



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:40 pm BST

PDB ID : 5VPP
Title : The 70S P-site tRNA SufA6 complex
Authors : Hong, S.; Sunita, S.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2017-05-05
Resolution : 3.90 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

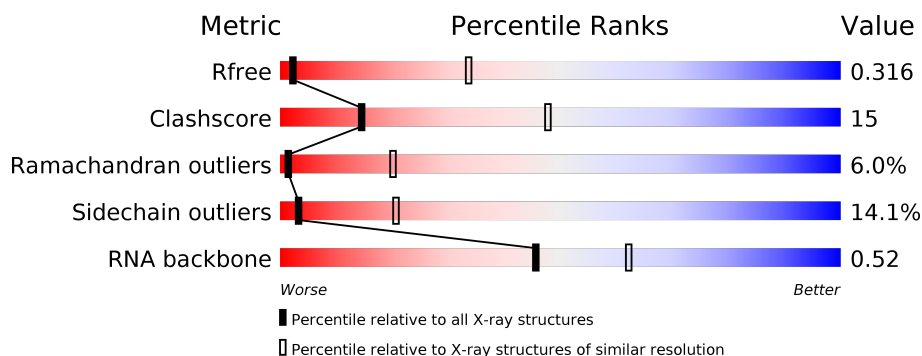
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	








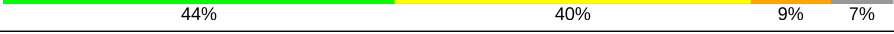



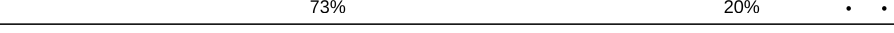



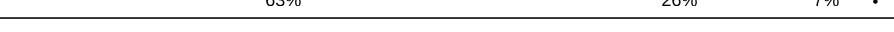



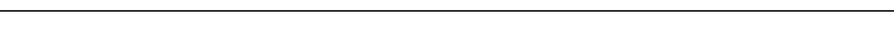
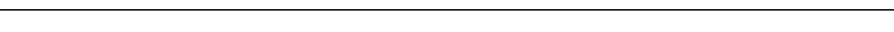

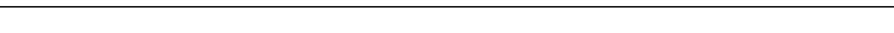
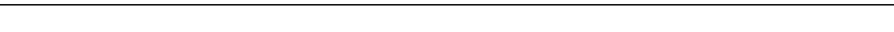

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Mol	Chain	Length	Quality of chain
4	RE	206	
4	YE	206	
5	RF	210	
5	YF	210	
6	RG	182	
6	YG	182	
7	RH	180	
7	YH	180	
8	RI	148	
8	YI	148	
9	RN	140	
9	YN	140	
10	RO	122	
10	YO	122	
11	RP	150	
11	YP	150	
12	RQ	141	
12	YQ	141	
13	RR	118	
13	YR	118	
14	RS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





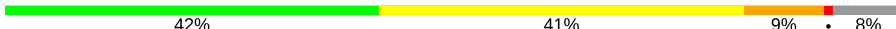
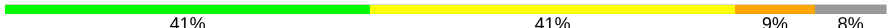
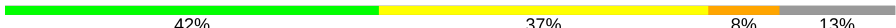


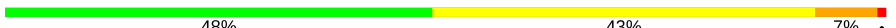










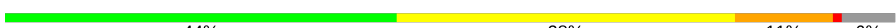

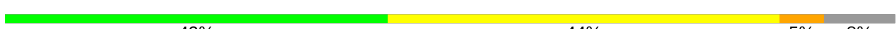


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Mol	Chain	Length	Quality of chain
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R5	60	
26	Y5	60	
27	R6	54	
27	Y6	54	
28	R7	49	
28	Y7	49	

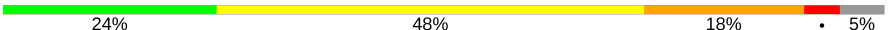

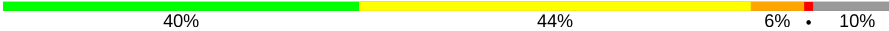








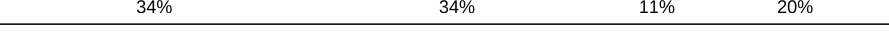




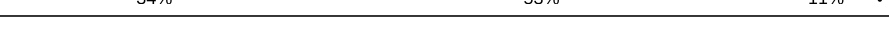

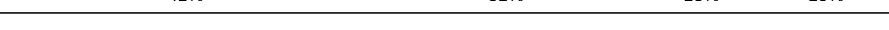
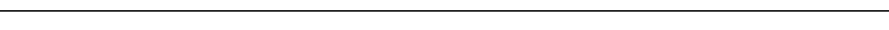
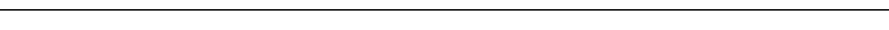
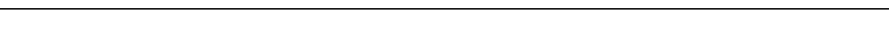
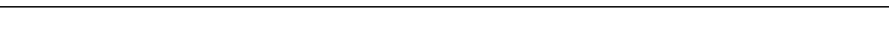
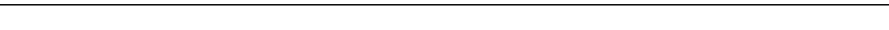

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Mol	Chain	Length	Quality of chain
29	R8	65	
29	Y8	65	
30	R9	37	
30	Y9	37	
31	QB	256	
31	XB	256	
32	QC	239	
32	XC	239	
33	QD	209	
33	XD	209	
34	QE	162	
34	XE	162	
35	QF	101	
35	XF	101	
36	QG	156	
36	XG	156	
37	QH	138	
37	XH	138	
38	QI	128	
38	XI	128	
39	QJ	105	
39	XJ	105	
40	QK	129	
40	XK	129	
41	QL	132	

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Mol	Chain	Length	Quality of chain
41	XL	132	
42	QM	126	
42	XM	126	
43	QN	61	
43	XN	61	
44	QO	89	
44	XO	89	
45	QP	88	
45	XP	88	
46	QQ	105	
46	XQ	105	
47	QR	88	
47	XR	88	
48	QT	106	
48	XT	106	
49	QA	1521	
49	XA	1521	
50	QS	93	
50	XS	93	
51	R4	71	
51	Y4	71	
52	QX	19	
52	XX	19	
53	QV	78	
53	XV	78	

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 291660 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
1	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

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

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

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

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

- 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	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
7	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	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	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- 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	0	0	0
			1122	715	212	188	7			
12	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- 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	0	0	0
			968	604	203	160	1			
13	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

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

- 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	0	0	0
			1141	710	234	196	1			
15	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- 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	0	0	0
			964	610	202	151	1			
16	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- 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	0	0	0
			779	501	142	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- 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	0	0	0
			900	566	177	155	2			
18	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
20	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
22	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	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	97	Total	C	N	O	S	0	0	0
			763	481	150	131	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	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- 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 L32.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
27	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
28	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	QB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			
31	XB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			
32	XC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6.

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

- Molecule 36 is a protein called 30S ribosomal protein S7.

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

- Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
37	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QI	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				
38	XI	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 39 is a protein called 30S ribosomal protein S10.

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

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
40	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
41	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

- Molecule 43 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
44	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

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

- Molecule 47 is a protein called 30S ribosomal protein S18.

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

- Molecule 48 is a protein called 30S ribosomal protein S20.

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

- Molecule 49 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QA	1511	Total	C	N	O	P	0	0	0
			32472	14454	6013	10495	1510			
49	XA	1515	Total	C	N	O	P	0	0	0
			32554	14491	6024	10525	1514			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	458C	G	C	conflict	GB 55771382
XA	458C	G	C	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	XS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			
50	QS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R4	34	Total	C	N	O	S	0	0	0
			262	169	43	48	2			
51	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 52 is a RNA chain called messenger RNA.

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

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

- Molecule 53 is a RNA chain called P-site tRNA SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	XV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			
53	QV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XV	38	1MG	-	insertion	GB 1151176235
QV	38	1MG	-	insertion	GB 1151176235

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	QA	131	Total	Mg	0	0
			131	131		
54	YA	379	Total	Mg	0	0
			379	379		
54	YR	1	Total	Mg	0	0
			1	1		
54	RT	3	Total	Mg	0	0
			3	3		
54	QD	3	Total	Mg	0	0
			3	3		
54	XE	1	Total	Mg	0	0
			1	1		
54	XO	1	Total	Mg	0	0
			1	1		
54	Y1	1	Total	Mg	0	0
			1	1		
54	YD	4	Total	Mg	0	0
			4	4		
54	RX	2	Total	Mg	0	0
			2	2		
54	Y8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	XA	128	Total 128	Mg 128	0	0
54	YY	1	Total 1	Mg 1	0	0
54	RQ	2	Total 2	Mg 2	0	0
54	R0	2	Total 2	Mg 2	0	0
54	QL	3	Total 3	Mg 3	0	0
54	YU	1	Total 1	Mg 1	0	0
54	RU	1	Total 1	Mg 1	0	0
54	RO	2	Total 2	Mg 2	0	0
54	XP	1	Total 1	Mg 1	0	0
54	Y0	1	Total 1	Mg 1	0	0
54	YQ	1	Total 1	Mg 1	0	0
54	RY	1	Total 1	Mg 1	0	0
54	QC	1	Total 1	Mg 1	0	0
54	R8	3	Total 3	Mg 3	0	0
54	YX	1	Total 1	Mg 1	0	0
54	RR	3	Total 3	Mg 3	0	0
54	RD	10	Total 10	Mg 10	0	0
54	R1	3	Total 3	Mg 3	0	0
54	YT	2	Total 2	Mg 2	0	0
54	XK	1	Total 1	Mg 1	0	0
54	QQ	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	RA	562	Total 562	Mg 562	0	0
54	YP	1	Total 1	Mg 1	0	0
54	RE	7	Total 7	Mg 7	0	0
54	XL	2	Total 2	Mg 2	0	0
54	YB	10	Total 10	Mg 10	0	0
54	QT	2	Total 2	Mg 2	0	0
54	XC	1	Total 1	Mg 1	0	0
54	RI	1	Total 1	Mg 1	0	0
54	R6	1	Total 1	Mg 1	0	0
54	QP	2	Total 2	Mg 2	0	0
54	RB	15	Total 15	Mg 15	0	0
54	YI	1	Total 1	Mg 1	0	0
54	XM	1	Total 1	Mg 1	0	0
54	QE	1	Total 1	Mg 1	0	0
54	XD	1	Total 1	Mg 1	0	0
54	RF	4	Total 4	Mg 4	0	0
54	R3	1	Total 1	Mg 1	0	0
54	YE	5	Total 5	Mg 5	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XD	1	Total 1	Zn 1	0	0

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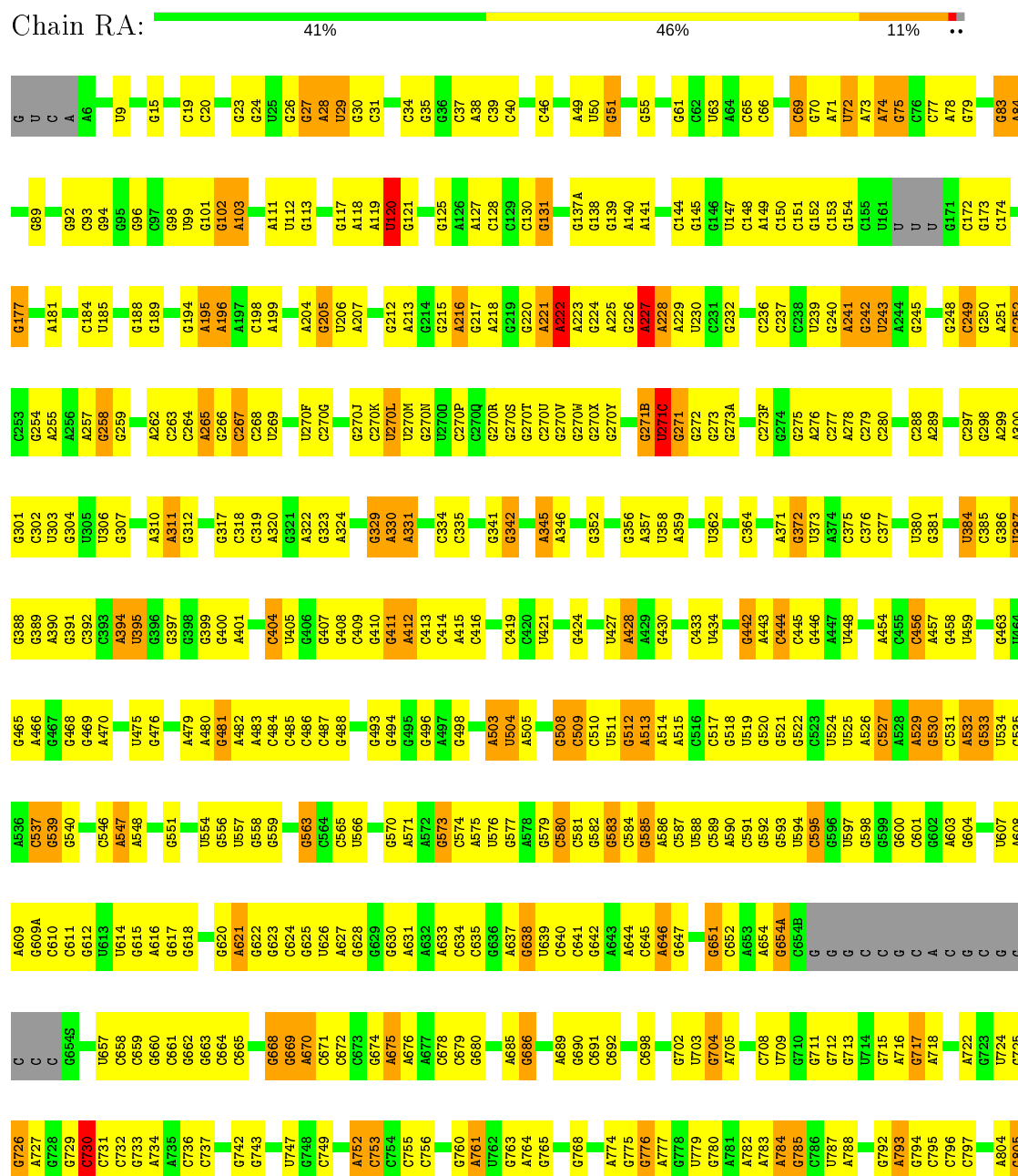
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	Y9	1	Total 1	Zn 1	0	0
55	QD	2	Total 2	Zn 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

