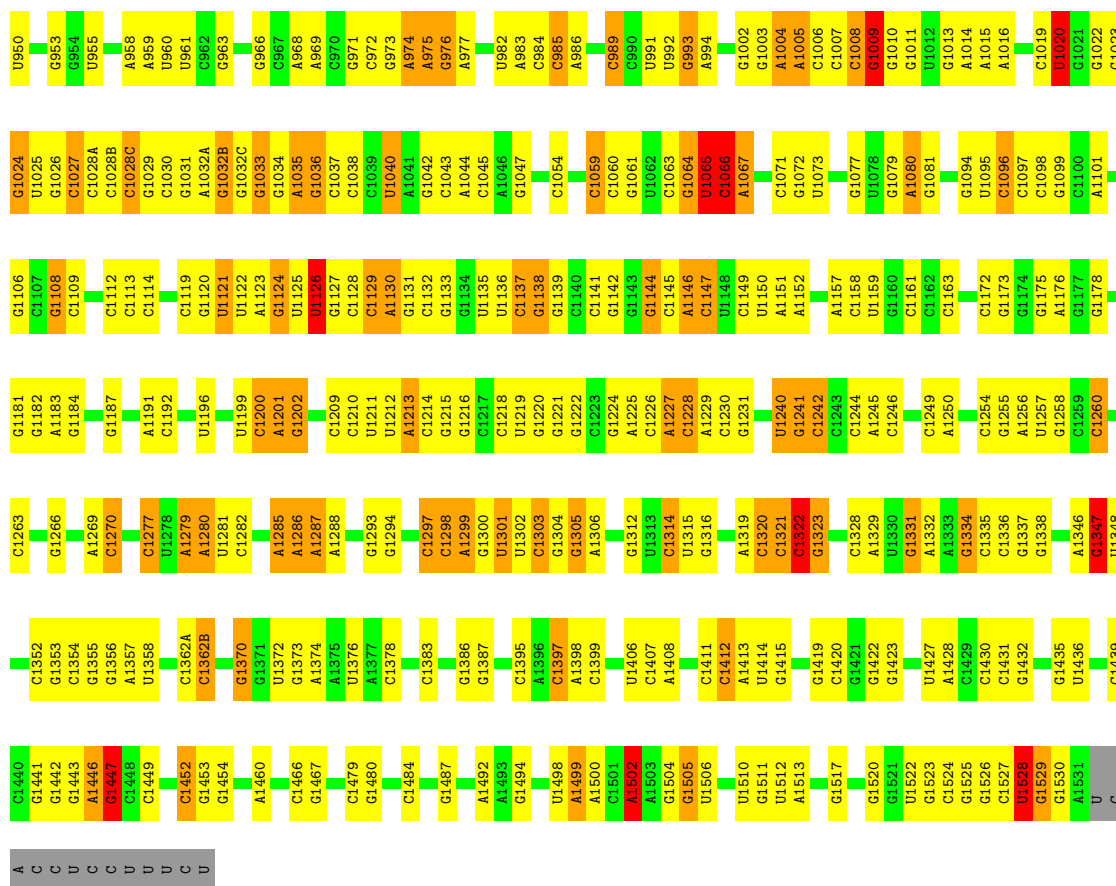
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	Y4	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		

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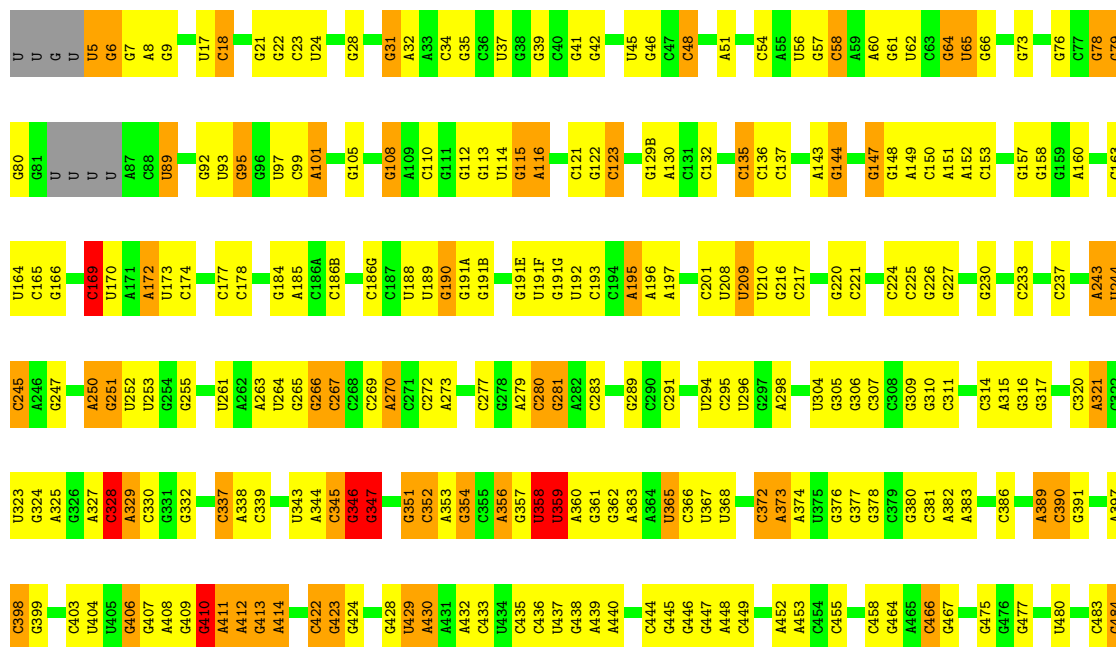
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R4	1	Total 1	Zn 1	0	0
57	R9	1	Total 1	Zn 1	0	0

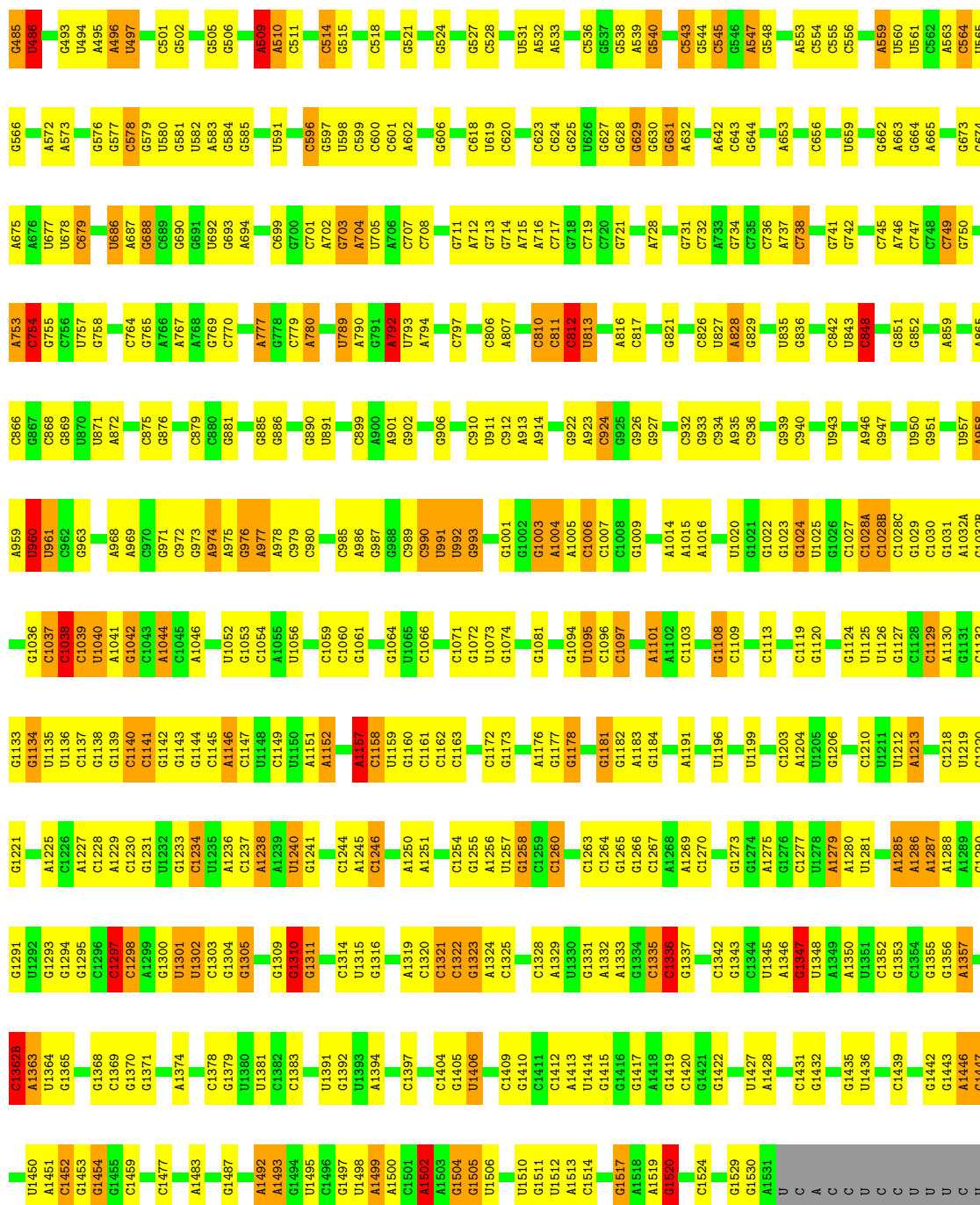




• Molecule 1: 16S rRNA

Chain XA:





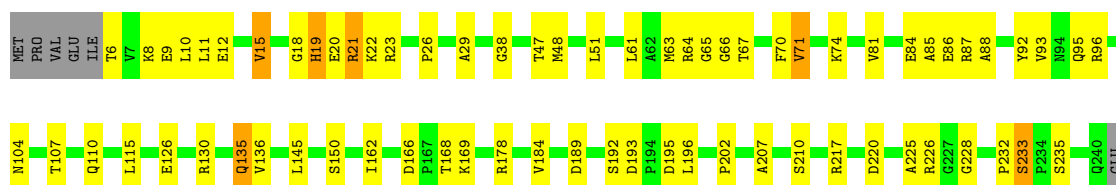
• Molecule 2: 30S ribosomal protein S2

Chain QB:

