wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2023 – 11:32 AM EDT

PDB ID	:	6NSH
Title	:	Modified ASL proline bound to Thermus thermophilus 70S (near-cognate)
Authors	:	Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.
Deposited on	:	2019-01-24
Resolution	:	3.40 Å(reported)

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

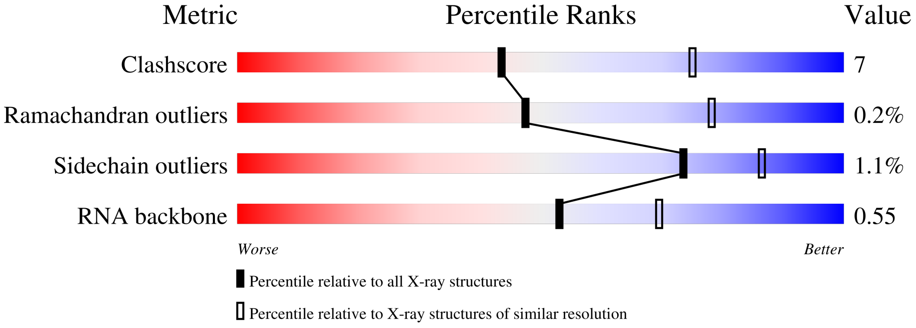
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	RA	2915	 55% 32% 10% ••
1	YA	2915	 54% 33% 11% ••
2	RB	122	 58% 27% 12% ••
2	YB	122	 58% 25% 16% •
3	RD	276	 83% 15% ••
3	YD	276	 83% 13% ••

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Mol	Chain	Length	Quality of chain
4	RE	206	
4	YE	206	
5	RF	210	
5	YF	210	
6	RG	182	
6	YG	182	
7	RH	180	
7	YH	180	
8	RI	148	
8	YI	148	
9	RN	140	
9	YN	140	
10	RO	122	
10	YO	122	
11	RP	150	
11	YP	150	
12	RQ	141	
12	YQ	141	
13	RR	118	
13	YR	118	
14	RS	112	
14	YS	112	
15	RT	146	
15	YT	146	
16	RU	118	

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Mol	Chain	Length	Quality of chain
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	
28	R6	54	
28	Y6	54	

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Mol	Chain	Length	Quality of chain
29	R7	49	 80% 14% • •
29	Y7	49	 82% 16% •
30	R8	65	 74% 18% 6% •
30	Y8	65	 69% 25% 5% •
31	R9	37	 73% 24% •
31	Y9	37	 70% 30%
32	QA	1521	 52% 37% 10% • •
32	XA	1521	 51% 37% 10% • •
33	QB	256	 62% 27% • 8%
33	XB	256	 67% 23% • 8%
34	QC	239	 64% 20% • 14%
34	XC	239	 64% 18% • 14%
35	QD	209	 68% 28% •
35	XD	209	 65% 31% •
36	QE	162	 73% 20% 7%
36	XE	162	 77% 16% 7%
37	QF	101	 75% 25%
37	XF	101	 89% 11%
38	QG	156	 76% 21% • •
38	XG	156	 73% 25% • •
39	QH	138	 75% 24% •
39	XH	138	 83% 17% •
40	QI	128	 66% 31% • •
40	XI	128	 59% 34% 6% •
41	QJ	105	 61% 30% • 6%

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Mol	Chain	Length	Quality of chain
41	XJ	105	56% 33% • 9%
42	QK	129	72% 16% • 10%
42	XK	129	73% 17% 10%
43	QL	132	70% 24% • 5%
43	XL	132	66% 25% • 8%
44	QM	126	62% 25% 9% 5%
44	XM	126	56% 36% • 6%
45	QN	61	72% 26% •
45	XN	61	56% 39% • •
46	QO	89	83% 16% •
46	XO	89	73% 24% • •
47	QP	88	70% 24% • 5%
47	XP	88	70% 23% • 5%
48	QQ	105	74% 20% • 5%
48	XQ	105	71% 23% • 5%
49	QR	88	61% 18% 20%
49	XR	88	60% 19% 20%
50	QS	93	55% 33% • 11%
50	XS	93	53% 33% • 10%
51	QT	106	68% 23% • 7%
51	XT	106	62% 28% • 7%
52	QU	27	56% 22% 11% • 7%
52	XU	27	41% 44% 7% 7%
53	QV	17	53% 47%
53	XV	17	47% 24% 18% 12%

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Mol	Chain	Length	Quality of chain
54	QX	19	
54	XX	19	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 290035 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 23S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
3	YD	273	Total 2126	C 1341	N 424	O 358	S 3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	RP	148	Total C N O S 1130 704 230 193 3	0	0	0
11	YP	147	Total C N O S 1122 698 229 192 3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	RR	118	Total C N O S 968 604 203 160 1	0	0	0
13	YR	117	Total C N O 960 599 202 159	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	RX	92	Total C N O 725 471 131 123	0	0	0
19	YX	94	Total C N O S 742 482 134 125 1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
21	YZ	201	Total	C	N	O	S	0	0	0
			1587	1012	281	291	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
22	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
24	Y2	72	Total	C	N	O	S	0	0	0
			606	375	122	107	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	36	Total	C	N	O	S	0	0	0
			302	186	67	45	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
32	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	QJ	99	Total C N O S 801 504 157 139 1	0	0	0
41	XJ	96	Total C N O S 777 487 153 136 1	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	QK	116	Total C N O S 864 537 164 160 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	116	Total 864	C 537	N 164	O 160	S 3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	120	Total 955	C 591	N 197	O 165	S 2	0	0	0
44	XM	119	Total 946	C 585	N 195	O 164	S 2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called 30S ribosomal protein Thx.

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

- Molecule 53 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	17	Total 365	C 163	N 65	O 120	P 17	0	0	0
53	XV	15	Total 322	C 144	N 57	O 106	P 15	0	0	0

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	18	Total 389	C 174	N 76	O 121	P 18	0	0	0
54	XX	19	Total 412	C 184	N 81	O 128	P 19	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RA	485	Total 485	Mg 485	0	0
55	RB	8	Total 8	Mg 8	0	0
55	RE	2	Total 2	Mg 2	0	0
55	RF	1	Total 1	Mg 1	0	0
55	RN	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	RP	2	Total 2	Mg 2	0	0
55	RQ	2	Total 2	Mg 2	0	0
55	RT	1	Total 1	Mg 1	0	0
55	RX	1	Total 1	Mg 1	0	0
55	R0	1	Total 1	Mg 1	0	0
55	R1	1	Total 1	Mg 1	0	0
55	R5	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0

Continued on next page...

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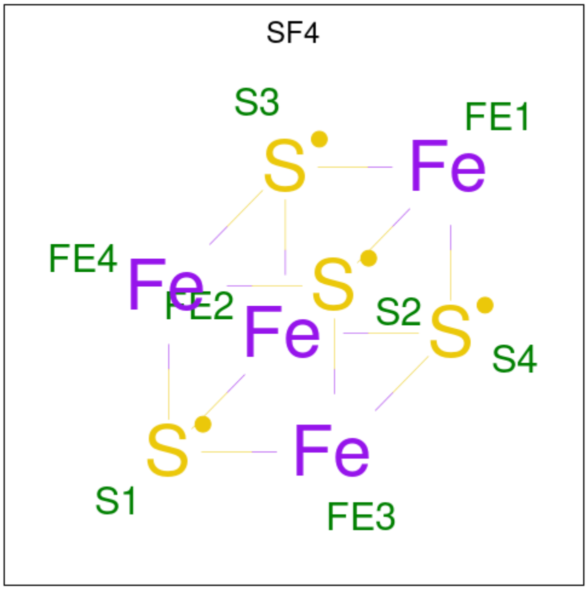
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	QA	66	Total Mg 66 66	0	0
55	QF	1	Total Mg 1 1	0	0
55	YA	510	Total Mg 510 510	0	0
55	YB	7	Total Mg 7 7	0	0
55	YD	1	Total Mg 1 1	0	0
55	YE	4	Total Mg 4 4	0	0
55	YO	1	Total Mg 1 1	0	0
55	YP	2	Total Mg 2 2	0	0
55	YQ	1	Total Mg 1 1	0	0
55	YR	1	Total Mg 1 1	0	0
55	Y0	2	Total Mg 2 2	0	0
55	Y1	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	1	Total Mg 1 1	0	0
55	Y8	1	Total Mg 1 1	0	0
55	XA	87	Total Mg 87 87	0	0
55	XE	1	Total Mg 1 1	0	0
55	XL	1	Total Mg 1 1	0	0
55	XQ	1	Total Mg 1 1	0	0
55	XS	1	Total Mg 1 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RY	1	Total Zn 1 1	0	0
56	R4	1	Total Zn 1 1	0	0
56	R5	1	Total Zn 1 1	0	0
56	R6	1	Total Zn 1 1	0	0
56	R9	1	Total Zn 1 1	0	0
56	QN	1	Total Zn 1 1	0	0
56	YY	1	Total Zn 1 1	0	0
56	Y4	1	Total Zn 1 1	0	0
56	Y5	1	Total Zn 1 1	0	0
56	Y6	1	Total Zn 1 1	0	0
56	Y9	1	Total Zn 1 1	0	0
56	XN	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

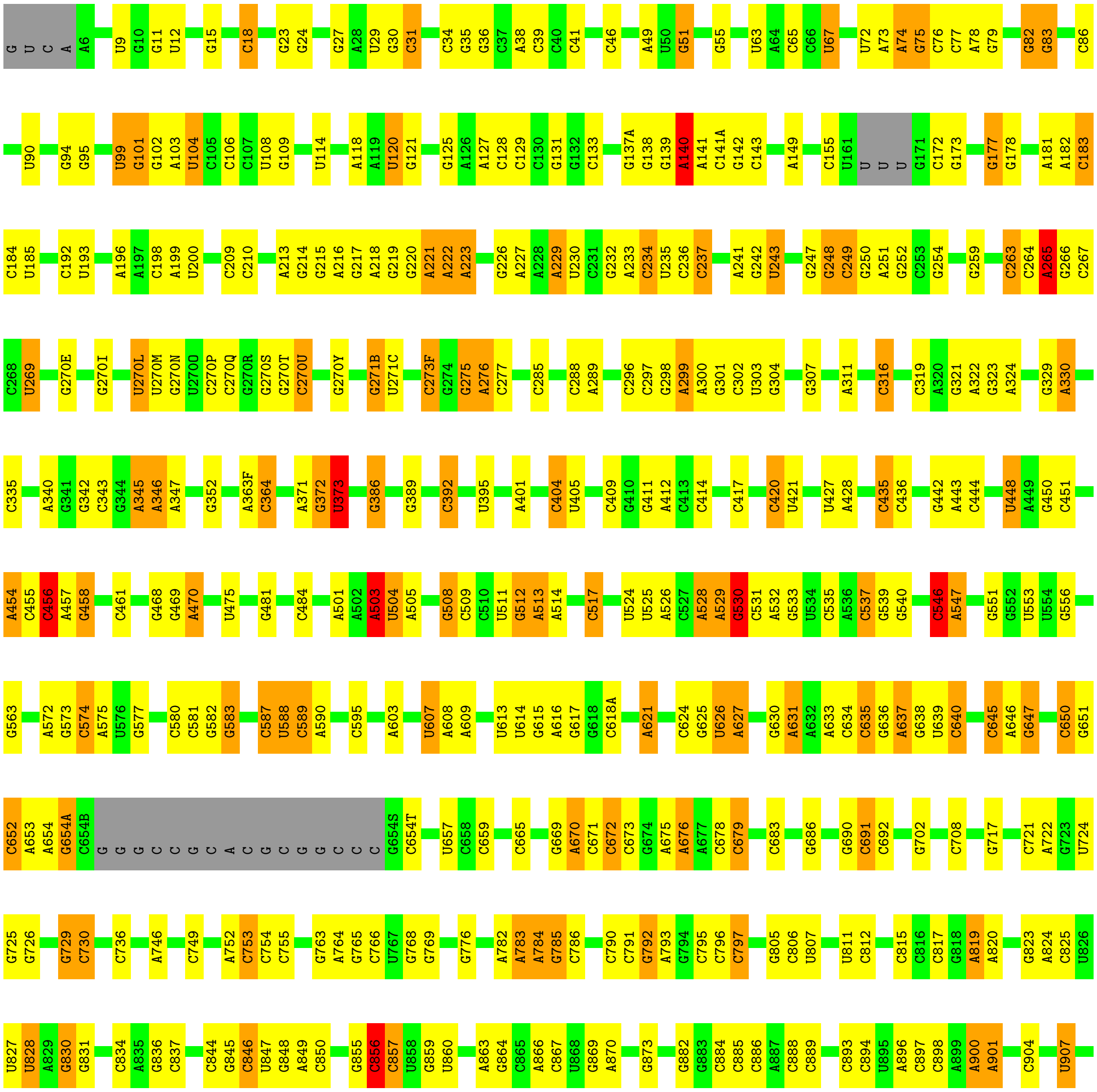
3 Residue-property plots

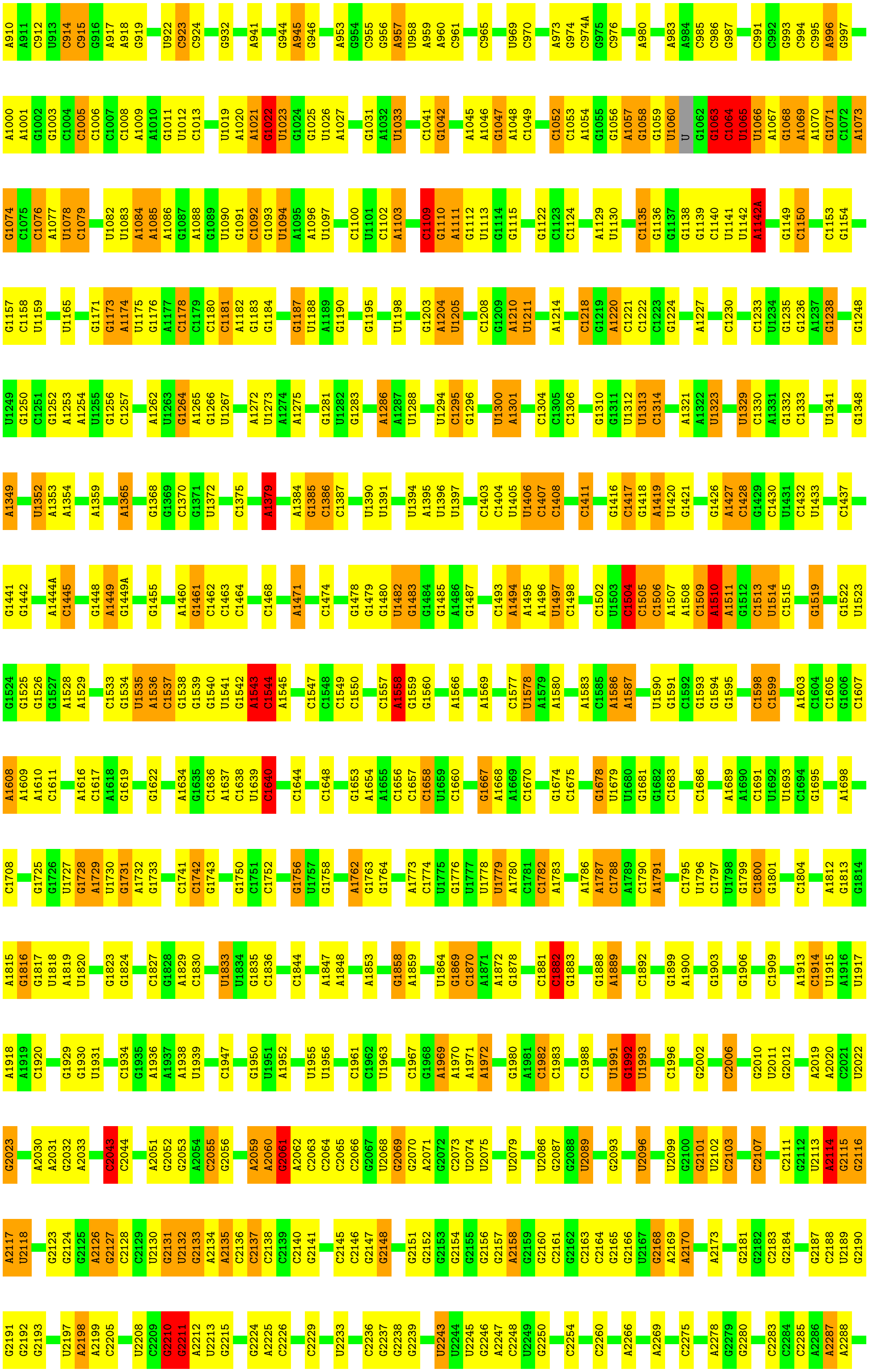
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: 23S rRNA

