



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 09:01 AM BST

PDB ID : 6OF6  
Title : Crystal structure of tRNA<sup>Ala</sup>(GGC) bound to cognate 70S A-site  
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.  
Deposited on : 2019-03-28  
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](mailto: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.

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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

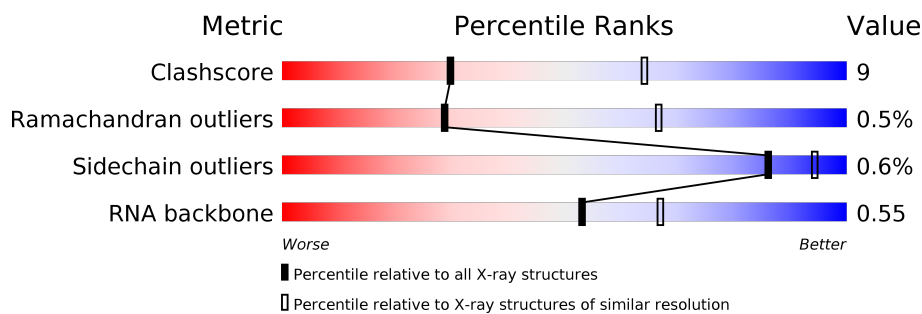
# 1 Overall quality at a glance

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  $\geq 3$ , 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	52% 38% 8% .
1	XA	1522	52% 38% 8% .
2	QB	256	74% 18% 7%
2	XB	256	65% 27% 7%
3	QC	239	63% 23% 14%
3	XC	239	65% 21% 14%
4	QD	209	80% 19% .

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Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	















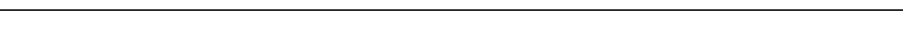




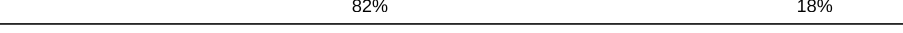





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	
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	
42	YH	180	
43	RI	148	
43	YI	148	
44	RN	140	
44	YN	140	
45	RO	122	
45	YO	122	
46	RP	150	
46	YP	150	
47	RQ	141	
47	YQ	141	
48	RR	118	
48	YR	118	
49	RS	112	
49	YS	112	
50	RT	146	
50	YT	146	
51	RU	118	
51	YU	118	
52	RV	101	
52	YV	101	
53	RW	113	
53	YW	113	
54	RX	96	

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Mol	Chain	Length	Quality of chain
54	YX	96	
55	RY	110	
55	YY	110	
56	RZ	206	
56	YZ	206	

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 298675 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<sup>fMet</sup>.

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<sup>Ala</sup>(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	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
			416	186	85	126	19			
24	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 25 is a RNA chain called A-site tRNA<sup>Ala</sup>(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	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			

- 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	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	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	124	Total	Mg	0	0
			124	124		
57	YV	1	Total	Mg	0	0
			1	1		
57	RP	3	Total	Mg	0	0
			3	3		
57	QX	1	Total	Mg	0	0
			1	1		
57	Y4	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YA	457	Total 457	Mg 457	0	0
57	QM	1	Total 1	Mg 1	0	0
57	YH	5	Total 5	Mg 5	0	0
57	YR	2	Total 2	Mg 2	0	0
57	RT	2	Total 2	Mg 2	0	0
57	QD	1	Total 1	Mg 1	0	0
57	RG	1	Total 1	Mg 1	0	0
57	YD	4	Total 4	Mg 4	0	0
57	XX	1	Total 1	Mg 1	0	0
57	QV	6	Total 6	Mg 6	0	0
57	YE	6	Total 6	Mg 6	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	123	Total 123	Mg 123	0	0
57	YY	5	Total 5	Mg 5	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QL	1	Total 1	Mg 1	0	0
57	YU	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	YG	2	Total 2	Mg 2	0	0