64%

25%

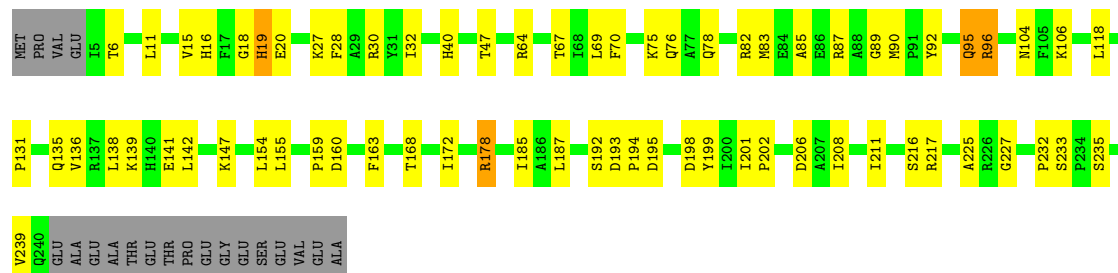
8%



ALA
GLU
ALA
THR
GLU
THR
PRO
GLY
GLU
SER
GLU
VAL
GLU
ALA

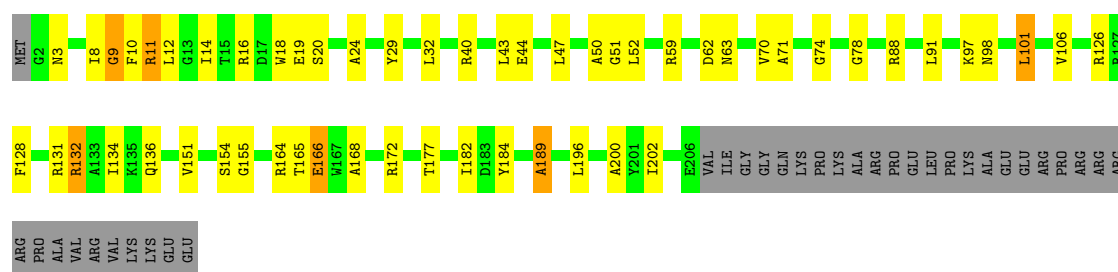
- Molecule 2: 30S ribosomal protein S2

Chain XB:  65% 25% 8%



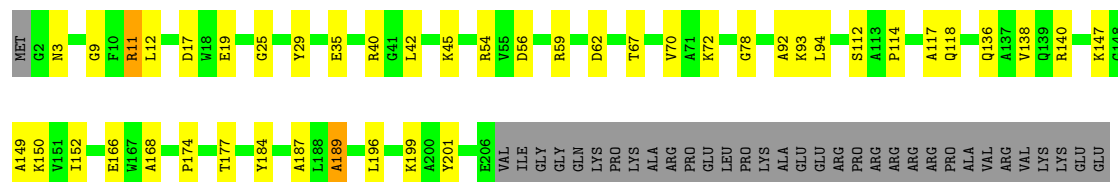
- Molecule 3: 30S ribosomal protein S3

Chain QC:  63% 21% 14%




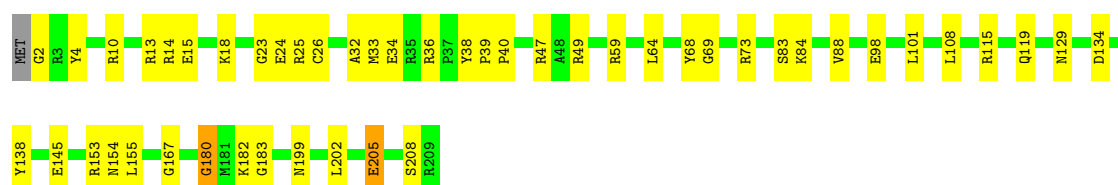
- Molecule 3: 30S ribosomal protein S3

Chain XC:  67% 18% 14%



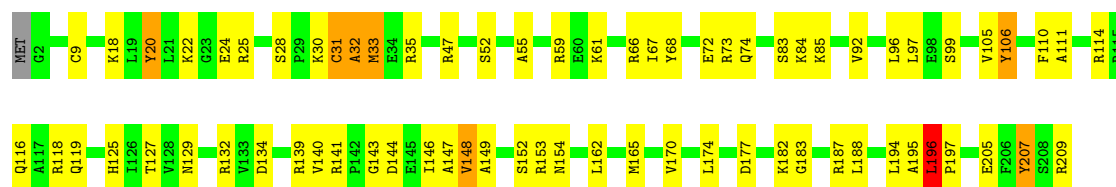
- Molecule 4: 30S ribosomal protein S4

Chain QD:  77% 22% 1%



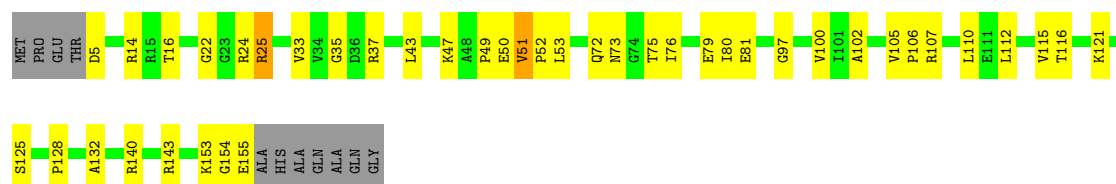
- Molecule 4: 30S ribosomal protein S4

Chain XD:  66% 30% .




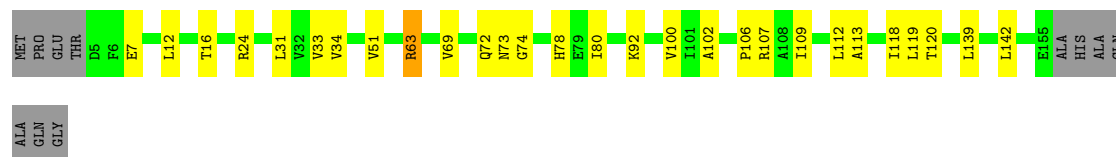
- Molecule 5: 30S ribosomal protein S5

Chain QE:  67% 25% . 7%




- Molecule 5: 30S ribosomal protein S5

Chain XE:  76% 17% . 7%




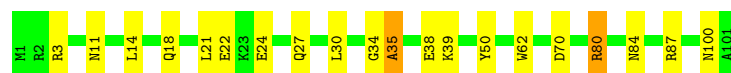
- Molecule 6: 30S ribosomal protein S6

Chain QF:  74% 25% .




- Molecule 6: 30S ribosomal protein S6

Chain XF:  80% 18% .

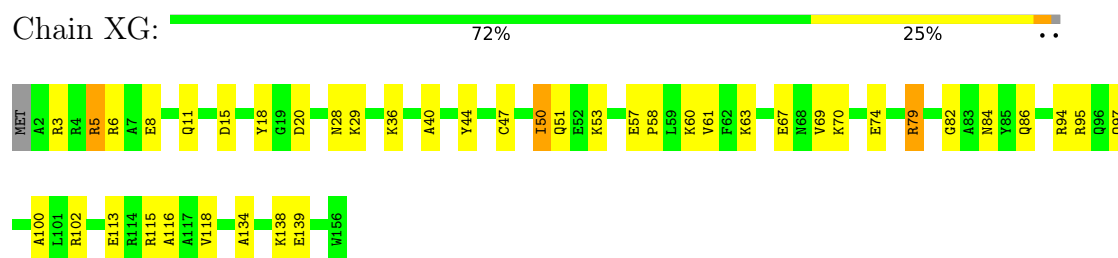


- Molecule 7: 30S ribosomal protein S7

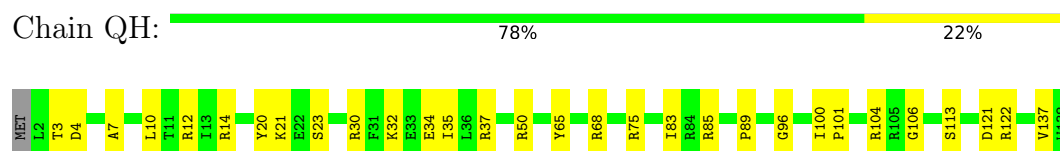
Chain QG:  79% 19% ..



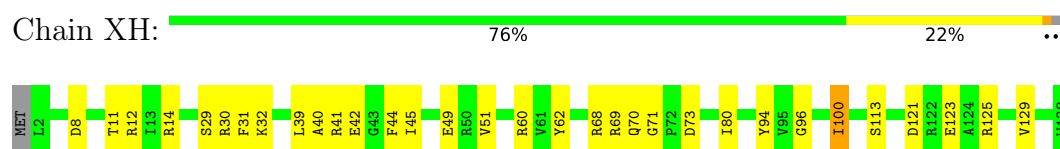
- Molecule 7: 30S ribosomal protein S7



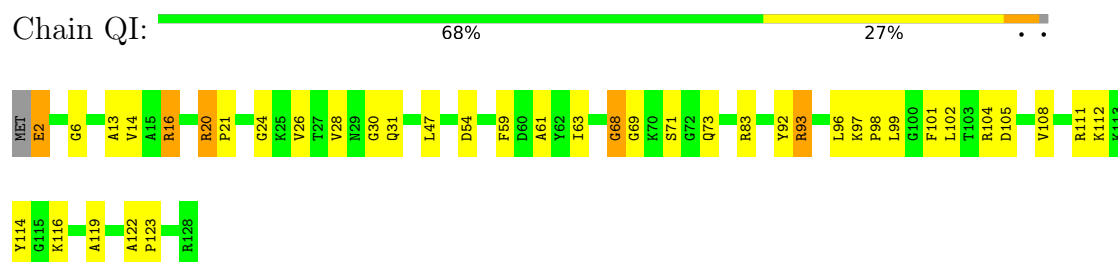
- Molecule 8: 30S ribosomal protein S8



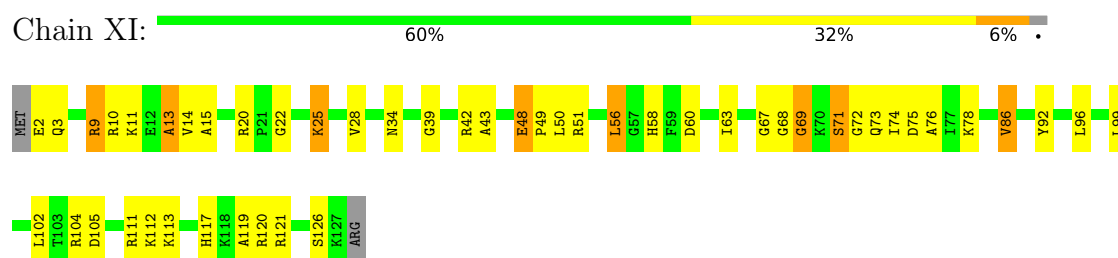
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

