



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 05:36 AM EDT

PDB ID : 6OJ2
Title : Crystal structure of tRNA^{Ala}(GGC) bound to the near-cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-10
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.35.1

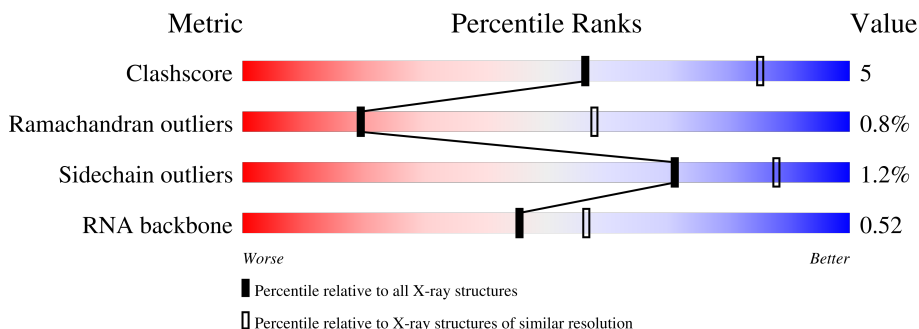
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)





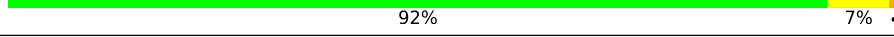



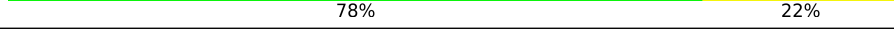

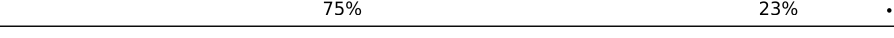
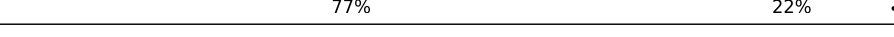

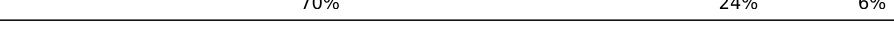


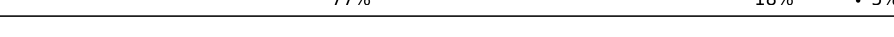

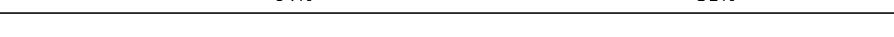






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	

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Mol	Chain	Length	Quality of chain
4	QD	209	 84% 14% .
4	XD	209	 79% 19% .
5	QE	162	 78% 15% 7%
5	XE	162	 73% 20% 7%
6	QF	101	 92% 7% .
6	XF	101	 86% 14%
7	QG	156	 85% 15% .
7	XG	156	 85% 14% .
8	QH	138	 78% 22%
8	XH	138	 75% 25%
9	QI	128	 75% 23% ..
9	XI	128	 77% 22% ..
10	QJ	105	 76% 18% 6%
10	XJ	105	 70% 24% 6%
11	QK	129	 80% 12% 8%
11	XK	129	 77% 16% 8%
12	QL	131	 77% 18% . 5%
12	XL	131	 76% 18% .. 5%
13	QM	126	 64% 31% . .
13	XM	126	 71% 24% . .
14	QN	61	 64% 31% . .
14	XN	61	 79% 20% .
15	QO	89	 87% 10% ..
15	XO	89	 98% ..
16	QP	88	 81% 14% . 5%


























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Mol	Chain	Length	Quality of chain
16	XP	88	82% 13% 5%
17	QQ	105	69% 27% 5%
17	XQ	105	82% 13% 5%
18	QR	88	65% 15% 20%
18	XR	88	67% 13% 20%
19	QS	93	72% 18% 10%
19	XS	93	65% 24% 10%
20	QT	106	82% 11% 7%
20	XT	106	78% 14% 7%
21	QU	27	70% 22% 7%
21	XU	27	74% 19% 7%
22	QV	77	69% 23% 8%
22	XV	77	74% 23% 3%
23	QW	76	51% 36% 11% 2%
23	XW	76	41% 42% 17%
24	QX	19	42% 47% 11%
24	XX	19	42% 32% 16% 10%
25	QY	76	49% 36% 13% 2%
25	XY	76	55% 32% 12% 1%
26	R0	85	86% 11% 3%
26	Y0	85	64% 33% 3%
27	R1	98	80% 18% 2% 2%
27	Y1	98	86% 10% 4% 2%
28	R2	72	83% 12% 5%
28	Y2	72	79% 17% 4%

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Mol	Chain	Length	Quality of chain
29	R3	60	 87% 12%
29	Y3	60	 87% 12%
30	R4	71	 68% 27% 6%
30	Y4	71	 72% 27%
31	R5	60	 70% 27%
31	Y5	60	 78% 20%
32	R6	54	 57% 26% 9%
32	Y6	54	 63% 26% 9%
33	R7	49	 84% 16%
33	Y7	49	 90% 10%
34	R8	65	 88% 11%
34	Y8	65	 68% 31%
35	R9	37	 70% 30%
35	Y9	37	 73% 27%
36	RA	2915	 66% 26% 6%
36	YA	2915	 68% 25% 6%
37	RB	122	 61% 30% 6%
37	YB	122	 66% 26% 5%
38	RD	276	 75% 22%
38	YD	276	 74% 22%
39	RE	206	 74% 24%
39	YE	206	 71% 26%
40	RF	210	 78% 19%
40	YF	210	 80% 16%
41	RG	182	 71% 27%

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Mol	Chain	Length	Quality of chain
41	YG	182	82% 17% ..
42	RH	180	77% 17% . 6%
42	YH	180	71% 23% . 6%
43	RI	148	86% 13% .
43	YI	148	79% 19% ..
44	RN	140	90% 9% .
44	YN	140	81% 14% ..
45	RO	122	79% 19% .
45	YO	122	76% 23% .
46	RP	150	79% 21% .
46	YP	150	83% 17% .
47	RQ	141	81% 18% ..
47	YQ	141	72% 27% .
48	RR	118	79% 19% .
48	YR	118	85% 14% .
49	RS	112	79% 18% ..
49	YS	112	79% 20% ..
50	RT	146	69% 24% . 6%
50	YT	146	70% 24% . 6%
51	RU	118	85% 13% ..
51	YU	118	75% 19% . . .
52	RV	101	84% 16%
52	YV	101	88% 12%
53	RW	113	86% 14%
53	YW	113	84% 16%

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Mol	Chain	Length	Quality of chain
54	RX	96	 82% 14%
54	YX	96	 82% 14%
55	RY	110	 72% 17% 7%
55	YY	110	 73% 18% 7%
56	RZ	206	 62% 26% 11%
56	YZ	206	 68% 18% 11%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298371 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
			Total	C	N	O	P			
1	QA	1500	Total 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1500	Total 32249	C 14354	N 5984	O 10412	P 1499	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	XB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	Total 1674	C 1050	N 333	O 284	S 7	0	0	0
4	XD	208	Total 1674	C 1050	N 333	O 284	S 7	0	0	0

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	121	964	597	199	166	2	0	0	0
13	XM	121	964	597	199	166	2	0	0	0

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

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

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

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

- 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 E-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			418	187	87	125	19			
24	XX	17	Total	C	N	O	P	0	0	0
			374	167	77	113	17			

- Molecule 25 is a RNA chain called A-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
30	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

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

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
36	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a protein called 50S ribosomal protein L2.

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

- Molecule 39 is a protein called 50S ribosomal protein L3.

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

- Molecule 40 is a protein called 50S ribosomal protein L4.

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

- Molecule 41 is a protein called 50S ribosomal protein L5.

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

- Molecule 42 is a protein called 50S ribosomal protein L6.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L9.

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

- Molecule 44 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RN	138	1104	712	206	182	4	0	0	0
44	YN	138	1104	712	206	182	4	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L14.

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

- Molecule 46 is a protein called 50S ribosomal protein L15.

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

- Molecule 47 is a protein called 50S ribosomal protein L16.

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

- Molecule 48 is a protein called 50S ribosomal protein L17.

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

- Molecule 49 is a protein called 50S ribosomal protein L18.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L20.

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

- Molecule 52 is a protein called 50S ribosomal protein L21.

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

- Molecule 53 is a protein called 50S ribosomal protein L22.

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

- Molecule 54 is a protein called 50S ribosomal protein L23.

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

- Molecule 55 is a protein called 50S ribosomal protein L24.

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

- Molecule 56 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	85	Total	Mg	0	0
			85	85		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	2	Total	Mg	0	0
			2	2		
57	QV	4	Total	Mg	0	0
			4	4		

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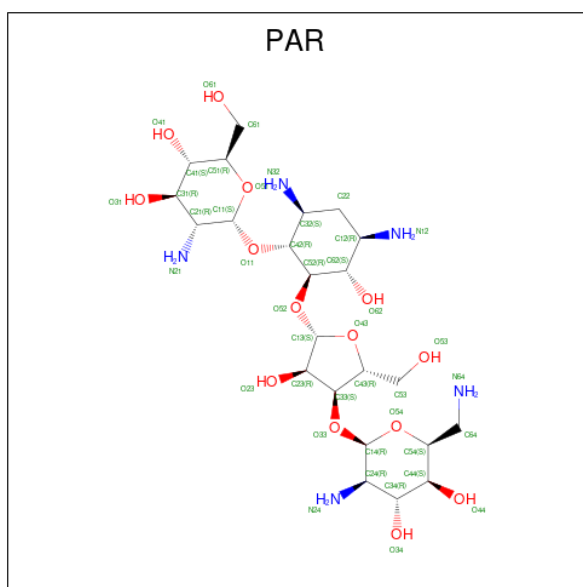
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RA	321	Total 321	Mg 321	0	0
57	RB	4	Total 4	Mg 4	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	3	Total 3	Mg 3	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	XA	94	Total 94	Mg 94	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	XY	1	Total 1	Mg 1	0	0

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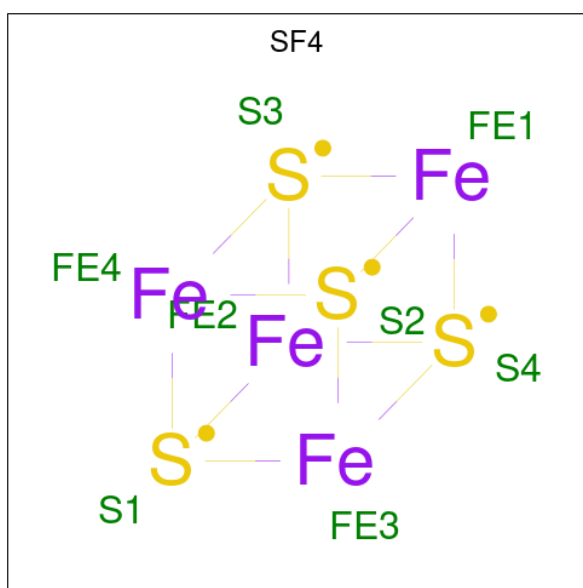
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y0	1	Total Mg 1 1	0	0
57	Y2	1	Total Mg 1 1	0	0
57	Y5	2	Total Mg 2 2	0	0
57	Y7	2	Total Mg 2 2	0	0
57	Y8	3	Total Mg 3 3	0	0
57	YA	379	Total Mg 379 379	0	0
57	YB	8	Total Mg 8 8	0	0
57	YD	3	Total Mg 3 3	0	0
57	YE	3	Total Mg 3 3	0	0
57	YH	1	Total Mg 1 1	0	0
57	YP	3	Total Mg 3 3	0	0
57	YQ	1	Total Mg 1 1	0	0
57	YR	2	Total Mg 2 2	0	0
57	YU	2	Total Mg 2 2	0	0
57	YV	1	Total Mg 1 1	0	0
57	YX	3	Total Mg 3 3	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	XN	1	Total 1	Zn 1	0	0

- Molecule 61 is water.

