



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 09:03 AM BST

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 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

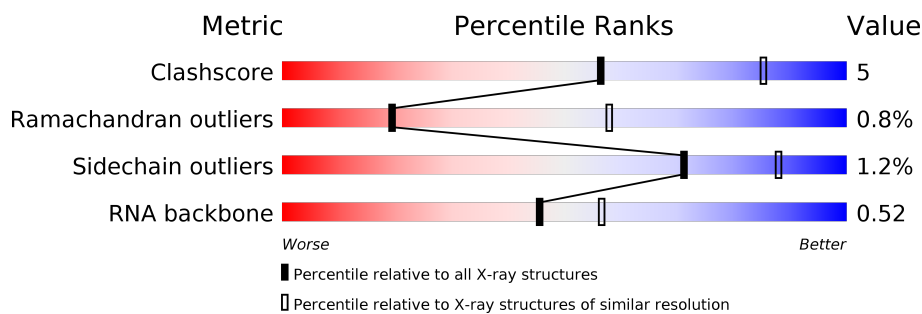
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)















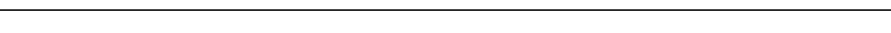




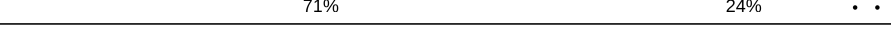



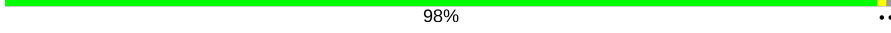

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	66% 27% 6% ..
1	XA	1522	64% 28% 5% ..
2	QB	256	71% 21% 7%
2	XB	256	72% 20% 7%
3	QC	239	73% 12% 14%
3	XC	239	70% 16% 14%
4	QD	209	84% 14% .

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Mol	Chain	Length	Quality of chain
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%
16	XP	88	 82% 13% . 5%















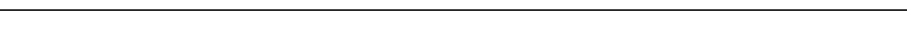




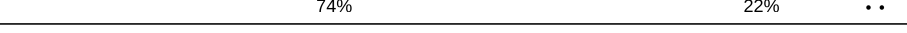





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	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















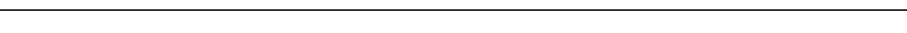




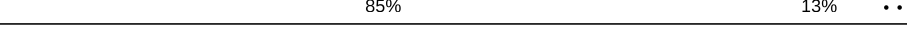





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Mol	Chain	Length	Quality of chain
29	Y3	60	
30	R4	71	
30	Y4	71	
31	R5	60	
31	Y5	60	
32	R6	54	
32	Y6	54	
33	R7	49	
33	Y7	49	
34	R8	65	
34	Y8	65	
35	R9	37	
35	Y9	37	
36	RA	2915	
36	YA	2915	
37	RB	122	
37	YB	122	
38	RD	276	
38	YD	276	
39	RE	206	
39	YE	206	
40	RF	210	
40	YF	210	
41	RG	182	
41	YG	182	






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Mol	Chain	Length	Quality of chain
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%
54	RX	96	 82% 14% •

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Mol	Chain	Length	Quality of chain
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
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 tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-site tRNA^{Ala}(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 tRNA^{Ala}(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
37	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
37	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	YV	1	Total	Mg	0	0
			1	1		
57	RP	2	Total	Mg	0	0
			2	2		
57	QX	1	Total	Mg	0	0
			1	1		
57	R7	1	Total	Mg	0	0
			1	1		

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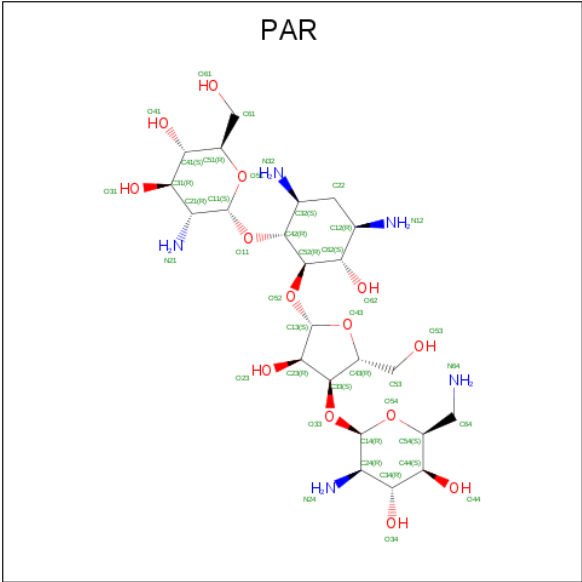
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YA	379	Total 379	Mg 379	0	0
57	QM	2	Total 2	Mg 2	0	0
57	YH	1	Total 1	Mg 1	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YD	3	Total 3	Mg 3	0	0
57	QV	4	Total 4	Mg 4	0	0
57	RX	1	Total 1	Mg 1	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	XA	94	Total 94	Mg 94	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	YU	2	Total 2	Mg 2	0	0
57	RU	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	YX	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	2	Total 2	Mg 2	0	0

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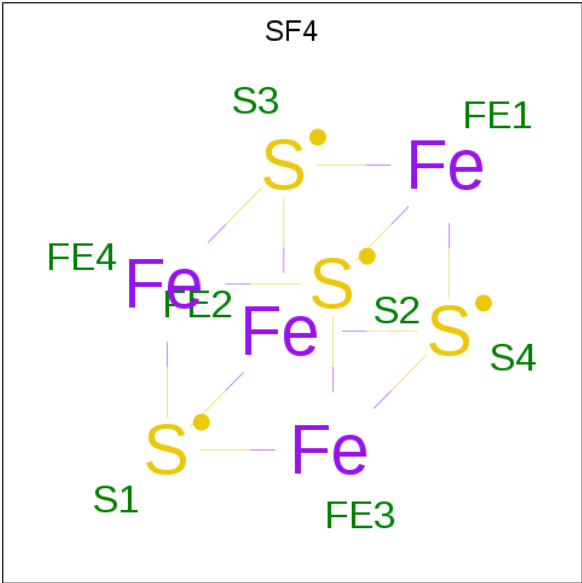
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	RA	321	Total 321	Mg 321	0	0
57	YP	3	Total 3	Mg 3	0	0
57	Y5	2	Total 2	Mg 2	0	0
57	RE	3	Total 3	Mg 3	0	0
57	YB	8	Total 8	Mg 8	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	4	Total 4	Mg 4	0	0
57	Y2	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RF	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	3	Total 3	Mg 3	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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



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

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

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

- Molecule 61 is water.

