



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 11:48 PM EDT

PDB ID : 6NDK
Title : Structure of ASLSufA6 A37.5 bound to the 70S A site
Authors : Nguyen, H.T.; Hoffer, E.D.; Dunham, C.M.
Deposited on : 2018-12-13
Resolution : 3.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

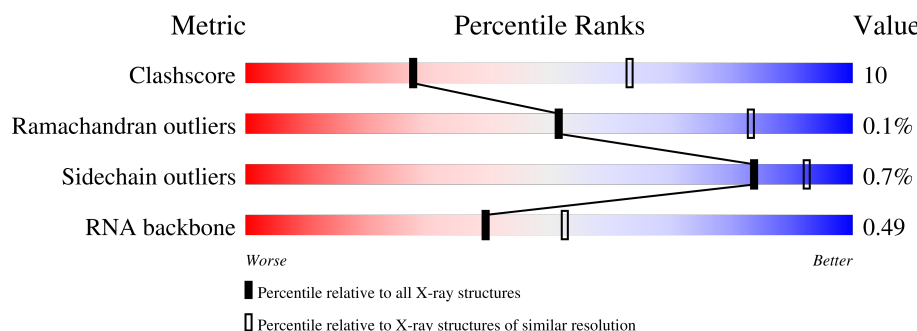
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	
1	XA	1521	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	










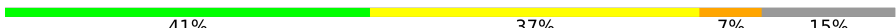
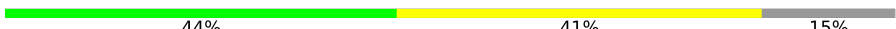
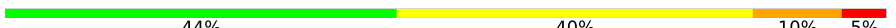




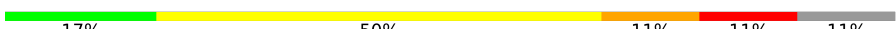
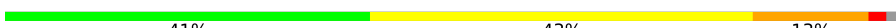

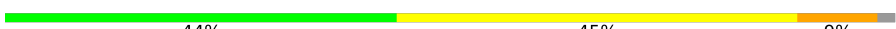





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Mol	Chain	Length	Quality of chain
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	

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Mol	Chain	Length	Quality of chain
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	26	
23	XX	26	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	

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Mol	Chain	Length	Quality of chain
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	

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Mol	Chain	Length	Quality of chain
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	

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Mol	Chain	Length	Quality of chain
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	ZA	3	
56	ZB	3	

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	MG	QN	101	-	-	X	-
57	MG	RB	203	-	-	X	-
57	MG	RD	303	-	-	X	-
58	SF4	QD	303	-	-	X	-
58	SF4	XD	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
1	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
5	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	XF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			
11	XK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
12	XL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	XM	114	Total	C	N	O	S	0	0	0
			916	566	189	159	2			

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

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

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

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			
16	XP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			743	458	159	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			759	469	162	126	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called P-site tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	11	Total	C	N	O	P	0	0	0
			233	105	43	74	11			

- Molecule 24 is a RNA chain called A-site ASLSufA6 A37.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			301	134	55	98	14			
24	XY	16	Total	C	N	O	P	0	0	0
			341	153	63	110	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2870	Total	C	N	O	P	0	0	0
			61819	27519	11565	19867	2868			
25	YA	2870	Total	C	N	O	P	0	0	0
			61822	27520	11565	19869	2868			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RD	275	Total	C	N	O	S	0	0	0
			2144	1353	428	360	3			
27	YD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
33	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
35	YP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
38	YS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	YT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	196	Total	C	N	O	S	0	0	0
			1552	988	273	288	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
46	Y0	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
48	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	Y3	59	Total	C	N	O	0	0	0
			468	298	90	80			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	58	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	124	Total	Mg	0	0
			124	124		
57	QC	1	Total	Mg	0	0
			1	1		
57	QD	2	Total	Mg	0	0
			2	2		
57	QE	2	Total	Mg	0	0
			2	2		
57	QL	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QM	2	Total 2	Mg 2	0	0
57	QN	2	Total 2	Mg 2	0	0
57	QO	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	RA	414	Total 414	Mg 414	0	0
57	RB	8	Total 8	Mg 8	0	0
57	RD	5	Total 5	Mg 5	0	0
57	RE	5	Total 5	Mg 5	0	0
57	RF	5	Total 5	Mg 5	0	0
57	RN	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RV	1	Total 1	Mg 1	0	0
57	RW	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	RZ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0

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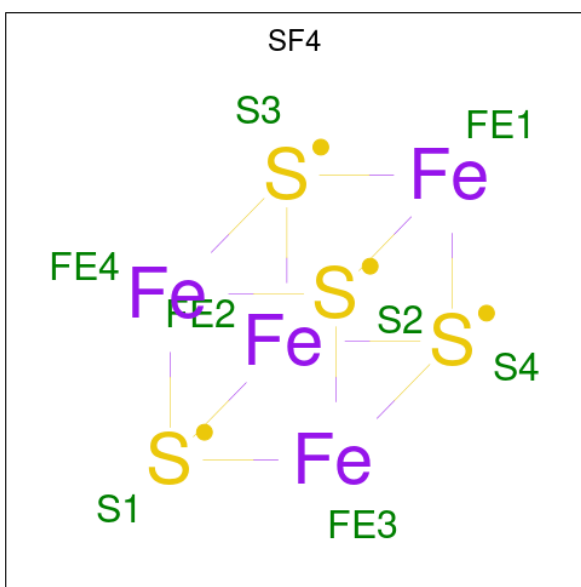
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R5	1	Total 1	Mg 1	0	0
57	R6	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	XA	128	Total 128	Mg 128	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XK	2	Total 2	Mg 2	0	0
57	XN	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	544	Total 544	Mg 544	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	8	Total 8	Mg 8	0	0
57	YE	7	Total 7	Mg 7	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	YQ	2	Total 2	Mg 2	0	0
57	YR	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YT	1	Total 1	Mg 1	0	0
57	YU	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YW	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y1	3	Total 3	Mg 3	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y6	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

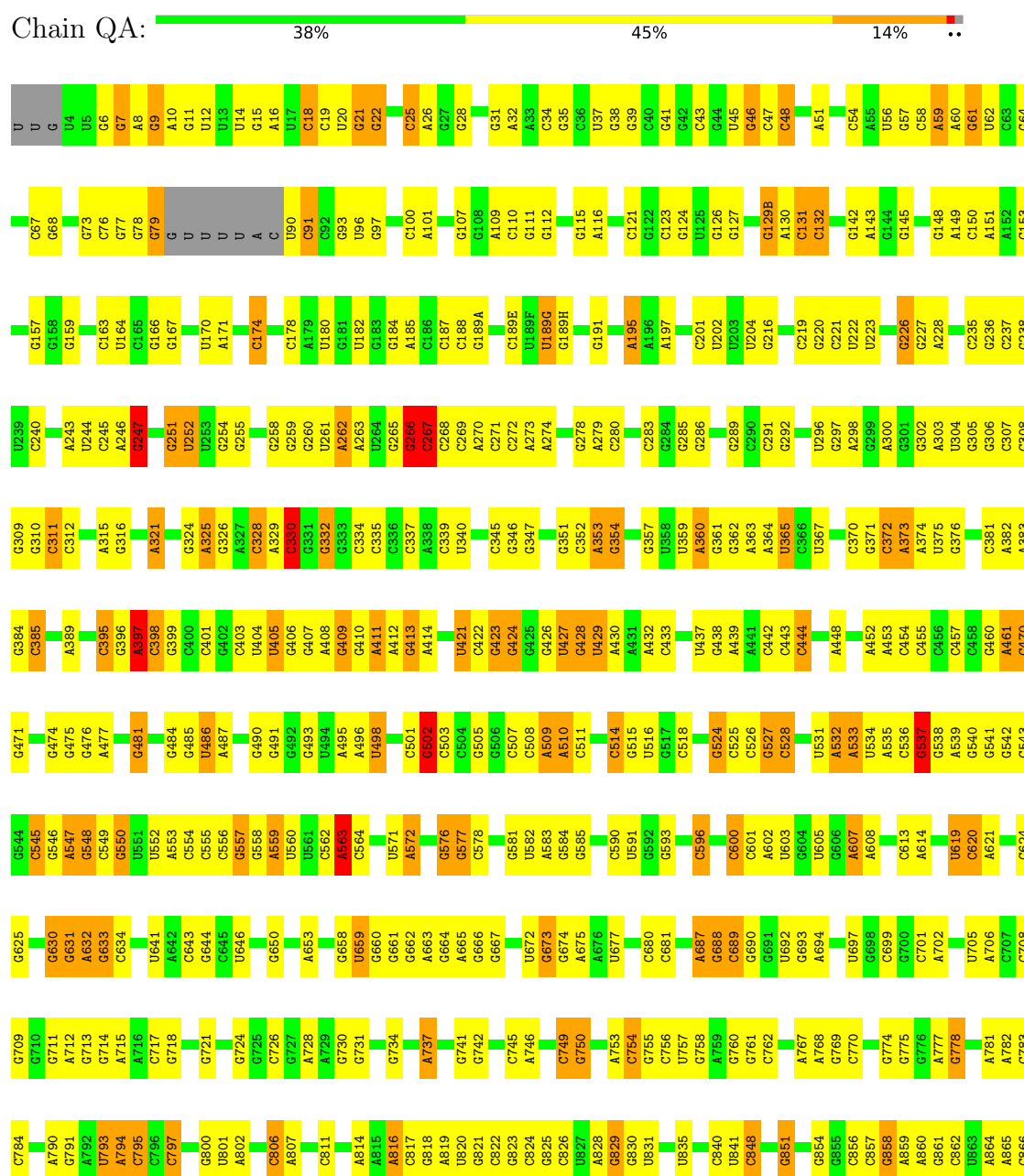
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		

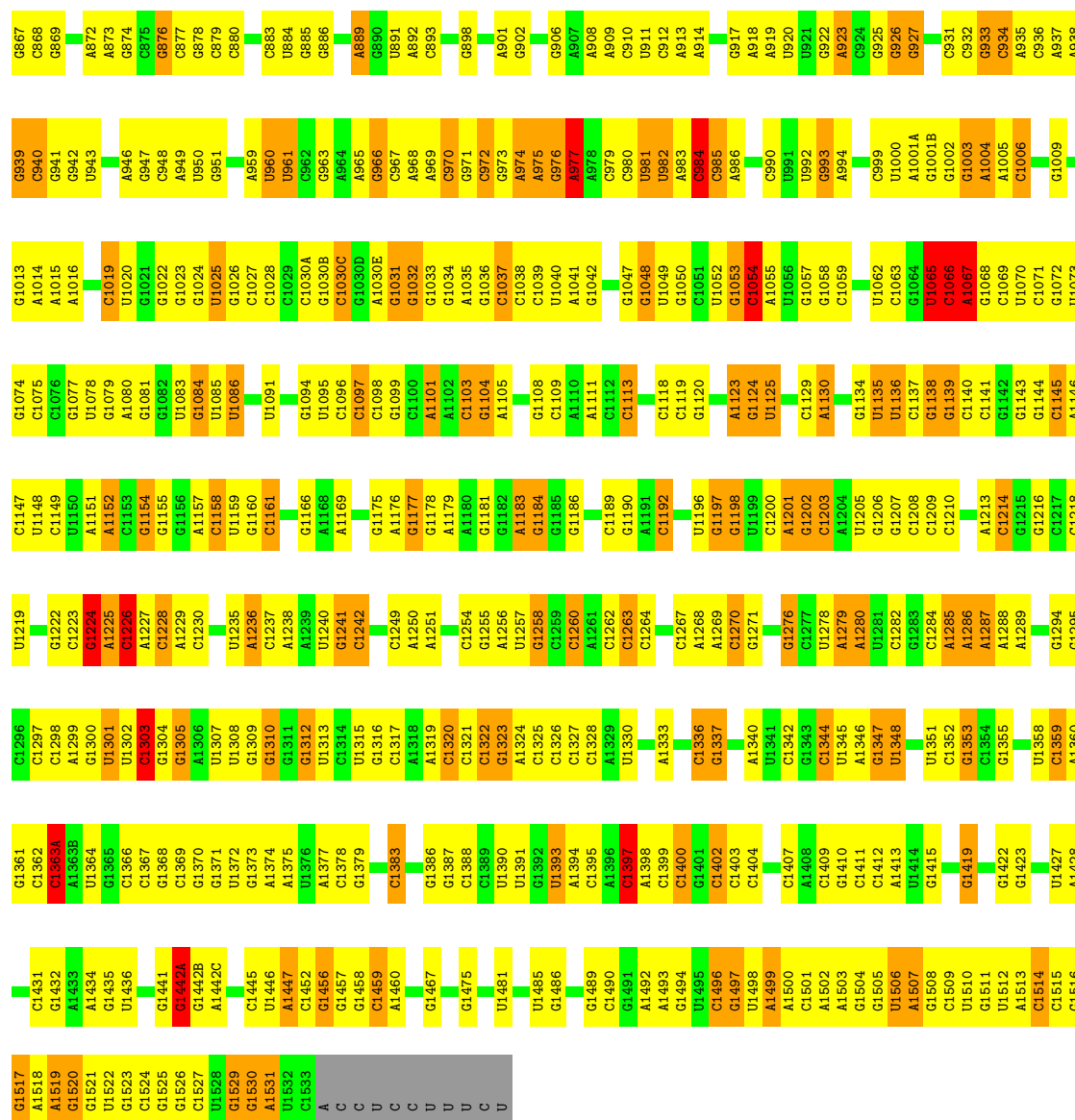
3 Residue-property plots

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.

