



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 08:42 AM BST

PDB ID : 6OPE
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to near-cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-24
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

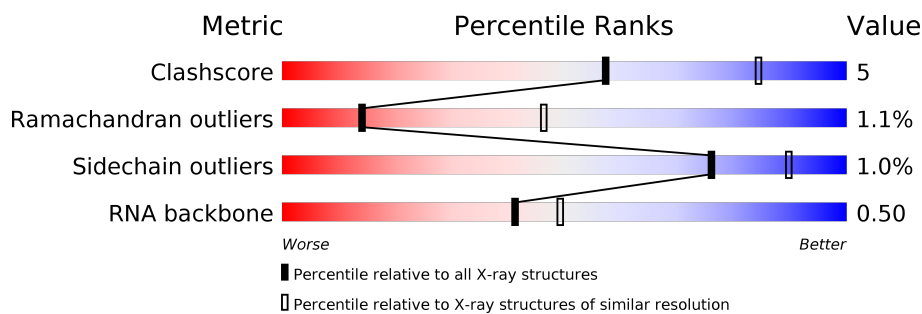
1 Overall quality at a glance

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)

















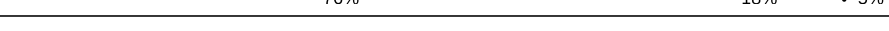

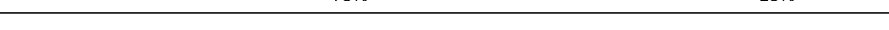
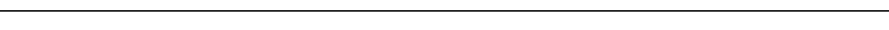
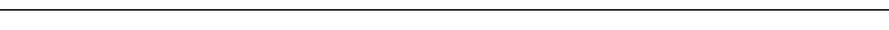
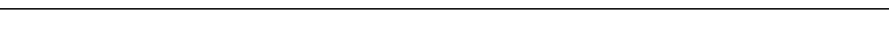
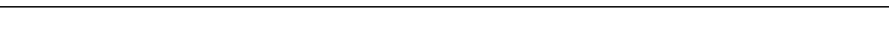
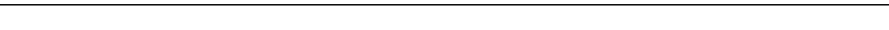

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	63% 29% 6% ..
1	XA	1522	64% 28% 6% ..
2	QB	256	74% 18% 7%
2	XB	256	74% 19% 7%
3	QC	239	67% 17% • 14%
3	XC	239	74% 12% 14%
4	QD	209	81% 17% •

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Mol	Chain	Length	Quality of chain
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	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	















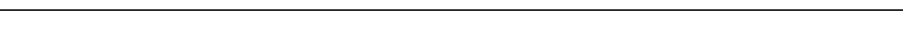




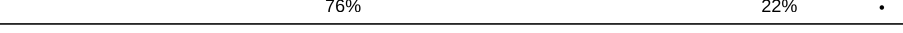





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	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









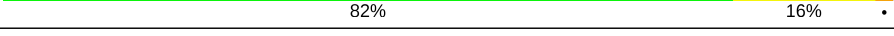


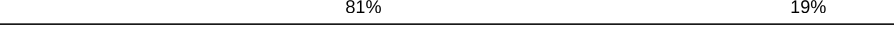

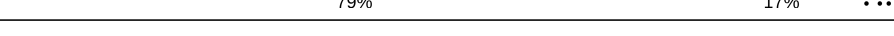


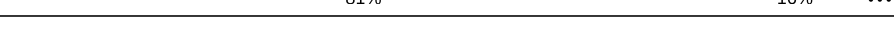

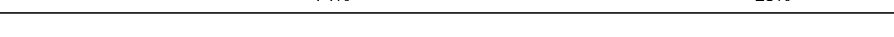
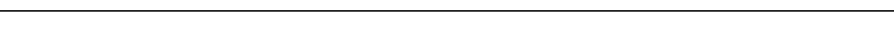

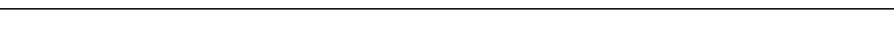
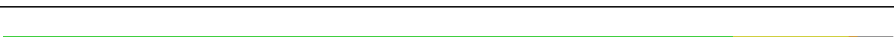


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Mol	Chain	Length	Quality of chain
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	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	 76%20%...
42	YI	148	 81%17%..
43	RN	140	 83%14%..
43	YN	140	 87%11%..
44	RO	122	 77%21%.
44	YO	122	 80%18%.
45	RP	150	 75%23%..
45	YP	150	 78%21%.
46	RQ	141	 82%16%.
46	YQ	141	 79%18%.
47	RR	118	 80%19%.
47	YR	118	 81%19%.
48	RS	112	 85%11%...
48	YS	112	 79%17%...
49	RT	146	 70%23%6%
49	YT	146	 67%25%6%
50	RU	118	 81%16%...
50	YU	118	 84%12%...
51	RV	101	 74%25%.
51	YV	101	 86%12%..
52	RW	113	 81%19%
52	YW	113	 81%19%
53	RX	96	 80%16%.
53	YX	96	 82%13%..
54	RY	110	 76%15%7%

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Mol	Chain	Length	Quality of chain
54	YY	110	<div><div></div><div>81%12%7%</div></div>
55	RZ	206	<div><div></div><div>65%22%•11%</div></div>
55	YZ	206	<div><div></div><div>67%20%•11%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	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
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

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

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

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

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

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

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

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

- 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	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- 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	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	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	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNAfMet.

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
			396	177	82	119	18			
23	XX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			

- Molecule 24 is a RNA chain called A-site tRNAAla(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			
24	XY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	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
			763	481	150	131	1			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- 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
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
29	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	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
			459	288	90	76	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
32	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
35	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- 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
			2573	1146	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	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	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
			1585	1011	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	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
			1474	942	268	260	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
41	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
43	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	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	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	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	111	Total	C	N	O	0	0	0
			882	556	176	150			
48	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
50	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	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
			779	501	142	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	73	Total	Mg	0	0
			73	73		
56	RP	3	Total	Mg	0	0
			3	3		
56	QX	2	Total	Mg	0	0
			2	2		
56	YA	347	Total	Mg	0	0
			347	347		
56	QM	1	Total	Mg	0	0
			1	1		
56	YR	1	Total	Mg	0	0
			1	1		
56	Y9	1	Total	Mg	0	0
			1	1		
56	Y1	1	Total	Mg	0	0
			1	1		
56	XX	1	Total	Mg	0	0
			1	1		

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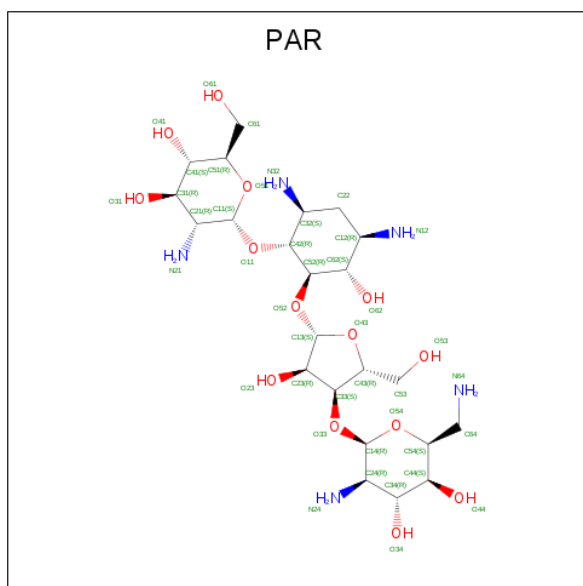
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QV	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	XA	91	Total 91	Mg 91	0	0
56	R0	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RD	1	Total 1	Mg 1	0	0
56	QF	1	Total 1	Mg 1	0	0
56	R5	1	Total 1	Mg 1	0	0
56	RA	281	Total 281	Mg 281	0	0
56	YP	3	Total 3	Mg 3	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	YB	6	Total 6	Mg 6	0	0
56	Y6	2	Total 2	Mg 2	0	0

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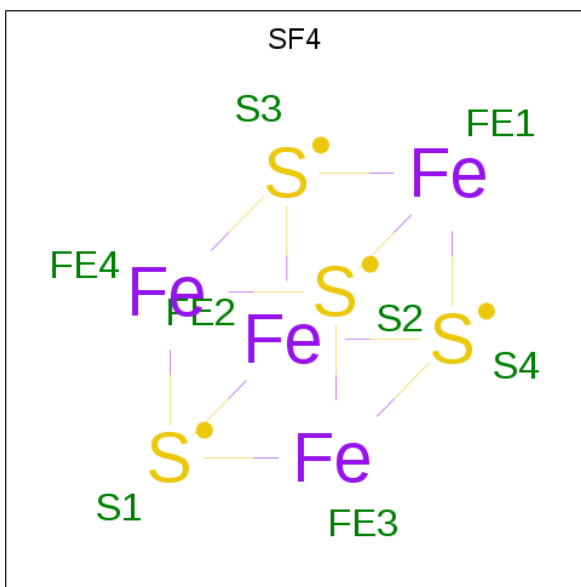
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XV	2	Total	Mg	0	0
			2	2		
56	RB	4	Total	Mg	0	0
			4	4		
56	Y2	1	Total	Mg	0	0
			1	1		
56	R8	1	Total	Mg	0	0
			1	1		
56	RF	1	Total	Mg	0	0
			1	1		
56	XM	1	Total	Mg	0	0
			1	1		
56	YE	3	Total	Mg	0	0
			3	3		

- 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: Fe_4S_4).



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).