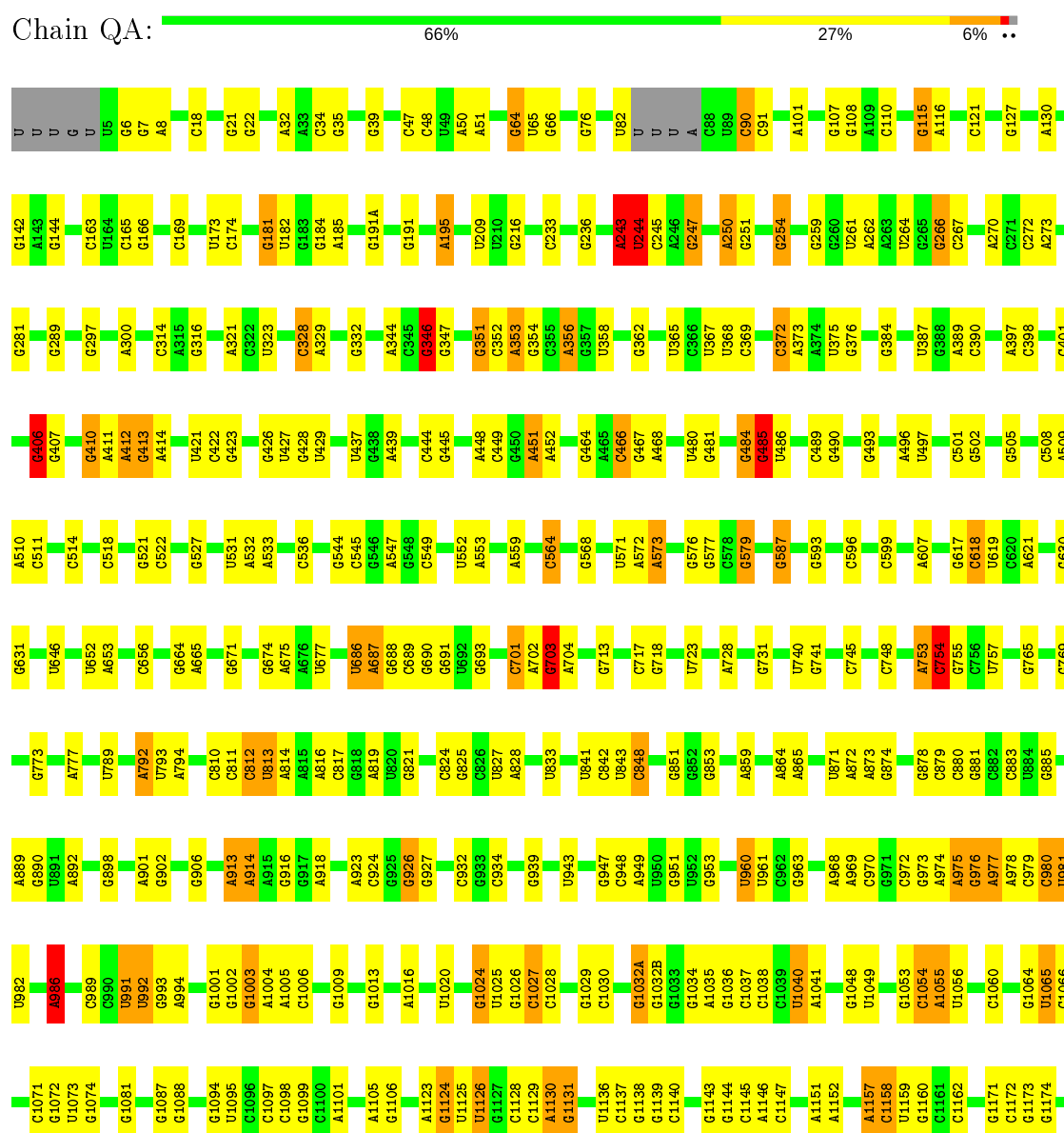
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	QA	1	Total	O	0	0
			1	1		
61	QX	1	Total	O	0	0
			1	1		

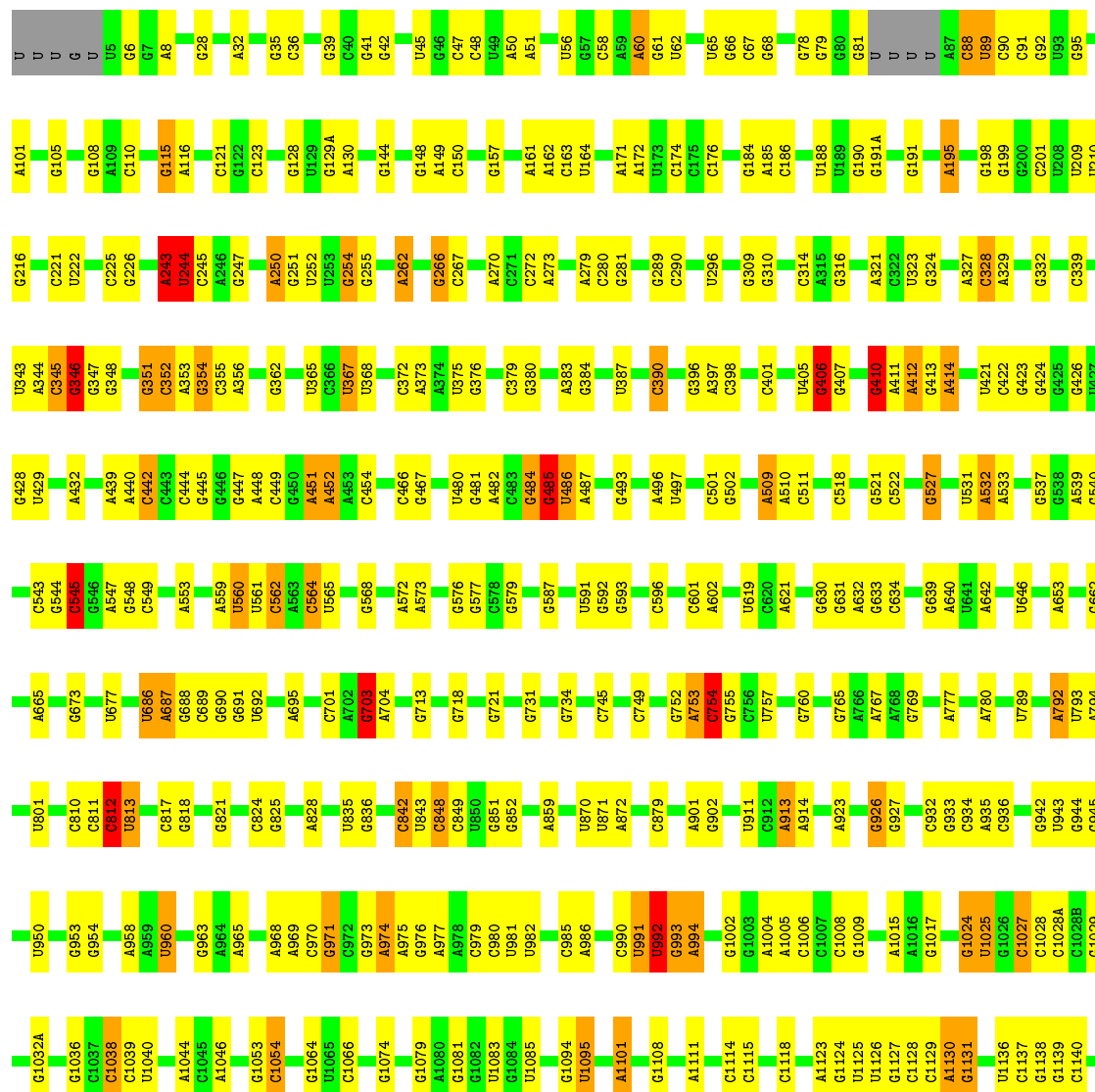
3 Residue-property plots

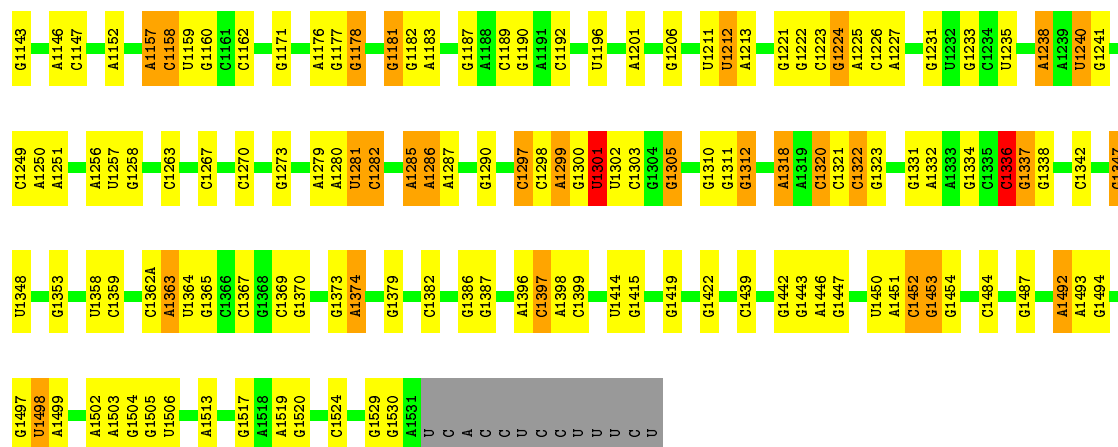
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