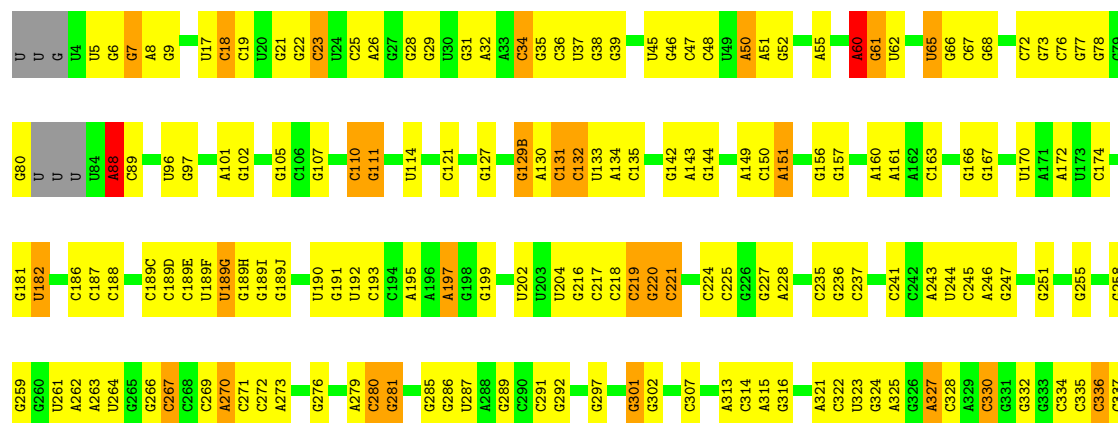
• Molecule 1: 16S rRNA





• Molecule 1: 16S rRNA

Chain XA: 43% 43% 12% ..

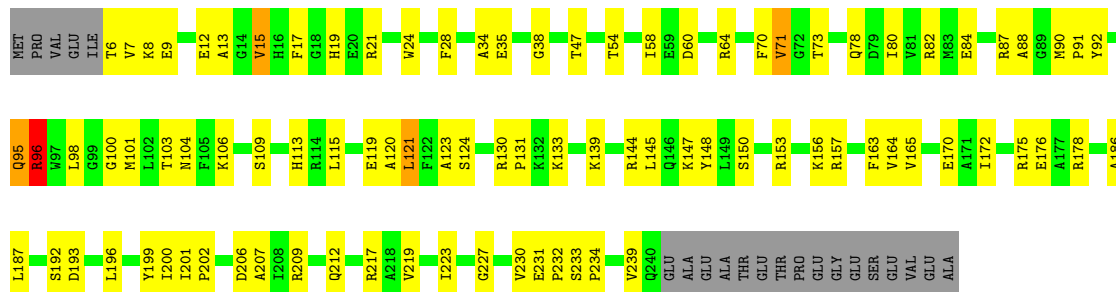


C1430	G1361	A1287	C1218	U1126	C1084	U981	G902	C811	A737	A653	C562	U486	U404	A338
C1431	C1362	A1288	U1219	G1127	A1085	U982	G903	C812	C738	G661	A563	A487	U405	C339
C1432	C1363A	A1289	G1220	C1128	G1088	C985	G906	U813	C739	U740	C488	G406	G406	C342
A1433	A1363B	G1290	G1221	C1129	G1089	A986	A907	A814	U741	A663	A408	A408	A408	A343
A1434	G1364	U1291	G1222	A1130	C1080	C989	A908	C817	G742	G664	G409	G409	G409	A344
G1435	G1365	U1292	C1223	U1136	G1061	C990	A909	G818	U743	A665	G410	G410	G410	C345
U1436	C1366	G1293	G1224	U1137	G1062	C991	A910	A819	G744	A675	A411	A411	A411	C346
C1437	C1367	G1294	A1225	C1138	U1082	U991	C910	U820	G745	G576	G412	G412	G412	G347
G1438	G1368	U1295	C1226	G1139	C1066	U992	U911	C821	U746	G577	G413	G413	G413	G348
C1439	C1369	C1296	A1227	C1140	C993	U993	A913	C822	C747	G578	C501	C501	C501	A349
	G1370	C1297	C1228	C1141	A1067	A994	A914	C823	C748	G579	G502	G502	G502	G350
G1442A	G1371	C1298	A1229	C1142	G1068	C999	A918	C824	G749	A676	U580	U580	U580	G351
G1442B	U1372	A1299	G1230	G1143	C1069	C999	A919	A828	G750	U677	C504	C504	C504	C352
G1447	A1374	G1300	G1231		U1070		A918	U829		U678	G505	G505	G505	A353
C1452	A1375	U1301	A1236	C1147	C1071	G1001B	A919	G829	C754	U678	U421	U421	U421	A354
G1456	C1302	U1302	G1237	U148	G1072	G1002	U920	U833	C755	C680	A509	A509	A509	C355
G1457	G1304	C1303	A1238	U148	G1073	G1003	U921	U834	G756	G689	A510	A510	A510	A356
G1458	U1381	G1305	A1239	A1152	G1074	A1004	C922	U835	U757	G683	C511	C511	C511	G357
C1459	C1382	A1306	U1240	C1158	C1075	A1005	C924	U836			U512	U512	U512	U358
	C1383	U1307	G1241	U1159	U1078	C1006	G925	G836	G761	A687	C513	C513	C513	U359
	G1384	U1308	C1244	G1160	G1079	G1010	G926	C840	G762	G688	C514	C514	C514	A360
	G1385	G1309	A1245	C1161	A1080	G1011	G927	U841	G763	C689	G515	G515	G515	G361
G1469	G1386		C1246		G1081		C931	C848	A766	U692	U516	U516	U516	A430
G1470	G1387		U1247	G1164	A1092	U1020	C932		A767	G693	A431	A431	A431	U365
			A1248	A1170	U1085	G1022	C933	G851		A694	A432	A432	A432	C366
G1475			C1249	A1170	U1086	G1023	G934	G852	C770	A602	C433	C433	C433	U367
G1476			G1185		U1087	U1024	C948	G853		A695	U434	U434	U434	U368
			G1186		C1098	U1025	A949	G854	G774	A696	C436	C436	C436	
G1480			C1259	G1178	A1092	G1026	U950	G855	G775	G698	C437	C437	C437	G371
U1481			A1261	A1179	A1093	G1027	C951	G855	A781	C609	A608	A608	A608	C372
			A1262		G1094	C1028	U952			A609	C438	C438	C438	A373
U1485	C1396	A1319	G1255	A1183	U1095	G1029	G953	A859	G776	G610	C525	C525	C525	C374
G1486	A1397	C1320	U1256	G1184	C1096	G1030A	U954	A860	A777	A611	C526	C526	C526	A374
G1487	C1398		G1257	G1185	C1097	C1030B	G955	A861			G527	G527	G527	U375
G1488	C1400	A1324	C1259	G1186	C1098	G1030C	U956	G862	C707	C618	C528	C528	C528	G376
G1489	G1401	C1325	C1260	G1190	G1099			U863		U619	A532	A532	A532	G377
C1490	C1402	C1326	A1261	G1191	C1100			A864	C783	C620	A533	A533	A533	G378
G1491	C1403		C1262	A1191	A1101			A865	G784	A621	U534	U534	U534	C379
A1492	C1404	C1329	C1263	C1192	A1102			A866	G785	G622	A535	A535	A535	G380
G1493	G1405	U1330	C1264		C1103			G867	G786	C623	A539	A539	A539	C381
G1494	U1406	C1331	G1265	U1196	G1104			C868		C624	C454	C454	C454	A382
			G1266	G1197				G869	A790	G625	G540	G540	G540	A383
G1497	C1407	A1340	C1267		G1108		U960	U870	G791	G717	C385	C385	C385	G384
U1498	C1408		A1268	C1200	C1109	G1031	U961	U871	A792	G718	A461	A461	A461	C386
A1499	G1410	C1343	A1269	A1201	C1112	G1032		A872	U793		C470	C470	C470	U387
A1500	C1411	G1344	C1270		C1113	G1036	G967	A873	A794	G721	G471	G471	G471	G388
C1501	C1412	U1345	G1271	C1203	G1114	G1037	A968			A722	A472	A472	A472	A389
A1502	A1413	A1346		A1204	C1115	C1038	A969	C877	G797	U723	G473	G473	G473	C390
A1503	U1414	G1347	G1274		C1116	C1039	C970	G878	G798	G724	G474	G474	G474	G391
G1504		U1348	A1275	G1207	C1117	U1040	G971			G725	G475	G475	G475	G392
G1505				C1208	C1118		C972	C883	A802		U552	U552	U552	
U1506			C1278	C1209	C1119	C1043	G973	U884	G803	A728	A553	A553	A553	G396
A1507			A1279	C1210	C1120	A1044	G974		G804	A729	C554	C554	C554	U397
			U1281	U1211	G1120			U891	U804		C479	C479	C479	C398
C1424			U1281	U1212	U1121	C1045	A975	A892	C805	G730	U480	U480	U480	G399
			C1282	A1213	U1122	A1046	G976	C893	C806	G731	G481	G481	G481	G400
				G1215	A1123	G1047	A977	C898	A807		A482	A482	A482	C401
			A1285		G1124		A978	G908	C908	G735	U560	U560	U560	G402
			A1286		U1125	G1053	C980	A900	C810		G483	G483	G483	C403



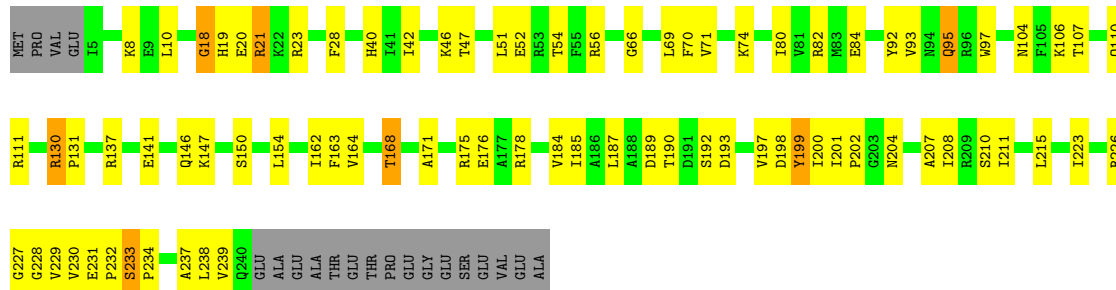
• Molecule 2: 30S ribosomal protein S2

Chain QB: 56% 34% 8%



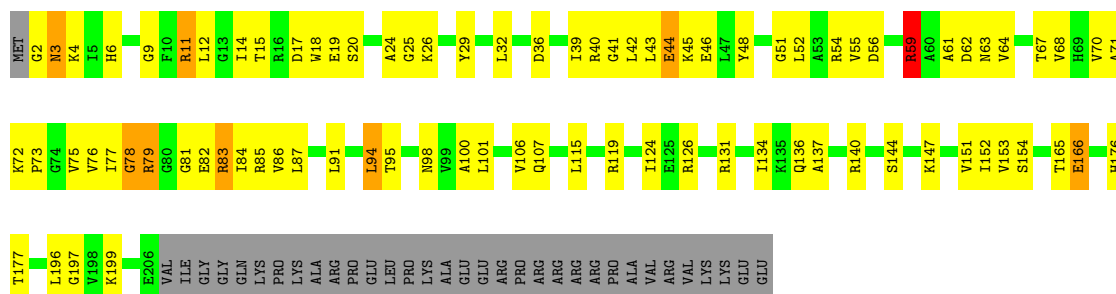
• Molecule 2: 30S ribosomal protein S2

Chain XB: 61% 29% 8%



• Molecule 3: 30S ribosomal protein S3

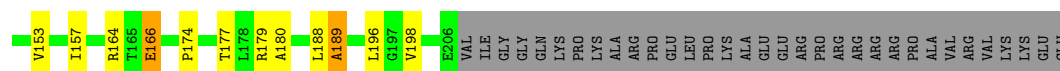
Chain QC: 50% 32% 14%



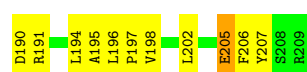
• Molecule 3: 30S ribosomal protein S3

Chain XC: 67% 17% 14%

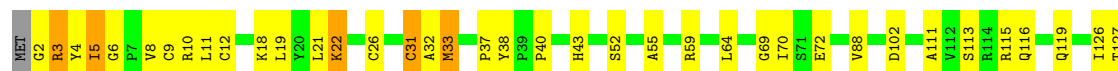




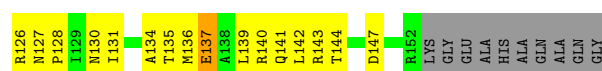
• Molecule 4: 30S ribosomal protein S4



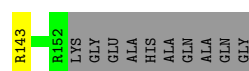
• Molecule 4: 30S ribosomal protein S4




• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5




• Molecule 6: 30S ribosomal protein S6

Chain QF:  73% 25% ..



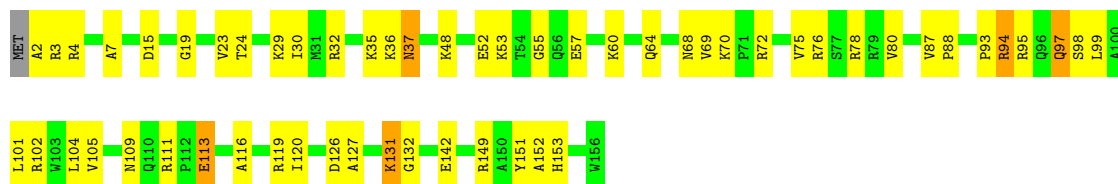
- Molecule 6: 30S ribosomal protein S6

Chain XF:  76% 23% .



- Molecule 7: 30S ribosomal protein S7

Chain QG:  63% 33% ..



- Molecule 7: 30S ribosomal protein S7

Chain XG:  72% 25% ..



- Molecule 8: 30S ribosomal protein S8

Chain QH:  59% 38% ..



- Molecule 8: 30S ribosomal protein S8

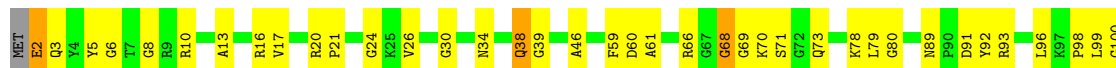
Chain XH:  68% 30% ..





- Molecule 9: 30S ribosomal protein S9

Chain QI: 53% 41% 5%



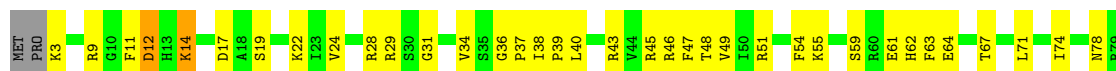
- Molecule 9: 30S ribosomal protein S9

Chain XI: 62% 35% ...