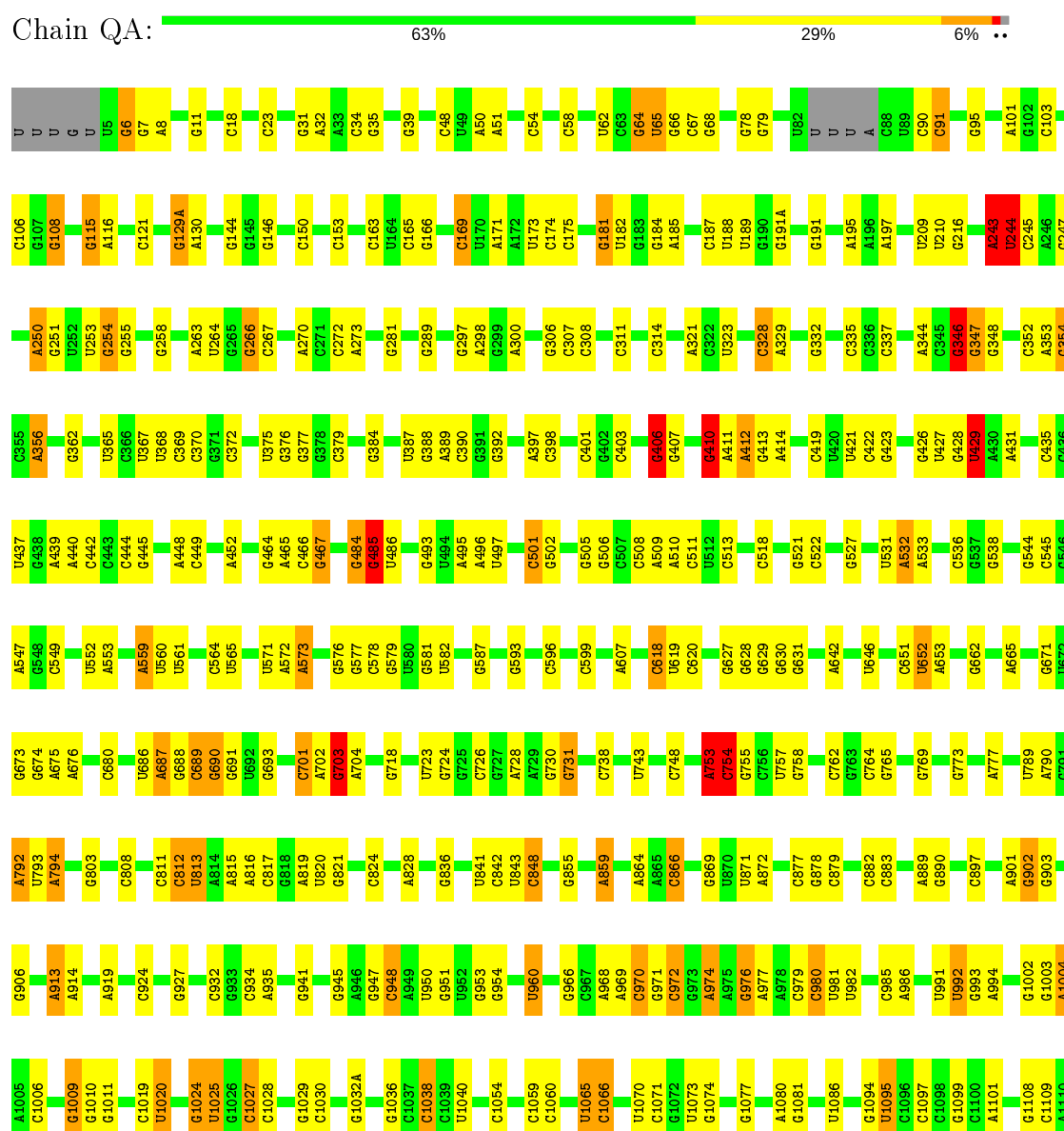
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

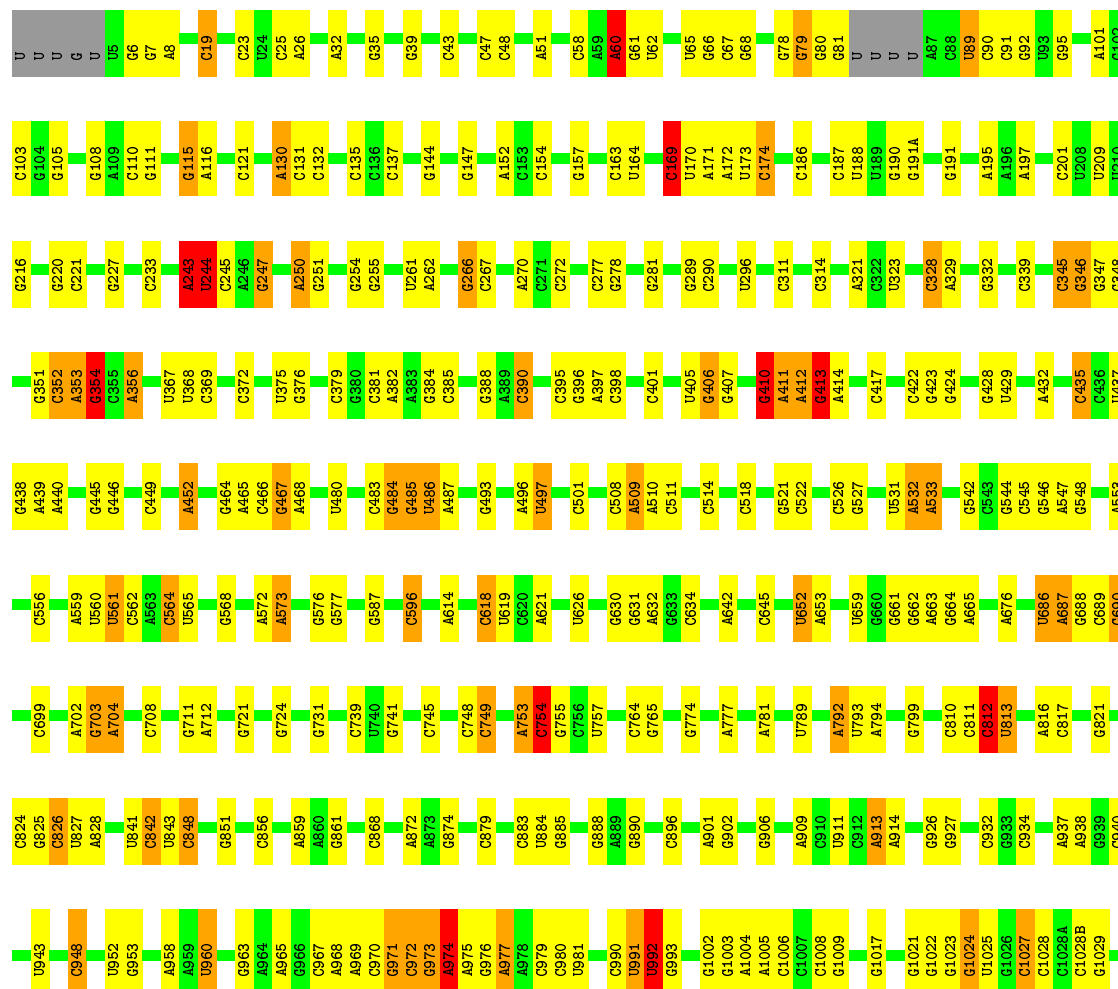
3 Residue-property plots

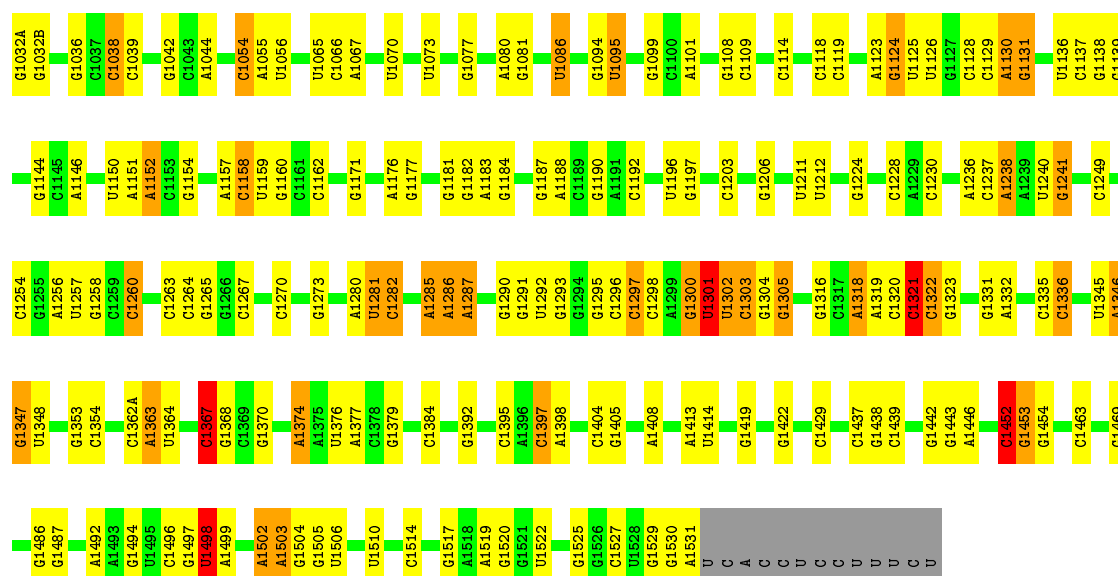
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

