



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 08:57 AM BST

PDB ID : 6ORD
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-30
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
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)	:	2.13

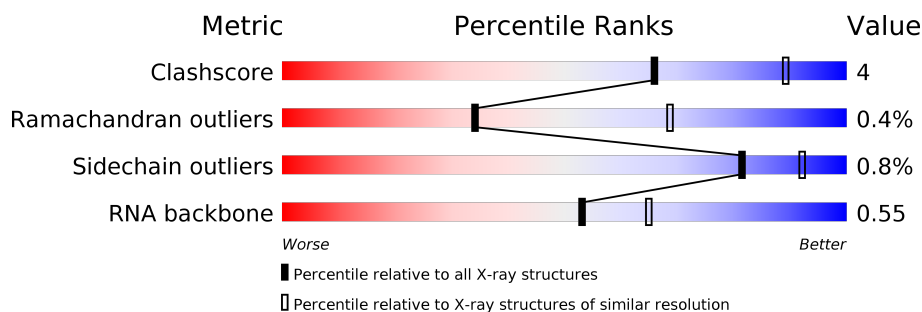
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)















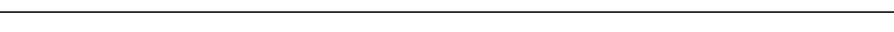

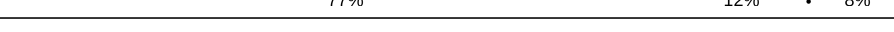

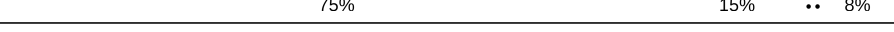



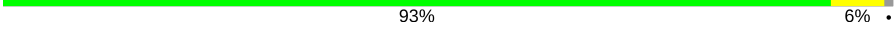


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	69% 25% . .
1	XA	1522	69% 25% . .
2	QB	256	71% 18% . 10%
2	XB	256	74% 16% 10%
3	QC	239	74% 11% . 14%
3	XC	239	75% 10% 14%
4	QD	209	80% 18% .

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Mol	Chain	Length	Quality of chain
4	XD	209	 84% 16%
5	QE	162	 76% 15% 9%
5	XE	162	 78% 14% 9%
6	QF	101	 87% 12% .
6	XF	101	 77% 20% ..
7	QG	156	 81% 17% ..
7	XG	156	 91% 8% .
8	QH	138	 80% 19% .
8	XH	138	 84% 15% .
9	QI	128	 74% 23% ..
9	XI	128	 73% 26% .
10	QJ	105	 78% 14% 8%
10	XJ	105	 74% 17% 9%
11	QK	129	 74% 14% 12%
11	XK	129	 76% 12% 12%
12	QL	132	 77% 12% . 8%
12	XL	132	 75% 16% .. 8%
13	QM	126	 75% 15% .. 8%
13	XM	126	 67% 22% . 10%
14	QN	61	 85% 13% .
14	XN	61	 84% 15% .
15	QO	89	 93% 6% .
15	XO	89	 92% 7% .
16	QP	88	 78% 13% . 7%
16	XP	88	 72% 18% .. 7%


























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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	

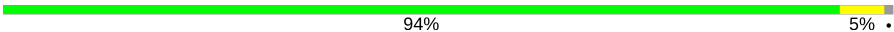













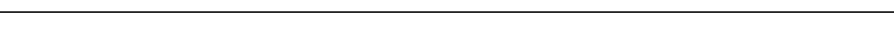

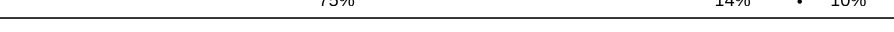

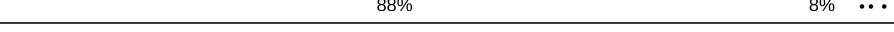

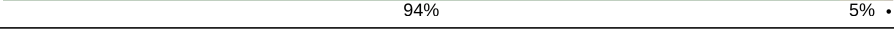




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Mol	Chain	Length	Quality of chain
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	
40	YG	182	
41	RH	180	
41	YH	180	

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Mol	Chain	Length	Quality of chain
42	RI	148	 94% 5% .
42	YI	148	 93% 6% .
43	RN	140	 84% 15% .
43	YN	140	 91% 9%
44	RO	122	 80% 20% .
44	YO	122	 79% 21%
45	RP	150	 81% 18% .
45	YP	150	 79% 20% .
46	RQ	141	 82% 18%
46	YQ	141	 87% 13%
47	RR	118	 92% 8%
47	YR	118	 89% 11%
48	RS	112	 84% 13% ..
48	YS	112	 88% 9% ..
49	RT	146	 73% 16% • 10%
49	YT	146	 75% 14% • 10%
50	RU	118	 85% 12% ...
50	YU	118	 88% 8% ...
51	RV	101	 79% 18% .
51	YV	101	 94% 5% .
52	RW	113	 88% 11% .
52	YW	113	 88% 12% .
53	RX	96	 85% 14% .
53	YX	96	 91% 8% .
54	RY	110	 86% 11% .

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Mol	Chain	Length	Quality of chain
54	YY	110	<div><div></div><div>79%</div><div>17%</div><div>••</div></div>
55	RZ	206	<div><div></div><div>74%</div><div>12%</div><div>14%</div></div>
55	YZ	206	<div><div></div><div>74%</div><div>11%</div><div>•</div><div>14%</div></div>

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 293819 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	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
2	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	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
			1665	1043	329	286	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	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
			814	516	144	151	3			
6	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			1235	769	244	216	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	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
			1098	694	210	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	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
			986	625	193	168				
9	XI	126	Total	C	N	O		0	0	0
			966	613	186	167				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	97	Total	C	N	O		0	0	0
			719	446	142	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O			
			710	442	137	131	0	0	0

- 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		
			834	520	156	155	3	0	0
11	XK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- 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		
			932	586	185	159	2	0	0
12	XL	122	Total	C	N	O	S		
			932	586	185	159	2	0	0

- 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		
			914	564	189	159	2	0	0
13	XM	114	Total	C	N	O	S		
			895	550	186	157	2	0	0

- 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		
			492	312	104	72	4	0	0
14	XN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- 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		
			728	456	144	126	2	0	0
15	XO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- 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
			681	433	134	113	1			
16	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	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
			648	415	120	111	2			
19	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	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
			732	449	157	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	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
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 24 is a RNA chain called A-site tRNA^{Ala}(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			
24	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
25	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
27	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O		0	0	0
			469	298	90	81				
28	Y3	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
31	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
35	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
36	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
37	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
41	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
43	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
48	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
49	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
52	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
54	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	178	Total	C	N	O	S	0	0	0
			1406	898	253	253	2			
55	YZ	177	Total	C	N	O	S	0	0	0
			1381	885	246	248	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	221	Total	Mg	0	0
			221	221		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	3	Total	Mg	0	0
			3	3		
56	R7	3	Total	Mg	0	0
			3	3		
56	YA	707	Total	Mg	0	0
			707	707		
56	Y5	1	Total	Mg	0	0
			1	1		
56	YR	2	Total	Mg	0	0
			2	2		
56	RT	4	Total	Mg	0	0
			4	4		
56	QD	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	2	Total 2	Mg 2	0	0
56	XE	2	Total 2	Mg 2	0	0
56	RG	4	Total 4	Mg 4	0	0
56	QI	1	Total 1	Mg 1	0	0
56	YD	7	Total 7	Mg 7	0	0
56	QV	5	Total 5	Mg 5	0	0
56	YE	5	Total 5	Mg 5	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	193	Total 193	Mg 193	0	0
56	Y1	2	Total 2	Mg 2	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	R0	3	Total 3	Mg 3	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QL	3	Total 3	Mg 3	0	0
56	RU	2	Total 2	Mg 2	0	0
56	QG	2	Total 2	Mg 2	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	Y7	2	Total 2	Mg 2	0	0
56	QH	2	Total 2	Mg 2	0	0

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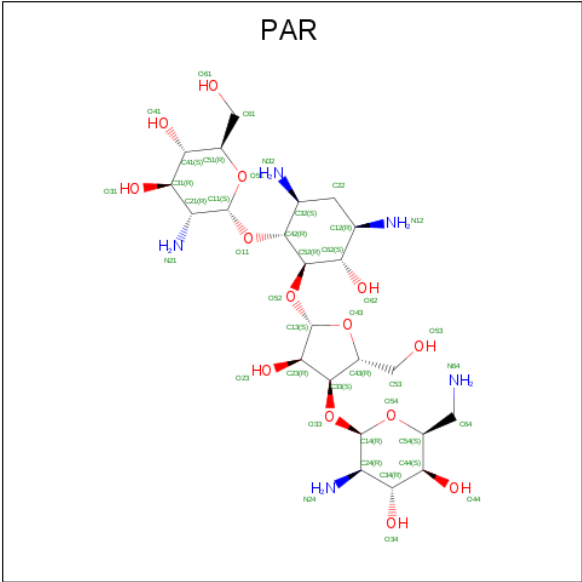
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YG	3	Total 3	Mg 3	0	0
56	XY	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	2	Total 2	Mg 2	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RD	8	Total 8	Mg 8	0	0
56	R1	1	Total 1	Mg 1	0	0
56	QO	2	Total 2	Mg 2	0	0
56	YT	3	Total 3	Mg 3	0	0
56	RV	3	Total 3	Mg 3	0	0
56	QF	2	Total 2	Mg 2	0	0
56	RH	2	Total 2	Mg 2	0	0
56	R5	2	Total 2	Mg 2	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	RA	709	Total 709	Mg 709	0	0
56	QK	1	Total 1	Mg 1	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YP	2	Total 2	Mg 2	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0

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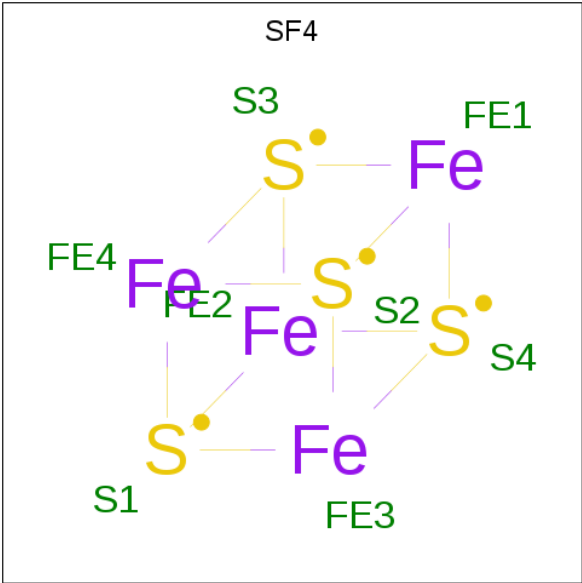
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R9	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	XL	2	Total 2	Mg 2	0	0
56	YB	20	Total 20	Mg 20	0	0
56	QT	1	Total 1	Mg 1	0	0
56	Y6	1	Total 1	Mg 1	0	0
56	QN	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	1	Total 1	Mg 1	0	0
56	R6	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	QP	1	Total 1	Mg 1	0	0
56	RB	17	Total 17	Mg 17	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	4	Total 4	Mg 4	0	0
56	XR	1	Total 1	Mg 1	0	0
56	RF	4	Total 4	Mg 4	0	0
56	R3	3	Total 3	Mg 3	0	0
56	Y3	1	Total 1	Mg 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	QA	1	Total	C	N	O	0	0
			42	23	5	14		
57	XA	1	Total	C	N	O	0	0
			42	23	5	14		

- 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).