Chain RA: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A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 G1031 A1032 U1033 C1041 G1042 A1045 A1046 G1047 A1048 C1049 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073
G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 C1100 U1101 C1102 A1103 C1109 G1110 A1111 G1112 U1113 G1114 G1115 G1122 C1123 C1124 A1129 U1130 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A G1149 C1150 C1153 G1154
G1157 C1158 U1159 U1165 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 G1187 U1188 A1189 G1190 G1195 U1198 G1203 A1204 U1205 C1208 G1209 A1210 U1211 A1214 C1218 G1219 A1220 C1221 C1222 C1223 G1224 A1227 C1230 C1233 U1234 G1235 G1236 A1237 G1238 G1248
U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 A1262 U1263 G1264 A1265 G1266 U1267 A1272 U1273 A1274 A1275 G1281 U1282 G1283 A1286 A1287 U1288 U1294 C1295 G1296 U1300 A1301 C1304 C1305 C1306 G1310 G1311 U1312 U1313 C1314 A1321 G1322 U1323 U1329 C1330 A1331 G1332 C1333 U1341 G1348
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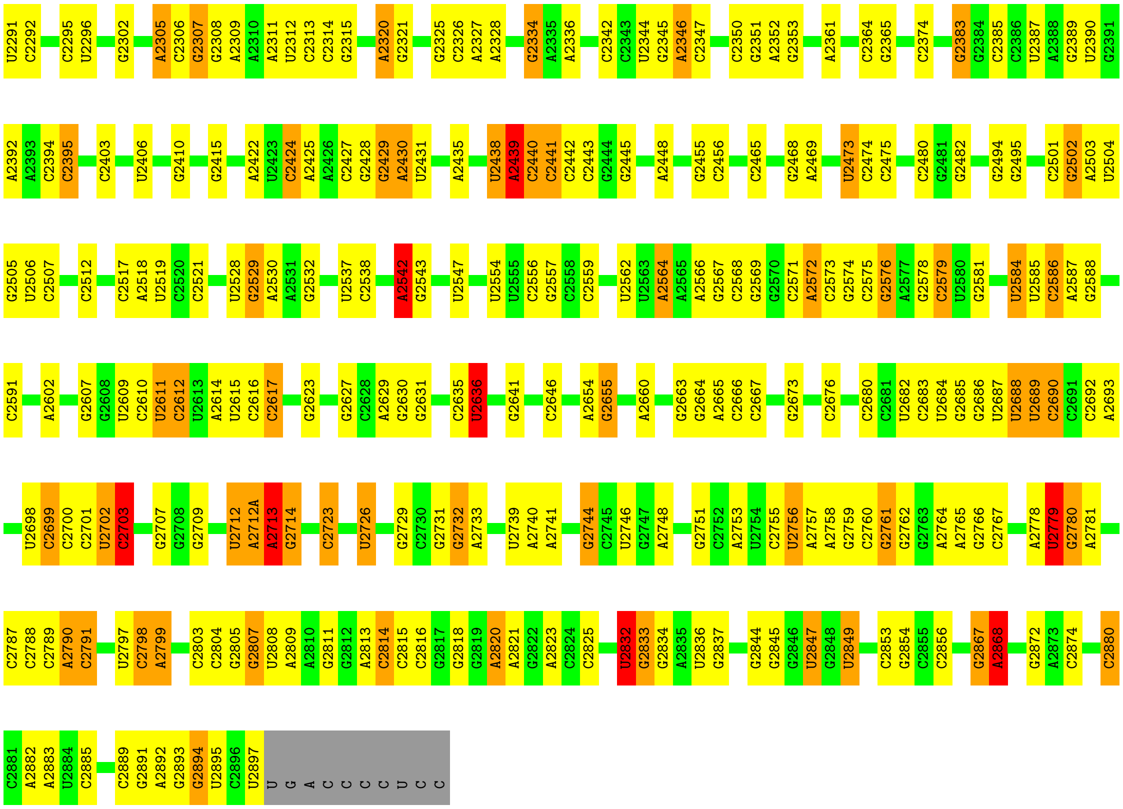
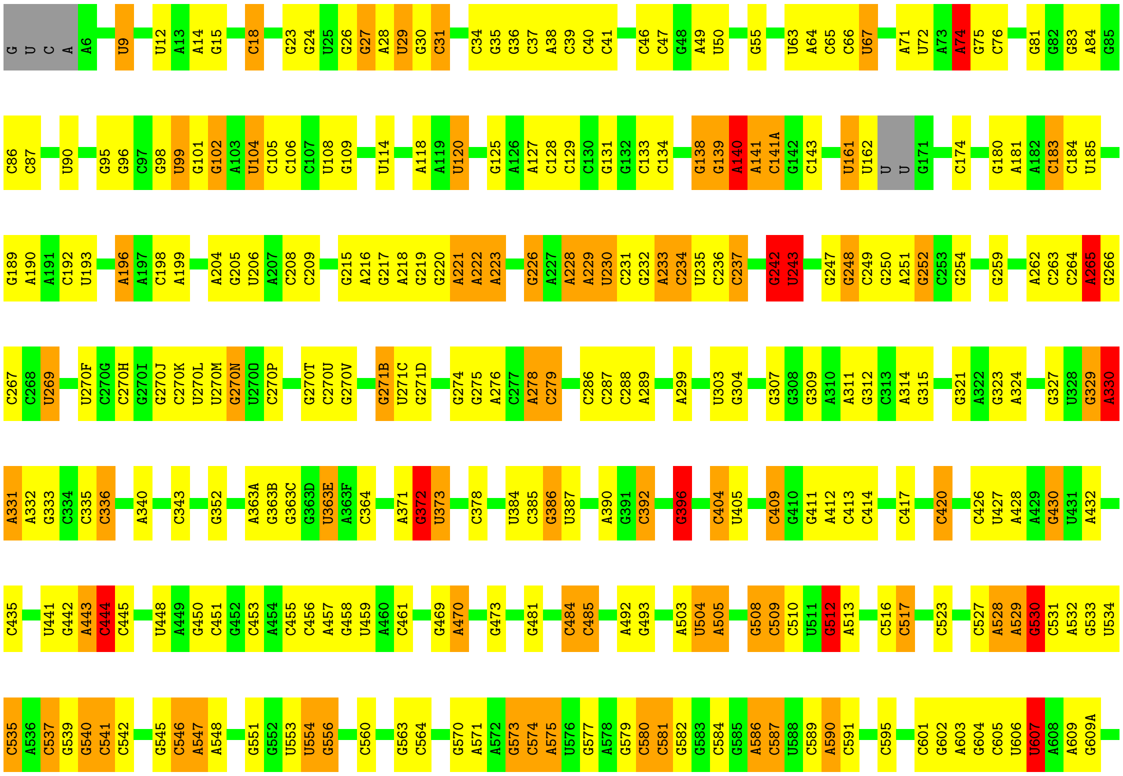
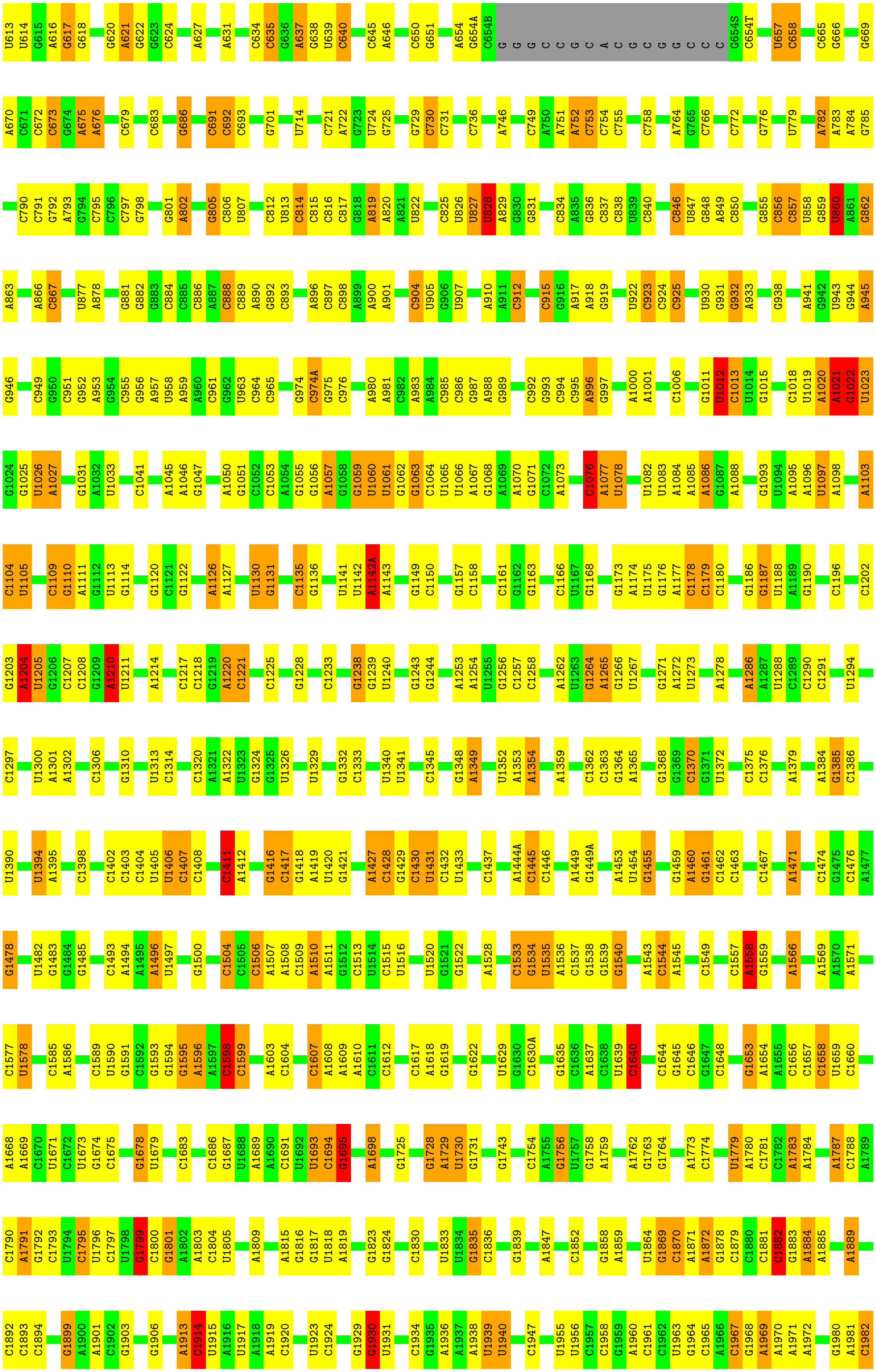
G1441 G1442 A1444A C1445 G1448 A1449 G1449A G1455 A1460 G1461 C1462 C1463 C1464 C1468 A1471 C1474 G1478 G1479 G1480 U1482 G1483 U1484 G1485 A1486 G1487 C1493 A1494 A1495 A1496 U1497 C1498 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 G1519 G1522 U1523
G1524 G1525 G1526 G1527 A1528 A1529 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1547 C1548 C1549 C1550 C1557 A1558 G1559 G1560 A1566 A1569 C1577 U1578 A1579 A1580 A1583 C1585 A1586 A1587 U1590 G1591 C1592 G1593 G1594 G1595 C1598 C1599 A1603 C1604 C1605 G1606 C1607
A1608 A1609 A1610 C1611 A1616 C1617 A1618 G1619 G1622 A1634 G1635 C1636 A1637 C1638 U1639 C1640 C1644 C1648 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1667 A1668 A1669 C1670 G1674 C1675 G1678 U1679 U1680 G1681 G1682 C1683 C1686 A1689 A1690 C1691 U1692 U1693 C1694 G1695 A1698
C1708 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1741 C1742 G1743 G1750 C1751 C1752 G1756 U1757 G1758 A1762 G1763 G1764 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1786 A1787 C1788 A1789 C1790 A1791 C1795 U1796 C1797 U1798 G1799 C1800 G1801 C1804 A1812 G1813 G1814
A1815 G1816 G1817 U1818 A1819 U1820 G1823 G1824 C1827 G1828 A1829 C1830 U1833 U1834 G1835 C1836 C1844 A1847 A1848 A1853 G1858 A1859 U1864 G1869 C1870 A1871 A1872 G1878 C1881 C1882 G1883 G1888 A1889 C1892 G1899 A1900 G1903 G1906 C1909 A1913 C1914 U1915 A1916 U1917
A1918 A1919 C1920 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 C1947 G1950 U1951 A1952 U1955 U1956 C1961 C1962 U1963 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 G1982 C1983 C1988 U1991 G1992 U1993 C1996 G2002 C2006 G2010 U2011 G2012 A2019 A2020 C2021 U2022
G2023 A2030 A2031 G2032 A2033 C2043 C2044 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 U2079 U2086 G2087 G2088 U2089 G2093 U2096 U2099 G2100 G2101 U2102 C2103 C2107 C2111 G2112 U2113 A2114 G2115 G2116
A2117 U2118 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2145 C2146 G2147 G2148 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2173 G2181 G2182 C2183 G2184 G2187 C2188 U2189 G2190
G2191 G2192 G2193 U2197 A2198 A2199 C2205 U2208 C2209 G2210 G2211 A2212 U2213 G2215 G2224 A2225 C2226 C2229 U2233 C2236 G2237 G2238 G2239 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 C2254 C2260 A2266 A2269 C2275 A2278 G2279 C2280 C2283 C2284 C2285 A2286 A2287 A2288



- Molecule 1: 23S rRNA

Chain YA:

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A670 C671 C672 C673 G674 A675 A676 C679 C683 G686 C691 C692 C693 G701 U714 C721 A722 G723 U724 G725 G729 C730 C731 C736 A746 C749 A750 A751 A752 C753 C754 C755 C758 A764 G765 C766 C772 G776 U779 A782 A783 A784 G785
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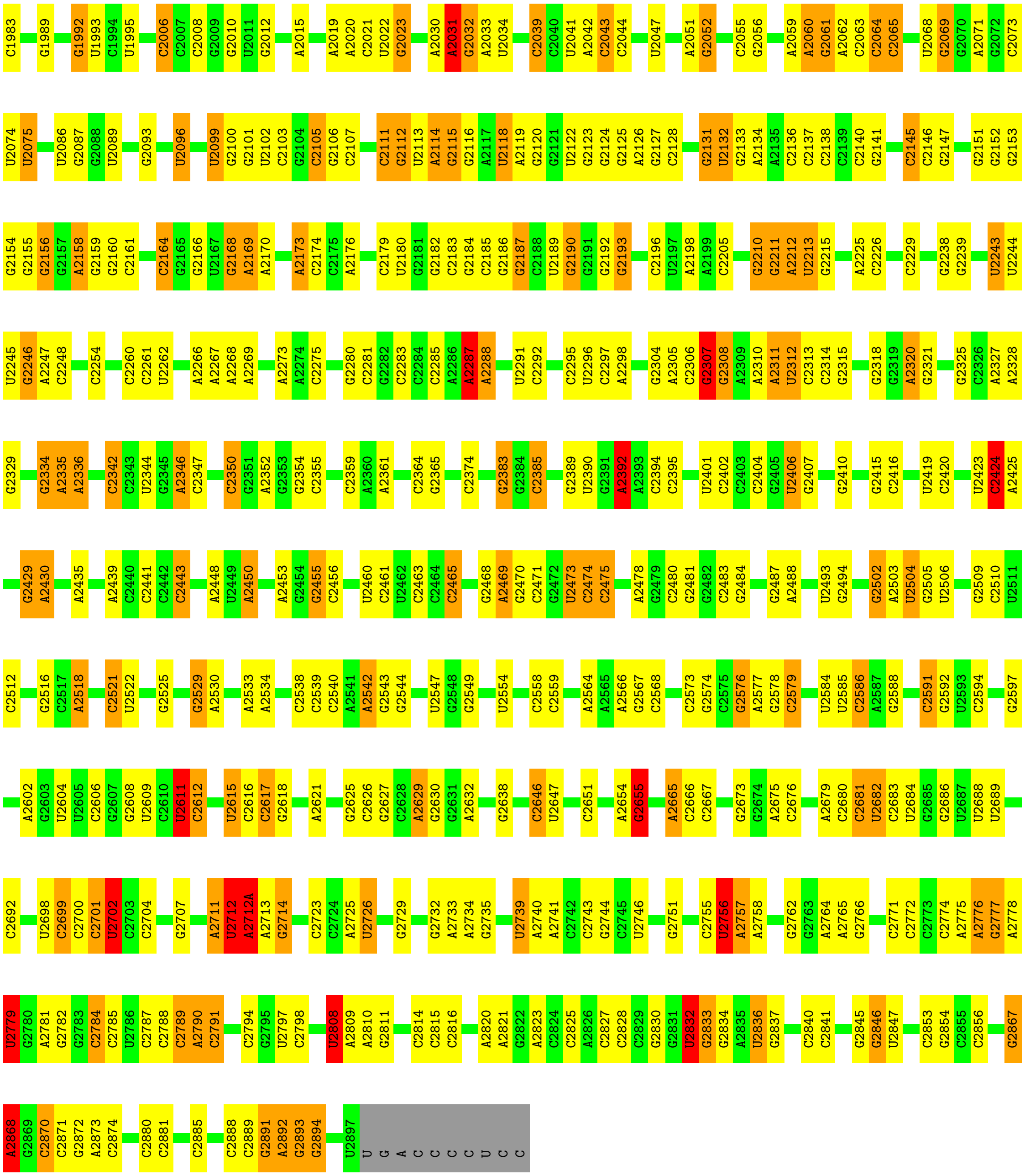
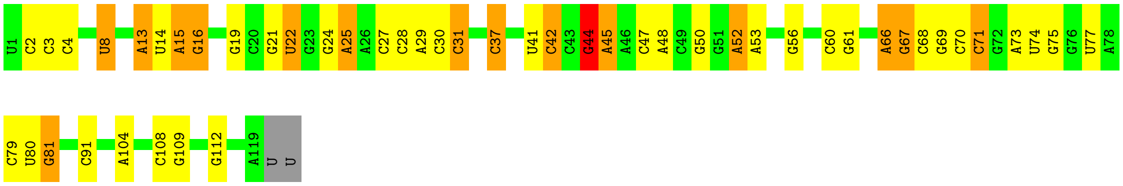