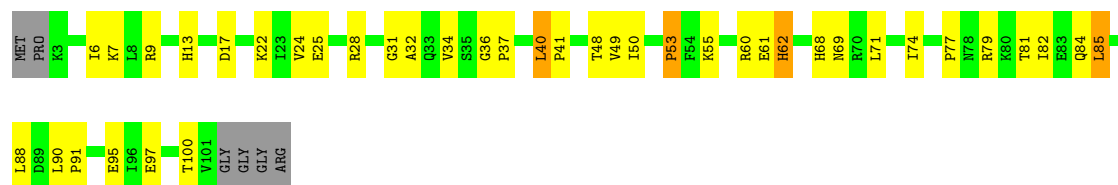


- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10





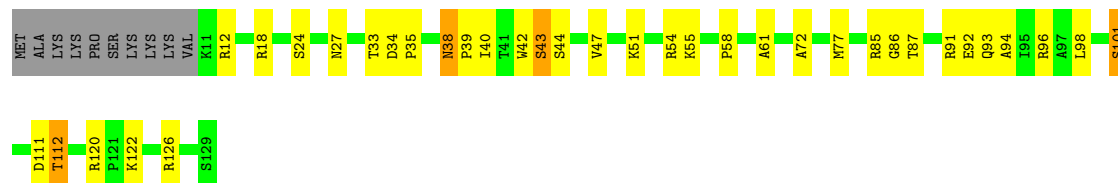
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 68% 21% 9%



- Molecule 11: 30S ribosomal protein S11

Chain QK: 64% 25% 8%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 71% 18% 10%



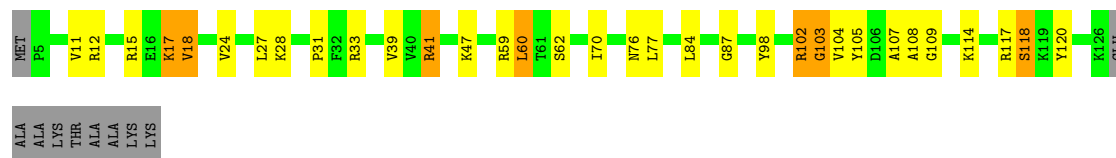
- Molecule 12: 30S ribosomal protein S12

Chain QL: 78% 15% 5%



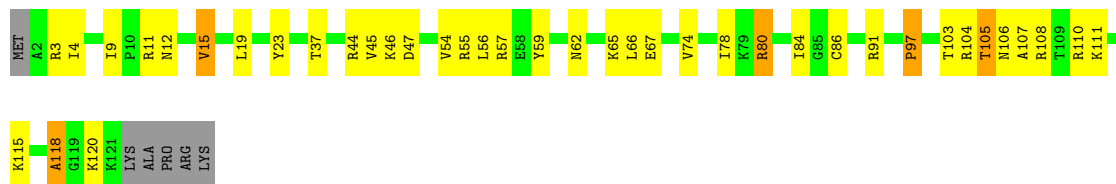
- Molecule 12: 30S ribosomal protein S12

Chain XL: 67% 20% 5% 8%



- Molecule 13: 30S ribosomal protein S13

Chain QM:  63% 28% 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  53% 37% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  51% 43% 5%




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  75% 18% 5%




- Molecule 15: 30S ribosomal protein S15

Chain QO:  88% 10% 2%



- Molecule 15: 30S ribosomal protein S15

Chain XO:  82% 16% 2%



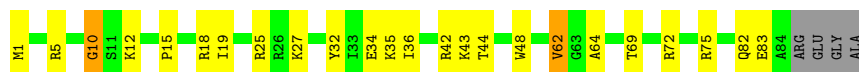
- Molecule 16: 30S ribosomal protein S16

Chain QP:  68% 26% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP: 68% 25% • 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ: 61% 32% • 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 79% 15% • 5%



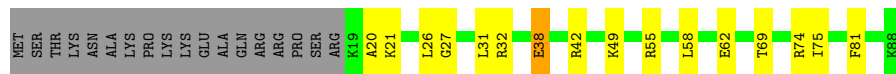
- Molecule 18: 30S ribosomal protein S18

Chain QR: 61% 18% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR: 61% 17% 20%



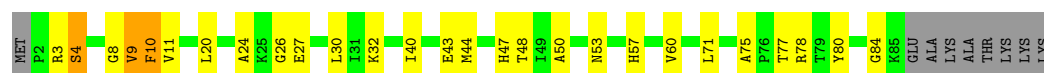
- Molecule 19: 30S ribosomal protein S19

Chain QS: 66% 22% • 11%



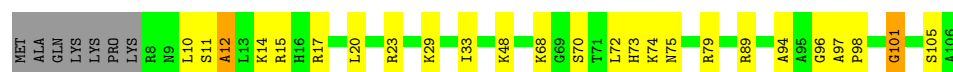
- Molecule 19: 30S ribosomal protein S19

Chain XS: 



- Molecule 20: 30S ribosomal protein S20

Chain QT: 70% 22% 7%




- Molecule 20: 30S ribosomal protein S20

Chain XT:  60% 31% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU:  78% 15% 7%