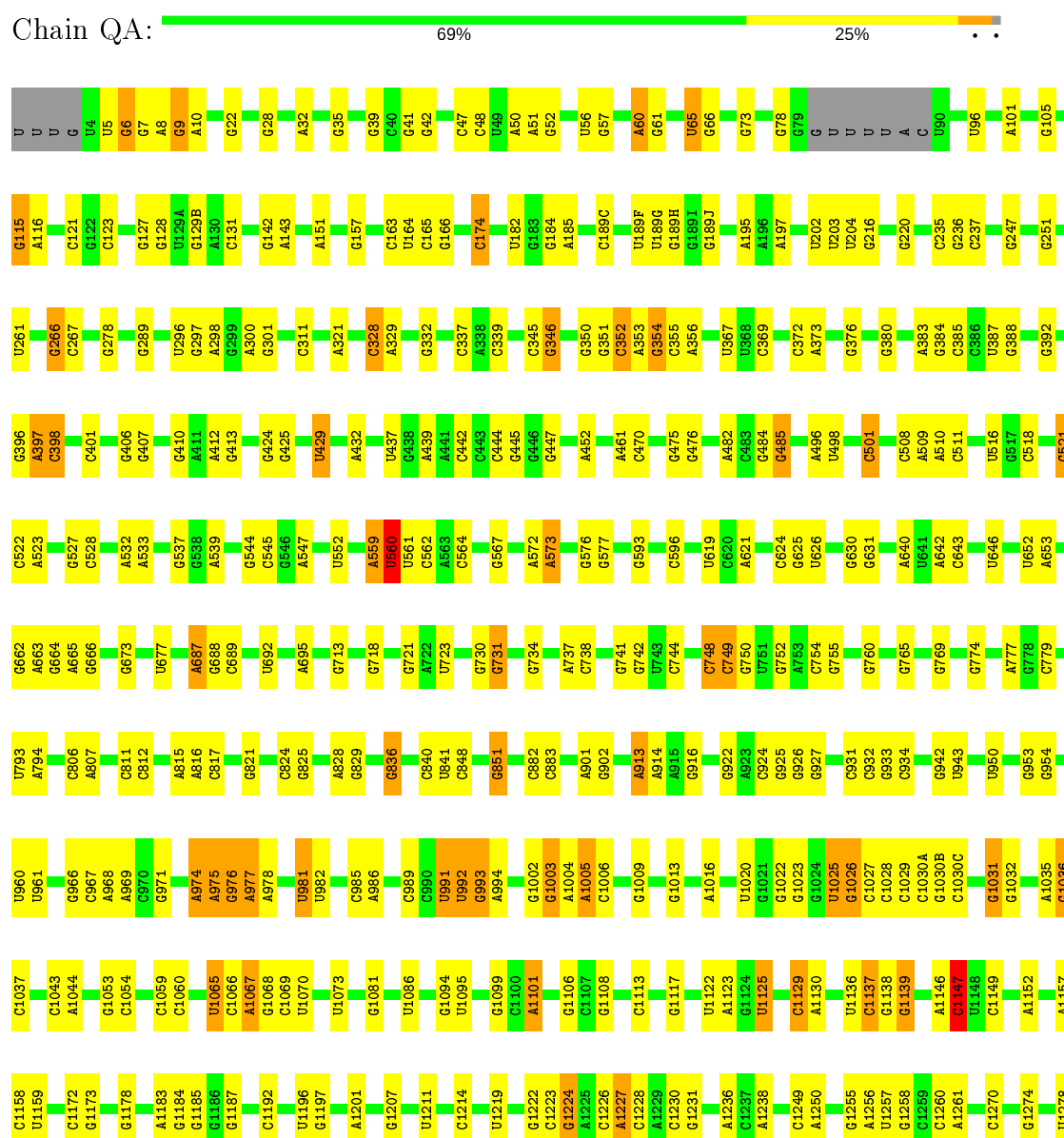
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	Y5	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0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

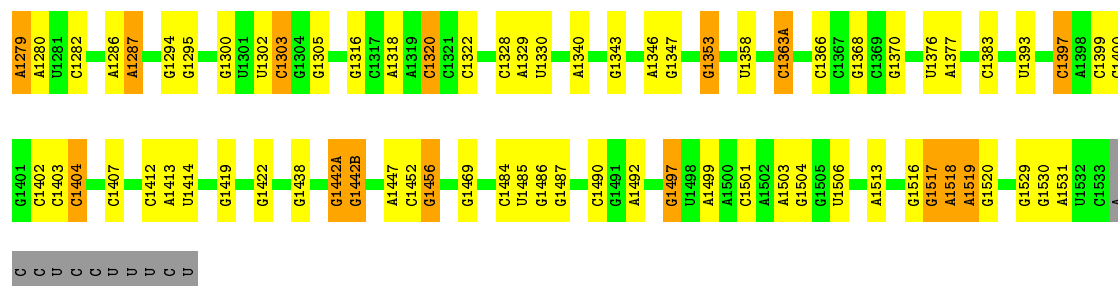
3 Residue-property plots [i](#)

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.

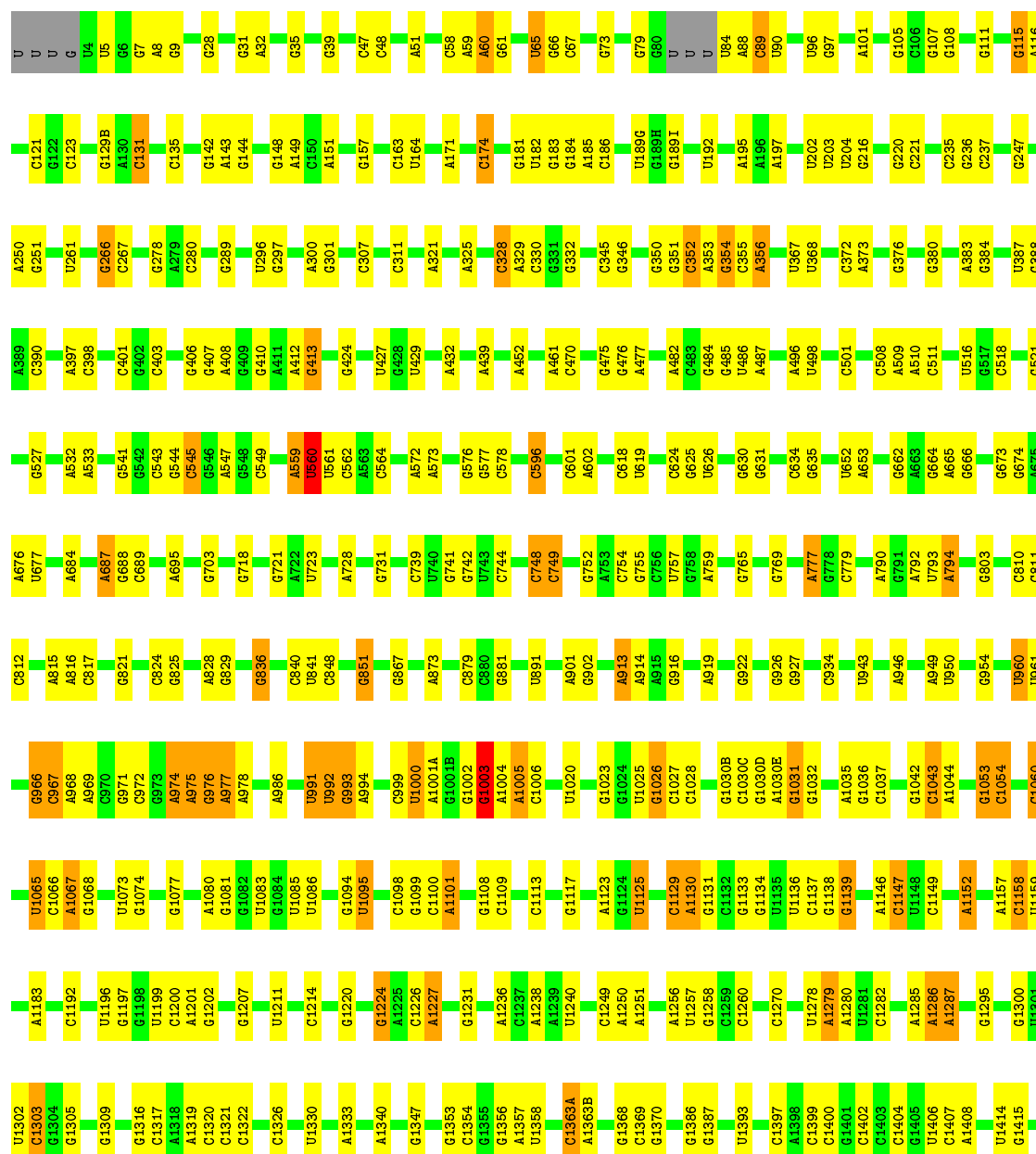
• Molecule 1: 16S rRNA

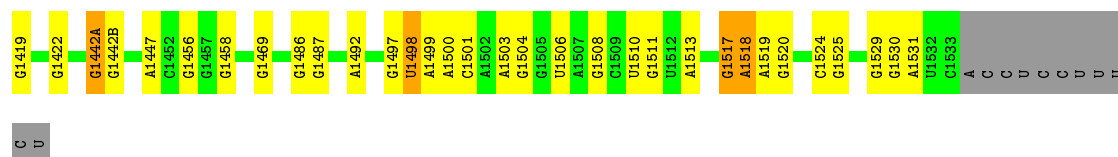




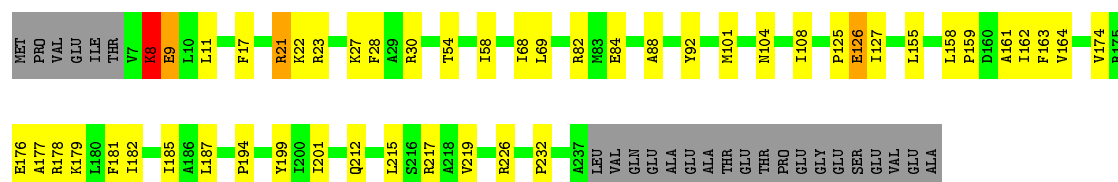
• Molecule 1: 16S rRNA

Chain XA:  69% 25% . .