- Molecule 2: 5S rRNA

Chain RB:

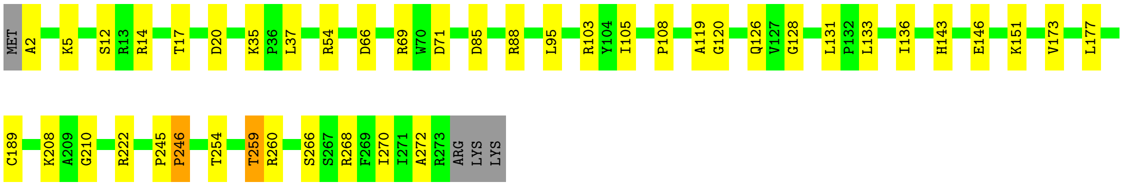


- Molecule 2: 5S rRNA

Chain YB:

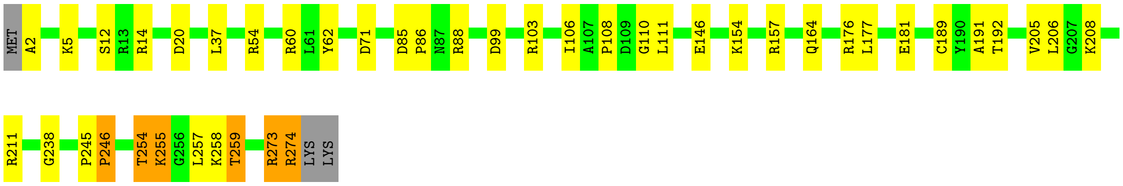
- Molecule 3: 50S ribosomal protein L2

Chain RD:



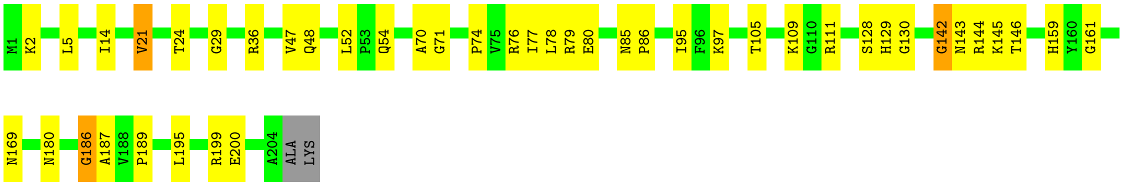
- Molecule 3: 50S ribosomal protein L2

Chain YD:



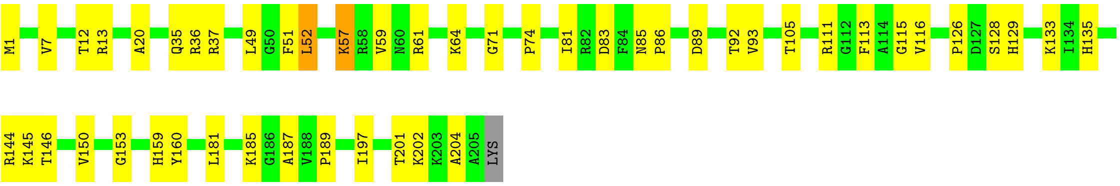
- Molecule 4: 50S ribosomal protein L3

Chain RE:



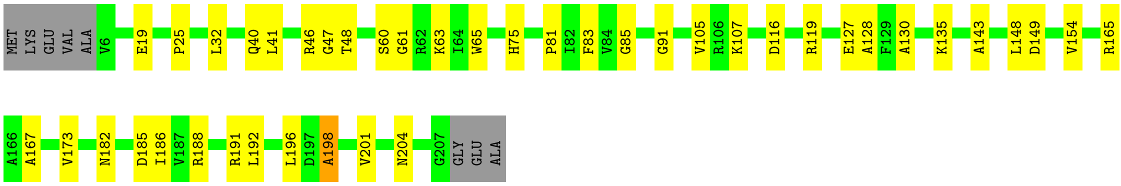
- Molecule 4: 50S ribosomal protein L3

Chain YE:



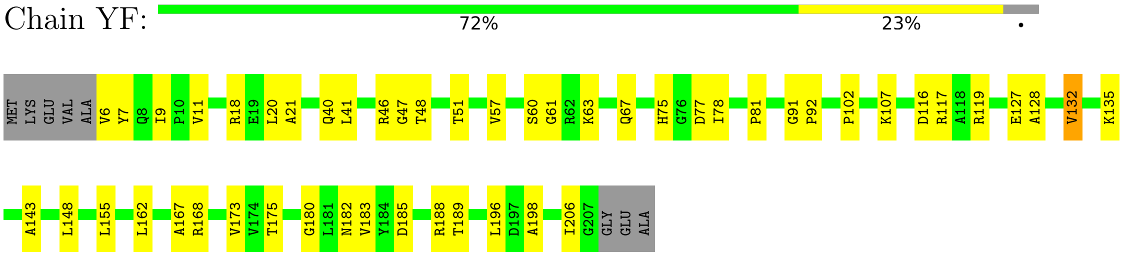
- Molecule 5: 50S ribosomal protein L4

Chain RF:



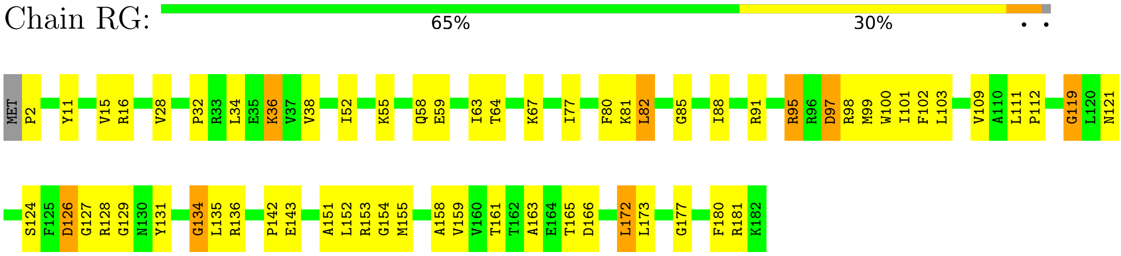
- Molecule 5: 50S ribosomal protein L4

Chain YF:



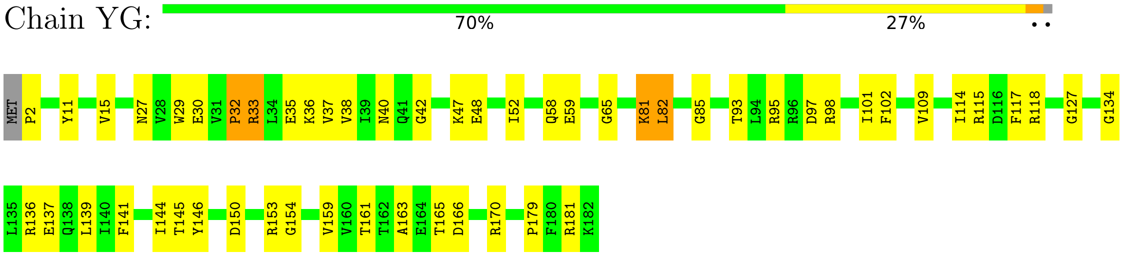
- Molecule 6: 50S ribosomal protein L5

Chain RG:



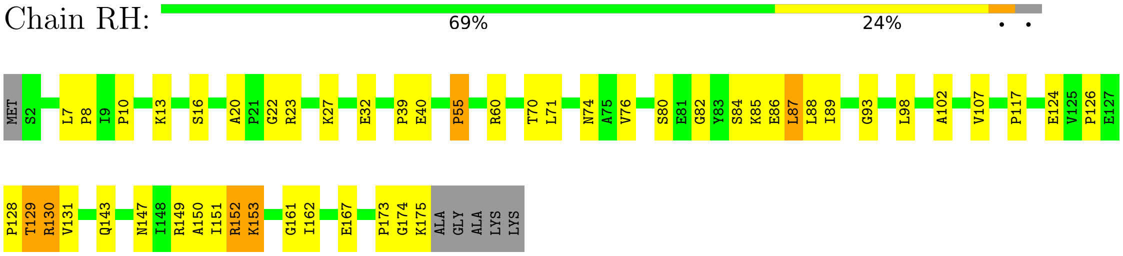
- Molecule 6: 50S ribosomal protein L5

Chain YG:



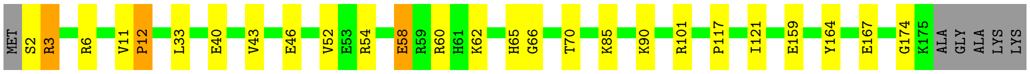
- Molecule 7: 50S ribosomal protein L6

Chain RH:



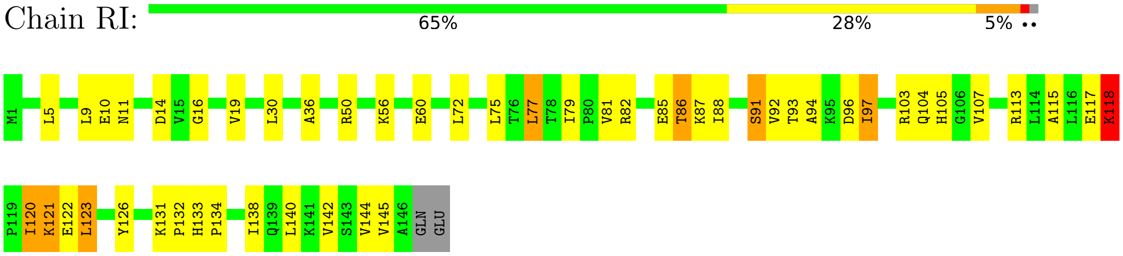
- Molecule 7: 50S ribosomal protein L6

Chain YH:



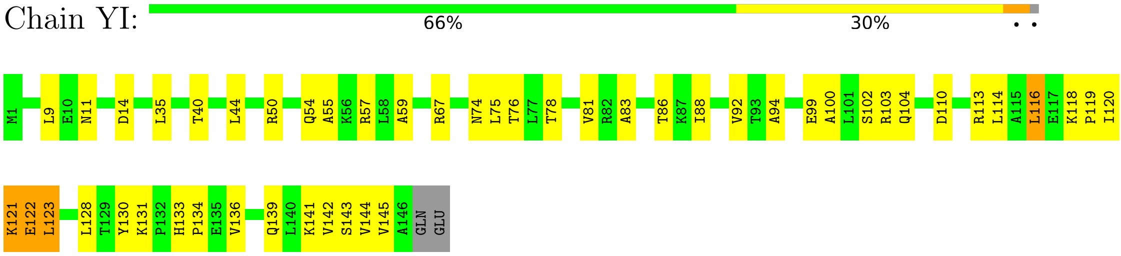
- Molecule 8: 50S ribosomal protein L9

Chain RI:



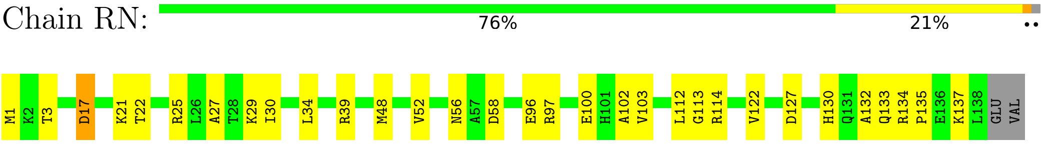
- Molecule 8: 50S ribosomal protein L9

Chain YI:



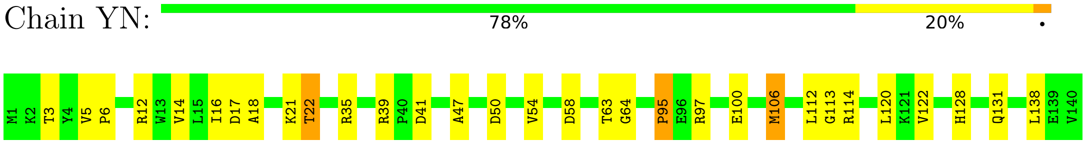
- Molecule 9: 50S ribosomal protein L13

Chain RN:



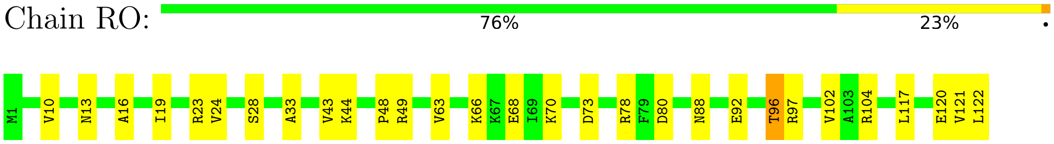
- Molecule 9: 50S ribosomal protein L13

Chain YN:



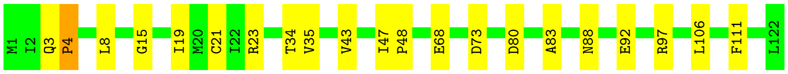
- Molecule 10: 50S ribosomal protein L14

Chain RO:



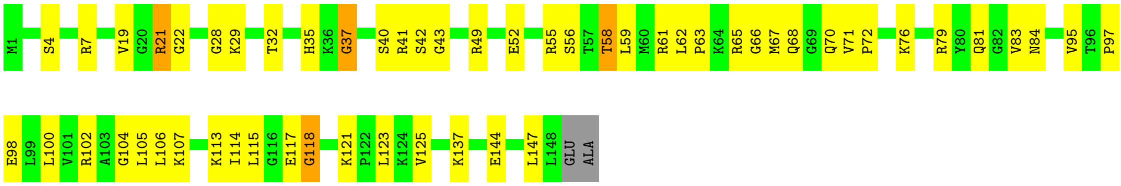
- Molecule 10: 50S ribosomal protein L14

Chain YO:



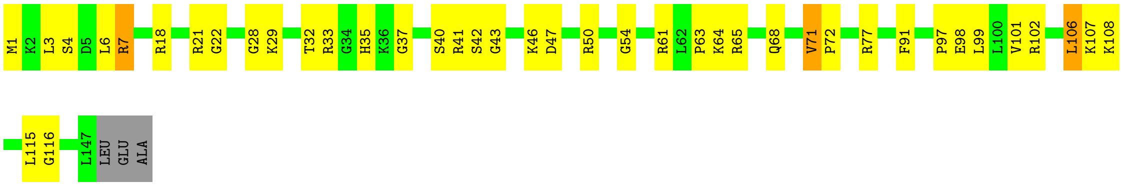
- Molecule 11: 50S ribosomal protein L15

Chain RP:



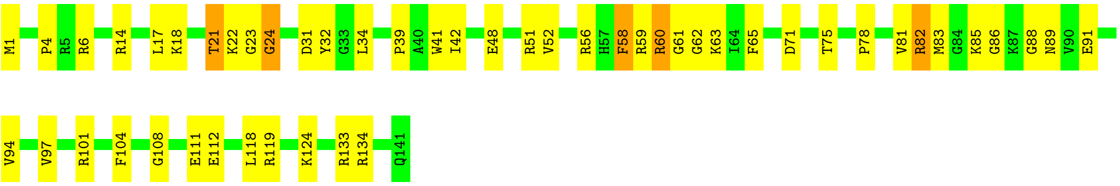
- Molecule 11: 50S ribosomal protein L15

Chain YP:



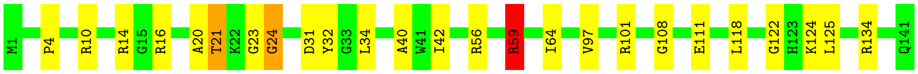
- Molecule 12: 50S ribosomal protein L16

Chain RQ:



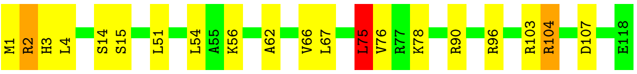
- Molecule 12: 50S ribosomal protein L16