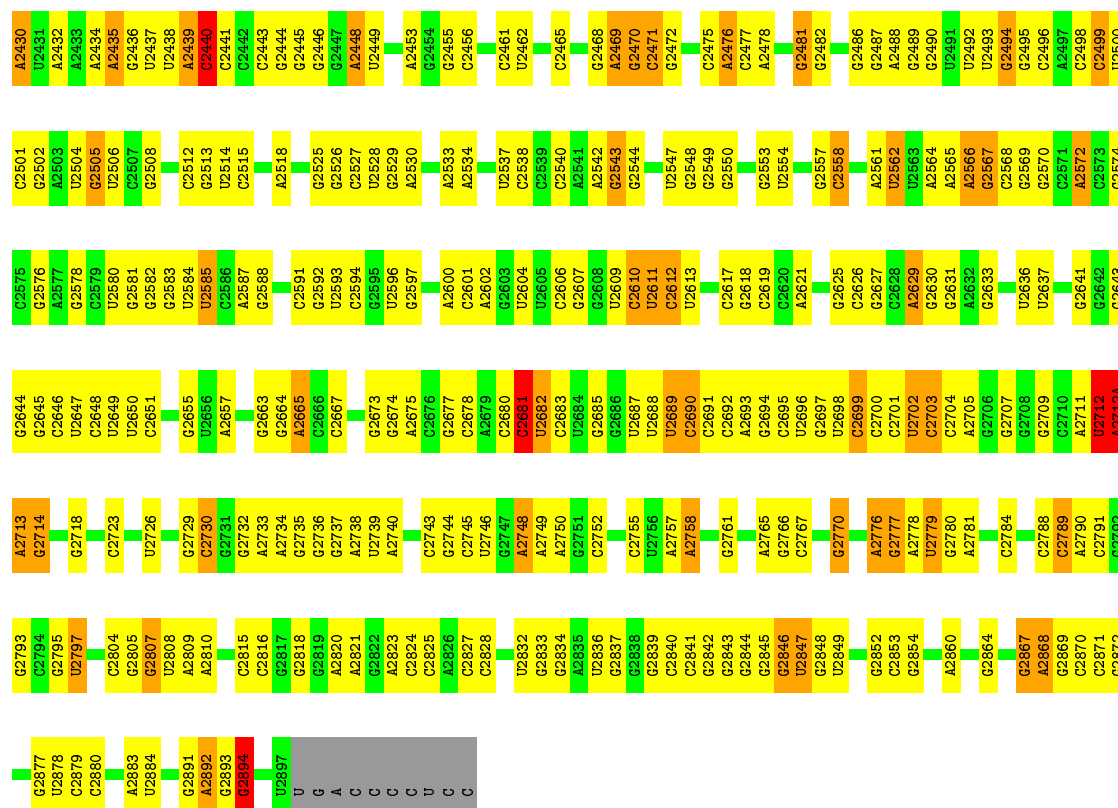
• Molecule 1: 23S rRNA



C1908	C1909	G1817	G1818	G1750	G1850	A1566	G1492	G1413	C1350	A1269	G1191	G1115	C965	U877	C806
A1918	A1919	U1818	U1819	C1751	G1651	A1569	C1493	G1414	C1351	C1270	G1192	C1116	G966	A878	U807
A1913	A1914	C1752	G1652	A1570	G1653	A1571	A1495	U1415	U1352	G1271	G1193	G1117	C967	G879	G808
C1914	C1915	G1753	A1654	A1572	U1496	A1573	A1496	G1417	A1354	U1272	G1195	G1120	U1035	G883	G809
A1918	A1919	G1754	C1754	A1572	U1497	A1573	U1497	G1418	G1355	A1274	G1196	G1121	G1036	G884	C812
A1918	A1919	G1755	C1755	A1572	U1498	A1573	U1498	G1419	G1356	A1275	G1197	G1122	C1041	G884	U813
A1919	A1920	G1756	U1659	A1572	C1499	A1573	C1499	U1420	U1357	A1275	G1198	G1123	C1042	G884	U814
C1920	C1921	G1757	G1500	A1572	G1500	A1573	G1500	U1421	U1358	A1276	G1199	G1124	G1043	A890	C814
U1923	U1924	A1760	C1506	A1572	C1506	A1573	C1506	G1422	A1359	G1280	U1198	G1125	G1044	A896	C815
U1923	U1924	C1761	C1507	A1573	A1507	A1573	A1507	G1423	A1360	C1201	U1199	C1126	G1045	C816	C817
C1924	C1925	A1762	A1508	A1573	A1508	A1573	A1508	G1424	G1361	G1202	U1200	A1127	C974A	C818	C819
A1927	A1928	G1763	C1509	A1573	C1509	A1573	C1509	G1425	C1362	G1203	G1203	A1127	C975	C819	C820
A1928	A1929	G1764	A1510	A1573	A1510	A1573	A1510	G1426	C1363	A1204	U1204	A1127	C975	C820	C821
G1930	G1931	C1765	A1511	A1573	A1511	A1573	A1511	G1427	G1364	A1205	U1205	A1127	C975	C821	C822
U1931	U1932	U1766	U1514	A1573	U1514	A1573	U1514	G1428	A1365	G1206	U1206	A1127	C975	C822	C823
C1934	C1935	C1767	C1518	A1573	C1518	A1573	C1518	G1429	A1366	A1210	U1210	A1127	C975	C823	C824
G1935	G1936	A1768	C1519	A1573	C1519	A1573	C1519	U1431	A1367	U1211	U1211	A1127	C975	C824	C825
A1936	A1937	G1769	U1519	A1573	U1519	A1573	U1519	G1432	A1368	U1212	U1212	A1127	C975	C825	C826
A1937	A1938	G1770	U1520	A1573	U1520	A1573	U1520	C1432	G1369	A1220	U1220	A1127	C975	C826	C827
A1938	A1939	G1771	U1521	A1573	U1521	A1573	U1521	U1433	G1370	C1221	U1221	A1127	C975	C827	C828
U1939	U1940	A1772	G1522	A1573	G1522	A1573	G1522	A1434	G1371	C1222	U1222	A1127	C975	C828	C829
C1942	C1943	C1774	C1532	A1573	C1532	A1573	C1532	G1443	U1300	C1223	U1223	A1127	C975	C829	C830
U1942	U1943	U1777	C1533	A1573	C1533	A1573	C1533	G1444	A1301	G1224	U1224	A1127	C975	C830	C831
A1943	A1944	U1778	U1534	A1573	U1534	A1573	U1534	G1445	A1302	A1227	U1227	A1127	C975	C831	C832
A1944	A1945	U1779	U1535	A1573	U1535	A1573	U1535	C1445	G1303	G1228	U1228	A1127	C975	C832	C833
A1945	A1946	C1780	U1536	A1573	U1536	A1573	U1536	G1446	C1304	A1229	U1229	A1127	C975	C833	C834
A1946	A1947	G1781	U1537	A1573	U1537	A1573	U1537	U1448	G1309	C1230	U1230	A1127	C975	C834	C835
A1947	A1948	C1782	U1538	A1573	U1538	A1573	U1538	G1449	G1310	G1231	U1231	A1127	C975	C835	C836
A1948	A1949	U1783	U1539	A1573	U1539	A1573	U1539	G1450	G1311	G1232	U1232	A1127	C975	C836	C837
A1949	A1950	C1784	U1540	A1573	U1540	A1573	U1540	G1451	G1312	G1233	U1233	A1127	C975	C837	C838
A1950	A1951	A1785	U1541	A1573	U1541	A1573	U1541	G1452	U1312	G1234	U1234	A1127	C975	C838	C839
A1951	A1952	C1786	U1542	A1573	U1542	A1573	U1542	G1453	A1313	G1235	U1235	A1127	C975	C839	C840
A1952	A1953	U1787	U1543	A1573	U1543	A1573	U1543	G1454	U1314	G1236	U1236	A1127	C975	C840	C841
A1953	A1954	U1788	U1544	A1573	U1544	A1573	U1544	G1455	G1385	G1237	U1237	A1127	C975	C841	C842
A1954	A1955	A1789	U1545	A1573	U1545	A1573	U1545	G1456	C1386	A1237	U1237	A1127	C975	C842	C843
A1955	A1956	U1790	U1546	A1573	U1546	A1573	U1546	G1457	U1387	C1004	U1004	A1127	C975	C843	C844
A1956	A1957	C1791	U1547	A1573	U1547	A1573	U1547	G1458	U1388	C1005	U1005	A1127	C975	C844	C845
A1957	A1958	U1792	U1548	A1573	U1548	A1573	U1548	G1459	U1389	C1006	U1006	A1127	C975	C845	C846
A1958	A1959	G1793	U1549	A1573	U1549	A1573	U1549	G1460	U1390	C1007	U1007	A1127	C975	C846	C847
A1959	A1960	C1794	U1550	A1573	U1550	A1573	U1550	G1461	U1391	C1008	U1008	A1127	C975	C847	C848
A1960	A1961	U1795	U1551	A1573	U1551	A1573	U1551	G1462	U1392	C1009	U1009	A1127	C975	C848	C849
A1961	A1962	U1796	U1552	A1573	U1552	A1573	U1552	G1463	U1393	G1087	U1087	A1127	C975	C849	C850
A1962	A1963	G1797	U1553	A1573	U1553	A1573	U1553	G1464	U1394	A1088	U1088	A1127	C975	C850	C851
A1963	A1964	U1798	U1554	A1573	U1554	A1573	U1554	G1465	U1395	U1090	U1090	A1127	C975	C851	C852
A1964	A1965	G1799	U1555	A1573	U1555	A1573	U1555	G1466	U1396	U1091	U1091	A1127	C975	C852	C853
A1965	A1966	C1800	U1556	A1573	U1556	A1573	U1556	G1467	C1398	U1092	U1092	A1127	C975	C853	C854
A1966	A1967	U1799	U1557	A1573	U1557	A1573	U1557	G1468	U1399	A1098	U1098	A1127	C975	C854	C855
A1967	A1968	G1801	U1558	A1573	U1558	A1573	U1558	G1469	U1400	A1099	U1099	A1127	C975	C855	C856
A1968	A1969	U1802	U1559	A1573	U1559	A1573	U1559	G1470	U1401	A1099	U1099	A1127	C975	C856	C857
A1969	A1970	C1803	U1560	A1573	U1560	A1573	U1560	G1471	U1402	A1099	U1099	A1127	C975	C857	C858
A1970	A1971	U1804	U1561	A1573	U1561	A1573	U1561	G1472	U1403	A1099	U1099	A1127	C975	C858	C859
A1971	A1972	G1805	U1562	A1573	U1562	A1573	U1562	G1473	U1404	A1099	U1099	A1127	C975	C859	C860
A1972	A1973	U1806	U1563	A1573	U1563	A1573	U1563	G1474	U1405	A1099	U1099	A1127	C975	C860	C861
A1973	A1974	C1807	U1564	A1573	U1564	A1573	U1564	G1475	U1406	A1099	U1099	A1127	C975	C861	C862
A1974	A1975	U1807	U1565	A1573	U1565	A1573	U1565	G1476	U1407	A1099	U1099	A1127	C975	C862	C863
A1975	A1976	G1808	U1566	A1573	U1566	A1573	U1566	G1477	U1408	A1099	U1099	A1127	C975	C863	C864
A1976	A1977	U1809	U1567	A1573	U1567	A1573	U1567	G1478	U1409	A1099	U1099	A1127	C975	C864	C865
A1977	A1978	C1809	U1568	A1573	U1568	A1573	U1568	G1479	U1410	A1099	U1099	A1127	C975	C865	C866
A1978	A1979	U1810	U1569	A1573	U1569	A1573	U1569	G1480	U1411	A1099	U1099	A1127	C975	C866	C867
A1979	A1980	G1811	U1570	A1573	U1570	A1573	U1570	G1481	U1412	A1099	U1099	A1127	C975	C867	C868
A1980	A1981	C1812	U1571	A1573	U1571	A1573	U1571	G1482	U1413	A1099	U1099	A1127	C975	C868	C869
A1981	A1982	U1813	U1572	A1573	U1572	A1573	U1572	G1483	U1414	A1099	U1099	A1127	C975	C869	C870
A1982	A1983	G1814	U1573	A1573	U1573	A1573	U1573	G1484	U1415	A1099	U1099	A1127	C975	C870	C871
A1983	A1984	U1815	U1574	A1573	U1574	A1573	U1574	G1485	U1416	A1099	U1099	A1127	C975	C871	C872
A1984	A1985	C1816	U1575	A1573	U1575	A1573	U1575	G1486	U1417	A1099	U1099	A1127	C975	C872	C873
A1985	A1986	U1816	U1576	A1573	U1576	A1573	U1576	G1487	U1418	A1099	U1099	A1127	C975	C873	C874
A1986	A1987	G1817	U1577	A1573	U1577	A1573	U1577	G1488	U1419	A1099	U1099	A1127	C975	C874	C875
A1987	A1988	C1818	U1578	A1573	U1578	A1573	U1578	G1489	U1420	A1099	U1099	A1127	C975	C875	C876
A1988	A1989	U1818	U1579	A1573	U1579	A1573	U1579	G1490	U1421	A1099	U1099	A1127	C975	C876	C877
A1989	A1990	G1819	U1580	A1573	U1580	A1573	U1580	G1491	U1422	A1099	U1099	A1127	C975	C877	C878
A1990	A1991	C1820	U1581	A1573	U1581	A1573	U1581	G1492	U1423	A1099	U1099	A1127	C975	C878	C879
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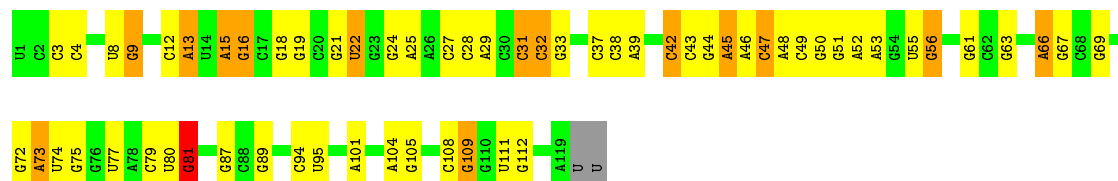
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A1085	C1013	C1013	A945	G886	U788	G713	C	C516	G442	G363B	C286	A251	G178
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U1088	C949	U1019	C949	U890	A793	G717	G	G520	U447	G372	C298	G258	U185
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					U839					A419			
	C994		C994	U922	C840					A420			
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	U1070		U1070	G926	C844					A424			
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				G928	G845					A426			
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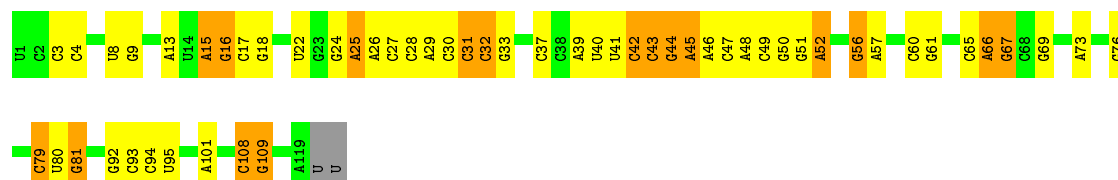
• Molecule 2: 5S rRNA

Chain RB: 48% 38% 11% ..



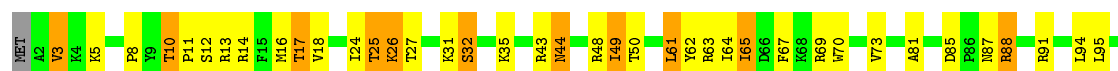
• Molecule 2: 5S rRNA

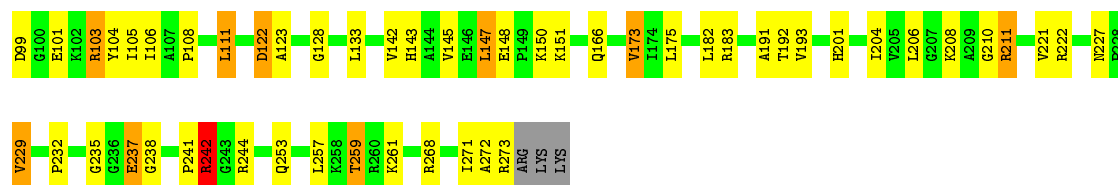
Chain YB: 53% 31% 14% .



• Molecule 3: 50S ribosomal protein L2

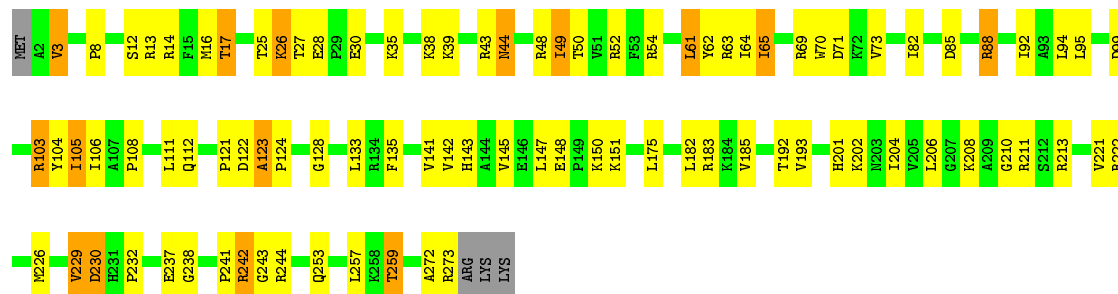
Chain RD: 66% 25% 7% .