- Molecule 10: 30S ribosomal protein S10

Chain QJ: 53% 39% 6%



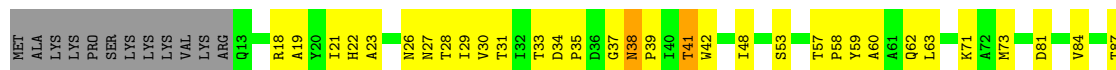
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 64% 28% 9%



- Molecule 11: 30S ribosomal protein S11

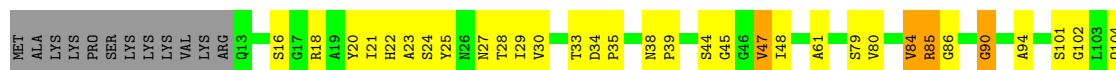
Chain QK: 57% 28% 12%





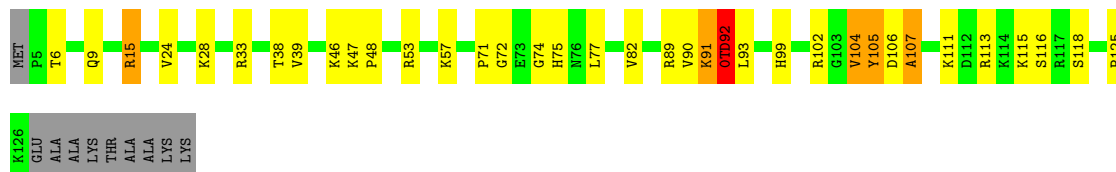
- Molecule 11: 30S ribosomal protein S11

Chain XK: 59% 26% 12%



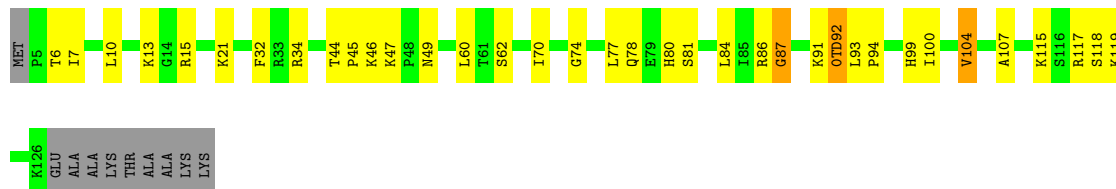
- Molecule 12: 30S ribosomal protein S12

Chain QL: 65% 23% 8%



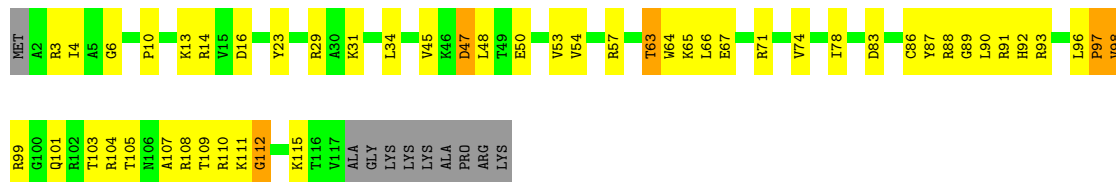
- Molecule 12: 30S ribosomal protein S12

Chain XL: 65% 25% 8%



- Molecule 13: 30S ribosomal protein S13

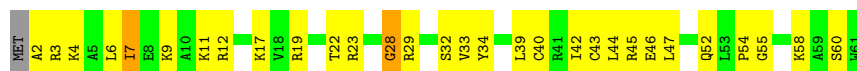
Chain QM: 52% 36% 8%



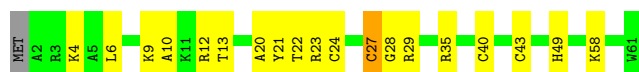
- Molecule 13: 30S ribosomal protein S13

Chain XM: 67% 21% 10%

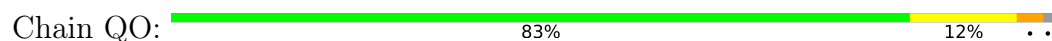
- Molecule 14: 30S ribosomal protein S14 type Z



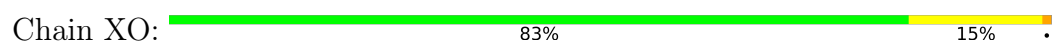
- Molecule 14: 30S ribosomal protein S14 type Z



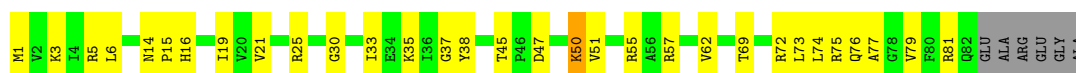
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

Chain QQ:  67% 24% 6%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  65% 29% 6%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  56% 22% 23%



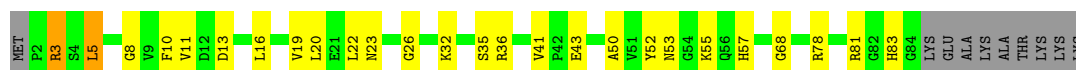
- Molecule 18: 30S ribosomal protein S18

Chain XR:  61% 15% 23%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  61% 26% 11%



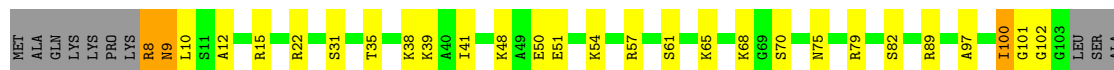
- Molecule 19: 30S ribosomal protein S19

Chain XS:  57% 30% 11%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  64% 24% 9%



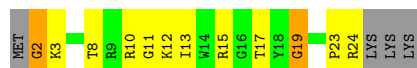
- Molecule 20: 30S ribosomal protein S20

Chain XT:  62% 30% 8%



- Molecule 21: 30S ribosomal protein Thx

Chain QU:  41% 37% 7% 15%



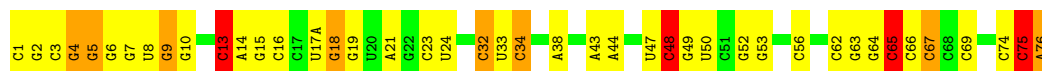
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  44% 41% 15%



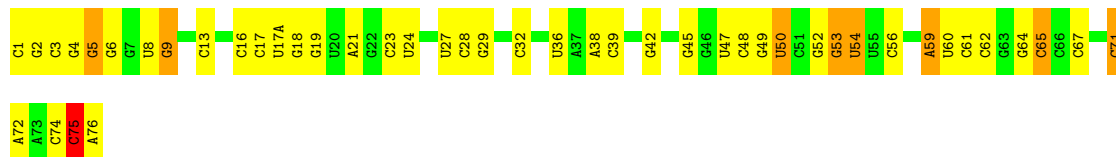
- Molecule 22: P-site tRNA^{fMet}

Chain QV:  44% 40% 10% 5%



- Molecule 22: P-site tRNA^{fMet}

Chain XV:  40% 48% 10% 2%



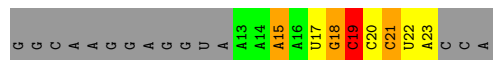
- Molecule 23: mRNA

Chain QX:  12% 19% 69%

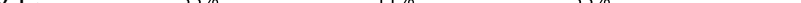


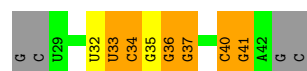
- Molecule 23: mRNA

Chain XX:  12% 15% 12% 58%

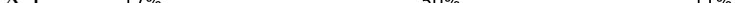


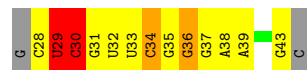
- Molecule 24: A-site ASLSufA6 A37.5

Chain QY: 



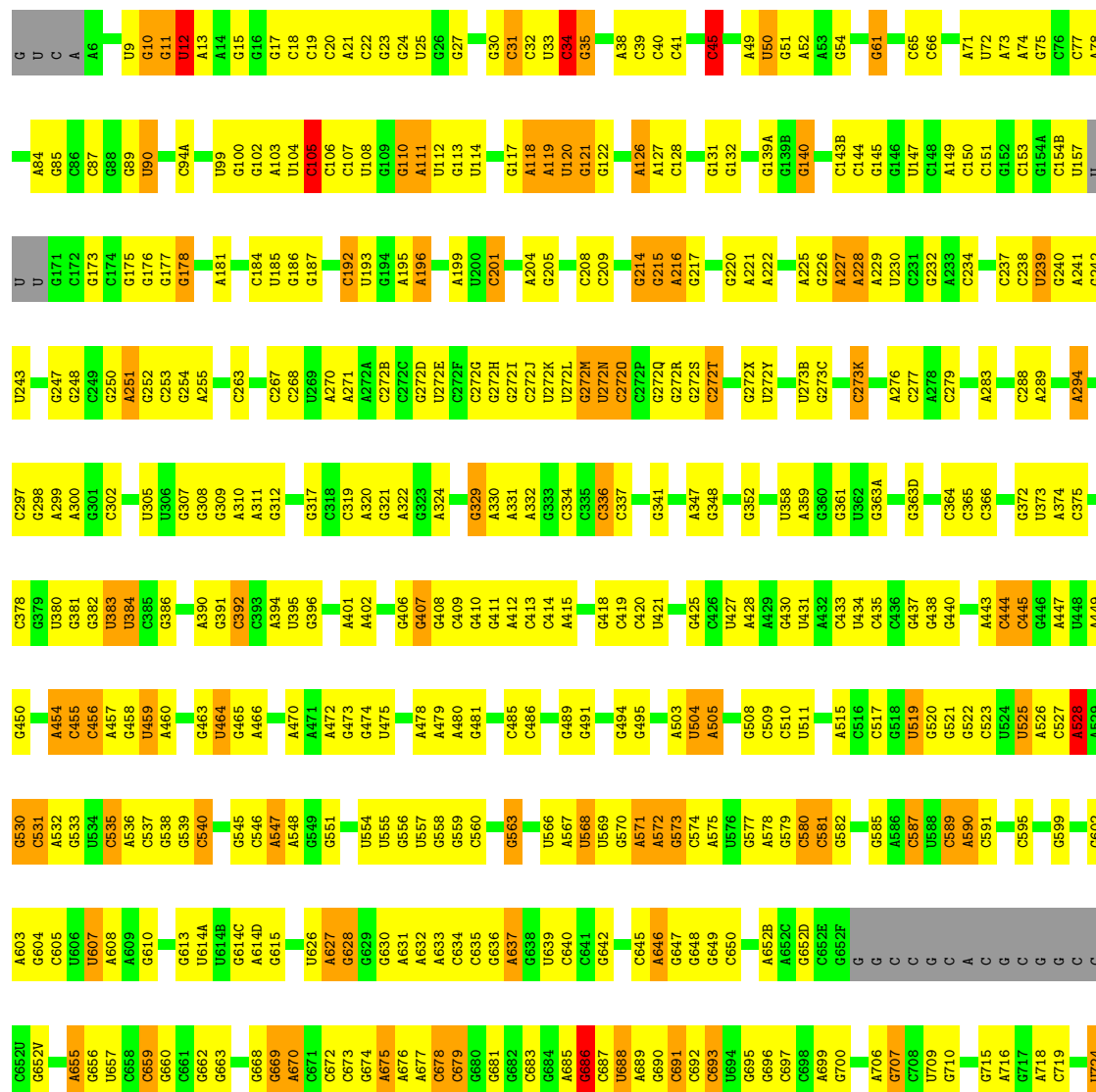
- Molecule 24: A-site ASLSufA6 A37.5

Chain XY:  17% 50% 11% 11% 11%



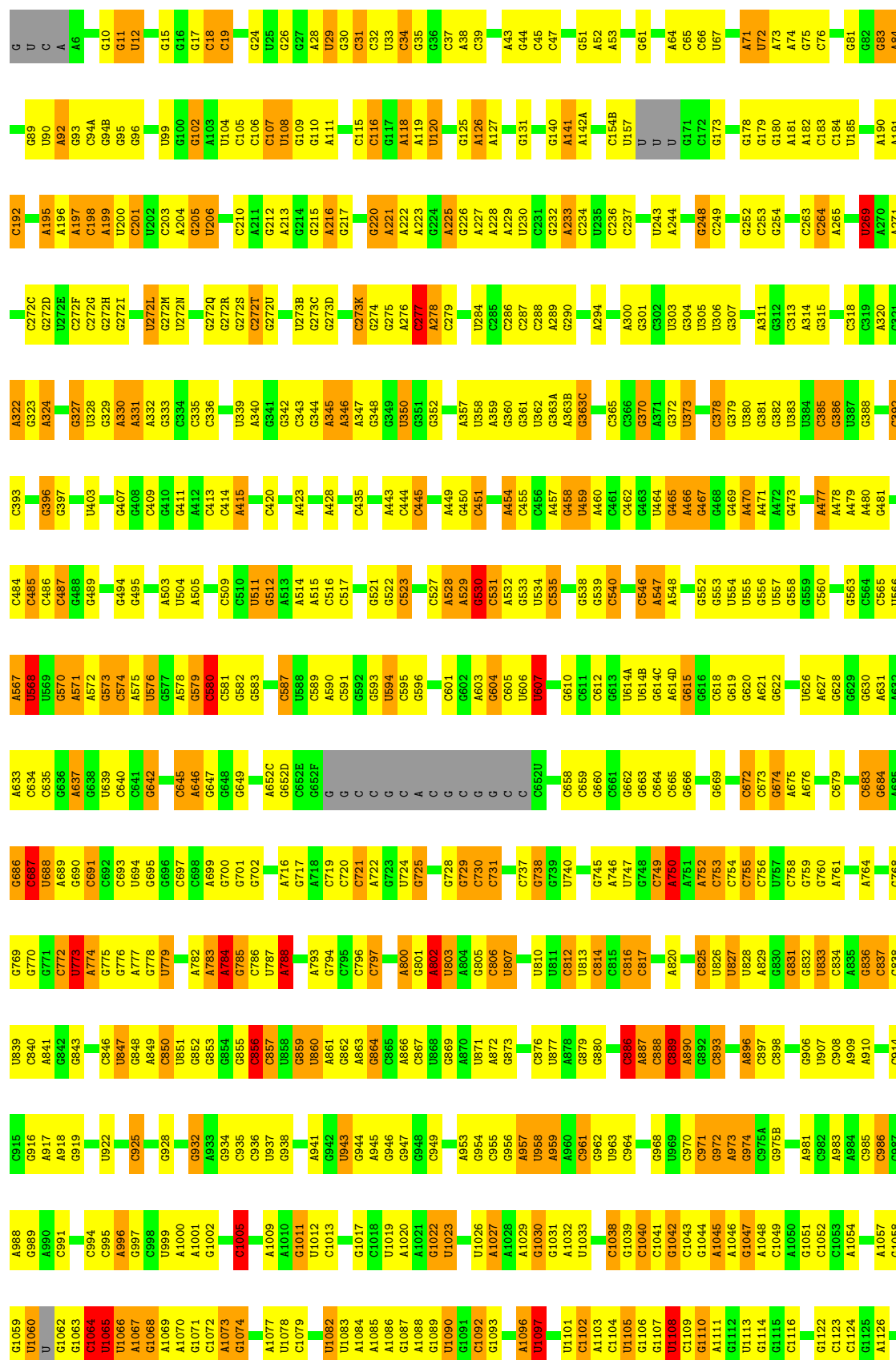
- Molecule 25: 23S rRNA

Chain RA:

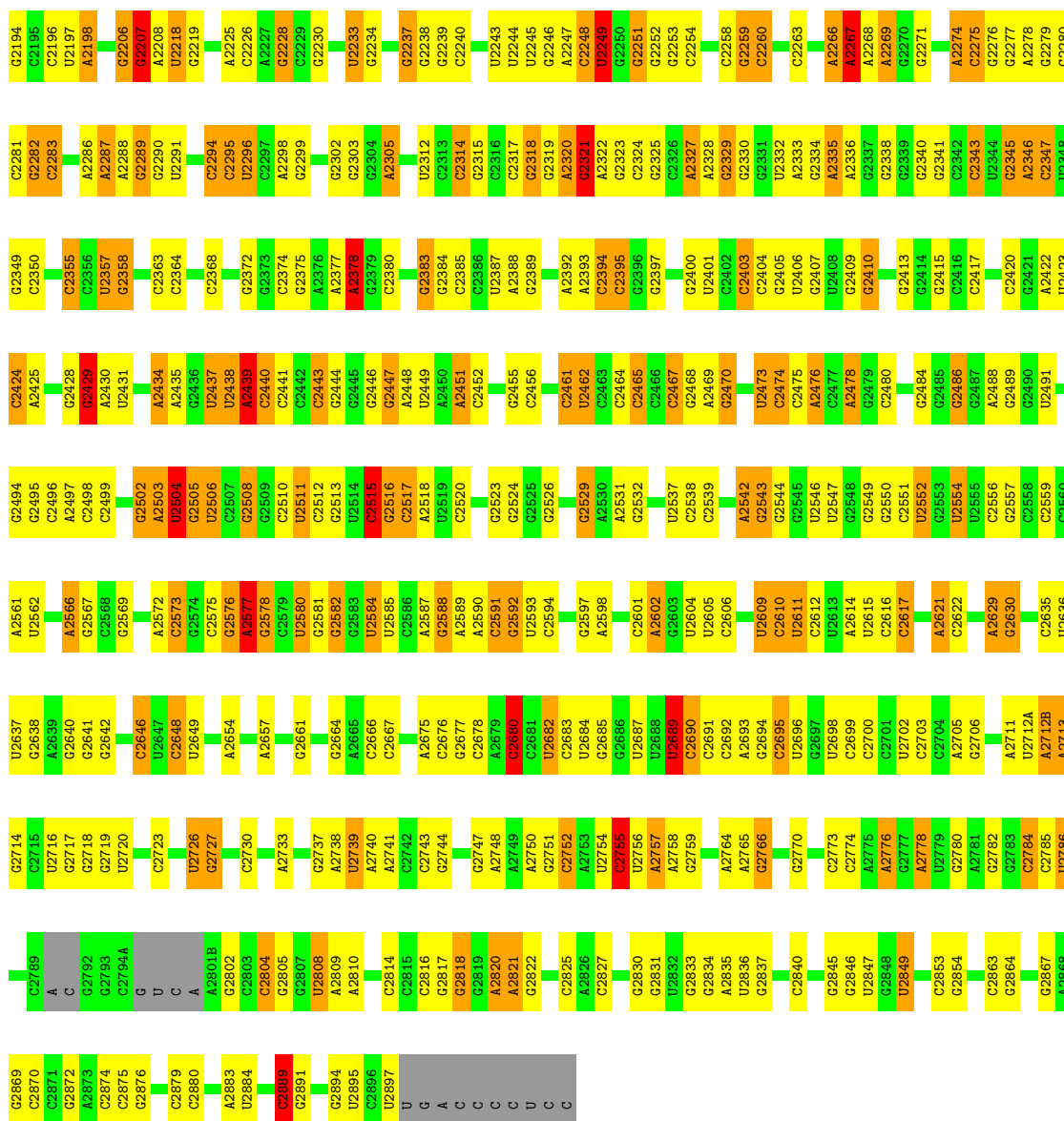


G1813	A1698	A1614	G1533	C1370	C1297	A1220	A1143	C1079	U1012	A941	G864	C797	G725
G1814	G1699	C1615	U1540	G1371	C1298	C1221A		U1082	C1013	G942	C865	G798	
A1815	A1616	A1616	G1541		U1299	C1221B	C1147	C1083	G1017	U943	A866	G799	G729
G1816	A1701	A1542	G1459	C1375	U1300	C1222	A1148	A1084	U1018	G945	C867	A800	G730
G1817	G1702	C1543	C1376	C1377	A1301	G1223	A1149	A1085	C1019	G946	U868	G801	C731
U1820	U1706	G1622	C1462	A1378	A1302	G1224	C1150	A1086	A1020	G947	A870	G802	C732
A1821			C1463	A1379	G1303	G1225	G1151	G1087	A1021	G948	U871	G805	G733
			C1464	G1380	C1304	G1226	G1152	A1088	G1022			C806	A734
			C1465		C1305	G1227	C1153	G1089	G1023			A735	C736
			C1466		C1306		C1154	U1090	U1024	G952	G881	U807	C737
			C1467				A1155	U1091	U1025			G808	
							A1156	C1092	U1026			G809	G739
							G1157	G1093	U1027			U810	
							C1158	A1095				U811	G742
							U1159	A1096	G1030	A959	C886	G743	
							G1160	G1097	G1031	A960	C887	G744	
							G1161	A1098	U1033	G962	C889	C961	A746
							G1162	A1099	U1034	G963	C890	U747	
							G1163	C1100	G1036	G964	C891	A819	
							G1164	C1101	G1037	G965	C892	A820	C748
							G1165	C1102	U1038	G966	C893	A821	C749
							G1166	C1103	U1039		C894	U822	A751
							G1167	C1104	G1038	U969	C895	A824	A752
							G1168	C1105	U1039	C970	C896	C825	
							G1169	C1106	C1040	C971	C897	U826	C755
							G1170	C1107	C1041	G972	C898	U827	C756
							G1171	C1108	G1042	A973	C899	U828	U757
							G1172	C1109	C1043	G974	C900	A829	C758
							G1173	C1110	U1044	C975A	C903	G830	
							G1174	C1111	A1045	G975B	C904	G831	G763
							G1175	C1112	A1046		C905	G832	A764
							G1176	C1113	G1047	G978	C906	U833	G765
							G1177	C1114	C1049	G979	A909	C834	C766
							G1178	C1115	U1052	A981	A910	A835	U767
							G1179	C1116	C1053	A982	C912	G836	G768
							G1180	C1117	A1054	A983	U913	G837	G769
							G1181	C1118	U1055	A984	C914	C838	G770
							G1182	C1119		C985	C915	U839	
							G1183	C1120	A1057	G986	G916	C840	A774
							G1184	C1121	U1060	G987	A917	A841	A775
							G1185	C1122	U1061	A988	A918	U846	G776
							G1186	C1123	U1062	A989	G919	C847	A777
							G1187	C1124	U1063	A990	U922	U848	G778
							G1188	C1125	C1064	C991	C923	A849	A781
							G1189	C1126	U1065	C992	C924	C850	A782
							G1190	C1127	U1066	C993	C925	U851	A783
							G1191	C1128	U1067	C994	C926	G852	A784
							G1192	C1129	A1067	C995	G927	G853	G785
							G1193	C1130	U1068	A996	G928	C854	C786
							G1194	C1131	U1069	G997	U930	U855	U787
							G1195	C1132	A1070	C998	U931	C856	A788
							G1196	C1133	G1071	C999	G932	C857	A789
							G1197	C1134	C1072	A1000	G933	U858	
							G1198	C1135	A1073	A1001	A933	G859	G792
							G1199	C1136	G1074	C1005	G934	U860	A793
							G1200	C1137	U1075		C935	A861	G794
							G1201	C1138	U1076		C936	G862	C796
							G1202	C1139	U1077				
							G1203	C1140	U1078				
							G1204	C1141					
							G1205	C1142					
							G1206	C1143					
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							G1299	C1					

- Molecule 25: 23S rRNA

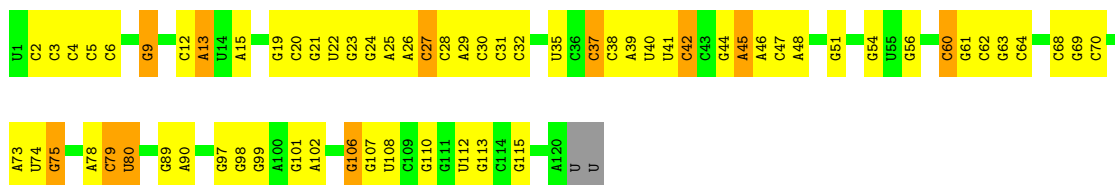
Chain YA: 

U2118	A2051	G1907	G1817	G1742	G1644	A1571	C1498	A1419	U1341	G1271	G1202	A1129
A2119	G2052	U1911	U1818	G1749	G1645	A1572	C1499	U1420	A1342	A1272	G1203	U1130
A2126	A2053	U1912	A1819	A1748	G1646	G1573	G1500	G1421	G1343	U1273	A1204	G1131
G2127	A2054	A1912	U1820	A1749	C1647	C1575	C1501	G1422	G1344	A1274	U1205	A1132
C2128	G2055	A1913	A1821	G1752	G1648	U1576	G1505	G1423	C1345	A1275	G1206	U1133
C2129	G2056	C1914	G1822	G1753	G1651	U1577	C1506	G1424	U1352	A1276	G1210	C1135
U2130	A2059	U1915	G1823	C1754	G1657	U1578	A1507	G1425	U1353	G1280	A1211	G1136
G2131	A2060	U1916	G1826	A1755	G1656	A1579	A1508	G1426	G1281	G1281	G1212	G1137
U2132	G2061	A1918	C1827	G1756	C1657	G1580	C1509A	A1427	G1354	U1282	G1212	G1138
G2133	A2062	A1919	G1828	G1757	C1657	G1581	A1509B	G1428	G1355	G1283	G1215	G1139
G2134	C2063	C1920	A1829	A1760	C1658	G1582	A1509C	G1429	G1356	G1284	G1216	C1140
+	C2064	G1921	C1761	G1761	U1659	G1583	G1510	C1430	U1357	A1286	C1217	U1141
C2137	C2065	G1922	G1831	A1762	C1660	C1584	C1511	U1431	G1358	A1287	C1218	U1142A
C2138	C2066	U1923	C1832	G1763	G1661	A1586	U1512	C1432	A1359	U1288	+	A1142B
C2139	C2067	C1925	U1833	G1764	G1662	A1587	C1513	U1433	A1360	C1291	C1221A	A1143
C2140	U2068	U1926	G1833	C1765	A1664	A1587	U1514	A1434	G1363	U1292	+	C1145
G2141	G2069	A1927	C1836	G1769	A1665	A1665	U1515	G1435	G1364	C1293	G1223	+
+	C2070	U1928	+	G1770	G1666	G1667	U1518	G1436	A1365	U1294	G1224	+
U2144	G2071	G1929	G1839	G1771	G1667	G1594	+	G1437	A1366	G1295	G1225	+
C2145	G2072	G1930	G1842	G1772	A1668	G1595	G1525	U1438	A1367	C1297	G1226	+
C2146	C2073	+	G1843	G1773	C1670	A1596	G1526	A1439	G1368	C1298	G1227	+
G2147	U2074	A1934	A1773	A1774	U1671	A1597	G1531	G1440	G1374	G1299	G1231	+
G2148	U2075	G1935	C1844	C1774	G1672	A1597	C1532	A1445A	G1375	U1300	G1232	+
+	U2076	A1936	+	+	U1673	C1599	C1533	C1445B	C1376	A1301	C1233	+
A2151	A2077	A1937	A1847	U1778	G1674	C1599	U	C1446	A1377	A1302	U1234	+
G2152	G2080	A1938	A1948	U1779	C1675	A1603	A	G1447	G1380	+	G1235	+
C2153	G2081	U1939	U1780	G1780	G1676	C1604	+	G1450A	A1306	+	G1236	+
G2154	C2081	U1940	C1852	G1781	C1677	C1605	+	+	A1307	+	G1164	+
G2155	A2082	C1941	A1853	C1782	G1678	G1606	C1536	U1452	G1308	+	U1165	+
G2156	G2085	G1942	A1853	A1783	+	C1607	G1537	A1453	G1309	+	+	+
G2157	U2086	U1943	G1857	A1784	G1681	A1608	U1538	G1455	G1310	+	G1239	+
A2158	+	U1944	G1858	A1785	G1682	A1609	G1539	G1456	A1241	+	U1240	+
C2159	+	G1945	U1864	A1786	C1683	A1610	+	G1465	G1242	+	A1241	+
G2160	U2091	U1946	U1865	G1788	C1684	A1610	A1542	U1467	G1387	+	G1243	+
C2161	U2092	U1947	C1866	A1789	G1687	G1611	C1543	C1462	G1388	+	A1246	+
G2162	G2093	G1948	A1876	C1790	+	G1612	A1544	C1463	U1394	C1314	A1247	+
C2163	G2094	G1949	A1877	A1791	A1690	G1613	A1545	C1464	U1395	U1316	+	+
C2164	C2095	U1950	G1878	G1792	C1691	A1614	C1546	G1465	A1317	A1317	G1250	+
+	U2096	A1952	C1879	C1793	U1692	A1616	C1547	G1466	C1318	+	C1251	+
G2168	C2097	+	C1882	G1794	U1693	+	C1549	C1467	U1397	+	G1252	+
A2169	U2098	G1954	U1882	C1795	G1694	G1619	C1550	+	G1398	A1321	A1253	+
A2170	G2100	U1955	U1798	+	G1695	+	+	G1470	C1399	A1322	A1254	+
A2171	+	U1956	A1889	U1798	G1696	G1622	A1553	A1471	G1400	+	U1255	+
U2172	G2101	C1957	C1892	G1799	G1697	C1625	A1554	A1472	G1401	G1325	G1256	+
A2173	C2103	C1958	C1893	G1800	A1698	G1626	+	G1473	C1402	U1326	C1257	+
C2174	G2032	+	C1894	G1801	G1699	U1629	+	+	U1405	G1327	C1258	+
+	A2033	+	U1894	A1802	A1701	+	A1557	C1476	U1406	U1328	G1259	+
C2178	C2105	C1961	U1897	A1803	G1702	+	A1558	+	U1329	+	G1260	+
C2179	+	U1962	U1898	G1804	+	G1633	G1560	G1482	C1407	C1330	C1261	+
+	C2036	U1963	U1899	+	C1712	A1634	G1561	+	G1408	A1331	A1262	+
C2185	G2037	G1964	G1899	U1808	+	A1635	A1562	U1490	C1409	G1332	U1263	+
G2186	U2109	C1965	G1900	A1809	G1719	G1636	G1563	G1491	G1333	G1333	G1264	+
G2187	C2039	A1966	A1901	A1810	U1719	A1637	C1564	G1492	C1411	G1334	A1265	+
C2188	G2040	C1967	C1902	U1810	U1720	+	C1565	G1493	A1412	+	G1267	+
U2189	U2041	G1968	G1903	G1813	C1721	G1638	A1666	A1494	G1416	A1335	U1197	+
C2190	A1969	+	U1902	G1814	U1722	G1639	+	A1495	G1417	A1336	U1198	+
G2191	U1970	A1815	G1904	G1815	A1722	C1640	A1569	A1496	C1417	G1337	A1268	+
G2192	C2044	+	G1906	G1816	U1739	+	+	U1497	+	+	C1200	+
G2193	+	+	+	+	+	A1641	A1570	+	+	U1340	C1270	+