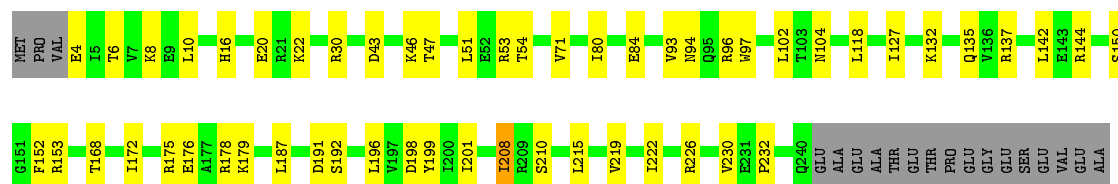






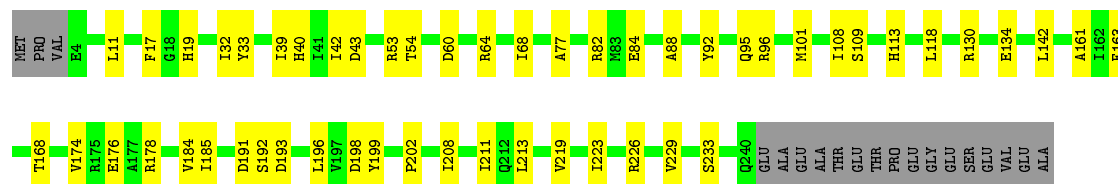
• Molecule 2: 30S ribosomal protein S2

Chain QB: 71% 21% 7%



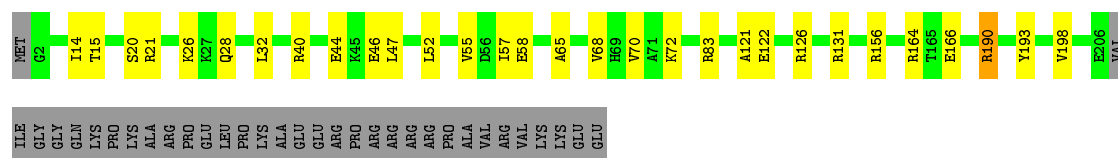
• Molecule 2: 30S ribosomal protein S2

Chain XB: 72% 20% 7%



• Molecule 3: 30S ribosomal protein S3

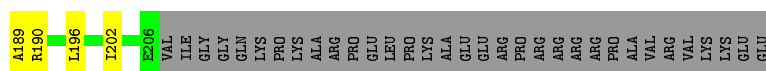
Chain QC: 73% 12% 14%



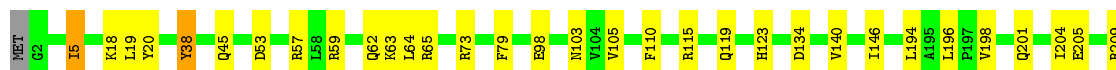
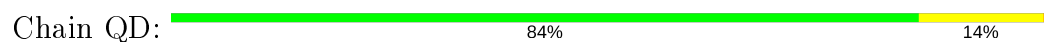
• Molecule 3: 30S ribosomal protein S3

Chain XC: 70% 16% 14%

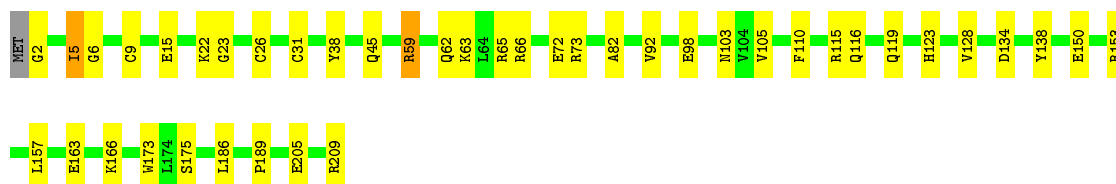




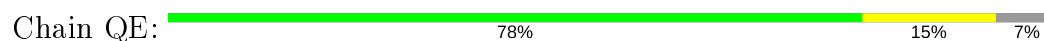
- Molecule 4: 30S ribosomal protein S4



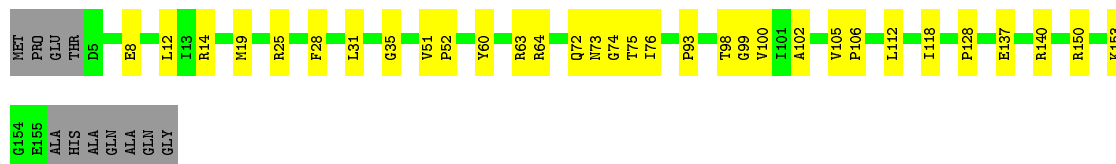
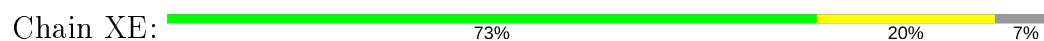
- Molecule 4: 30S ribosomal protein S4



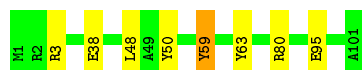
- Molecule 5: 30S ribosomal protein S5



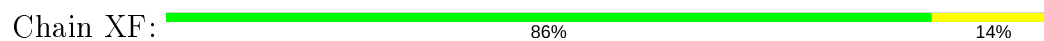
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6





- Molecule 7: 30S ribosomal protein S7

Chain QG: 85% 15%



- Molecule 7: 30S ribosomal protein S7

Chain XG: 85% 14%



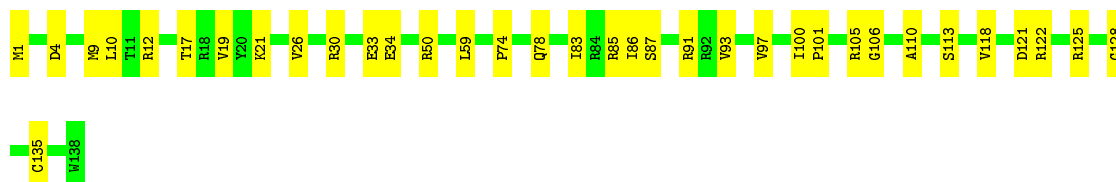
- Molecule 8: 30S ribosomal protein S8

Chain QH: 78% 22%



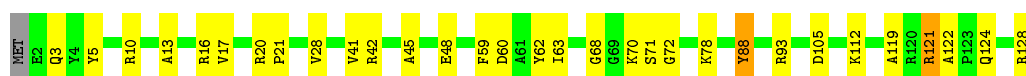
- Molecule 8: 30S ribosomal protein S8

Chain XH: 75% 25%



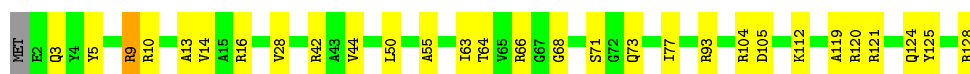
- Molecule 9: 30S ribosomal protein S9

Chain QI: 75% 23%




- Molecule 9: 30S ribosomal protein S9

Chain XI: 77% 22%



- 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%




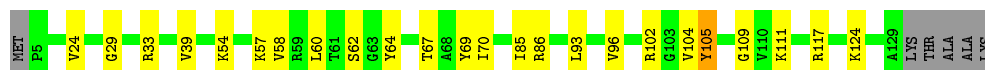
- Molecule 11: 30S ribosomal protein S11