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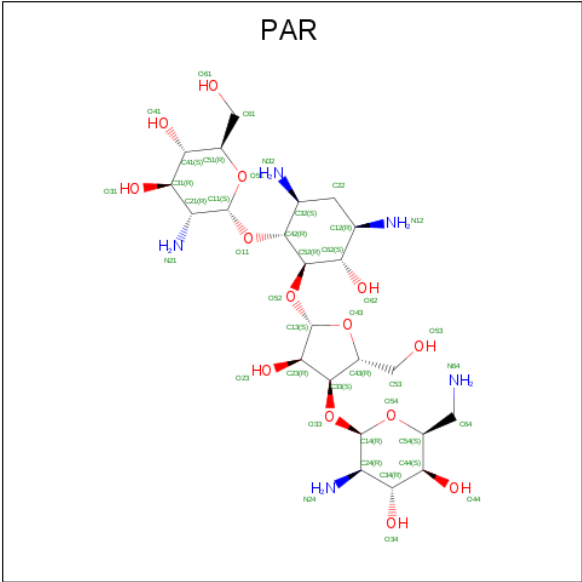
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YQ	4	Total 4	Mg 4	0	0
57	YN	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	2	Total 2	Mg 2	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	2	Total 2	Mg 2	0	0
57	R1	1	Total 1	Mg 1	0	0
57	XL	2	Total 2	Mg 2	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	XB	2	Total 2	Mg 2	0	0
57	YT	2	Total 2	Mg 2	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	3	Total 3	Mg 3	0	0
57	RA	378	Total 378	Mg 378	0	0
57	QK	2	Total 2	Mg 2	0	0
57	YF	5	Total 5	Mg 5	0	0
57	YP	7	Total 7	Mg 7	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	RE	8	Total 8	Mg 8	0	0

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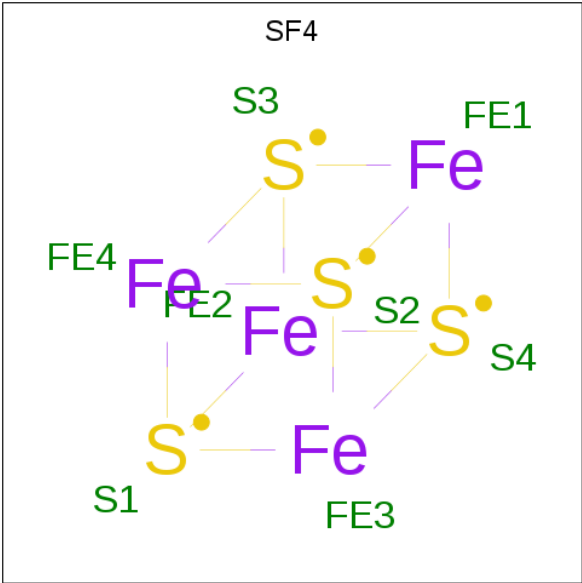
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XK	1	Total 1	Mg 1	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YW	1	Total 1	Mg 1	0	0
57	RI	1	Total 1	Mg 1	0	0
57	XV	7	Total 7	Mg 7	0	0
57	RB	4	Total 4	Mg 4	0	0
57	Y2	3	Total 3	Mg 3	0	0
57	YI	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RF	2	Total 2	Mg 2	0	0
57	XM	1	Total 1	Mg 1	0	0
57	Y3	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



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: Fe<sub>4</sub>S<sub>4</sub>).

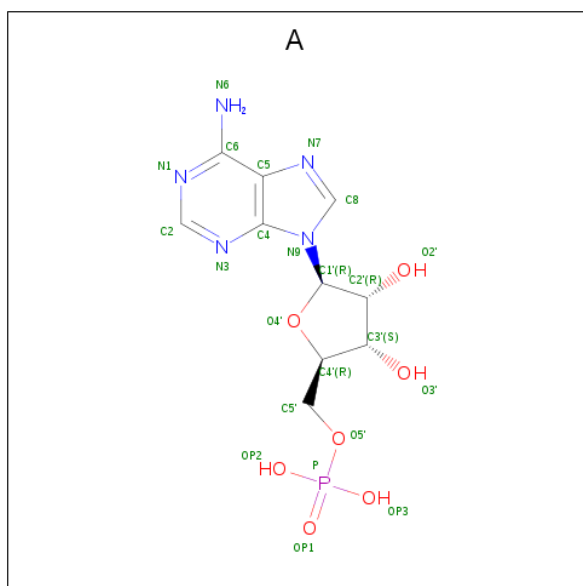


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	QD	1	Total	Fe	S	0	0
			8	4	4		
59	XD	1	Total	Fe	S	0	0
			8	4	4		

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

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

- Molecule 61 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	QY	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 62 is water.