• Molecule 26: 5S rRNA

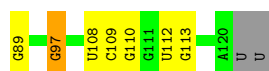
Chain RB: 44% 45% 9%



• Molecule 26: 5S rRNA

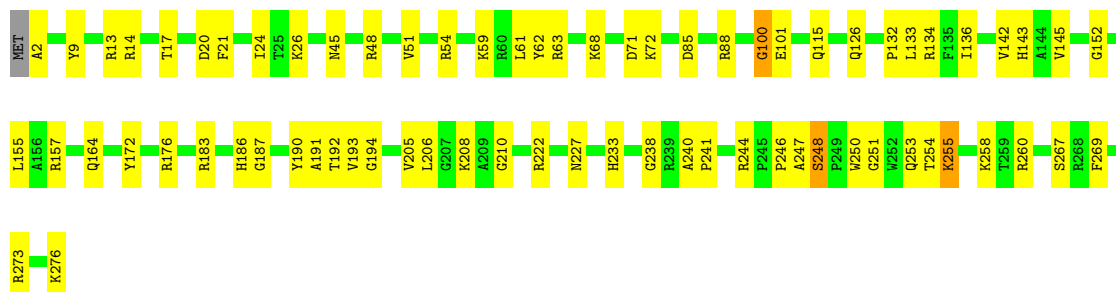
Chain YB: 58% 29% 10%





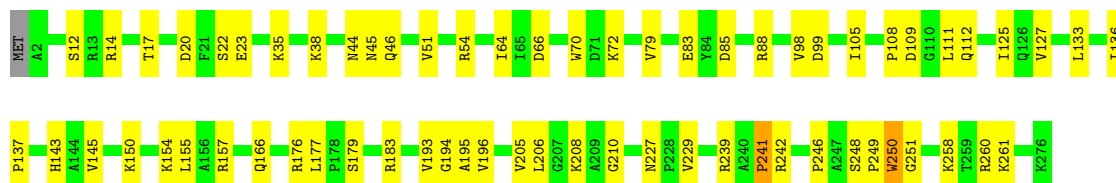
- Molecule 27: 50S ribosomal protein L2

Chain RD: 74% 25% .



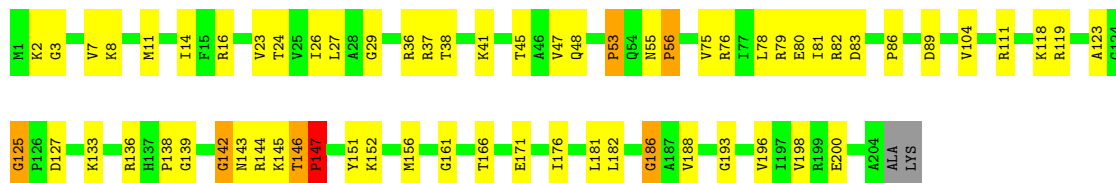
- Molecule 27: 50S ribosomal protein L2

Chain YD: 76% 23% .



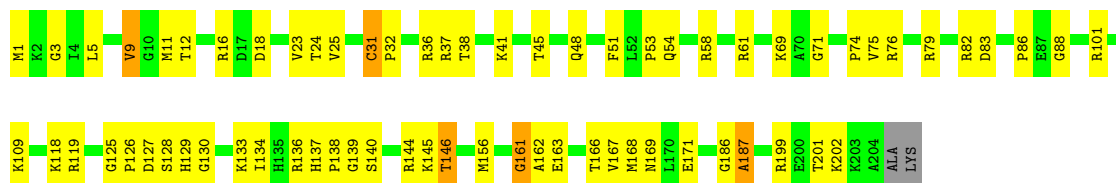
- Molecule 28: 50S ribosomal protein L3

Chain RE: 68% 28% . .



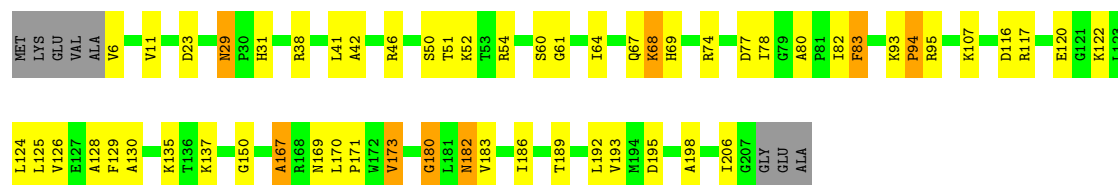
- Molecule 28: 50S ribosomal protein L3

Chain YE: 66% 31% . .



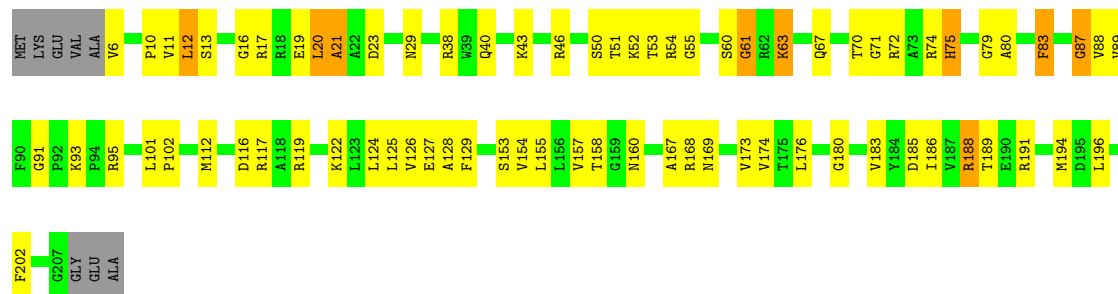
- Molecule 29: 50S ribosomal protein L4

Chain RF: 69% 23% . .



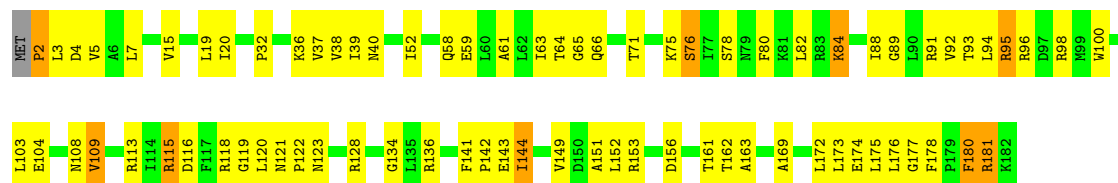
- Molecule 29: 50S ribosomal protein L4

Chain YF: 60% 31% . .



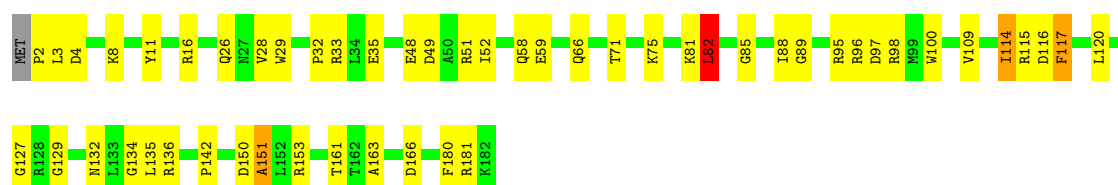
- Molecule 30: 50S ribosomal protein L5

Chain RG: 57% 37% 5% .



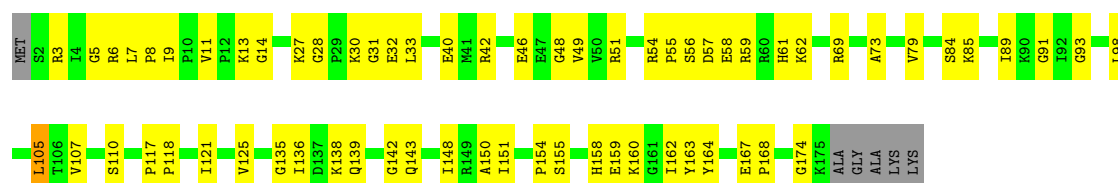
- Molecule 30: 50S ribosomal protein L5

Chain YG: 71% 26% . .



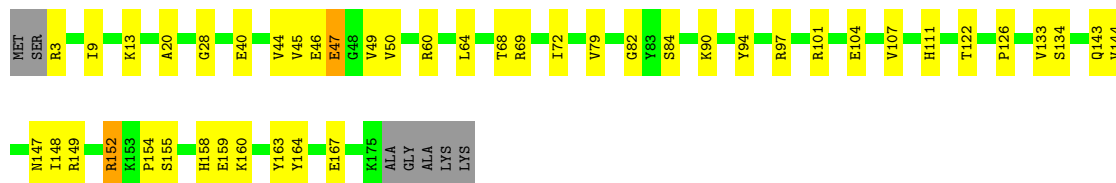
- Molecule 31: 50S ribosomal protein L6

Chain RH: 61% 36% . .



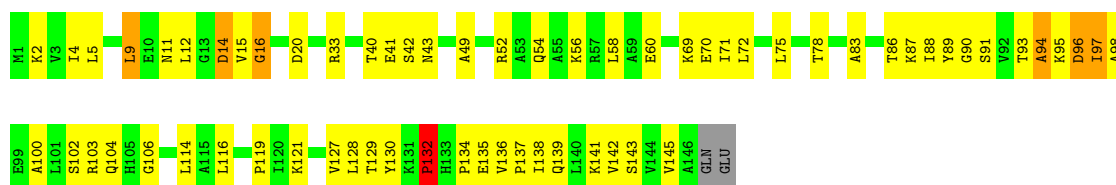
- Molecule 31: 50S ribosomal protein L6

Chain YH:  71% 24% ..




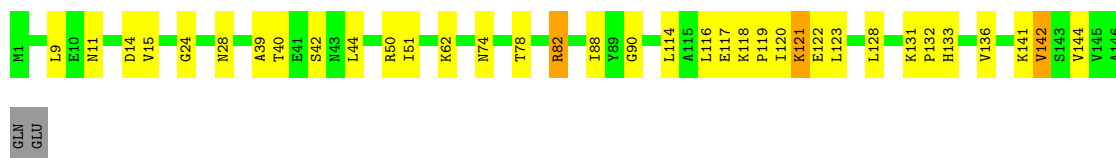
- Molecule 32: 50S ribosomal protein L9

Chain RI:  55% 39% ..



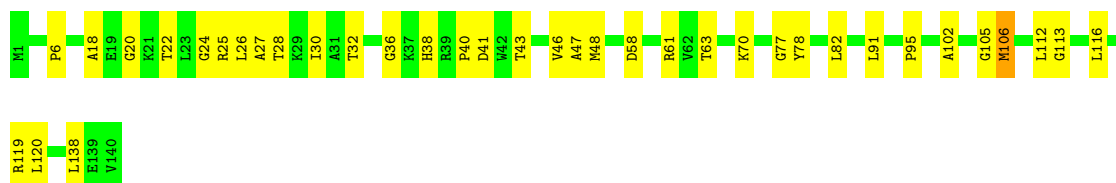
- Molecule 32: 50S ribosomal protein L9

Chain YI:  75% 22% ..




- Molecule 33: 50S ribosomal protein L13

Chain RN:  74% 26% .



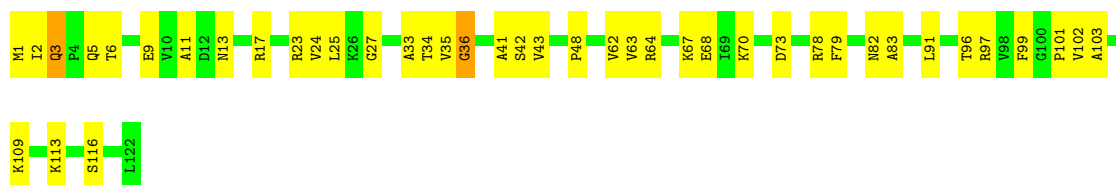
- Molecule 33: 50S ribosomal protein L13

Chain YN:  84% 16%



- Molecule 34: 50S ribosomal protein L14

Chain RO:  66% 33% .



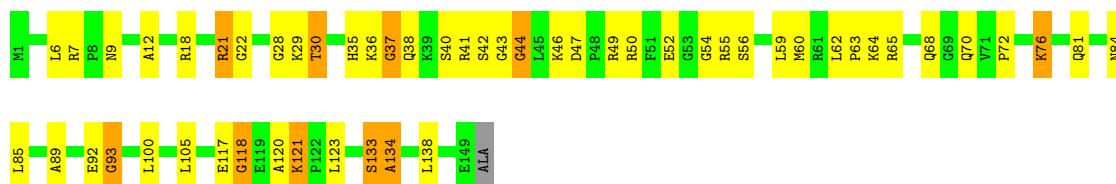
- Molecule 34: 50S ribosomal protein L14

Chain YO: 79% 20% .