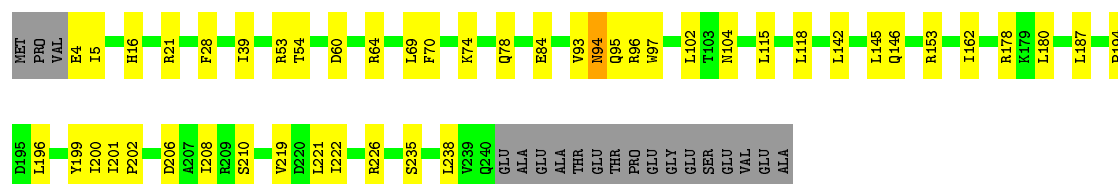






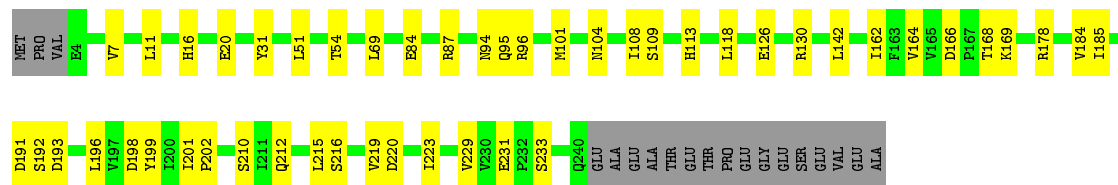
• Molecule 2: 30S ribosomal protein S2

Chain QB: 74% 18% 7%



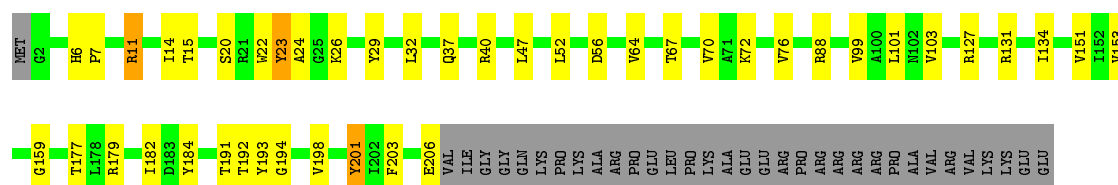
• Molecule 2: 30S ribosomal protein S2

Chain XB: 74% 19% 7%




• Molecule 3: 30S ribosomal protein S3

Chain QC: 67% 17% 14%




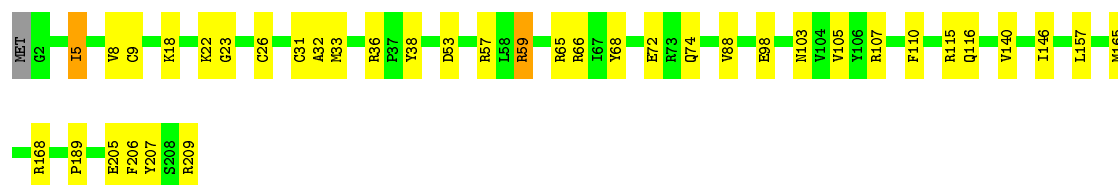
• Molecule 3: 30S ribosomal protein S3

Chain XC:  74% 12% 14%




- Molecule 4: 30S ribosomal protein S4

Chain QD:  81% 17%




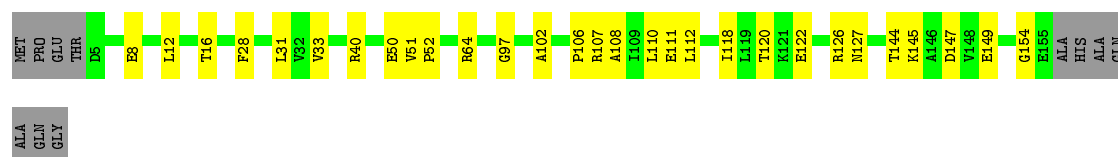
- Molecule 4: 30S ribosomal protein S4

Chain XD:  85% 14%




- Molecule 5: 30S ribosomal protein S5

Chain QE:  75% 18% 7%




- Molecule 5: 30S ribosomal protein S5

Chain XE:  83% 10% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  87% 13%



- Molecule 6: 30S ribosomal protein S6

Chain XF:  87% 13%



- Molecule 7: 30S ribosomal protein S7

Chain QG:  88% 12%




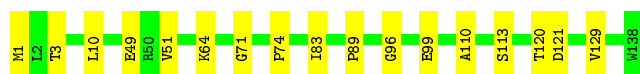
- Molecule 7: 30S ribosomal protein S7

Chain XG:  91% 8%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  88% 12%



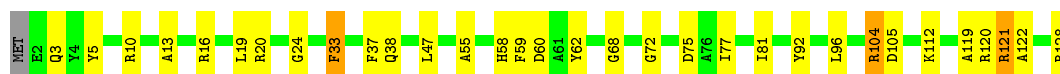
- Molecule 8: 30S ribosomal protein S8

Chain XH:  77% 23%



- Molecule 9: 30S ribosomal protein S9

Chain QI:  74% 23%



- Molecule 9: 30S ribosomal protein S9

Chain XI:  73% 27%




- Molecule 10: 30S ribosomal protein S10

Chain QJ: 



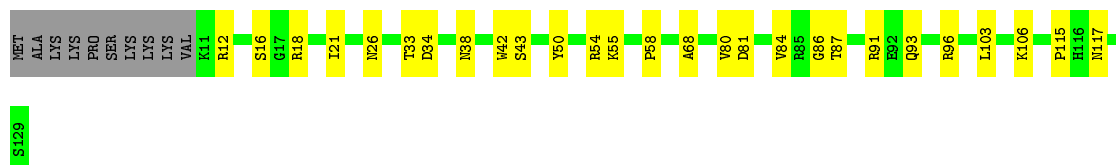
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 




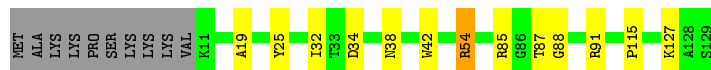
- Molecule 11: 30S ribosomal protein S11

Chain QK: 




- Molecule 11: 30S ribosomal protein S11

Chain XK: 




- Molecule 12: 30S ribosomal protein S12

Chain QL: 



- Molecule 12: 30S ribosomal protein S12

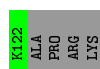
Chain XL: 



- Molecule 13: 30S ribosomal protein S13

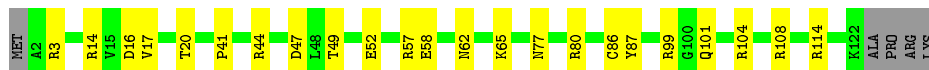
Chain QM: 





- Molecule 13: 30S ribosomal protein S13

Chain XM: 78% 18% .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 75% 23% .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 85% 13% .



- Molecule 15: 30S ribosomal protein S15

Chain QO: 84% 13% ..



- Molecule 15: 30S ribosomal protein S15

Chain XO: 92% 7% .



- Molecule 16: 30S ribosomal protein S16

Chain QP: 70% 24% . 5%

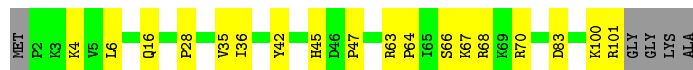
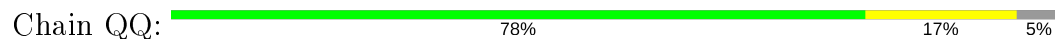


- Molecule 16: 30S ribosomal protein S16

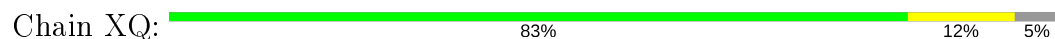
Chain XP: 80% 15% . 5%



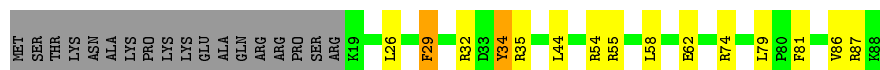
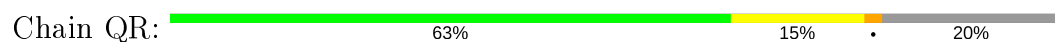
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



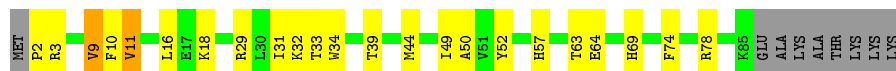
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



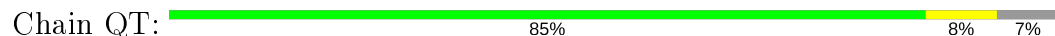
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20

Chain XT: 75% 15% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 70% 22% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain XU: 78% 15% 7%



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

Chain QV: 70% 26% 1%



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

Chain XV: 74% 22% 1%



- Molecule 23: mRNA

Chain QX: 26% 63% 5% 5%

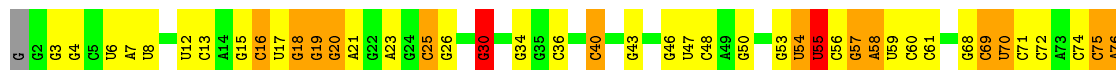


- Molecule 23: mRNA

Chain XX: 42% 42% 11% 5%



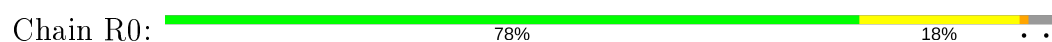
- Molecule 24: A-site tRNAAla(GGC) U32-A38



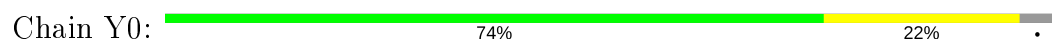
- Molecule 24: A-site tRNAAla(GGC) U32-A38



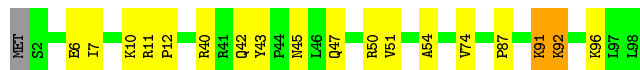
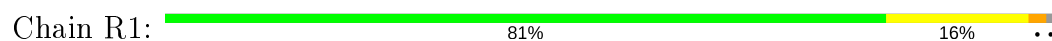
- Molecule 25: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29

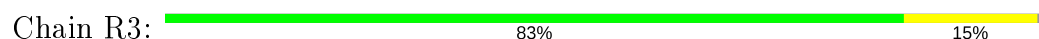




- Molecule 27: 50S ribosomal protein L29



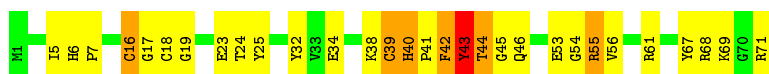
- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



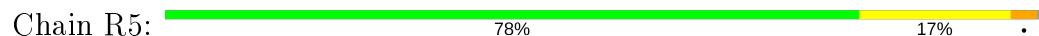
- Molecule 29: 50S ribosomal protein L31



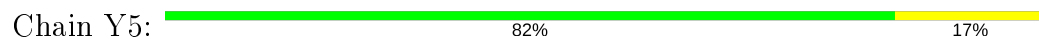
- Molecule 29: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L32

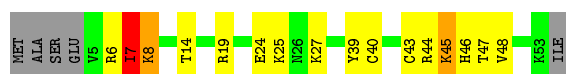




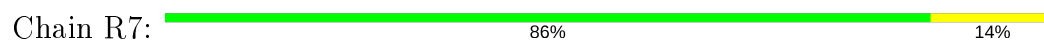
- Molecule 31: 50S ribosomal protein L33



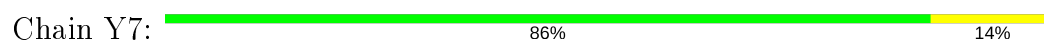
- Molecule 31: 50S ribosomal protein L33



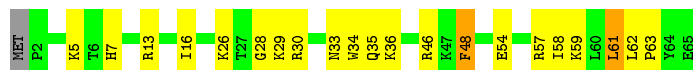
- Molecule 32: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L34



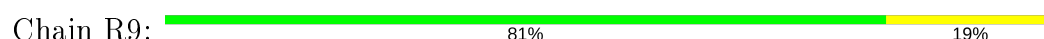
- Molecule 33: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L35