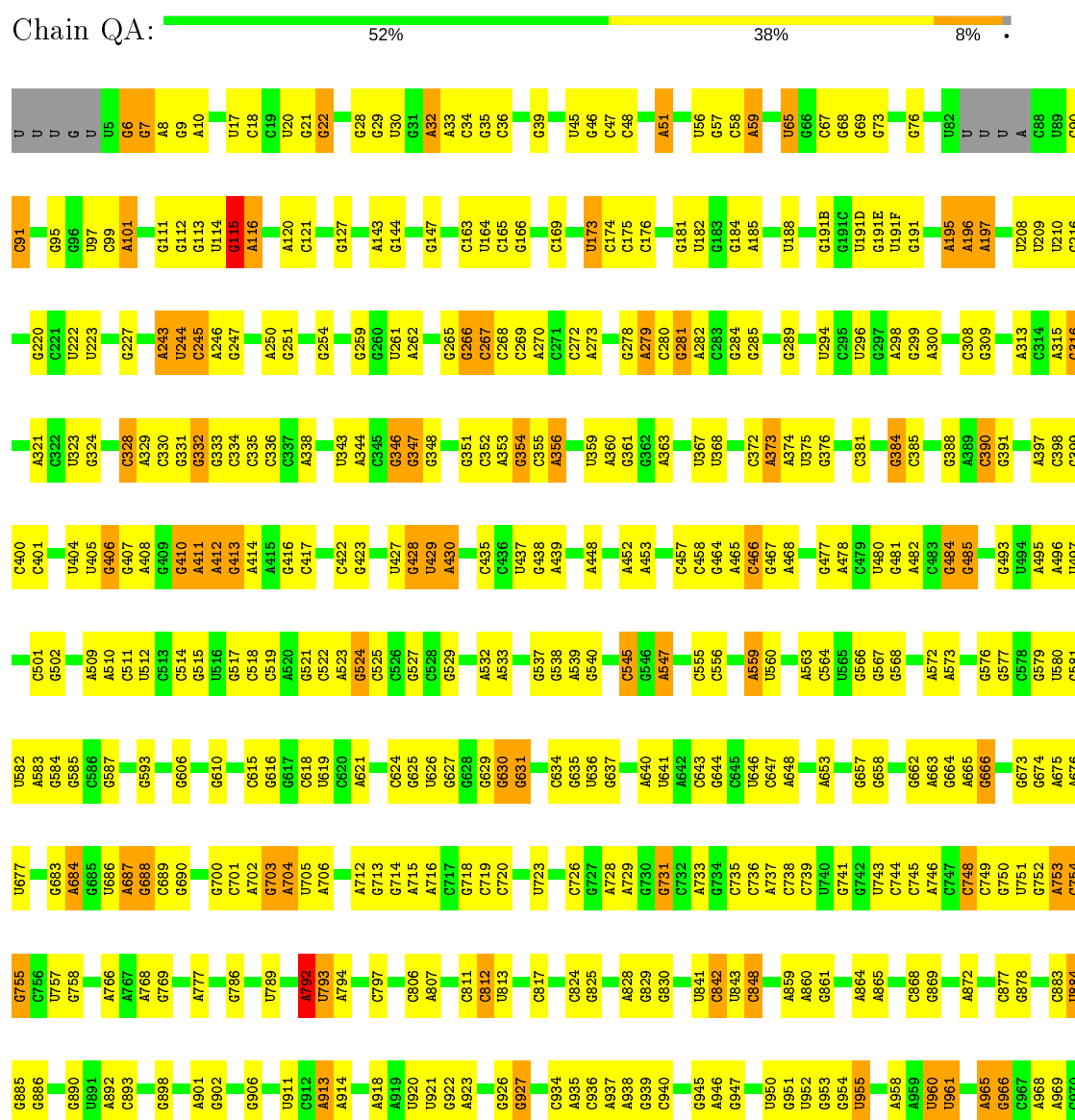
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	QA	1	Total	O	0	0
			1	1		
62	QX	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