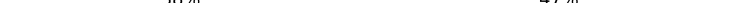


- Molecule 21: 30S ribosomal protein Thx

Chain XU:  56% 33% 7%



- Molecule 22: P-site tRNA-Pro

Chain QV:  38% 47% 13% 2%

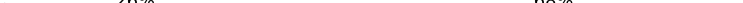


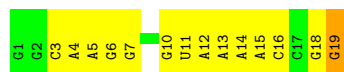
- Molecule 22: P-site tRNA-Pro

Chain XV: 45% 43% 9%



- Molecule 23: mRNA

Chain QX:  26% 68% 5%



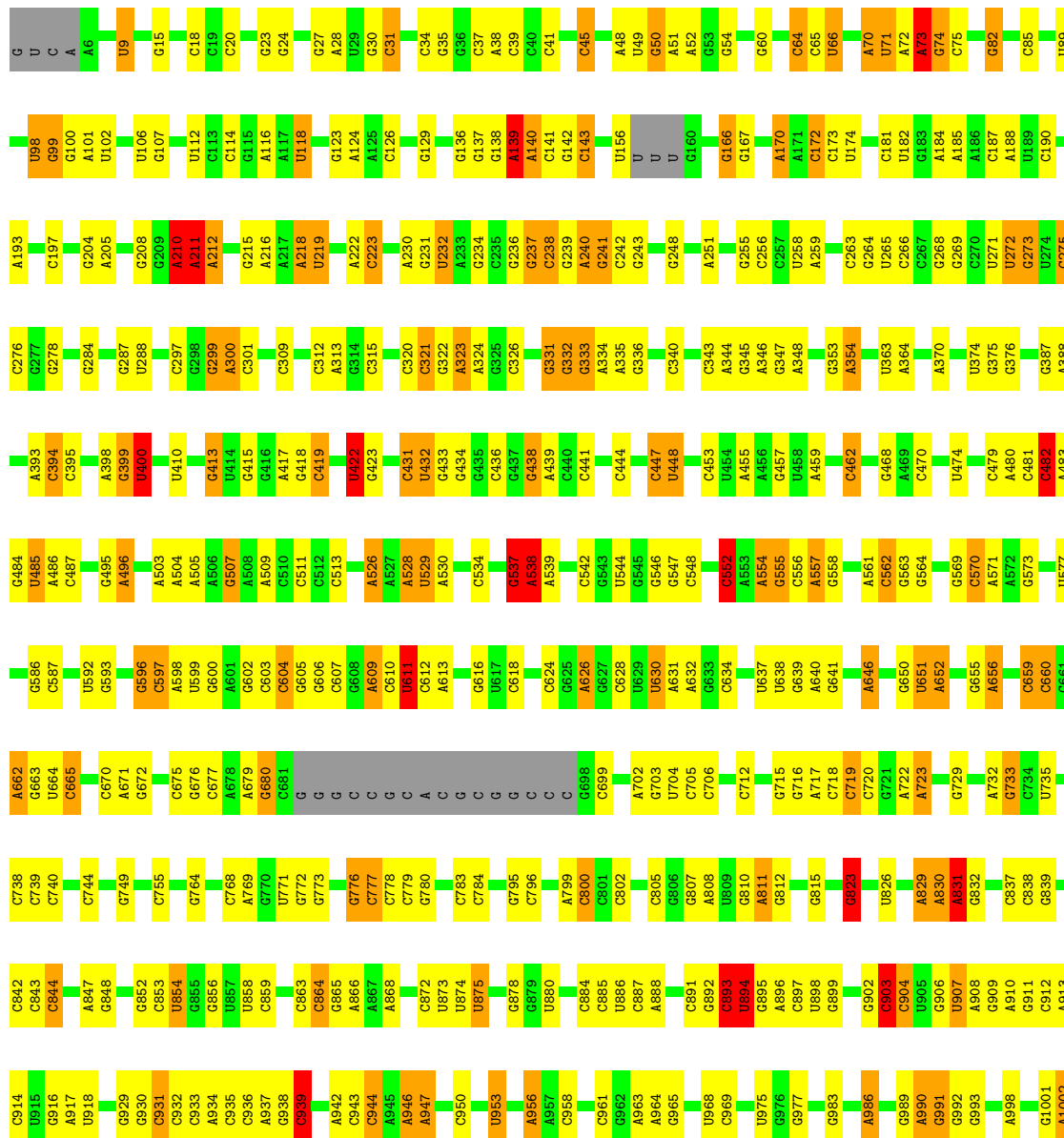
- Molecule 23: mRNA

Chain XX: 26% 58% 11% 5%

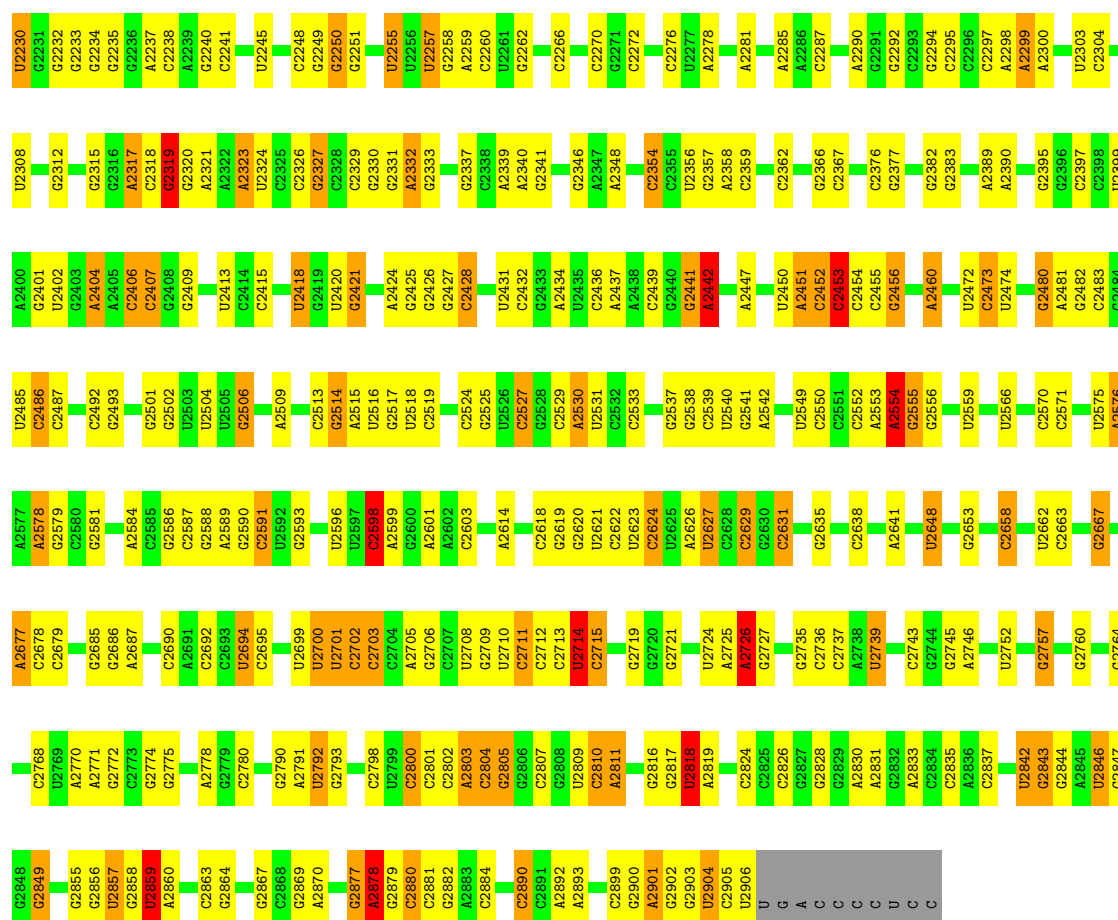


- Molecule 24: 23S rRNA

Chain RA: 

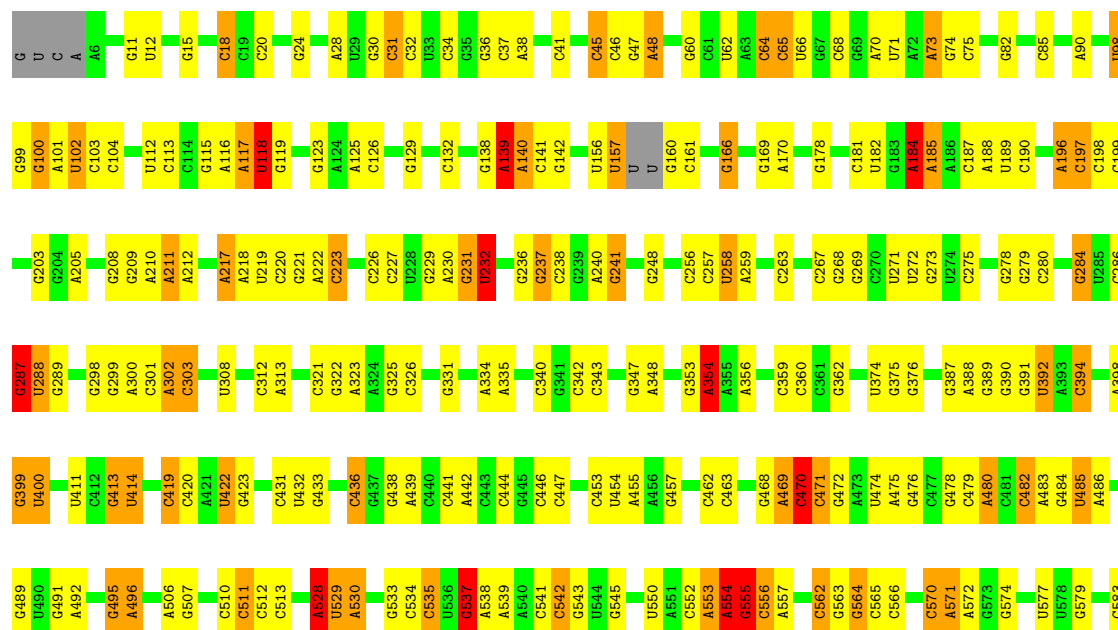




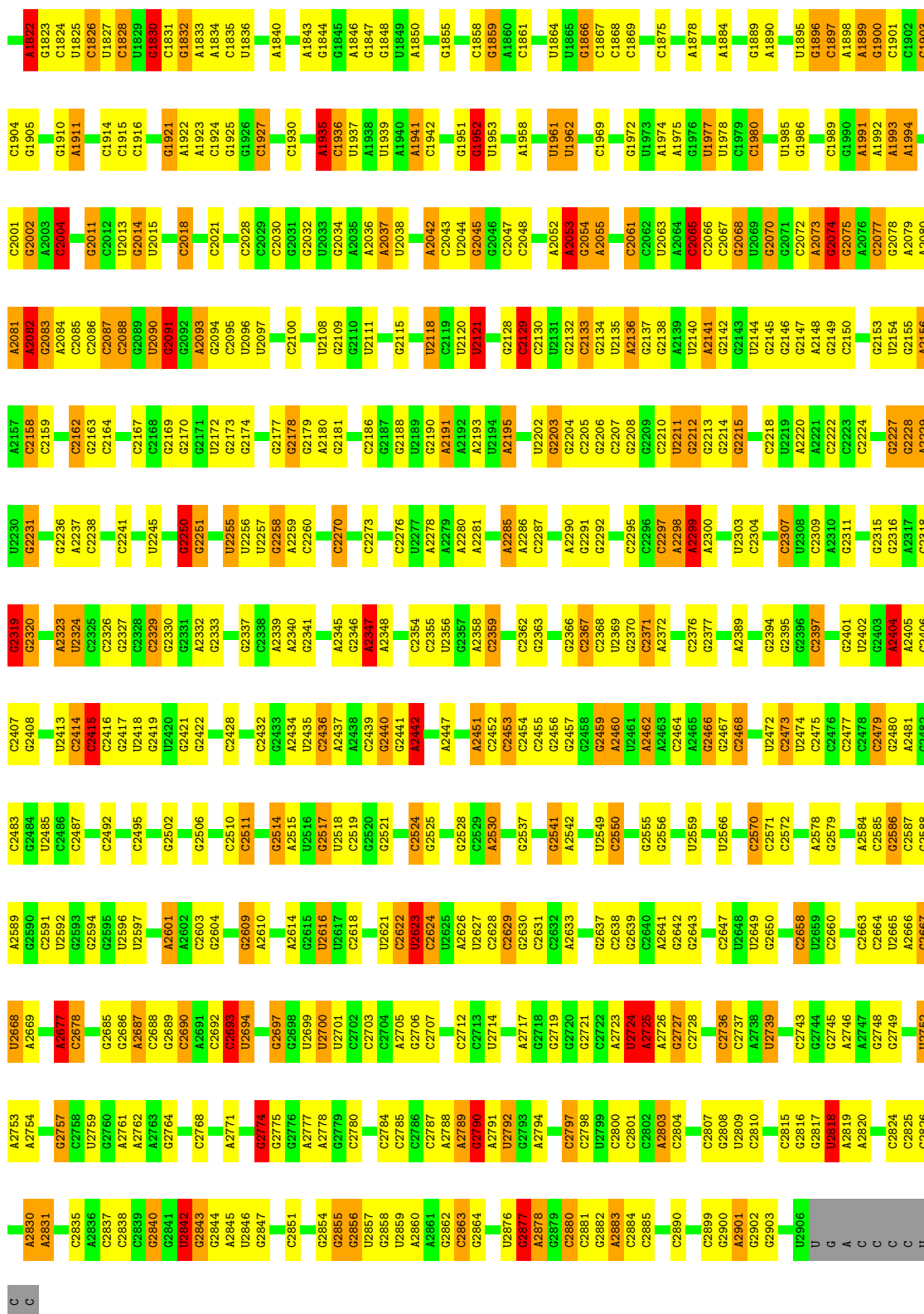


• Molecule 24: 23S rRNA

Chain YA: 50% 35% 11% ..