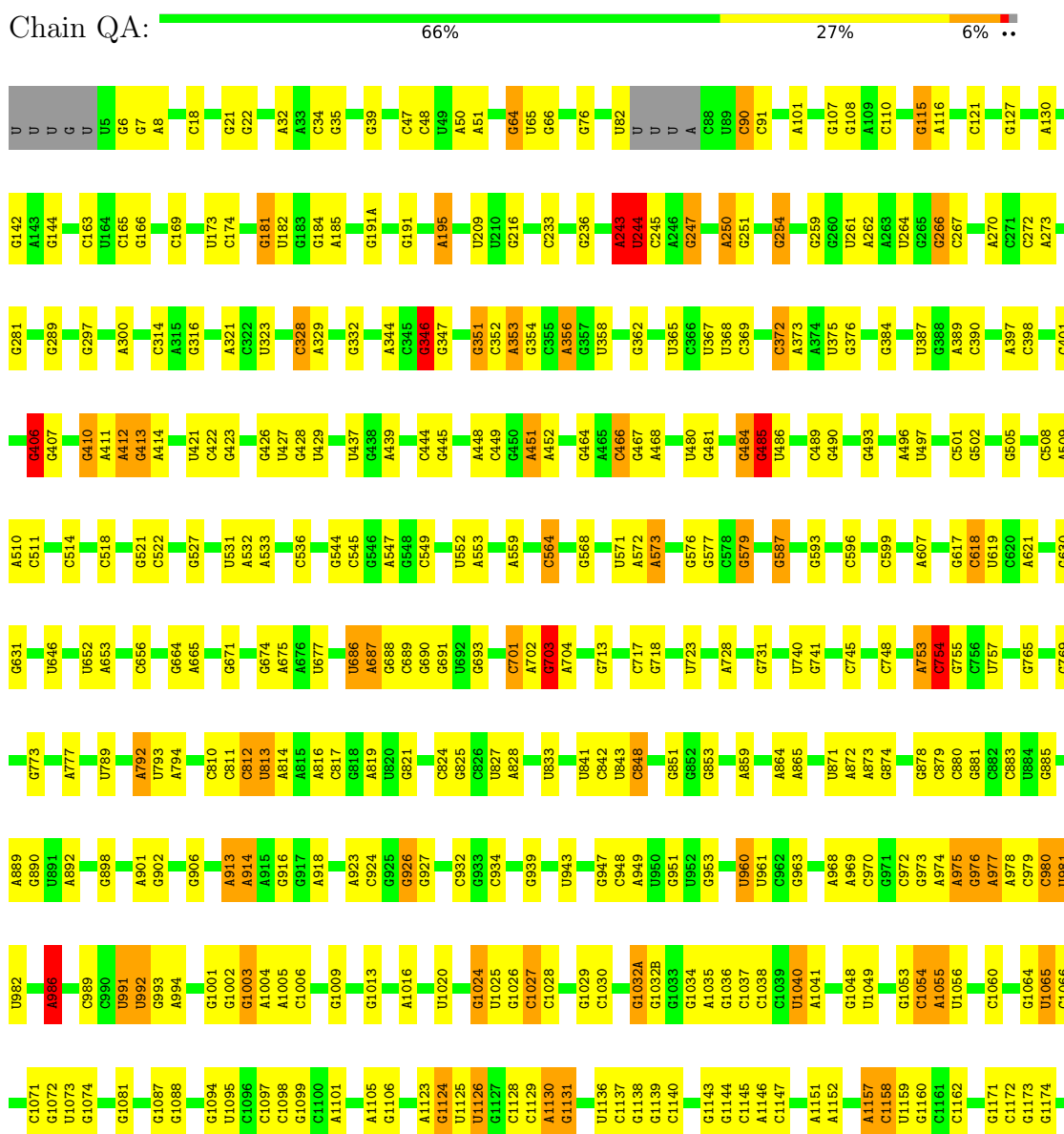
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	QA	1	Total 1	O 1	0	0
61	QX	1	Total 1	O 1	0	0

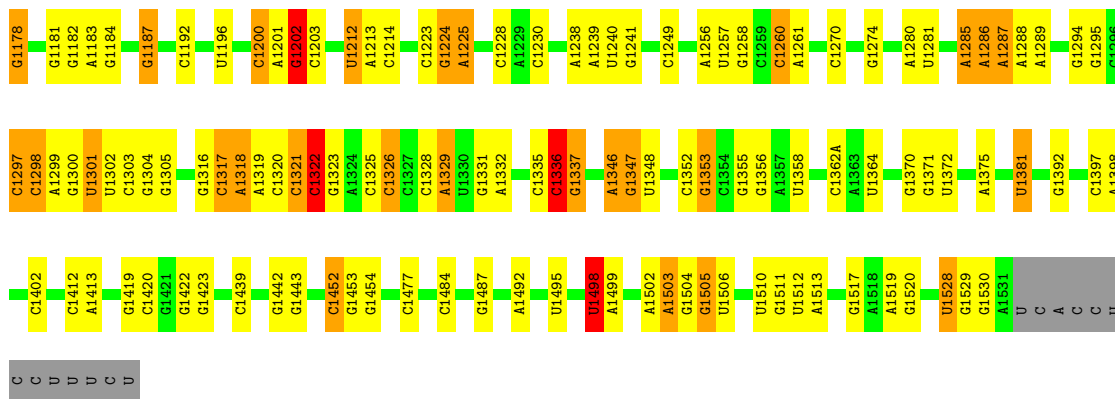
3 Residue-property plots [i](#)

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.

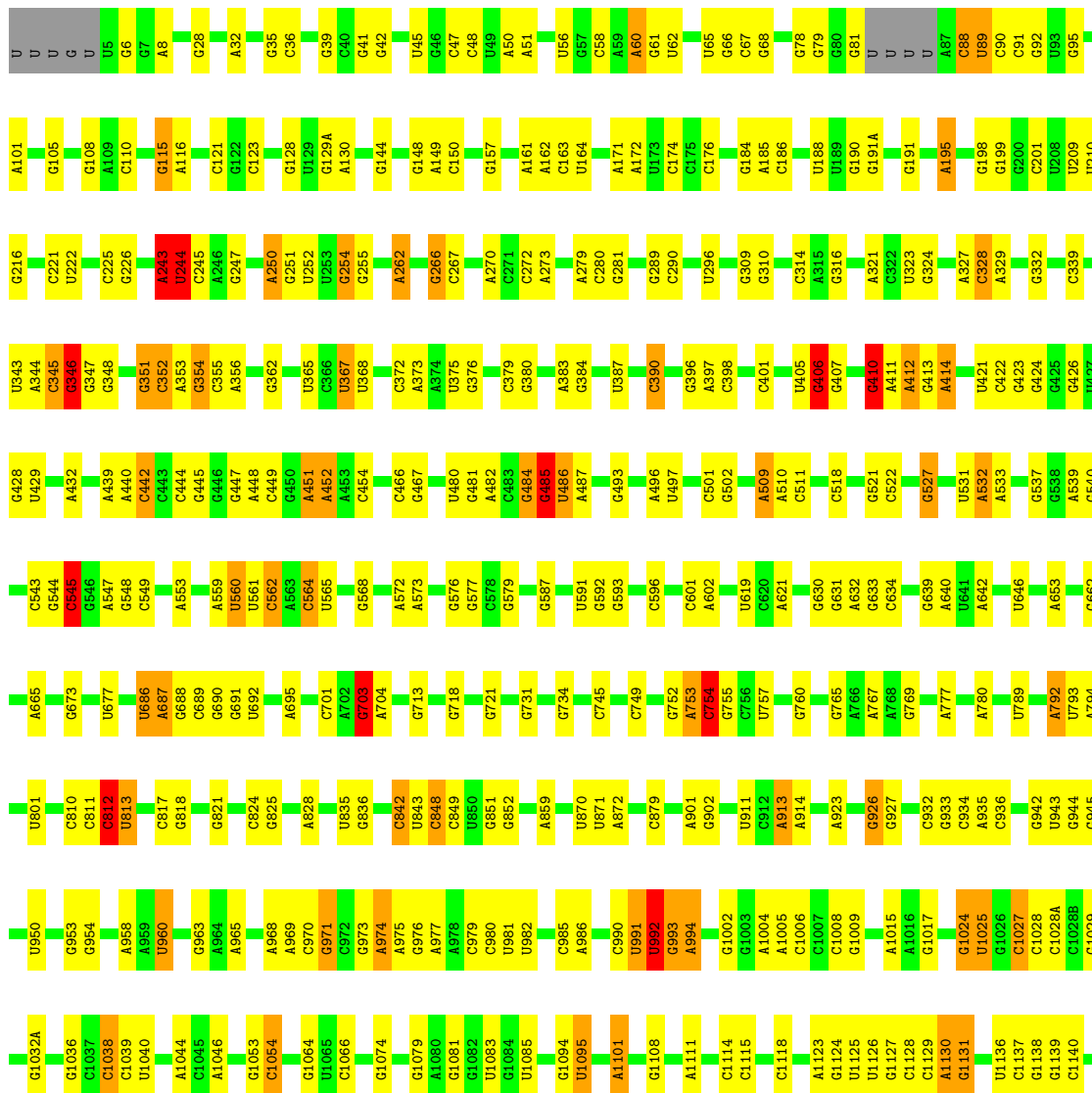
Note EDS failed to run properly.