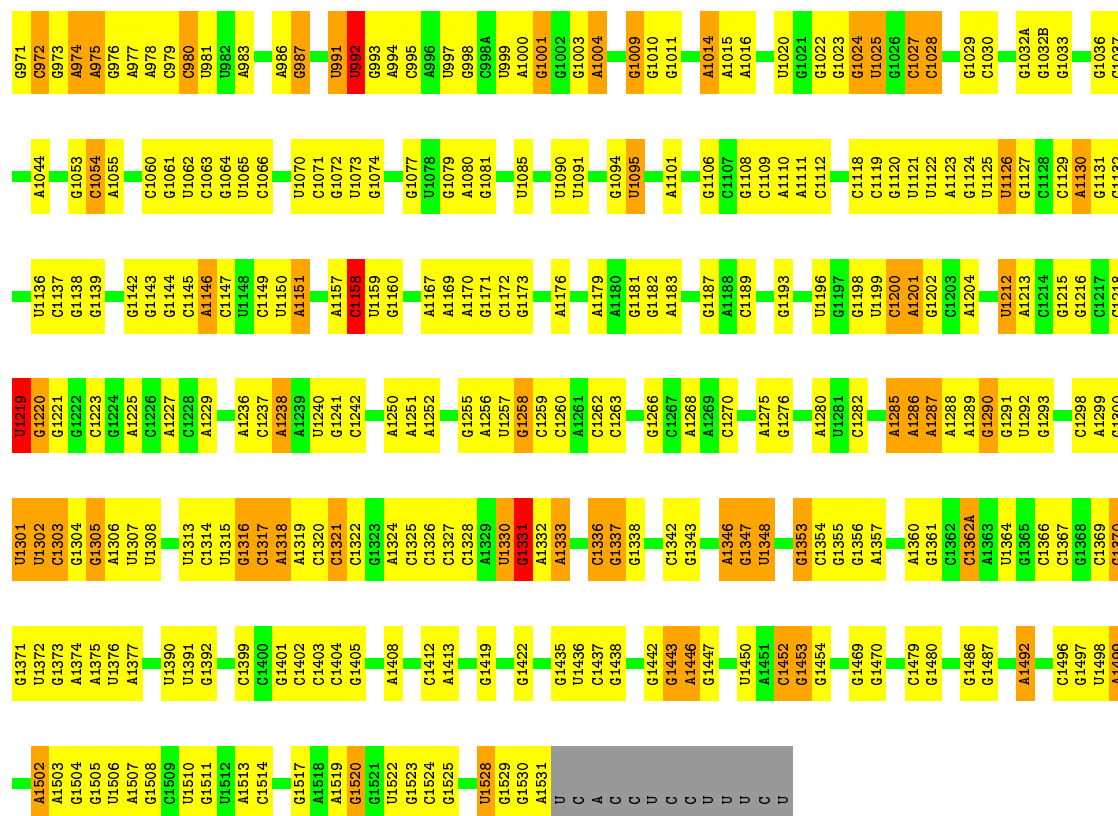
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