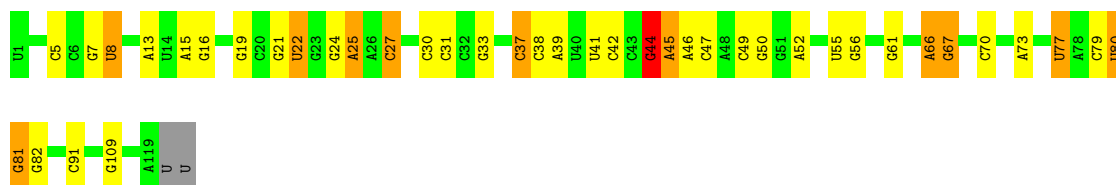






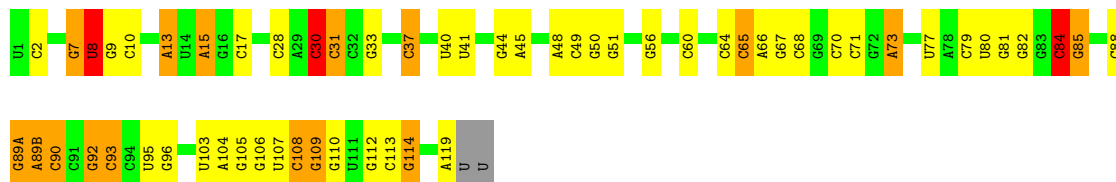
● Molecule 25: 5S rRNA

Chain RB:



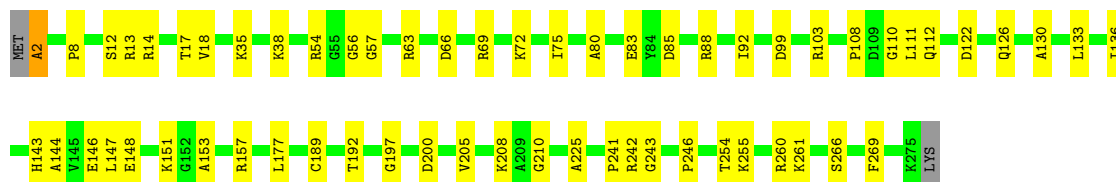
• Molecule 25: 5S rRNA

Chain YB: 51% 32% 13% ..



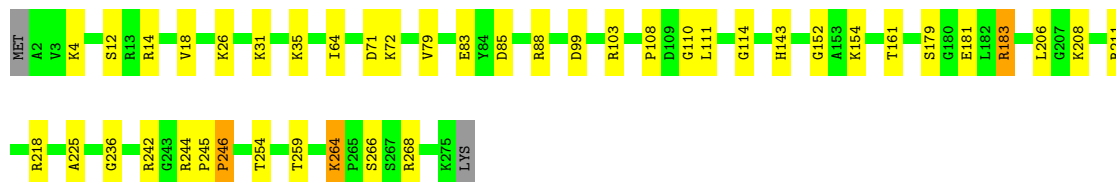
• Molecule 26: 50S ribosomal protein L2

Chain RD: 78% 21% .



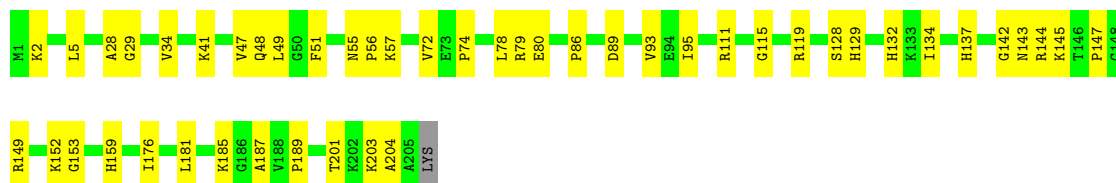
• Molecule 26: 50S ribosomal protein L2

Chain YD: 84% 14% ..



• Molecule 27: 50S ribosomal protein L3

Chain RE: 77% 23%



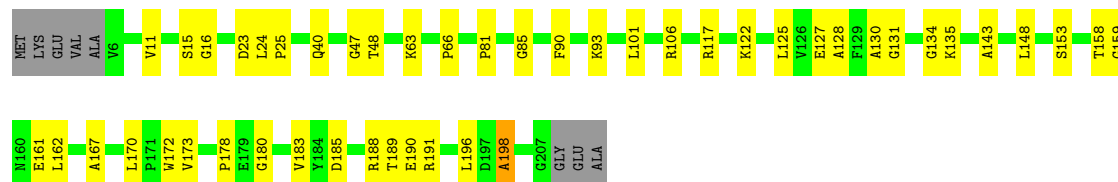
• Molecule 27: 50S ribosomal protein L3

Chain YE: 78% 20% ..



- Molecule 28: 50S ribosomal protein L4

Chain RF: 74% 22% .



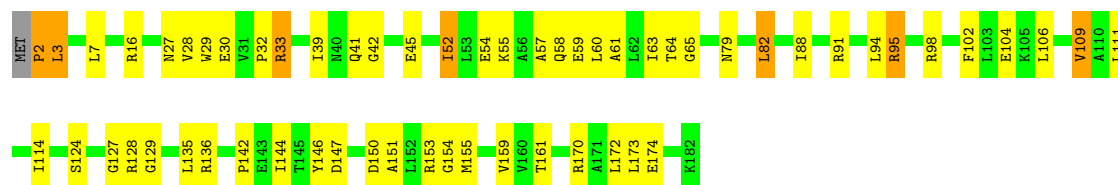
- Molecule 28: 50S ribosomal protein L4

Chain YF: 73% 23% .



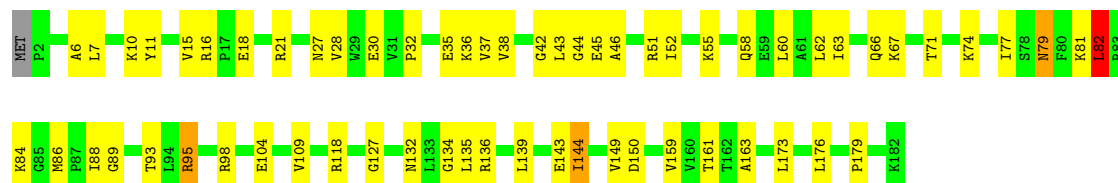
- Molecule 29: 50S ribosomal protein L5

Chain RG: 67% 29% . .



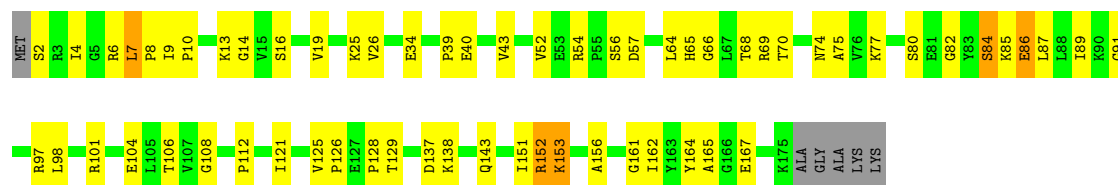
- Molecule 29: 50S ribosomal protein L5

Chain YG: 65% 32% . . .



- Molecule 30: 50S ribosomal protein L6

Chain RH: 62% 32% . . .



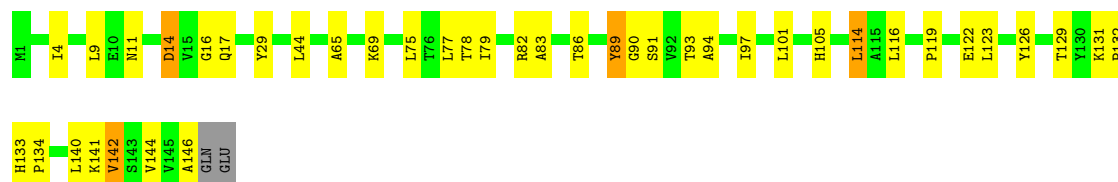
- Molecule 30: 50S ribosomal protein L6

Chain YH: 82% 14% ..



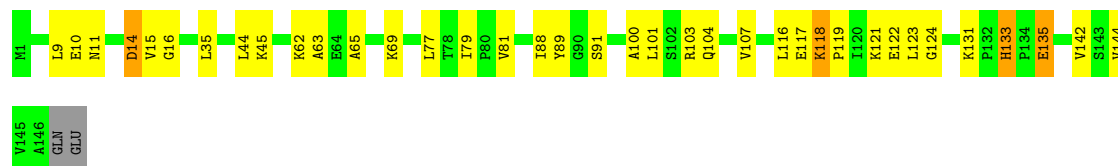
- Molecule 31: 50S ribosomal protein L9

Chain RI: 71% 25% ..



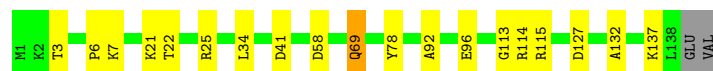
- Molecule 31: 50S ribosomal protein L9

Chain YI: 74% 22% ..



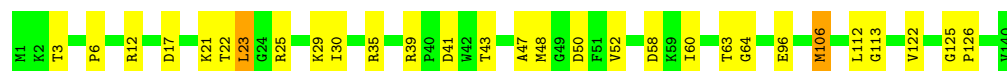
- Molecule 32: 50S ribosomal protein L13

Chain RN: 85% 13% ..




- Molecule 32: 50S ribosomal protein L13

Chain YN: 79% 19% ..




- Molecule 33: 50S ribosomal protein L14

Chain RO:  75% 23%




- Molecule 33: 50S ribosomal protein L14

Chain YO:  80% 19%




- Molecule 34: 50S ribosomal protein L15

Chain RP:  78% 19%



ALA

- Molecule 34: 50S ribosomal protein L15

Chain YP:  74% 24%



S133
A141
L147
LEU
GLU
ALA

- Molecule 35: 50S ribosomal protein L16

Chain RQ:  62% 35%




V102
M103
F104
E105
G108
V109
T110
E111
E112
Q113
E116
A117
L118
R119
K130
R134
D135
A136
Y137
Q141

- Molecule 35: 50S ribosomal protein L16

Chain YQ:  86% 14%


M1
R14
G15
R16
L17
K18
K22
D31
Y32
G33
L34
A40
R59
G62
G108
V109
T110
E111
E112
Q113
L118
G122
L125
K128
R134
Q141

- Molecule 36: 50S ribosomal protein L17

Chain RR:  75% 23% ..



- Molecule 36: 50S ribosomal protein L17

Chain YR:  82% 15% ..