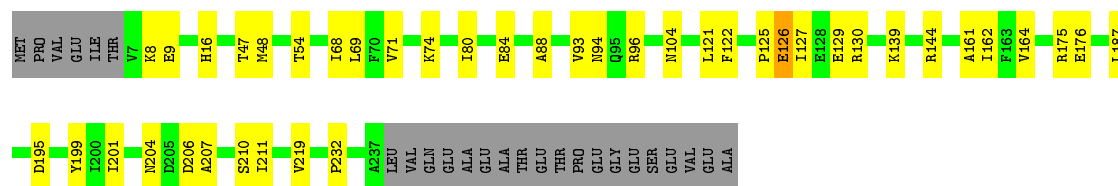
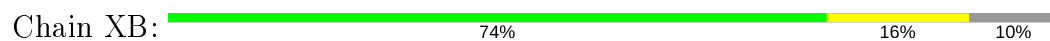




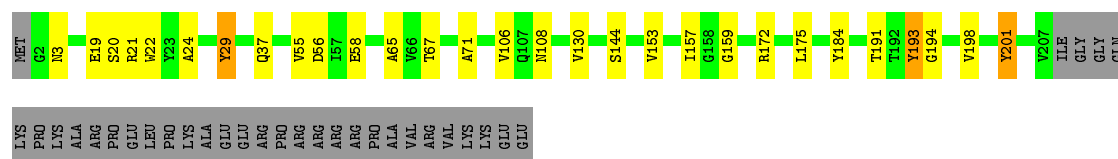
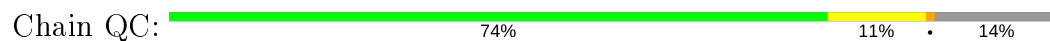
- Molecule 2: 30S ribosomal protein S2



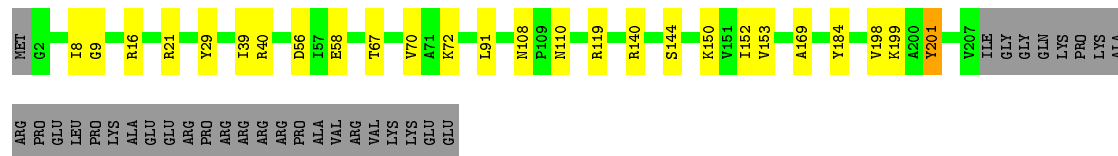
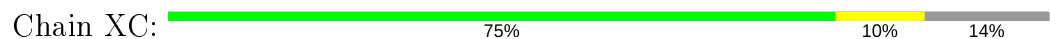
- Molecule 2: 30S ribosomal protein S2



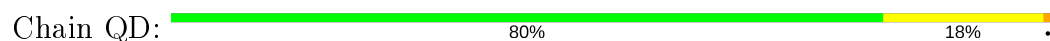
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



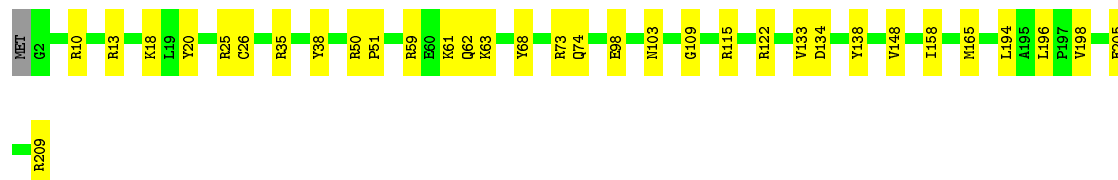
- Molecule 4: 30S ribosomal protein S4





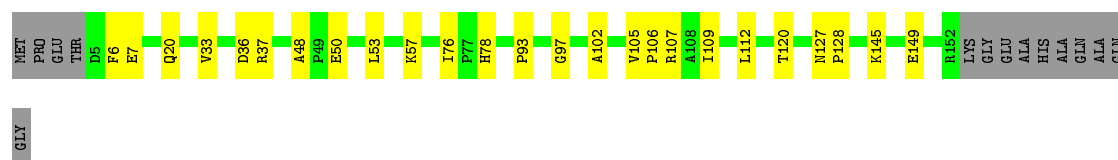
- Molecule 4: 30S ribosomal protein S4

Chain XD: 84% 16%



- Molecule 5: 30S ribosomal protein S5

Chain QE: 76% 15% 9%



- Molecule 5: 30S ribosomal protein S5

Chain XE: 78% 14% 9%



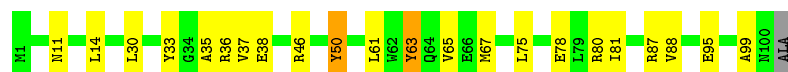
- Molecule 6: 30S ribosomal protein S6

Chain QF: 87% 12%




- Molecule 6: 30S ribosomal protein S6

Chain XF: 77% 20%



- Molecule 7: 30S ribosomal protein S7

Chain QG:  81% 17% ..




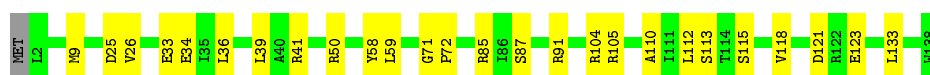
- Molecule 7: 30S ribosomal protein S7

Chain XG:  91% 8% .




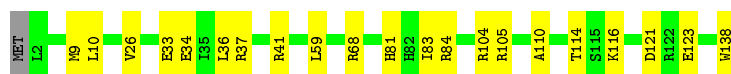
- Molecule 8: 30S ribosomal protein S8

Chain QH:  80% 19% .



- Molecule 8: 30S ribosomal protein S8

Chain XH:  84% 15% .



- Molecule 9: 30S ribosomal protein S9

Chain QI:  74% 23% ..




- Molecule 9: 30S ribosomal protein S9

Chain XI:  73% 26% .



- Molecule 10: 30S ribosomal protein S10

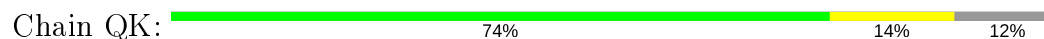
Chain QJ:  78% 14% 8%



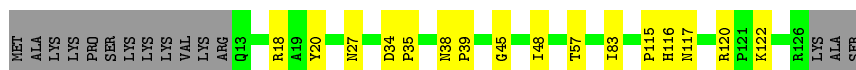
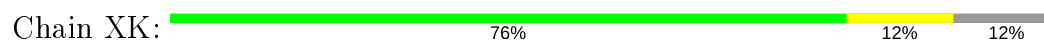
- Molecule 10: 30S ribosomal protein S10



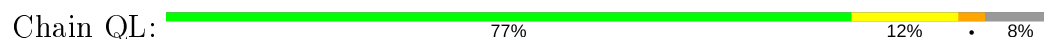
- Molecule 11: 30S ribosomal protein S11



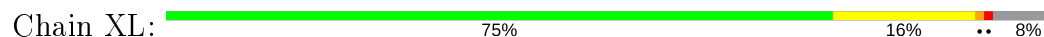
- Molecule 11: 30S ribosomal protein S11



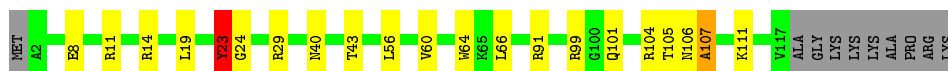
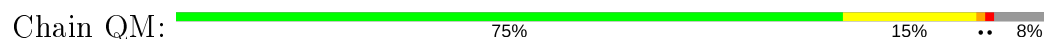
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



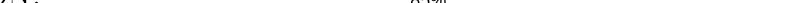
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13




- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 



- Molecule 15: 30S ribosomal protein S15

Chain QO:  93% 6%




- Molecule 15: 30S ribosomal protein S15

Chain XO: 92% 7%



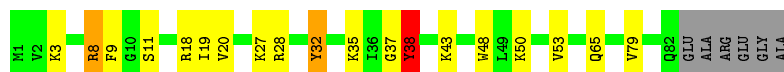
- Molecule 16: 30S ribosomal protein S16

Chain QP:  78% 13% 7%




- Molecule 16: 30S ribosomal protein S16

Chain XP: 72% 18% 7%




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  81% 13% 6%



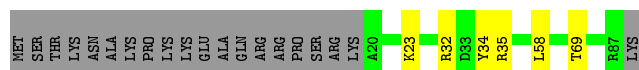
- Molecule 17: 30S ribosomal protein S17

Chain XQ:  78% 16% 6%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  70% 7% 23%




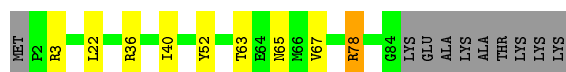
- Molecule 18: 30S ribosomal protein S18

Chain XR:  64% 14% 23%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  80% 9% 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  76% 13% 11%




- Molecule 20: 30S ribosomal protein S20

Chain QT:  79% 11% 9%




- Molecule 20: 30S ribosomal protein S20

Chain XT:  86% 7% 8%




- Molecule 21: 30S ribosomal protein Thx

Chain QU:  81% 15%



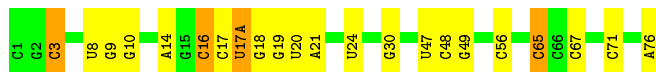
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  85% 15%




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

Chain QV:  71% 23% 5%



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

Chain XV:  77% 18% 5% 2%



- Molecule 23: mRNA

Chain QX:  53% 37% 5% 5%



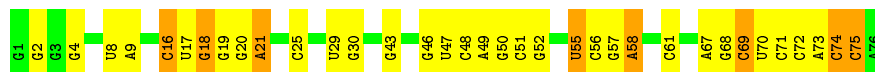
- Molecule 23: mRNA

Chain XX:  42% 47% 5% 5%



- Molecule 24: A-site tRNA^{Ala}(GGC) U32-A38

Chain QY:  54% 36% 11%




- Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain XY:  47% 43% 9%



- Molecule 25: 50S ribosomal protein L27

Chain R0:  76% 13% 9%




- Molecule 25: 50S ribosomal protein L27

Chain Y0:  71% 19% 9%



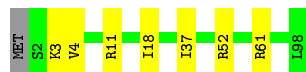
- Molecule 26: 50S ribosomal protein L28

Chain R1:  86% 13% 1%




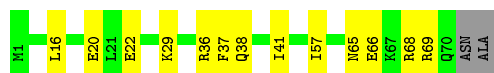
- Molecule 26: 50S ribosomal protein L28

Chain Y1:  92% 7% 1%




- Molecule 27: 50S ribosomal protein L29

Chain R2:  79% 18% 3%



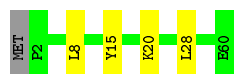
- Molecule 27: 50S ribosomal protein L29

Chain Y2:  85% 13% .




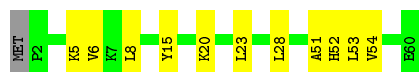
- Molecule 28: 50S ribosomal protein L30

Chain R3:  92% 7% .




- Molecule 28: 50S ribosomal protein L30

Chain Y3:  80% 18% .



- Molecule 29: 50S ribosomal protein L31

Chain R4:  77% 20% .




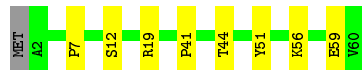
- Molecule 29: 50S ribosomal protein L31

Chain Y4:  68% 24% . . .




- Molecule 30: 50S ribosomal protein L32

Chain R5:  85% 13% .



- Molecule 30: 50S ribosomal protein L32

Chain Y5:  85% 13% .




- Molecule 31: 50S ribosomal protein L33

Chain R6:  89% 9%




- Molecule 31: 50S ribosomal protein L33

Chain Y6:  85% 13%




- Molecule 32: 50S ribosomal protein L34

Chain R7:  86% 12%



- Molecule 32: 50S ribosomal protein L34

Chain Y7:  84% 14%




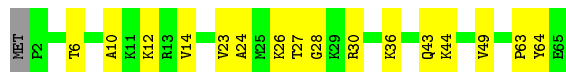
- Molecule 33: 50S ribosomal protein L35

Chain R8:  72% 26%




- Molecule 33: 50S ribosomal protein L35

Chain Y8:  74% 25%



- Molecule 34: 50S ribosomal protein L36

Chain R9:  78% 22%



- Molecule 34: 50S ribosomal protein L36

Chain Y9:  73% 27%

M1 V16 R22 V25 I26 E28 Q34 R35 Q36 G37

• Molecule 35: 23S rRNA

Chain RA:  71% 23%

G U C A G G10 G15 A221 C18 C34 C39 C45 G51 A71 A74 G75 G83 A84 G102 C116 G117 A118 A119 U120 A126 G131 G139A G143A U157 U A277 U G171 A181 A182 G188 A195 A196 A197 C198 A199

U200 G205 G214 G215 A216 G220 A221 A222 A223 A229 U230 A233 C237 G242 G248 C249 G252 A265 U269 A270 A271 U272L U272M U272N G272Q G272R G273B G273C A276 C277 C297 G298 A299 G307 G310 G311 G312 G313 G317

G318 C319 A320 G321 A322 G323 A324 G329 A330 A331 G338 G339 A340 G341 G342 A345 G352 U362 G363A G365 G372 G386 A390 G391 C392 G396 U405 C409 G411 G412 C420 A428 C435 G442 A443 C444 C451 C452 C453 A454 C455 C456

A457 G458 U459 A460 C461 C462 G463 A466 G468 G469 A470 A475 U479 A480 G481 G491 G500 G503 U504 A505 G508 U514B G510 G521 G522 G526 G527 A528 A529 G530 A532 G533 U534 C535 G545 C A G546 A G549 A622C G622D C652E G652F G G C C G