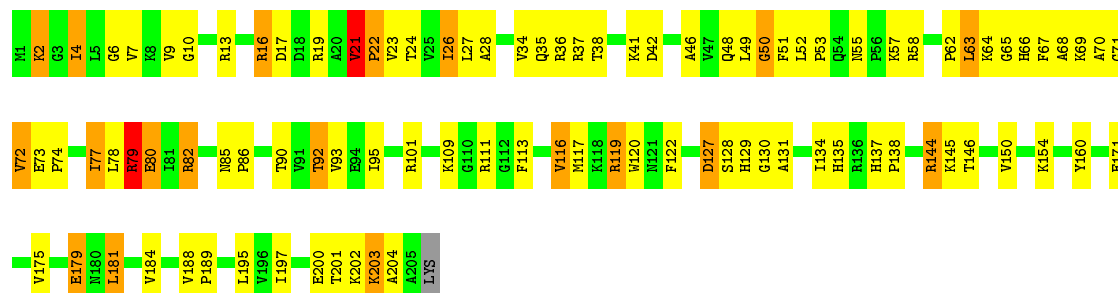
• Molecule 3: 50S ribosomal protein L2

Chain YD: 66% 28% 5% .



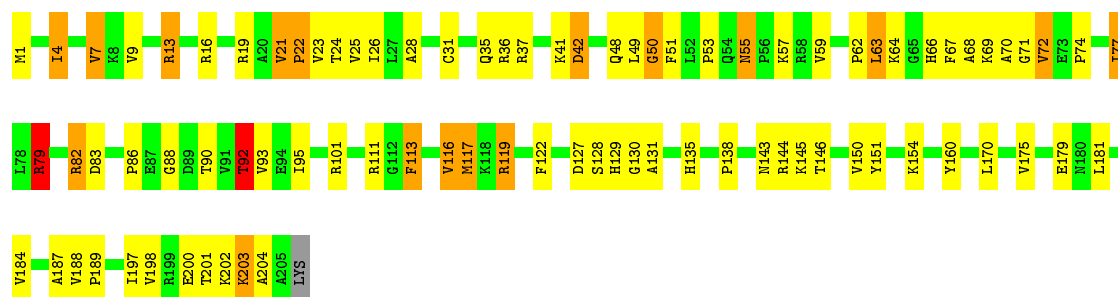
• Molecule 4: 50S ribosomal protein L3

Chain RE: 53% 36% 9% .



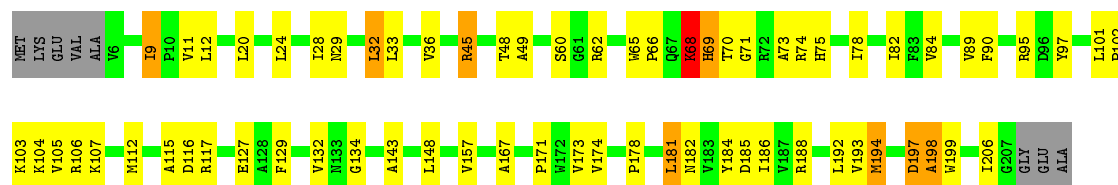
• Molecule 4: 50S ribosomal protein L3

Chain YE: 58% 33% 8% .



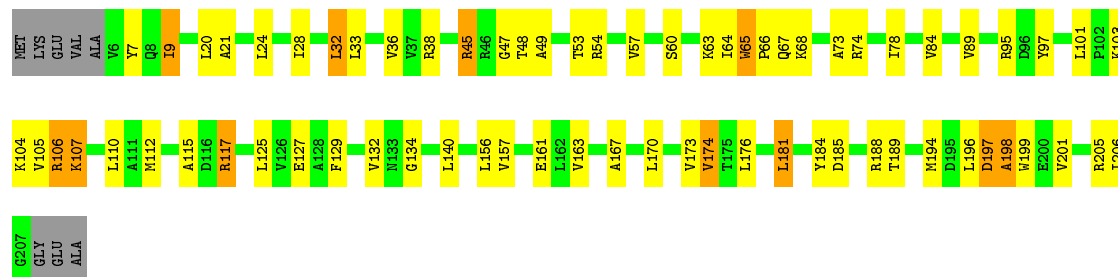
• Molecule 5: 50S ribosomal protein L4

Chain RF: 64% 28% 8% .



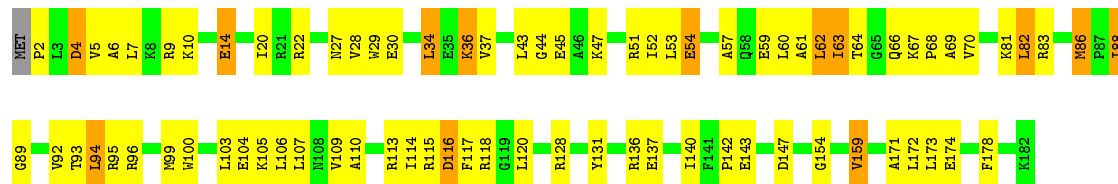
- Molecule 5: 50S ribosomal protein L4

Chain YF: 63% 28% 5% •



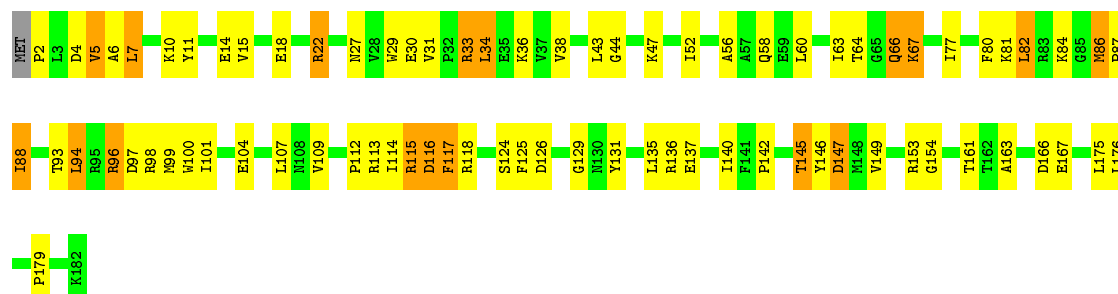
- Molecule 6: 50S ribosomal protein L5

Chain RG: 56% 36% 7% •



- Molecule 6: 50S ribosomal protein L5

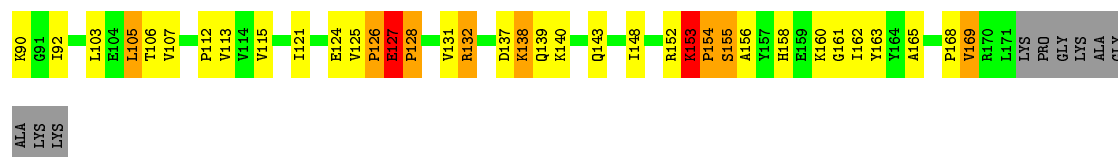
Chain YG: 56% 34% 9% •



- Molecule 7: 50S ribosomal protein L6

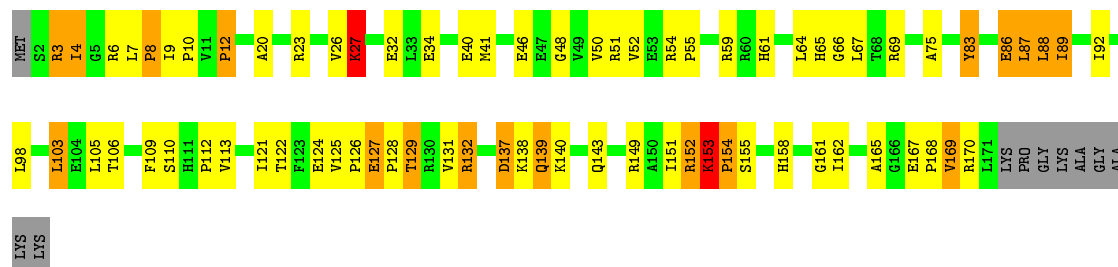
Chain RH: 53% 31% 9% 6% •





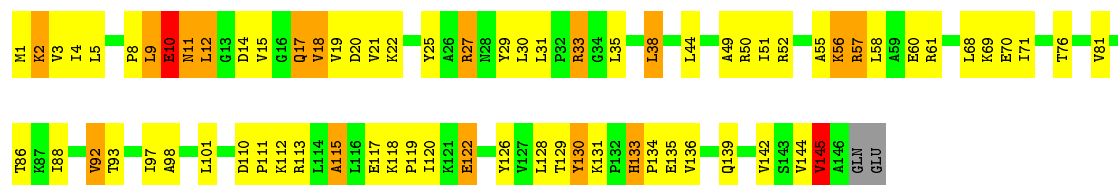
• Molecule 7: 50S ribosomal protein L6

Chain YH: 53% 30% 10% 6%



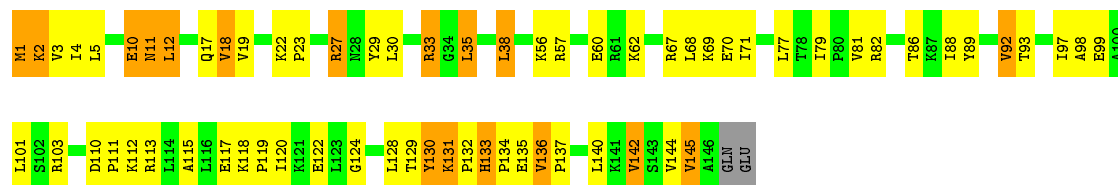
• Molecule 8: 50S ribosomal protein L9

Chain RI: 49% 37% 11% ..



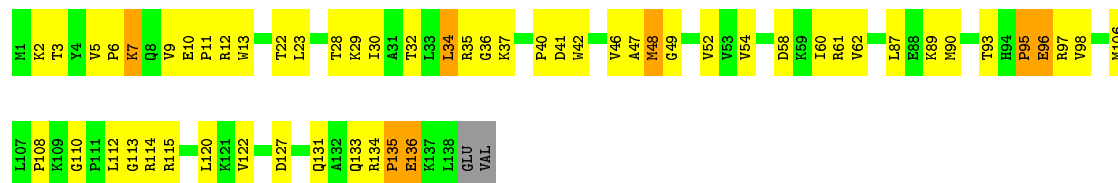
• Molecule 8: 50S ribosomal protein L9

Chain YI: 53% 34% 11% .



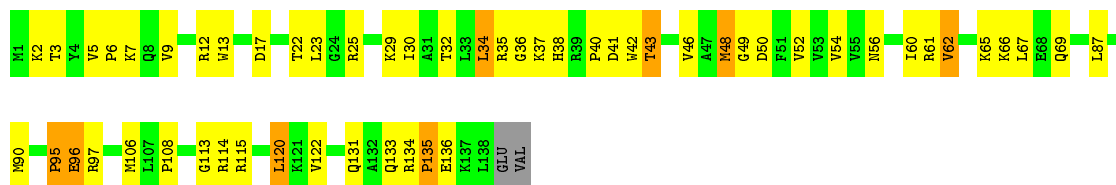
• Molecule 9: 50S ribosomal protein L13

Chain RN: 59% 35% 5% .




• Molecule 9: 50S ribosomal protein L13

Chain YN:  59% 34% 6% •




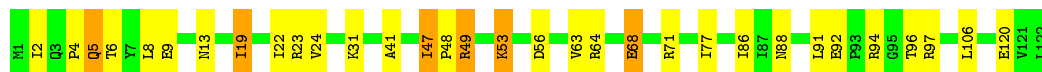
- Molecule 10: 50S ribosomal protein L14

Chain RO:  80% 16% •



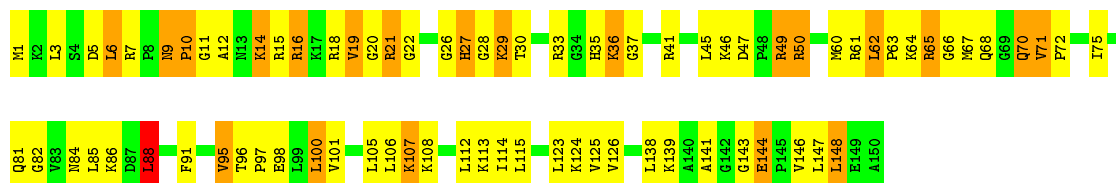
- Molecule 10: 50S ribosomal protein L14

Chain YO:  74% 21% 5% •



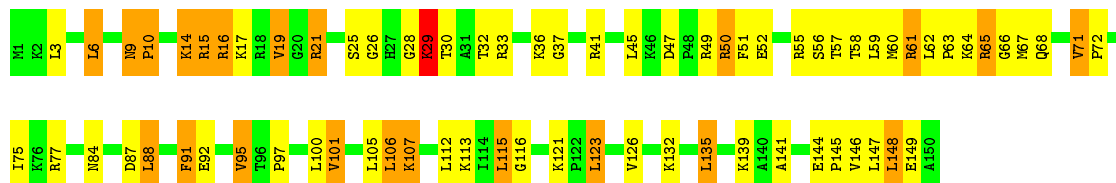
- Molecule 11: 50S ribosomal protein L15

Chain RP:  48% 37% 14% •



- Molecule 11: 50S ribosomal protein L15

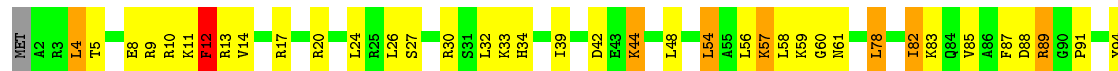
Chain YP:  51% 33% 15% •



- Molecule 12: 50S ribosomal protein L16

Chain RQ:  57% 35% 6% •



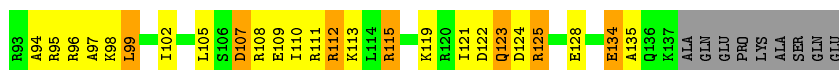
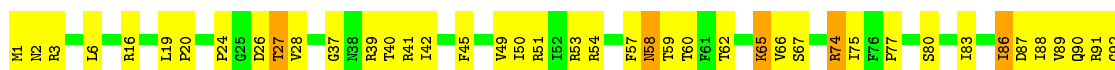




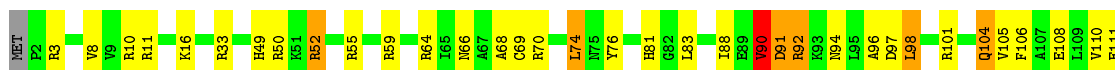
- Molecule 15: 50S ribosomal protein L19



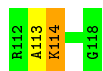
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



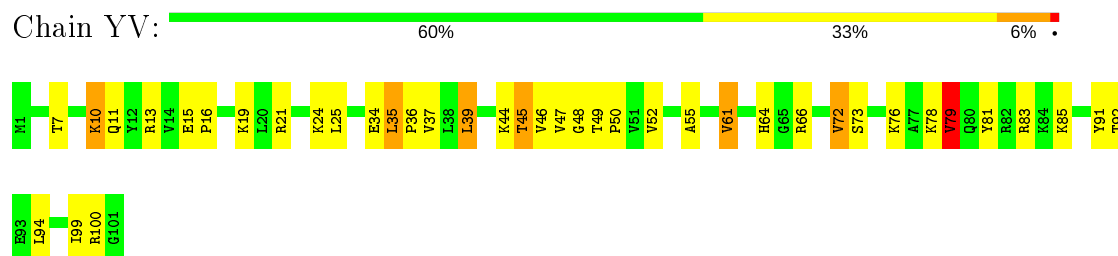
- Molecule 16: 50S ribosomal protein L20