Chain XK:  77% 16% 8%



- Molecule 12: 30S ribosomal protein S12

Chain QL:  77% 18% 5%



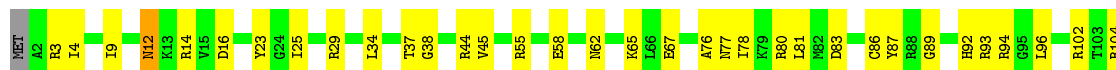
- Molecule 12: 30S ribosomal protein S12

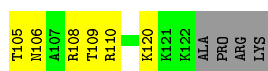
Chain XL:  76% 18% 5%



- Molecule 13: 30S ribosomal protein S13

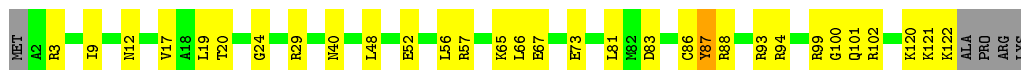
Chain QM:  64% 31% 5%





- Molecule 13: 30S ribosomal protein S13

Chain XM: 71% 24% ..



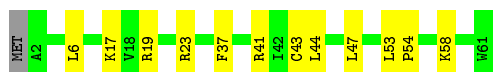
- Molecule 14: 30S ribosomal protein S14 type Z

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

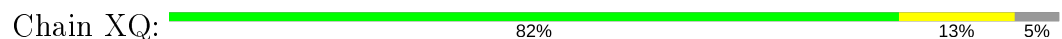
Chain XP: 82% 13% 5%



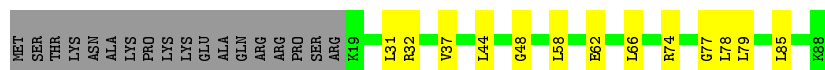
- Molecule 17: 30S ribosomal protein S17



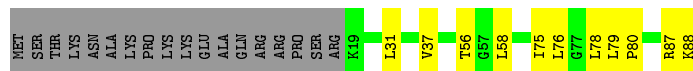
- Molecule 17: 30S ribosomal protein S17



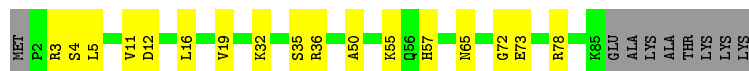
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



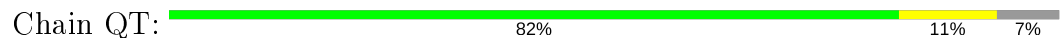
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



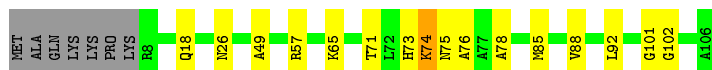
- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20

Chain XT: 78% 14% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 70% 22% 7%



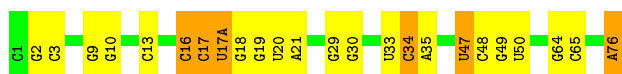
- Molecule 21: 30S ribosomal protein Thx

Chain XU: 74% 19% 7%



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

Chain QV: 69% 23% 8%



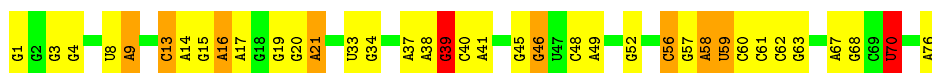
- Molecule 22: P-site tRNA^{fMet}

Chain XV: 74% 23% 3%



- Molecule 23: E-site tRNA^{Ala}(GGC)

Chain QW: 51% 36% 11%

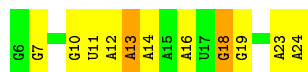


- Molecule 23: E-site tRNA^{Ala}(GGC)

Chain XW: 41% 42% 17%



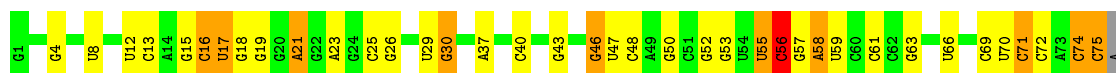
- Molecule 24: mRNA



- Molecule 24: mRNA



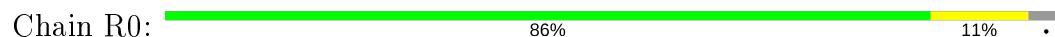
- Molecule 25: A-site tRNAAla(GGC)



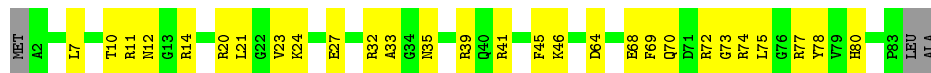
- Molecule 25: A-site tRNAAla(GGC)



- Molecule 26: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28





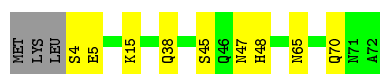
- Molecule 27: 50S ribosomal protein L28

Chain Y1: 86% 10% . .



- Molecule 28: 50S ribosomal protein L29

Chain R2: 83% 13% .



- Molecule 28: 50S ribosomal protein L29

Chain Y2: 79% 17% .



- Molecule 29: 50S ribosomal protein L30

Chain R3: 87% 12% .



- Molecule 29: 50S ribosomal protein L30

Chain Y3: 87% 12% .



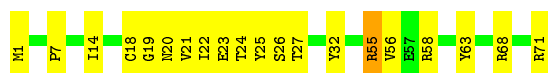
- Molecule 30: 50S ribosomal protein L31

Chain R4: 68% 27% 6%



- Molecule 30: 50S ribosomal protein L31

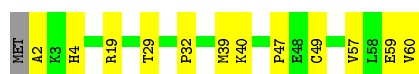
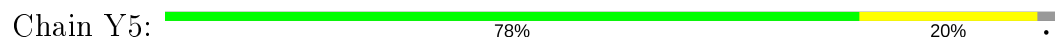
Chain Y4: 72% 27% .



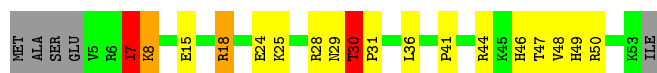
- Molecule 31: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L32



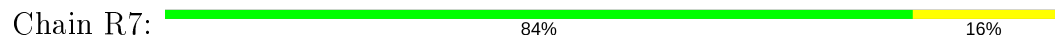
- Molecule 32: 50S ribosomal protein L33



- Molecule 32: 50S ribosomal protein L33



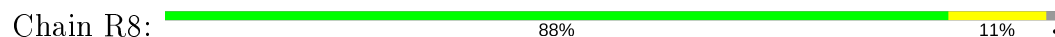
- Molecule 33: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L34