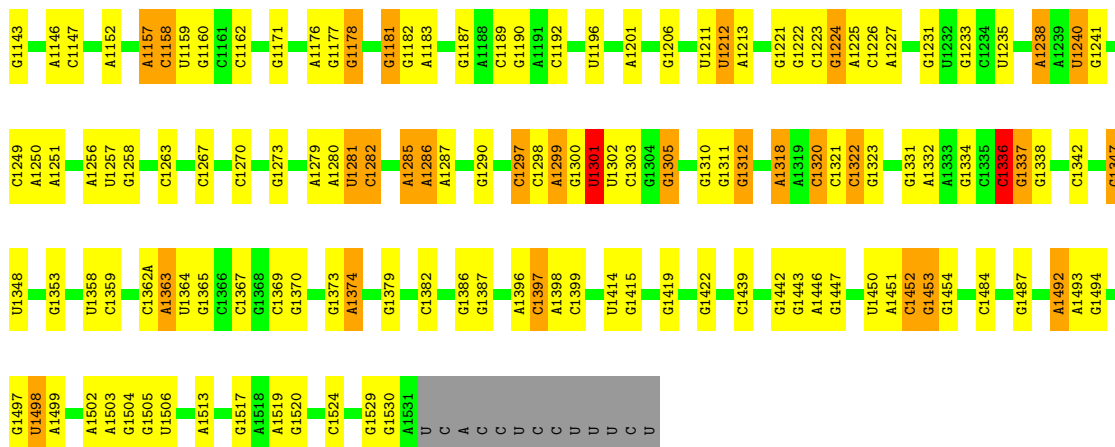
- Molecule 1: 16S rRNA



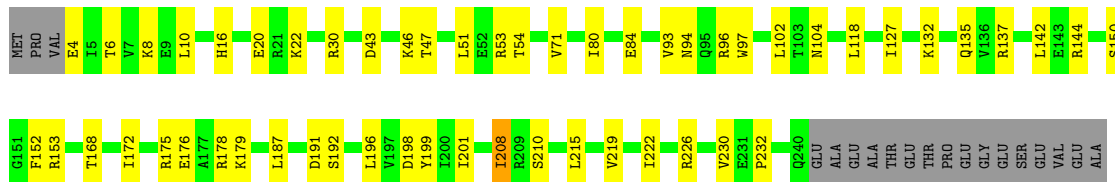


• Molecule 1: 16S rRNA

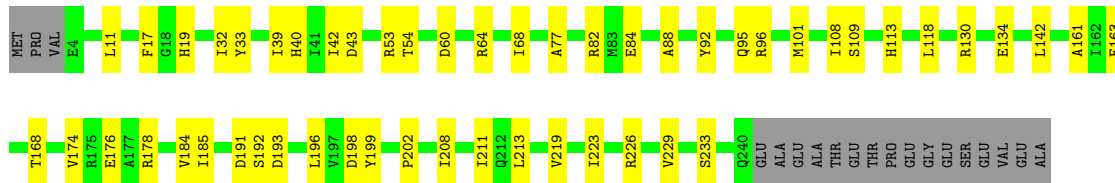




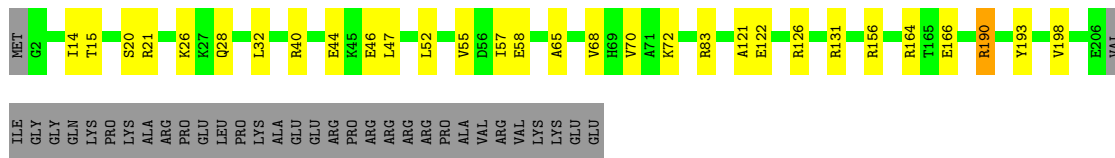
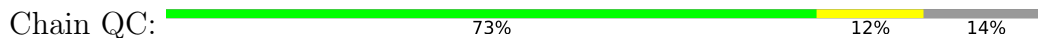
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

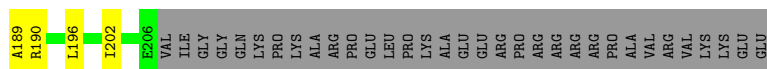


• Molecule 3: 30S ribosomal protein S3

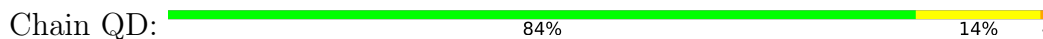


• Molecule 3: 30S ribosomal protein S3

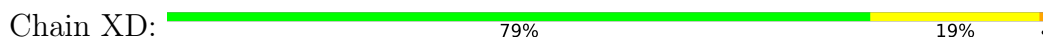




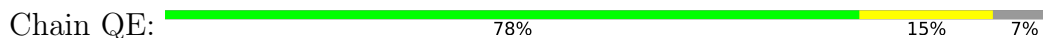
- Molecule 4: 30S ribosomal protein S4



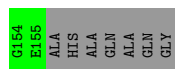
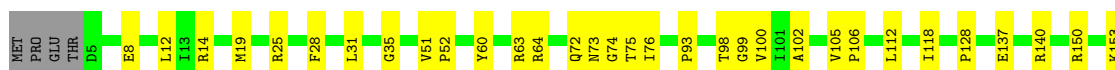
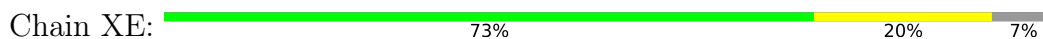
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



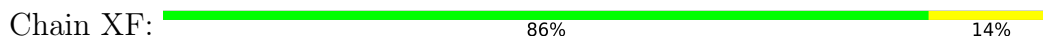
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

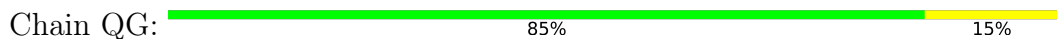


- Molecule 6: 30S ribosomal protein S6

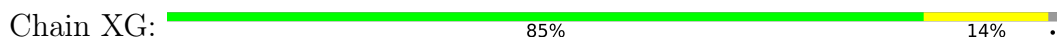




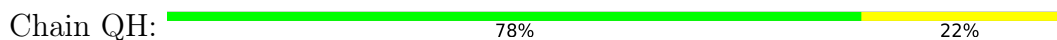
- Molecule 7: 30S ribosomal protein S7



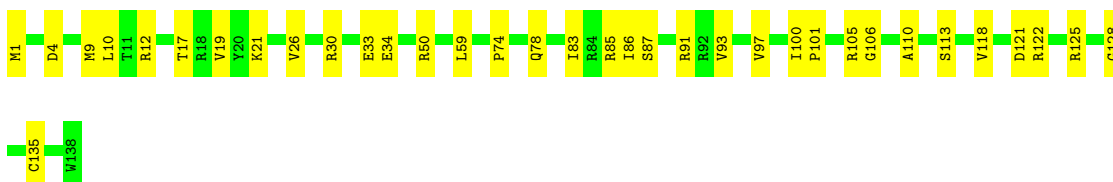
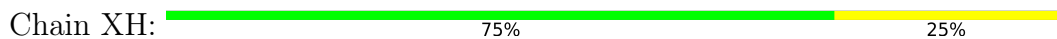
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



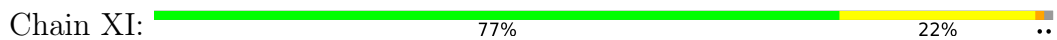
- Molecule 8: 30S ribosomal protein S8




- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

Chain QJ:  76% 18% 6%




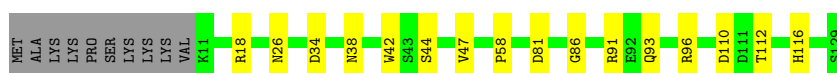
- Molecule 10: 30S ribosomal protein S10

Chain XJ:  70% 24% 6%




- Molecule 11: 30S ribosomal protein S11

Chain QK:  80% 12% 8%




- Molecule 11: 30S ribosomal protein S11

Chain XK:  77% 16% 8%




- Molecule 12: 30S ribosomal protein S12

Chain QL:  77% 18% 5%



- Molecule 12: 30S ribosomal protein S12

Chain XL:  76% 18% 6%



- Molecule 13: 30S ribosomal protein S13

Chain QM:  64% 31% 5%





- Molecule 13: 30S ribosomal protein S13

Chain XM: 71% 24% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 64% 31% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 79% 20% ..



- Molecule 15: 30S ribosomal protein S15

Chain QO: 87% 10% ..



- Molecule 15: 30S ribosomal protein S15

Chain XO: 98% ..



- Molecule 16: 30S ribosomal protein S16

Chain QP: 81% 14% 5% ..



- Molecule 16: 30S ribosomal protein S16

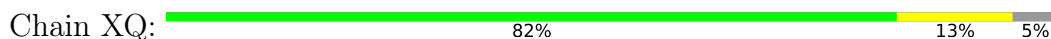
Chain XP: 82% 13% 5% ..



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



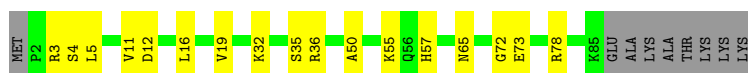
- Molecule 18: 30S ribosomal protein S18



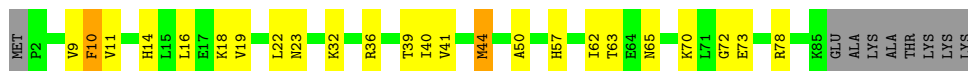
- Molecule 18: 30S ribosomal protein S18



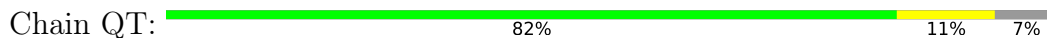
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

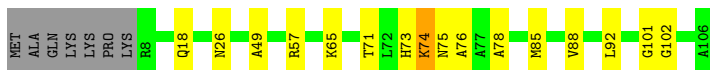
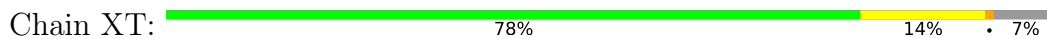


- Molecule 20: 30S ribosomal protein S20





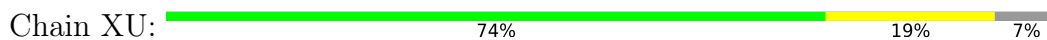
- Molecule 20: 30S ribosomal protein S20



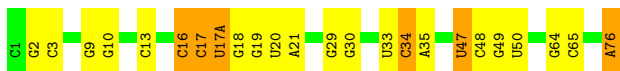
- Molecule 21: 30S ribosomal protein Thx



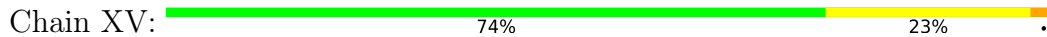
- Molecule 21: 30S ribosomal protein Thx



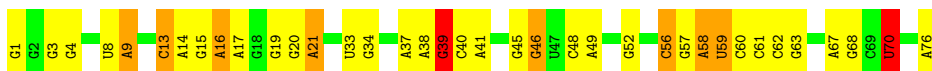
- Molecule 22: P-site tRNAfMet



- Molecule 22: P-site tRNAfMet



- Molecule 23: E-site tRNAAla(GGC)

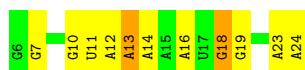


- Molecule 23: E-site tRNAAla(GGC)