G573 C574 A575 U576 G577 A578 G579 C580 C581 A586 C587 U588 G600 G601 G602 A603 C605 U606 U607 A608 A609 G613 U614A G614B G614C A614D G615 G620 G624 A627 A631 G634 G635 G636 A637 G645 A646 G647 A652C G652D C652E G652F G G C C G

C A C G C G C C C652U G652V A655 G660 G666 G669 C679 G680 G685 G686 G693 G698 A861 G717 G726 A727 G728 G729 C730 A734 G743 A752 C753 A764 G765 C766 A774 G775 G776 A782 A783 A784 G785 A788 A789

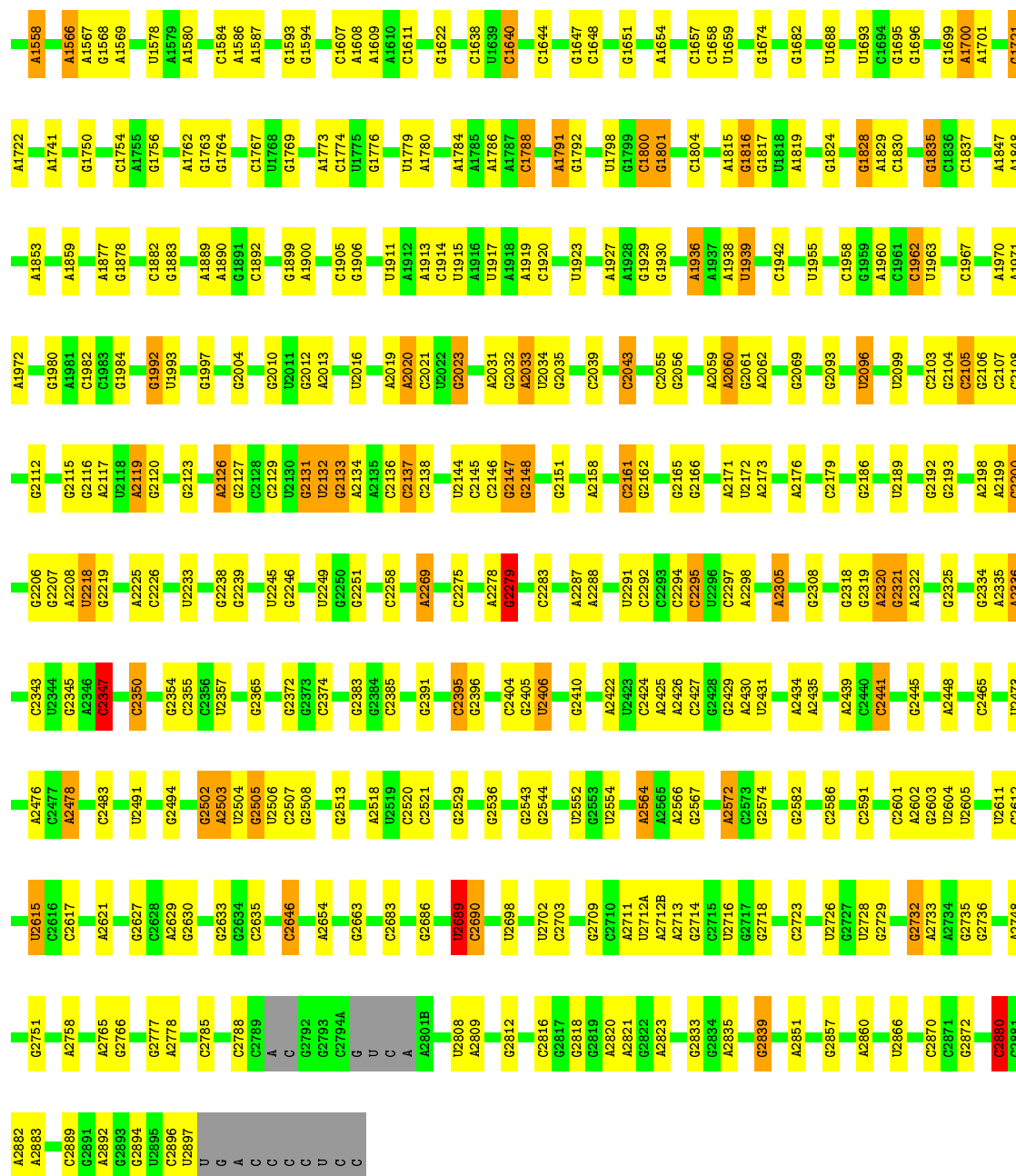
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A918 G919 U922 G932 A941 G944 A945 G946 A953 G954 G955 G956 G957 U958 A959 G961 G974 C975A G975B C976 A983 U980 A984 A985 G986 G987 G988 G989 A1000 G1005 G1006 C1007 G1008 A1009 U1012 C1013 A1021 G1022 U1023 G1024 G1025 U1026 U1033 C1038

C1041 G1042 G1043 G1044 A1045 A1046 G1047 A1048 G1051 C1052 G1053 A1054 G1055 G1056 G1057 A1058 U1059 U1060 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 G1072 A1073 G1074 C1075 A1076 A1077 U1078 C1079 U1082 A1083 A1084 A1085 A1086 A1087 A1088 G1089 U1090 G1091 C1092 G1093 A1094 A1095 A1096 U1097 A1098 C1102 A1103

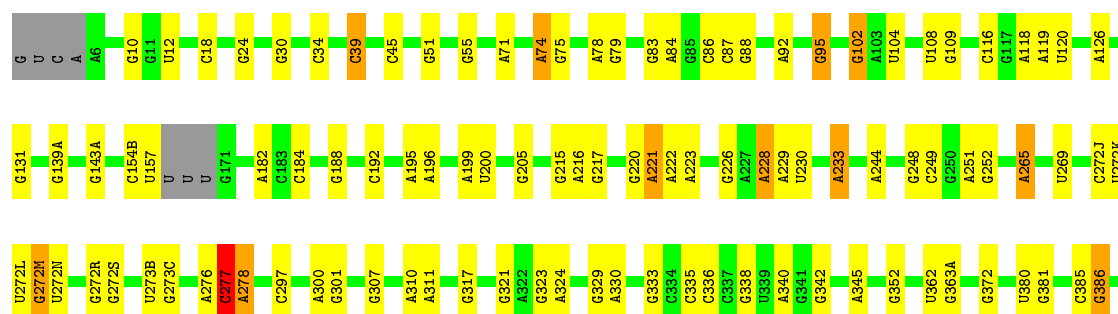
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A1253 A1254 U1255 G1256 C1257 G1284 A1285 G1286 G1271 A1272 U1273 U1288 U1300 A1301 G1309 G1310 G1311 U1312 U1313 C1314 G1333 U1341 A1352 A1353 A1359 A1360 A1365 A1366 A1367 G1368 G1369 C1370 C1376 G1514 G1515 G1516 G1517 G1533 U A C1536 A1542 C1543 C1546 G1418 A1554




• Molecule 35: 23S rRNA

Chain YA: 71% 23% • •




A2225	U2118	G1816	G1533	U1394	A1220	C1082	A1009	G692	G775	G649	G549	G396
A2119	A2119	G1824	U	A1395	G1223	C1082	U1012	C893	G776	A652C	U557	U405
G2120	C1536	G1674	A	G1400	A1226	A1095	C1013	U895	A782	G652D	U557	G411
G2121	G1537	G1828	G1538	G1401	G1236	U1097	G1022	A896	A783	C652E	C560	A412
G2122	G1539	A1829	G1539	U1415	G1243	A1098	U1023	C997	A784	G652F	G563	C413
A2126	U1540	C1830	U1540	G1416	G1243	G1099	G1024	G906	G786	G	C564	C414
G2127	G1541	G1835	G1541	G1418	G1243	C1102	G1025	U907	C786	G	C565	A415
C2128	A1542	G1835	A1542	G1419	G1243	C1103	U1026	U907	U787	C	C574	C420
C2129	C1543	G1835	C1543	U1420	G1250	A1103	U1026	U907	U788	C	C574	C420
U2130	G1697	A1847	G1697	G1421	A1253	U1104	U1033	A910	A789	C	A575	A428
G2131	A1546	A1848	C1547	G1422	A1253	U1105	G1034	A910	A789	C	A575	A428
U2132	C1547	A1853	C1547	G1423	G1256	G1107	U1035	C915	G792	C	A575	A428
A2134	A1558	A1701	A1558	G1424	G1256	U1108	C1038	G916	A793	G	A575	A428
A2135	A1566	G1721	A1566	G1425	G1266	C1109	C1038	A917	G794	C	A575	A428
C2136	A1567	A1722	A1567	G1426	G1266	G1110	C1041	A918	C795	G	A575	A428
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C2138	A1569	G1750	A1569	C1437	A1272	U1112	A1045	G932	A802	C	A575	A428
U2144	A1572	G1754	U1578	A1445A	A1273	U1113	A1046	G932	A802	C	A575	A428
C2145	U1578	A1755	U1578	G1450A	A1278	U1114	G1047	A941	A802	C	A575	A428
C2146	A1579	A1755	A1579	G1450A	A1278	U1114	G1047	A941	A802	C	A575	A428
G2147	A1580	U1757	A1580	U1453	U1288	A1129	G1055	A944	A802	C	A575	A428
G2148	A1584	A1762	A1584	G1455	U1300	U1130	A1057	A945	A802	C	A575	A428
G2149	A1586	G1763	A1586	G1459	A1301	G1135	G1059	A945	A802	C	A575	A428
C2150	G1594	G1764	G1594	A1460	G1309	G1136	U1060	A945	A802	C	A575	A428
C2151	A1603	C1773	A1603	G1466	U1313	A1143	U	A945	A802	C	A575	A428
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C2154	C1611	A1780	C1611	A1471	U1316	G1154	A1067	A945	A802	C	A575	A428
C2155	G1622	A1784	G1622	G1471	A1317	C1155	G1068	A945	A802	C	A575	A428
C2156	C1640	A1785	C1640	A1493	U1327	G1156	A1069	A945	A802	C	A575	A428
C2157	A1786	A1786	A1786	A1494	U1352	A1156	A1070	A945	A802	C	A575	A428
C2158	C1788	C1788	C1788	U1497	A1353	G1171	G1071	A945	A802	C	A575	A428
C2159	A1789	C1790	A1789	G1500	A1365	C1178	C1072	A945	A802	C	A575	A428
C2160	C1790	A1791	C1790	A1508	A1368	U1188	A1073	A945	A802	C	A575	A428
C2161	U1955	G1792	U1955	C1509A	U1372	A1189	C1074	A945	A802	C	A575	A428
C2162	C1962	C1962	C1962	A1509B	A1378	G1206	C1076	A945	A802	C	A575	A428
C2163	U1963	U1963	U1963	G1520	A1379	U1081	C1076	A945	A802	C	A575	A428
C2164	C1967	C1967	C1967	G1525	G1380	A1210	U1073	A945	A802	C	A575	A428
C2165	A1970	A1970	A1970	C1531	A1384	U1211	A1085	A945	A802	C	A575	A428
C2166	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
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C2193	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
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C2195	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
C2196	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
C2197	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
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C2232	A1972	A1972	A1972	C1532	G1385	A1214	A1086	A945	A802	C	A575	A428
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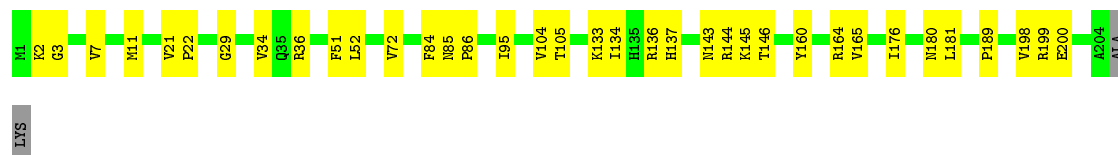
- Molecule 38: 50S ribosomal protein L3