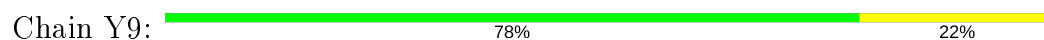


- Molecule 34: 50S ribosomal protein L36

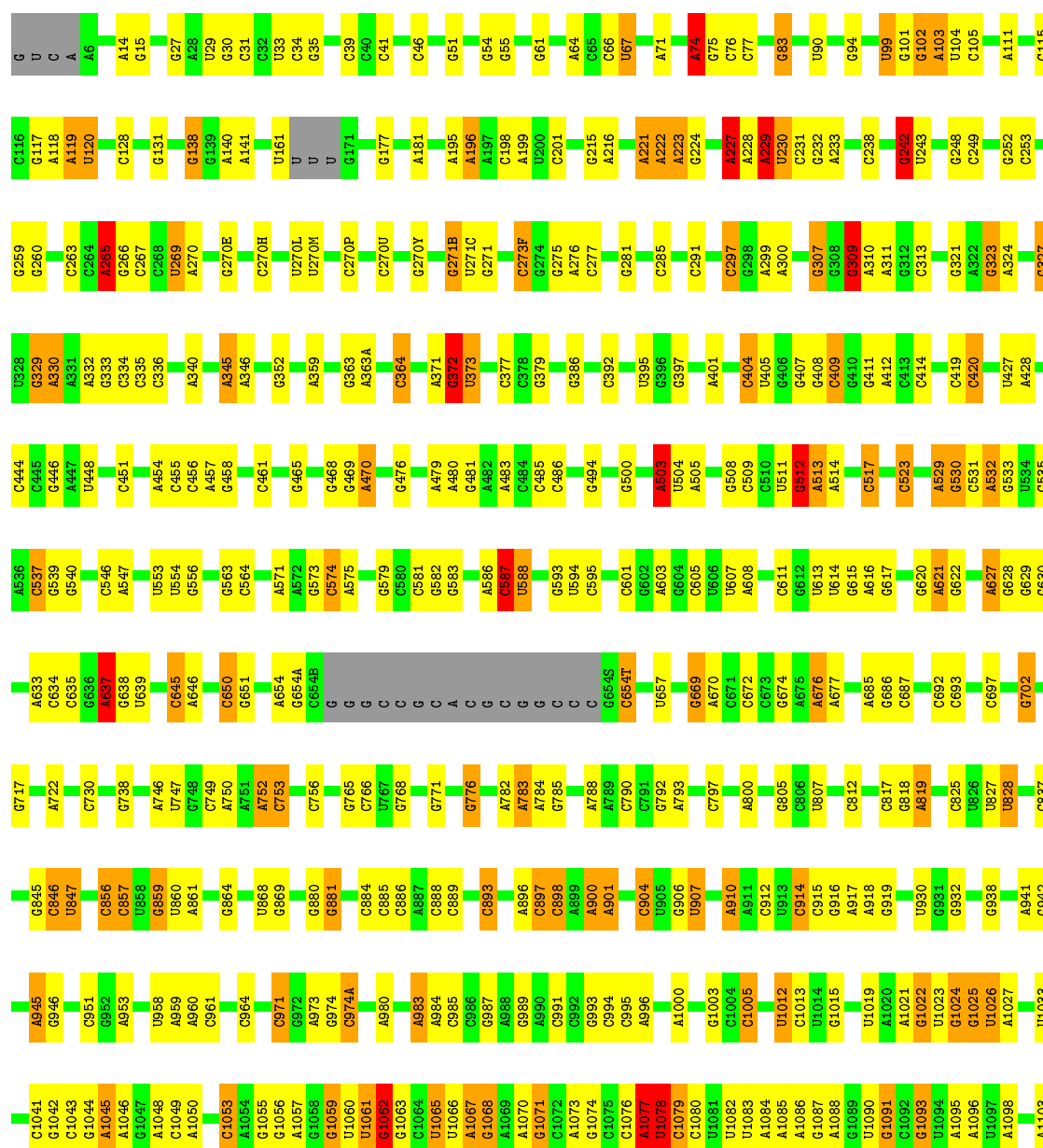




- Molecule 34: 50S ribosomal protein L36

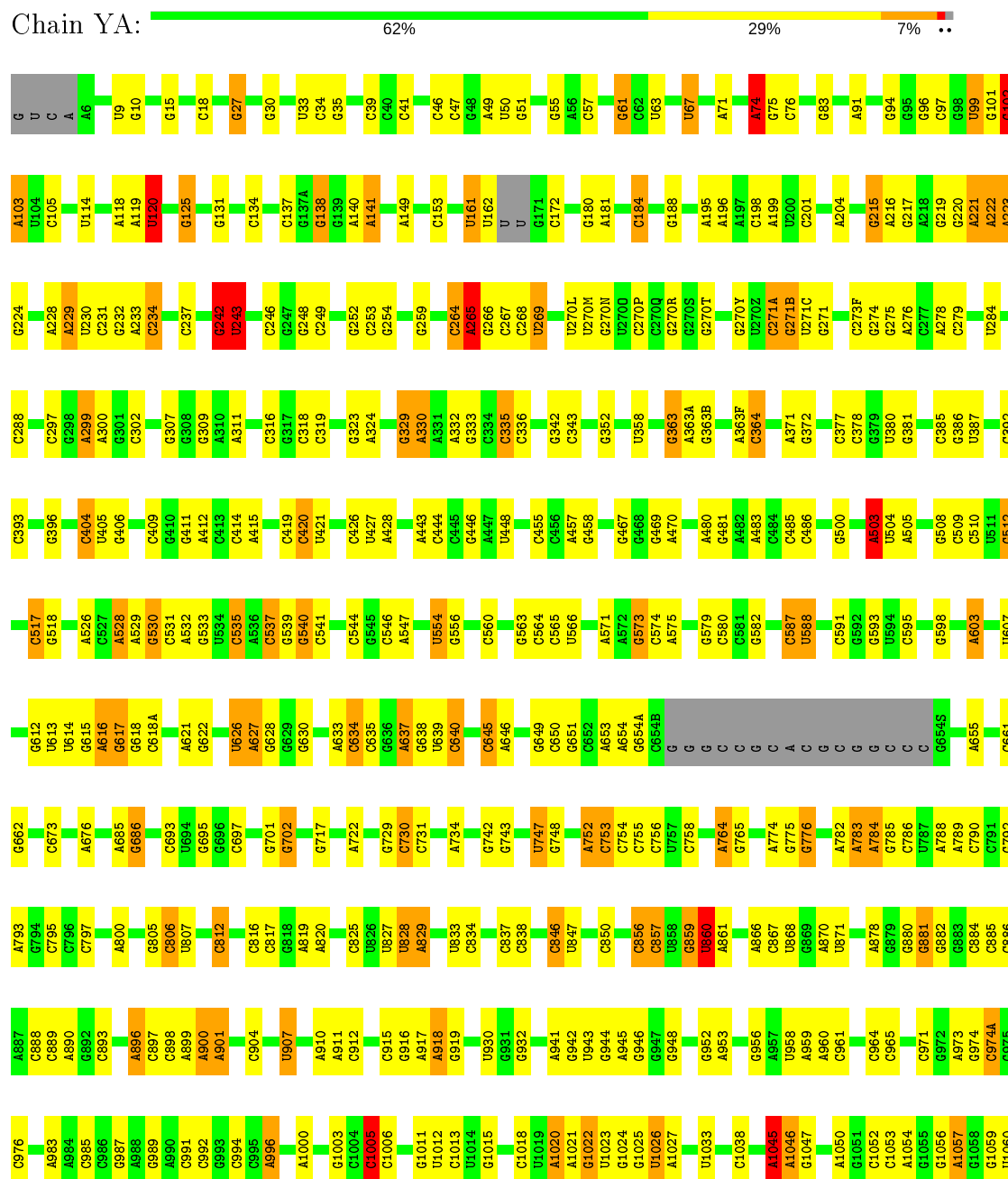


- Molecule 35: 23S rRNA

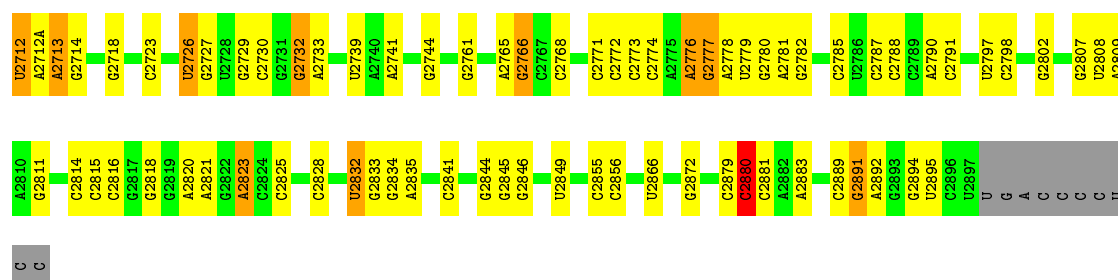


G2554	G2416	C2313	G2210	G2120	G2012	C1892	A1786	G1666	A1558	C1458	G1332	C1217	C1104
G2555	G2417	G2318	G2211	G2121	A2019	G1899	A1787	G1667	G1559	G1459	G1333	C1218	U1105
C2559	C2420	G2319	A2212	G2122	A2020	A1900	A1791	A1668	A1566	A1460	U1341	A1220	G1110
C2421	G2421	A2320	G2215	G2123	G2023	C1901	G1792	A1567	G1568	C1467	A1349	G1228	G1112
A2422	U2422	G2321	G2219	C2126	A2024	G1902	U1794	C1675	A1569	C1468	C1352	C1233	U1113
U2423	A2423	G2325	G2224	C2127	A2031	G1906	C1795	G1681	C1574	A1471	U1353	C1234	G1122
C2424	C2424	G2326	G2225	C2128	G2032	G1907	U1796	C1686	C1575	A1353	G1236	G1237	C1123
A2425	C2425	G2334	A2226	U2130	A2033	C1908	C1797	U1688	C1474	A1365	G1238	G1239	C1124
G2426	A2426	A2335	A2227	G2131	G2036	A1913	U1798	U1689	G1479	G1368	G1239	U1240	U1130
C2427	C2427	G2345	G2228	U2132	G2037	C1914	G1799	U1690	G1480	G1369	G1240	U1241	G1131
G2428	G2428	A2346	C2229	A2133	G2038	C1915	C1800	A1689	U1482	G1370	G1241	C1242	C1135
G2429	G2429	C2347	U2232	A2136	C2039	C1920	C1804	A1690	G1485	C1375	G1252	G1253	G1136
A2430	A2430	C2347	U2233	G2137	C2040	G1921	G1811	C1691	A1495	C1376	A1254	U1255	G1138
A2435	A2435	C2350	G2238	C2137	C2041	G1922	U1812	G1694	A1384	C1377	A1256	G1257	C1140
C2436	C2436	G2358	G2239	G2145	C2042	G1923	A1815	G1695	A1385	C1378	G1258	C1259	A1142A
G2439	G2439	G2355	U2243	C2146	G2052	G1930	A1816	C1698	A1386	C1379	G1259	U1260	A1155
C2440	C2440	C2355	U2244	G2147	C2053	U1931	U1817	A1698	C1598	A1387	A1262	G1263	G1168
G2441	G2441	G2358	U2245	G2148	C2054	A1936	U1818	G1703	C1599	G1380	A1264	A1265	G1169
C2445	C2445	G2361	G2246	G2151	C2056	A1937	A1820	C1708	C1600	A1494	G1266	G1267	G1170
A2448	A2448	G2362	U2249	G2152	A2059	A1938	G1827	C1711	A1603	A1495	A1268	C1269	G1171
G2468	G2468	C2363	G2250	G2156	A2060	U1939	U1828	G1725	C1607	C1502	A1269	G1270	G1172
A2469	A2469	C2364	G2251	G2157	G2061	C1940	A1829	A1728	A1608	U1503	A1271	A1272	A1174
C2470	C2470	G2371	C2258	A2158	C2062	A1962	U1832	A1730	A1609	C1504	A1273	U1273	U1175
C2471	C2471	G2372	G2259	G2166	C2063	G1964	U1833	G1731	C1505	C1506	A1407	A1408	G1176
C2475	C2475	G2373	C2260	C2161	C2064	U1955	U1834	C1734	C1611	C1507	C1411	A1278	A1177
G2478	G2478	G2376	C2261	G2162	U2068	C1962	U1835	C1742	C1615	A1511	G1416	A1284	C1179
C2483	C2483	A2376	U2265	A2163	G2069	A1969	U1836	G1743	A1616	G1512	A1419	C1290	G1183
G2484	G2484	A2377	A2266	G2166	A2071	A1970	U1858	A1762	C1636	C1513	U1420	C1295	G1187
C2485	C2485	A2378	G2269	U2167	C2072	A1971	A1859	G1765	A1637	U1514	G1421	G1296	U1188
G2486	G2486	G2381	A2269	G2168	C2073	A1972	G1860	U1766	C1638	G1525	A1427	U1300	A1189
C2487	C2487	G2382	C2275	A2169	G2076	A1981	U1863	G1767	U1639	C1533	C1428	G1300	G1190
G2494	G2494	G2383	C2276	A2170	U2076	C1982	U1864	C1764	C1640	U1535	A1301	A1301	G1191
C2495	C2495	G2384	A2283	G2171	C2084	C1983	G1869	C1765	C1644	A1536	C1437	C1305	G1192
G2498	G2498	C2385	C2284	U2172	C2084	C1990	A1872	U1766	C1644	C1537	G1441	G1306	A1194
C2499	C2499	G2386	A2285	A2173	U2086	U1991	G1878	A1773	C1648	G1538	G1442	G1309	G1195
G2502	G2502	U2387	A2286	G2176	C2097	G1981	C1881	U1775	G1649	A1444A	A1444A	A1204	A1204
A2503	A2503	A2392	A2287	C2177	C2097	C1982	C1882	U1776	G1650	C1544	U1312	U1312	U1205
C2504	C2504	C2393	G2288	C2178	G2100	C1983	G1883	G1767	C1651	C1445	U1313	G1206	G1206
G2505	G2505	G2394	U2291	G2187	G2101	C1983	A1884	U1779	A1652	A1546A	C1314	C1314	A1210
U2506	U2506	G2395	U2102	U2183	U2102	C1990	A1885	A1780	G1653	C1546	A1449	G1319	U1211
C2518	C2518	G2396	C2107	G2190	C2107	G1993	A1886	C1782	A1654	C1549	U1454	U1329	A1212
U2519	U2519	C2402	C2111	G2193	C2111	C1999	C1887	A1783	C1657	A1554	G1455	U1329	A1214
G2520	G2520	C2403	G2112	G2193	G2112	C1999	G1888	A1784	C1658	A1554	U1329	U1329	A1214
C2527	C2527	U2404	U2113	A2198	U2113	C1999	G1889	A1785	C1658	A1554	U1329	U1329	A1214
U2528	U2528	G2405	G2114	A2199	G2114	C2006	A1884	C1782	C1657	A1554	U1329	U1329	A1214
G2529	G2529	U2406	G2115	C2205	G2115	C2006	A1885	A1783	C1657	A1554	U1329	U1329	A1214
C2535	C2535	G2406	G2116	C2206	G2116	C2008	A1886	A1784	C1657	A1554	U1329	U1329	A1214
G2542	G2542	U2411	U2117	C2207	U2117	C2009	A1888	A1785	C1657	A1554	U1329	U1329	A1214
C2543	C2543	A2411	U2118	C2207	U2118	G2010	A1889	A1785	C1657	A1554	U1329	U1329	A1214
G2543	G2543	A2411	U2119	C2207	U2119	U2011	A1889	A1785	C1657	A1554	U1329	U1329	A1214