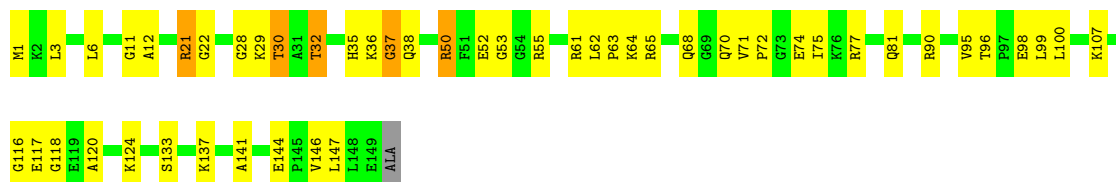
- Molecule 35: 50S ribosomal protein L15

Chain RP: 64% 29% 7% .



- Molecule 35: 50S ribosomal protein L15

Chain YP: 66% 30% . .



- Molecule 36: 50S ribosomal protein L16

Chain RQ: 67% 33%

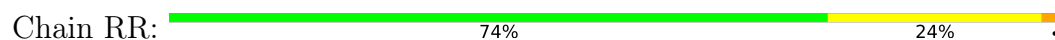


- Molecule 36: 50S ribosomal protein L16

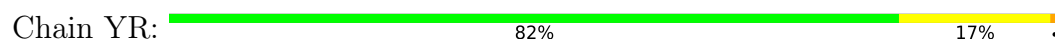
Chain YQ: 79% 21%



- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17



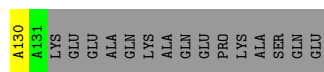
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



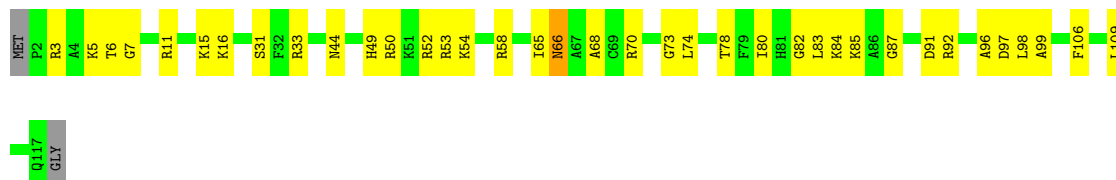
- Molecule 39: 50S ribosomal protein L19





- Molecule 40: 50S ribosomal protein L20

Chain RU: 67% 31% ..



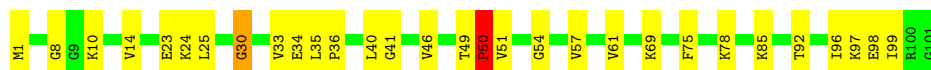
- Molecule 40: 50S ribosomal protein L20

Chain YU: 78% 20% .



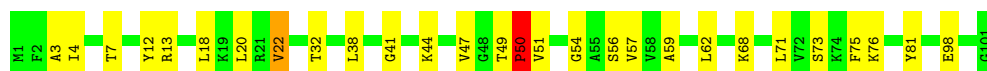
- Molecule 41: 50S ribosomal protein L21

Chain RV: 70% 28% ..



- Molecule 41: 50S ribosomal protein L21

Chain YV: 72% 26% ..



- Molecule 42: 50S ribosomal protein L22

Chain RW: 77% 22% .



- Molecule 42: 50S ribosomal protein L22

Chain YW: 79% 19% ..



- Molecule 43: 50S ribosomal protein L23

Chain RX: 72% 25% ..



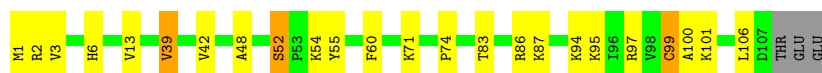
- Molecule 43: 50S ribosomal protein L23

Chain YX: 86% 12% .



- Molecule 44: 50S ribosomal protein L24

Chain RY: 75% 19% . .



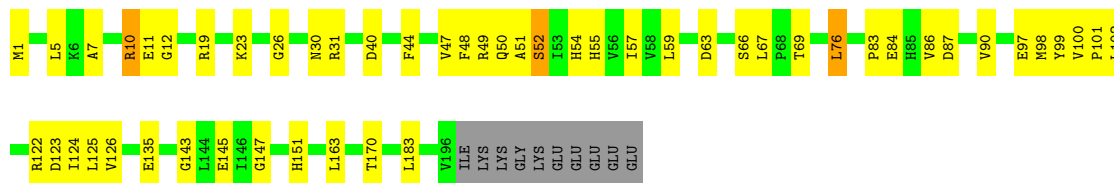
- Molecule 44: 50S ribosomal protein L24

Chain YY: 68% 27% . .



- Molecule 45: 50S ribosomal protein L25

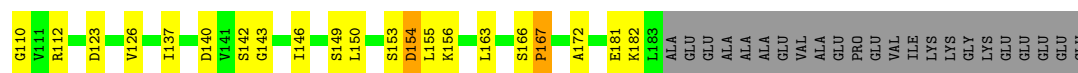
Chain RZ: 70% 24% . 5%



- Molecule 45: 50S ribosomal protein L25

Chain YZ: 62% 25% . 11%

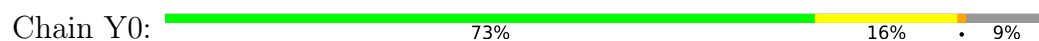




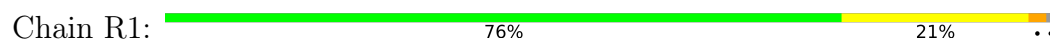
- Molecule 46: 50S ribosomal protein L27



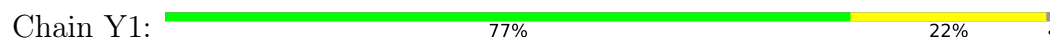
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



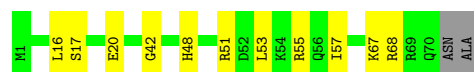
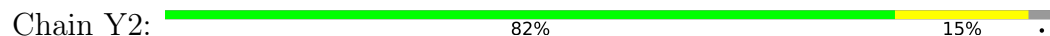
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

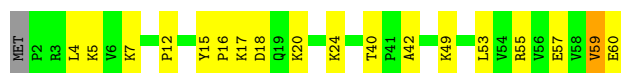


- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30

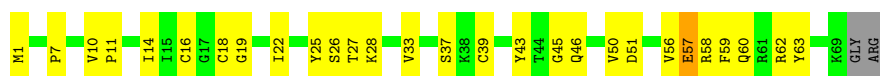




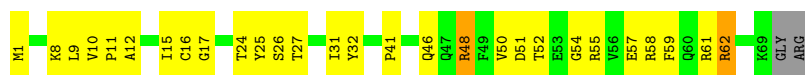
- Molecule 49: 50S ribosomal protein L30



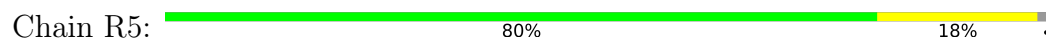
- Molecule 50: 50S ribosomal protein L31



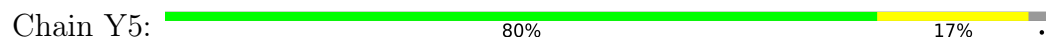
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33

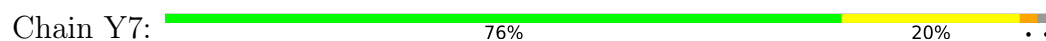




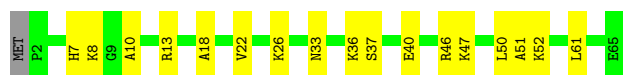
- Molecule 53: 50S ribosomal protein L34



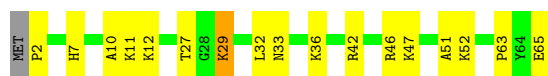
- Molecule 53: 50S ribosomal protein L34



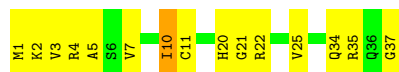
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic





- Molecule 56: tRNA acceptor end mimic

Chain ZB:  33% 67%



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	208.91Å 445.91Å 617.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.64	Depositor
% Data completeness (in resolution range)	93.4 (49.17-3.64)	Depositor
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.208 , 0.250	Depositor
Wilson B-factor (Å ²)	123.8	Xtriage
Anisotropy	0.381	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291822	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: SF4, PPU, 0TD, MA6, OMG, OMU, 5MU, ZN, M2G, 2MA, 2MG, OMC, 5MC, 4OC, MG, UR3, PSU, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.92	1/35795 (0.0%)	1.25	264/55864 (0.5%)
1	XA	1.03	8/35890 (0.0%)	1.25	234/56012 (0.4%)
2	QB	0.36	0/1942	0.64	0/2619
2	XB	0.39	0/1950	0.59	0/2630
3	QC	0.36	0/1629	0.60	1/2195 (0.0%)
3	XC	0.42	0/1629	0.59	0/2195
4	QD	0.47	0/1733	0.66	0/2318
4	XD	0.48	0/1733	0.61	0/2318
5	QE	0.40	0/1149	0.61	0/1548
5	XE	0.47	0/1149	0.59	0/1548
6	QF	0.40	0/850	0.56	0/1147
6	XF	0.49	0/850	0.60	1/1147 (0.1%)
7	QG	0.36	0/1276	0.55	0/1709
7	XG	0.43	0/1276	0.56	0/1709
8	QH	0.43	0/1128	0.59	0/1517
8	XH	0.44	0/1128	0.59	0/1517
9	QI	0.38	0/1029	0.62	0/1379
9	XI	0.42	0/1017	0.64	0/1365
10	QJ	0.37	0/814	0.61	0/1095
10	XJ	0.40	0/790	0.52	0/1063
11	QK	0.42	0/859	0.54	0/1162
11	XK	0.41	0/859	0.52	0/1162
12	QL	0.49	0/963	0.65	0/1287
12	XL	0.52	0/963	0.60	0/1287
13	QM	0.41	0/938	0.64	0/1258
13	XM	0.45	0/926	0.61	0/1241
14	QN	0.40	0/501	0.59	0/664
14	XN	0.48	0/501	0.60	0/664
15	QO	0.38	0/745	0.55	0/992
15	XO	0.45	0/745	0.62	0/992
16	QP	0.50	0/707	0.56	0/951

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.43	0/707	0.57	0/951
17	QQ	0.45	0/836	0.58	0/1117
17	XQ	0.45	0/836	0.56	0/1117
18	QR	0.38	0/560	0.58	0/746
18	XR	0.45	0/560	0.60	0/746
19	QS	0.33	0/680	0.57	0/915
19	XS	0.44	0/680	0.58	0/915
20	QT	0.43	0/745	0.57	0/981
20	XT	0.34	0/762	0.57	0/1003
21	QU	0.37	0/203	0.54	0/266
21	XU	0.41	0/203	0.47	0/266
22	QV	0.90	1/1836 (0.1%)	1.28	31/2859 (1.1%)
22	XV	1.16	1/1836 (0.1%)	1.40	25/2859 (0.9%)
23	QX	0.71	0/185	1.34	1/285 (0.4%)
23	XX	0.89	0/260	1.69	8/402 (2.0%)
24	QY	0.69	0/336	1.25	3/522 (0.6%)
24	XY	0.71	0/381	1.39	7/593 (1.2%)
25	RA	1.20	15/68971 (0.0%)	1.33	622/107656 (0.6%)
25	YA	1.36	49/68976 (0.1%)	1.43	918/107668 (0.9%)
26	RB	0.78	0/2876	1.27	26/4486 (0.6%)
26	YB	1.09	0/2878	1.27	18/4490 (0.4%)
27	RD	0.60	0/2194	0.59	0/2955
27	YD	0.67	0/2195	0.62	0/2955
28	RE	0.57	0/1596	0.59	0/2153
28	YE	0.61	0/1596	0.65	0/2153
29	RF	0.60	1/1620 (0.1%)	0.61	0/2194
29	YF	0.65	0/1620	0.64	1/2194 (0.0%)
30	RG	0.40	0/1499	0.69	0/2016
30	YG	0.53	0/1499	0.67	1/2016 (0.0%)
31	RH	0.38	0/1362	0.58	0/1841
31	YH	0.55	0/1356	0.58	0/1833
32	RI	0.42	0/1151	0.68	1/1558 (0.1%)
32	YI	0.44	0/1151	0.67	0/1558
33	RN	0.51	0/1148	0.55	0/1547
33	YN	0.58	0/1148	0.54	0/1547
34	RO	0.56	0/943	0.67	1/1269 (0.1%)
34	YO	0.64	0/943	0.67	2/1269 (0.2%)
35	RP	0.50	0/1156	0.60	0/1537
35	YP	0.56	0/1156	0.62	0/1537
36	RQ	0.50	0/1143	0.58	0/1527
36	YQ	0.59	0/1143	0.59	0/1527
37	RR	0.56	0/982	0.66	0/1312
37	YR	0.54	0/982	0.62	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RS	0.39	0/887	0.63	1/1180 (0.1%)
38	YS	0.49	0/887	0.62	0/1180
39	RT	0.52	0/1105	0.57	0/1477
39	YT	0.58	0/1105	0.58	0/1477
40	RU	0.52	0/977	0.52	0/1301
40	YU	0.61	0/977	0.54	0/1301
41	RV	0.48	0/790	0.64	0/1057
41	YV	0.59	0/790	0.67	0/1057
42	RW	0.60	0/901	0.55	0/1209
42	YW	0.62	0/901	0.54	0/1209
43	RX	0.54	0/764	0.57	1/1025 (0.1%)
43	YX	0.63	0/764	0.59	0/1025
44	RY	0.49	0/831	0.59	0/1108
44	YY	0.57	0/831	0.61	0/1108
45	RZ	0.42	0/1585	0.61	1/2153 (0.0%)
45	YZ	0.50	0/1493	0.65	1/2026 (0.0%)
46	R0	0.47	0/619	0.55	0/825
46	Y0	0.59	0/619	0.57	0/825
47	R1	0.52	0/770	0.58	0/1022
47	Y1	0.59	1/770 (0.1%)	0.60	0/1022
48	R2	0.40	0/594	0.52	0/785
48	Y2	0.47	0/594	0.51	0/785
49	R3	0.52	0/474	0.61	0/635
49	Y3	0.52	0/473	0.62	0/635
50	R4	0.36	0/578	0.60	0/776
50	Y4	0.42	0/578	0.63	1/776 (0.1%)
51	R5	0.58	0/473	0.61	0/639
51	Y5	0.57	0/465	0.57	0/629
52	R6	0.32	0/460	0.56	0/613
52	Y6	0.33	0/460	0.64	0/613
53	R7	0.58	0/426	0.59	0/561
53	Y7	0.62	0/426	0.63	0/561
54	R8	0.52	0/525	0.58	0/691
54	Y8	0.59	0/525	0.65	0/691
55	R9	0.29	0/310	0.56	0/407
55	Y9	0.38	0/310	0.59	0/407
56	ZA	0.64	0/40	1.52	4/60 (6.7%)
56	ZB	1.26	0/40	1.60	0/60
All	All	1.02	77/314471 (0.0%)	1.18	2174/470119 (0.5%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	XA	0	1
2	QB	0	30
2	XB	0	23
3	QC	0	24
3	XC	0	16
4	QD	0	18
4	XD	0	8
5	QE	0	13
5	XE	0	15
6	QF	0	6
6	XF	0	5
7	QG	0	10
7	XG	0	10
8	QH	0	14
8	XH	0	6
9	QI	0	22
9	XI	0	9
10	QJ	0	10
10	XJ	0	8
11	QK	0	6
11	XK	0	11
12	QL	0	13
12	XL	0	10
13	QM	0	12
13	XM	0	7
14	QN	0	5
14	XN	0	6
15	QO	0	4
15	XO	0	3
16	QP	0	10
16	XP	0	4
17	QQ	0	7
17	XQ	0	5
18	QR	0	3
18	XR	0	1
19	QS	0	10
19	XS	0	8
20	QT	0	6
20	XT	0	4
21	QU	0	3
21	XU	0	2
25	YA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	RD	0	17
27	YD	0	9
28	RE	0	14
28	YE	0	16
29	RF	0	15
29	YF	0	19
30	RG	0	29
30	YG	0	19
31	RH	0	20
31	YH	0	5
32	RI	0	26
32	YI	0	19
33	RN	0	7
33	YN	0	5
34	RO	0	5
34	YO	0	1
35	RP	0	23
35	YP	0	18
36	RQ	0	4
36	YQ	0	4
37	RR	0	5
37	YR	0	5
38	RS	0	5
38	YS	0	5
39	RT	0	5
39	YT	0	5
40	RU	0	6
40	YU	0	1
41	RV	0	8
41	YV	0	9
42	RW	0	2
42	YW	0	5
43	RX	0	4
43	YX	0	3
44	RY	0	6
44	YY	0	6
45	RZ	0	13
45	YZ	0	22
46	R0	0	5
46	Y0	0	3
47	R1	0	5
47	Y1	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	R2	0	3
48	Y2	0	1
49	R3	0	2
49	Y3	0	4
50	R4	0	10
50	Y4	0	11
51	R5	0	2
51	Y5	0	3
52	R6	0	5
52	Y6	0	5
53	R7	0	4
53	Y7	0	2
54	R8	0	1
54	Y8	0	4
55	R9	0	4
55	Y9	0	1
All	All	0	858