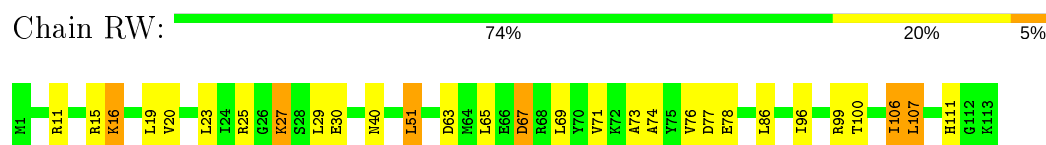
- Molecule 17: 50S ribosomal protein L21



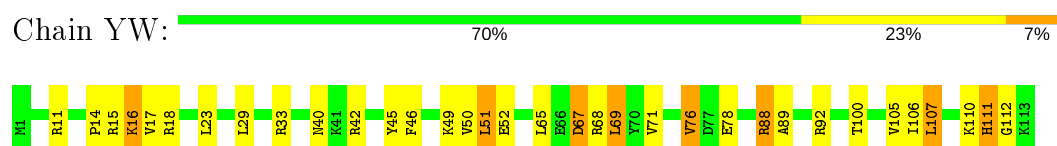
- Molecule 17: 50S ribosomal protein L21



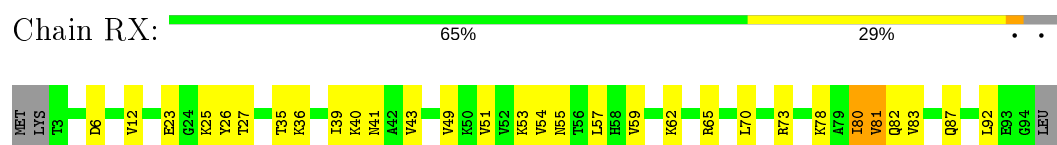
- Molecule 18: 50S ribosomal protein L22



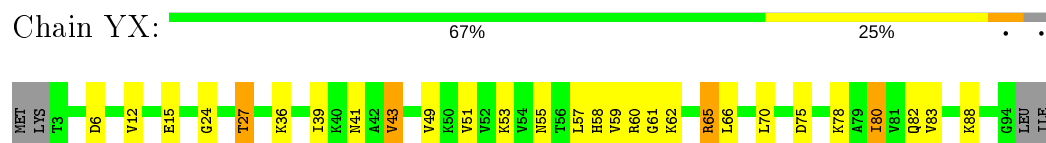
- Molecule 18: 50S ribosomal protein L22



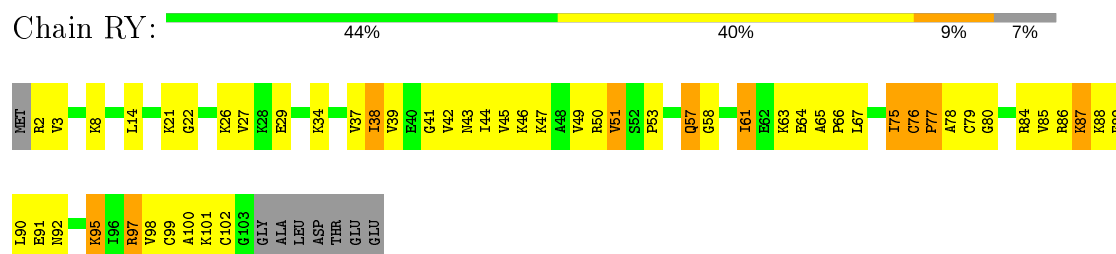
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24



Chain R1:  66% 29% ..



- Molecule 23: 50S ribosomal protein L28

Chain Y1:  65% 27% 6% ..



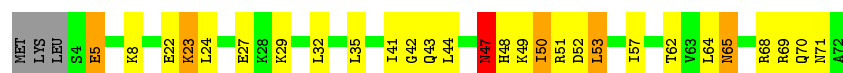
- Molecule 24: 50S ribosomal protein L29

Chain R2:  63% 26% 7% .




- Molecule 24: 50S ribosomal protein L29

Chain Y2:  57% 31% 7% . .




- Molecule 25: 50S ribosomal protein L30

Chain R3:  75% 22% . .



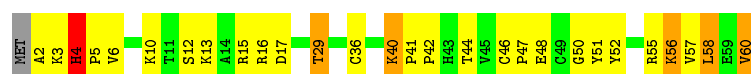
- Molecule 25: 50S ribosomal protein L30

Chain Y3:  87% 8% . .



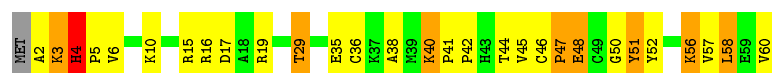
- Molecule 26: 50S ribosomal protein L32

Chain R5:  52% 37% 8% . .



- Molecule 26: 50S ribosomal protein L32

Chain Y5: 



- Molecule 27: 50S ribosomal protein L33

Chain R6: 



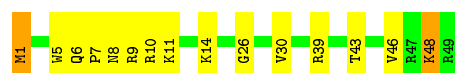
- Molecule 27: 50S ribosomal protein L33

Chain Y6: 



- Molecule 28: 50S ribosomal protein L34

Chain R7: 



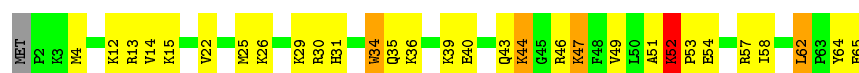
- Molecule 28: 50S ribosomal protein L34

Chain Y7: 



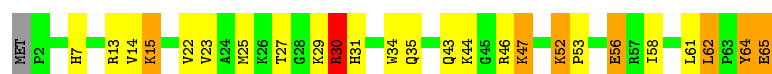
- Molecule 29: 50S ribosomal protein L35

Chain R8: 



- Molecule 29: 50S ribosomal protein L35

Chain Y8: 




- Molecule 30: 50S ribosomal protein L36

Chain R9:  70% 30%



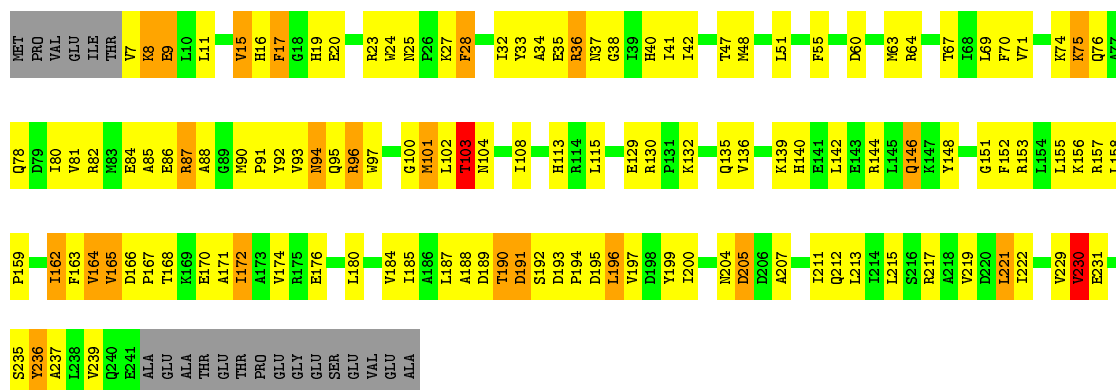
- Molecule 30: 50S ribosomal protein L36

Chain Y9:  76% 24%



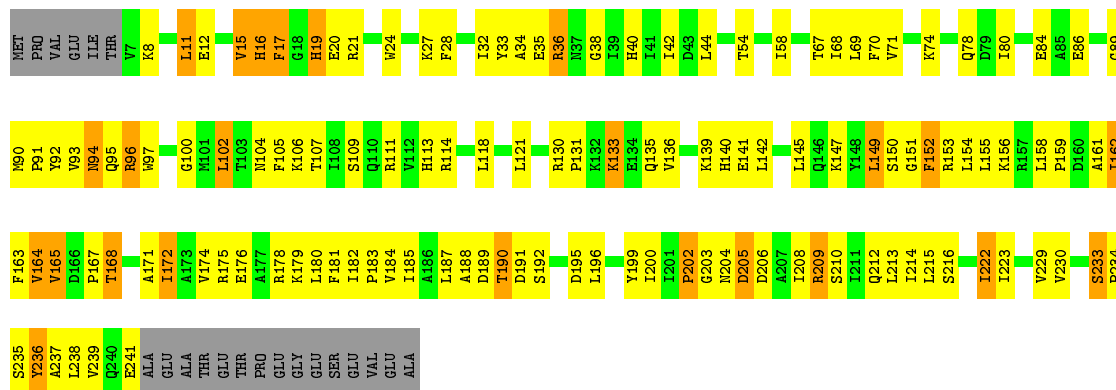
- Molecule 31: 30S ribosomal protein S2

Chain QB:  42% 41% 9% 8%



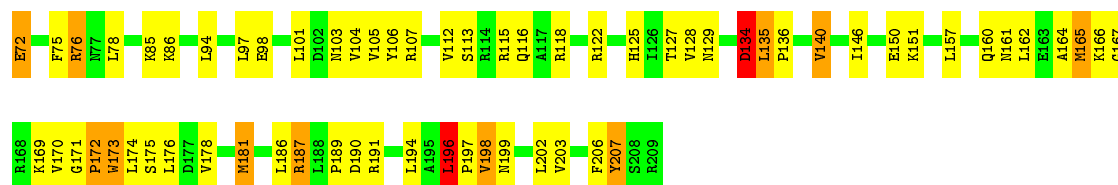
- Molecule 31: 30S ribosomal protein S2

Chain XB:  41% 41% 9% 8%



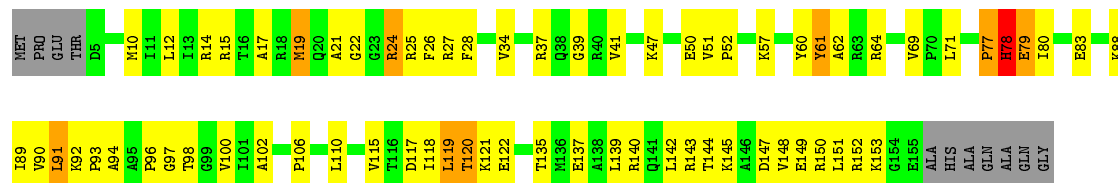
- Molecule 32: 30S ribosomal protein S3

Chain QC:  42% 37% 8% 13%



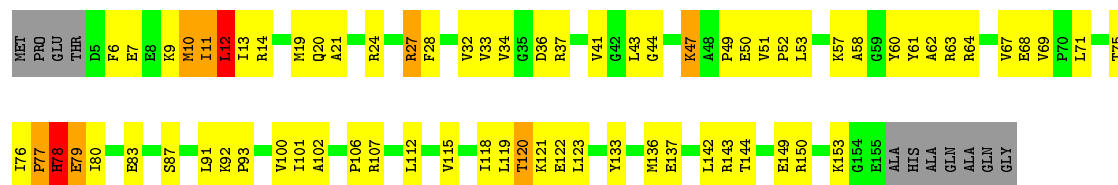
- Molecule 34: 30S ribosomal protein S5

Chain QE: 51% 37% 5% 7%



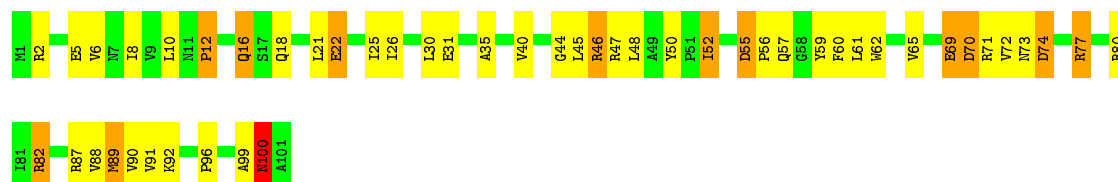
- Molecule 34: 30S ribosomal protein S5

Chain XE: 49% 39% 7%



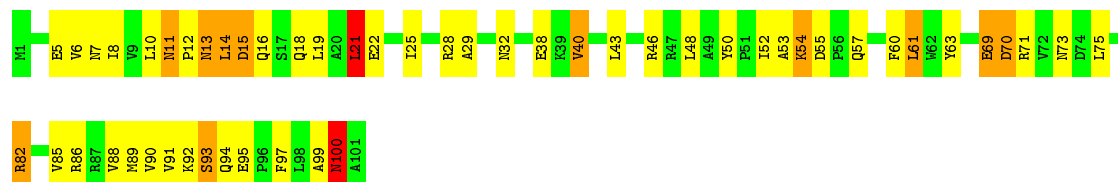
- Molecule 35: 30S ribosomal protein S6

Chain QF: 51% 36% 12%



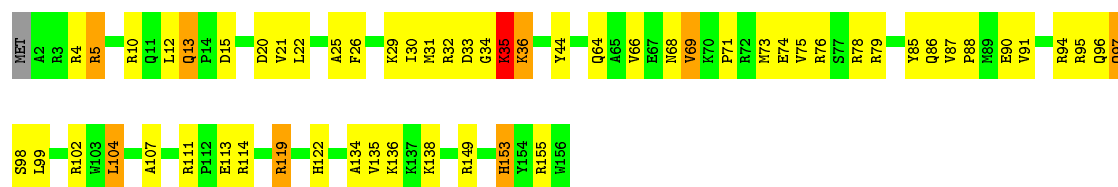
- Molecule 35: 30S ribosomal protein S6

Chain XF: 49% 39% 11%



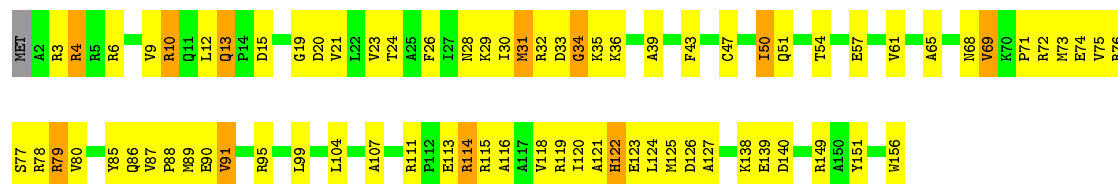
- Molecule 36: 30S ribosomal protein S7

Chain QG:  62% 31% 5% ..



- Molecule 36: 30S ribosomal protein S7

Chain XG:  51% 42% 7% .



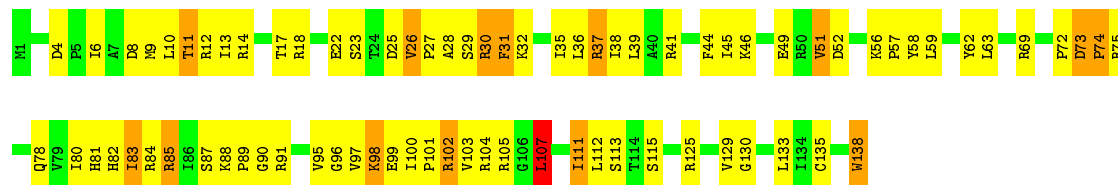
- Molecule 37: 30S ribosomal protein S8

Chain QH:  48% 43% 9% .



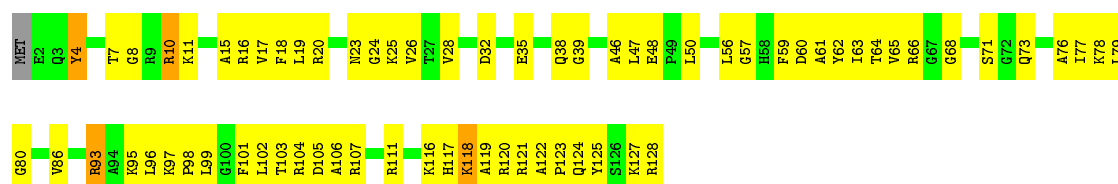
- Molecule 37: 30S ribosomal protein S8

Chain XH:  43% 46% 10% .