- Molecule 34: 50S ribosomal protein L35

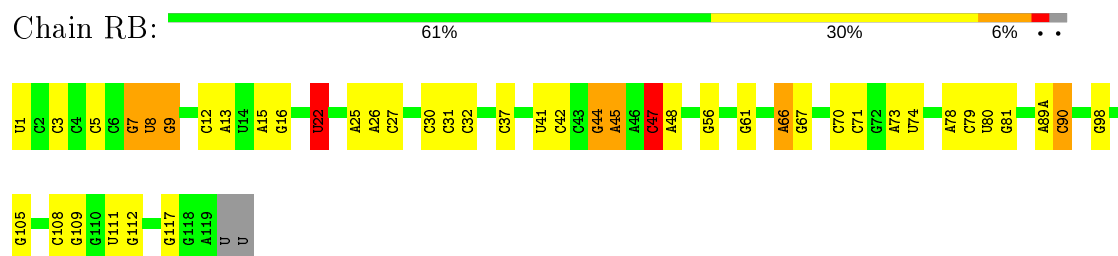




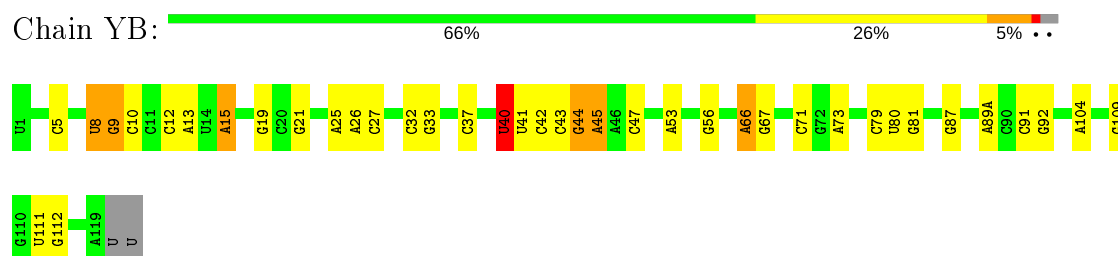
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G2319	G2211	G2212	G2112	C1980	G1559	G1449A	A1321	A1174	C1079	A1003	C904	A784
A2320	U2213	U2214	U2113	A1981	C1565	U1454	G1327	U1175	U1082	G1008	C906	G785
G2445	G2215	G2216	A2114	G1689	A1567	G1455	A1328	A1177	A1084	C1013	C907	C790
G2325	G2115	G2116	G2115	C1684	A1568	C1458	U1329	C1178	A1085	G1011	C910	C791
A2333	A2217	A2218	A2117	G1695	A1569	G1460	C1330	C1179	A1086	U1012	A911	C792
G2334	U2118	U2119	A2118	A1698	A1570	G1461	A1331	C1180	A1087	U1014	C912	A793
A2335	G2120	G2121	G2120	A1698	U1576	C1462	G1332	G1184	A1088	G1015	A915	A800
C2342	G2238	G2239	G2121	G1703	U1577	C1467	U1341	A1189	G1091	G1015	C915	G805
A2346	A2235	A2236	A2126	U1725	U1578	C1467	A1342	A1190	C1092	G1015	C916	C806
C2347	U2243	U2244	G2127	G1728	A1579	A1471	A1349	A1191	G1093	U1019	A917	U807
C2476	U2243	U2244	G2127	G1728	A1581	A1471	A1349	G1192	U1094	A1020	A918	C812
C2477	U2244	U2245	G2128	A1858	A1581	G1479	U1352	G1195	A1095	A1021	A919	C812
C2350	G2245	G2246	U2129	A1858	A1586	G1479	U1352	G1195	A1096	G1022	U930	A819
G2484	U2130	U2131	U2130	U1730	A1586	U1482	A1353	A1204	U1023	G1024	U932	U827
G2354	G2131	G2132	G2131	G1731	G1595	G1483	A1385	U1205	A1098	G1025	U933	U828
G2355	U2132	U2133	U2132	C1742	C1598	G1483	A1385	U1206	C1104	G1026	U938	U829
G2356	G2012	G2013	A2013	G1743	C1599	A1486	G1388	A1210	U1105	A1027	U938	A829
G2371	A2013	A2014	A2013	G1743	C1599	A1486	G1388	A1210	U1105	A1027	U938	G830
C2498	A2135	A2136	A2135	G1756	C1600	A1490	A1378	U1211	G1110	U1033	A941	G831
G2374	A2266	A2267	C2137	A1762	A1603	G1491	A1379	U1211	G1110	U1033	A941	G832
A2377	A2269	A2270	C2138	G1763	A1603	G1491	A1379	U1211	G1110	U1033	A941	G832
G2378	C2022	C2023	C2138	G1764	A1607	G1492	A1384	G1217	G1112	G1036	A945	C838
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G2383	G2147	G2148	A2147	A1889	A1608	A1494	G1385	A1220	G1114	G1039	A947	U847
G2384	G2148	G2149	G2148	A1889	A1609	U1497	G1388	G1236	G1115	C1043	U948	C846
C2385	G2280	G2281	A2148	G1773	A1610	U1497	G1388	A1237	G1116	G1044	U958	U860
G2386	G2281	G2282	A2149	G1774	A1611	U1497	G1388	A1237	G1117	A1045	A959	A861
A2392	C2283	C2284	G2155	G1776	C1617	C1506	U1391	G1238	G1122	A1046	A960	G862
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C2420	C2294	C2295	G2166	A1786	A1638	U1514	C1407	G1256	G1131	C1053	C961	G862
G2421	U2296	U2297	U2167	A1787	U1639	U1514	C1407	G1256	G1131	C1053	C961	A863
A2422	C2297	C2298	G2168	A1788	U1639	U1514	C1407	G1256	G1131	C1053	C961	A863
C2424	A2298	A2299	A2170	C1788	C1640	G1522	C1411	U1263	C1135	A1054	U969	A866
A2425	A2305	A2306	A2171	A1791	C1644	G1522	C1411	U1263	C1135	A1054	U969	A866
A2426	C2307	C2308	A2176	C1795	C1648	G1525	G1446	G1266	G1136	A1057	A973	G869
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G2428	U2086	U2087	C2188	G1800	G1651	A1533	U1420	G1271	C1140	G1059	C974	G881
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A2561	U2431	U2432	G2190	A1966	G1653	U1535	G1422	U1273	U1142	U1061	A980	G882
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U2563	G2192	G2193	G2191	A1815	A1654	C1537	G1427	G1286	G1151	U1066	A984	C884
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A2566	A2316	A2317	A2199	A1971	A1668	A1544	G1444A	A1301	A1156	G1071	A989	C889
C2567	C2317	C2318	A2199	A1972	A1668	A1545	G1445	A1316	U1165	A1073	A896	A896
												C897
												C898
												C899
												A900