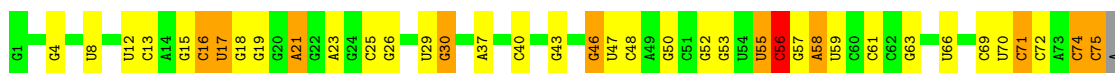
- Molecule 24: mRNA



- Molecule 24: mRNA



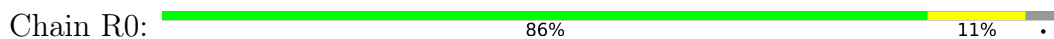
- Molecule 25: A-site tRNAAla(GGC)



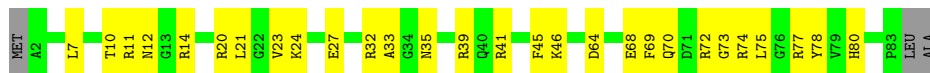
- Molecule 25: A-site tRNAAla(GGC)



- Molecule 26: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L27

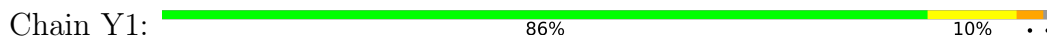


- Molecule 27: 50S ribosomal protein L28

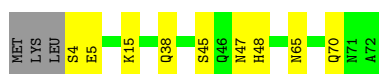
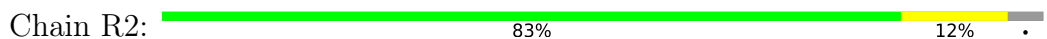




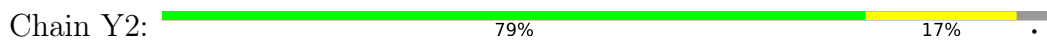
- Molecule 27: 50S ribosomal protein L28



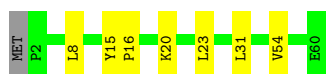
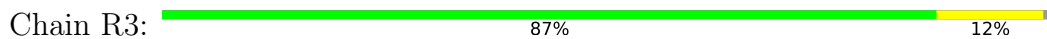
- Molecule 28: 50S ribosomal protein L29



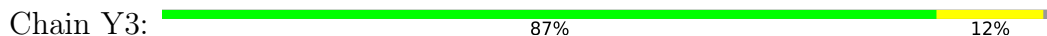
- Molecule 28: 50S ribosomal protein L29



- Molecule 29: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L30

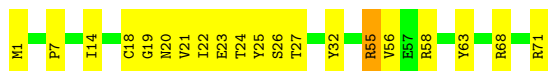


- Molecule 30: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L31

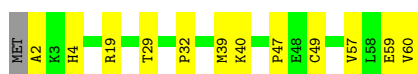
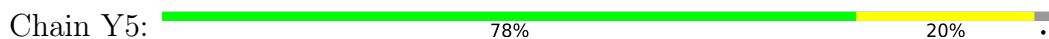




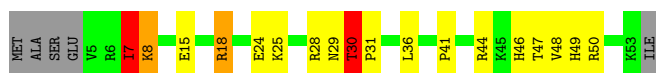
- Molecule 31: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L32



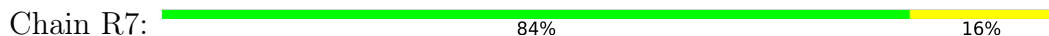
- Molecule 32: 50S ribosomal protein L33



- Molecule 32: 50S ribosomal protein L33



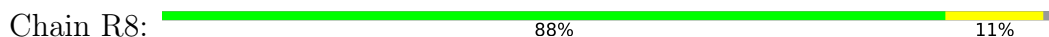
- Molecule 33: 50S ribosomal protein L34

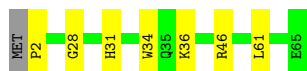


- Molecule 33: 50S ribosomal protein L34

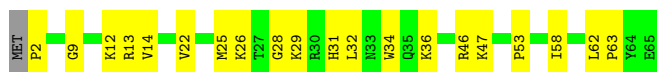


- Molecule 34: 50S ribosomal protein L35





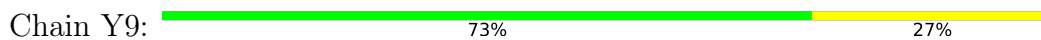
• Molecule 34: 50S ribosomal protein L35



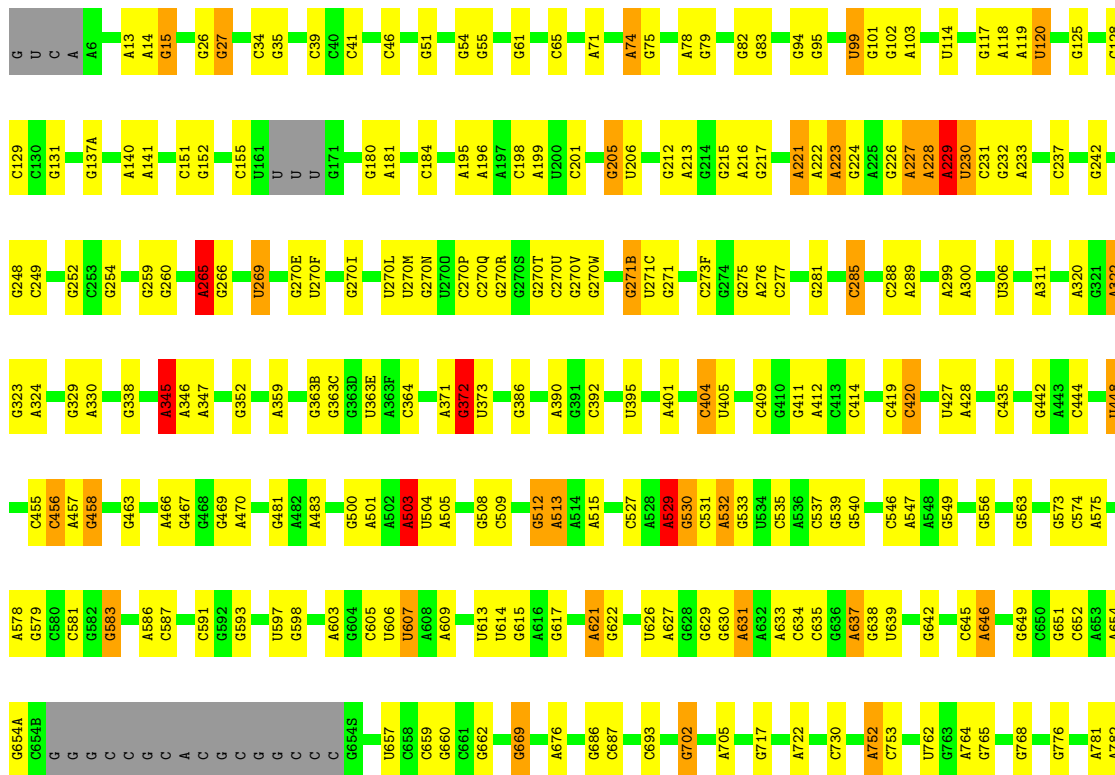
• Molecule 35: 50S ribosomal protein L36



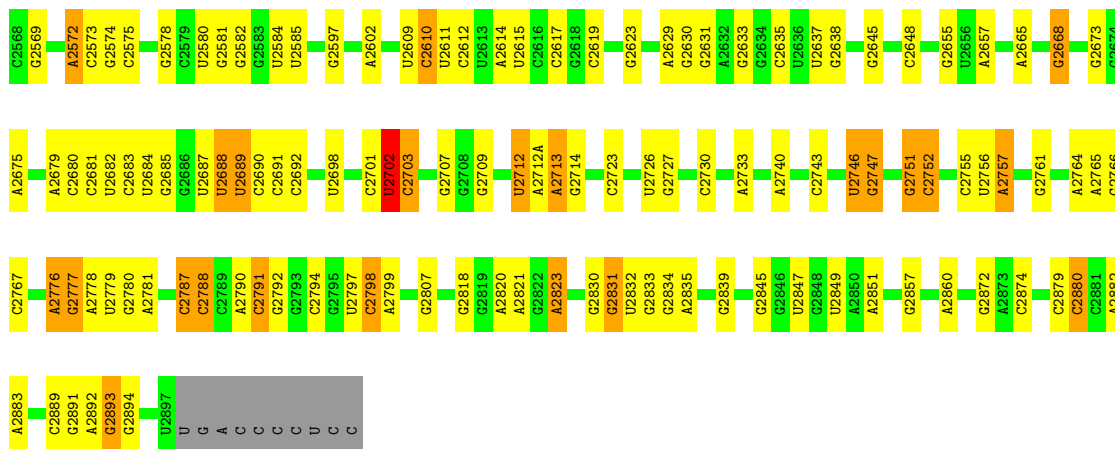
• Molecule 35: 50S ribosomal protein L36