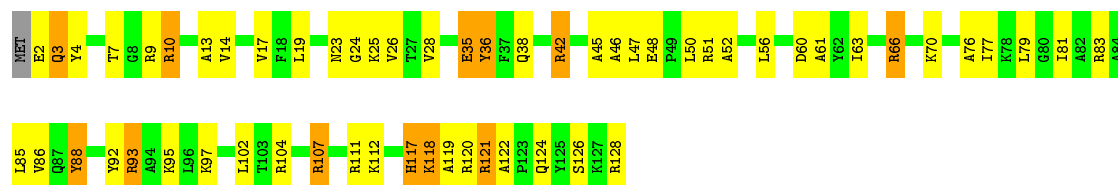
- Molecule 38: 30S ribosomal protein S9

Chain QI:  45% 51% ..



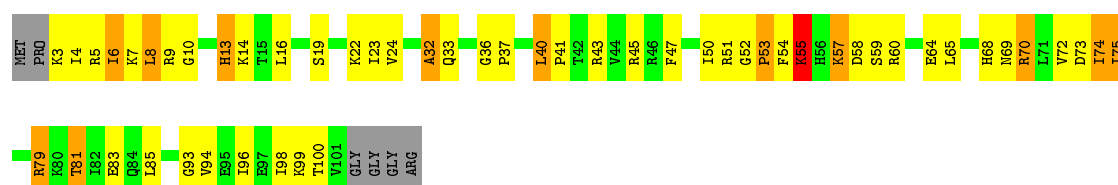
- Molecule 38: 30S ribosomal protein S9

Chain XI: 



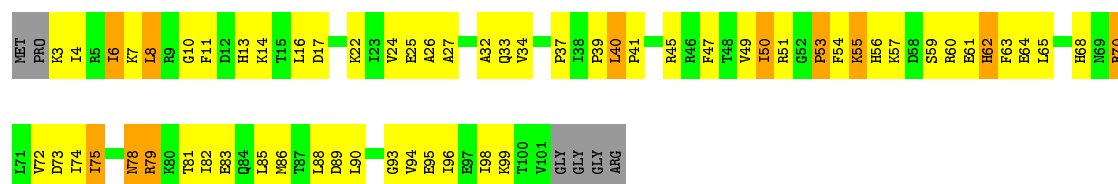
- Molecule 39: 30S ribosomal protein S10

Chain QJ: 



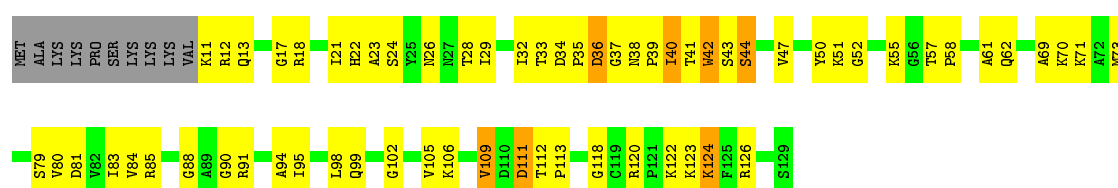
- Molecule 39: 30S ribosomal protein S10

Chain XJ: 



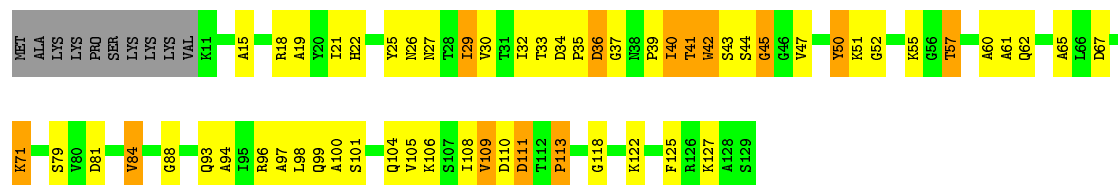
- Molecule 40: 30S ribosomal protein S11

Chain QK: 



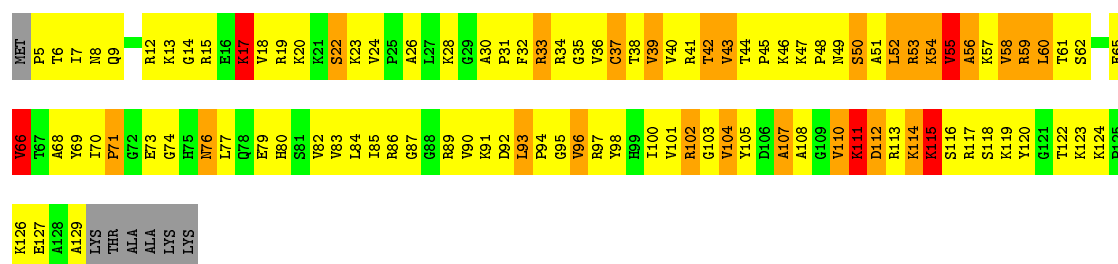
- Molecule 40: 30S ribosomal protein S11

Chain XK: 



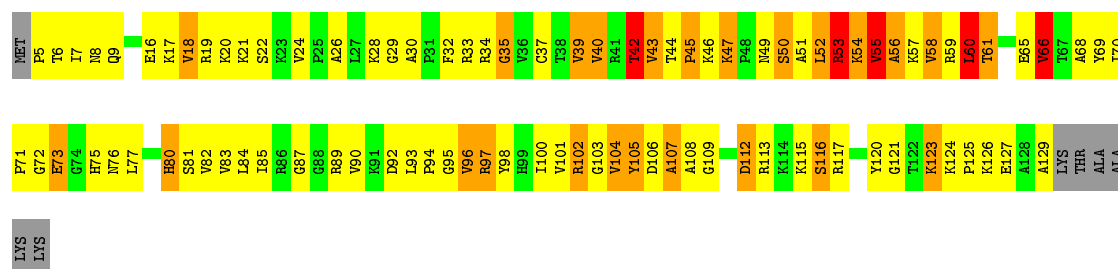
- Molecule 41: 30S ribosomal protein S12

Chain QL: 



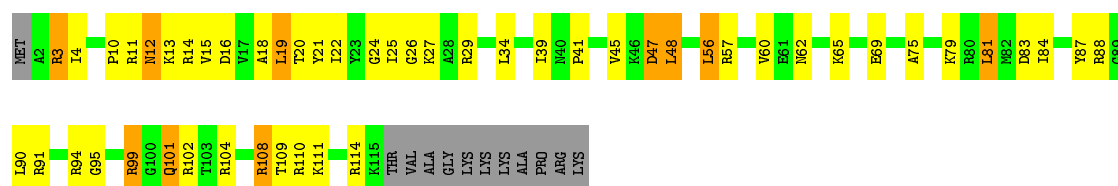
- Molecule 41: 30S ribosomal protein S12

Chain XL: 



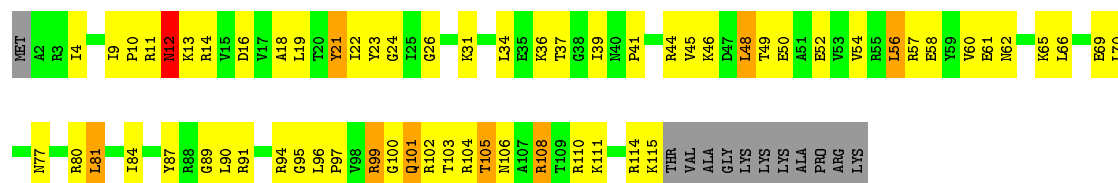
- Molecule 42: 30S ribosomal protein S13

Chain QM: 



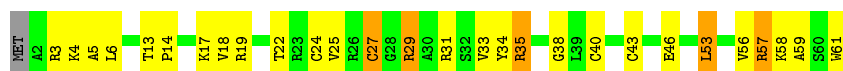
- Molecule 42: 30S ribosomal protein S13

Chain XM:



- Molecule 43: 30S ribosomal protein S14 type Z

Chain QN: 



- Molecule 43: 30S ribosomal protein S14 type Z



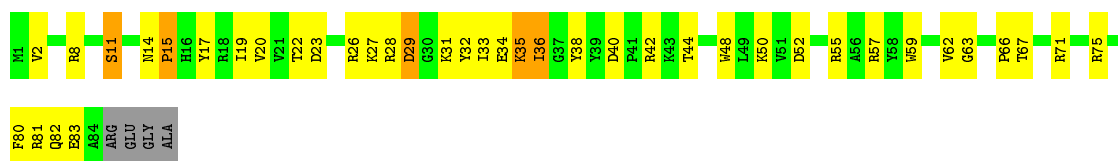
- Molecule 44: 30S ribosomal protein S15



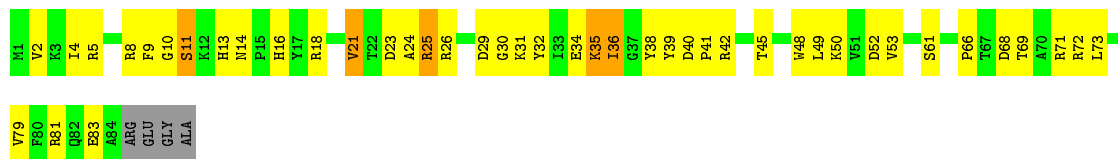
- Molecule 44: 30S ribosomal protein S15



- Molecule 45: 30S ribosomal protein S16

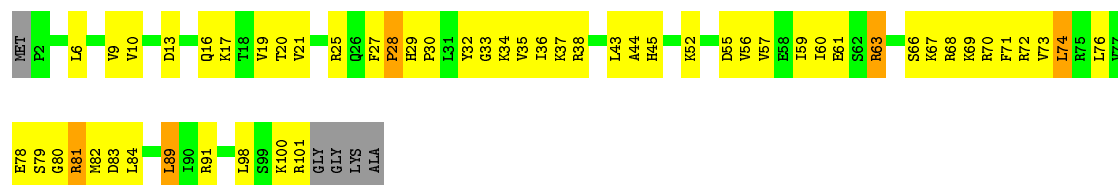


- Molecule 45: 30S ribosomal protein S16

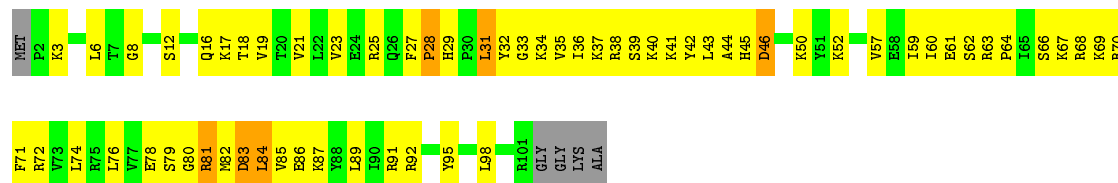


- Molecule 46: 30S ribosomal protein S17

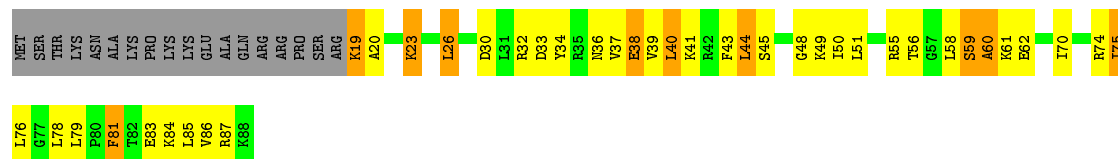




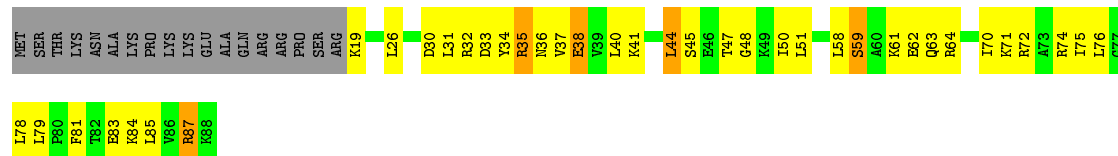
- Molecule 46: 30S ribosomal protein S17



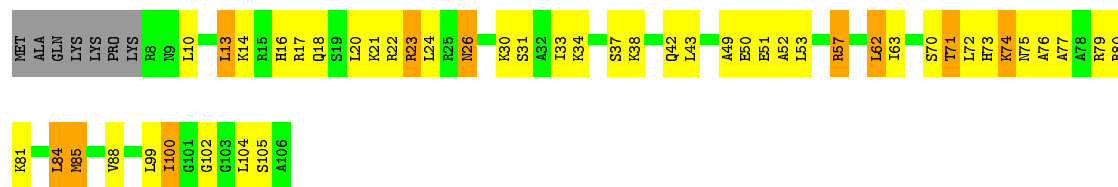
- Molecule 47: 30S ribosomal protein S18



- Molecule 47: 30S ribosomal protein S18



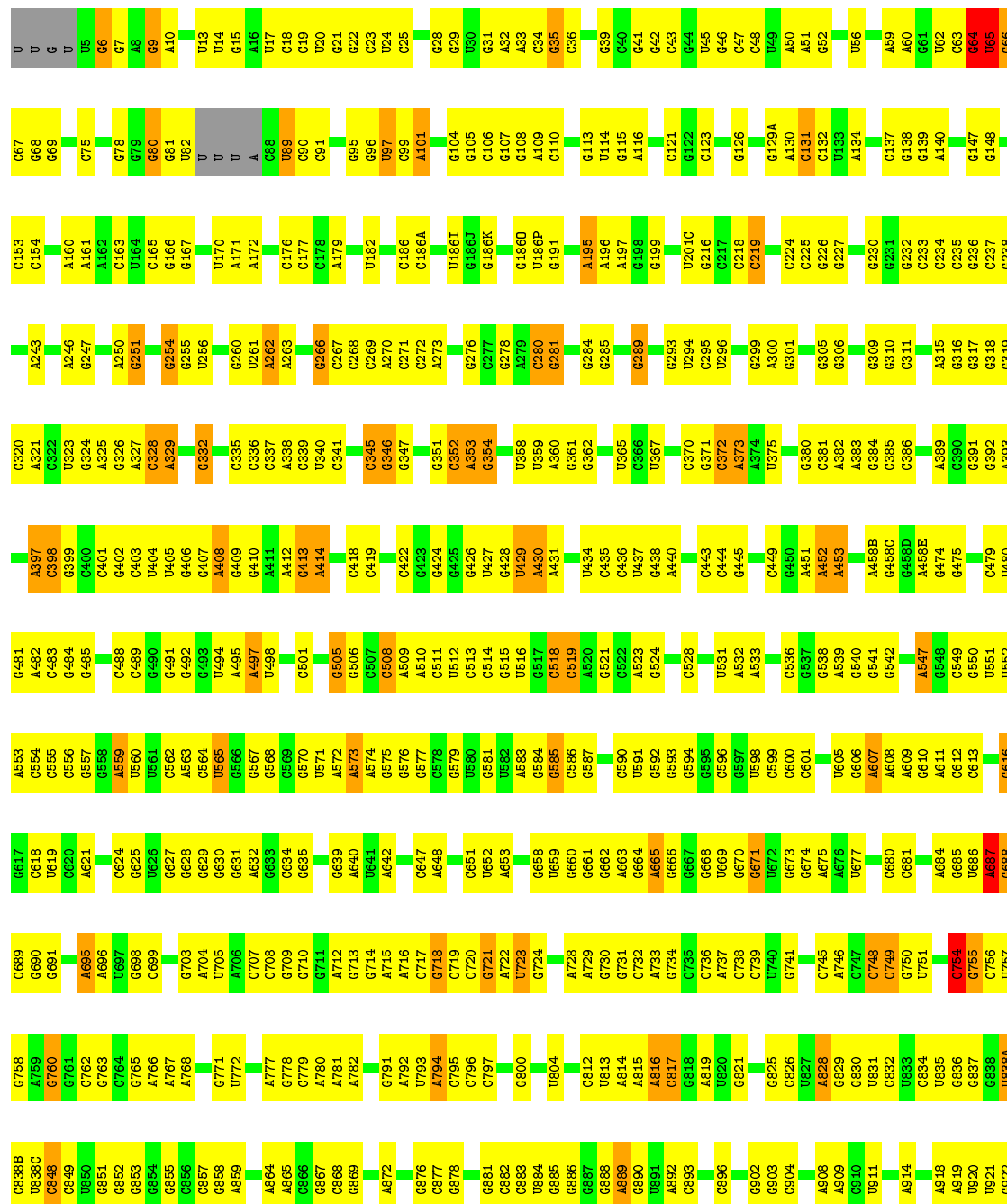
- Molecule 48: 30S ribosomal protein S20