C2773	G2673	A2425	A2311	G2043	A1918	C1781	C1638	U1514	U1406	A1262	C1135
A2776	G2674	A2426	C2314	C2055	A1919	A1786	U1639	C1407	C1407	U1263	G1136
G2777	A2675	G2427	G2315	G2056	G2168	A1787	C1640	C1408	C1408	A1264	G1137
A2778	C2680	G2428	G2316	A2059	A2169	C1788	G1647	C1411	C1411	G1266	G1138
G2780	C2681	A2430	G2319	A2060	A2170	A1791	C1648	G1416	G1416	C1270	C1140
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C	C2683	C	G2321	A2173	U1931	C1799	G1653	G1418	G1418	G1272	U1142
U	U2562	U	A2436	G2192	A1936	G1799	A1654	U1420	U1420	U1273	A1142A
C	A2566	A2439	G2325	A2176	A1937	G1800	C1657	G1421	G1421	U1288	A1143
C	G2567	C2440	G2334	U2189	A1938	A1800	A1543	A1427	A1427	U1300	G1151
C	A2572	C2441	A2335	G2190	U1939	A1802	A1544	C1428	C1428	A1301	G1171
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C	C2582	U2449	C2343	A2199	A1960	A1816	A1569	G1442	G1442	C1314	A1177
C	G2583	A2450	G2210	G2211	U1963	A1819	C1565	A1444	A1444	U1325	A1178
C	U2584	G2468	A2212	U2113	G1964	U1820	C1566	C1445	C1445	G1326	U1188
C	U2585	A2469	A2213	A2114	A1965	G1824	A1567	C1446	C1446	C1327	A1194
C	C2586	G2470	G2215	G2115	A1966	A1829	G1568	A1449	A1449	U1328	G1195
C	A2590	C2474	G2225	G2116	C1967	G1835	A1569	G1455	G1455	G1332	C1196
C	G2597	A2475	A2225	A2117	G1968	A1835	U1578	U1341	U1341	U1341	A1203
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C	A2602	C2477	G2239	A2119	A1970	A1858	C1585	G1459	G1459	A1210	G1218
C	G2603	G2478	G2243	A2120	A1971	A1859	A1586	A1461	A1461	U1211	G1219
C	U2604	C2479	U2243	G2123	A1972	U1864	A1587	C1464	C1464	A1220	A1225
C	G2609	C2480	G2250	G2124	G1973	G1869	G1591	A1378	A1378	C1225	G1228
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C	C2617	G2495	A2278	G2132	U1993	C1882	A1607	A1490	A1490	G1385	A1283
C	A2629	C	A2278	G2133	G2004	G1883	A1608	C1493	C1493	U1391	A1286
C	G2632	G2502	C2283	A2134	G2010	G1888	A1609	U1497	U1497	A1395	G1243
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C	G2634	G2505	C2284	G2148	U2022	G1763	A1611	A1508	A1508	C1402	A1283
C	C2635	U2506	C2285	G2149	G2023	G1764	C1611	C1509	C1509	U1405	G1256
C	U2636	C2507	A2288	U2150	A2031	A1773	A1616	A1510	A1510		
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C	C2646	A2518	C2292	G2152	A2033	U1775	A1618				
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C	G2656	U2519	C2294	U2150	A2035	A1914	A1618				
C	A2657	C2520	C2295	G2151	G2034		A1618				
C	C2662	U2527	C2297	G2152	G2035		A1618				
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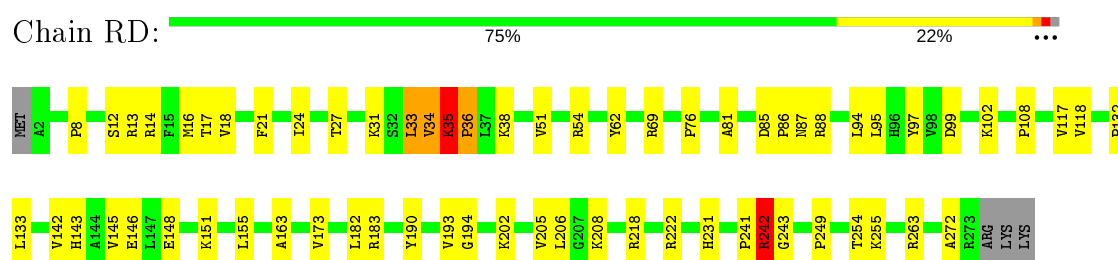
- Molecule 37: 5S rRNA