Chain YQ:



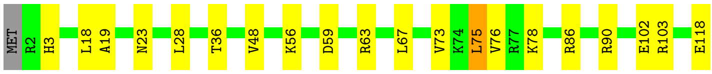
- Molecule 13: 50S ribosomal protein L17

Chain RR:



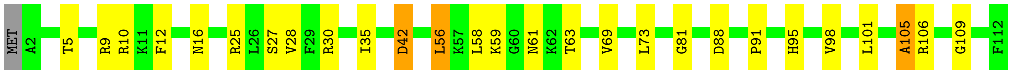
- Molecule 13: 50S ribosomal protein L17

Chain YR:



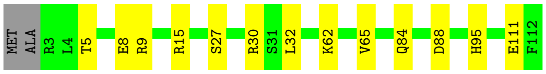
- Molecule 14: 50S ribosomal protein L18

Chain RS:



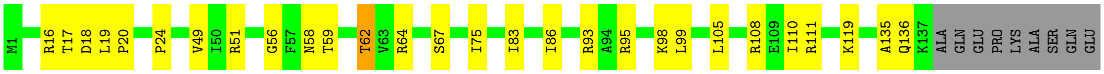
- Molecule 14: 50S ribosomal protein L18

Chain YS:



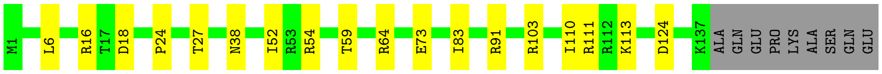
- Molecule 15: 50S ribosomal protein L19

Chain RT:



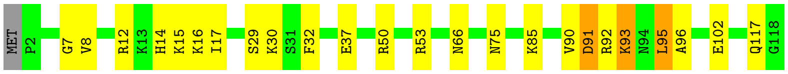
- Molecule 15: 50S ribosomal protein L19

Chain YT:



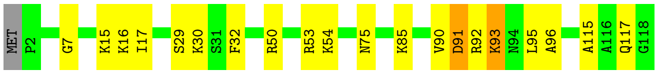
- Molecule 16: 50S ribosomal protein L20

Chain RU:



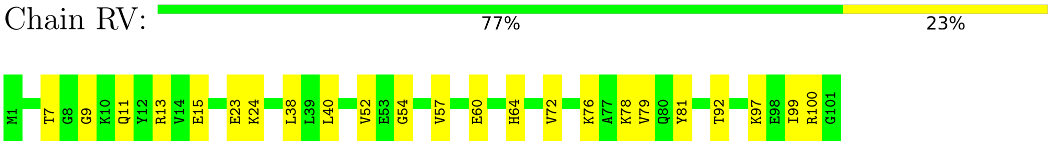
- Molecule 16: 50S ribosomal protein L20

Chain YU:



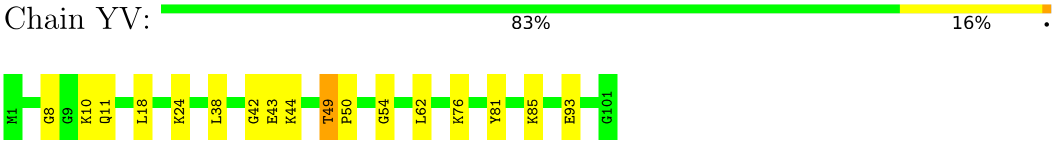
- Molecule 17: 50S ribosomal protein L21

Chain RV:



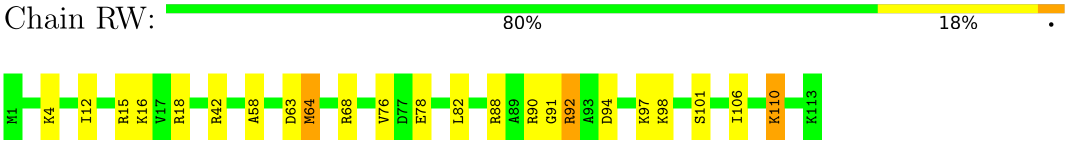
- Molecule 17: 50S ribosomal protein L21

Chain YV:



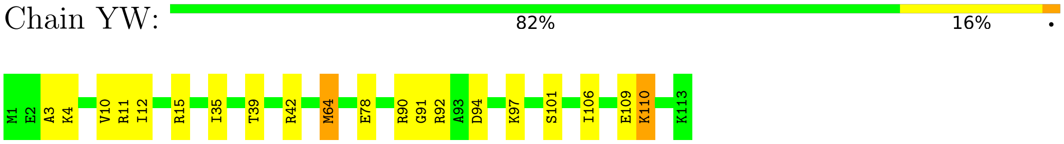
- Molecule 18: 50S ribosomal protein L22

Chain RW:



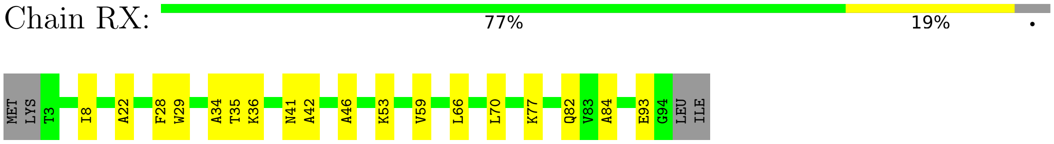
- Molecule 18: 50S ribosomal protein L22

Chain YW:



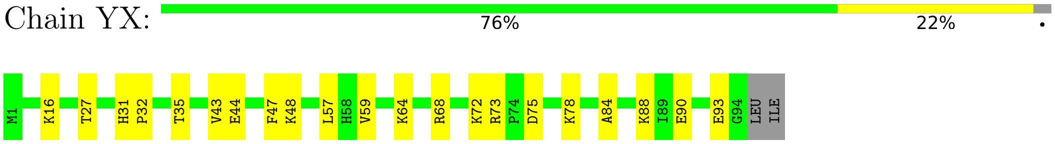
- Molecule 19: 50S ribosomal protein L23

Chain RX:



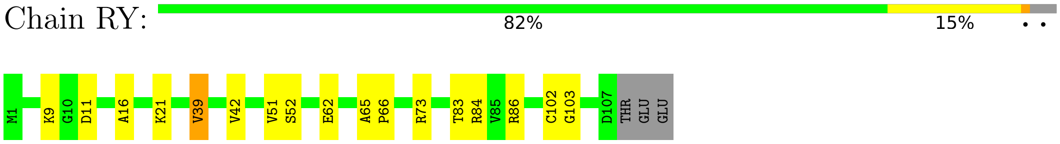
- Molecule 19: 50S ribosomal protein L23

Chain YX:



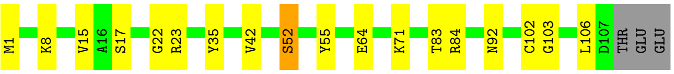
- Molecule 20: 50S ribosomal protein L24

Chain RY:



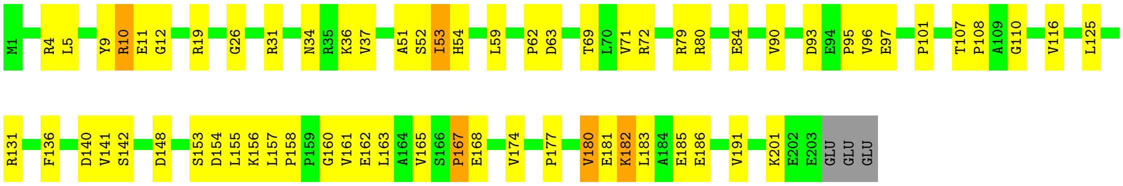
- Molecule 20: 50S ribosomal protein L24

Chain YY:



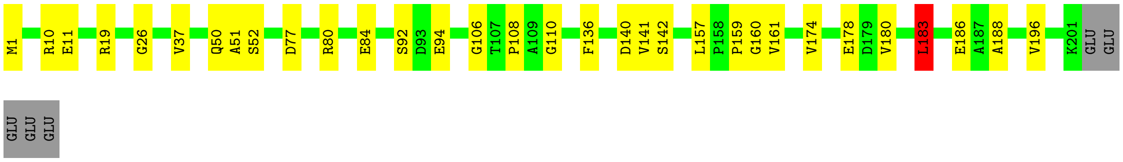
- Molecule 21: 50S ribosomal protein L25

Chain RZ:



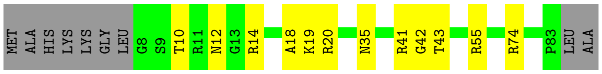
- Molecule 21: 50S ribosomal protein L25

Chain YZ:



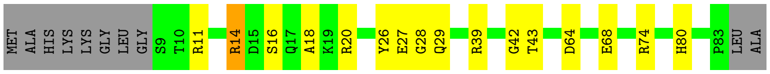
- Molecule 22: 50S ribosomal protein L27

Chain R0:



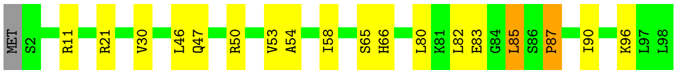
- Molecule 22: 50S ribosomal protein L27

Chain Y0:



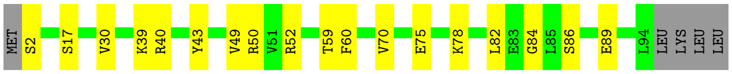
- Molecule 23: 50S ribosomal protein L28

Chain R1:



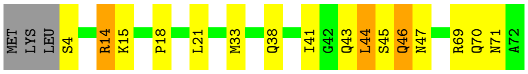
- Molecule 23: 50S ribosomal protein L28

Chain Y1:



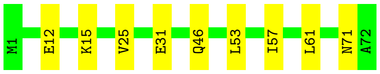
- Molecule 24: 50S ribosomal protein L29

Chain R2:



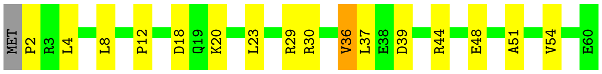
- Molecule 24: 50S ribosomal protein L29

Chain Y2:



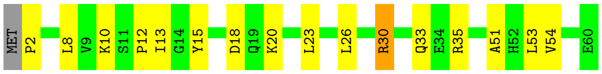
- Molecule 25: 50S ribosomal protein L30

Chain R3:



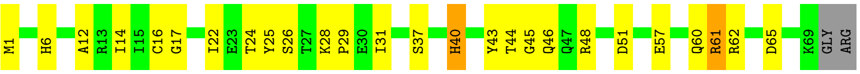
- Molecule 25: 50S ribosomal protein L30

Chain Y3:



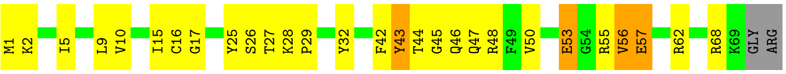
- Molecule 26: 50S ribosomal protein L31

Chain R4:



- Molecule 26: 50S ribosomal protein L31

Chain Y4:



- Molecule 27: 50S ribosomal protein L32

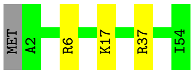
Chain R5:

- Molecule 27: 50S ribosomal protein L32

Chain Y5:

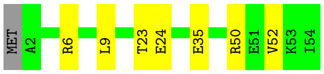
- Molecule 28: 50S ribosomal protein L33

Chain R6:



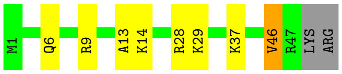
- Molecule 28: 50S ribosomal protein L33

Chain Y6:



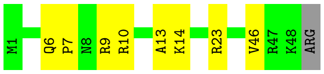
- Molecule 29: 50S ribosomal protein L34

Chain R7:



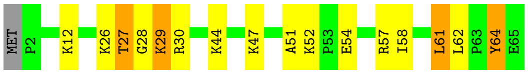
- Molecule 29: 50S ribosomal protein L34

Chain Y7:



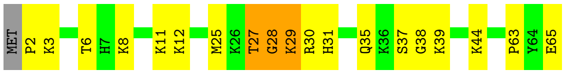
- Molecule 30: 50S ribosomal protein L35

Chain R8:



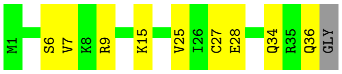
- Molecule 30: 50S ribosomal protein L35

Chain Y8:



- Molecule 31: 50S ribosomal protein L36

Chain R9:

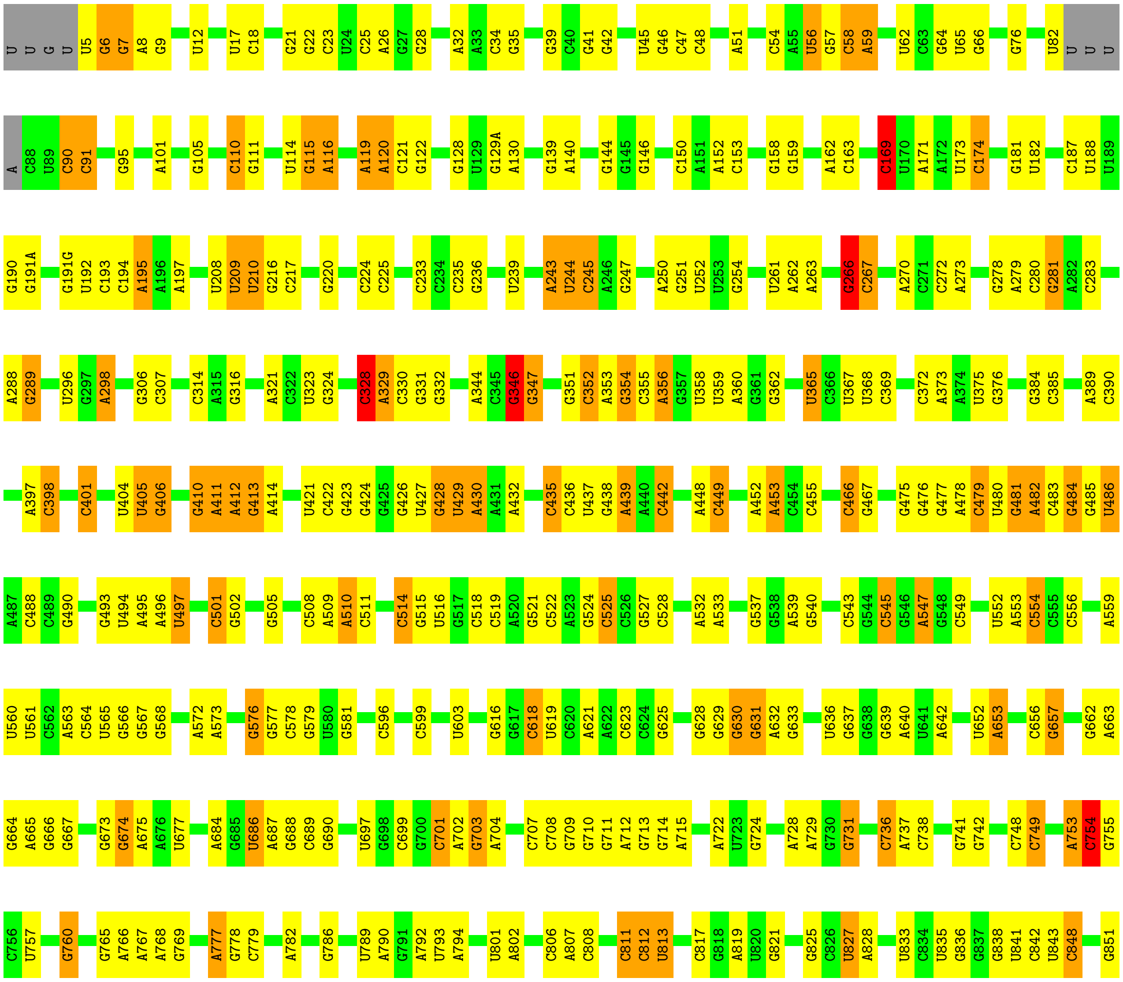


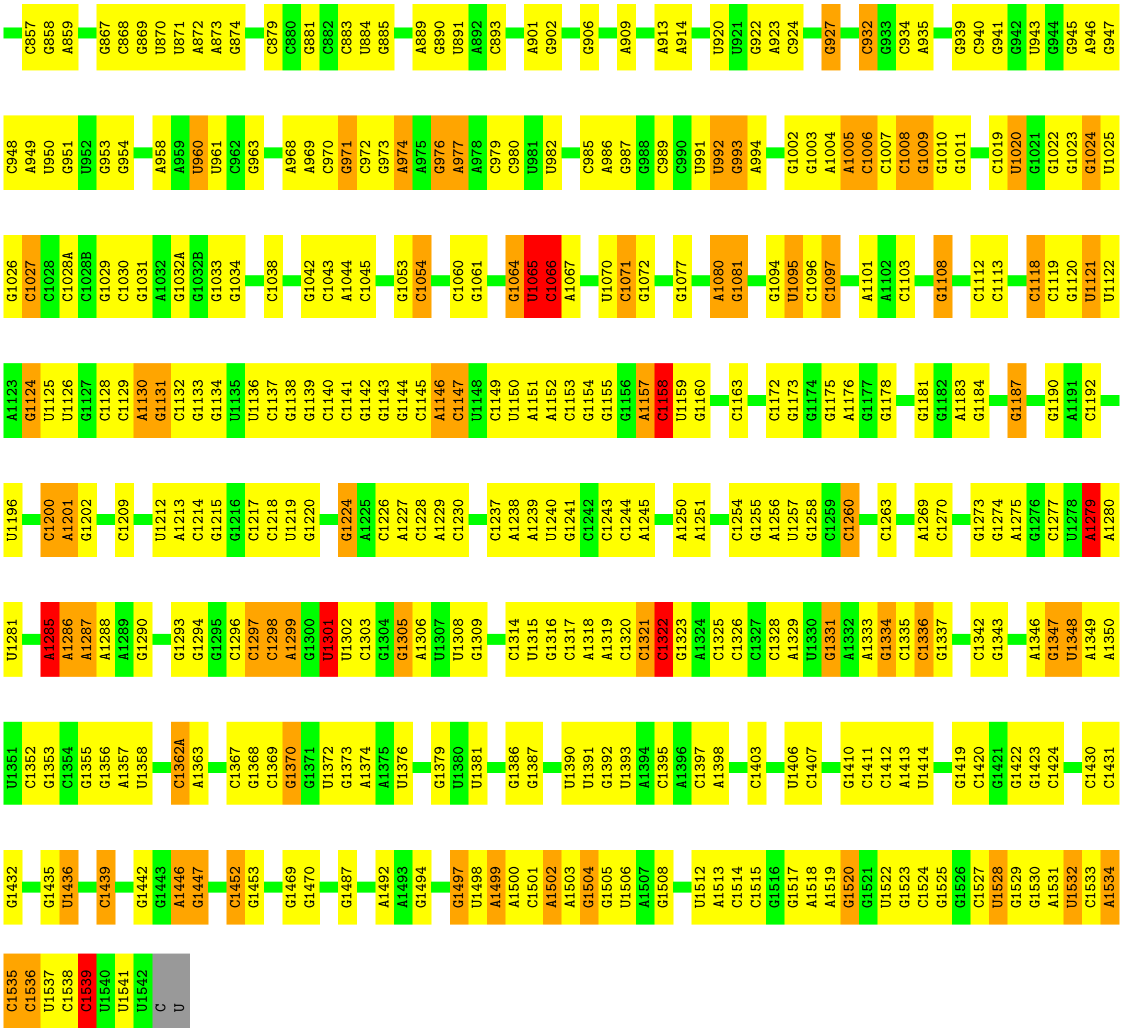
- Molecule 31: 50S ribosomal protein L36

Chain Y9:

- Molecule 32: 16S rRNA

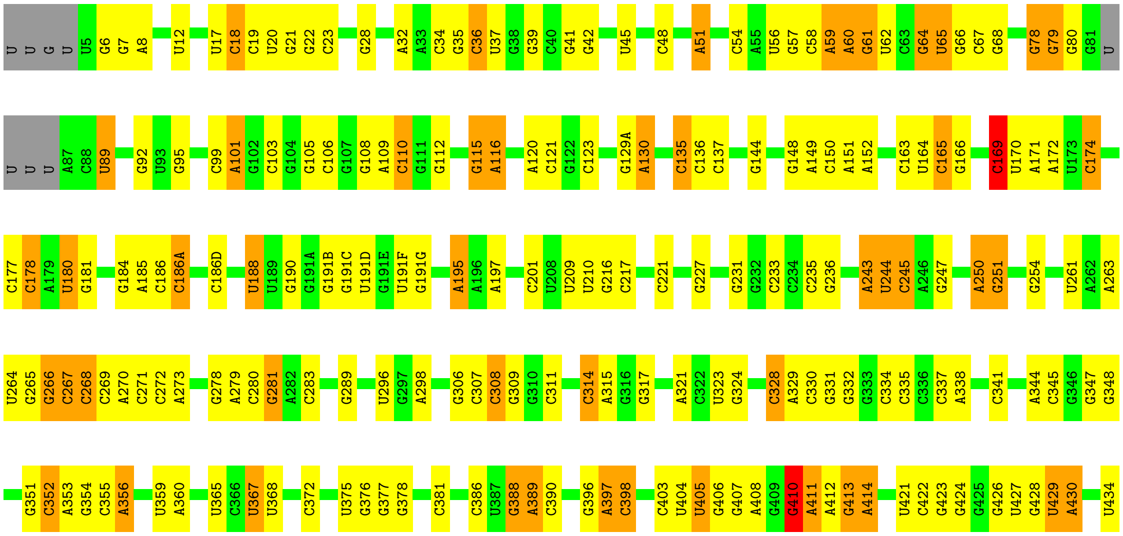
Chain QA:

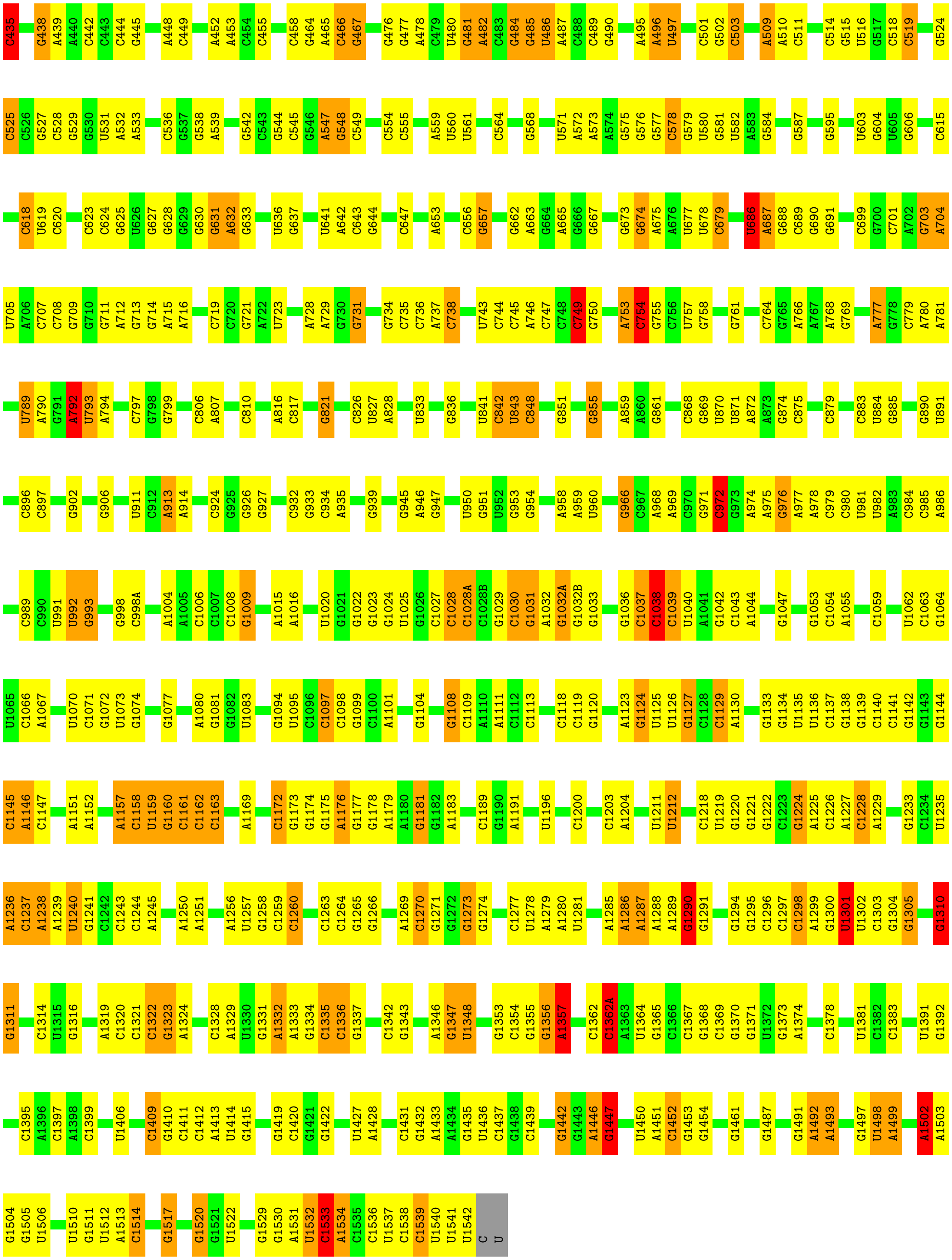




- Molecule 32: 16S rRNA

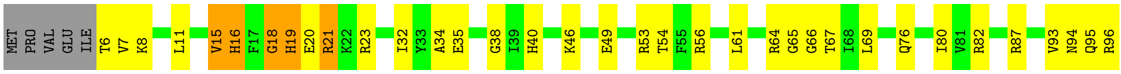
Chain XA:

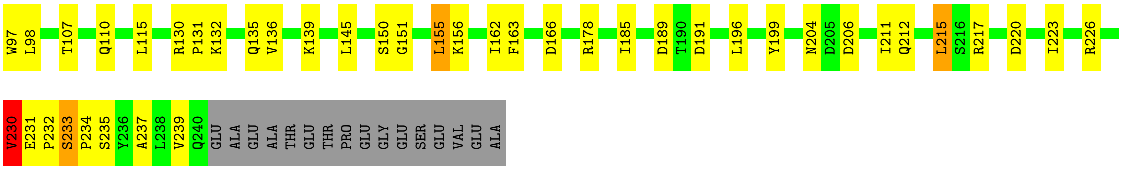




- Molecule 33: 30S ribosomal protein S2

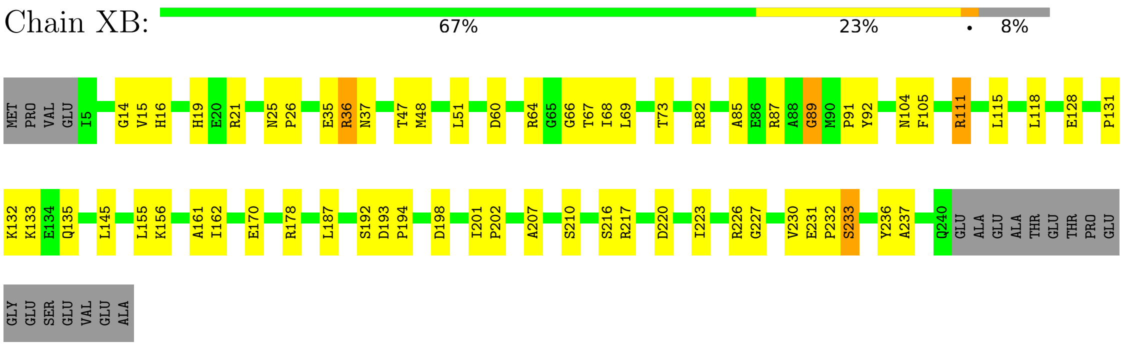
Chain QB:





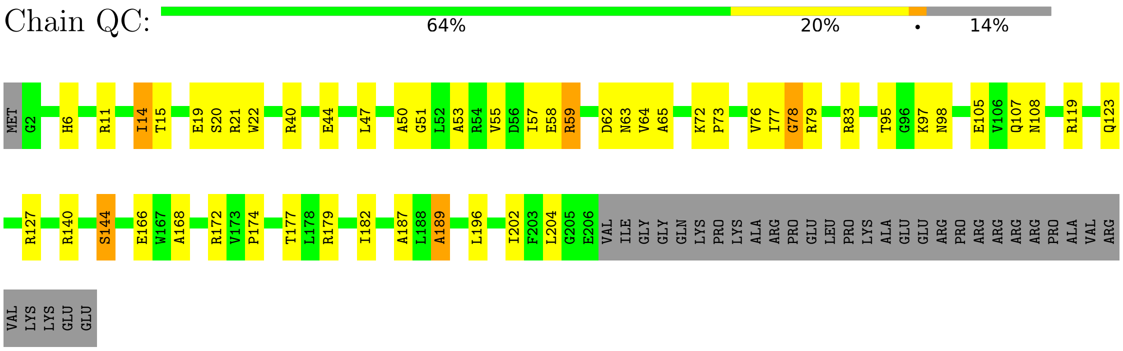
- Molecule 33: 30S ribosomal protein S2

Chain XB:



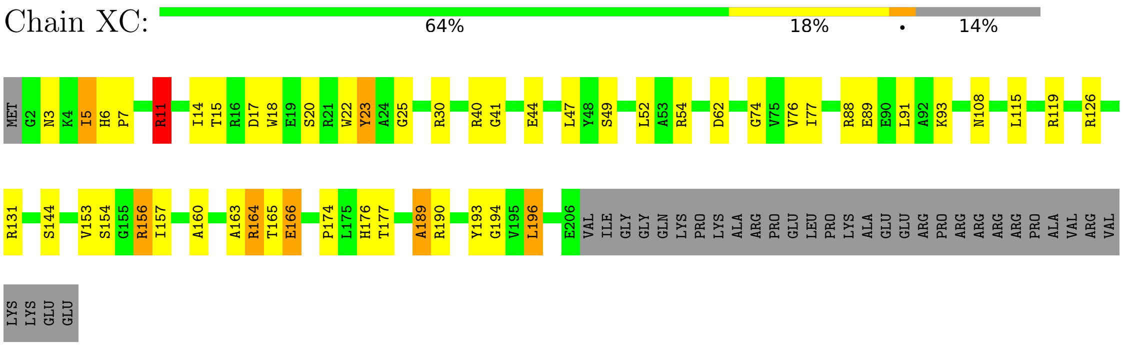
- Molecule 34: 30S ribosomal protein S3

Chain QC:



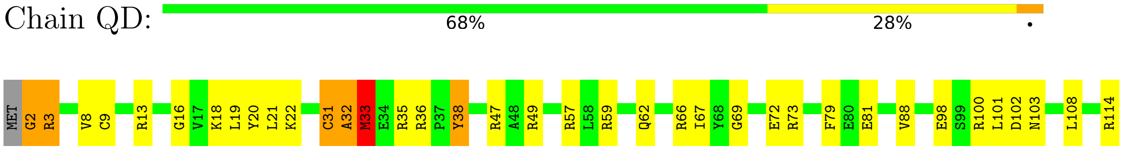
- Molecule 34: 30S ribosomal protein S3

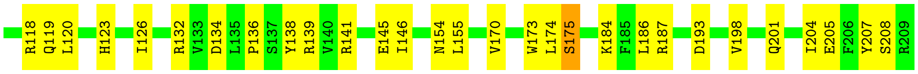
Chain XC:



- Molecule 35: 30S ribosomal protein S4

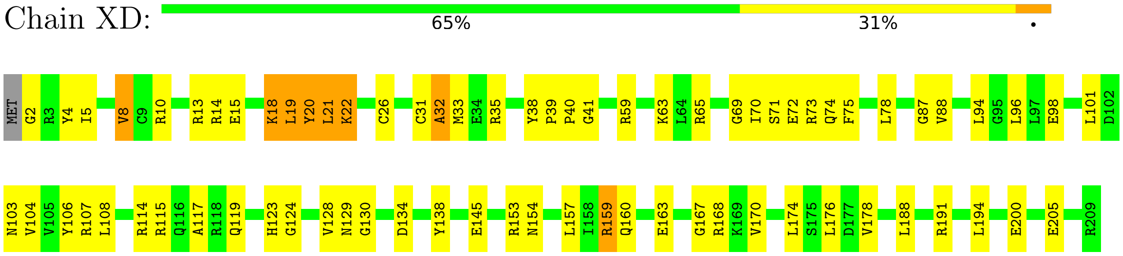
Chain QD:





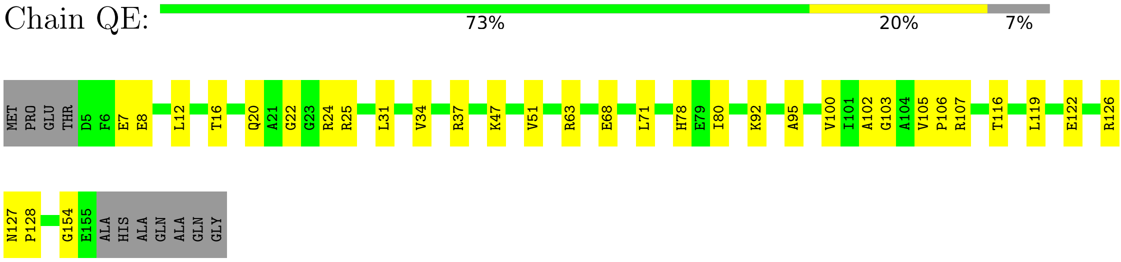
- Molecule 35: 30S ribosomal protein S4

Chain XD:



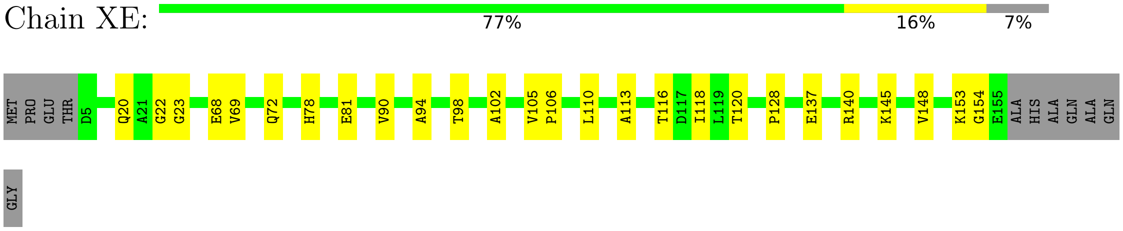
- Molecule 36: 30S ribosomal protein S5

Chain QE:



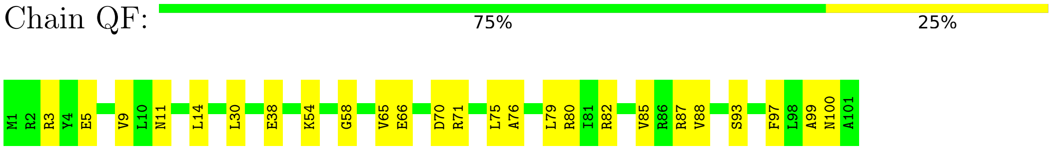
- Molecule 36: 30S ribosomal protein S5

Chain XE:



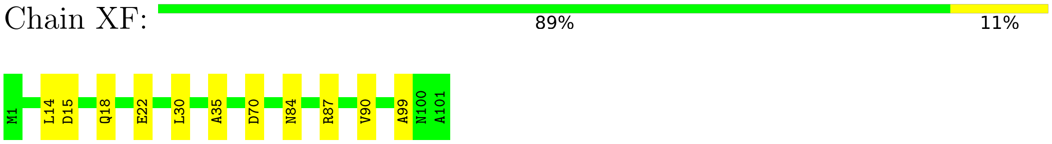
- Molecule 37: 30S ribosomal protein S6

Chain QF:



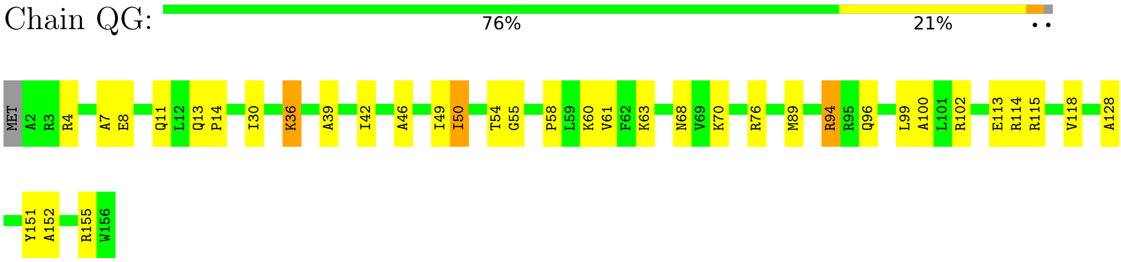
- Molecule 37: 30S ribosomal protein S6

Chain XF:



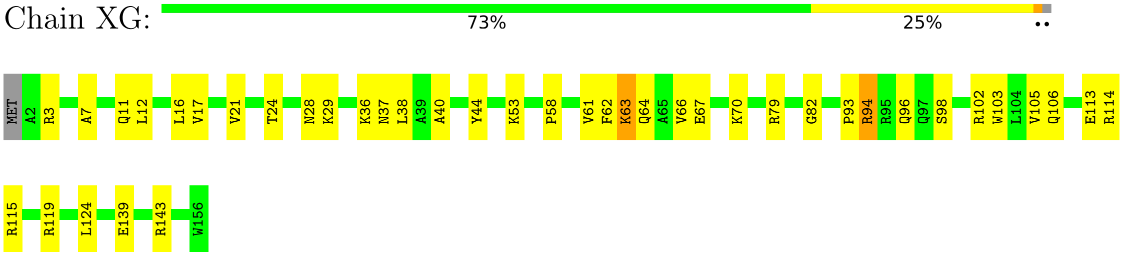
- Molecule 38: 30S ribosomal protein S7

Chain QG:



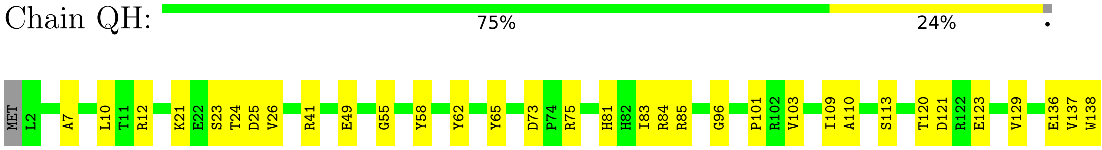
- Molecule 38: 30S ribosomal protein S7

Chain XG:



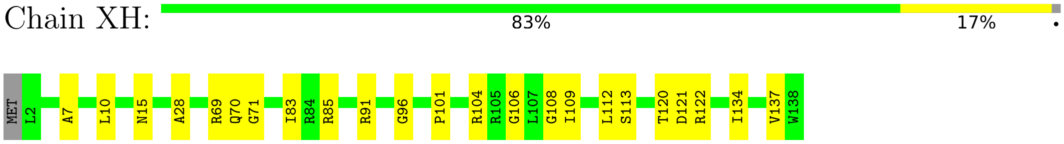
- Molecule 39: 30S ribosomal protein S8

Chain QH:



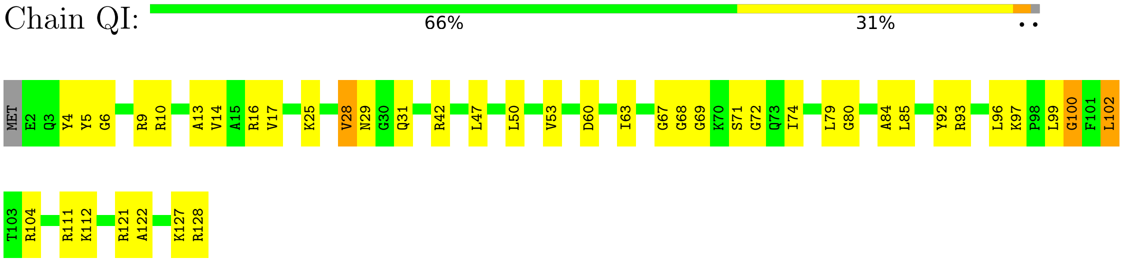
- Molecule 39: 30S ribosomal protein S8

Chain XH:



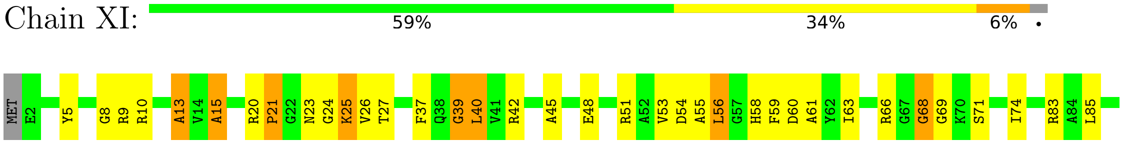
- Molecule 40: 30S ribosomal protein S9

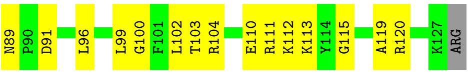
Chain QI:



- Molecule 40: 30S ribosomal protein S9

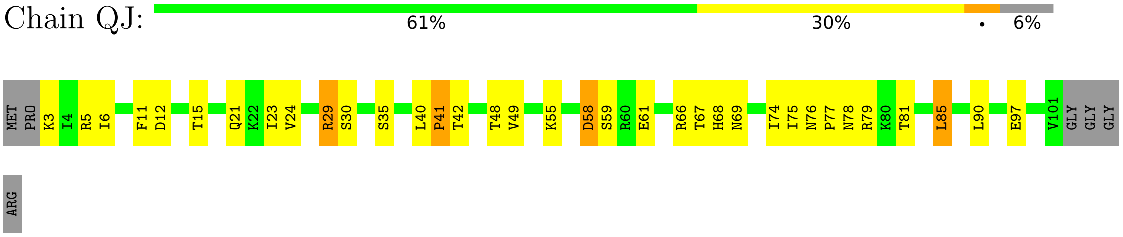
Chain XI:





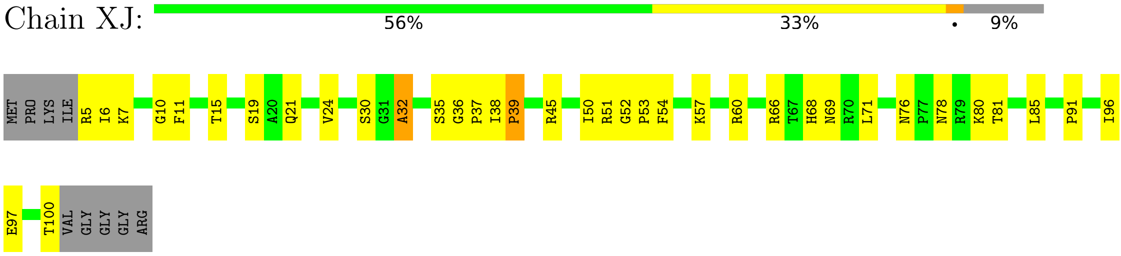
- Molecule 41: 30S ribosomal protein S10

Chain QJ:



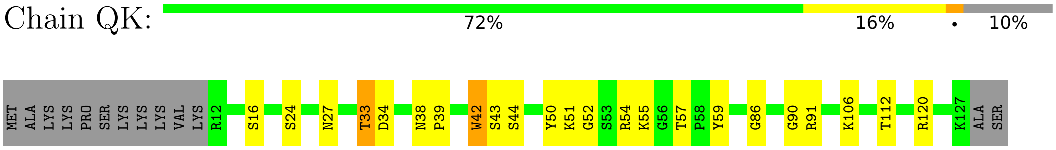
- Molecule 41: 30S ribosomal protein S10

Chain XJ:



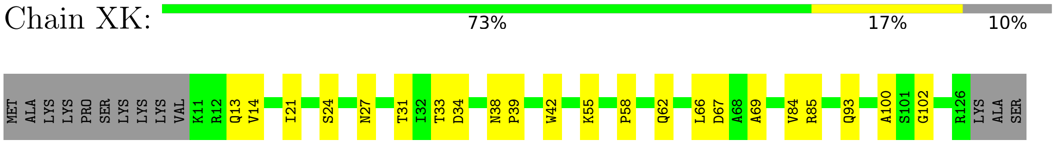
- Molecule 42: 30S ribosomal protein S11

Chain QK:



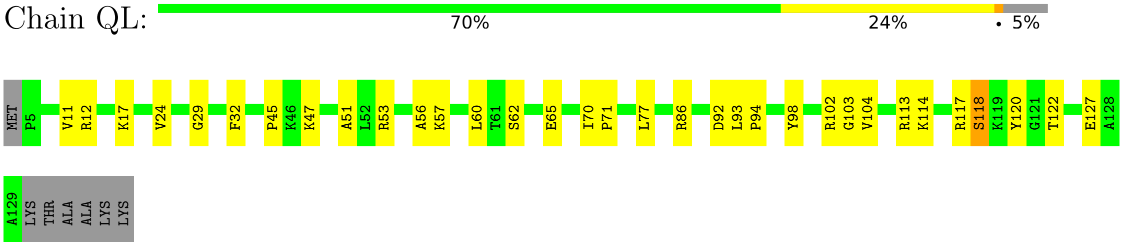
- Molecule 42: 30S ribosomal protein S11

Chain XK:



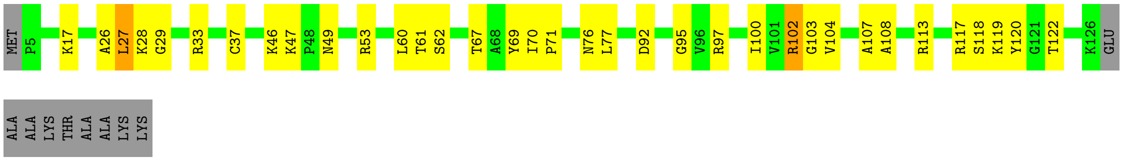
- Molecule 43: 30S ribosomal protein S12

Chain QL:



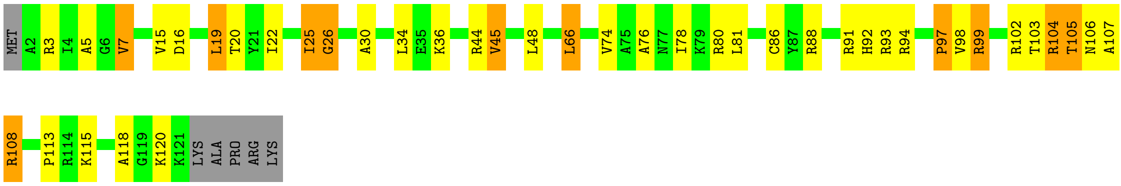
- Molecule 43: 30S ribosomal protein S12

Chain XL:



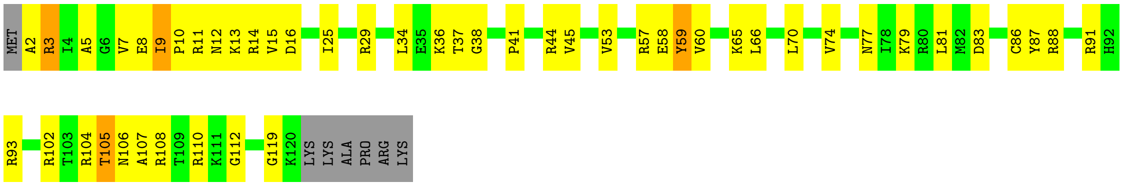
- Molecule 44: 30S ribosomal protein S13

Chain QM:



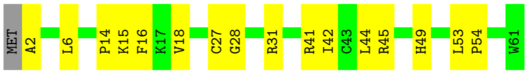
- Molecule 44: 30S ribosomal protein S13

Chain XM:



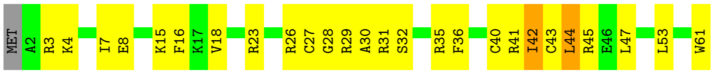
- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:



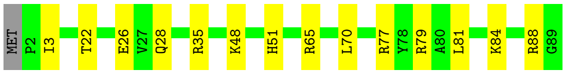
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN:



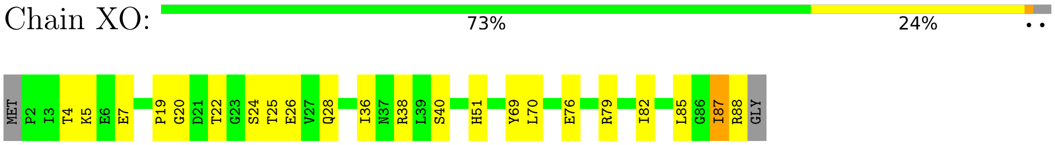
- Molecule 46: 30S ribosomal protein S15

Chain QO:



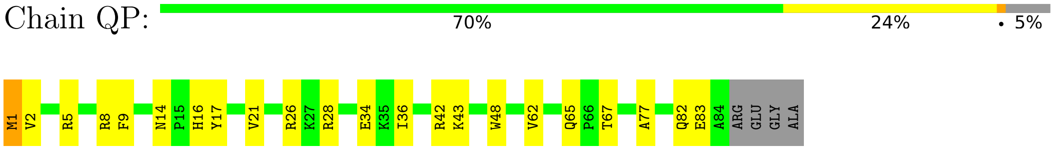
- Molecule 46: 30S ribosomal protein S15

Chain XO:



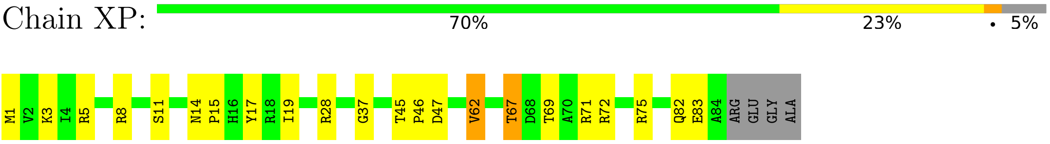
- Molecule 47: 30S ribosomal protein S16

Chain QP:



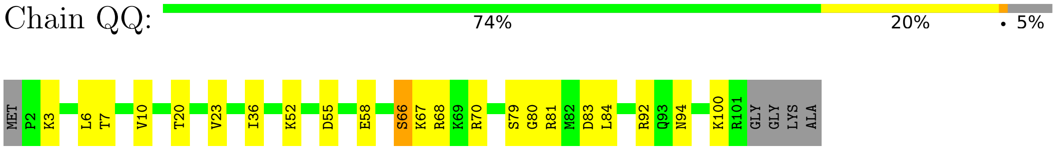
- Molecule 47: 30S ribosomal protein S16