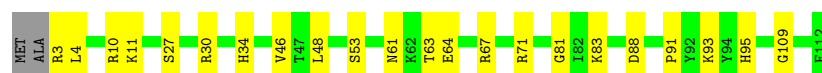
- Molecule 37: 50S ribosomal protein L18

Chain RS:  71% 25% ..



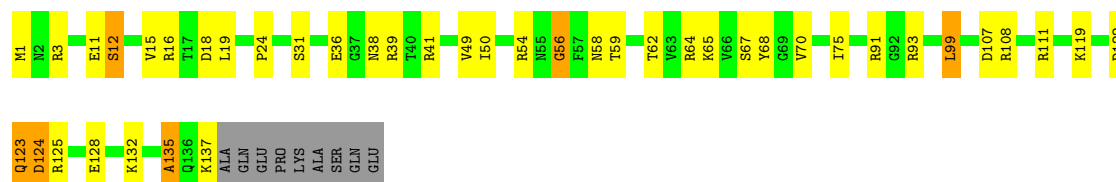
- Molecule 37: 50S ribosomal protein L18

Chain YS:  79% 20% .



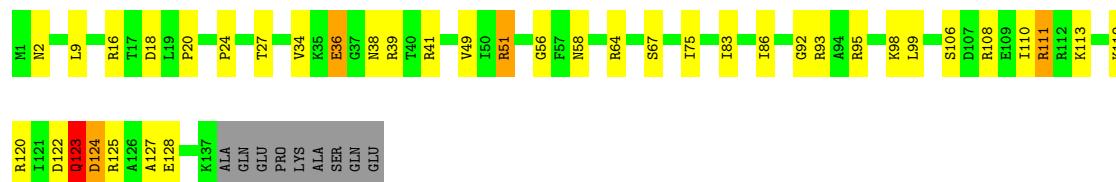
- Molecule 38: 50S ribosomal protein L19

Chain RT:  65% 25% . 6%




- Molecule 38: 50S ribosomal protein L19

Chain YT:  67% 23% . 6%



- Molecule 39: 50S ribosomal protein L20

Chain RU:  78% 19% ..



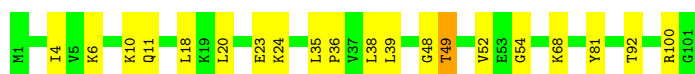
- Molecule 39: 50S ribosomal protein L20

Chain YU: 82% 14% . .



- Molecule 40: 50S ribosomal protein L21

Chain RV: 80% 19% .



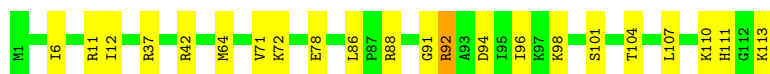
- Molecule 40: 50S ribosomal protein L21

Chain YV: 82% 13% 5%



- Molecule 41: 50S ribosomal protein L22

Chain RW: 81% 19% .



- Molecule 41: 50S ribosomal protein L22

Chain YW: 82% 17% .



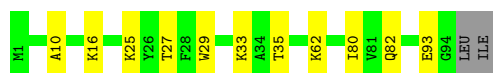
- Molecule 42: 50S ribosomal protein L23

Chain RX: 82% 14% .



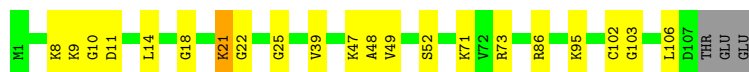
- Molecule 42: 50S ribosomal protein L23

Chain YX: 86% 11% .



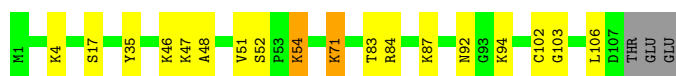
- Molecule 43: 50S ribosomal protein L24

Chain RY: 78% 18% ..



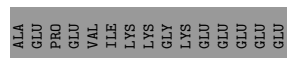
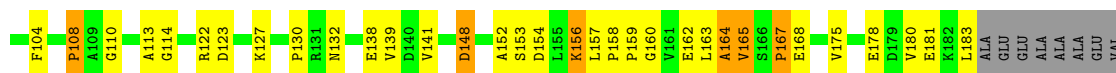
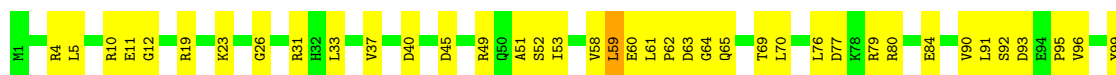
- Molecule 43: 50S ribosomal protein L24

Chain YY: 81% 15% ..



- Molecule 44: 50S ribosomal protein L25

Chain RZ: 54% 32% 11%



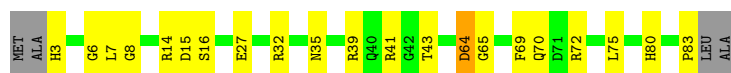
- Molecule 44: 50S ribosomal protein L25

Chain YZ: 67% 21% 11%



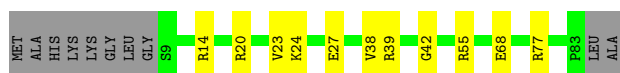
- Molecule 45: 50S ribosomal protein L27

Chain R0: 71% 24% 5%



- Molecule 45: 50S ribosomal protein L27

Chain Y0: 75% 13% 12%



- Molecule 46: 50S ribosomal protein L28

Chain R1: 79% 16% . .



- Molecule 46: 50S ribosomal protein L28

Chain Y1: 72% 20% . 5%



- Molecule 47: 50S ribosomal protein L29

Chain R2: 72% 24% .



- Molecule 47: 50S ribosomal protein L29

Chain Y2: 69% 22% 8%



- Molecule 48: 50S ribosomal protein L30

Chain R3: 72% 27% .



- Molecule 48: 50S ribosomal protein L30

Chain Y3: 78% 20% .

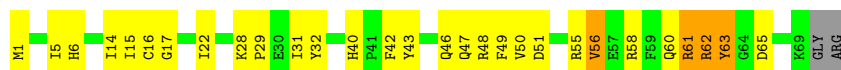


- Molecule 49: 50S ribosomal protein L31

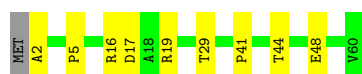
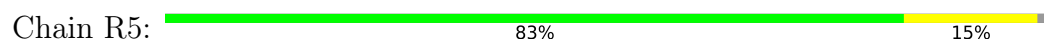
Chain R4: 58% 37% . .



- Molecule 49: 50S ribosomal protein L31



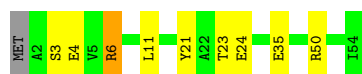
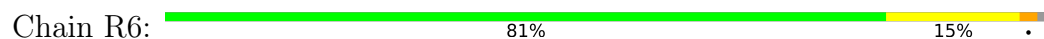
- Molecule 50: 50S ribosomal protein L32



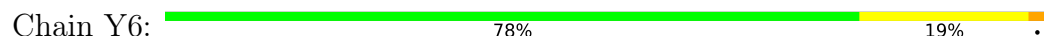
- Molecule 50: 50S ribosomal protein L32



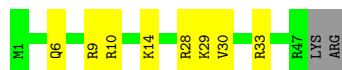
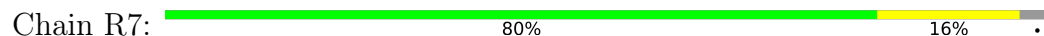
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34