- Molecule 35: 23S rRNA

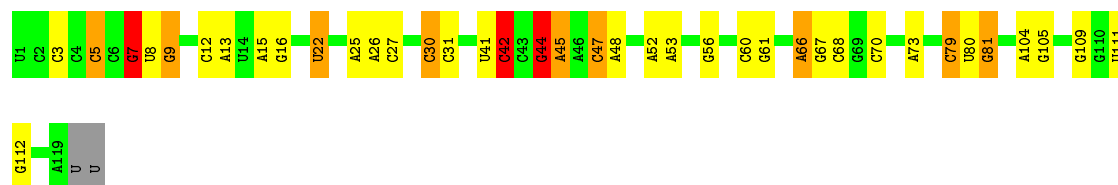


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G2481	U2609	G2384	C2283	A2062	G1964	C1836	G1733	A1609	A1496	U1394	G1266	U1141	G1062
G2483	C2610	C2385		C2065	C1965	A1847	C1742	C1617	U1497	A1395	A1272	U1142	G1063
G2490	U2611	G2391	A2287	C2066	C1967	A1853	G1743	A1618	C1504	U1396	C1290	C1153	U1065
U2491	C2612	A2382	G2185	U2068	A1969	G1858	C1764	G1622	C1506		C1291	U1158	U1066
G2494	U2615	C2383	G2186	G2069	A1970	A1859	A1765	A1631	A1507	C1402	C1295	C1158	A1067
C2498	C2617	A2384	U2167	G2070	A1971	A1869	G1756		C1508		G1296	G1173	A1068
	G2618	C2402	A2169	G2072	A1972	G1869	A1762	C1638	C1509	C1407	G1296	A1174	A1070
G2502	G2619	C2403	A2170	C2073	G1979	A1872	G1763	A1639	A1510	C1408	U1300	U1175	G1071
A2503		C2404	U2171	U2074	A1981	G1878	G1764	C1640	A1511		A1301	G1176	
U2504		G2405	U2172	G2075	C1982	C1879	C1765		U1514			A1177	G1074
G2506	A2632	U2406	A2173	U2076	C1983	C1880	G1769	C1644	U1523		C1306	C1178	G1075
		G2410	A2176	U2079	C1988	C1881		C1648	U1528	G1416	G1309	C1179	C1076
A2518		C2416	C2177	U2080	U1991	C1882	A1773		A1529		G1310		A1077
	C2646		C2178	G2090	G1992	G1883	G1776	G1651	G1530		U1313	G1187	U1082
G2524	U2653	C2420	C2185	G2093	C1994	A1884		A1652			C1314	U1188	U1083
G2525	A2654	U2423	G2186	U2096	U1995	A1889	U1779	G1653	G1535	C1427	C1315	G1190	A1084
	U2655	C2424	G2187	C2097	C1996	A1892	A1780	A1654	A1536	C1428		G1195	A1085
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G2543	G2659	C2427	G2191	U2100	G2010	G1896	A1785		G1539	U1434	U1329		A1088
G2544	A2660	G2428	G2192	U2101	U2011	A1897	A1786	C1662	G1540	C1437	G1332	G1203	G1089
G2545	G2661	C2429	G2193	U2102	C2012	G1899	C1788	G1667	U1541	U1438	C1333	A1204	U1093
U2547	A2662	A2430	A2198	U2103	A2013	A1900	A1789	A1669	G1542	A1444	G1338	U1205	U1094
				C2111	A2014	A1901	C1790	C1670	A1543	C1445		U1206	A1095
U2554		A2435	G2210	G2112	U2016	C1902	A1791		G1544		U1341	A1210	A1096
C2559	C2667	U2439	G2211	U2113	A2019	G1905	C1797	G1674	A1545		A1342	U1211	U1097
A2561		C2441	U2212	A2114	A2020	G1906	U1798	C1675	C1549	G1449	G1343	A1214	A1103
U2562	G2673	G2442	G2215	G2116	C2021	C1914	C1800			U1454	G1344		C1104
U2563	A2679	C2443	A2225	G2117	G2023		G1801	C1682	G1559			G1218	U1105
A2564	C2680	G2444	U2233	U2118	U2022	C1919	U1805	C1686	C1565	U1454	A1349	G1219	G1106
A2565	U2682	G2446	G2234	A2119	G2023	A1919	U1806		C1566	C1468		A1220	G1110
A2566	C2683	G2447	G2235	G2120	A2031	C1920	U1807	A1690	A1567	G1469	U1352	C1221	A1111
G2567		C2448	C2236	G2125	A2032	G1929	U1808	C1691	G1568	A1460	A1353	C1222	G1112
A2572	U2687	U2449	G2237	A2126	A2033	G1930	U1809	U1692	A1569	C1461	G1363	C1223	U1113
C2573	U2688	U2344	G2238	G2127	U2034	U1931	G1811		A1570	C1463	G1364		
G2574	U2689	C2445	G2239	C2128	G2035	A1937	G1816	G1695	A1571		A1365	G1238	C1121
C2575	C2690	A2346	U2243	C2129	G2039	A1938	G1817		U1578	C1467	G1366	G1239	G1122
G2576	C2691	C2347	G2246	U2130		U1939	U1818	A1698	A1579		A1367	U1240	G1123
A2577	C2692			U2132	C2043	U1940	U1819	G1699	A1580		G1368	G1124	G1125
G2578		G2468	G2246	G2133	C2044		U1820	A1700	G1581		C1370	A1246	A1126
C2579	U2698	A2469	U2249	C2138	G2053	C1947	U1821			G1478			
U2580		G2470	U2249	G2139	A2054		G1824	C1712	C1585	G1479	C1376	G1250	A1129
U2584	C2701	C2471	G2253	G1950	C2055	G1950	A1825	G1725	A1586	G1483	A1379	C1251	U1130
C2585	U2702	U2472	G2253	G2146	C2056	U1955	A1826			G1484	A1253	G1252	G1131
C2586		C2473	C2258	G2147	G2056	U1956	G1827	G1728	G1595	G1485	A1384	G1256	C1135
G2592	G2706	C2474		G2148	A2057	U1957	C1827				G1385		G1136
	C2709	C2475	C2261	G2149	A2058	C1957	G1828	U1729	C1598	A1490	C1386	G1264	G1138
	C2710	U2150		U2150	A2059	C1958	A1829				C1387		G1139
G2597		G2151	A2269	G2151	A2060			G1731	C1607				



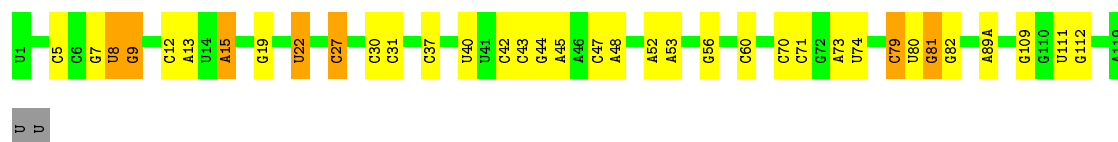
• Molecule 36: 5S rRNA

Chain RB: 66% 22% 7% . .



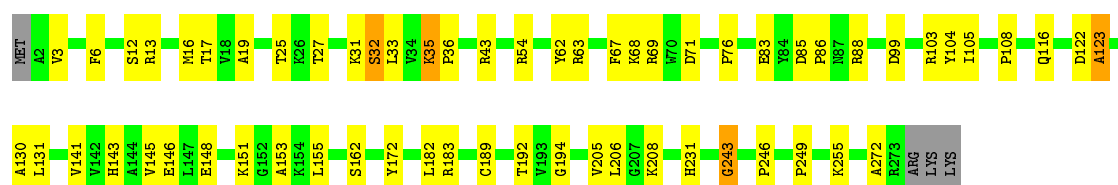
• Molecule 36: 5S rRNA

Chain YB: 69% 24% 6% .