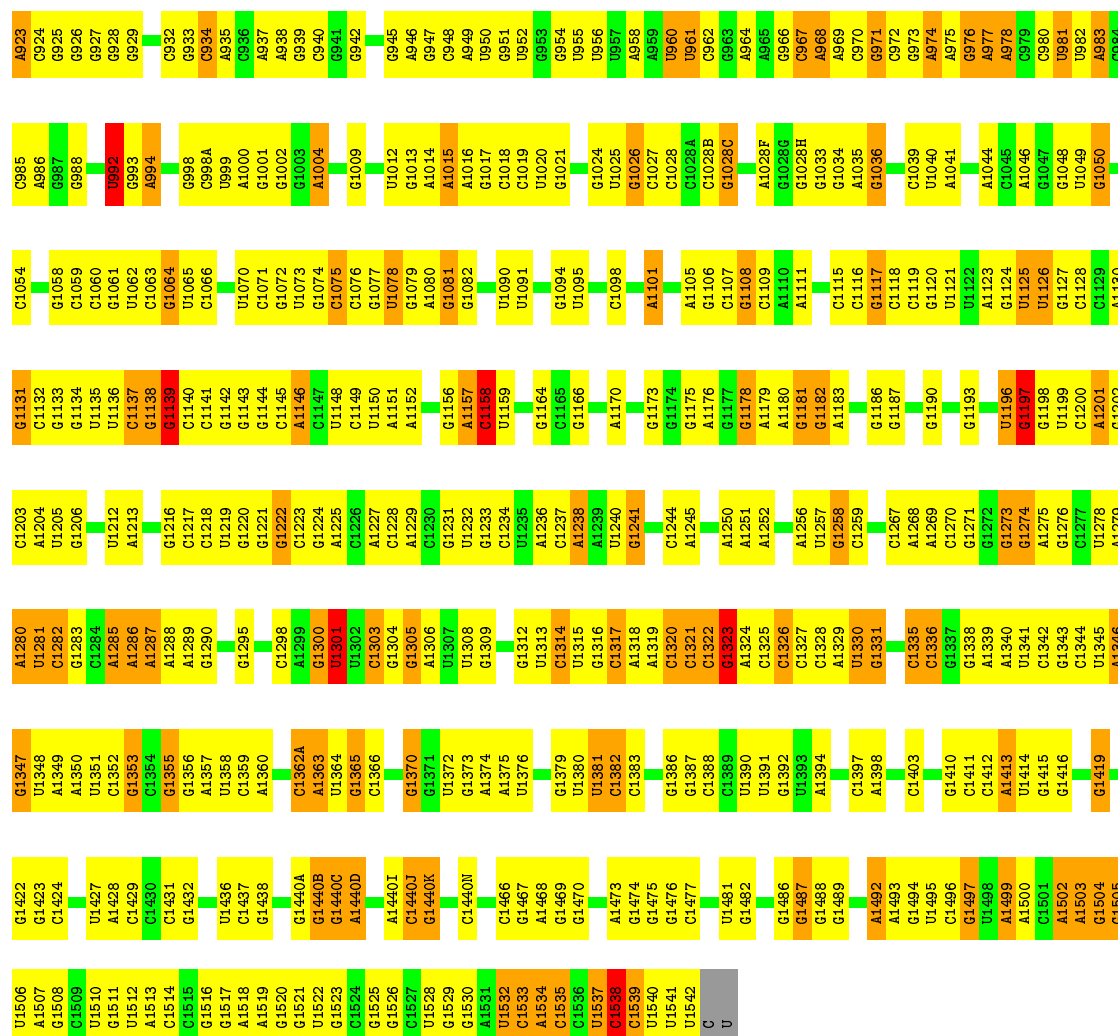


- Molecule 48: 30S ribosomal protein S20

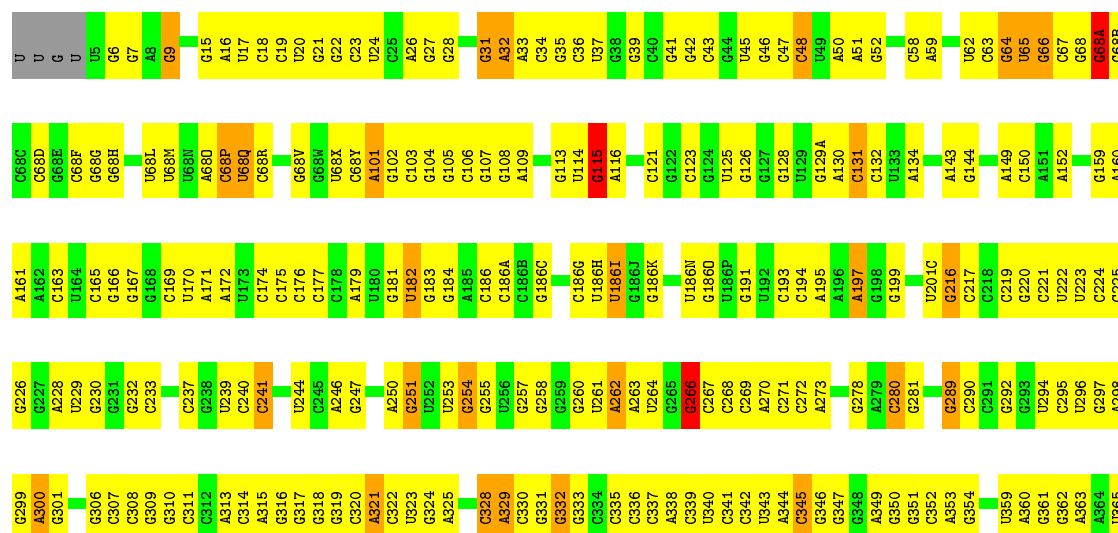


- Molecule 49: 16S rRNA





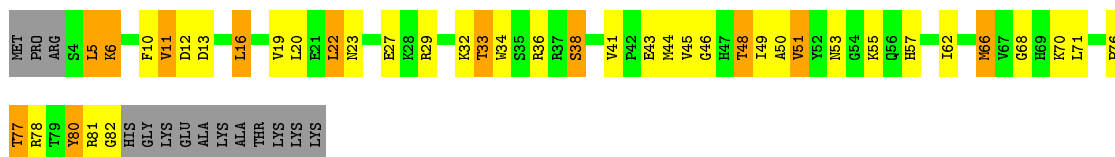
Chain XA: 34% 53% 11%



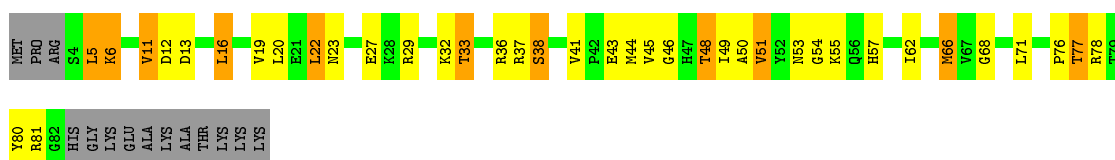
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A1394	C1328	U1257	A1183	G1108	G1033	G972	G903	G821	C745	G674	U605	A535	U437	U367
C1397	A1329	C1258	C1109	G973	G1034	G973	G906	G822	C748	A675	G606	A536	G438	C370
C1400	G1331	C1259	C1112	A974	A1035	A974	G906	C824	C749	A676	A607	A537	A440	G371
C1409	A1332	C1261	G1187	G975	G1036	G975	A908	C825	G750	G677	A609	A538	C443	C372
G1410	A1333	C1262	C1189	G976	G1038	G976	A909	C826	G751	C680	A609	A539	C444	A373
C1411	G1334	C1263	G1116	A977	C1039	A977	G910	U827	U751	C681	G610	A540	G445	A374
C1412	C1335	C1264	C1118	A978	U1040	A978	U911	U828	G752	G682	G612	A541	G446	U375
A1413	C1336	G1265	G1119	G979	G1042	G979	U911	G829	A753	G683	C613	A542		G376
U1414	G1337	G1266	C1120	U981	G1043	U981	A914	C832	C754	G684	G614	A543	A452	G377
G1414	C1342	C1267	G1120	U982	G1044	U982	A918	C833	C755	G685	C615	A453	G378	G378
G1415	G1343	A1268	U1121	A983	G1045	A983	A919	U834	G756	U686	U616		A454	C379
	C1344	A1269	U1122	C984	C1046	C984	U920	U835	G757	A687	G617		G458A	G380
G1419	U1345	C1270	G1124	C985	A1046	C985	U921	C836A	A759	G688	C618	U551	A458B	C381
C1420	G1271	C1270	U1125	A986	G1047	A986	U921	C837B	A760	G689	U619	U552	G458C	A382
G1421	G1272	A1201	U1126	G987	U1048	G987	U922	C838C	G761	G690	C620	A553	G458D	A383
G1422	A1347	G1273	G1127	U1049	G1049	U1049	A923	U838C	G762	G691	C621	A554	A458E	G384
G1423	C1274	G1274	C1128	G1050	G1050	G1050	G924	C848	G763	U692	A622	A555	G474	C385
C1424			C1129	G1051	G1051	G1051	G925	C849	C764	G693	G623	A556		G388
C1425	A1279	A1280	U1135	U1052	G1052	U1052	G926	C850	G765	G694	C624	A557	U480	
C1426	U1281	U1281	G1131	G1053	G1053	A994	G927	G851	A766	A695	G625	A558	G481	A389
U1427	C1352	C1282	G1132	C995	G1054	C995	G928	G852	A767		U626	A559	A482	
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		G1283	U1136	C988A	U1056	C988A	C930	G854	G769	A702		U561	G484	A393
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G1432	A1285	A1285	G1138	U999	G1058	U999	G932	C856	C771	A704	C634	A563		C395
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		U1219	C1145	G1003	U1062	G1003			C779	C708	G639	A567	G494	G399
	C1362		U1146	A1004	C1063	A1004	G939	A864	A780	G711	A642	A573	A495	C400
G1440B	C1362A	C1286	C1147	C1007	G1064	C1007	C940	A865	A781	A712	C643	A574	A497	C401
A1440C	A1363	C1287	U1148	C1008	U1065	C1008	G941	A866	C784	G713	C644	A575	U498	G402
G1440D	U1364	C1288	C1149	G1009	C1066	G1009	A946	G867		G714	C645	A576	G499	C403
G1440E	G1365	A1290	U1150	G1010	U1073	G1010	G947	G868	A787	A715	U646	A577	G500	U404
C1440F	C1365	A1291	A1151	G1011	G1074	G1011	C948	G869	U788	A716	C647	A578	G501	U405
C1440G	U1301	A1227	A1152	U1012	C1075	U1012	A949	U870	U789	G717	A648	A579	G407	G406
U1440H	U1302	C1228	A1157	U1013	G1076	G1013	U950	A872	A790	G718	G649	A580	A408	A407
C1440I	G1303	C1229	C1158	G1014	C1077	G1014	G951		G791	C719	G650	A581	G409	G409
G1440J	G1373	G1304	U1159	A1015	U1078	A1015	U952	C875	A792	C720	C651	A582	A510	A412
G1440K	A1374	G1305	G1160	A1016	G1079	A1016	G953	G876	U793	G721	U652	A583	A511	G413
	A1375	A1306	C1161	G1017	A1080	G1017	G954	C877	A794	A722	A653	A584	C514	A414
C1463	U1376		G1161	G1018	G1081	C1018	U955	G878		U723	G654	A585	C515	
G1464	A1377	G1309	G1166	C1019	G1082	C1019	U956	C879	G799	G727	G658	A586	C518	C422
C1465	C1378	G1310	A1167	U1020	U1083	U1020	U957	C880	G800	A728	U659	A587	C519	G423
G1466	U1380	C1237	A1169	G1021	G1084	U1021	A958	G881		A729	G660	A588	C514	G424
G1467	U1381	C1238	A1170	G1022		G1022	A959		C806	G730	G661	A589	C515	G425
G1468	U1382	A1239	G1171	G1023	G1094	G1023	U960	G888	A807	G731	G662	C590	C518	G426
G1470	C1383	U1240	C1172	U1024	U1095	U1024	U961	A889		G732	A663	C591	C519	U427
	A1384	G1241	G1173	U1025	C1096	U1025	G962	G890	C811	G733	G664	C592	C521	G428
G1476	C1385	C1242	G1174	G1026	G1097	G1026	G963		C812	A734	A665	C593	C522	U429
C1477	G1386	C1243	G1175	C1027	C1098	C1027	A964	C893	U813	G735	G666	C594	A430	A430
	G1387	C1244	A1176	G1028	G1099	G1028	A965	C896	A814	C736	G667	C595	A523	A431
G1480	C1388	A1245	G1177	C1028A	G1100	C1028A	G966	C897	A815	G737	G668	C596	G524	G524
U1481	C1389	G1323	G1178	C1028B	A1101	C1028B	C967	C899	A816	A738	G669	C597	G525	A432
G1482	A1394	C1324	A1179	G1028C	A1101	C1028C	A968	A900	C817	G739		C601		C433
A1483	U1391	C1254	A1180	G1029	A1105	G1029	A969		G818		G671	A532	A532	U434
C1484	G1392	C1326	G1181	G1029G	G1106	G1029G	C970	A901	A819	U743	U672	U603	A533	C435



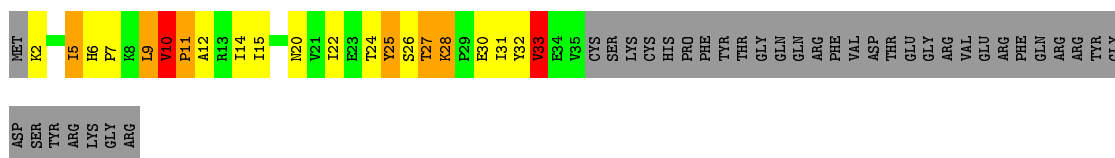
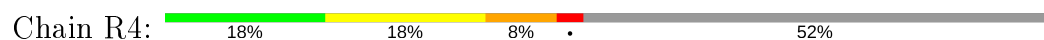
- Molecule 50: 30S ribosomal protein S19



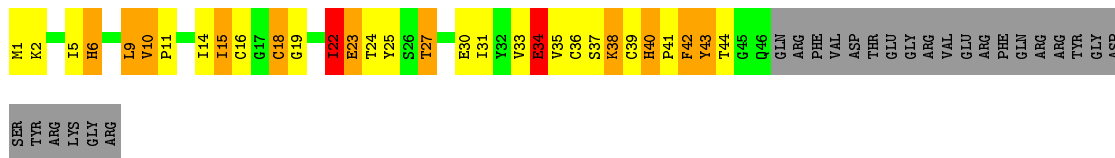
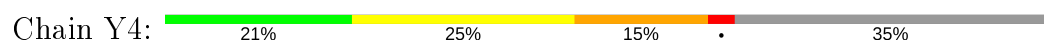
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: messenger RNA