• Molecule 36: 23S rRNA

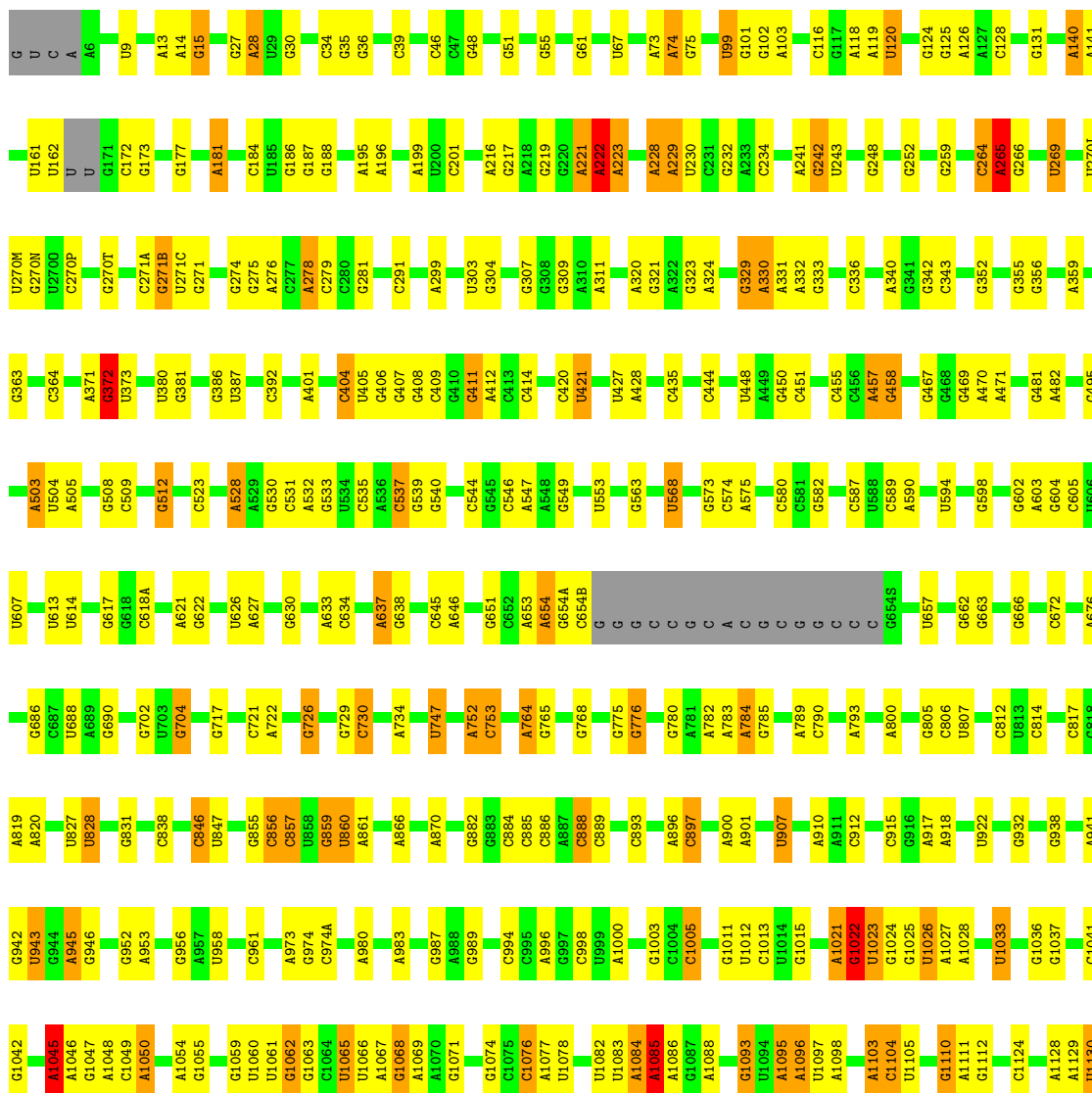


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G2444	G2319	G2211	G2112	C1686	G1449A	A1454	A1174	C1079	C904	A784
G2445	A1981	A1826	A1981	C1686	U1454	G1455	U1175	U1082	G905	G785
A2448	C1982	A1689	C1827	A1689	G1455	A1177	G1176	A1083	G906	C790
C2467	U1981	G1694	A1567	C1458	C1458	C1178	C1178	A1084	U907	G791
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A2564	G1967	G1817	G1817	U1535	G1423	G1423	A1287	A1067	C985	C885
A2565	A1969	A1817	A1817	A1536	A1427	A1427	G1296	A1068	C986	C886
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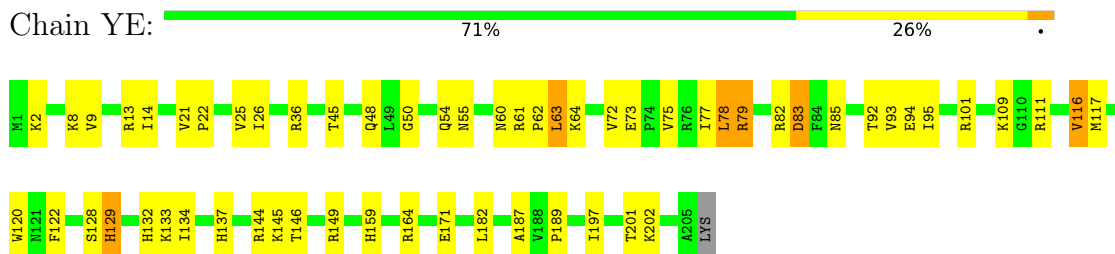
• Molecule 36: 23S rRNA

Chain YA: 68% 25% 6%

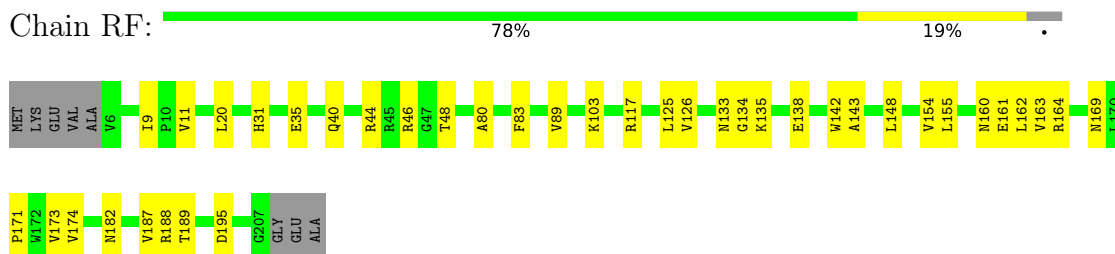


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G	C2777	A2675	G2428	G2315	G2188	G2066	C1920	A1787	C1640	C1408	G1264	A1265	A1137
A	A2778	C2429	G2429	G2316	A2169	A2059	G1929	C1788	G1647	C1411	G1266	G1265	G1138
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C	C2780	A2435	A2435	C2319	A2171	A2061	G1931	C1795	A1652	G1417	G1271	U1141	U1142
C	A2781	A2436	A2436	G2320	A2172	G2062	U1931	C1796	G1653	G1418	A1272	U1143	U1144
C	U2782	A2437	A2437	G2321	A2173	A2063	A1931	C1797	A1654	G1419	A1424	A1143	U1145
U	C2783	A2438	A2438	G2322	A2174	A2064	A1932	G1798	G1655	G1420	U1273	A1144	U1146
U	U2688	A2439	A2439	G2323	A2175	U2068	A1933	G1799	C1657	G1421	U1288	G1151	G1152
U	U2689	C2440	C2440	G2324	U2189	G2069	A1934	C1800	G1666	A1427	U1300	U1300	G1171
C	C2690	C2441	C2441	A2199	G2190	G2070	U1939	G1801	A1667	C1428	A1301	G1173	G1174
C	U2698	C2442	C2442	G2192	G2191	A2071	G1950	A1802	A1668	A1434	C1306	U1175	A1174
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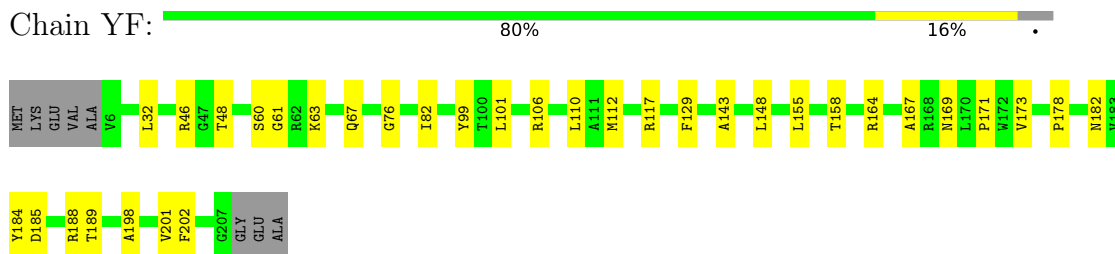
- Molecule 39: 50S ribosomal protein L3



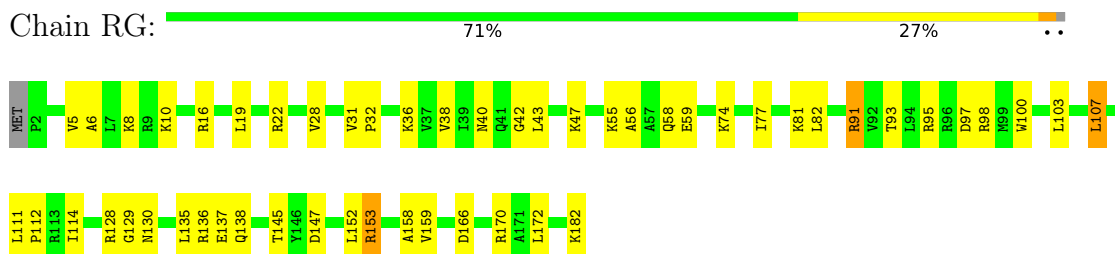
- Molecule 40: 50S ribosomal protein L4



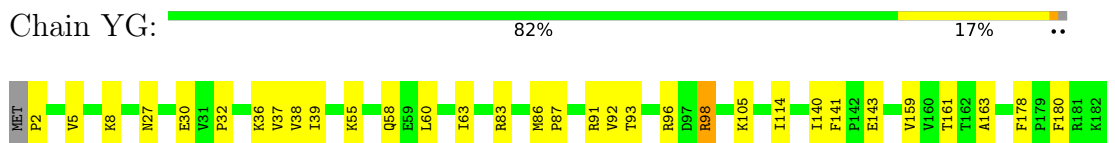
- Molecule 40: 50S ribosomal protein L4




- Molecule 41: 50S ribosomal protein L5



- Molecule 41: 50S ribosomal protein L5



- Molecule 42: 50S ribosomal protein L6

Chain RH:  77% 17% 6%




- Molecule 42: 50S ribosomal protein L6

Chain YH:  71% 23% 6%




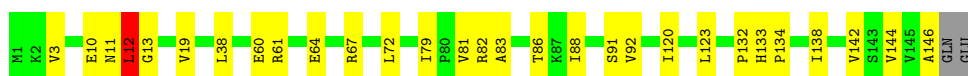
- Molecule 43: 50S ribosomal protein L9

Chain RI:  86% 13%



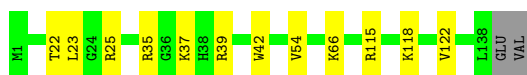
- Molecule 43: 50S ribosomal protein L9

Chain YI:  79% 19%




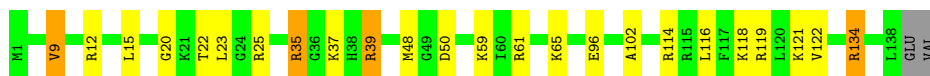
- Molecule 44: 50S ribosomal protein L13

Chain RN:  90% 9%




- Molecule 44: 50S ribosomal protein L13

Chain YN:  81% 14%

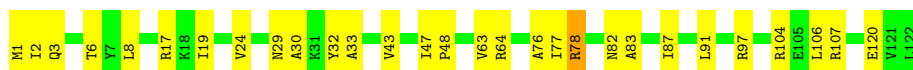
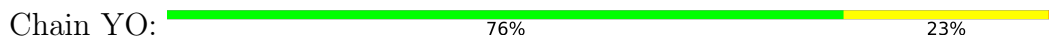


- Molecule 45: 50S ribosomal protein L14

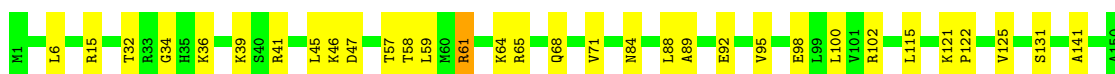
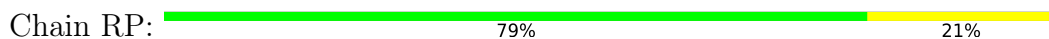
Chain RO:  79% 19%



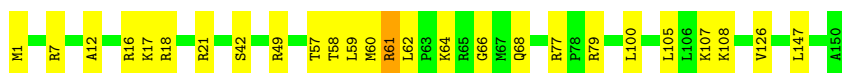
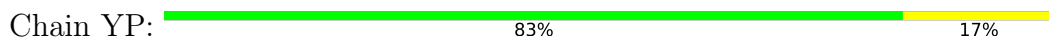
- Molecule 45: 50S ribosomal protein L14