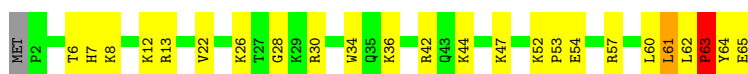




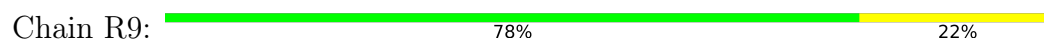
- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 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	210.17Å 451.47Å 620.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.46 – 3.20	Depositor
% Data completeness (in resolution range)	99.1 (152.46-3.20)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.224 , 0.256	Depositor
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.167	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291964	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.96	1/36098 (0.0%)	1.22	232/56341 (0.4%)
1	XA	0.95	3/36101 (0.0%)	1.23	252/56346 (0.4%)
2	QB	0.42	0/1942	0.63	0/2619
2	XB	0.42	0/1950	0.57	0/2630
3	QC	0.38	0/1629	0.62	1/2195 (0.0%)
3	XC	0.37	0/1629	0.58	0/2195
4	QD	0.52	0/1733	0.58	0/2318
4	XD	0.54	1/1733 (0.1%)	0.64	0/2318
5	QE	0.45	0/1171	0.62	0/1576
5	XE	0.49	0/1171	0.57	0/1576
6	QF	0.45	0/856	0.59	0/1154
6	XF	0.55	0/856	0.54	0/1154
7	QG	0.37	0/1276	0.55	0/1709
7	XG	0.37	0/1276	0.54	0/1709
8	QH	0.51	0/1128	0.61	0/1517
8	XH	0.54	0/1128	0.62	0/1517
9	QI	0.34	0/1029	0.64	1/1379 (0.1%)
9	XI	0.39	0/1017	0.64	0/1365
10	QJ	0.36	0/814	0.62	0/1095
10	XJ	0.34	0/790	0.60	0/1063
11	QK	0.47	0/900	0.61	0/1213
11	XK	0.49	0/879	0.54	0/1187
12	QL	0.62	0/991	0.61	0/1327
12	XL	0.57	0/972	0.64	1/1301 (0.1%)
13	QM	0.37	0/965	0.64	0/1292
13	XM	0.33	0/956	0.65	0/1281
14	QN	0.43	0/501	0.70	1/664 (0.2%)
14	XN	0.44	0/501	0.63	1/664 (0.2%)
15	QO	0.46	0/745	0.59	0/992
15	XO	0.49	0/740	0.52	0/987
16	QP	0.55	0/721	0.60	0/970
16	XP	0.46	0/721	0.60	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.54	0/847	0.60	0/1131
17	XQ	0.55	0/847	0.58	0/1131
18	QR	0.46	0/579	0.64	0/768
18	XR	0.49	0/579	0.60	0/768
19	QS	0.36	0/680	0.66	0/915
19	XS	0.35	0/689	0.65	0/926
20	QT	0.43	0/765	0.57	0/1007
20	XT	0.36	0/765	0.58	0/1007
21	QU	0.39	0/221	0.88	1/288 (0.3%)
21	XU	0.34	0/221	0.58	0/288
22	QV	0.62	1/1814 (0.1%)	1.10	6/2825 (0.2%)
22	XV	0.57	1/1814 (0.1%)	1.21	8/2825 (0.3%)
23	QX	0.46	0/470	1.00	1/733 (0.1%)
23	XX	0.52	0/470	1.22	6/733 (0.8%)
24	RA	1.32	53/69498 (0.1%)	1.31	773/108491 (0.7%)
24	YA	1.59	262/69543 (0.4%)	1.39	981/108563 (0.9%)
25	RB	0.92	0/2878	1.24	26/4490 (0.6%)
25	YB	1.86	31/2878 (1.1%)	6.09	81/4490 (1.8%)
26	RD	0.75	1/2185 (0.0%)	0.62	0/2944
26	YD	0.87	1/2185 (0.0%)	0.67	0/2944
27	RE	0.71	0/1601	0.61	0/2160
27	YE	0.83	1/1596 (0.1%)	0.66	0/2153
28	RF	0.68	0/1620	0.61	0/2194
28	YF	0.85	0/1620	0.63	0/2194
29	RG	0.41	0/1499	0.64	0/2016
29	YG	0.51	0/1499	0.63	1/2016 (0.0%)
30	RH	0.48	0/1362	0.65	1/1841 (0.1%)
30	YH	0.72	0/1356	0.59	0/1833
31	RI	0.44	0/1151	0.69	1/1558 (0.1%)
31	YI	0.50	0/1151	0.70	1/1558 (0.1%)
32	RN	0.60	0/1131	0.59	0/1525
32	YN	0.82	1/1148 (0.1%)	0.67	0/1547
33	RO	0.73	0/943	0.61	0/1269
33	YO	0.82	1/943 (0.1%)	0.66	1/1269 (0.1%)
34	RP	0.61	0/1156	0.62	0/1537
34	YP	0.74	0/1139	0.64	0/1514
35	RQ	0.60	0/1143	0.63	0/1527
35	YQ	0.82	0/1143	0.59	0/1527
36	RR	0.67	0/974	0.64	1/1302 (0.1%)
36	YR	0.77	0/974	0.72	0/1302
37	RS	0.49	0/892	0.73	1/1187 (0.1%)
37	YS	0.68	0/887	0.58	0/1180
38	RT	0.62	0/1155	0.66	1/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.70	0/1155	0.67	1/1542 (0.1%)
39	RU	0.68	0/982	0.61	0/1306
39	YU	0.93	0/982	0.62	0/1306
40	RV	0.62	0/790	0.61	0/1057
40	YV	0.86	0/790	0.67	0/1057
41	RW	0.69	0/911	0.61	0/1220
41	YW	0.89	0/911	0.64	0/1220
42	RX	0.67	0/739	0.61	0/993
42	YX	0.83	0/756	0.57	0/1014
43	RY	0.60	0/831	0.58	0/1108
43	YY	0.74	0/831	0.60	0/1108
44	RZ	0.48	0/1493	0.71	2/2026 (0.1%)
44	YZ	0.63	0/1493	0.57	0/2026
45	R0	0.60	0/652	0.60	0/867
45	Y0	0.84	0/607	0.63	0/809
46	R1	0.67	0/770	0.65	0/1022
46	Y1	0.78	0/736	0.65	0/978
47	R2	0.47	0/583	0.52	0/771
47	Y2	0.65	0/560	0.61	0/741
48	R3	0.62	1/474 (0.2%)	0.61	0/635
48	Y3	0.73	0/474	0.67	0/635
49	R4	0.39	0/578	0.64	0/776
49	Y4	0.41	0/578	0.68	0/776
50	R5	0.71	0/473	0.58	0/639
50	Y5	0.91	1/473 (0.2%)	0.65	1/639 (0.2%)
51	R6	0.62	0/460	0.65	1/613 (0.2%)
51	Y6	0.75	0/460	0.65	1/613 (0.2%)
52	R7	0.74	0/417	0.57	0/550
52	Y7	0.91	0/426	0.61	0/561
53	R8	0.68	0/525	0.71	0/691
53	Y8	0.77	0/525	0.76	1/691 (0.1%)
54	R9	0.62	0/310	0.53	0/407
54	Y9	0.84	0/310	0.55	0/407
All	All	1.14	360/315985 (0.1%)	1.30	2387/472446 (0.5%)

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
1	XA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	22
2	XB	0	15
3	QC	0	15
3	XC	0	9
4	QD	0	12
4	XD	0	15
5	QE	0	7
5	XE	0	6
6	QF	0	5
6	XF	0	3
7	QG	0	9
7	XG	0	10
8	QH	0	3
8	XH	0	5
9	QI	0	15
9	XI	0	16
10	QJ	0	12
10	XJ	0	8
11	QK	0	5
11	XK	0	4
12	QL	0	8
12	XL	0	11
13	QM	0	13
13	XM	0	18
14	QN	0	6
14	XN	0	2
15	QO	0	1
15	XO	0	2
16	QP	0	5
16	XP	0	10
17	QQ	0	3
17	XQ	0	1
18	QR	0	5
18	XR	0	6
19	QS	0	13
19	XS	0	14
20	QT	0	10
20	XT	0	12
21	XU	0	4
24	YA	0	2
26	RD	0	13
26	YD	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	RE	0	7
27	YE	0	10
28	RF	0	12
28	YF	0	15
29	RG	0	17
29	YG	0	20
30	RH	0	23
30	YH	0	1
31	RI	0	17
31	YI	0	21
32	RN	0	10
32	YN	0	7
33	RO	0	2
33	YO	0	1
34	RP	0	8
34	YP	0	5
35	RQ	0	18
35	YQ	0	6
36	RR	0	4
36	YR	0	5
37	RS	0	11
37	YS	0	1
38	RT	0	15
38	YT	0	11
39	RU	0	5
39	YU	0	5
40	RV	0	6
40	YV	0	7
41	RW	0	5
41	YW	0	5
42	RX	0	2
42	YX	0	1
43	RY	0	7
43	YY	0	5
44	RZ	0	38
44	YZ	0	10
45	R0	0	2
45	Y0	0	1
46	R1	0	10
46	Y1	0	7
47	R2	0	5
47	Y2	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	R3	0	1
48	Y3	0	2
49	R4	0	15
49	Y4	0	11
50	R5	0	1
52	R7	0	1
53	R8	0	11
53	Y8	0	6
All	All	0	781

The worst 5 of 360 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	YB	112	G	N9-C4	30.70	1.62	1.38
25	YB	114	G	N9-C4	28.24	1.60	1.38
25	YB	112	G	N9-C8	-27.57	1.18	1.37
25	YB	114	G	N9-C8	-26.21	1.19	1.37
25	YB	112	G	C8-N7	14.77	1.39	1.30

The worst 5 of 2387 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YB	114	G	C4-C5-N7	-176.50	40.20	110.80
25	YB	112	G	C4-C5-N7	-173.34	41.46	110.80
25	YB	114	G	N7-C8-N9	-148.48	38.86	113.10
25	YB	112	G	N7-C8-N9	-146.23	39.98	113.10
25	YB	112	G	C8-N9-C4	-129.76	54.49	106.40

There are no chirality outliers.

5 of 781 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	18	GLY	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	38	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	448	0
1	XA	32249	0	16278	456	3
2	QB	1907	0	1958	34	0
2	XB	1915	0	1969	35	0
3	QC	1605	0	1668	29	0
3	XC	1605	0	1668	21	0
4	QD	1703	0	1766	27	0
4	XD	1703	0	1764	37	0
5	QE	1155	0	1213	27	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	14	0
6	XF	843	0	857	11	0
7	QG	1257	0	1296	15	0
7	XG	1257	0	1296	22	0
8	QH	1108	0	1165	19	0
8	XH	1108	0	1165	23	0
9	QI	1010	0	1037	19	0
9	XI	998	0	1024	28	0
10	QJ	801	0	849	23	0
10	XJ	777	0	816	15	0
11	QK	885	0	904	28	0
11	XK	864	0	881	13	0
12	QL	975	0	1062	13	0
12	XL	956	0	1046	22	0
13	QM	955	0	1021	21	0
13	XM	946	0	1008	24	0
14	QN	492	0	529	19	0
14	XN	492	0	529	11	0
15	QO	734	0	771	9	0
15	XO	729	0	768	8	0
16	QP	705	0	725	15	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	24	0
17	XQ	834	0	904	15	0
18	QR	574	0	644	7	0
18	XR	574	0	644	7	0
19	QS	665	0	686	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	10	0
20	QT	763	0	861	13	0
20	XT	763	0	861	22	0
21	QU	217	0	234	4	0
21	XU	217	0	234	4	0
22	QV	1648	0	834	28	0
22	XV	1648	0	834	23	0
23	QX	418	0	209	7	0
23	XX	418	0	209	7	0
24	RA	62051	0	31279	607	3
24	YA	62091	0	31292	530	0
25	RB	2573	0	1306	22	0
25	YB	2573	0	1304	41	0
26	RD	2135	0	2221	35	0
26	YD	2135	0	2221	32	0
27	RE	1568	0	1634	29	0
27	YE	1563	0	1628	27	0
28	RF	1585	0	1632	23	0
28	YF	1585	0	1632	24	0
29	RG	1474	0	1535	35	0
29	YG	1474	0	1535	30	0
30	RH	1336	0	1418	27	0
30	YH	1330	0	1413	18	0
31	RI	1136	0	1223	13	2
31	YI	1136	0	1223	12	0
32	RN	1104	0	1180	8	0
32	YN	1121	0	1194	15	0
33	RO	933	0	996	25	0
33	YO	933	0	995	17	0
34	RP	1139	0	1223	26	0
34	YP	1122	0	1206	26	0
35	RQ	1122	0	1179	27	0
35	YQ	1122	0	1179	10	0
36	RR	960	0	1021	18	0
36	YR	960	0	1021	11	0
37	RS	882	0	943	17	0
37	YS	877	0	938	15	0
38	RT	1141	0	1202	23	0
38	YT	1141	0	1202	26	0
39	RU	964	0	1022	25	0
39	YU	964	0	1021	19	0
40	RV	779	0	852	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YV	779	0	852	12	0
41	RW	900	0	964	11	0
41	YW	900	0	964	11	0
42	RX	725	0	778	7	0
42	YX	742	0	803	8	0
43	RY	818	0	909	11	0
43	YY	818	0	909	13	0
44	RZ	1461	0	1493	26	0
44	YZ	1461	0	1493	22	0
45	R0	643	0	667	12	0
45	Y0	599	0	617	7	0
46	R1	763	0	848	9	0
46	Y1	729	0	801	10	0
47	R2	581	0	629	7	0
47	Y2	558	0	610	5	2
48	R3	469	0	517	7	0
48	Y3	469	0	518	8	0
49	R4	565	0	558	9	0
49	Y4	565	0	557	13	0
50	R5	459	0	476	7	0
50	Y5	459	0	476	9	0
51	R6	453	0	473	7	0
51	Y6	453	0	473	10	0
52	R7	409	0	454	6	0
52	Y7	418	0	467	3	0
53	R8	517	0	582	12	0
53	Y8	517	0	582	13	0
54	R9	307	0	335	6	0
54	Y9	307	0	335	7	0
55	QA	64	0	0	0	0
55	QV	1	0	0	0	0
55	R0	2	0	0	0	0
55	R8	2	0	0	0	0
55	RA	444	0	0	0	0
55	RB	7	0	0	0	0
55	RE	5	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RQ	1	0	0	0	0
55	RR	1	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XA	78	0	0	0	0
55	XE	1	0	0	0	0
55	XM	2	0	0	0	0
55	XV	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	2	0	0	0	0
55	Y3	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	510	0	0	0	0
55	YB	7	0	0	0	0
55	YD	2	0	0	0	0
55	YE	5	0	0	0	0
55	YP	3	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	1	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	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	Y4	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	0	0
All	All	291964	0	197872	3283	5