- Molecule 52: messenger RNA

Chain QX:  63% 32% 5%

G1 G2 C3 A4 A5 G6 C7 A8 G9 G10 U11 A12 A13 A14 A15 C16 C17 C18 U19

- Molecule 53: P-site tRNA SufA6

Chain XV:  47% 37% 14%

C1 G2 U8 G9 G10 C11 G15 C16 C17 U18 G19 G20 U21 G23 A22 C24 G25 C31 G32 C35 G36 G37 G38 G39 A40 C41 G42 A43 A44 G45 G46 U49 C50 G51 C58 G59 A60 A61 U62 C63 U67 A68 C72 A75 C76 C77 A78

- Molecule 53: P-site tRNA SufA6

Chain QV:  49% 32% 14% 5%

C1 G2 U8 G9 G10 C11 A14 C16 C17 U18 G19 G20 U21 G23 A22 C24 G25 C31 G32 C35 G36 G37 G38 G39 A40 C41 G42 A43 A44 G45 G46 U49 C50 G51 A60 A61 U62 C63 U67 A68 C73 G74 A75 C76 C77 A78

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.75Å 450.05Å 626.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.60 – 3.90 49.96 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (16.60-3.90) 98.2 (49.96-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.272 , 0.316	Depositor DCC
R_{free} test set	23266 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	291660	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: ZN, MG, 1MG

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	0.31	11/69520 (0.0%)	0.97	171/108525 (0.2%)
1	YA	0.29	1/69543 (0.0%)	0.96	137/108563 (0.1%)
2	RB	0.29	0/2878	0.99	11/4490 (0.2%)
2	YB	0.29	0/2878	0.99	9/4490 (0.2%)
3	RD	0.28	0/2165	0.54	0/2919
3	YD	0.27	0/2165	0.53	0/2919
4	RE	0.29	0/1601	0.60	2/2160 (0.1%)
4	YE	0.32	1/1601 (0.1%)	0.59	1/2160 (0.0%)
5	RF	0.28	0/1620	0.55	1/2194 (0.0%)
5	YF	0.27	0/1620	0.51	0/2194
6	RG	0.28	0/1499	0.55	0/2016
6	YG	0.26	0/1499	0.51	0/2016
7	RH	0.28	0/1332	0.56	0/1802
7	YH	0.30	0/1332	0.61	1/1802 (0.1%)
8	RI	0.26	0/1151	0.61	0/1558
8	YI	0.27	0/1151	0.60	0/1558
9	RN	0.26	0/1131	0.51	0/1525
9	YN	0.26	0/1131	0.50	0/1525
10	RO	0.26	0/943	0.51	0/1269
10	YO	0.26	0/943	0.51	0/1269
11	RP	0.28	0/1162	0.65	1/1544 (0.1%)
11	YP	0.28	0/1162	0.63	0/1544
12	RQ	0.31	0/1143	0.58	0/1527
12	YQ	0.28	0/1143	0.55	0/1527
13	RR	0.26	0/982	0.55	0/1312
13	YR	0.29	0/982	0.57	0/1312
14	RS	0.27	0/892	0.58	0/1187
14	YS	0.27	0/892	0.60	0/1187
15	RT	0.35	0/1155	0.65	2/1542 (0.1%)
15	YT	0.32	0/1155	0.59	0/1542
16	RU	0.28	0/982	0.54	0/1306
16	YU	0.25	0/982	0.47	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.26	0/790	0.55	0/1057
17	YV	0.27	0/790	0.58	1/1057 (0.1%)
18	RW	0.26	0/911	0.48	0/1220
18	YW	0.26	0/911	0.51	0/1220
19	RX	0.28	0/739	0.49	0/993
19	YX	0.30	0/739	0.51	0/993
20	RY	0.31	0/798	0.61	0/1064
20	YY	0.30	0/798	0.60	0/1064
21	RZ	0.28	0/1493	0.57	0/2026
21	YZ	0.27	0/1493	0.58	1/2026 (0.0%)
22	R0	0.26	0/657	0.53	0/874
22	Y0	0.33	0/657	0.56	0/874
23	R1	0.31	0/770	0.58	0/1022
23	Y1	0.29	0/770	0.55	0/1022
24	R2	0.25	0/583	0.53	0/771
24	Y2	0.23	0/583	0.49	0/771
25	R3	0.27	0/474	0.51	0/635
25	Y3	0.22	0/474	0.44	0/635
26	R5	0.26	0/473	0.57	0/639
26	Y5	0.27	0/473	0.55	0/639
27	R6	0.27	0/431	0.63	0/575
27	Y6	0.25	0/431	0.61	0/575
28	R7	0.24	0/438	0.48	0/575
28	Y7	0.23	0/438	0.45	0/575
29	R8	0.27	0/525	0.58	0/691
29	Y8	0.33	0/525	0.60	0/691
30	R9	0.24	0/310	0.51	0/407
30	Y9	0.23	0/310	0.48	0/407
31	QB	0.28	0/1944	0.58	0/2621
31	XB	0.27	0/1944	0.59	0/2621
32	QC	0.26	0/1644	0.57	0/2216
32	XC	0.27	0/1644	0.60	0/2216
33	QD	0.45	2/1733 (0.1%)	0.70	4/2318 (0.2%)
33	XD	0.30	0/1733	0.62	0/2318
34	QE	0.28	0/1171	0.58	0/1576
34	XE	0.26	0/1171	0.58	1/1576 (0.1%)
35	QF	0.25	0/856	0.59	0/1154
35	XF	0.27	0/856	0.60	1/1154 (0.1%)
36	QG	0.25	0/1276	0.51	0/1709
36	XG	0.26	0/1276	0.51	0/1709
37	QH	0.26	0/1136	0.58	0/1527
37	XH	0.27	0/1136	0.58	0/1527
38	QI	0.29	0/1029	0.55	0/1379

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XI	0.26	0/1029	0.55	0/1379
39	QJ	0.26	0/814	0.53	0/1095
39	XJ	0.26	0/814	0.57	0/1095
40	QK	0.28	0/900	0.54	0/1213
40	XK	0.27	0/900	0.54	0/1213
41	QL	0.28	0/991	0.68	0/1327
41	XL	0.30	0/991	0.74	1/1327 (0.1%)
42	QM	0.25	0/924	0.57	0/1238
42	XM	0.29	0/924	0.64	0/1238
43	QN	0.28	0/501	0.56	0/664
43	XN	0.30	0/501	0.59	0/664
44	QO	0.24	0/745	0.55	0/992
44	XO	0.34	1/745 (0.1%)	0.55	0/992
45	QP	0.26	0/721	0.62	0/970
45	XP	0.26	0/721	0.60	0/970
46	QQ	0.28	0/847	0.61	0/1131
46	XQ	0.27	0/847	0.59	0/1131
47	QR	0.28	0/579	0.62	0/768
47	XR	0.28	0/579	0.65	0/768
48	QT	0.23	0/765	0.53	0/1007
48	XT	0.24	0/765	0.50	0/1007
49	QA	0.25	0/36347	0.90	37/56727 (0.1%)
49	XA	0.31	6/36439 (0.0%)	0.96	86/56872 (0.2%)
50	QS	0.23	0/646	0.49	0/870
50	XS	0.24	0/646	0.49	0/870
51	R4	0.34	0/267	0.63	0/362
51	Y4	0.27	0/366	0.57	0/495
52	QX	0.22	0/459	0.89	2/715 (0.3%)
52	XX	0.21	0/459	0.89	2/715 (0.3%)
53	QV	0.22	0/1839	0.87	9/2866 (0.3%)
53	XV	0.17	0/1839	0.78	2/2866 (0.1%)
All	All	0.29	22/315578 (0.0%)	0.87	483/472056 (0.1%)

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	RA	0	2
3	RD	0	1
7	RH	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	YH	0	2
11	RP	0	1
15	RT	0	1
21	YZ	0	1
23	R1	0	1
29	R8	0	1
33	QD	0	1
33	XD	0	1
49	XA	0	2
53	QV	0	1
All	All	0	17

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	XA	771	G	C1'-N9	18.11	1.75	1.48
1	RA	1558	A	C1'-N9	17.07	1.74	1.48
1	RA	1913	A	C5'-C4'	16.54	1.71	1.51
49	XA	771	G	C4'-O4'	14.31	1.64	1.45
1	RA	1463	C	C5'-C4'	12.46	1.66	1.51

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	XA	771	G	O4'-C1'-N9	26.71	129.57	108.20
1	RA	1558	A	C8-N9-C1'	-26.16	80.62	127.70
1	RA	1558	A	O4'-C1'-N9	-24.62	88.50	108.20
1	RA	1463	C	C2-N1-C1'	24.24	145.47	118.80
1	RA	1762	A	N1-C6-N6	-24.02	104.19	118.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	RA	1558	A	Sidechain
1	RA	1765	C	Sidechain
3	RD	235	GLY	Mainchain
7	RH	127	GLU	Peptide
7	RH	153	LYS	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	RA	62071	0	31249	1298	0
1	YA	62091	0	31283	1245	0
2	RB	2573	0	1299	53	0
2	YB	2573	0	1304	49	0
3	RD	2115	0	2191	68	0
3	YD	2115	0	2194	63	0
4	RE	1568	0	1632	58	0
4	YE	1568	0	1633	51	0
5	RF	1585	0	1630	48	0
5	YF	1585	0	1632	53	0
6	RG	1474	0	1535	68	0
6	YG	1474	0	1535	56	0
7	RH	1307	0	1382	54	0
7	YH	1307	0	1382	54	0
8	RI	1136	0	1223	44	0
8	YI	1136	0	1223	42	0
9	RN	1104	0	1180	33	0
9	YN	1104	0	1180	35	0
10	RO	933	0	995	13	0
10	YO	933	0	996	22	0
11	RP	1145	0	1228	54	0
11	YP	1145	0	1228	69	0
12	RQ	1122	0	1179	39	0
12	YQ	1122	0	1179	35	0
13	RR	968	0	1032	34	0
13	YR	968	0	1031	28	0
14	RS	882	0	943	33	0
14	YS	882	0	943	36	0
15	RT	1141	0	1200	39	0
15	YT	1141	0	1201	45	0
16	RU	964	0	1022	30	0
16	YU	964	0	1022	32	0
17	RV	779	0	852	22	0
17	YV	779	0	852	22	0
18	RW	900	0	964	13	0
18	YW	900	0	964	21	0
19	RX	725	0	778	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	YX	725	0	778	21	0
20	RY	785	0	877	30	0
20	YY	785	0	877	30	0
21	RZ	1461	0	1493	46	0
21	YZ	1461	0	1493	51	0
22	R0	648	0	671	18	0
22	Y0	648	0	672	18	0
23	R1	763	0	846	21	0
23	Y1	763	0	847	26	0
24	R2	581	0	629	15	0
24	Y2	581	0	629	14	0
25	R3	469	0	518	10	0
25	Y3	469	0	518	3	0
26	R5	459	0	480	25	0
26	Y5	459	0	479	25	0
27	R6	424	0	450	26	0
27	Y6	424	0	450	23	0
28	R7	430	0	480	11	0
28	Y7	430	0	480	12	0
29	R8	517	0	582	23	0
29	Y8	517	0	582	24	0
30	R9	307	0	338	7	0
30	Y9	307	0	335	5	0
31	QB	1909	0	1957	99	0
31	XB	1909	0	1957	100	0
32	QC	1620	0	1688	63	0
32	XC	1620	0	1687	74	0
33	QD	1703	0	1762	97	0
33	XD	1703	0	1765	83	0
34	QE	1155	0	1213	52	0
34	XE	1155	0	1213	47	0
35	QF	843	0	857	32	0
35	XF	843	0	857	42	0
36	QG	1257	0	1296	34	0
36	XG	1257	0	1296	56	0
37	QH	1116	0	1177	52	0
37	XH	1116	0	1177	73	0
38	QI	1010	0	1035	58	0
38	XI	1010	0	1037	55	0
39	QJ	801	0	849	51	0
39	XJ	801	0	849	46	0
40	QK	885	0	904	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	XK	885	0	904	47	0
41	QL	975	0	1062	109	0
41	XL	975	0	1061	88	0
42	QM	914	0	971	33	0
42	XM	914	0	971	54	0
43	QN	492	0	533	26	0
43	XN	492	0	533	34	0
44	QO	734	0	771	39	0
44	XO	734	0	768	27	0
45	QP	705	0	724	38	0
45	XP	705	0	725	39	0
46	QQ	834	0	903	48	0
46	XQ	834	0	904	59	0
47	QR	574	0	644	35	0
47	XR	574	0	644	40	0
48	QT	763	0	861	33	0
48	XT	763	0	861	44	0
49	QA	32472	0	16387	843	0
49	XA	32554	0	16414	909	0
50	QS	633	0	655	28	0
50	XS	633	0	655	28	0
51	R4	262	0	272	25	0
51	Y4	357	0	362	29	0
52	QX	409	0	209	49	0
52	XX	409	0	209	53	0
53	QV	1670	0	845	49	0
53	XV	1670	0	845	30	0
54	QA	131	0	0	0	0
54	QC	1	0	0	0	0
54	QD	3	0	0	0	0
54	QE	1	0	0	0	0
54	QL	3	0	0	0	0
54	QP	2	0	0	0	0
54	QQ	2	0	0	0	0
54	QT	2	0	0	0	0
54	R0	2	0	0	0	0
54	R1	3	0	0	0	0
54	R3	1	0	0	0	0
54	R6	1	0	0	0	0
54	R8	3	0	0	0	0
54	RA	562	0	0	0	0
54	RB	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	RD	10	0	0	0	0
54	RE	7	0	0	0	0
54	RF	4	0	0	0	0
54	RI	1	0	0	0	0
54	RO	2	0	0	0	0
54	RQ	2	0	0	0	0
54	RR	3	0	0	0	0
54	RT	3	0	0	0	0
54	RU	1	0	0	0	0
54	RX	2	0	0	0	0
54	RY	1	0	0	0	0
54	XA	128	0	0	0	0
54	XC	1	0	0	0	0
54	XD	1	0	0	0	0
54	XE	1	0	0	0	0
54	XK	1	0	0	0	0
54	XL	2	0	0	0	0
54	XM	1	0	0	0	0
54	XO	1	0	0	0	0
54	XP	1	0	0	0	0
54	Y0	1	0	0	0	0
54	Y1	1	0	0	0	0
54	Y8	1	0	0	0	0
54	YA	379	0	0	0	0
54	YB	10	0	0	0	0
54	YD	4	0	0	0	0
54	YE	5	0	0	0	0
54	YI	1	0	0	0	0
54	YP	1	0	0	0	0
54	YQ	1	0	0	0	0
54	YR	1	0	0	0	0
54	YT	2	0	0	0	0
54	YU	1	0	0	0	0
54	YX	1	0	0	0	0
54	YY	1	0	0	0	0
55	QD	2	0	0	0	0
55	XD	1	0	0	0	0
55	Y9	1	0	0	0	0
All	All	291660	0	197069	7411	0

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 15.