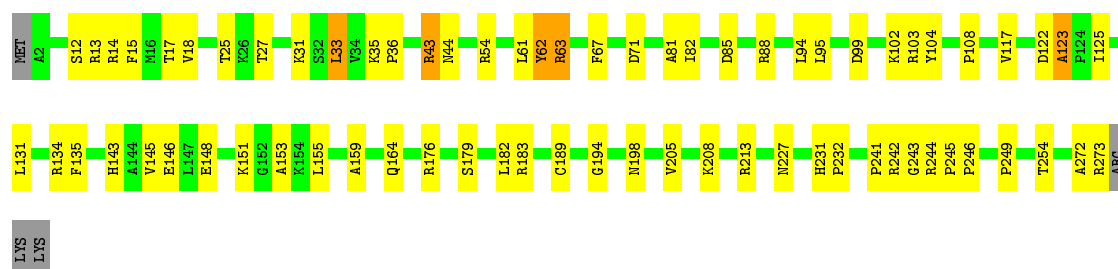
• Molecule 37: 50S ribosomal protein L2

Chain RD: 76% 21% . .

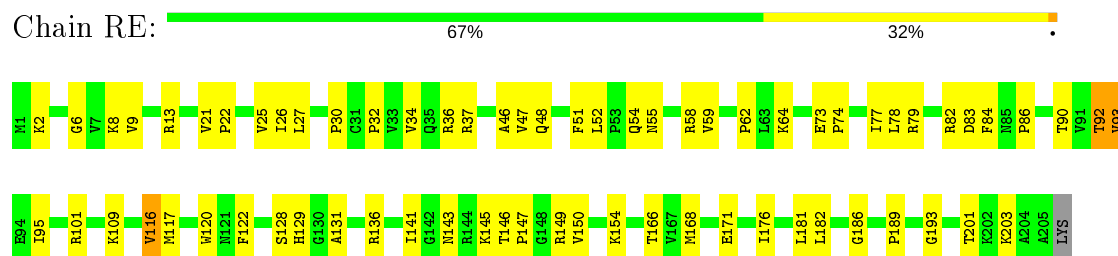


• Molecule 37: 50S ribosomal protein L2

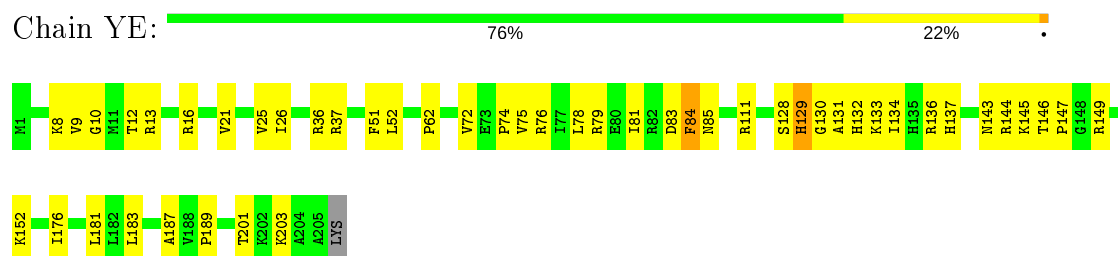
Chain YD: 73% 24% . .



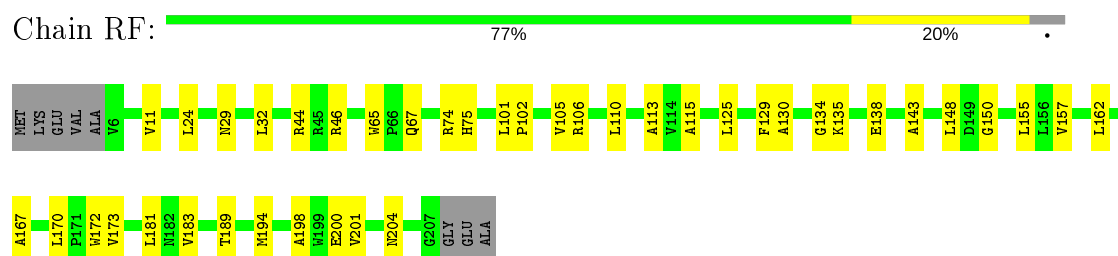
- Molecule 38: 50S ribosomal protein L3



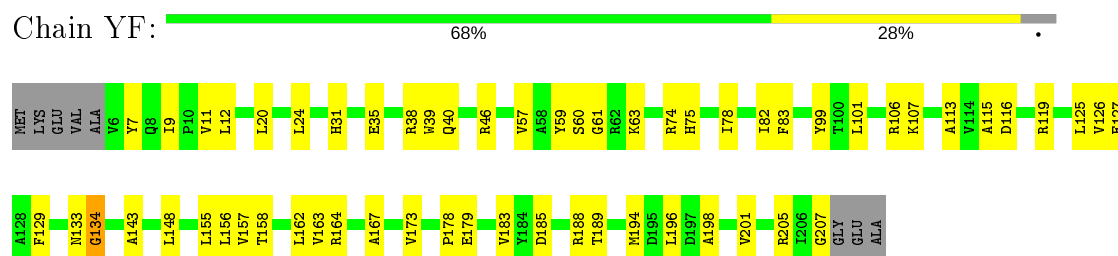
- Molecule 38: 50S ribosomal protein L3



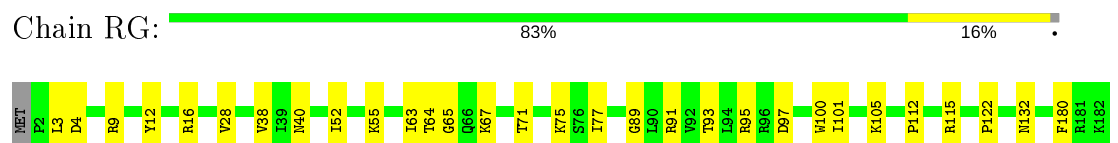
- Molecule 39: 50S ribosomal protein L4



- Molecule 39: 50S ribosomal protein L4



- Molecule 40: 50S ribosomal protein L5



- Molecule 40: 50S ribosomal protein L5

- | GLY | ALA | LYS | LYS |
|-----|-----|-----|------|
| Met | S2 | R3 | I4 |
| | | | P8 |
| | | | E18 |
| | | | R23 |
| | | | V24 |
| | | | K25 |
| | | | V35 |
| | | | P36 |
| | | | E40 |
| | | | M41 |
| | | | P45 |
| | | | R69 |
| | | | G82 |
| | | | K85 |
| | | | E86 |
| | | | I89 |
| | | | L103 |
| | | | V107 |
| | | | F123 |
| | | | E124 |
| | | | V125 |
| | | | P126 |
| | | | R130 |
| | | | V131 |
| | | | Q139 |
| | | | R152 |
| | | | K153 |
| | | | P154 |
| | | | S155 |
| | | | I162 |
| | | | P168 |
| | | | V169 |
| | | | R170 |
| | | | L171 |
| | | | LYS |
| | | | P190 |
| | | | GLY |
| | | | LYS |
| | | | ALA |


- | GLY | ALA | LYS | LYS | MET |
|-----|-----|-----|-----|------|
| S2 | R3 | I4 | G5 | R6 |
| | | | | M41 |
| | | | | E46 |
| | | | | R51 |
| | | | | V52 |
| | | | | E53 |
| | | | | R54 |
| | | | | P55 |
| | | | | S56 |
| | | | | D57 |
| | | | | H61 |
| | | | | L64 |
| | | | | H65 |
| | | | | G82 |
| | | | | Y83 |
| | | | | R101 |
| | | | | A102 |
| | | | | L103 |
| | | | | V115 |
| | | | | F123 |
| | | | | P126 |
| | | | | R130 |
| | | | | V131 |
| | | | | R132 |
| | | | | R149 |
| | | | | K153 |
| | | | | P154 |
| | | | | S155 |
| | | | | A156 |
| | | | | Y157 |
| | | | | H158 |
| | | | | T162 |
| | | | | P168 |
| | | | | L171 |
| | | | | LYS |
| | | | | PRO |
| | | | | GLY |
| | | | | LYS |
| | | | | ALA |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|--|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|------|------|------|------|--|------|------|------|--|------|------|------|------|------|------|------|------|--|------|--|------|-----|-----|
| M1 | K2 | V3 | | N11 | L12 | G13 | D14 | V15 | G16 | | V21 | | L30 | R33 | A36 | V37 | L38 | E64 | R67 | L68 | K69 | E73 | I79 | T86 | G90 | S91 | V92 | | K118 | P119 | I120 | K121 | | Y126 | V127 | L128 | | K131 | P132 | H133 | P134 | E135 | V136 | P137 | I138 | | V142 | | A146 | G1N | C1U |
|----|----|----|--|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|------|------|------|------|--|------|------|------|--|------|------|------|------|------|------|------|------|--|------|--|------|-----|-----|

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|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|
| M1 | I4 | L5 | E10 | N11 | G13 | D14 | V15 | G16 | Q17 | V18 | V19 | A26 | L30 | A36 | T40 | M43 | L68 | I71 | L77 | T78 | I79 | L101 | L114 | Y130 | K131 | V136 | V142 | A146 | GLN | G11 |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|


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|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|
| M1 | K2 | T3 | E10 | P11 | T22 | T23 | G24 | R25 | T28 | K29 | M48 | K66 | E96 | R97 | V98 | L99 | E100 | H101 | A102 | V103 | M106 | L107 | P108 | G113 | V122 | Q133 | R134 | P135 | L138 | GLU | VAL |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|

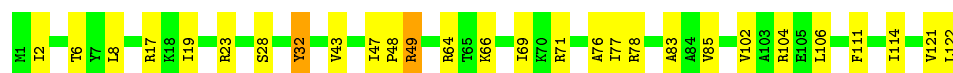
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Chain YN:  87% 11% ..




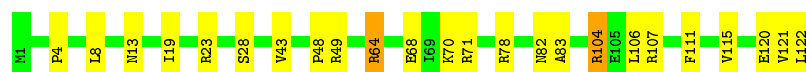
- Molecule 44: 50S ribosomal protein L14

Chain RO:  77% 21% .



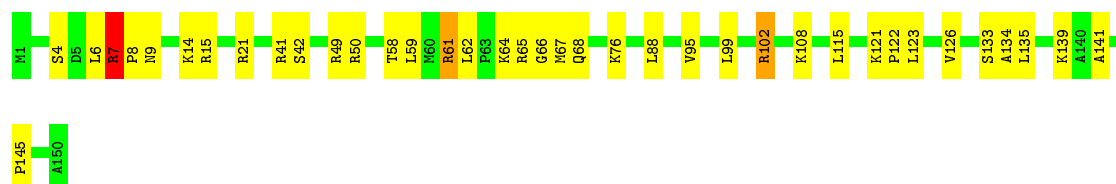
- Molecule 44: 50S ribosomal protein L14

Chain YO:  80% 18% .