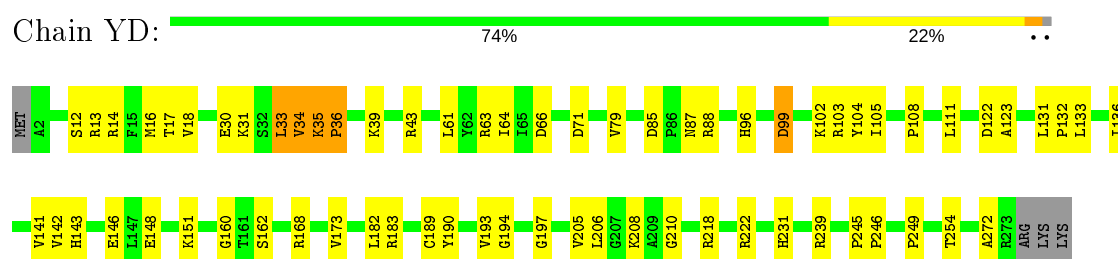
- Molecule 37: 5S rRNA



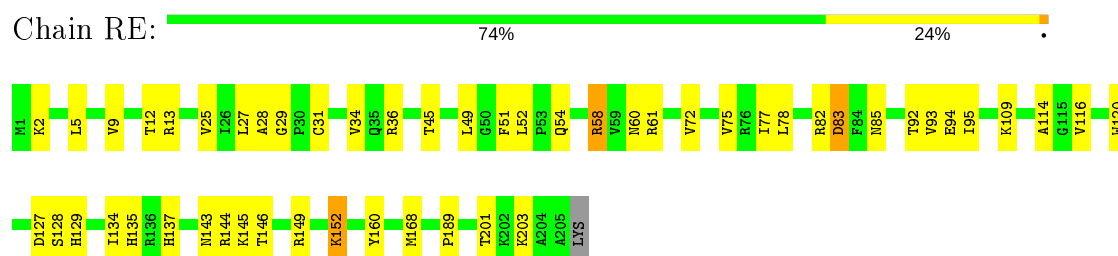
- Molecule 38: 50S ribosomal protein L2



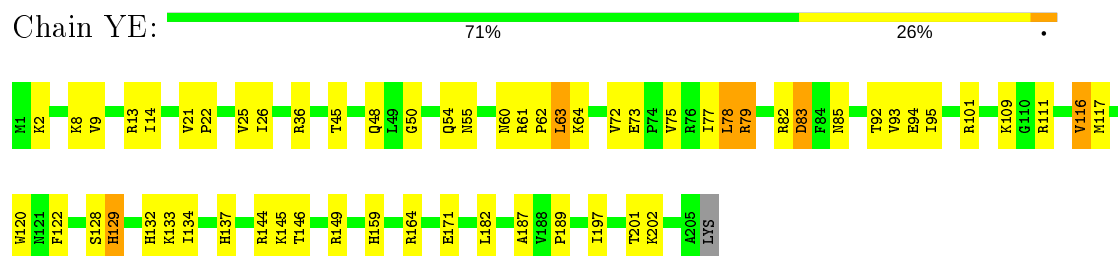
- Molecule 38: 50S ribosomal protein L2



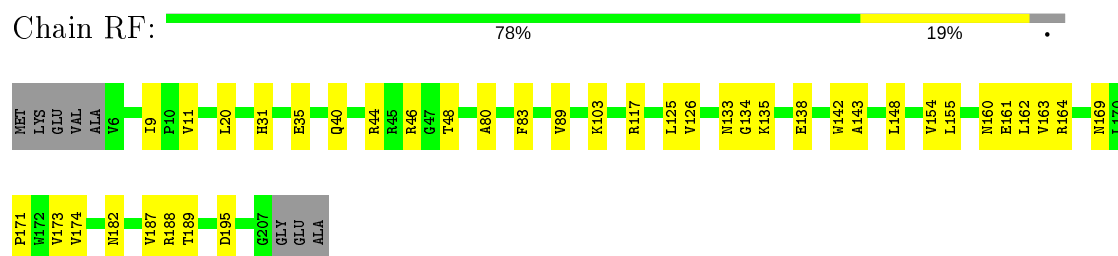
- Molecule 39: 50S ribosomal protein L3



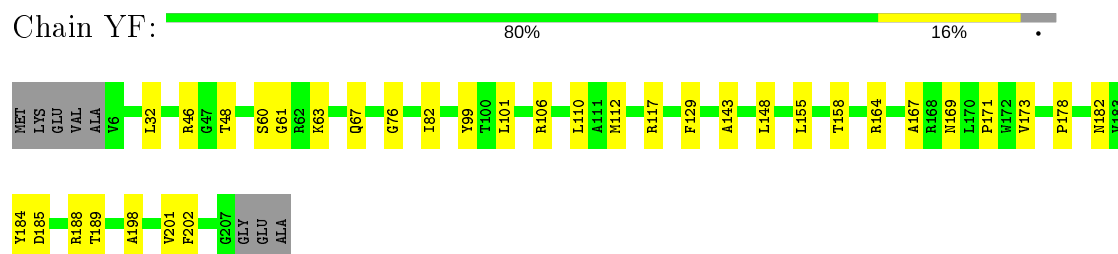
- Molecule 39: 50S ribosomal protein L3



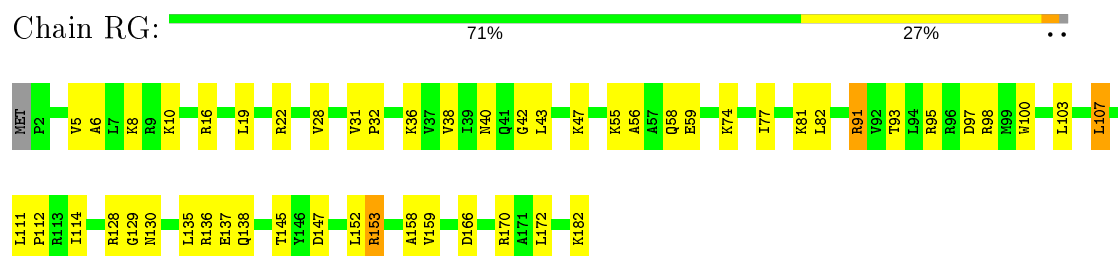
- Molecule 40: 50S ribosomal protein L4



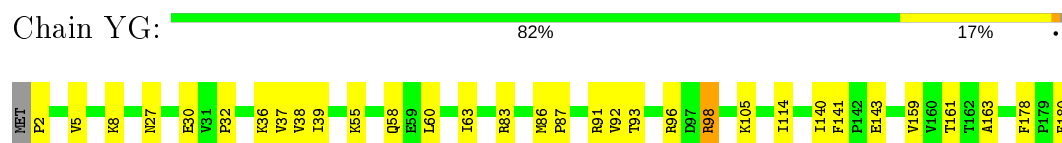
- Molecule 40: 50S ribosomal protein L4




- Molecule 41: 50S ribosomal protein L5



- Molecule 41: 50S ribosomal protein L5



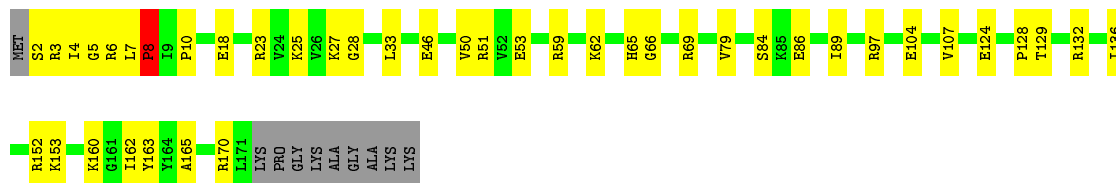
- Molecule 42: 50S ribosomal protein L6

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% ••




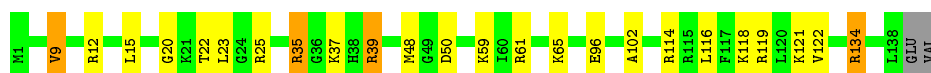
- Molecule 44: 50S ribosomal protein L13

Chain RN:  90% 9% •




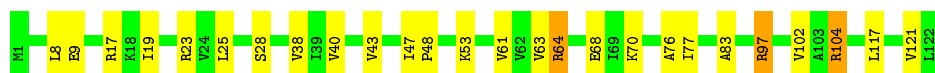
- Molecule 44: 50S ribosomal protein L13

Chain YN:  81% 14% ••



- Molecule 45: 50S ribosomal protein L14

Chain RO:  79% 19% •



- Molecule 45: 50S ribosomal protein L14

Chain YO: 76% 23% .



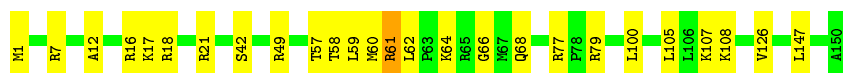
- Molecule 46: 50S ribosomal protein L15

Chain RP: 79% 21% .



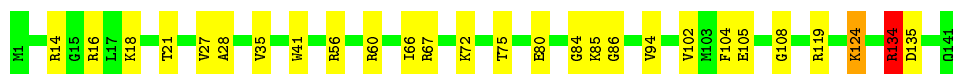
- Molecule 46: 50S ribosomal protein L15

Chain YP: 83% 17% .



- Molecule 47: 50S ribosomal protein L16

Chain RQ: 81% 18% ..



- Molecule 47: 50S ribosomal protein L16

Chain YQ: 72% 27% .



- Molecule 48: 50S ribosomal protein L17

Chain RR: 79% 19% .



- Molecule 48: 50S ribosomal protein L17

M1	R2	H3	L4	K5		R8		N11	V38		R63	F80		Y87		R90		R96		R103	R104	R105	G106	D107		A112		E115		E118
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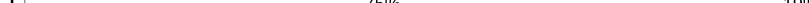
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|-----|----|----|--|----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|--|-----|--|-----|--|-----|--|------|------|------|
| MET | A2 | R3 | | R9 | R10 | | R13 | V14 | R15 | | T21 | G22 | R23 | L24 | R25 | | R30 | | H34 | | Q38 | I39 | L40 | | T47 | L48 | V49 | | S53 | | A77 | | R89 | | R97 | | L110 | E111 | F112 |
|-----|----|----|--|----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|--|-----|--|-----|--|-----|--|------|------|------|

- | MET |
|------|
| A2 |
| Y7 |
| E8 |
| R9 |
| R10 |
| R11 |
| R12 |
| R13 |
| V14 |
| R15 |
| R16 |
| R17 |
| R25 |
| L39 |
| K62 |
| R67 |
| L73 |
| Q84 |
| F87 |
| K93 |
| Y94 |
| H95 |
| K99 |
| A102 |
| E103 |
| L110 |
| E111 |
| F112 |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|
| R1 | K137 | ALA | GLN | GLU | PRO | LYS | ALA | LYS | SER | GLN | GLU | R41 | I42 | Q43 | D44 | F45 | E46 | I50 | R51 | I52 | R53 | G56 | T62 | V66 | V70 | G71 | R74 | I75 | H79 | R91 | G92 | K98 | L99 | Y100 | L105 | R112 | R115 | A116 | D117 | R118 | K119 | R120 | I121 | D122 |
|----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|

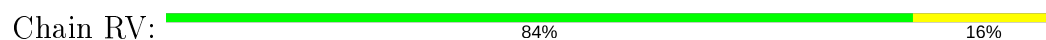
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|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| D117 | R118 | I121 | K137 | ALA | GLN | GLU | PRO | LYS | ALA | SER | GLN | GLU | R1 | R2 | R3 | L6 | R16 | L19 | P20 | P24 | K33 | E36 | R39 | T40 | R41 | I42 | Q43 | V49 | I50 | R51 | I52 | R63 | T62 | R63 | R64 | R65 | V66 | S67 | G71 | V72 | E73 | R74 | I75 | L82 | I86 | G92 | K98 | L99 | R103 | S106 | I110 | L114 | R115 | A116 |
|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

- | MET |
|------|
| P2 |
| K15 |
| S31 |
| E37 |
| R50 |
| R53 |
| K54 |
| R55 |
| R58 |
| W61 |
| I62 |
| V63 |
| R64 |
| N75 |
| F79 |
| V90 |
| D91 |
| R92 |
| K93 |
| N94 |
| G118 |

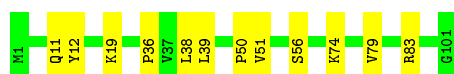
- Chain YU:  75% 19% ..