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	88	A	C3'-C2'	11.98	1.66	1.52
22	XV	1	C	OP3-P	-9.54	1.49	1.61
22	QV	1	C	OP3-P	-9.31	1.50	1.61
1	XA	88	A	C1'-N9	7.29	1.59	1.48
1	XA	88	A	C4'-O4'	7.00	1.54	1.45

The worst 5 of 2174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	88	A	O4'-C1'-C2'	16.46	122.42	107.60
1	XA	359	U	C2-N1-C1'	15.95	136.84	117.70
25	YA	2415	G	N3-C2-N2	-15.63	108.96	119.90
23	XX	19	C	N1-C2-O2	13.47	126.98	118.90
1	XA	358	U	N1-C1'-C2'	-12.81	97.35	114.00

There are no chirality outliers.

5 of 858 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	13	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	17	PHE	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16294	685	0
1	XA	32331	0	16338	595	14
2	QB	1907	0	1958	42	0
2	XB	1915	0	1969	45	0
3	QC	1605	0	1668	48	0
3	XC	1605	0	1668	20	1
4	QD	1703	0	1762	81	0
4	XD	1703	0	1763	52	6
5	QE	1133	0	1190	32	0
5	XE	1133	0	1191	23	0
6	QF	837	0	852	11	1
6	XF	837	0	852	15	0
7	QG	1257	0	1296	34	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	33	0
8	XH	1108	0	1165	27	0
9	QI	1010	0	1037	36	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	29	0
10	XJ	777	0	815	16	0
11	QK	844	0	855	29	1
11	XK	844	0	855	22	0
12	QL	958	0	1047	23	0
12	XL	958	0	1047	19	0
13	QM	928	0	987	37	0
13	XM	916	0	973	20	0
14	QN	492	0	530	30	0
14	XN	492	0	528	11	0
15	QO	734	0	771	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	734	0	771	10	0
16	QP	691	0	714	17	0
16	XP	691	0	714	19	0
17	QQ	823	0	891	24	0
17	XQ	823	0	891	20	0
18	QR	555	0	618	11	0
18	XR	555	0	618	8	0
19	QS	665	0	686	13	0
19	XS	665	0	686	20	0
20	QT	743	0	840	22	0
20	XT	759	0	861	24	0
21	QU	199	0	208	10	0
21	XU	199	0	208	8	0
22	QV	1644	0	835	29	0
22	XV	1644	0	836	26	0
23	QX	167	0	86	2	0
23	XX	233	0	120	4	0
24	QY	301	0	152	5	0
24	XY	341	0	175	8	0
25	RA	61819	0	31179	950	3
25	YA	61822	0	31176	961	3
26	RB	2572	0	1305	44	0
26	YB	2573	0	1306	28	0
27	RD	2144	0	2233	57	3
27	YD	2145	0	2234	53	0
28	RE	1563	0	1629	44	0
28	YE	1563	0	1628	44	0
29	RF	1585	0	1632	35	0
29	YF	1585	0	1632	43	0
30	RG	1474	0	1535	40	0
30	YG	1474	0	1535	29	0
31	RH	1336	0	1418	30	0
31	YH	1330	0	1413	28	13
32	RI	1136	0	1223	26	14
32	YI	1136	0	1223	13	0
33	RN	1121	0	1195	25	0
33	YN	1121	0	1195	16	0
34	RO	933	0	996	32	0
34	YO	933	0	996	22	0
35	RP	1139	0	1222	35	0
35	YP	1139	0	1222	36	0
36	RQ	1122	0	1179	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	YQ	1122	0	1179	20	0
37	RR	968	0	1033	22	0
37	YR	968	0	1033	17	0
38	RS	877	0	938	26	0
38	YS	877	0	938	28	0
39	RT	1091	0	1151	25	0
39	YT	1091	0	1151	32	0
40	RU	959	0	1019	28	0
40	YU	959	0	1019	25	0
41	RV	779	0	852	16	0
41	YV	779	0	852	13	6
42	RW	890	0	951	17	1
42	YW	890	0	951	17	0
43	RX	750	0	814	16	0
43	YX	750	0	814	7	0
44	RY	818	0	913	13	0
44	YY	818	0	911	15	14
45	RZ	1552	0	1573	31	0
45	YZ	1461	0	1493	24	0
46	R0	611	0	631	13	0
46	Y0	611	0	631	12	0
47	R1	763	0	848	15	0
47	Y1	763	0	848	11	0
48	R2	592	0	654	10	0
48	Y2	592	0	654	6	1
49	R3	469	0	518	12	0
49	Y3	468	0	518	15	0
50	R4	565	0	556	14	0
50	Y4	565	0	557	13	0
51	R5	459	0	480	8	0
51	Y5	451	0	471	6	3
52	R6	453	0	477	6	0
52	Y6	453	0	477	8	0
53	R7	418	0	467	12	0
53	Y7	418	0	467	8	0
54	R8	517	0	582	15	0
54	Y8	517	0	582	12	0
55	R9	307	0	335	10	0
55	Y9	307	0	338	8	0
56	ZA	74	0	51	13	0
56	ZB	74	0	51	5	0
57	QA	124	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	QC	1	0	0	0	0
57	QD	2	0	0	0	0
57	QE	2	0	0	0	0
57	QL	2	0	0	0	0
57	QM	2	0	0	0	0
57	QN	2	0	0	2	0
57	QO	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	2	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	R9	1	0	0	0	0
57	RA	414	0	0	2	0
57	RB	8	0	0	2	0
57	RD	5	0	0	2	0
57	RE	5	0	0	2	0
57	RF	5	0	0	0	0
57	RN	2	0	0	0	0
57	RO	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	RV	1	0	0	0	0
57	RW	1	0	0	0	0
57	RX	1	0	0	0	0
57	RZ	1	0	0	0	0
57	XA	128	0	0	0	0
57	XD	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XK	2	0	0	0	0
57	XN	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	3	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	544	0	0	1	0
57	YB	8	0	0	0	0
57	YD	8	0	0	0	0
57	YE	7	0	0	1	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	1	0	0	0	0
57	YT	1	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	YX	1	0	0	0	0
58	QD	8	0	0	6	0
58	XD	8	0	0	4	0
59	QN	1	0	0	1	0
59	R4	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
All	All	291822	0	197739	4729	42

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 10.

The worst 5 of 4729 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)
28:RE:152:LYS:HG3	33:RN:77:GLY:O	1.40	1.18
49:Y3:10:LYS:NZ	49:Y3:15:TYR:OH	1.81	1.13
25:YA:2228:G:OP1	27:YD:261:LYS:NZ	1.83	1.12
1:QA:982:U:H3	1:QA:1223:C:N4	1.52	1.08
1:QA:1055:A:H62	1:QA:1200:C:N4	1.56	1.04

The worst 5 of 42 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:YH:46:GLU:CG	44:YY:22:GLY:O[4_445]	1.23	0.97
31:YH:46:GLU:CB	44:YY:22:GLY:O[4_445]	1.41	0.79
32:RI:89:TYR:CD2	1:XA:55:A:C2[4_555]	1.42	0.78
27:RD:134:ARG:NE	4:XD:166:LYS:NZ[4_555]	1.53	0.67
32:RI:89:TYR:CE2	1:XA:55:A:N3[4_555]	1.58	0.62

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	204 (88%)	29 (12%)	0	100	100
2	XB	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	QC	203/239 (85%)	184 (91%)	19 (9%)	0	100	100
3	XC	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	QD	206/209 (99%)	183 (89%)	21 (10%)	2 (1%)	15	54
4	XD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
5	QE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	XE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
11	XK	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	QL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
12	XL	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
13	QM	114/126 (90%)	108 (95%)	6 (5%)	0	100	100
13	XM	112/126 (89%)	102 (91%)	10 (9%)	0	100	100
14	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
20	QT	94/106 (89%)	89 (95%)	5 (5%)	0	100	100
20	XT	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	21 (100%)	0	0	100	100
27	RD	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
27	YD	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
28	RE	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	29	67
28	YE	202/206 (98%)	181 (90%)	21 (10%)	0	100	100
29	RF	200/210 (95%)	192 (96%)	8 (4%)	0	100	100
29	YF	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
30	RG	179/182 (98%)	156 (87%)	23 (13%)	0	100	100
30	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	63
31	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	25	63
32	RI	144/148 (97%)	115 (80%)	28 (19%)	1 (1%)	22	61
32	YI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
33	RN	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
33	YN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
34	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
34	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	RP	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	61
35	YP	147/150 (98%)	135 (92%)	12 (8%)	0	100	100
36	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	YQ	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
37	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
37	YR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
38	YS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
39	RT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
39	YT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
40	RU	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
40	YU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
41	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	54
41	YV	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	54
42	RW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
42	YW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
43	RX	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
43	YX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	194/206 (94%)	181 (93%)	13 (7%)	0	100	100
45	YZ	181/206 (88%)	154 (85%)	27 (15%)	0	100	100
46	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
46	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	Y1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
49	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	Y3	57/60 (95%)	57 (100%)	0	0	100	100
50	R4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
50	Y4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	R7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
53	Y7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
54	R8	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
54	Y8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
55	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11420/12128 (94%)	10610 (93%)	801 (7%)	9 (0%)	51	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	32	ALA
4	QD	31	CYS
30	YG	81	LYS
32	RI	132	PRO
41	RV	50	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	
2	QB	203/220 (92%)	201 (99%)	2 (1%)	76	88
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	83
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	94
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	85
4	QD	180/181 (99%)	175 (97%)	5 (3%)	43	71
4	XD	180/181 (99%)	175 (97%)	5 (3%)	43	71
5	QE	114/123 (93%)	114 (100%)	0	100	100
5	XE	114/123 (93%)	113 (99%)	1 (1%)	78	89
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	87
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	87
7	QG	126/127 (99%)	123 (98%)	3 (2%)	49	74
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	96 (99%)	1 (1%)	76	88
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	86/99 (87%)	85 (99%)	1 (1%)	71	86
11	XK	86/99 (87%)	86 (100%)	0	100	100
12	QL	102/108 (94%)	102 (100%)	0	100	100
12	XL	102/108 (94%)	102 (100%)	0	100	100
13	QM	94/101 (93%)	93 (99%)	1 (1%)	73	87
13	XM	93/101 (92%)	93 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	78 (99%)	1 (1%)	69	85
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	85
16	QP	71/74 (96%)	71 (100%)	0	100	100
16	XP	71/74 (96%)	71 (100%)	0	100	100
17	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	94/97 (97%)	93 (99%)	1 (1%)	73	87
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	58 (98%)	1 (2%)	60	81
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	72/80 (90%)	72 (100%)	0	100	100
20	QT	74/82 (90%)	74 (100%)	0	100	100
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	85
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
27	RD	217/218 (100%)	217 (100%)	0	100	100
27	YD	217/218 (100%)	217 (100%)	0	100	100
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	163 (99%)	2 (1%)	71	86
29	RF	161/166 (97%)	161 (100%)	0	100	100
29	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
30	RG	155/156 (99%)	155 (100%)	0	100	100
30	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
31	RH	145/148 (98%)	145 (100%)	0	100	100
31	YH	144/148 (97%)	142 (99%)	2 (1%)	67	84
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	119/119 (100%)	117 (98%)	2 (2%)	60	81
33	YN	119/119 (100%)	119 (100%)	0	100	100
34	RO	100/100 (100%)	100 (100%)	0	100	100
34	YO	100/100 (100%)	100 (100%)	0	100	100
35	RP	116/116 (100%)	116 (100%)	0	100	100
35	YP	116/116 (100%)	115 (99%)	1 (1%)	78	89
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	89
37	RR	101/101 (100%)	99 (98%)	2 (2%)	55	78
37	YR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	87
38	YS	87/88 (99%)	87 (100%)	0	100	100
39	RT	115/127 (91%)	115 (100%)	0	100	100
39	YT	115/127 (91%)	115 (100%)	0	100	100
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	92 (99%)	1 (1%)	73	87
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	81 (99%)	1 (1%)	71	86
42	RW	91/92 (99%)	91 (100%)	0	100	100
42	YW	91/92 (99%)	91 (100%)	0	100	100
43	RX	77/78 (99%)	77 (100%)	0	100	100
43	YX	77/78 (99%)	77 (100%)	0	100	100
44	RY	88/91 (97%)	87 (99%)	1 (1%)	73	87
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	170/179 (95%)	169 (99%)	1 (1%)	86	94
45	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	86
46	R0	62/67 (92%)	61 (98%)	1 (2%)	62	82
46	Y0	62/67 (92%)	62 (100%)	0	100	100
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	82/83 (99%)	82 (100%)	0	100	100
48	R2	66/67 (98%)	65 (98%)	1 (2%)	65	83
48	Y2	66/67 (98%)	66 (100%)	0	100	100
49	R3	51/52 (98%)	49 (96%)	2 (4%)	32	64
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	62 (100%)	0	100	100
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	62	82
51	R5	51/52 (98%)	50 (98%)	1 (2%)	55	78
51	Y5	50/52 (96%)	49 (98%)	1 (2%)	55	78
52	R6	51/52 (98%)	50 (98%)	1 (2%)	55	78
52	Y6	51/52 (98%)	48 (94%)	3 (6%)	19	54
53	R7	41/42 (98%)	40 (98%)	1 (2%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	33 (97%)	1 (3%)	42	71
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9676/10064 (96%)	9608 (99%)	68 (1%)	84	92