Chain RE:  86% 13%




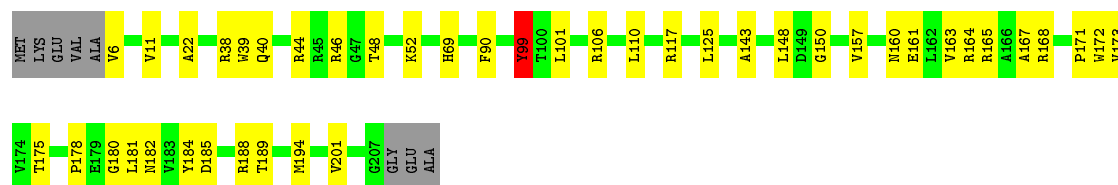
- Molecule 38: 50S ribosomal protein L3

Chain YE:  82% 17%




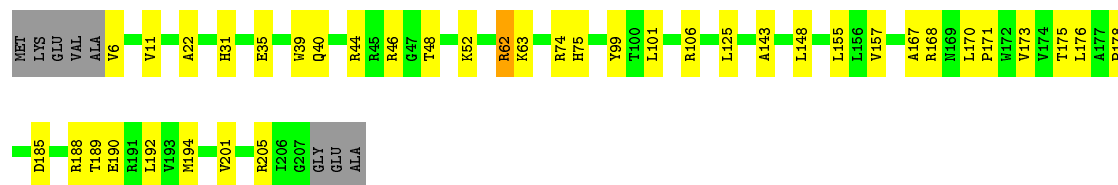
- Molecule 39: 50S ribosomal protein L4

Chain RF:  76% 20%




- Molecule 39: 50S ribosomal protein L4

Chain YF:  78% 18%




- Molecule 40: 50S ribosomal protein L5

Chain RG:  87% 12%



- Molecule 40: 50S ribosomal protein L5

Chain YG:  80% 19%





- Molecule 41: 50S ribosomal protein L6

Chain RH: 86% 10% ..



- Molecule 41: 50S ribosomal protein L6

Chain YH: 84% 12% ..



- Molecule 42: 50S ribosomal protein L9

Chain RI: 94% 5% .



- Molecule 42: 50S ribosomal protein L9

Chain YI: 93% 6% .



- Molecule 43: 50S ribosomal protein L13

Chain RN: 84% 15% .



- Molecule 43: 50S ribosomal protein L13

Chain YN: 91% 9%

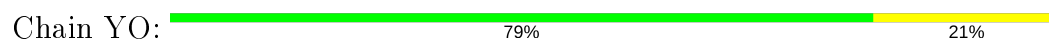


- Molecule 44: 50S ribosomal protein L14

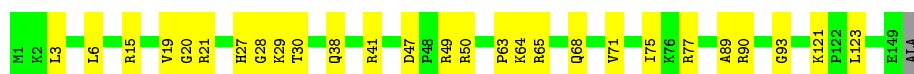
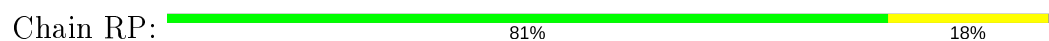
Chain RO: 80% 20%



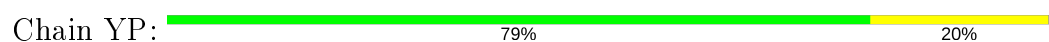
- Molecule 44: 50S ribosomal protein L14



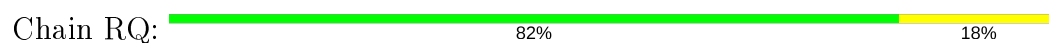
- Molecule 45: 50S ribosomal protein L15



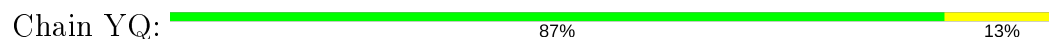
- Molecule 45: 50S ribosomal protein L15



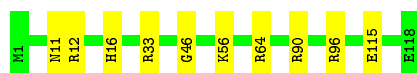
- Molecule 46: 50S ribosomal protein L16



- Molecule 46: 50S ribosomal protein L16



- Molecule 47: 50S ribosomal protein L17



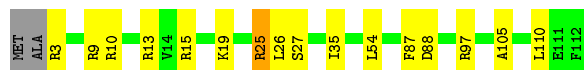
- Molecule 47: 50S ribosomal protein L17





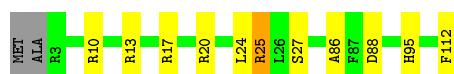
- Molecule 48: 50S ribosomal protein L18

Chain RS: 84% 13% ..



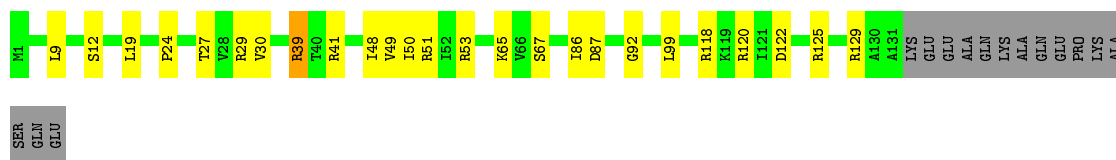
- Molecule 48: 50S ribosomal protein L18

Chain YS: 88% 9% ..



- Molecule 49: 50S ribosomal protein L19

Chain RT: 73% 16% • 10%



- Molecule 49: 50S ribosomal protein L19

Chain YT: 75% 14% • 10%



- Molecule 50: 50S ribosomal protein L20

Chain RU: 85% 12% ...




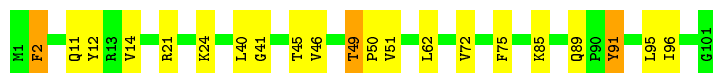
- Molecule 50: 50S ribosomal protein L20

Chain YU: 88% 8% ...



- Molecule 51: 50S ribosomal protein L21

Chain RV:  79% 18% .



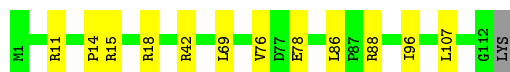
- Molecule 51: 50S ribosomal protein L21

Chain YV:  94% 5% .



- Molecule 52: 50S ribosomal protein L22

Chain RW:  88% 11% .




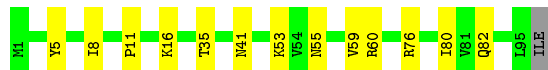
- Molecule 52: 50S ribosomal protein L22

Chain YW:  88% 12% .



- Molecule 53: 50S ribosomal protein L23

Chain RX:  85% 14% .




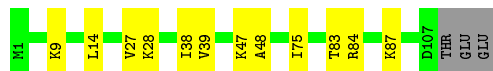
- Molecule 53: 50S ribosomal protein L23

Chain YX:  91% 8% .



- Molecule 54: 50S ribosomal protein L24

Chain RY:  86% 11% .



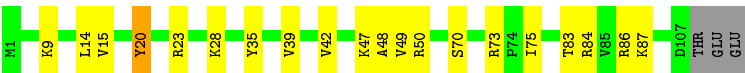
- Molecule 54: 50S ribosomal protein L24

Chain YY:

79%

17%

••



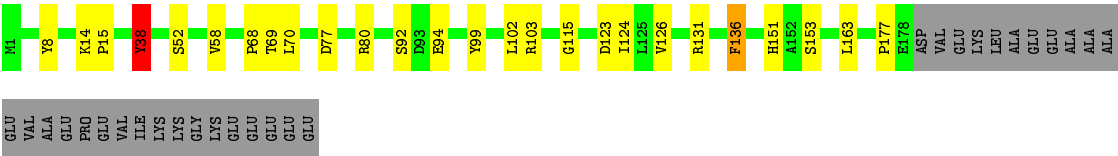
• Molecule 55: 50S ribosomal protein L25

Chain RZ:

74%

12%

14%



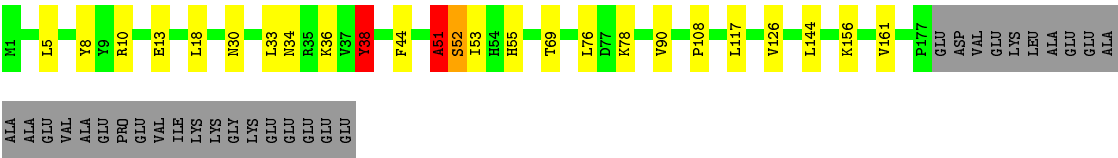
• Molecule 55: 50S ribosomal protein L25

Chain YZ:

74%

11%

14%



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	209.38Å 445.83Å 616.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10	Depositor
% Data completeness (in resolution range)	95.2 (50.00-3.10)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.231 , 0.268	Depositor
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.273	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	293819	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: 5MU, OMC, PAR, M2G, OMG, 5MC, MA6, G7M, SF4, 0TD, MG, 2MA, 2MG, OMU, UR3, 4OC, ZN, PSU