The worst 5 of 7411 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)
49:QA:1339:A:C2	53:QV:32:G:H1'	1.41	1.52
1:RA:1558:A:C1'	1:RA:1558:A:N9	1.74	1.48
49:XA:771:G:C1'	49:XA:771:G:N9	1.75	1.46
49:XA:1531:A:C5	49:XA:1532:U:O4	1.70	1.42
49:XA:771:G:C4'	49:XA:771:G:O4'	1.64	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	270/276 (98%)	235 (87%)	28 (10%)	7 (3%)	5	35
3	YD	270/276 (98%)	234 (87%)	30 (11%)	6 (2%)	6	38
4	RE	203/206 (98%)	158 (78%)	29 (14%)	16 (8%)	1	15
4	YE	203/206 (98%)	154 (76%)	33 (16%)	16 (8%)	1	15
5	RF	200/210 (95%)	173 (86%)	21 (10%)	6 (3%)	4	33
5	YF	200/210 (95%)	177 (88%)	18 (9%)	5 (2%)	5	36
6	RG	179/182 (98%)	149 (83%)	20 (11%)	10 (6%)	2	21
6	YG	179/182 (98%)	151 (84%)	18 (10%)	10 (6%)	2	21
7	RH	168/180 (93%)	129 (77%)	22 (13%)	17 (10%)	0	10
7	YH	168/180 (93%)	126 (75%)	25 (15%)	17 (10%)	0	10
8	RI	144/148 (97%)	109 (76%)	25 (17%)	10 (7%)	1	17
8	YI	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	2	21
9	RN	136/140 (97%)	113 (83%)	15 (11%)	8 (6%)	1	20
9	YN	136/140 (97%)	114 (84%)	13 (10%)	9 (7%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	RO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	57
10	YO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	57
11	RP	148/150 (99%)	105 (71%)	32 (22%)	11 (7%)	1	16
11	YP	148/150 (99%)	106 (72%)	32 (22%)	10 (7%)	1	18
12	RQ	139/141 (99%)	104 (75%)	21 (15%)	14 (10%)	0	10
12	YQ	139/141 (99%)	105 (76%)	17 (12%)	17 (12%)	0	6
13	RR	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	43
13	YR	116/118 (98%)	104 (90%)	9 (8%)	3 (3%)	5	35
14	RS	109/112 (97%)	81 (74%)	19 (17%)	9 (8%)	1	14
14	YS	109/112 (97%)	83 (76%)	17 (16%)	9 (8%)	1	14
15	RT	135/146 (92%)	109 (81%)	19 (14%)	7 (5%)	2	23
15	YT	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	2	25
16	RU	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	43
16	YU	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	43
17	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	20
17	YV	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	1	20
18	RW	111/113 (98%)	105 (95%)	4 (4%)	2 (2%)	8	42
18	YW	111/113 (98%)	105 (95%)	4 (4%)	2 (2%)	8	42
19	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
19	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
20	RY	100/110 (91%)	73 (73%)	16 (16%)	11 (11%)	0	8
20	YY	100/110 (91%)	73 (73%)	17 (17%)	10 (10%)	0	10
21	RZ	181/206 (88%)	133 (74%)	29 (16%)	19 (10%)	0	9
21	YZ	181/206 (88%)	139 (77%)	26 (14%)	16 (9%)	1	13
22	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
22	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
23	R1	95/98 (97%)	75 (79%)	15 (16%)	5 (5%)	2	22
23	Y1	95/98 (97%)	75 (79%)	15 (16%)	5 (5%)	2	22
24	R2	67/72 (93%)	58 (87%)	4 (6%)	5 (8%)	1	16
24	Y2	67/72 (93%)	58 (87%)	4 (6%)	5 (8%)	1	16
25	R3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	42
26	R5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	8	42
26	Y5	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	3	30
27	R6	47/54 (87%)	21 (45%)	18 (38%)	8 (17%)	0	3
27	Y6	47/54 (87%)	24 (51%)	17 (36%)	6 (13%)	0	5
28	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	39
28	Y7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	39
29	R8	62/65 (95%)	53 (86%)	5 (8%)	4 (6%)	1	19
29	Y8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	24
30	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
30	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	QB	233/256 (91%)	181 (78%)	38 (16%)	14 (6%)	1	20
31	XB	233/256 (91%)	190 (82%)	31 (13%)	12 (5%)	2	23
32	QC	205/239 (86%)	152 (74%)	33 (16%)	20 (10%)	0	10
32	XC	205/239 (86%)	157 (77%)	34 (17%)	14 (7%)	1	18
33	QD	206/209 (99%)	153 (74%)	40 (19%)	13 (6%)	1	19
33	XD	206/209 (99%)	149 (72%)	41 (20%)	16 (8%)	1	15
34	QE	149/162 (92%)	128 (86%)	17 (11%)	4 (3%)	5	35
34	XE	149/162 (92%)	123 (83%)	18 (12%)	8 (5%)	2	22
35	QF	99/101 (98%)	80 (81%)	15 (15%)	4 (4%)	3	27
35	XF	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	2	23
36	QG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	5	35
36	XG	153/156 (98%)	127 (83%)	18 (12%)	8 (5%)	2	23
37	QH	136/138 (99%)	105 (77%)	25 (18%)	6 (4%)	2	25
37	XH	136/138 (99%)	106 (78%)	24 (18%)	6 (4%)	2	25
38	QI	125/128 (98%)	106 (85%)	16 (13%)	3 (2%)	6	37
38	XI	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	4	32
39	QJ	97/105 (92%)	77 (79%)	15 (16%)	5 (5%)	2	23
39	XJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	3	27
40	QK	117/129 (91%)	86 (74%)	22 (19%)	9 (8%)	1	16
40	XK	117/129 (91%)	84 (72%)	23 (20%)	10 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QL	123/132 (93%)	44 (36%)	47 (38%)	32 (26%)	0	1
41	XL	123/132 (93%)	47 (38%)	44 (36%)	32 (26%)	0	1
42	QM	112/126 (89%)	95 (85%)	11 (10%)	6 (5%)	2	22
42	XM	112/126 (89%)	96 (86%)	10 (9%)	6 (5%)	2	22
43	QN	58/61 (95%)	44 (76%)	11 (19%)	3 (5%)	2	23
43	XN	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	9
44	QO	86/89 (97%)	74 (86%)	9 (10%)	3 (4%)	3	30
44	XO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	13	49
45	QP	82/88 (93%)	62 (76%)	13 (16%)	7 (8%)	1	13
45	XP	82/88 (93%)	62 (76%)	14 (17%)	6 (7%)	1	16
46	QQ	98/105 (93%)	80 (82%)	17 (17%)	1 (1%)	15	52
46	XQ	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	4	32
47	QR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	16
47	XR	68/88 (77%)	54 (79%)	11 (16%)	3 (4%)	2	25
48	QT	97/106 (92%)	81 (84%)	13 (13%)	3 (3%)	4	32
48	XT	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	7	39
50	QS	77/93 (83%)	43 (56%)	25 (32%)	9 (12%)	0	6
50	XS	77/93 (83%)	43 (56%)	25 (32%)	9 (12%)	0	6
51	R4	32/71 (45%)	16 (50%)	13 (41%)	3 (9%)	0	12
51	Y4	44/71 (62%)	22 (50%)	11 (25%)	11 (25%)	0	1
All	All	11338/12074 (94%)	9058 (80%)	1601 (14%)	679 (6%)	1	20

5 of 679 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	RD	26	LYS
3	RD	122	ASP
3	RD	242	ARG
4	RE	22	PRO
4	RE	53	PRO

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%)	184 (86%)	30 (14%)	3	21
3	YD	214/218 (98%)	187 (87%)	27 (13%)	4	23
4	RE	165/166 (99%)	137 (83%)	28 (17%)	2	14
4	YE	165/166 (99%)	142 (86%)	23 (14%)	3	21
5	RF	161/166 (97%)	147 (91%)	14 (9%)	10	37
5	YF	161/166 (97%)	145 (90%)	16 (10%)	8	31
6	RG	155/156 (99%)	141 (91%)	14 (9%)	9	36
6	YG	155/156 (99%)	135 (87%)	20 (13%)	4	23
7	RH	142/148 (96%)	126 (89%)	16 (11%)	6	27
7	YH	142/148 (96%)	123 (87%)	19 (13%)	4	22
8	RI	122/124 (98%)	99 (81%)	23 (19%)	1	10
8	YI	122/124 (98%)	102 (84%)	20 (16%)	2	15
9	RN	117/119 (98%)	102 (87%)	15 (13%)	4	23
9	YN	117/119 (98%)	103 (88%)	14 (12%)	5	25
10	RO	100/100 (100%)	92 (92%)	8 (8%)	12	41
10	YO	100/100 (100%)	91 (91%)	9 (9%)	9	36
11	RP	116/116 (100%)	88 (76%)	28 (24%)	0	5
11	YP	116/116 (100%)	92 (79%)	24 (21%)	1	7
12	RQ	111/111 (100%)	97 (87%)	14 (13%)	4	23
12	YQ	111/111 (100%)	98 (88%)	13 (12%)	5	26
13	RR	101/101 (100%)	89 (88%)	12 (12%)	5	25
13	YR	101/101 (100%)	90 (89%)	11 (11%)	6	28
14	RS	87/88 (99%)	72 (83%)	15 (17%)	2	14
14	YS	87/88 (99%)	75 (86%)	12 (14%)	3	21
15	RT	120/127 (94%)	107 (89%)	13 (11%)	6	29
15	YT	120/127 (94%)	102 (85%)	18 (15%)	3	18
16	RU	93/94 (99%)	82 (88%)	11 (12%)	5	25
16	YU	93/94 (99%)	84 (90%)	9 (10%)	8	32
17	RV	82/82 (100%)	70 (85%)	12 (15%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	YV	82/82 (100%)	69 (84%)	13 (16%)	2	17
18	RW	92/92 (100%)	78 (85%)	14 (15%)	3	17
18	YW	92/92 (100%)	79 (86%)	13 (14%)	3	21
19	RX	74/78 (95%)	64 (86%)	10 (14%)	4	22
19	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18
20	RY	85/91 (93%)	66 (78%)	19 (22%)	1	6
20	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
21	RZ	162/179 (90%)	140 (86%)	22 (14%)	3	22
21	YZ	162/179 (90%)	139 (86%)	23 (14%)	3	20
22	R0	65/67 (97%)	60 (92%)	5 (8%)	13	42
22	Y0	65/67 (97%)	63 (97%)	2 (3%)	40	64
23	R1	82/83 (99%)	77 (94%)	5 (6%)	18	48
23	Y1	82/83 (99%)	75 (92%)	7 (8%)	10	39
24	R2	64/67 (96%)	58 (91%)	6 (9%)	8	33
24	Y2	64/67 (96%)	52 (81%)	12 (19%)	1	11
25	R3	51/52 (98%)	46 (90%)	5 (10%)	8	31
25	Y3	51/52 (98%)	48 (94%)	3 (6%)	19	49
26	R5	51/52 (98%)	40 (78%)	11 (22%)	1	7
26	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
27	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
27	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
28	R7	42/42 (100%)	38 (90%)	4 (10%)	8	33
28	Y7	42/42 (100%)	38 (90%)	4 (10%)	8	33
29	R8	54/55 (98%)	45 (83%)	9 (17%)	2	15
29	Y8	54/55 (98%)	42 (78%)	12 (22%)	1	6
30	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
30	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49
31	QB	203/220 (92%)	170 (84%)	33 (16%)	2	16
31	XB	203/220 (92%)	169 (83%)	34 (17%)	2	15
32	QC	161/188 (86%)	141 (88%)	20 (12%)	4	24
32	XC	161/188 (86%)	136 (84%)	25 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	QD	180/181 (99%)	154 (86%)	26 (14%)	3	20
33	XD	180/181 (99%)	155 (86%)	25 (14%)	3	21
34	QE	116/123 (94%)	100 (86%)	16 (14%)	3	21
34	XE	116/123 (94%)	98 (84%)	18 (16%)	2	17
35	QF	90/90 (100%)	73 (81%)	17 (19%)	1	10
35	XF	90/90 (100%)	75 (83%)	15 (17%)	2	15
36	QG	126/127 (99%)	111 (88%)	15 (12%)	5	25
36	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
37	QH	119/119 (100%)	101 (85%)	18 (15%)	3	18
37	XH	119/119 (100%)	102 (86%)	17 (14%)	3	20
38	QI	98/99 (99%)	89 (91%)	9 (9%)	9	34
38	XI	98/99 (99%)	83 (85%)	15 (15%)	2	17
39	QJ	89/92 (97%)	74 (83%)	15 (17%)	2	14
39	XJ	89/92 (97%)	72 (81%)	17 (19%)	1	10
40	QK	90/99 (91%)	83 (92%)	7 (8%)	12	41
40	XK	90/99 (91%)	80 (89%)	10 (11%)	6	27
41	QL	104/109 (95%)	83 (80%)	21 (20%)	1	8
41	XL	104/109 (95%)	85 (82%)	19 (18%)	1	11
42	QM	92/101 (91%)	80 (87%)	12 (13%)	4	23
42	XM	92/101 (91%)	75 (82%)	17 (18%)	1	11
43	QN	49/50 (98%)	42 (86%)	7 (14%)	3	20
43	XN	49/50 (98%)	36 (74%)	13 (26%)	0	4
44	QO	79/80 (99%)	60 (76%)	19 (24%)	0	5
44	XO	79/80 (99%)	71 (90%)	8 (10%)	7	30
45	QP	72/74 (97%)	71 (99%)	1 (1%)	67	81
45	XP	72/74 (97%)	65 (90%)	7 (10%)	8	32
46	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	33
46	XQ	95/97 (98%)	84 (88%)	11 (12%)	5	26
47	QR	61/77 (79%)	49 (80%)	12 (20%)	1	9
47	XR	61/77 (79%)	55 (90%)	6 (10%)	8	31
48	QT	76/82 (93%)	63 (83%)	13 (17%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	XT	76/82 (93%)	60 (79%)	16 (21%)	1	7
50	QS	69/80 (86%)	55 (80%)	14 (20%)	1	8
50	XS	69/80 (86%)	55 (80%)	14 (20%)	1	8
51	R4	30/63 (48%)	20 (67%)	10 (33%)	0	1
51	Y4	41/63 (65%)	32 (78%)	9 (22%)	1	6
All	All	9589/10022 (96%)	8239 (86%)	1350 (14%)	3	21

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	YV	7	THR
31	QB	36	ARG
43	XN	40	CYS
18	YW	67	ASP
22	Y0	36	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
15	YT	58	ASN
31	QB	16	HIS
32	XC	104	GLN
7	YH	147	ASN
13	YR	24	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2878/2915 (98%)	573 (19%)	52 (1%)
1	YA	2880/2915 (98%)	590 (20%)	55 (1%)
2	RB	119/122 (97%)	19 (15%)	2 (1%)
2	YB	119/122 (97%)	20 (16%)	2 (1%)
49	QA	1509/1521 (99%)	296 (19%)	15 (0%)
49	XA	1514/1521 (99%)	288 (19%)	19 (1%)
52	QX	18/19 (94%)	7 (38%)	1 (5%)
52	XX	18/19 (94%)	7 (38%)	1 (5%)
53	QV	77/78 (98%)	27 (35%)	4 (5%)
53	XV	77/78 (98%)	26 (33%)	5 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9209/9310 (98%)	1853 (20%)	156 (1%)

5 of 1853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	9	U
1	RA	15	G
1	RA	28	A
1	RA	34	C
1	RA	35	G

5 of 156 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	653	A
1	YA	1558	A
49	XA	1537	U
1	YA	752	A
1	YA	1022	G

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
53	1MG	QV	38	53	18,26,27	1.19	2 (11%)	19,39,42	1.72	3 (15%)
53	1MG	XV	38	53	18,26,27	1.20	2 (11%)	19,39,42	1.73	3 (15%)

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	38	53	-	3/3/25/26	0/3/3/3
53	1MG	XV	38	53	-	3/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	38	1MG	C6-C5	3.93	1.47	1.41
53	QV	38	1MG	C6-C5	3.86	1.47	1.41
53	XV	38	1MG	C5-C4	2.31	1.47	1.40
53	QV	38	1MG	C5-C4	2.30	1.47	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	XV	38	1MG	C2-N3-C4	5.90	122.10	115.36
53	QV	38	1MG	C2-N3-C4	5.89	122.08	115.36
53	XV	38	1MG	C6-C5-C4	-2.51	118.35	119.96
53	QV	38	1MG	C4-C5-N7	-2.47	106.83	109.40
53	QV	38	1MG	C6-C5-C4	-2.46	118.38	119.96

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	QV	38	1MG	C4'-C5'-O5'-P
53	QV	38	1MG	O4'-C4'-C5'-O5'
53	XV	38	1MG	C4'-C5'-O5'-P
53	XV	38	1MG	O4'-C4'-C5'-O5'
53	QV	38	1MG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	QV	38	1MG	1	0
53	XV	38	1MG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1319 ligands modelled in this entry, 1319 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	RA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RA	1052:C	O3'	1053:C	P	3.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.