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 3283 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)
24:RA:1712:A:C2'	24:RA:1713:G:H5'	1.74	1.18
43:YY:92:ASN:ND2	43:YY:94:LYS:HG2	1.60	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1405:A:N6	24:YA:1418:U:H3	1.48	1.10
24:RA:2818:U:C2	24:RA:2901:A:N6	2.27	1.02
24:RA:2226:C:H1'	24:RA:2232:G:N2	1.74	1.01

All (5) 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)
31:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.00	0.20
24:RA:331:G:OP2	47:Y2:17:SER:CA[3_555]	2.01	0.19
31:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	2.10	0.10
24:RA:331:G:OP2	47:Y2:17:SER:CB[3_555]	2.10	0.10
24:RA:2158:C:O2'	1:XA:1042:G:O2'[4_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	205 (88%)	28 (12%)	0	100	100
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
4	XD	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	10	44
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	88 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	101 (86%)	16 (14%)	0	100	100
11	XK	114/129 (88%)	102 (90%)	12 (10%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	13 (11%)	0	100	100
12	XL	120/132 (91%)	100 (83%)	20 (17%)	0	100	100
13	QM	118/126 (94%)	102 (86%)	16 (14%)	0	100	100
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	17	56
14	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
14	XN	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	QO	86/89 (97%)	83 (96%)	3 (4%)	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%)	74 (90%)	8 (10%)	0	100	100
17	QQ	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	272/276 (99%)	259 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	YD	272/276 (99%)	253 (93%)	19 (7%)	0	100	100
27	RE	203/206 (98%)	187 (92%)	16 (8%)	0	100	100
27	YE	202/206 (98%)	189 (94%)	13 (6%)	0	100	100
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
29	RG	179/182 (98%)	155 (87%)	24 (13%)	0	100	100
29	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	64
30	RH	172/180 (96%)	142 (83%)	29 (17%)	1 (1%)	25	64
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
31	YI	144/148 (97%)	120 (83%)	24 (17%)	0	100	100
32	RN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
32	YN	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
33	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	RP	147/150 (98%)	142 (97%)	5 (3%)	0	100	100
34	YP	145/150 (97%)	138 (95%)	6 (4%)	1 (1%)	22	61
35	RQ	139/141 (99%)	116 (84%)	22 (16%)	1 (1%)	22	61
35	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
36	RR	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	56
36	YR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
37	RS	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
37	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
38	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	44
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	44
39	RU	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	56
40	RV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
41	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
42	YX	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
43	YY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
44	RZ	181/206 (88%)	143 (79%)	38 (21%)	0	100	100
44	YZ	181/206 (88%)	176 (97%)	4 (2%)	1 (1%)	25	64
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	84 (92%)	7 (8%)	0	100	100
47	R2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
47	Y2	64/72 (89%)	61 (95%)	3 (5%)	0	100	100
48	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
49	Y4	67/71 (94%)	55 (82%)	12 (18%)	0	100	100
50	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	53 (86%)	8 (13%)	1 (2%)	9	43
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11453/12128 (94%)	10502 (92%)	935 (8%)	16 (0%)	51	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	RR	4	LEU
4	XD	31	CYS

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Mol	Chain	Res	Type
44	YZ	52	SER
38	RT	123	GLN
38	RT	124	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	88	95
2	XB	204/220 (93%)	203 (100%)	1 (0%)	88	95
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%)	179 (99%)	1 (1%)	86	94
4	XD	180/181 (99%)	172 (96%)	8 (4%)	28	64
5	QE	116/123 (94%)	114 (98%)	2 (2%)	60	83
5	XE	116/123 (94%)	113 (97%)	3 (3%)	46	76
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%)	123 (98%)	3 (2%)	49	77
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	84
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	88
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%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	94 (98%)	2 (2%)	53	79
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	66
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	80
15	QO	79/80 (99%)	78 (99%)	1 (1%)	69	87
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	86
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	88
17	XQ	95/97 (98%)	95 (100%)	0	100	100
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%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	60
26	RD	216/218 (99%)	216 (100%)	0	100	100
26	YD	216/218 (99%)	214 (99%)	2 (1%)	78	91
27	RE	165/166 (99%)	164 (99%)	1 (1%)	86	94
27	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
29	RG	155/156 (99%)	153 (99%)	2 (1%)	69	87
29	YG	155/156 (99%)	155 (100%)	0	100	100
30	RH	145/148 (98%)	145 (100%)	0	100	100
30	YH	144/148 (97%)	142 (99%)	2 (1%)	67	86
31	RI	122/124 (98%)	121 (99%)	1 (1%)	81	93
31	YI	122/124 (98%)	121 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
32	YN	119/119 (100%)	119 (100%)	0	100	100
33	RO	100/100 (100%)	98 (98%)	2 (2%)	55	80
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	115 (99%)	1 (1%)	78	91
34	YP	114/116 (98%)	113 (99%)	1 (1%)	78	91
35	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
35	YQ	111/111 (100%)	111 (100%)	0	100	100
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	90
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	120 (100%)	0	100	100
38	YT	120/127 (94%)	119 (99%)	1 (1%)	81	93
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
39	YU	93/94 (99%)	91 (98%)	2 (2%)	52	79
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	79 (96%)	3 (4%)	34	68
41	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	76/78 (97%)	76 (100%)	0	100	100
43	RY	88/91 (97%)	87 (99%)	1 (1%)	73	88
43	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
44	RZ	162/179 (90%)	162 (100%)	0	100	100
44	YZ	162/179 (90%)	162 (100%)	0	100	100
45	R0	65/67 (97%)	63 (97%)	2 (3%)	40	72
45	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Y2	62/67 (92%)	62 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	55	80
48	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	80
49	R4	62/63 (98%)	62 (100%)	0	100	100
49	Y4	62/63 (98%)	61 (98%)	1 (2%)	62	84
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	50 (98%)	1 (2%)	55	80
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	53 (98%)	1 (2%)	57	81
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	57	81
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9692/10066 (96%)	9620 (99%)	72 (1%)	84	94

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	R0	64	ASP
4	XD	33	MET
43	YY	54	LYS
48	R3	30	ARG
4	XD	18	LYS

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

Mol	Chain	Res	Type
38	RT	58	ASN
45	R0	35	ASN
27	YE	129	HIS
33	RO	3	GLN
28	YF	40	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	289 (19%)	39 (2%)
1	XA	1499/1521 (98%)	271 (18%)	33 (2%)
22	QV	76/77 (98%)	22 (28%)	1 (1%)
22	XV	76/77 (98%)	18 (23%)	1 (1%)
23	QX	18/19 (94%)	7 (38%)	1 (5%)
23	XX	18/19 (94%)	6 (33%)	0
24	RA	2877/2915 (98%)	591 (20%)	37 (1%)
24	YA	2880/2915 (98%)	551 (19%)	43 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9181/9308 (98%)	1794 (19%)	157 (1%)

5 of 1794 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	47	C

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	RA	2148	A
1	XA	250	A
24	YA	1830	G
24	RA	2578	A
1	XA	5	U

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

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	XV	37	22	18,26,27	1.37	3 (16%)	19,39,42	1.70	3 (15%)
22	1MG	QV	37	22	18,26,27	1.34	2 (11%)	19,39,42	1.72	4 (21%)

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	XV	37	22	-	0/3/25/26	0/3/3/3
22	1MG	QV	37	22	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	37	1MG	C6-C5	4.46	1.48	1.41
22	QV	37	1MG	C6-C5	4.44	1.48	1.41
22	QV	37	1MG	C5-C4	2.53	1.47	1.40
22	XV	37	1MG	C5-C4	2.48	1.47	1.40
22	XV	37	1MG	C6-N1	2.07	1.41	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	C2-N3-C4	5.60	121.76	115.36
22	QV	37	1MG	C2-N3-C4	5.47	121.61	115.36
22	QV	37	1MG	C6-C5-C4	-2.94	118.07	119.96
22	XV	37	1MG	C6-C5-C4	-2.93	118.08	119.96
22	XV	37	1MG	C4-C5-N7	-2.91	106.36	109.40

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
22	QV	37	1MG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1166 ligands modelled in this entry, 1164 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	QD	301	4	0,12,12	0.00	-	-		
56	SF4	XD	301	4	0,12,12	0.00	-	-		

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	QD	301	4	-	-	0/6/5/5
56	SF4	XD	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.