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	0.71	0/35795	0.97	64/55864 (0.1%)
1	XA	0.76	3/35890 (0.0%)	0.99	84/56012 (0.1%)
2	QB	0.45	0/1876	0.78	3/2533 (0.1%)
2	XB	0.44	0/1860	0.75	2/2518 (0.1%)
3	QC	0.42	0/1582	0.65	2/2137 (0.1%)
3	XC	0.49	0/1566	0.70	2/2119 (0.1%)
4	QD	0.54	0/1695	0.71	1/2274 (0.0%)
4	XD	0.48	0/1698	0.66	1/2277 (0.0%)
5	QE	0.40	0/1149	0.63	0/1548
5	XE	0.42	0/1149	0.63	0/1548
6	QF	0.53	0/827	0.69	2/1120 (0.2%)
6	XF	0.54	0/829	0.67	1/1123 (0.1%)
7	QG	0.44	0/1254	0.61	0/1683
7	XG	0.49	0/1248	0.63	0/1676
8	QH	0.45	0/1118	0.66	0/1506
8	XH	0.45	0/1108	0.64	0/1494
9	QI	0.42	1/1005 (0.1%)	0.70	1/1351 (0.1%)
9	XI	0.41	0/985	0.67	0/1329
10	QJ	0.42	0/732	0.72	0/993
10	XJ	0.45	0/723	0.65	0/984
11	QK	0.42	0/849	0.60	0/1150
11	XK	0.41	0/848	0.60	1/1149 (0.1%)
12	QL	0.55	0/937	0.81	3/1260 (0.2%)
12	XL	0.58	1/937 (0.1%)	0.84	3/1260 (0.2%)
13	QM	0.44	0/924	0.76	2/1242 (0.2%)
13	XM	0.47	0/905	0.76	1/1217 (0.1%)
14	QN	0.44	0/501	0.66	0/664
14	XN	0.46	0/501	0.66	0/664
15	QO	0.45	0/739	0.64	0/985
15	XO	0.43	0/739	0.62	0/985
16	QP	0.48	0/697	0.77	2/939 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.49	0/693	0.76	1/935 (0.1%)
17	QQ	0.48	0/836	0.62	0/1117
17	XQ	0.47	0/836	0.66	1/1117 (0.1%)
18	QR	0.42	0/560	0.59	0/746
18	XR	0.48	0/560	0.60	0/746
19	QS	0.44	0/663	0.67	0/895
19	XS	0.41	0/660	0.68	0/893
20	QT	0.37	0/734	0.60	0/969
20	XT	0.37	0/736	0.56	0/976
21	QU	0.38	0/203	0.58	0/266
21	XU	0.39	0/203	0.59	0/266
22	QV	0.64	0/1832	1.00	6/2855 (0.2%)
22	XV	0.70	0/1832	1.01	6/2855 (0.2%)
23	QX	0.59	0/443	1.07	3/690 (0.4%)
23	XX	0.61	0/443	1.12	2/690 (0.3%)
24	QY	0.56	0/1816	1.07	8/2830 (0.3%)
24	XY	0.58	0/1816	1.08	11/2830 (0.4%)
25	R0	0.49	0/616	0.72	0/821
25	Y0	0.52	0/616	0.74	0/821
26	R1	0.47	0/761	0.61	0/1013
26	Y1	0.51	0/766	0.61	0/1018
27	R2	0.45	0/590	0.57	0/781
27	Y2	0.48	0/594	0.65	0/785
28	R3	0.45	0/474	0.64	0/635
28	Y3	0.51	0/469	0.63	0/630
29	R4	0.54	0/559	0.85	1/754 (0.1%)
29	Y4	0.54	0/549	0.94	5/741 (0.7%)
30	R5	0.59	1/473 (0.2%)	0.68	0/639
30	Y5	0.54	0/469	0.64	0/635
31	R6	0.55	0/460	0.67	0/613
31	Y6	0.57	0/456	0.65	0/608
32	R7	0.50	0/426	0.69	0/561
32	Y7	0.52	0/426	0.69	0/561
33	R8	0.47	0/525	0.58	0/691
33	Y8	0.50	0/525	0.59	0/691
34	R9	0.54	0/310	0.66	0/407
34	Y9	0.58	0/310	0.66	0/407
35	RA	0.83	0/68903	1.02	168/107552 (0.2%)
35	YA	0.92	0/68903	1.03	186/107552 (0.2%)
36	RB	0.71	0/2876	1.03	13/4486 (0.3%)
36	YB	0.84	0/2878	1.05	11/4490 (0.2%)
37	RD	0.54	0/2181	0.71	1/2940 (0.0%)
37	YD	0.57	0/2186	0.70	1/2944 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RE	0.48	0/1592	0.67	0/2149
38	YE	0.53	0/1592	0.68	0/2149
39	RF	0.54	0/1618	0.68	1/2191 (0.0%)
39	YF	0.54	0/1614	0.66	0/2186
40	RG	0.47	0/1451	0.67	1/1961 (0.1%)
40	YG	0.47	0/1449	0.67	0/1957
41	RH	0.45	0/1356	0.65	1/1834 (0.1%)
41	YH	0.53	0/1350	0.61	0/1826
42	RI	0.43	0/1109	0.68	0/1512
42	YI	0.48	0/1091	0.63	1/1490 (0.1%)
43	RN	0.49	1/1148 (0.1%)	0.58	0/1547
43	YN	0.51	0/1144	0.61	0/1543
44	RO	0.51	0/943	0.66	0/1269
44	YO	0.55	0/943	0.65	0/1269
45	RP	0.47	0/1152	0.70	0/1533
45	YP	0.53	0/1152	0.70	0/1533
46	RQ	0.45	0/1143	0.65	0/1527
46	YQ	0.49	0/1143	0.66	1/1527 (0.1%)
47	RR	0.45	0/982	0.65	0/1312
47	YR	0.47	0/982	0.65	0/1312
48	RS	0.45	0/887	0.66	0/1180
48	YS	0.48	0/880	0.61	0/1172
49	RT	0.47	0/1105	0.65	0/1477
49	YT	0.48	0/1097	0.66	0/1468
50	RU	0.49	0/977	0.69	2/1301 (0.2%)
50	YU	0.54	0/977	0.71	3/1301 (0.2%)
51	RV	0.55	0/786	0.78	3/1053 (0.3%)
51	YV	0.54	0/782	0.69	0/1049
52	RW	0.47	0/897	0.59	0/1205
52	YW	0.51	0/897	0.59	0/1205
53	RX	0.49	0/764	0.63	0/1025
53	YX	0.49	0/764	0.64	0/1025
54	RY	0.46	0/823	0.66	0/1099
54	YY	0.53	0/823	0.67	0/1100
55	RZ	0.45	0/1438	0.76	1/1955 (0.1%)
55	YZ	0.50	0/1413	0.77	2/1924 (0.1%)
All	All	0.74	7/316097 (0.0%)	0.94	615/473222 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1042	G	C5-C4	9.41	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1042	G	C6-N1	6.72	1.44	1.39
30	R5	59	GLU	CD-OE1	5.69	1.31	1.25
1	XA	1042	G	N9-C4	-5.68	1.33	1.38
9	QI	121	ARG	C-N	-5.32	1.21	1.34

The worst 5 of 615 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	999	C	N1-C2-O2	15.66	128.30	118.90
1	XA	999	C	C5-C6-N1	13.88	127.94	121.00
1	XA	1042	G	C6-N1-C2	12.73	132.74	125.10
2	QB	232	PRO	C-N-CA	12.22	152.25	121.70
1	XA	1042	G	C5-C6-N1	-12.10	105.45	111.50

There are no chirality outliers.

There are no planarity outliers.

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	16295	169	0
1	XA	32331	0	16337	177	0
2	QB	1842	0	1861	26	0
2	XB	1825	0	1828	22	0
3	QC	1558	0	1557	29	0
3	XC	1542	0	1517	16	0
4	QD	1665	0	1691	33	0
4	XD	1668	0	1707	26	0
5	QE	1133	0	1191	16	0
5	XE	1133	0	1191	14	0
6	QF	814	0	808	7	0
6	XF	816	0	808	19	0
7	QG	1235	0	1249	17	0
7	XG	1229	0	1238	8	0
8	QH	1098	0	1143	18	0
8	XH	1088	0	1126	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	QI	986	0	990	24	0
9	XI	966	0	953	24	0
10	QJ	719	0	672	10	0
10	XJ	710	0	661	13	0
11	QK	834	0	838	12	0
11	XK	833	0	836	11	0
12	QL	932	0	981	17	0
12	XL	932	0	981	11	0
13	QM	914	0	954	14	0
13	XM	895	0	920	22	0
14	QN	492	0	529	10	0
14	XN	492	0	529	10	0
15	QO	728	0	760	2	0
15	XO	728	0	760	3	0
16	QP	681	0	697	20	0
16	XP	677	0	686	22	0
17	QQ	823	0	891	10	0
17	XQ	823	0	891	10	0
18	QR	555	0	618	4	0
18	XR	555	0	618	11	0
19	QS	648	0	658	7	0
19	XS	645	0	635	15	0
20	QT	732	0	809	8	0
20	XT	733	0	795	8	0
21	QU	199	0	208	1	0
21	XU	199	0	208	0	0
22	QV	1640	0	837	5	0
22	XV	1640	0	837	5	0
23	QX	394	0	197	1	0
23	XX	394	0	197	1	0
24	QY	1625	0	822	5	0
24	XY	1625	0	822	5	0
25	R0	608	0	622	8	0
25	Y0	608	0	622	12	0
26	R1	754	0	823	10	0
26	Y1	759	0	837	5	0
27	R2	588	0	643	8	0
27	Y2	592	0	654	6	0
28	R3	469	0	518	2	0
28	Y3	464	0	514	8	0
29	R4	546	0	522	9	0
29	Y4	536	0	514	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	R5	459	0	476	8	0
30	Y5	455	0	465	6	0
31	R6	453	0	473	3	0
31	Y6	449	0	469	4	0
32	R7	418	0	466	5	0
32	Y7	418	0	466	4	0
33	R8	517	0	582	14	0
33	Y8	517	0	582	13	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	7	0
35	RA	61758	0	31137	265	0
35	YA	61758	0	31138	256	0
36	RB	2572	0	1304	3	0
36	YB	2573	0	1306	6	0
37	RD	2131	0	2205	41	0
37	YD	2136	0	2217	43	0
38	RE	1559	0	1618	20	0
38	YE	1559	0	1618	33	0
39	RF	1583	0	1624	43	0
39	YF	1579	0	1618	27	0
40	RG	1426	0	1445	13	0
40	YG	1424	0	1441	22	0
41	RH	1330	0	1407	16	0
41	YH	1324	0	1402	14	0
42	RI	1094	0	1127	4	0
42	YI	1076	0	1094	4	0
43	RN	1121	0	1195	16	0
43	YN	1117	0	1184	8	0
44	RO	933	0	996	15	0
44	YO	933	0	996	18	0
45	RP	1135	0	1212	22	0
45	YP	1135	0	1212	24	0
46	RQ	1122	0	1179	19	0
46	YQ	1122	0	1179	14	0
47	RR	968	0	1033	8	0
47	YR	968	0	1033	10	0
48	RS	877	0	938	10	0
48	YS	870	0	923	8	0
49	RT	1091	0	1151	16	0
49	YT	1083	0	1136	15	0
50	RU	959	0	1019	15	0
50	YU	959	0	1019	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	RV	775	0	841	14	0
51	YV	771	0	830	8	0
52	RW	886	0	940	8	0
52	YW	886	0	940	9	0
53	RX	750	0	814	11	0
53	YX	750	0	814	6	0
54	RY	810	0	892	7	0
54	YY	810	0	887	14	0
55	RZ	1406	0	1418	17	0
55	YZ	1381	0	1386	15	0
56	QA	221	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
56	QE	4	0	0	0	0
56	QF	2	0	0	0	0
56	QG	2	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QK	1	0	0	0	0
56	QL	3	0	0	0	0
56	QN	1	0	0	0	0
56	QO	2	0	0	0	0
56	QP	1	0	0	0	0
56	QT	1	0	0	0	0
56	QV	5	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R3	3	0	0	0	0
56	R5	2	0	0	0	0
56	R6	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	709	0	0	0	0
56	RB	17	0	0	0	0
56	RD	8	0	0	0	0
56	RE	4	0	0	0	0
56	RF	4	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RQ	4	0	0	0	0
56	RR	2	0	0	0	0
56	RT	4	0	0	0	0
56	RU	2	0	0	0	0
56	RV	3	0	0	0	0
56	RW	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	193	0	0	0	0
56	XE	2	0	0	0	0
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	2	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y3	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y7	2	0	0	0	0
56	Y8	1	0	0	0	0
56	YA	707	0	0	0	0
56	YB	20	0	0	0	0
56	YD	7	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	2	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	2	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
57	QA	42	0	45	1	0
57	XA	42	0	45	1	0
58	QD	8	0	0	0	0
58	XD	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	293819	0	196213	1738	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1738 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)
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CE1	1.78	1.17
16:QP:20:VAL:HG21	16:QP:32:TYR:HD2	1.09	1.13
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CD1	1.90	1.07
35:RA:660:G:H5'	39:RF:99:TYR:CE2	1.94	1.03
16:QP:20:VAL:HG21	16:QP:32:TYR:CD2	1.94	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	20
2	XB	229/256 (90%)	204 (89%)	22 (10%)	3 (1%)	12	42
3	QC	204/239 (85%)	197 (97%)	7 (3%)	0	100	100
3	XC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
5	QE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
5	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
6	QF	98/101 (97%)	98 (100%)	0	0	100	100
6	XF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	22
10	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	7	30
11	QK	112/129 (87%)	107 (96%)	5 (4%)	0	100	100
11	XK	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
12	QL	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	9	36
12	XL	119/132 (90%)	109 (92%)	6 (5%)	4 (3%)	3	21
13	QM	114/126 (90%)	107 (94%)	4 (4%)	3 (3%)	5	26
13	XM	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
14	QN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	44
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	66 (100%)	0	0	100	100
19	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
20	QT	94/106 (89%)	91 (97%)	3 (3%)	0	100	100
20	XT	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
25	R0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	Y0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	Y1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
27	R2	68/72 (94%)	68 (100%)	0	0	100	100
27	Y2	68/72 (94%)	68 (100%)	0	0	100	100
28	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	R4	67/71 (94%)	59 (88%)	7 (10%)	1 (2%)	10	39
29	Y4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	6
30	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
31	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
37	YD	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
38	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YE	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	64
39	RF	200/210 (95%)	196 (98%)	4 (2%)	0	100	100
39	YF	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
40	RG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	9	36
40	YG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	46
41	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
41	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
42	RI	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
42	YI	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
43	RN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
43	YN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
45	RP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
45	YP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
46	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
46	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	RR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
47	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
48	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
49	RT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
49	YT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
50	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
50	YU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
51	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	49
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	49
52	RW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
52	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
53	RX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
53	YX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
54	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
55	RZ	176/206 (85%)	164 (93%)	11 (6%)	1 (1%)	25	59
55	YZ	175/206 (85%)	165 (94%)	8 (5%)	2 (1%)	14	46
All	All	11389/12128 (94%)	10866 (95%)	478 (4%)	45 (0%)	34	69