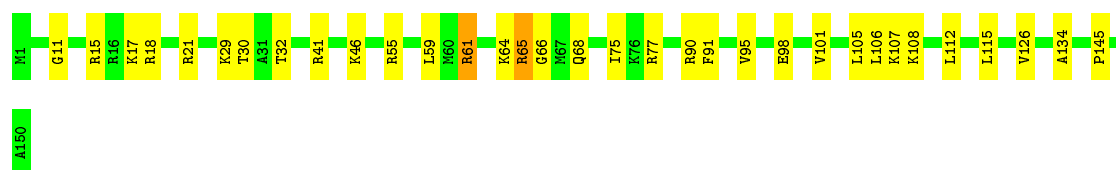
- Molecule 45: 50S ribosomal protein L15

Chain RP:  75% 23% ..




- Molecule 45: 50S ribosomal protein L15

Chain YP:  78% 21% .




- Molecule 46: 50S ribosomal protein L16

Chain RQ:  82% 16% .

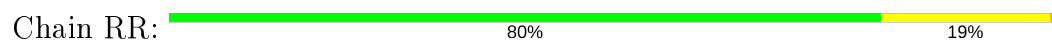


- Molecule 46: 50S ribosomal protein L16

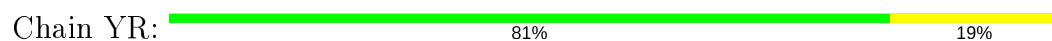
Chain YQ:  79% 18% .



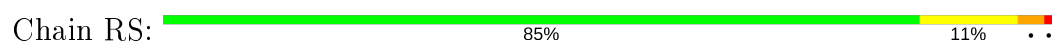
- Molecule 47: 50S ribosomal protein L17



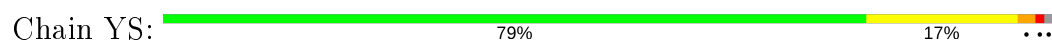
- Molecule 47: 50S ribosomal protein L17



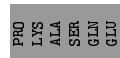
- Molecule 48: 50S ribosomal protein L18



- Molecule 48: 50S ribosomal protein L18




- Molecule 49: 50S ribosomal protein L19



- Molecule 49: 50S ribosomal protein L19




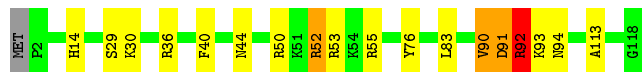
- Molecule 50: 50S ribosomal protein L20

Chain RU:  81% 16% ...




- Molecule 50: 50S ribosomal protein L20

Chain YU:  84% 12% ..




- Molecule 51: 50S ribosomal protein L21

Chain RV:  74% 25% .




- Molecule 51: 50S ribosomal protein L21

Chain YV:  86% 12% ..




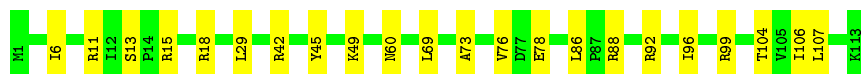
- Molecule 52: 50S ribosomal protein L22

Chain RW:  81% 19%



- Molecule 52: 50S ribosomal protein L22

Chain YW:  81% 19%




- Molecule 53: 50S ribosomal protein L23

Chain RX:  80% 16% .




- Molecule 53: 50S ribosomal protein L23

Chain YX:  82% 13% . .




- Molecule 54: 50S ribosomal protein L24

Chain RY:  76% 15% . 7%



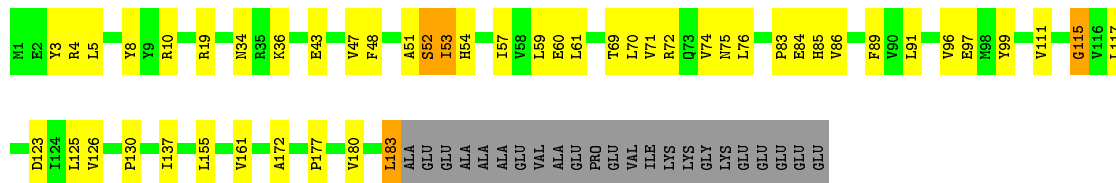
- Molecule 54: 50S ribosomal protein L24

Chain YY:  81% 12% 7%



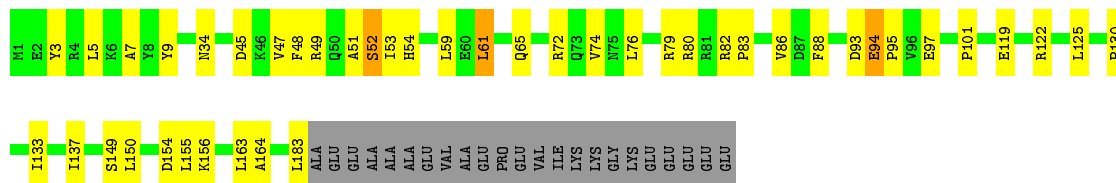
- Molecule 55: 50S ribosomal protein L25

Chain RZ:  65% 22% . 11%



- Molecule 55: 50S ribosomal protein L25

Chain YZ:  67% 20% . 11%



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 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10	Depositor
% Data completeness (in resolution range)	97.2 (49.74-3.10)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266	Depositor
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.328	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	1.05	0/36098	1.14	177/56341 (0.3%)
1	XA	1.14	0/36101	1.18	234/56346 (0.4%)
2	QB	0.48	0/1959	0.68	0/2642
2	XB	0.55	0/1959	0.68	0/2642
3	QC	0.50	0/1629	0.69	2/2195 (0.1%)
3	XC	0.52	0/1629	0.66	0/2195
4	QD	0.58	0/1704	0.63	0/2284
4	XD	0.58	0/1704	0.65	0/2284
5	QE	0.55	1/1171 (0.1%)	0.67	0/1576
5	XE	0.54	0/1171	0.65	1/1576 (0.1%)
6	QF	0.60	0/856	0.62	0/1154
6	XF	0.58	0/856	0.66	0/1154
7	QG	0.51	0/1276	0.65	1/1709 (0.1%)
7	XG	0.52	0/1276	0.65	0/1709
8	QH	0.51	0/1136	0.66	0/1527
8	XH	0.59	0/1136	0.66	0/1527
9	QI	0.53	0/1029	0.77	0/1379
9	XI	0.53	0/1029	0.72	0/1379
10	QJ	0.46	0/814	0.64	0/1095
10	XJ	0.53	0/814	0.63	0/1095
11	QK	0.55	0/900	0.64	0/1213
11	XK	0.53	0/900	0.63	0/1213
12	QL	0.56	0/991	0.76	3/1327 (0.2%)
12	XL	0.63	0/991	0.75	1/1327 (0.1%)
13	QM	0.52	0/974	0.79	1/1303 (0.1%)
13	XM	0.50	0/974	0.72	0/1303
14	QN	0.55	0/501	0.67	0/664
14	XN	0.62	0/501	0.75	0/664
15	QO	0.50	0/745	0.59	0/992
15	XO	0.48	0/745	0.59	0/992
16	QP	0.58	0/721	0.75	2/970 (0.2%)
16	XP	0.55	0/721	0.76	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.60	0/847	0.65	1/1131 (0.1%)
17	XQ	0.59	0/847	0.64	1/1131 (0.1%)
18	QR	0.59	0/579	0.73	0/768
18	XR	0.57	0/579	0.65	0/768
19	QS	0.47	0/689	0.70	0/926
19	XS	0.62	0/689	0.97	2/926 (0.2%)
20	QT	0.48	0/765	0.66	0/1007
20	XT	0.44	0/765	0.71	1/1007 (0.1%)
21	QU	0.59	0/221	0.73	0/288
21	XU	0.67	0/221	0.81	1/288 (0.3%)
22	QV	0.91	0/1832	1.23	17/2855 (0.6%)
22	XV	1.07	0/1832	1.13	7/2855 (0.2%)
23	QX	0.77	0/446	1.06	2/695 (0.3%)
23	XX	0.87	0/446	1.17	1/695 (0.1%)
24	QY	0.74	0/1790	1.20	15/2789 (0.5%)
24	XY	0.78	0/1790	1.20	10/2789 (0.4%)
25	R0	0.59	0/657	0.68	1/874 (0.1%)
25	Y0	0.69	0/657	0.69	0/874
26	R1	0.63	0/770	0.79	2/1022 (0.2%)
26	Y1	0.64	0/770	0.76	1/1022 (0.1%)
27	R2	0.52	0/583	0.68	0/771
27	Y2	0.56	0/583	0.75	0/771
28	R3	0.50	0/474	0.57	0/635
28	Y3	0.57	0/474	0.58	0/635
29	R4	0.61	0/594	1.05	2/795 (0.3%)
29	Y4	0.56	0/594	1.05	3/795 (0.4%)
30	R5	0.60	0/473	0.92	2/639 (0.3%)
30	Y5	0.68	0/473	0.74	0/639
31	R6	0.70	0/431	1.14	2/575 (0.3%)
31	Y6	0.73	0/431	1.04	2/575 (0.3%)
32	R7	0.66	0/438	0.66	0/575
32	Y7	0.71	0/438	0.71	0/575
33	R8	0.64	0/525	0.86	1/691 (0.1%)
33	Y8	0.78	1/525 (0.2%)	0.84	0/691
34	R9	0.61	0/310	0.54	0/407
34	Y9	0.67	0/310	0.60	0/407
35	RA	1.23	8/69521 (0.0%)	1.22	496/108529 (0.5%)
35	YA	1.38	19/69543 (0.0%)	1.26	627/108563 (0.6%)
36	RB	0.99	0/2878	1.19	16/4490 (0.4%)
36	YB	1.23	0/2878	1.22	17/4490 (0.4%)
37	RD	0.71	0/2165	0.76	1/2919 (0.0%)
37	YD	0.75	0/2165	0.78	2/2919 (0.1%)
38	RE	0.63	0/1601	0.82	4/2160 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YE	0.71	0/1601	0.85	1/2160 (0.0%)
39	RF	0.65	0/1620	0.67	0/2194
39	YF	0.72	1/1620 (0.1%)	0.71	1/2194 (0.0%)
40	RG	0.51	0/1499	0.72	0/2016
40	YG	0.55	0/1499	0.70	1/2016 (0.0%)
41	RH	0.50	0/1332	0.81	2/1802 (0.1%)
41	YH	0.63	0/1332	0.84	3/1802 (0.2%)
42	RI	0.59	2/1151 (0.2%)	0.90	7/1558 (0.4%)
42	YI	0.52	0/1151	0.83	2/1558 (0.1%)
43	RN	0.57	0/1131	0.71	1/1525 (0.1%)
43	YN	0.63	0/1131	0.74	2/1525 (0.1%)
44	RO	0.62	0/943	0.66	1/1269 (0.1%)
44	YO	0.72	0/943	0.76	2/1269 (0.2%)
45	RP	0.59	0/1162	0.89	0/1544
45	YP	0.61	0/1162	0.85	1/1544 (0.1%)
46	RQ	0.63	0/1143	0.83	2/1527 (0.1%)
46	YQ	0.71	0/1143	0.87	3/1527 (0.2%)
47	RR	0.62	0/982	0.69	0/1312
47	YR	0.64	0/982	0.72	0/1312
48	RS	0.55	0/892	0.92	5/1187 (0.4%)
48	YS	0.59	0/892	0.78	1/1187 (0.1%)
49	RT	0.61	0/1155	0.78	3/1542 (0.2%)
49	YT	0.66	0/1155	0.82	4/1542 (0.3%)
50	RU	0.61	0/982	0.67	1/1306 (0.1%)
50	YU	0.70	0/982	0.69	1/1306 (0.1%)
51	RV	0.58	0/790	0.82	2/1057 (0.2%)
51	YV	0.76	0/790	0.88	2/1057 (0.2%)
52	RW	0.66	0/911	0.70	0/1220
52	YW	0.64	0/911	0.66	0/1220
53	RX	0.66	0/739	0.70	0/993
53	YX	0.71	0/739	0.67	0/993
54	RY	0.59	0/798	0.69	0/1064
54	YY	0.70	0/798	0.76	0/1064
55	RZ	0.52	0/1493	0.81	4/2026 (0.2%)
55	YZ	0.56	0/1493	0.78	2/2026 (0.1%)
All	All	1.08	32/319657 (0.0%)	1.11	1714/478147 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
48	RS	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y8	23	VAL	CB-CG1	-8.00	1.36	1.52
35	YA	528	A	N9-C4	-7.92	1.33	1.37
35	YA	1021	A	N9-C4	-7.85	1.33	1.37
35	YA	1142(A)	A	N9-C4	-7.78	1.33	1.37
35	YA	2287	A	N9-C4	-7.34	1.33	1.37