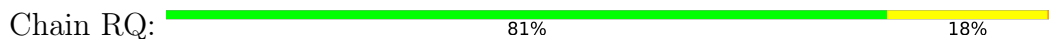
- Molecule 46: 50S ribosomal protein L15



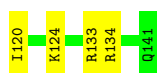
- Molecule 46: 50S ribosomal protein L15



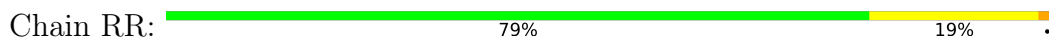
- Molecule 47: 50S ribosomal protein L16




- Molecule 47: 50S ribosomal protein L16



- Molecule 48: 50S ribosomal protein L17




- Molecule 48: 50S ribosomal protein L17

Chain YR:  85% 14%




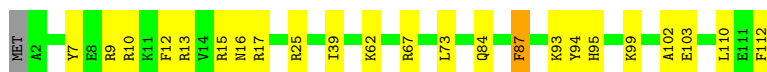
- Molecule 49: 50S ribosomal protein L18

Chain RS:  79% 18%



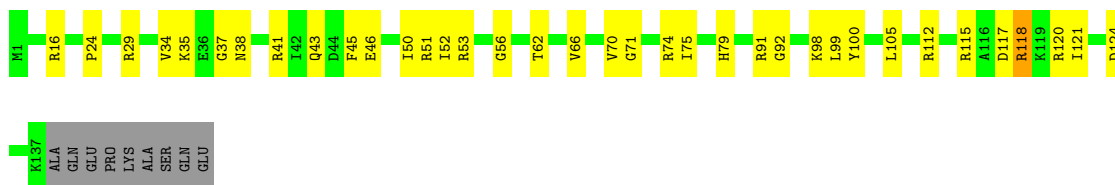
- Molecule 49: 50S ribosomal protein L18

Chain YS:  79% 20%



- Molecule 50: 50S ribosomal protein L19

Chain RT:  69% 24% 6%




- Molecule 50: 50S ribosomal protein L19

Chain YT:  70% 24% 6%




- Molecule 51: 50S ribosomal protein L20

Chain RU:  85% 13%

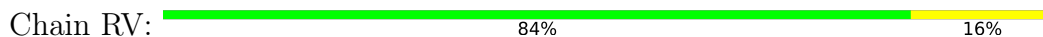


- Molecule 51: 50S ribosomal protein L20

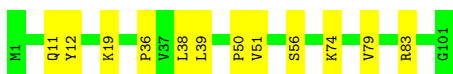
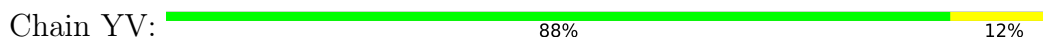
Chain YU:  75% 19%



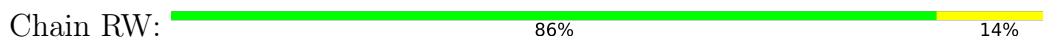
- Molecule 52: 50S ribosomal protein L21



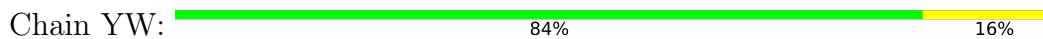
- Molecule 52: 50S ribosomal protein L21



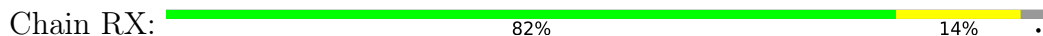
- Molecule 53: 50S ribosomal protein L22



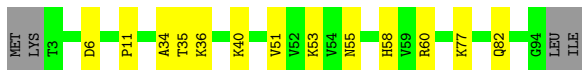
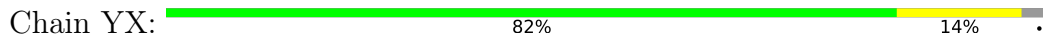
- Molecule 53: 50S ribosomal protein L22



- Molecule 54: 50S ribosomal protein L23

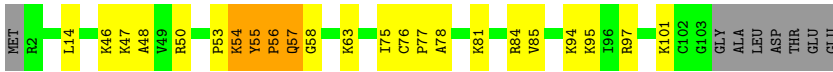


- Molecule 54: 50S ribosomal protein L23

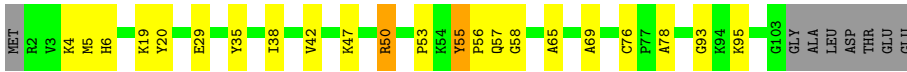
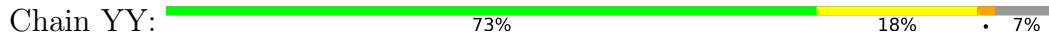


- Molecule 55: 50S ribosomal protein L24

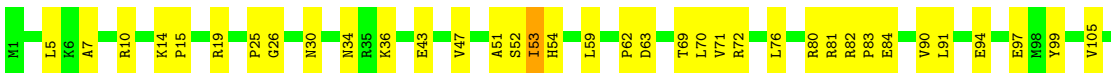
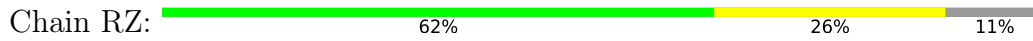




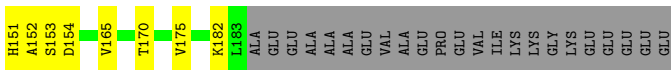
- Molecule 55: 50S ribosomal protein L24



- Molecule 56: 50S ribosomal protein L25



- Molecule 56: 50S ribosomal protein L25



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	211.00Å 453.48Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.20	Depositor
% Data completeness (in resolution range)	99.5 (49.99-3.20)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.237 , 0.270	Depositor
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.308	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298371	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.54	0/36098	1.04	122/56341 (0.2%)
1	XA	0.55	0/36101	1.02	113/56346 (0.2%)
2	QB	0.38	0/1959	0.68	4/2642 (0.2%)
2	XB	0.34	0/1959	0.65	0/2642
3	QC	0.37	0/1629	0.67	0/2195
3	XC	0.32	0/1629	0.63	0/2195
4	QD	0.43	0/1704	0.61	1/2284 (0.0%)
4	XD	0.43	0/1704	0.64	0/2284
5	QE	0.33	0/1171	0.62	0/1576
5	XE	0.37	0/1171	0.66	1/1576 (0.1%)
6	QF	0.39	0/856	0.72	2/1154 (0.2%)
6	XF	0.37	0/856	0.66	0/1154
7	QG	0.33	0/1276	0.56	0/1709
7	XG	0.33	0/1276	0.60	0/1709
8	QH	0.34	0/1136	0.62	0/1527
8	XH	0.33	0/1136	0.61	0/1527
9	QI	0.36	0/1029	0.71	1/1379 (0.1%)
9	XI	0.36	0/1029	0.70	0/1379
10	QJ	0.34	0/814	0.62	0/1095
10	XJ	0.33	0/814	0.62	0/1095
11	QK	0.37	0/900	0.58	0/1213
11	XK	0.36	0/900	0.64	1/1213 (0.1%)
12	QL	0.38	0/991	0.70	1/1327 (0.1%)
12	XL	0.41	0/991	0.74	2/1327 (0.2%)
13	QM	0.37	0/974	0.80	0/1303
13	XM	0.35	0/974	0.77	1/1303 (0.1%)
14	QN	0.43	0/501	0.71	0/664
14	XN	0.50	0/501	0.81	1/664 (0.2%)
15	QO	0.32	0/745	0.56	0/992
15	XO	0.32	0/745	0.53	0/992
16	QP	0.44	0/721	0.74	1/970 (0.1%)
16	XP	0.37	0/721	0.75	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.45	1/847 (0.1%)	0.64	0/1131
17	XQ	0.33	0/847	0.61	0/1131
18	QR	0.31	0/579	0.59	0/768
18	XR	0.36	0/579	0.61	0/768
19	QS	0.34	0/689	0.66	0/926
19	XS	0.55	0/689	0.87	2/926 (0.2%)
20	QT	0.29	0/765	0.61	0/1007
20	XT	0.30	0/765	0.68	0/1007
21	QU	0.47	0/221	0.68	1/288 (0.3%)
21	XU	0.42	0/221	0.68	1/288 (0.3%)
22	QV	0.49	0/1832	1.04	6/2855 (0.2%)
22	XV	0.53	0/1832	1.02	4/2855 (0.1%)
23	QW	0.49	1/1826 (0.1%)	1.11	12/2845 (0.4%)
23	XW	0.51	1/1826 (0.1%)	1.14	10/2845 (0.4%)
24	QX	0.47	0/471	1.06	2/734 (0.3%)
24	XX	0.46	0/421	0.90	1/656 (0.2%)
25	QY	0.39	0/1791	1.09	8/2791 (0.3%)
25	XY	0.40	0/1816	1.11	14/2830 (0.5%)
26	R0	0.35	0/657	0.62	0/874
26	Y0	0.43	0/657	0.65	0/874
27	R1	0.40	0/770	0.70	1/1022 (0.1%)
27	Y1	0.49	0/770	0.70	0/1022
28	R2	0.33	0/583	0.64	0/771
28	Y2	0.34	0/583	0.69	0/771
29	R3	0.30	0/474	0.55	0/635
29	Y3	0.34	0/474	0.56	0/635
30	R4	0.51	1/594 (0.2%)	0.91	1/795 (0.1%)
30	Y4	0.48	0/594	0.81	1/795 (0.1%)
31	R5	0.39	0/473	0.82	1/639 (0.2%)
31	Y5	0.56	1/473 (0.2%)	0.80	0/639
32	R6	0.69	1/431 (0.2%)	1.10	2/575 (0.3%)
32	Y6	0.46	0/431	0.86	2/575 (0.3%)
33	R7	0.43	0/438	0.65	0/575
33	Y7	0.36	0/438	0.66	0/575
34	R8	0.42	0/525	0.72	0/691
34	Y8	0.43	0/525	0.72	0/691
35	R9	0.29	0/310	0.64	0/407
35	Y9	0.29	0/310	0.53	0/407
36	RA	0.60	0/69521	1.04	215/108529 (0.2%)
36	YA	0.64	1/69543 (0.0%)	1.04	216/108563 (0.2%)
37	RB	0.52	0/2878	1.07	14/4490 (0.3%)
37	YB	0.55	0/2878	1.04	5/4490 (0.1%)
38	RD	0.52	1/2165 (0.0%)	0.79	6/2919 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YD	0.48	0/2165	0.71	0/2919
39	RE	0.55	3/1601 (0.2%)	0.81	2/2160 (0.1%)
39	YE	0.49	0/1601	0.83	3/2160 (0.1%)
40	RF	0.42	0/1620	0.65	0/2194
40	YF	0.44	0/1620	0.68	1/2194 (0.0%)
41	RG	0.42	0/1499	0.74	1/2016 (0.0%)
41	YG	0.35	0/1499	0.70	3/2016 (0.1%)
42	RH	0.35	0/1332	0.76	0/1802
42	YH	0.43	0/1332	0.75	1/1802 (0.1%)
43	RI	0.49	0/1151	0.80	3/1558 (0.2%)
43	YI	0.43	0/1151	0.87	4/1558 (0.3%)
44	RN	0.37	0/1131	0.68	0/1525
44	YN	0.44	0/1131	0.76	4/1525 (0.3%)
45	RO	0.41	0/943	0.64	0/1269
45	YO	0.44	0/943	0.66	0/1269
46	RP	0.41	0/1162	0.77	0/1544
46	YP	0.43	0/1162	0.79	0/1544
47	RQ	0.43	0/1143	0.77	2/1527 (0.1%)
47	YQ	0.44	0/1143	0.76	0/1527
48	RR	0.34	0/982	0.67	0/1312
48	YR	0.35	0/982	0.70	0/1312
49	RS	0.45	0/892	0.80	2/1187 (0.2%)
49	YS	0.42	0/892	0.78	0/1187
50	RT	0.41	0/1155	0.73	0/1542
50	YT	0.37	0/1155	0.72	0/1542
51	RU	0.40	0/982	0.64	1/1306 (0.1%)
51	YU	0.47	1/982 (0.1%)	0.69	1/1306 (0.1%)
52	RV	0.38	0/790	0.70	2/1057 (0.2%)
52	YV	0.43	0/790	0.75	1/1057 (0.1%)
53	RW	0.40	0/911	0.65	0/1220
53	YW	0.36	0/911	0.62	0/1220
54	RX	0.38	0/739	0.62	0/993
54	YX	0.46	0/739	0.63	0/993
55	RY	0.43	0/798	0.82	1/1064 (0.1%)
55	YY	0.44	0/798	0.80	1/1064 (0.1%)
56	RZ	0.36	0/1493	0.79	3/2026 (0.1%)
56	YZ	0.40	0/1493	0.78	4/2026 (0.2%)
All	All	0.54	12/323336 (0.0%)	0.96	817/483880 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QW	1	G	OP3-P	-10.86	1.48	1.61
23	XW	1	G	OP3-P	-10.84	1.48	1.61
38	RD	35	LYS	C-N	7.52	1.48	1.34
39	RE	58	ARG	CZ-NH1	6.79	1.41	1.33
51	YU	69	CYS	CB-SG	-6.60	1.71	1.82