Chain XP:



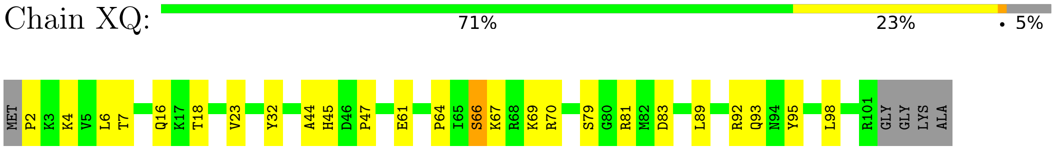
- Molecule 48: 30S ribosomal protein S17

Chain QQ:



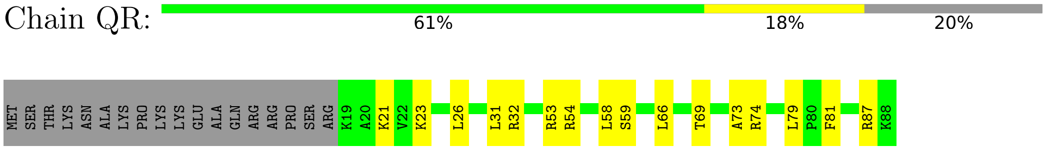
- Molecule 48: 30S ribosomal protein S17

Chain XQ:



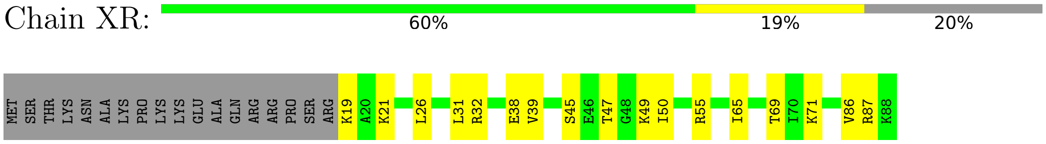
- Molecule 49: 30S ribosomal protein S18

Chain QR:



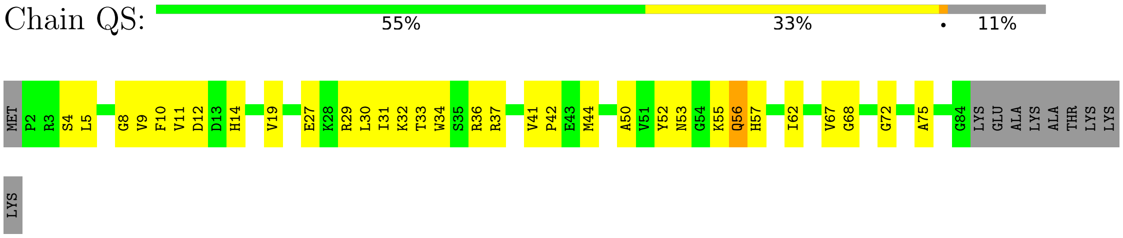
- Molecule 49: 30S ribosomal protein S18

Chain XR:



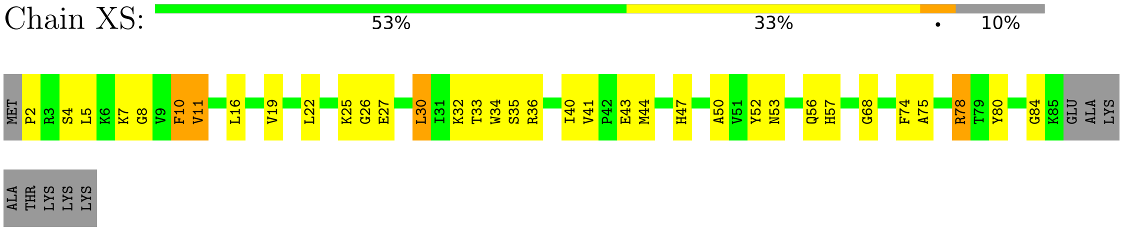
- Molecule 50: 30S ribosomal protein S19

Chain QS:



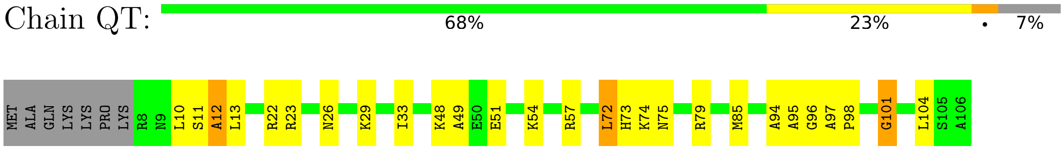
- Molecule 50: 30S ribosomal protein S19

Chain XS:



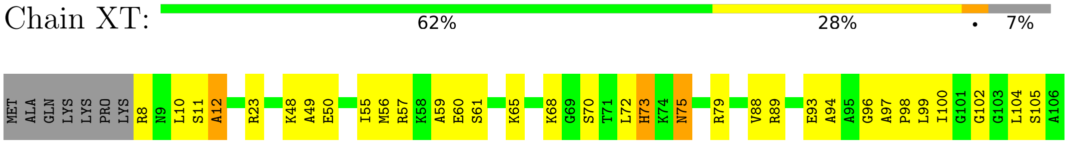
- Molecule 51: 30S ribosomal protein S20

Chain QT:



- Molecule 51: 30S ribosomal protein S20

Chain XT:

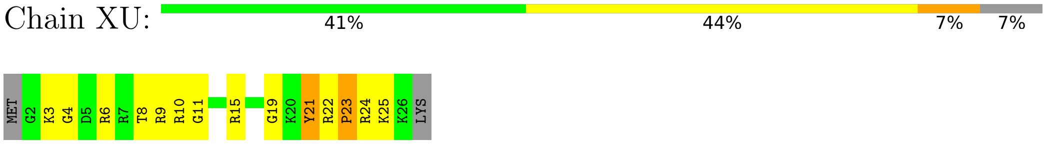


- Molecule 52: 30S ribosomal protein Thx

Chain QU:

- Molecule 52: 30S ribosomal protein Thx

Chain XU:

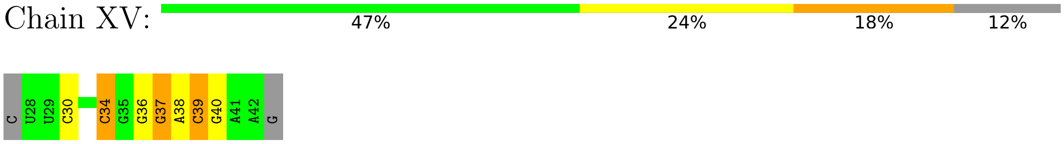


- Molecule 53: P-site ASLPro

Chain QV:

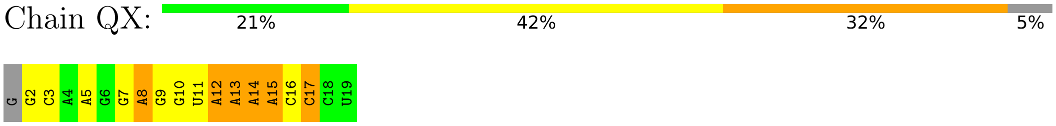
- Molecule 53: P-site ASLPro

Chain XV:



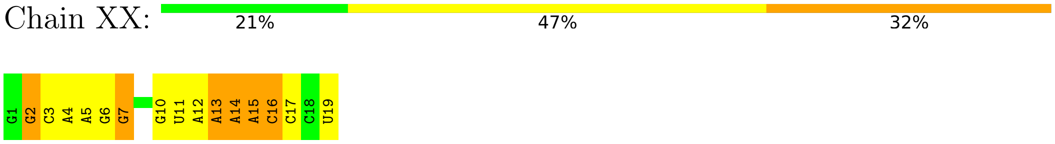
- Molecule 54: mRNA

Chain QX:



- Molecule 54: mRNA

Chain XX:



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	210.12Å 451.80Å 622.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.68 – 3.40	Depositor
% Data completeness (in resolution range)	98.8 (188.68-3.40)	Depositor
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.237	Depositor
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.210	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	290035	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 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 1MG, SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	RA	1.16	19/69498 (0.0%)	1.25	634/108491 (0.6%)
1	YA	1.43	115/69543 (0.2%)	1.33	828/108563 (0.8%)
2	RB	0.85	0/2878	1.24	33/4490 (0.7%)
2	YB	1.23	0/2878	1.34	43/4490 (1.0%)
3	RD	0.68	0/2165	0.60	0/2919
3	YD	0.80	0/2176	0.63	0/2933
4	RE	0.66	0/1596	0.60	0/2153
4	YE	0.77	0/1601	0.68	0/2160
5	RF	0.64	0/1620	0.59	0/2194
5	YF	0.79	1/1620 (0.1%)	0.63	0/2194
6	RG	0.36	0/1499	0.64	1/2016 (0.0%)
6	YG	0.45	0/1499	0.60	0/2016
7	RH	0.44	0/1362	0.59	0/1841
7	YH	0.63	0/1362	0.56	0/1841
8	RI	0.48	0/1151	0.68	0/1558
8	YI	0.47	0/1151	0.66	0/1558
9	RN	0.59	0/1131	0.58	0/1525
9	YN	0.73	1/1148 (0.1%)	0.61	0/1547
10	RO	0.67	0/943	0.60	0/1269
10	YO	0.77	0/943	0.63	0/1269
11	RP	0.56	0/1147	0.68	1/1525 (0.1%)
11	YP	0.70	0/1139	0.70	1/1514 (0.1%)
12	RQ	0.59	1/1143 (0.1%)	0.65	0/1527
12	YQ	0.75	0/1143	0.60	0/1527
13	RR	0.58	0/982	0.65	1/1312 (0.1%)
13	YR	0.70	0/974	0.69	0/1302
14	RS	0.43	0/892	0.68	1/1187 (0.1%)
14	YS	0.61	0/887	0.57	0/1180
15	RT	0.58	0/1155	0.64	2/1542 (0.1%)
15	YT	0.65	0/1155	0.55	0/1542
16	RU	0.61	0/982	0.57	0/1306
16	YU	0.83	0/982	0.63	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	RV	0.54	0/790	0.58	0/1057
17	YV	0.77	0/790	0.66	0/1057
18	RW	0.66	0/911	0.56	0/1220
18	YW	0.80	0/911	0.60	0/1220
19	RX	0.60	0/739	0.60	0/993
19	YX	0.76	0/756	0.64	0/1014
20	RY	0.55	0/831	0.52	0/1108
20	YY	0.72	1/831 (0.1%)	0.56	0/1108
21	RZ	0.45	0/1634	0.65	1/2216 (0.0%)
21	YZ	0.57	0/1620	0.55	0/2197
22	R0	0.56	0/611	0.58	0/814
22	Y0	0.76	0/607	0.60	0/809
23	R1	0.58	0/770	0.61	0/1022
23	Y1	0.70	0/736	0.57	0/978
24	R2	0.41	0/583	0.49	0/771
24	Y2	0.57	0/608	0.52	0/803
25	R3	0.52	0/474	0.54	0/635
25	Y3	0.66	0/474	0.62	0/635
26	R4	0.35	0/578	0.59	0/776
26	Y4	0.38	0/578	0.67	0/776
27	R5	0.70	0/473	0.57	0/639
27	Y5	0.80	0/473	0.62	1/639 (0.2%)
28	R6	0.57	0/460	0.56	0/613
28	Y6	0.71	0/460	0.63	0/613
29	R7	0.69	0/417	0.52	0/550
29	Y7	0.85	1/426 (0.2%)	0.58	0/561
30	R8	0.57	0/525	0.62	0/691
30	Y8	0.71	0/525	0.65	0/691
31	R9	0.54	0/305	0.48	0/402
31	Y9	0.71	0/310	0.52	0/407
32	QA	0.87	1/36343 (0.0%)	1.17	200/56720 (0.4%)
32	XA	0.88	0/36346	1.17	213/56725 (0.4%)
33	QB	0.39	0/1942	0.62	1/2619 (0.0%)
33	XB	0.39	0/1950	0.58	0/2630
34	QC	0.35	0/1629	0.62	0/2195
34	XC	0.35	0/1629	0.57	0/2195
35	QD	0.51	0/1733	0.55	0/2318
35	XD	0.47	0/1733	0.56	0/2318
36	QE	0.45	0/1171	0.58	0/1576
36	XE	0.46	0/1171	0.54	0/1576
37	QF	0.48	0/856	0.56	0/1154
37	XF	0.46	0/856	0.52	0/1154
38	QG	0.33	0/1276	0.56	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	XG	0.34	0/1276	0.53	0/1709
39	QH	0.51	0/1128	0.56	0/1517
39	XH	0.48	0/1128	0.57	0/1517
40	QI	0.32	0/1029	0.63	2/1379 (0.1%)
40	XI	0.34	0/1017	0.63	1/1365 (0.1%)
41	QJ	0.35	0/814	0.61	0/1095
41	XJ	0.32	0/790	0.53	0/1063
42	QK	0.44	0/879	0.54	0/1187
42	XK	0.44	0/879	0.53	0/1187
43	QL	0.56	0/991	0.59	0/1327
43	XL	0.51	0/972	0.62	0/1301
44	QM	0.36	0/965	0.64	1/1292 (0.1%)
44	XM	0.37	0/956	0.67	0/1281
45	QN	0.41	0/501	0.68	1/664 (0.2%)
45	XN	0.40	0/501	0.61	1/664 (0.2%)
46	QO	0.42	0/745	0.55	0/992
46	XO	0.44	0/740	0.47	0/987
47	QP	0.49	0/721	0.56	0/970
47	XP	0.44	0/721	0.57	0/970
48	QQ	0.51	0/847	0.55	0/1131
48	XQ	0.49	0/847	0.58	0/1131
49	QR	0.45	0/579	0.62	0/768
49	XR	0.44	0/579	0.60	0/768
50	QS	0.30	0/680	0.56	0/915
50	XS	0.31	0/689	0.65	2/926 (0.2%)
51	QT	0.39	0/765	0.52	0/1007
51	XT	0.35	0/765	0.52	0/1007
52	QU	0.34	0/221	0.66	0/288
52	XU	0.36	0/221	0.62	0/288
53	QV	0.55	0/380	1.09	2/590 (0.3%)
53	XV	0.56	0/332	1.15	5/515 (1.0%)
54	QX	0.61	0/436	1.06	1/678 (0.1%)
54	XX	0.52	0/462	1.17	5/719 (0.7%)
All	All	1.02	140/313742 (0.0%)	1.11	1982/468899 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	RD	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	YD	0	10
4	RE	0	10
4	YE	0	13
5	RF	0	13
5	YF	0	9
6	RG	0	17
6	YG	0	18
7	RH	0	24
7	YH	0	5
8	RI	0	13
8	YI	0	18
9	RN	0	10
9	YN	0	6
10	RO	0	2
10	YO	0	2
11	RP	0	19
11	YP	0	18
12	RQ	0	11
12	YQ	0	8
13	RR	0	6
13	YR	0	5
14	RS	0	8
14	YS	0	2
15	RT	0	6
15	YT	0	4
16	RU	0	3
16	YU	0	5
17	RV	0	8
17	YV	0	4
18	RW	0	5
18	YW	0	5
19	RX	0	5
19	YX	0	4
20	RY	0	5
20	YY	0	2
21	RZ	0	22
21	YZ	0	9
22	R0	0	2
22	Y0	0	3
23	R1	0	6
23	Y1	0	2
24	R2	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	R3	0	3
25	Y3	0	1
26	R4	0	10
26	Y4	0	12
27	R5	0	1
27	Y5	0	2
29	R7	0	2
30	R8	0	7
30	Y8	0	4
31	Y9	0	1
33	QB	0	21
33	XB	0	18
34	QC	0	14
34	XC	0	17
35	QD	0	13
35	XD	0	13
36	QE	0	5
36	XE	0	5
37	QF	0	2
37	XF	0	1
38	QG	0	9
38	XG	0	6
39	QH	0	4
39	XH	0	8
40	QI	0	11
40	XI	0	19
41	QJ	0	6
41	XJ	0	9
42	QK	0	4
42	XK	0	5
43	QL	0	8
43	XL	0	12
44	QM	0	17
44	XM	0	14
45	QN	0	6
45	XN	0	5
46	QO	0	2
46	XO	0	3
47	QP	0	6
47	XP	0	7
48	QQ	0	2
48	XQ	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	QR	0	4
49	XR	0	4
50	QS	0	11
50	XS	0	14
51	QT	0	13
51	XT	0	13
52	QU	0	3
52	XU	0	5
All	All	0	749

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	528	A	N9-C4	-9.09	1.32	1.37
1	YA	1021	A	N9-C4	-8.37	1.32	1.37
1	YA	1142(A)	A	N9-C4	-8.06	1.33	1.37
1	YA	676	A	N9-C4	-7.65	1.33	1.37
1	YA	1783	A	N9-C4	-6.76	1.33	1.37

The worst 5 of 1982 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	YA	856	C	C6-N1-C2	-13.93	114.73	120.30
1	YA	856	C	C5-C6-N1	13.46	127.73	121.00
1	YA	1535	U	N1-C2-O2	13.33	132.13	122.80
1	RA	856	C	C6-N1-C2	-13.11	115.06	120.30
1	YA	2868	A	N7-C8-N9	12.59	120.10	113.80

There are no chirality outliers.