The worst 5 of 1714 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	XS	10	PHE	CB-CG-CD1	12.46	129.52	120.80
1	QA	1301	U	N1-C2-O2	11.86	131.10	122.80
35	RA	2506	U	C2-N1-C1'	11.85	131.92	117.70
1	QA	1301	U	C2-N1-C1'	11.78	131.83	117.70
35	YA	2506	U	C2-N1-C1'	11.73	131.77	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	208	0
1	XA	32249	0	16279	169	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	28	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	16	0
4	QD	1674	0	1718	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1674	0	1718	21	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	19	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	18	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	15	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	17	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0
19	XS	674	0	699	13	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	396	0	197	2	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y0	648	0	672	10	0
26	R1	763	0	847	13	0
26	Y1	763	0	848	12	0
27	R2	581	0	629	15	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	16	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	10	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	11	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	6	0
33	R8	517	0	582	17	0
33	Y8	517	0	582	30	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	341	0
35	YA	62091	0	31290	289	0
36	RB	2573	0	1306	15	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	51	0
38	RE	1568	0	1633	45	0
38	YE	1568	0	1634	31	0
39	RF	1585	0	1632	22	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0
40	YG	1474	0	1535	18	0
41	RH	1307	0	1382	20	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	11	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	8	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	27	0
46	RQ	1122	0	1179	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	YQ	1122	0	1177	20	0
47	RR	968	0	1033	17	0
47	YR	968	0	1033	16	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	23	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	19	0
51	RV	779	0	852	17	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	17	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	27	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y1	1	0	0	0	0
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199665	2182	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 5.

The worst 5 of 2182 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:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.13	1.11
35:RA:2055:C:H5'	35:RA:2056:G:H5''	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	17	52
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	57
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	57
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	54
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	19	54
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	3	16
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	19	54
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	36
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	3	19
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	23
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	4	22
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	30
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10	39
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	4	24
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	8
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	8
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	22
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	9	37
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	8	33
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	34	69
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	10	39
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	5	27
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	10	39
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	49
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	25	59
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	6	27
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	13	44
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	2	11
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	3	16
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	57
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	57
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	54
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5	25
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	11	40
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	57
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	4	24
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	36
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9	36
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	5	25
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	17	52
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	22	57
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5	26
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	7	31
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	49
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	14	46
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	5	25
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	6	29
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	14	46

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS

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	205/220 (93%)	203 (99%)	2 (1%)	76	90
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	87
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	171 (99%)	2 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	173/181 (96%)	172 (99%)	1 (1%)	86	94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	118 (99%)	1 (1%)	81	92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	70
9	XI	98/99 (99%)	97 (99%)	1 (1%)	76	90
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	88 (99%)	1 (1%)	73	89
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	89
11	XK	90/99 (91%)	89 (99%)	1 (1%)	73	89
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76	90
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	86
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	89
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	70 (96%)	3 (4%)	30	64
19	XS	73/80 (91%)	71 (97%)	2 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	59
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	62 (97%)	2 (3%)	40	70
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	59 (94%)	4 (6%)	18	48
29	Y4	63/63 (100%)	62 (98%)	1 (2%)	62	84
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	R6	48/52 (92%)	47 (98%)	1 (2%)	53	79
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	41 (98%)	1 (2%)	49	76
33	R8	54/55 (98%)	53 (98%)	1 (2%)	57	81
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	66
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%)	212 (99%)	2 (1%)	78	91
37	YD	214/218 (98%)	211 (99%)	3 (1%)	67	86
38	RE	165/166 (99%)	163 (99%)	2 (1%)	71	88
38	YE	165/166 (99%)	163 (99%)	2 (1%)	71	88
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
41	RH	142/148 (96%)	141 (99%)	1 (1%)	84	93
41	YH	142/148 (96%)	141 (99%)	1 (1%)	84	93
42	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	98 (98%)	2 (2%)	55	80
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	80
45	RP	116/116 (100%)	113 (97%)	3 (3%)	46	74
45	YP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
46	YQ	111/111 (100%)	108 (97%)	3 (3%)	44	74
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	100 (99%)	1 (1%)	76	90
48	RS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	69
49	RT	120/127 (94%)	118 (98%)	2 (2%)	60	83
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	89
51	RV	82/82 (100%)	81 (99%)	1 (1%)	71	88
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	89
52	YW	92/92 (100%)	92 (100%)	0	100	100
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	67	86
54	RY	85/91 (93%)	84 (99%)	1 (1%)	71	88
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
55	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9688/10064 (96%)	9587 (99%)	101 (1%)	76	90

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	RS	29	PHE
8	XH	104	ARG
49	YT	65	LYS
49	RT	115	ARG
54	RY	101	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
49	RT	58	ASN
2	XB	94	ASN
49	YT	38	ASN
50	RU	44	ASN
52	RW	60	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	270 (18%)	29 (1%)
1	XA	1498/1522 (98%)	279 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	7 (41%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	587 (20%)	47 (1%)
35	YA	2880/2915 (98%)	587 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1859 (19%)	150 (1%)

5 of 1859 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	RA	2060	A
1	XA	244	U
35	YA	1955	U
35	RA	2405	G
35	RA	2832	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 855 ligands modelled in this entry, 851 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	501	-	0,12,12	0.00	-	-		
58	SF4	XD	501	4	0,12,12	0.00	-	-		
57	PAR	QA	1663	-	45,45,45	0.80	0	64,67,67	1.30	8 (12%)
57	PAR	XA	1670	-	45,45,45	0.86	1 (2%)	64,67,67	1.28	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	501	-	-	-	0/6/5/5
58	SF4	XD	501	4	-	-	0/6/5/5
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4
57	PAR	XA	1670	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.01	1.44	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1663	PAR	C13-O52-C52	-3.20	110.03	117.96
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	XA	1670	PAR	C13-O52-C52	-2.87	110.85	117.96
57	QA	1663	PAR	C64-C54-C44	-2.68	107.82	113.10
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.81

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

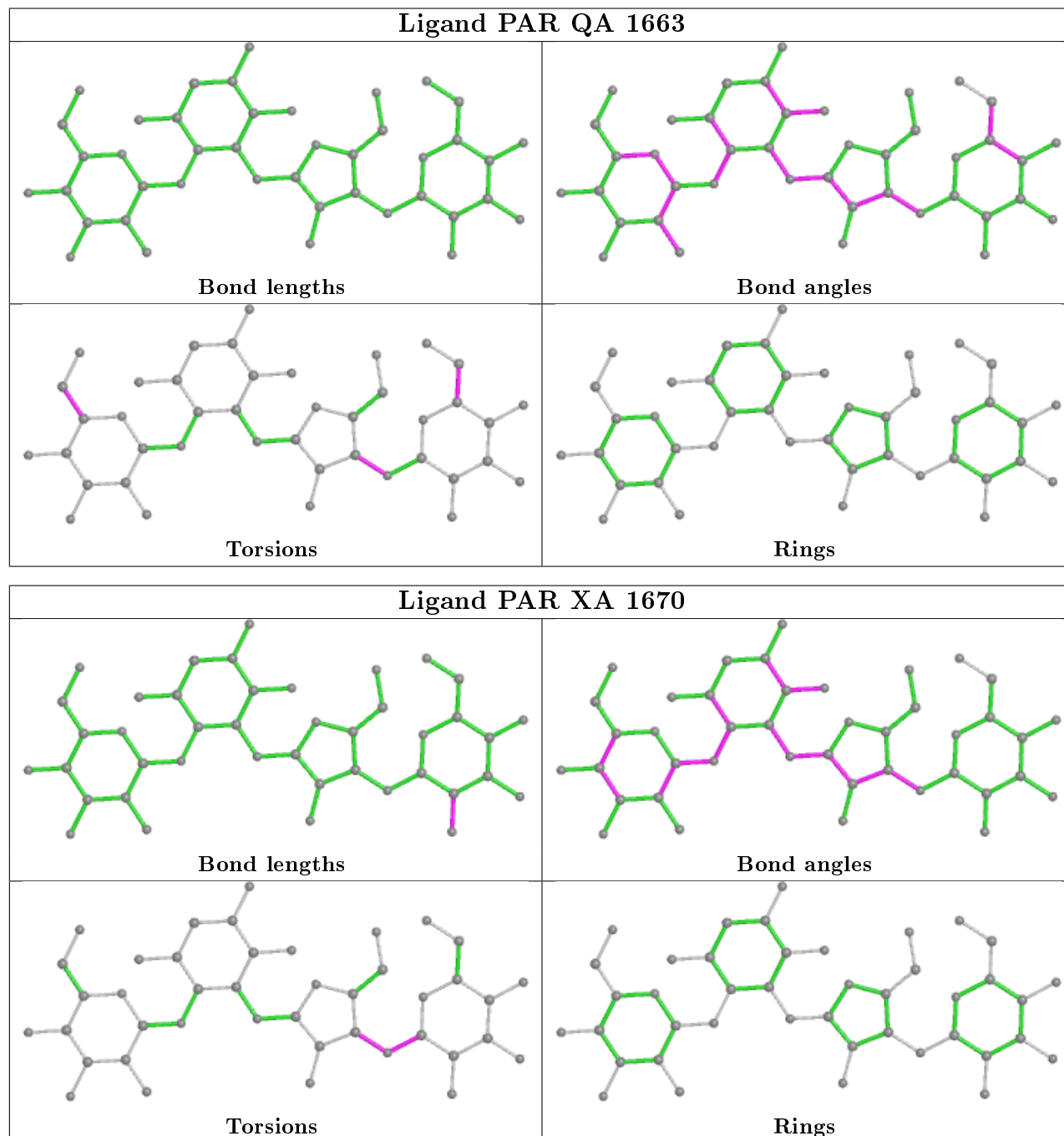
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	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.