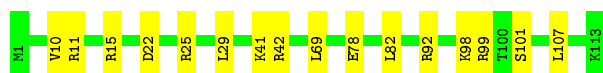
- Molecule 52: 50S ribosomal protein L21



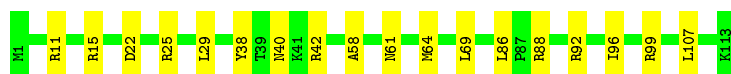
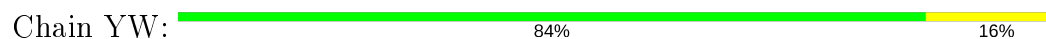
- Molecule 52: 50S ribosomal protein L21



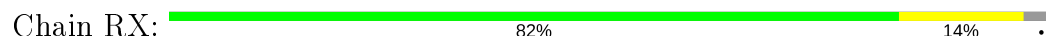
- Molecule 53: 50S ribosomal protein L22



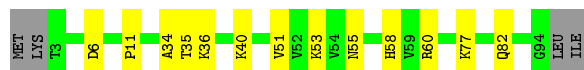
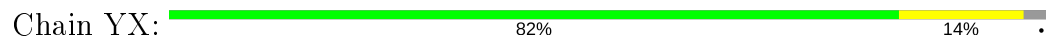
- Molecule 53: 50S ribosomal protein L22



- Molecule 54: 50S ribosomal protein L23

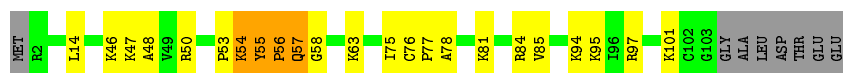


- Molecule 54: 50S ribosomal protein L23



- Molecule 55: 50S ribosomal protein L24





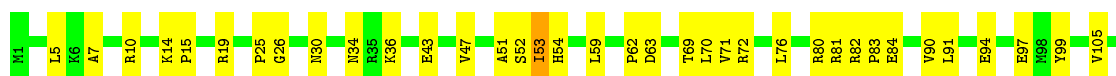
- Molecule 55: 50S ribosomal protein L24

Chain YY: 73% 18% 7%



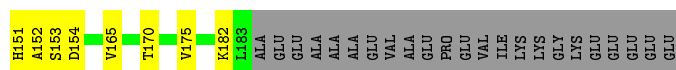
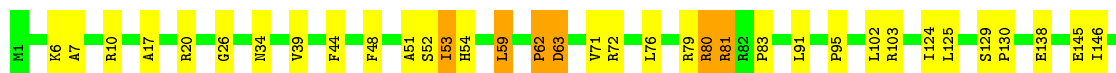
- Molecule 56: 50S ribosomal protein L25

Chain RZ: 62% 26% 11%



- Molecule 56: 50S ribosomal protein L25

Chain YZ: 68% 18% 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	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 ⓘ

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	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

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 ⓘ

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
50	RT	112	ARG
4	XD	59	ARG
51	YU	52	ARG
50	RT	115	ARG
55	RY	81	LYS

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

Mol	Chain	Res	Type
6	XF	7	ASN
9	XI	124	GLN
53	YW	34	ASN
7	XG	68	ASN
9	XI	3	GLN

5.3.3 RNA ⓘ

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
36	RA	2439	A
1	XA	250	A
36	YA	1930	G
36	RA	2566	A
36	RA	2787	C

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	0.00	-	-		
59	SF4	QD	501	4	0,12,12	0.00	-	-		
58	PAR	QA	1667	-	45,45,45	0.69	0	64,67,67	1.20	6 (9%)
58	PAR	XA	1679	-	45,45,45	0.65	0	64,67,67	1.41	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
59	SF4	QD	501	4	-	-	0/6/5/5
58	PAR	QA	1667	-	-	4/18/94/94	0/4/4/4
58	PAR	XA	1679	-	-	7/18/94/94	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	XA	1679	PAR	C44-C54-C64-N64
58	XA	1679	PAR	O54-C54-C64-N64
58	QA	1667	PAR	O54-C54-C64-N64
58	XA	1679	PAR	O51-C51-C61-O61
58	QA	1667	PAR	O51-C51-C61-O61

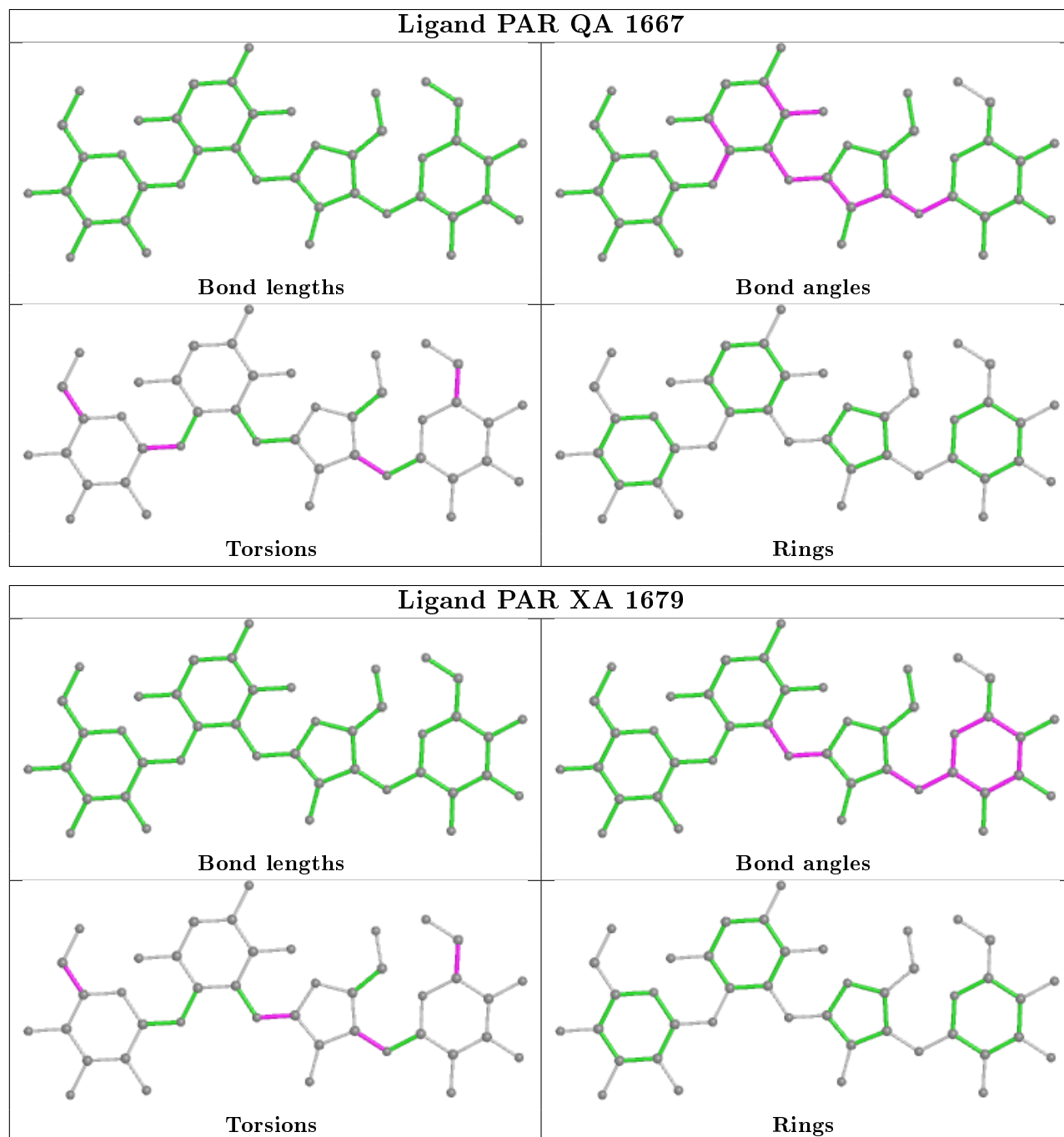
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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