5 of 749 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	RD	119	ALA	Peptide
3	RD	120	GLY	Peptide
3	RD	126	GLN	Peptide
3	RD	2	ALA	Peptide
3	RD	246	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	62051	0	31279	531	1
1	YA	62091	0	31300	497	0
2	RB	2573	0	1306	25	0
2	YB	2573	0	1306	16	0
3	RD	2115	0	2195	31	0
3	YD	2126	0	2208	39	0
4	RE	1563	0	1629	28	0
4	YE	1568	0	1633	30	0
5	RF	1585	0	1632	21	0
5	YF	1585	0	1632	28	0
6	RG	1474	0	1535	38	0
6	YG	1474	0	1535	26	0
7	RH	1336	0	1418	21	0
7	YH	1336	0	1418	23	1
8	RI	1136	0	1223	35	2
8	YI	1136	0	1223	21	0
9	RN	1104	0	1179	14	0
9	YN	1121	0	1194	16	0
10	RO	933	0	996	22	0
10	YO	933	0	995	14	0
11	RP	1130	0	1217	26	0
11	YP	1122	0	1206	23	0
12	RQ	1122	0	1178	48	0
12	YQ	1122	0	1179	16	0
13	RR	968	0	1033	10	0
13	YR	960	0	1021	10	0
14	RS	882	0	943	13	0
14	YS	877	0	938	9	0
15	RT	1141	0	1202	15	0
15	YT	1141	0	1202	11	0
16	RU	964	0	1022	21	0
16	YU	964	0	1022	19	0
17	RV	779	0	852	12	0
17	YV	779	0	852	17	0
18	RW	900	0	964	16	1
18	YW	900	0	964	12	0
19	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	YX	742	0	803	9	0
20	RY	818	0	909	11	0
20	YY	818	0	909	9	2
21	RZ	1601	0	1630	43	0
21	YZ	1587	0	1622	16	0
22	R0	603	0	619	7	0
22	Y0	599	0	617	9	0
23	R1	763	0	848	10	0
23	Y1	729	0	802	12	0
24	R2	581	0	629	9	0
24	Y2	606	0	665	5	1
25	R3	469	0	518	7	0
25	Y3	469	0	518	12	0
26	R4	565	0	557	11	0
26	Y4	565	0	557	16	0
27	R5	459	0	476	10	0
27	Y5	459	0	476	9	0
28	R6	453	0	473	3	0
28	Y6	453	0	473	3	0
29	R7	409	0	454	6	0
29	Y7	418	0	466	4	0
30	R8	517	0	582	12	0
30	Y8	517	0	582	15	0
31	R9	302	0	332	7	0
31	Y9	307	0	335	9	0
32	QA	32469	0	16393	418	0
32	XA	32471	0	16393	441	2
33	QB	1907	0	1958	36	0
33	XB	1915	0	1969	28	0
34	QC	1605	0	1668	27	0
34	XC	1605	0	1668	28	0
35	QD	1703	0	1763	63	0
35	XD	1703	0	1764	50	0
36	QE	1155	0	1213	18	0
36	XE	1155	0	1213	11	0
37	QF	843	0	857	16	0
37	XF	843	0	857	13	0
38	QG	1257	0	1296	20	0
38	XG	1257	0	1296	24	0
39	QH	1108	0	1165	17	0
39	XH	1108	0	1165	11	0
40	QI	1010	0	1037	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	XI	998	0	1024	28	0
41	QJ	801	0	849	21	0
41	XJ	777	0	816	24	0
42	QK	864	0	881	15	0
42	XK	864	0	881	12	0
43	QL	975	0	1062	18	0
43	XL	956	0	1046	18	0
44	QM	955	0	1021	25	0
44	XM	946	0	1008	32	0
45	QN	492	0	529	10	0
45	XN	492	0	529	17	0
46	QO	734	0	771	11	0
46	XO	729	0	768	14	0
47	QP	705	0	725	12	0
47	XP	705	0	725	11	0
48	QQ	834	0	904	16	0
48	XQ	834	0	904	15	0
49	QR	574	0	644	9	0
49	XR	574	0	644	9	0
50	QS	665	0	686	16	0
50	XS	674	0	699	16	0
51	QT	763	0	861	12	0
51	XT	763	0	861	16	0
52	QU	217	0	234	9	0
52	XU	217	0	234	10	0
53	QV	365	0	186	5	0
53	XV	322	0	164	6	0
54	QX	389	0	197	27	0
54	XX	412	0	208	12	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	485	0	0	0	0
55	RB	8	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	XA	87	0	0	0	0
55	XE	1	0	0	0	0
55	XL	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	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	1	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	1	0	0	0	0
56	QN	1	0	0	0	0
56	R4	1	0	0	0	0
56	R5	1	0	0	0	0
56	R6	1	0	0	0	0
56	R9	1	0	0	0	0
56	RY	1	0	0	0	0
56	XN	1	0	0	0	0
56	Y4	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	3	0
All	All	290035	0	196997	3129	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 3129 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)
32:QA:1535:C:N4	54:QX:9:G:C2	1.91	1.37
32:QA:1535:C:N4	54:QX:9:G:N2	1.78	1.30
17:YV:49:THR:OG1	17:YV:50:PRO:HD2	1.30	1.25
21:RZ:182:LYS:O	21:RZ:186:GLU:HG2	1.39	1.22
32:QA:1535:C:C4	54:QX:9:G:N2	2.07	1.22

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)
1:RA:307:G:O6	24:Y2:71:ASN:O[3_555]	1.47	0.73
7:YH:46:GLU:CB	20:YY:22:GLY:O[4_445]	1.82	0.38
8:RI:82:ARG:NH1	32:XA:56:U:O2'[4_555]	2.05	0.15
8:RI:91:SER:OG	32:XA:368:U:OP1[4_555]	2.07	0.13
18:RW:63:ASP:OD1	20:YY:92:ASN:ND2[3_555]	2.08	0.12

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	
3	RD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
3	YD	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
4	RE	202/206 (98%)	190 (94%)	12 (6%)	0	100	100
4	YE	203/206 (98%)	170 (84%)	32 (16%)	1 (0%)	29	61
5	RF	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
5	YF	200/210 (95%)	182 (91%)	18 (9%)	0	100	100
6	RG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	25	57
6	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	57
7	RH	172/180 (96%)	149 (87%)	21 (12%)	2 (1%)	13	41
7	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	RI	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	22	55
8	YI	144/148 (97%)	122 (85%)	22 (15%)	0	100	100
9	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
9	YN	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	22	55
10	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	RP	146/150 (97%)	122 (84%)	24 (16%)	0	100	100
11	YP	145/150 (97%)	129 (89%)	15 (10%)	1 (1%)	22	55
12	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	55
12	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	RR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	YR	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
14	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
14	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
15	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
15	YT	135/146 (92%)	127 (94%)	8 (6%)	0	100	100
16	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
16	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	49
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	46
18	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
18	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
19	YX	92/96 (96%)	84 (91%)	8 (9%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	RZ	201/206 (98%)	180 (90%)	20 (10%)	1 (0%)	29	61
21	YZ	199/206 (97%)	188 (94%)	9 (4%)	2 (1%)	15	46
22	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
22	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y1	91/98 (93%)	91 (100%)	0	0	100	100
24	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
24	Y2	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
25	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
26	Y4	67/71 (94%)	58 (87%)	9 (13%)	0	100	100
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	45/49 (92%)	45 (100%)	0	0	100	100
29	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	R8	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
30	Y8	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
31	R9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
31	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	QB	233/256 (91%)	201 (86%)	32 (14%)	0	100	100
33	XB	234/256 (91%)	205 (88%)	29 (12%)	0	100	100
34	QC	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
34	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
35	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	46
36	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	XE	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
37	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
37	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
38	QG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	XG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
39	QH	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
40	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
41	QJ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
41	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
42	QK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
42	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
43	QL	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
43	XL	120/132 (91%)	106 (88%)	14 (12%)	0	100	100
44	QM	118/126 (94%)	104 (88%)	13 (11%)	1 (1%)	19	51
44	XM	117/126 (93%)	105 (90%)	10 (8%)	2 (2%)	9	34
45	QN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
47	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	XP	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
48	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
48	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
49	QR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
49	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
50	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	XS	82/93 (88%)	68 (83%)	13 (16%)	1 (1%)	13	41
51	QT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
51	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
52	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
52	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	11486/12128 (95%)	10518 (92%)	945 (8%)	23 (0%)	47	78

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	YV	49	THR
35	XD	32	ALA

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Mol	Chain	Res	Type
21	YZ	52	SER
16	RU	93	LYS
35	QD	32	ALA

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	
3	RD	214/218 (98%)	214 (100%)	0	100	100
3	YD	215/218 (99%)	213 (99%)	2 (1%)	78	90
4	RE	165/166 (99%)	163 (99%)	2 (1%)	71	85
4	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
5	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
5	YF	161/166 (97%)	159 (99%)	2 (1%)	71	85
6	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
6	YG	155/156 (99%)	153 (99%)	2 (1%)	69	84
7	RH	145/148 (98%)	145 (100%)	0	100	100
7	YH	145/148 (98%)	143 (99%)	2 (1%)	67	83
8	RI	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	YI	122/124 (98%)	121 (99%)	1 (1%)	81	91
9	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
9	YN	119/119 (100%)	118 (99%)	1 (1%)	81	91
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	113 (98%)	2 (2%)	60	80
11	YP	114/116 (98%)	113 (99%)	1 (1%)	78	90
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	63
12	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	79
13	RR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	YR	100/101 (99%)	100 (100%)	0	100	100
14	RS	87/88 (99%)	87 (100%)	0	100	100
14	YS	87/88 (99%)	87 (100%)	0	100	100
15	RT	120/127 (94%)	119 (99%)	1 (1%)	81	91
15	YT	120/127 (94%)	120 (100%)	0	100	100
16	RU	93/94 (99%)	93 (100%)	0	100	100
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	86
17	RV	82/82 (100%)	81 (99%)	1 (1%)	71	85
17	YV	82/82 (100%)	82 (100%)	0	100	100
18	RW	92/92 (100%)	92 (100%)	0	100	100
18	YW	92/92 (100%)	92 (100%)	0	100	100
19	RX	74/78 (95%)	73 (99%)	1 (1%)	67	83
19	YX	76/78 (97%)	73 (96%)	3 (4%)	32	61
20	RY	88/91 (97%)	88 (100%)	0	100	100
20	YY	88/91 (97%)	87 (99%)	1 (1%)	73	86
21	RZ	174/179 (97%)	169 (97%)	5 (3%)	42	69
21	YZ	173/179 (97%)	171 (99%)	2 (1%)	71	85
22	R0	61/67 (91%)	60 (98%)	1 (2%)	62	81
22	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	81
23	R1	82/83 (99%)	82 (100%)	0	100	100
23	Y1	78/83 (94%)	78 (100%)	0	100	100
24	R2	64/67 (96%)	64 (100%)	0	100	100
24	Y2	67/67 (100%)	67 (100%)	0	100	100
25	R3	51/52 (98%)	49 (96%)	2 (4%)	32	61
25	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	77
26	R4	62/63 (98%)	60 (97%)	2 (3%)	39	67
26	Y4	62/63 (98%)	62 (100%)	0	100	100
27	R5	51/52 (98%)	51 (100%)	0	100	100
27	Y5	51/52 (98%)	51 (100%)	0	100	100
28	R6	51/52 (98%)	51 (100%)	0	100	100
28	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	R7	40/42 (95%)	40 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	53 (98%)	1 (2%)	57	78
30	Y8	54/55 (98%)	54 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	203/220 (92%)	201 (99%)	2 (1%)	76	88
33	XB	204/220 (93%)	204 (100%)	0	100	100
34	QC	159/188 (85%)	159 (100%)	0	100	100
34	XC	159/188 (85%)	157 (99%)	2 (1%)	69	84
35	QD	180/181 (99%)	178 (99%)	2 (1%)	73	86
35	XD	180/181 (99%)	173 (96%)	7 (4%)	32	61
36	QE	116/123 (94%)	113 (97%)	3 (3%)	46	72
36	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
37	QF	90/90 (100%)	90 (100%)	0	100	100
37	XF	90/90 (100%)	90 (100%)	0	100	100
38	QG	126/127 (99%)	124 (98%)	2 (2%)	62	81
38	XG	126/127 (99%)	124 (98%)	2 (2%)	62	81
39	QH	118/119 (99%)	118 (100%)	0	100	100
39	XH	118/119 (99%)	118 (100%)	0	100	100
40	QI	98/99 (99%)	97 (99%)	1 (1%)	76	88
40	XI	97/99 (98%)	97 (100%)	0	100	100
41	QJ	89/92 (97%)	86 (97%)	3 (3%)	37	65
41	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	85
42	QK	88/99 (89%)	87 (99%)	1 (1%)	73	86
42	XK	88/99 (89%)	88 (100%)	0	100	100
43	QL	104/109 (95%)	104 (100%)	0	100	100
43	XL	103/109 (94%)	103 (100%)	0	100	100
44	QM	96/101 (95%)	93 (97%)	3 (3%)	40	68
44	XM	95/101 (94%)	92 (97%)	3 (3%)	39	67
45	QN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	XN	49/50 (98%)	49 (100%)	0	100	100
46	QO	79/80 (99%)	78 (99%)	1 (1%)	69	84
46	XO	79/80 (99%)	79 (100%)	0	100	100
47	QP	72/74 (97%)	70 (97%)	2 (3%)	43	70
47	XP	72/74 (97%)	70 (97%)	2 (3%)	43	70
48	QQ	95/97 (98%)	95 (100%)	0	100	100
48	XQ	95/97 (98%)	95 (100%)	0	100	100
49	QR	61/77 (79%)	61 (100%)	0	100	100
49	XR	61/77 (79%)	61 (100%)	0	100	100
50	QS	72/80 (90%)	72 (100%)	0	100	100
50	XS	73/80 (91%)	71 (97%)	2 (3%)	44	70
51	QT	76/82 (93%)	76 (100%)	0	100	100
51	XT	76/82 (93%)	76 (100%)	0	100	100
52	QU	20/22 (91%)	18 (90%)	2 (10%)	7	27
52	XU	20/22 (91%)	20 (100%)	0	100	100
All	All	9712/10066 (96%)	9607 (99%)	105 (1%)	73	86

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	QP	67	THR
11	YP	71	VAL
44	XM	7	VAL
52	QU	24	ARG
6	YG	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
41	QJ	69	ASN
6	YG	40	ASN
50	XS	83	HIS
39	XH	78	GLN
50	XS	53	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2877/2915 (98%)	581 (20%)	41 (1%)
1	YA	2880/2915 (98%)	558 (19%)	40 (1%)
2	RB	119/122 (97%)	19 (15%)	1 (0%)
2	YB	119/122 (97%)	23 (19%)	2 (1%)
32	QA	1510/1521 (99%)	292 (19%)	37 (2%)
32	XA	1509/1521 (99%)	277 (18%)	29 (1%)
53	QV	16/17 (94%)	1 (6%)	0
53	XV	14/17 (82%)	0	0
54	QX	17/19 (89%)	5 (29%)	1 (5%)
54	XX	18/19 (94%)	9 (50%)	1 (5%)
All	All	9079/9188 (98%)	1765 (19%)	152 (1%)

5 of 1765 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	34	C
1	RA	35	G
1	RA	46	C

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	2712	U
32	XA	992	U
1	YA	2867	G
32	XA	388	G
32	XA	1537	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	1MG	QV	37	53	18,26,27	0.67	0	19,39,42	1.09	3 (15%)
53	1MG	XV	37	53	18,26,27	0.66	0	19,39,42	1.00	2 (10%)

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
53	1MG	QV	37	53	-	0/3/25/26	0/3/3/3
53	1MG	XV	37	53	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	QV	37	1MG	C8-N7-C5	2.46	107.67	102.99
53	XV	37	1MG	C8-N7-C5	2.37	107.51	102.99
53	XV	37	1MG	C5-C6-N1	2.28	117.33	113.90
53	QV	37	1MG	C5-C6-N1	2.06	117.00	113.90
53	QV	37	1MG	CM1-N1-C6	2.04	120.35	117.55

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
53	XV	37	1MG	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1213 ligands modelled in this entry, 1211 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
57	SF4	XD	301	35	0,12,12	-	-	-		
57	SF4	QD	301	35	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	35	-	-	0/6/5/5
57	SF4	QD	301	35	-	-	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.

2 monomers are involved in 4 short contacts:

Mol	**Chain**	**Res**	**Type**	**Clashes**	**Symm-Clashes**
57	XD	301	SF4	3	0
57	QD	301	SF4	1	0

5.7 Other polymers ⓘ

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.