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	17	PHE
2	QB	127	ILE
4	QD	5	ILE
10	QJ	32	ALA
10	QJ	79	ARG

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	191/220 (87%)	188 (98%)	3 (2%)	62	84
2	XB	187/220 (85%)	184 (98%)	3 (2%)	62	84
3	QC	144/188 (77%)	143 (99%)	1 (1%)	84	93
3	XC	140/188 (74%)	138 (99%)	2 (1%)	67	86
4	QD	171/181 (94%)	168 (98%)	3 (2%)	59	82
4	XD	172/181 (95%)	172 (100%)	0	100	100
5	QE	114/123 (93%)	113 (99%)	1 (1%)	78	91
5	XE	114/123 (93%)	113 (99%)	1 (1%)	78	91
6	QF	85/90 (94%)	85 (100%)	0	100	100
6	XF	85/90 (94%)	84 (99%)	1 (1%)	71	88
7	QG	120/127 (94%)	118 (98%)	2 (2%)	60	83
7	XG	119/127 (94%)	117 (98%)	2 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	116/119 (98%)	116 (100%)	0	100	100
8	XH	114/119 (96%)	113 (99%)	1 (1%)	78	91
9	QI	91/99 (92%)	91 (100%)	0	100	100
9	XI	88/99 (89%)	88 (100%)	0	100	100
10	QJ	68/92 (74%)	68 (100%)	0	100	100
10	XJ	68/92 (74%)	68 (100%)	0	100	100
11	QK	83/99 (84%)	83 (100%)	0	100	100
11	XK	83/99 (84%)	82 (99%)	1 (1%)	71	88
12	QL	96/108 (89%)	95 (99%)	1 (1%)	76	90
12	XL	96/108 (89%)	95 (99%)	1 (1%)	76	90
13	QM	90/101 (89%)	89 (99%)	1 (1%)	73	89
13	XM	87/101 (86%)	85 (98%)	2 (2%)	50	77
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	78/80 (98%)	77 (99%)	1 (1%)	69	87
15	XO	78/80 (98%)	77 (99%)	1 (1%)	69	87
16	QP	69/74 (93%)	67 (97%)	2 (3%)	42	72
16	XP	68/74 (92%)	65 (96%)	3 (4%)	28	61
17	QQ	94/97 (97%)	94 (100%)	0	100	100
17	XQ	94/97 (97%)	94 (100%)	0	100	100
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	59 (100%)	0	100	100
19	QS	68/80 (85%)	67 (98%)	1 (2%)	65	85
19	XS	67/80 (84%)	67 (100%)	0	100	100
20	QT	71/82 (87%)	71 (100%)	0	100	100
20	XT	70/82 (85%)	70 (100%)	0	100	100
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
25	R0	61/67 (91%)	59 (97%)	2 (3%)	38	69
25	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
26	R1	79/83 (95%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Y1	81/83 (98%)	81 (100%)	0	100	100
27	R2	65/67 (97%)	64 (98%)	1 (2%)	65	85
27	Y2	66/67 (98%)	65 (98%)	1 (2%)	65	85
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	49 (98%)	1 (2%)	55	80
29	R4	58/63 (92%)	58 (100%)	0	100	100
29	Y4	54/63 (86%)	52 (96%)	2 (4%)	34	66
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	50/52 (96%)	49 (98%)	1 (2%)	55	80
31	R6	51/52 (98%)	51 (100%)	0	100	100
31	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	80
32	R7	41/42 (98%)	41 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
37	YD	215/218 (99%)	214 (100%)	1 (0%)	88	94
38	RE	164/166 (99%)	164 (100%)	0	100	100
38	YE	164/166 (99%)	164 (100%)	0	100	100
39	RF	160/166 (96%)	158 (99%)	2 (1%)	69	87
39	YF	159/166 (96%)	157 (99%)	2 (1%)	69	87
40	RG	144/156 (92%)	143 (99%)	1 (1%)	84	93
40	YG	142/156 (91%)	142 (100%)	0	100	100
41	RH	144/148 (97%)	144 (100%)	0	100	100
41	YH	143/148 (97%)	142 (99%)	1 (1%)	84	93
42	RI	111/124 (90%)	111 (100%)	0	100	100
42	YI	108/124 (87%)	107 (99%)	1 (1%)	78	91
43	RN	119/119 (100%)	117 (98%)	2 (2%)	60	83
43	YN	118/119 (99%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	90
44	YO	100/100 (100%)	99 (99%)	1 (1%)	76	90
45	RP	115/116 (99%)	115 (100%)	0	100	100
45	YP	115/116 (99%)	115 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100
48	RS	87/88 (99%)	86 (99%)	1 (1%)	73	89
48	YS	85/88 (97%)	84 (99%)	1 (1%)	71	88
49	RT	115/127 (91%)	113 (98%)	2 (2%)	60	83
49	YT	113/127 (89%)	112 (99%)	1 (1%)	78	91
50	RU	93/94 (99%)	91 (98%)	2 (2%)	52	78
50	YU	93/94 (99%)	91 (98%)	2 (2%)	52	78
51	RV	81/82 (99%)	80 (99%)	1 (1%)	71	88
51	YV	80/82 (98%)	79 (99%)	1 (1%)	69	87
52	RW	90/92 (98%)	90 (100%)	0	100	100
52	YW	90/92 (98%)	90 (100%)	0	100	100
53	RX	77/78 (99%)	77 (100%)	0	100	100
53	YX	77/78 (99%)	77 (100%)	0	100	100
54	RY	86/91 (94%)	86 (100%)	0	100	100
54	YY	86/91 (94%)	84 (98%)	2 (2%)	50	77
55	RZ	152/179 (85%)	149 (98%)	3 (2%)	55	80
55	YZ	148/179 (83%)	146 (99%)	2 (1%)	67	86
All	All	9329/10064 (93%)	9254 (99%)	75 (1%)	81	92

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	RZ	131	ARG
6	XF	50	TYR
50	YU	55	ARG
55	RZ	136	PHE
3	XC	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
39	RF	40	GLN
52	RW	61	ASN
53	YX	41	ASN
41	RH	74	ASN
53	RX	41	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1494/1522 (98%)	238 (15%)	15 (1%)
1	XA	1498/1522 (98%)	230 (15%)	15 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	13 (17%)	0
23	QX	17/19 (89%)	6 (35%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	75/76 (98%)	31 (41%)	0
24	XY	75/76 (98%)	33 (44%)	0
35	RA	2857/2915 (98%)	452 (15%)	16 (0%)
35	YA	2857/2915 (98%)	454 (15%)	15 (0%)
36	RB	119/122 (97%)	10 (8%)	0
36	YB	119/122 (97%)	11 (9%)	0
All	All	9280/9462 (98%)	1501 (16%)	63 (0%)

5 of 1501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	RA	2172	U
1	XA	266	G
35	YA	2126	A
35	RA	2406	U
35	RA	2689	U

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

48 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$
35	PSU	YA	1917	56,35	17,21,22	1.69	5 (29%)	20,30,33	3.05	5 (25%)
35	5MC	YA	1962	56,35	15,22,23	1.21	1 (6%)	19,32,35	1.28	3 (15%)
1	2MG	QA	1207	1	19,26,27	1.13	2 (10%)	21,38,41	2.21	7 (33%)
1	4OC	XA	1402	1	16,23,24	0.85	1 (6%)	17,32,35	1.39	1 (5%)
35	PSU	RA	2605	35	17,21,22	1.69	5 (29%)	20,30,33	3.10	6 (30%)
1	2MG	XA	1207	1	19,26,27	1.07	2 (10%)	21,38,41	2.22	7 (33%)
35	5MU	RA	1939	35	15,22,23	1.08	2 (13%)	16,32,35	1.74	2 (12%)
1	PSU	QA	516	1	17,21,22	1.76	5 (29%)	20,30,33	3.25	5 (25%)
35	PSU	YA	1911	35	17,21,22	1.61	5 (29%)	20,30,33	3.07	5 (25%)
35	5MC	YA	1942	35	15,22,23	1.22	1 (6%)	19,32,35	1.31	2 (10%)
1	5MC	XA	1404	1	15,22,23	1.21	1 (6%)	19,32,35	1.34	3 (15%)
35	OMC	YA	1920	35	15,22,23	0.94	1 (6%)	17,31,34	1.62	4 (23%)
35	2MA	YA	2503	56,35	17,25,26	1.22	2 (11%)	19,37,40	2.13	3 (15%)
1	MA6	QA	1518	1	19,26,27	0.97	1 (5%)	18,38,41	1.81	4 (22%)
1	G7M	QA	527	1,56	20,26,27	2.60	4 (20%)	20,39,42	2.02	5 (25%)
12	0TD	XL	92	12	4,9,10	0.57	0	3,11,13	1.85	1 (33%)
1	M2G	XA	966	1	20,27,28	1.17	3 (15%)	22,40,43	2.09	5 (22%)
1	M2G	QA	966	1	20,27,28	1.26	3 (15%)	22,40,43	2.02	6 (27%)
35	5MC	RA	1942	35	15,22,23	1.26	1 (6%)	19,32,35	1.29	3 (15%)
35	PSU	RA	1911	35	17,21,22	1.76	5 (29%)	20,30,33	3.00	6 (30%)
35	OMC	RA	1920	35	15,22,23	0.83	0	17,31,34	1.69	3 (17%)
1	MA6	XA	1518	1	19,26,27	0.99	1 (5%)	18,38,41	1.90	4 (22%)
1	5MC	XA	1400	1	15,22,23	1.23	1 (6%)	19,32,35	1.44	3 (15%)
12	0TD	QL	92	12	4,9,10	0.56	0	3,11,13	1.85	1 (33%)
1	5MC	QA	1404	1	15,22,23	1.21	1 (6%)	19,32,35	1.28	3 (15%)
35	PSU	RA	1917	56,35	17,21,22	1.67	5 (29%)	20,30,33	3.11	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	5MU	YA	1915	35	15,22,23	1.03	2 (13%)	16,32,35	2.01	2 (12%)
35	OMU	RA	2552	56,35	14,22,23	1.06	1 (7%)	14,31,34	0.92	1 (7%)
35	OMG	YA	2251	56,22,35	18,26,27	1.11	2 (11%)	20,38,41	2.04	6 (30%)
1	4OC	QA	1402	1	16,23,24	0.81	1 (6%)	17,32,35	1.39	1 (5%)
1	PSU	XA	516	1	17,21,22	1.62	5 (29%)	20,30,33	3.02	6 (30%)
1	5MC	QA	1407	1	15,22,23	1.23	1 (6%)	19,32,35	1.44	2 (10%)
1	G7M	XA	527	1,56	20,26,27	2.61	4 (20%)	20,39,42	2.08	5 (25%)
1	5MC	QA	967	1	15,22,23	1.32	1 (6%)	19,32,35	1.25	2 (10%)
35	5MU	RA	1915	35	15,22,23	1.03	2 (13%)	16,32,35	2.01	2 (12%)
1	5MC	QA	1400	1	15,22,23	1.23	1 (6%)	19,32,35	1.37	3 (15%)
35	2MA	RA	2503	56,35	17,25,26	1.26	1 (5%)	19,37,40	2.15	3 (15%)
1	MA6	QA	1519	1	19,26,27	0.90	1 (5%)	18,38,41	1.85	6 (33%)
1	UR3	XA	1498	1	14,22,23	0.92	1 (7%)	15,32,35	0.69	0
35	OMG	RA	2251	56,22,35	18,26,27	1.09	2 (11%)	20,38,41	2.05	6 (30%)
35	5MU	YA	1939	35	15,22,23	1.12	2 (13%)	16,32,35	1.80	2 (12%)
35	PSU	YA	2605	35	17,21,22	1.63	5 (29%)	20,30,33	2.99	5 (25%)
1	UR3	QA	1498	1	14,22,23	0.75	0	15,32,35	0.67	0
1	5MC	XA	967	1	15,22,23	1.15	1 (6%)	19,32,35	1.35	3 (15%)
35	5MC	RA	1962	56,35	15,22,23	1.15	1 (6%)	19,32,35	1.41	3 (15%)
35	OMU	YA	2552	56,35	14,22,23	1.03	2 (14%)	14,31,34	0.82	1 (7%)
1	5MC	XA	1407	1	15,22,23	1.13	1 (6%)	19,32,35	1.39	2 (10%)
1	MA6	XA	1519	1	19,26,27	0.90	1 (5%)	18,38,41	1.96	6 (33%)