The worst 5 of 817 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1317	C	O5'-P-OP1	-31.67	72.70	110.70
1	QA	1317	C	O5'-P-OP2	-24.74	81.02	110.70
1	QA	1317	C	OP1-P-OP2	13.74	140.21	119.60
1	QA	1301	U	N1-C2-O2	11.96	131.17	122.80
1	QA	1158	C	C2-N1-C1'	11.80	131.78	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16273	201	0
1	XA	32249	0	16278	200	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	32	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	25	0
4	QD	1674	0	1718	27	0
4	XD	1674	0	1718	30	0
5	QE	1155	0	1213	19	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	14	0
8	QH	1116	0	1177	20	0
8	XH	1116	0	1177	22	0
9	QI	1010	0	1037	25	0
9	XI	1010	0	1037	23	0
10	QJ	801	0	849	12	0
10	XJ	801	0	848	16	0
11	QK	885	0	904	11	0
11	XK	885	0	904	12	0
12	QL	975	0	1062	18	0
12	XL	975	0	1062	21	0
13	QM	964	0	1034	28	0
13	XM	964	0	1034	21	0
14	QN	492	0	533	18	0
14	XN	492	0	530	8	0
15	QO	734	0	771	7	0
15	XO	734	0	771	0	0
16	QP	705	0	725	10	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	10	0
18	QR	574	0	644	10	0
18	XR	574	0	644	8	0
19	QS	674	0	699	14	0
19	XS	674	0	699	19	0
20	QT	763	0	861	10	0
20	XT	763	0	861	11	0
21	QU	217	0	234	5	0
21	XU	217	0	234	3	0
22	QV	1640	0	837	9	0
22	XV	1640	0	837	6	0
23	QW	1632	0	824	12	0
23	XW	1632	0	824	10	0
24	QX	418	0	207	4	0
24	XX	374	0	186	2	0
25	QY	1603	0	811	12	0
25	XY	1625	0	822	6	0
26	R0	648	0	672	6	0
26	Y0	648	0	672	21	0
27	R1	763	0	848	11	0
27	Y1	763	0	848	7	0
28	R2	581	0	629	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Y2	581	0	628	7	0
29	R3	469	0	518	5	0
29	Y3	469	0	518	4	0
30	R4	581	0	577	23	0
30	Y4	581	0	577	13	0
31	R5	459	0	479	11	0
31	Y5	459	0	480	8	0
32	R6	424	0	450	16	0
32	Y6	424	0	450	10	0
33	R7	430	0	480	7	0
33	Y7	430	0	480	4	0
34	R8	517	0	582	6	0
34	Y8	517	0	582	13	0
35	R9	307	0	338	6	0
35	Y9	307	0	338	8	0
36	RA	62071	0	31280	311	0
36	YA	62091	0	31292	289	0
37	RB	2573	0	1306	19	0
37	YB	2573	0	1306	22	0
38	RD	2115	0	2195	53	0
38	YD	2115	0	2195	60	0
39	RE	1568	0	1634	36	0
39	YE	1568	0	1634	39	0
40	RF	1585	0	1632	26	0
40	YF	1585	0	1632	20	0
41	RG	1474	0	1535	38	0
41	YG	1474	0	1535	20	0
42	RH	1307	0	1382	25	0
42	YH	1307	0	1382	38	0
43	RI	1136	0	1223	16	0
43	YI	1136	0	1223	12	0
44	RN	1104	0	1180	7	0
44	YN	1104	0	1180	13	0
45	RO	933	0	996	22	0
45	YO	933	0	996	21	0
46	RP	1145	0	1226	24	0
46	YP	1145	0	1228	22	0
47	RQ	1122	0	1179	22	0
47	YQ	1122	0	1179	29	0
48	RR	968	0	1033	21	0
48	YR	968	0	1033	12	0
49	RS	882	0	943	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	YS	882	0	943	16	0
50	RT	1141	0	1202	25	0
50	YT	1141	0	1202	25	0
51	RU	964	0	1022	14	0
51	YU	964	0	1022	26	0
52	RV	779	0	852	9	0
52	YV	779	0	852	7	0
53	RW	900	0	964	10	0
53	YW	900	0	964	13	0
54	RX	725	0	777	10	0
54	YX	725	0	778	12	0
55	RY	785	0	878	13	0
55	YY	785	0	878	11	0
56	RZ	1461	0	1493	32	0
56	YZ	1461	0	1493	23	0
57	QA	85	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	2	0	0	0	0
57	QV	4	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	321	0	0	0	0
57	RB	4	0	0	0	0
57	RD	1	0	0	0	0
57	RE	3	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RU	1	0	0	0	0
57	RX	1	0	0	0	0
57	XA	94	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y2	1	0	0	0	0
57	Y5	2	0	0	0	0
57	Y7	2	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	379	0	0	0	0
57	YB	8	0	0	0	0
57	YD	3	0	0	0	0
57	YE	3	0	0	0	0
57	YH	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	2	0	0	0	0
57	YU	2	0	0	0	0
57	YV	1	0	0	0	0
57	YX	3	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	XN	1	0	0	0	0
61	QA	1	0	0	0	0
61	QX	1	0	0	0	0
All	All	298371	0	201332	2196	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 2196 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)
36:YA:1112:G:H5'	42:YH:3:ARG:HD3	1.20	1.19
36:YA:1112:G:H5'	42:YH:3:ARG:CD	1.79	1.12
43:RI:92:VAL:CG1	43:RI:120:ILE:HG23	1.82	1.09
42:RH:6:ARG:HD3	42:RH:6:ARG:H	1.19	1.07
38:YD:33:LEU:H	38:YD:33:LEU:HD23	1.19	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%)	26 (11%)	3 (1%)	12	47
2	XB	235/256 (92%)	205 (87%)	29 (12%)	1 (0%)	34	69
3	QC	203/239 (85%)	182 (90%)	20 (10%)	1 (0%)	29	67
3	XC	203/239 (85%)	187 (92%)	15 (7%)	1 (0%)	29	67
4	QD	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	67
4	XD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	67
5	QE	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	8 (5%)	2 (1%)	12	47
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	97/105 (92%)	82 (84%)	15 (16%)	0	100	100
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
12	QL	123/131 (94%)	109 (89%)	13 (11%)	1 (1%)	19	58
12	XL	123/131 (94%)	107 (87%)	13 (11%)	3 (2%)	6	34
13	QM	119/126 (94%)	100 (84%)	16 (13%)	3 (2%)	5	32
13	XM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	42
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	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%)	66 (97%)	2 (3%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	69 (84%)	12 (15%)	1 (1%)	13	49
20	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	6 (6%)	2 (2%)	7	37
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
26	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
27	R1	95/98 (97%)	84 (88%)	9 (10%)	2 (2%)	7	37
27	Y1	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	7	37
28	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
28	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	44
29	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	Y3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	R4	69/71 (97%)	45 (65%)	21 (30%)	3 (4%)	2	20
30	Y4	69/71 (97%)	47 (68%)	21 (30%)	1 (1%)	11	46
31	R5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
31	Y5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
32	R6	47/54 (87%)	24 (51%)	20 (43%)	3 (6%)	1	10
32	Y6	47/54 (87%)	31 (66%)	16 (34%)	0	100	100
33	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Y7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	R8	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
34	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	26
35	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
38	RD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	22	61
38	YD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	22	61
39	RE	203/206 (98%)	172 (85%)	28 (14%)	3 (2%)	10	44
39	YE	203/206 (98%)	174 (86%)	21 (10%)	8 (4%)	3	22
40	RF	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	29	67
40	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	15	54
41	RG	179/182 (98%)	159 (89%)	20 (11%)	0	100	100
41	YG	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
42	RH	168/180 (93%)	141 (84%)	26 (16%)	1 (1%)	25	64
42	YH	168/180 (93%)	141 (84%)	25 (15%)	2 (1%)	13	49
43	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	46
43	YI	144/148 (97%)	125 (87%)	15 (10%)	4 (3%)	5	29
44	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
44	YN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
45	RO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
45	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
46	RP	148/150 (99%)	125 (84%)	23 (16%)	0	100	100
46	YP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	11	46
47	RQ	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
47	YQ	139/141 (99%)	118 (85%)	19 (14%)	2 (1%)	11	46
48	RR	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	42
48	YR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	42
49	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
49	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	56
50	RT	135/146 (92%)	118 (87%)	17 (13%)	0	100	100
50	YT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
51	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	YU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	9	42
52	RV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
52	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	54
53	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
53	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
54	RX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
54	YX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
55	RY	100/110 (91%)	71 (71%)	24 (24%)	5 (5%)	2	16
55	YY	100/110 (91%)	73 (73%)	22 (22%)	5 (5%)	2	16
56	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	14	51
56	YZ	181/206 (88%)	154 (85%)	23 (13%)	4 (2%)	6	35
All	All	11470/12126 (95%)	10262 (90%)	1114 (10%)	94 (1%)	19	58