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	YP	32	THR
40	YU	95	LEU
52	Y6	6	ARG
45	RZ	55	HIS
44	RY	99	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
30	YG	58	GLN
32	YI	133	HIS
52	Y6	49	HIS
35	RP	9	ASN
14	XN	52	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1494/1521 (98%)	292 (19%)	14 (0%)
1	XA	1498/1521 (98%)	287 (19%)	14 (0%)
22	QV	76/77 (98%)	18 (23%)	0
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	7/26 (26%)	1 (14%)	1 (14%)
23	XX	10/26 (38%)	7 (70%)	1 (10%)
24	QY	13/18 (72%)	5 (38%)	2 (15%)
24	XY	15/18 (83%)	9 (60%)	1 (6%)
25	RA	2860/2915 (98%)	599 (20%)	21 (0%)
25	YA	2861/2915 (98%)	580 (20%)	19 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	RB	119/122 (97%)	17 (14%)	0
26	YB	119/122 (97%)	24 (20%)	0
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	1 (100%)	0
All	All	9150/9364 (97%)	1857 (20%)	74 (0%)

5 of 1857 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	11	G
1	QA	21	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	752	A
25	YA	2439	A
25	YA	856	C
25	YA	1900	A
25	RA	1073	A

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

50 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
1	M2G	QA	966	1	20,27,28	1.34	3 (15%)	22,40,43	0.99	2 (9%)
1	MA6	XA	1519	1	18,26,27	0.84	0	19,38,41	2.05	6 (31%)
1	4OC	QA	1402	1	20,23,24	0.78	0	26,32,35	0.95	1 (3%)
1	5MC	QA	1407	1	18,22,23	0.88	2 (11%)	26,32,35	1.10	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	OMG	YA	2251	22,25,57	18,26,27	1.19	1 (5%)	19,38,41	1.21	4 (21%)
1	M2G	XA	966	1	20,27,28	1.21	2 (10%)	22,40,43	1.11	3 (13%)
25	PSU	RA	2605	25	18,21,22	1.71	4 (22%)	22,30,33	2.10	5 (22%)
1	MA6	QA	1519	1	18,26,27	0.91	1 (5%)	19,38,41	1.90	6 (31%)
1	5MC	XA	1407	1	18,22,23	0.96	2 (11%)	26,32,35	1.39	5 (19%)
1	UR3	XA	1498	1	19,22,23	1.01	2 (10%)	26,32,35	1.39	2 (7%)
1	5MC	XA	1404	1	18,22,23	1.02	1 (5%)	26,32,35	1.35	3 (11%)
25	PSU	YA	1911	25	18,21,22	1.56	5 (27%)	22,30,33	1.89	4 (18%)
25	5MC	YA	1962	25	18,22,23	1.00	1 (5%)	26,32,35	2.27	8 (30%)
25	PSU	RA	1911	25	18,21,22	1.55	5 (27%)	22,30,33	2.01	4 (18%)
25	OMC	YA	1920	25	19,22,23	0.92	1 (5%)	26,31,34	1.81	5 (19%)
25	OMG	RA	2251	22,25,57	18,26,27	1.13	1 (5%)	19,38,41	1.19	2 (10%)
25	PSU	YA	2605	25	18,21,22	1.60	4 (22%)	22,30,33	2.19	4 (18%)
12	0TD	XL	92	12	7,9,10	1.38	2 (28%)	6,11,13	1.40	1 (16%)
1	2MG	QA	1207	1	18,26,27	1.00	1 (5%)	16,38,41	1.16	3 (18%)
25	5MU	YA	1939	25,57	19,22,23	1.55	4 (21%)	28,32,35	2.20	6 (21%)
1	5MC	XA	967	1	18,22,23	0.96	1 (5%)	26,32,35	1.33	2 (7%)
56	PPU	ZB	3	56,25	32,40,41	0.89	0	33,57,60	1.57	7 (21%)
56	PPU	ZA	3	56,25,57	32,40,41	0.96	1 (3%)	33,57,60	1.82	7 (21%)
1	5MC	QA	1404	1	18,22,23	0.92	1 (5%)	26,32,35	1.42	4 (15%)
25	5MU	RA	1939	25,57	19,22,23	1.45	4 (21%)	28,32,35	2.31	6 (21%)
25	PSU	RA	1917	25	18,21,22	1.47	4 (22%)	22,30,33	2.08	4 (18%)
1	5MC	QA	967	1	18,22,23	0.96	2 (11%)	26,32,35	1.30	2 (7%)
25	2MA	RA	2503	25,57	17,25,26	1.10	1 (5%)	17,37,40	0.98	2 (11%)
25	2MA	YA	2503	25,57	17,25,26	1.26	2 (11%)	17,37,40	0.96	1 (5%)
25	5MU	RA	1915	25	19,22,23	1.57	5 (26%)	28,32,35	2.43	9 (32%)
1	G7M	QA	527	1	20,26,27	2.53	4 (20%)	17,39,42	1.04	1 (5%)
1	PSU	QA	516	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	5 (22%)
1	5MC	XA	1400	1	18,22,23	0.99	2 (11%)	26,32,35	1.25	2 (7%)
1	MA6	QA	1518	1	18,26,27	0.87	1 (5%)	19,38,41	1.92	7 (36%)
25	OMU	RA	2552	25	19,22,23	1.38	3 (15%)	26,31,34	1.95	6 (23%)
25	OMU	YA	2552	25,57	19,22,23	1.41	3 (15%)	26,31,34	2.01	7 (26%)
25	5MC	RA	1942	25	18,22,23	1.07	1 (5%)	26,32,35	1.39	2 (7%)
25	5MC	RA	1962	25,57	18,22,23	0.98	1 (5%)	26,32,35	1.60	7 (26%)
1	PSU	XA	516	57,1	18,21,22	1.37	4 (22%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	QA	1498	1	19,22,23	0.96	2 (10%)	26,32,35	1.34	2 (7%)
1	2MG	XA	1207	1	18,26,27	1.08	1 (5%)	16,38,41	1.25	3 (18%)
1	MA6	XA	1518	1	18,26,27	0.94	1 (5%)	19,38,41	1.72	4 (21%)
1	5MC	QA	1400	1	18,22,23	0.93	1 (5%)	26,32,35	1.22	1 (3%)
25	5MU	YA	1915	25	19,22,23	1.52	5 (26%)	28,32,35	2.51	9 (32%)
25	PSU	YA	1917	25	18,21,22	1.44	3 (16%)	22,30,33	2.01	4 (18%)
25	OMC	RA	1920	25	19,22,23	0.95	1 (5%)	26,31,34	1.87	8 (30%)
1	4OC	XA	1402	1	20,23,24	0.85	1 (5%)	26,32,35	0.95	2 (7%)
12	0TD	QL	92	12	7,9,10	1.40	1 (14%)	6,11,13	2.18	3 (50%)
25	5MC	YA	1942	25	18,22,23	1.17	2 (11%)	26,32,35	1.54	2 (7%)
1	G7M	XA	527	1	20,26,27	2.49	4 (20%)	17,39,42	1.00	1 (5%)

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
1	M2G	QA	966	1	-	0/7/29/30	0/3/3/3
1	MA6	XA	1519	1	-	6/7/29/30	0/3/3/3
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	QA	1407	1	-	0/7/25/26	0/2/2/2
25	OMG	YA	2251	22,25,57	-	0/5/27/28	0/3/3/3
1	M2G	XA	966	1	-	2/7/29/30	0/3/3/3
25	PSU	RA	2605	25	-	0/7/25/26	0/2/2/2
1	MA6	QA	1519	1	-	5/7/29/30	0/3/3/3
1	5MC	XA	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	XA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	XA	1404	1	-	0/7/25/26	0/2/2/2
25	PSU	YA	1911	25	-	0/7/25/26	0/2/2/2
25	5MC	YA	1962	25	-	4/7/25/26	0/2/2/2
25	PSU	RA	1911	25	-	0/7/25/26	0/2/2/2
25	OMC	YA	1920	25	-	4/9/27/28	0/2/2/2
25	OMG	RA	2251	22,25,57	-	0/5/27/28	0/3/3/3
25	PSU	YA	2605	25	-	0/7/25/26	0/2/2/2
12	0TD	XL	92	12	-	4/7/12/14	-
1	2MG	QA	1207	1	-	0/5/27/28	0/3/3/3
25	5MU	YA	1939	25,57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	XA	967	1	-	0/7/25/26	0/2/2/2
56	PPU	ZB	3	56,25	-	5/21/43/44	0/4/4/4
56	PPU	ZA	3	56,25,57	-	5/21/43/44	0/4/4/4
1	5MC	QA	1404	1	-	0/7/25/26	0/2/2/2
25	5MU	RA	1939	25,57	-	0/7/25/26	0/2/2/2
25	PSU	RA	1917	25	-	0/7/25/26	0/2/2/2
1	5MC	QA	967	1	-	0/7/25/26	0/2/2/2
25	2MA	RA	2503	25,57	-	1/3/25/26	0/3/3/3
25	2MA	YA	2503	25,57	-	2/3/25/26	0/3/3/3
25	5MU	RA	1915	25	-	3/7/25/26	0/2/2/2
1	G7M	QA	527	1	-	2/3/25/26	0/3/3/3
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
1	5MC	XA	1400	1	-	4/7/25/26	0/2/2/2
1	MA6	QA	1518	1	-	1/7/29/30	0/3/3/3
25	OMU	RA	2552	25	-	3/9/27/28	0/2/2/2
25	OMU	YA	2552	25,57	-	2/9/27/28	0/2/2/2
25	5MC	RA	1942	25	-	0/7/25/26	0/2/2/2
25	5MC	RA	1962	25,57	-	0/7/25/26	0/2/2/2
1	PSU	XA	516	57,1	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	2/7/25/26	0/2/2/2
1	2MG	XA	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	XA	1518	1	-	1/7/29/30	0/3/3/3
1	5MC	QA	1400	1	-	5/7/25/26	0/2/2/2
25	5MU	YA	1915	25	-	4/7/25/26	0/2/2/2
25	PSU	YA	1917	25	-	0/7/25/26	0/2/2/2
25	OMC	RA	1920	25	-	4/9/27/28	0/2/2/2
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	QL	92	12	-	4/7/12/14	-
25	5MC	YA	1942	25	-	0/7/25/26	0/2/2/2
1	G7M	XA	527	1	-	2/3/25/26	0/3/3/3

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	QA	527	G7M	C8-N9	7.06	1.46	1.33
1	XA	527	G7M	C8-N9	7.02	1.46	1.33
1	QA	527	G7M	C8-N7	6.58	1.45	1.33
1	XA	527	G7M	C8-N7	6.18	1.44	1.33
25	RA	1915	5MU	C4-N3	-3.96	1.31	1.38

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1917	PSU	N1-C2-N3	6.22	122.18	115.13
25	RA	1915	5MU	N3-C2-N1	6.21	123.14	114.89
25	RA	2605	PSU	N1-C2-N3	6.14	122.09	115.13
25	RA	1911	PSU	N1-C2-N3	6.13	122.08	115.13
25	YA	1917	PSU	N1-C2-N3	6.11	122.06	115.13

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	QL	92	0TD	O-C-CA-CB
12	QL	92	0TD	CA-CB-SB-CSB
12	QL	92	0TD	CG-CB-SB-CSB
1	QA	527	G7M	O4'-C4'-C5'-O5'
1	QA	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	QA	966	M2G	1	0
1	QA	1402	4OC	1	0
25	YA	2251	OMG	1	0
1	QA	1519	MA6	1	0
1	XA	1407	5MC	1	0
1	XA	1404	5MC	2	0
25	YA	1962	5MC	1	0
25	YA	1920	OMC	2	0
25	RA	2251	OMG	2	0
12	XL	92	0TD	1	0
25	YA	1939	5MU	1	0
1	XA	967	5MC	1	0
56	ZB	3	PPU	4	0
56	ZA	3	PPU	10	0
25	RA	2503	2MA	2	0
25	YA	2503	2MA	1	0
25	RA	2552	OMU	3	0
25	YA	2552	OMU	2	0
25	RA	1942	5MC	1	0
1	XA	1207	2MG	2	0
1	XA	1518	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	QA	1400	5MC	1	0
25	YA	1917	PSU	1	0
25	RA	1920	OMC	1	0
1	XA	1402	4OC	1	0
12	QL	92	0TD	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1328 ligands modelled in this entry, 1326 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	XD	302	4	0,12,12	-	-	-		
58	SF4	QD	303	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	XD	302	4	-	-	0/6/5/5
58	SF4	QD	303	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XD	302	SF4	4	0
58	QD	303	SF4	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.