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
35	PSU	YA	1917	56,35	-	0/7/25/26	0/2/2/2
35	5MC	YA	1962	56,35	-	1/5/25/26	0/2/2/2
1	2MG	QA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
35	PSU	RA	2605	35	-	0/7/25/26	0/2/2/2
1	2MG	XA	1207	1	-	0/5/27/28	0/3/3/3
35	5MU	RA	1939	35	-	0/5/25/26	0/2/2/2
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	YA	1911	35	-	0/7/25/26	0/2/2/2
35	5MC	YA	1942	35	-	0/5/25/26	0/2/2/2
1	5MC	XA	1404	1	-	0/5/25/26	0/2/2/2
35	OMC	YA	1920	35	-	0/7/27/28	0/2/2/2
35	2MA	YA	2503	56,35	-	1/3/25/26	0/3/3/3
1	MA6	QA	1518	1	-	3/7/29/30	0/3/3/3
1	G7M	QA	527	1,56	-	2/3/25/26	0/3/3/3
12	0TD	XL	92	12	-	1/3/12/14	-
1	M2G	XA	966	1	-	0/7/29/30	0/3/3/3
1	M2G	QA	966	1	-	2/7/29/30	0/3/3/3
35	5MC	RA	1942	35	-	0/5/25/26	0/2/2/2
35	PSU	RA	1911	35	-	0/7/25/26	0/2/2/2
35	OMC	RA	1920	35	-	0/7/27/28	0/2/2/2
1	MA6	XA	1518	1	-	3/7/29/30	0/3/3/3
1	5MC	XA	1400	1	-	2/5/25/26	0/2/2/2
12	0TD	QL	92	12	-	1/3/12/14	-
1	5MC	QA	1404	1	-	2/5/25/26	0/2/2/2
35	PSU	RA	1917	56,35	-	0/7/25/26	0/2/2/2
35	5MU	YA	1915	35	-	0/5/25/26	0/2/2/2
35	OMU	RA	2552	56,35	-	1/7/27/28	0/2/2/2
35	OMG	YA	2251	56,22,35	-	0/5/27/28	0/3/3/3
1	4OC	QA	1402	1	-	3/9/29/30	0/2/2/2
1	PSU	XA	516	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	1407	1	-	0/5/25/26	0/2/2/2
1	G7M	XA	527	1,56	-	3/3/25/26	0/3/3/3
1	5MC	QA	967	1	-	0/5/25/26	0/2/2/2
35	5MU	RA	1915	35	-	0/5/25/26	0/2/2/2
1	5MC	QA	1400	1	-	2/5/25/26	0/2/2/2
35	2MA	RA	2503	56,35	-	1/3/25/26	0/3/3/3
1	MA6	QA	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	XA	1498	1	-	0/5/25/26	0/2/2/2
35	OMG	RA	2251	56,22,35	-	0/5/27/28	0/3/3/3
35	5MU	YA	1939	35	-	0/5/25/26	0/2/2/2
35	PSU	YA	2605	35	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	0/5/25/26	0/2/2/2
1	5MC	XA	967	1	-	0/5/25/26	0/2/2/2
35	5MC	RA	1962	56,35	-	1/5/25/26	0/2/2/2
35	OMU	YA	2552	56,35	-	0/7/27/28	0/2/2/2
1	5MC	XA	1407	1	-	0/5/25/26	0/2/2/2
1	MA6	XA	1519	1	-	3/7/29/30	0/3/3/3

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	QA	527	G7M	C8-N9	7.12	1.46	1.33
1	XA	527	G7M	C8-N9	7.09	1.46	1.33
1	QA	527	G7M	C8-N7	6.53	1.45	1.33
1	XA	527	G7M	C8-N7	6.25	1.44	1.33
1	XA	527	G7M	C5-C4	5.50	1.47	1.39

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	516	PSU	N1-C2-N3	-9.00	121.28	128.43
35	RA	2605	PSU	N1-C2-N3	-8.90	121.36	128.43
35	RA	1917	PSU	N1-C2-N3	-8.67	121.54	128.43
35	YA	1911	PSU	N1-C2-N3	-8.54	121.64	128.43
35	YA	1917	PSU	N1-C2-N3	-8.46	121.71	128.43

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	QA	1518	MA6	C5-C6-N6-C9
1	QA	1518	MA6	C5-C6-N6-C10
12	XL	92	0TD	CG-CB-SB-CSB
1	XA	1518	MA6	C5-C6-N6-C9
1	XA	1518	MA6	C5-C6-N6-C10

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	YA	1962	5MC	1	0
35	RA	1939	5MU	1	0
35	YA	2503	2MA	2	0
1	QA	1518	MA6	1	0
1	XA	966	M2G	1	0
1	XA	1518	MA6	1	0
12	QL	92	0TD	1	0
35	RA	2503	2MA	2	0
1	QA	1519	MA6	1	0
1	XA	1498	UR3	1	0
1	XA	967	5MC	1	0
35	RA	1962	5MC	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2027 ligands modelled in this entry, 2023 are monoatomic - leaving 4 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	QD	302	-	0,12,12	0.00	-	-		
57	PAR	XA	1794	-	45,45,45	0.66	0	64,67,67	1.23	6 (9%)
57	PAR	QA	1821	-	45,45,45	0.68	0	64,67,67	1.49	11 (17%)
58	SF4	XD	301	-	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	-	-	-	0/6/5/5
57	PAR	XA	1794	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1821	-	-	4/18/94/94	0/4/4/4
58	SF4	XD	301	-	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1821	PAR	C44-C34-C24	4.78	119.30	111.07
57	QA	1821	PAR	O52-C13-C23	3.44	115.09	107.96
57	XA	1794	PAR	C13-O52-C52	-3.34	109.70	117.96
57	QA	1821	PAR	C13-O52-C52	-3.33	109.73	117.96
57	XA	1794	PAR	C14-O33-C33	-2.90	110.79	117.96

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

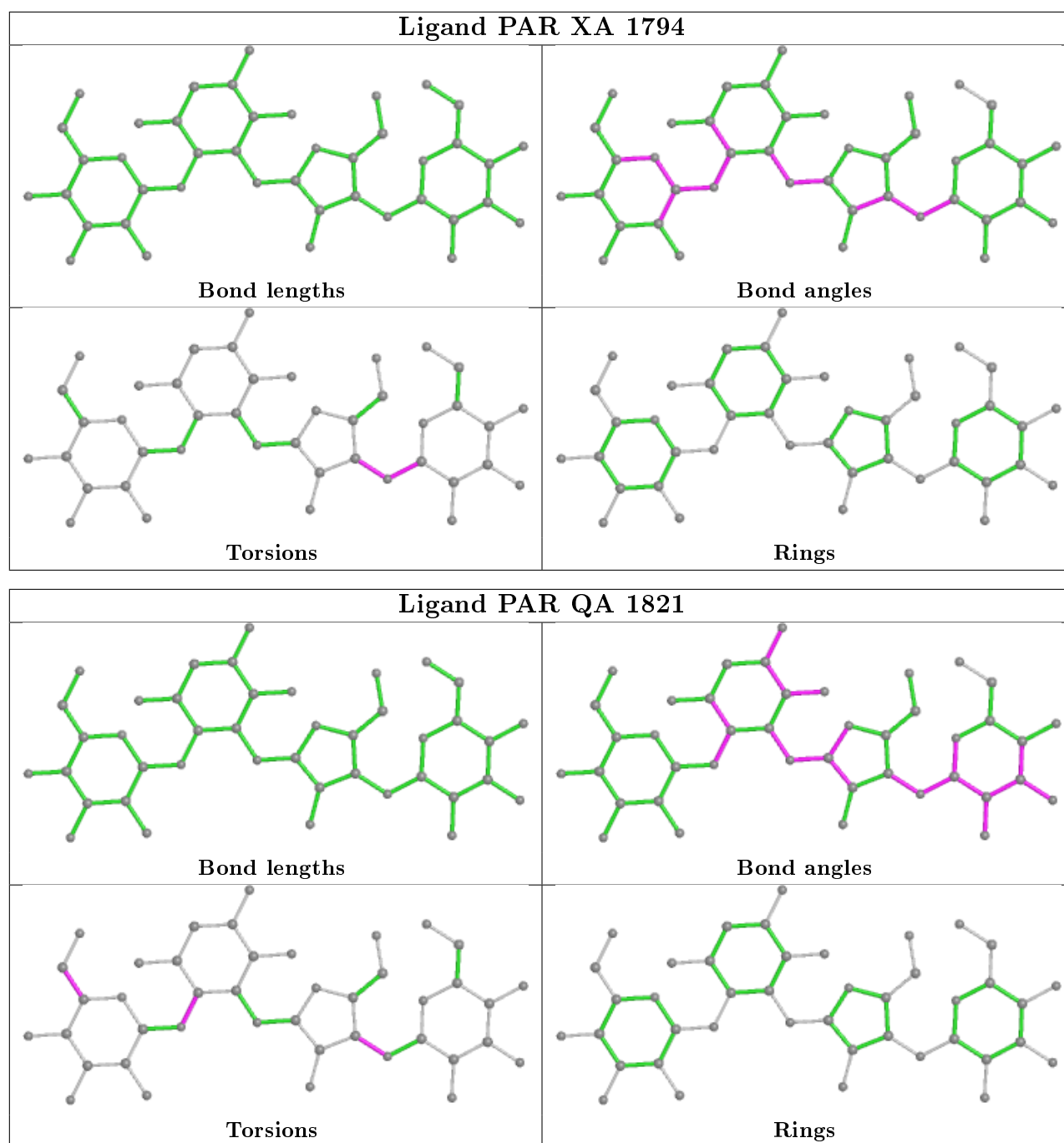
Mol	Chain	Res	Type	Atoms
57	QA	1821	PAR	O51-C51-C61-O61
57	QA	1821	PAR	C41-C51-C61-O61
57	QA	1821	PAR	C23-C33-O33-C14
57	XA	1794	PAR	O54-C14-O33-C33
57	QA	1821	PAR	C52-C42-O11-C11

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1794	PAR	1	0
57	QA	1821	PAR	1	0
58	XD	301	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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