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
30	R4	24	THR
30	R4	43	TYR
32	R6	8	LYS
32	R6	30	THR

5.3.2 Protein sidechains [i](#)

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%)	200 (98%)	5 (2%)	49	77
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88	95
3	QC	159/188 (85%)	156 (98%)	3 (2%)	57	81
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	173/181 (96%)	170 (98%)	3 (2%)	60	83
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	88
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%)	125 (99%)	1 (1%)	81	93
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	80
9	XI	98/99 (99%)	96 (98%)	2 (2%)	55	80
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	88
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	88 (98%)	2 (2%)	52	79
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	103 (99%)	1 (1%)	76	90
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	94 (97%)	3 (3%)	40	72
14	QN	49/50 (98%)	46 (94%)	3 (6%)	18	54
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	77
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	87
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%)	93 (98%)	2 (2%)	53	79
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	60 (98%)	1 (2%)	62	84
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	87
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%)	20 (100%)	0	100	100
26	R0	65/67 (97%)	65 (100%)	0	100	100
26	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	63
27	R1	82/83 (99%)	82 (100%)	0	100	100
27	Y1	82/83 (99%)	80 (98%)	2 (2%)	49	77
28	R2	64/67 (96%)	62 (97%)	2 (3%)	40	72
28	Y2	64/67 (96%)	64 (100%)	0	100	100
29	R3	51/52 (98%)	51 (100%)	0	100	100
29	Y3	51/52 (98%)	51 (100%)	0	100	100
30	R4	63/63 (100%)	61 (97%)	2 (3%)	39	71
30	Y4	63/63 (100%)	62 (98%)	1 (2%)	62	84
31	R5	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	80
32	R6	48/52 (92%)	47 (98%)	1 (2%)	53	79
32	Y6	48/52 (92%)	48 (100%)	0	100	100
33	R7	42/42 (100%)	42 (100%)	0	100	100
33	Y7	42/42 (100%)	42 (100%)	0	100	100
34	R8	54/55 (98%)	54 (100%)	0	100	100
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	32 (94%)	2 (6%)	19	54
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	213 (100%)	1 (0%)	88	95
38	YD	214/218 (98%)	210 (98%)	4 (2%)	57	81
39	RE	165/166 (99%)	164 (99%)	1 (1%)	86	94
39	YE	165/166 (99%)	165 (100%)	0	100	100
40	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	YF	161/166 (97%)	161 (100%)	0	100	100
41	RG	155/156 (99%)	152 (98%)	3 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
42	RH	142/148 (96%)	140 (99%)	2 (1%)	67	86
42	YH	142/148 (96%)	137 (96%)	5 (4%)	36	69
43	RI	122/124 (98%)	121 (99%)	1 (1%)	81	93
43	YI	122/124 (98%)	122 (100%)	0	100	100
44	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
44	YN	117/119 (98%)	115 (98%)	2 (2%)	60	83
45	RO	100/100 (100%)	97 (97%)	3 (3%)	41	73
45	YO	100/100 (100%)	99 (99%)	1 (1%)	76	90
46	RP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	YP	116/116 (100%)	114 (98%)	2 (2%)	60	83
47	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
47	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100
49	RS	87/88 (99%)	84 (97%)	3 (3%)	37	70
49	YS	87/88 (99%)	85 (98%)	2 (2%)	50	78
50	RT	120/127 (94%)	115 (96%)	5 (4%)	30	65
50	YT	120/127 (94%)	119 (99%)	1 (1%)	81	93
51	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
51	YU	93/94 (99%)	89 (96%)	4 (4%)	29	64
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	81 (99%)	1 (1%)	71	88
53	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	73 (99%)	1 (1%)	67	86
54	YX	74/78 (95%)	74 (100%)	0	100	100
55	RY	85/91 (93%)	83 (98%)	2 (2%)	49	77
55	YY	85/91 (93%)	84 (99%)	1 (1%)	71	88
56	RZ	162/179 (90%)	160 (99%)	2 (1%)	71	88
56	YZ	162/179 (90%)	159 (98%)	3 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9688/10064 (96%)	9575 (99%)	113 (1%)	71 88

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	RY	81	LYS
56	YZ	34	ASN
13	XM	40	ASN
55	YY	50	ARG
47	YQ	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
34	Y8	31	HIS
45	YO	29	ASN
38	YD	227	ASN
41	YG	58	GLN
53	YW	34	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	274 (18%)	34 (2%)
1	XA	1498/1522 (98%)	285 (19%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	24 (32%)	1 (1%)
23	XW	75/76 (98%)	38 (50%)	2 (2%)
24	QX	18/19 (94%)	8 (44%)	1 (5%)
24	XX	16/19 (84%)	7 (43%)	1 (6%)
25	QY	74/76 (97%)	28 (37%)	0
25	XY	75/76 (98%)	31 (41%)	0
36	RA	2879/2915 (98%)	607 (21%)	47 (1%)
36	YA	2880/2915 (98%)	578 (20%)	44 (1%)
37	RB	119/122 (97%)	24 (20%)	1 (0%)
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1950 (20%)	162 (1%)

5 of 1950 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	XW	58	A
36	YA	1558	A
36	YA	222	A
36	YA	827	U
36	YA	1980	G

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 955 ligands modelled in this entry, 951 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	$\# Z > 2$
59	SF4	XD	501	4	0,12,12	-	-	-		
58	PAR	XA	1679	-	45,45,45	0.65	0	64,67,67	1.41	6 (9%)
59	SF4	QD	501	4	0,12,12	-	-	-		
58	PAR	QA	1667	-	45,45,45	0.69	0	64,67,67	1.20	6 (9%)

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
59	SF4	XD	501	4	-	-	0/6/5/5
58	PAR	XA	1679	-	-	7/18/94/94	0/4/4/4
59	SF4	QD	501	4	-	-	0/6/5/5
58	PAR	QA	1667	-	-	4/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1679	PAR	C14-O33-C33	-4.13	107.75	117.96
58	QA	1667	PAR	C13-O52-C52	-3.60	109.04	117.96
58	XA	1679	PAR	C13-O52-C52	-3.48	109.35	117.96
58	XA	1679	PAR	O33-C14-C24	3.38	114.03	108.22
58	XA	1679	PAR	C44-C34-C24	3.23	116.63	111.07

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1667	PAR	O54-C54-C64-N64
58	XA	1679	PAR	C44-C54-C64-N64
58	XA	1679	PAR	O54-C54-C64-N64
58	XA	1679	PAR	O51-C51-C61-O61
58	QA	1667	PAR	O51-C51-C61-O61

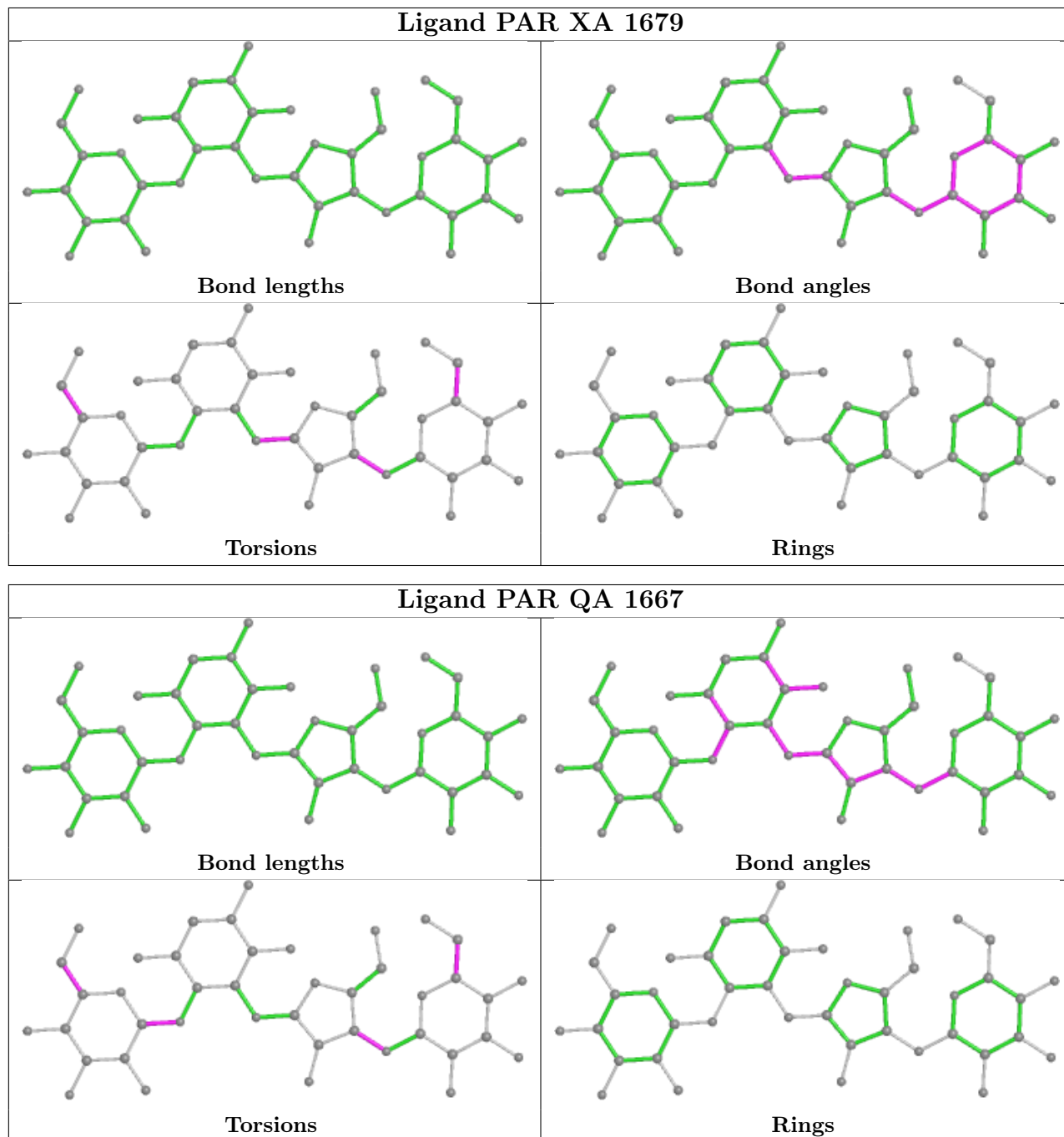
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1679	PAR	1	0
58	QA	1667	PAR	2	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.