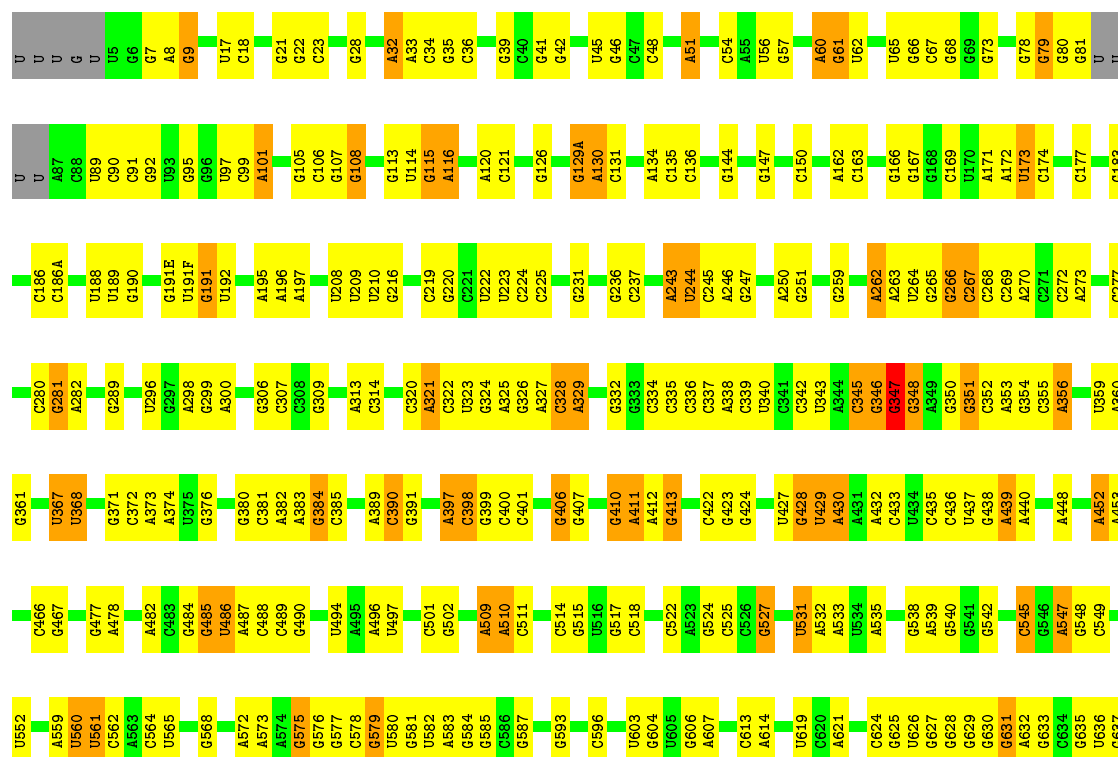


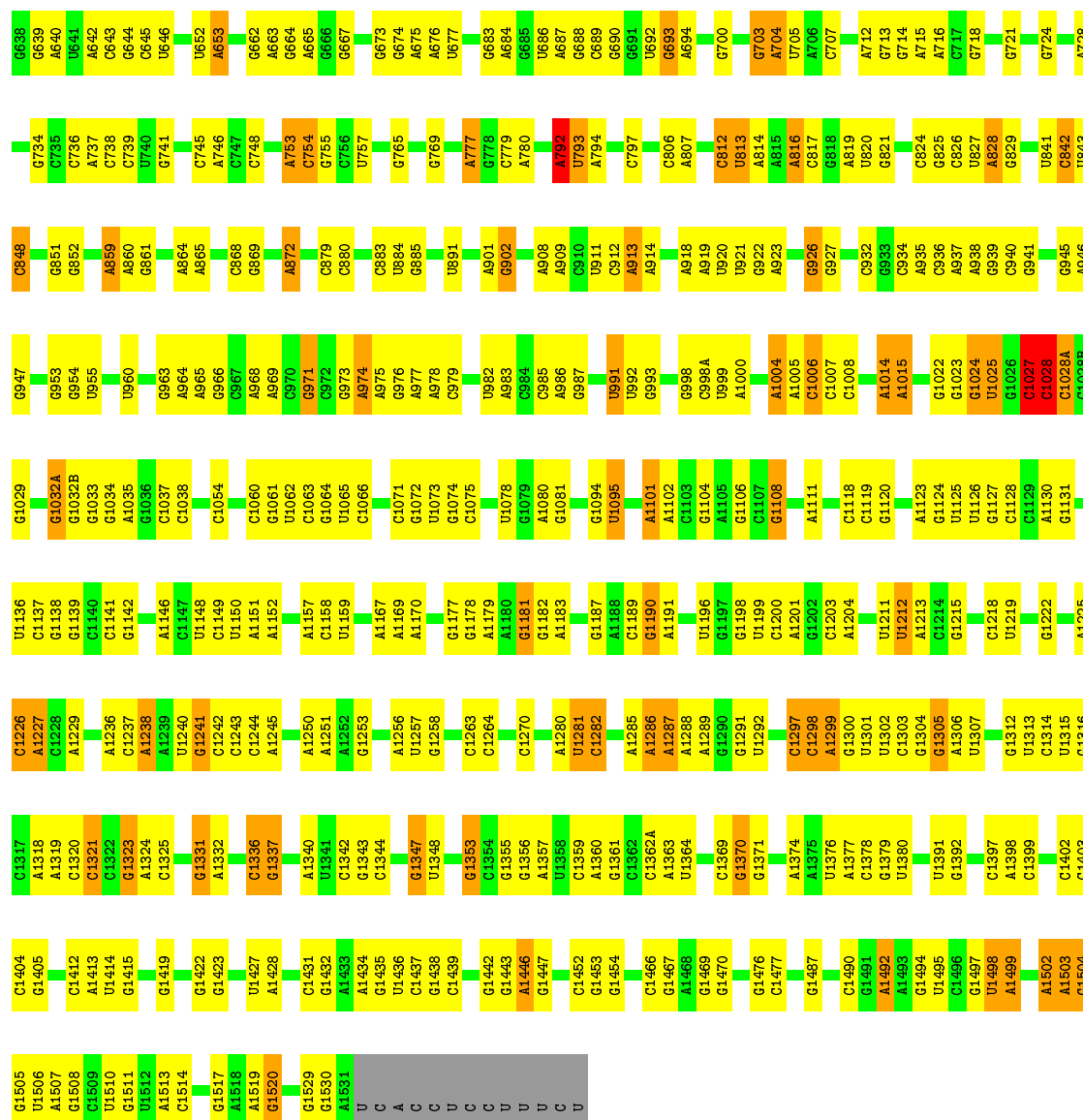




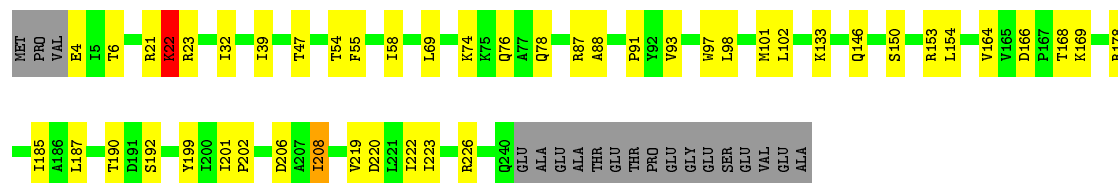
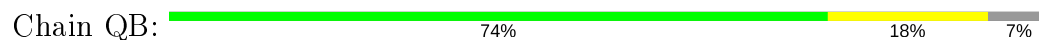
• Molecule 1: 16S rRNA

Chain XA:



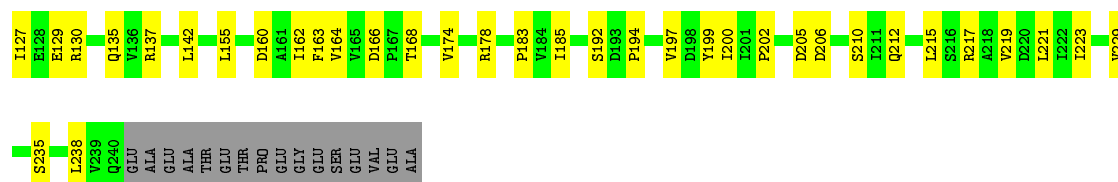


• Molecule 2: 30S ribosomal protein S2

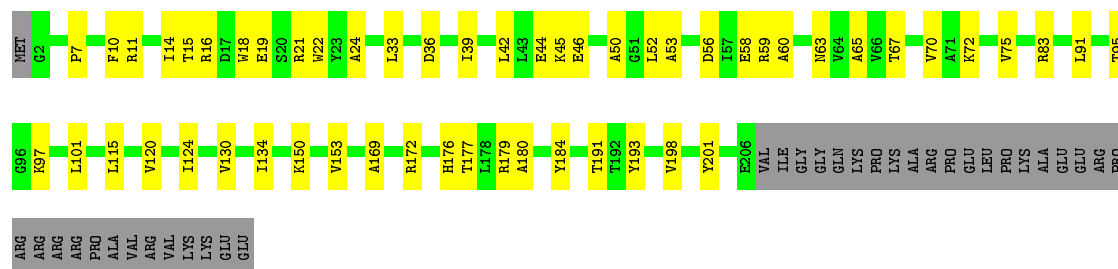


• Molecule 2: 30S ribosomal protein S2

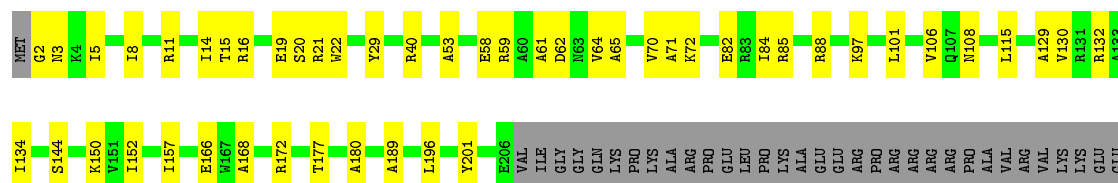




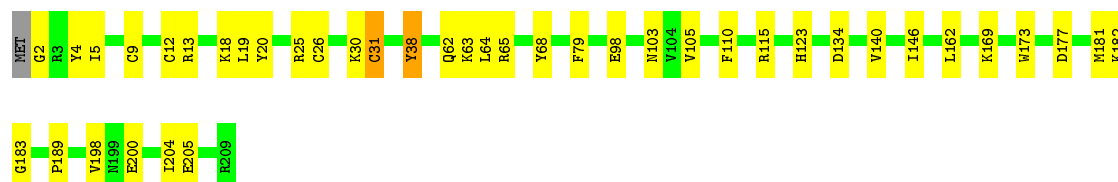
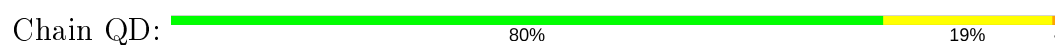
- Molecule 3: 30S ribosomal protein S3



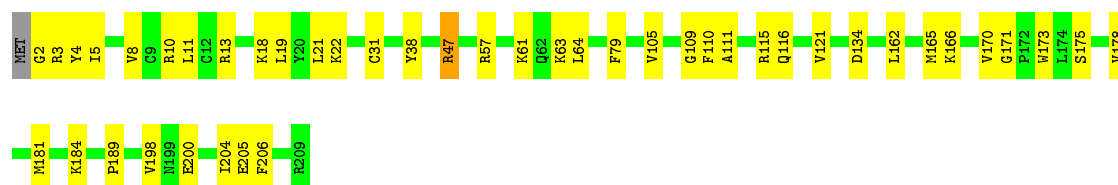
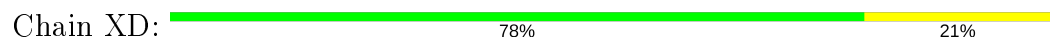
- Molecule 3: 30S ribosomal protein S3




- Molecule 4: 30S ribosomal protein S4

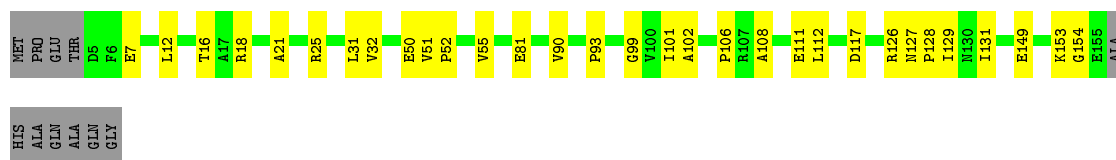


- Molecule 4: 30S ribosomal protein S4



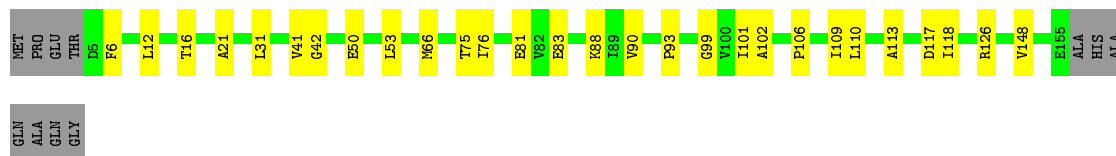
- Molecule 5: 30S ribosomal protein S5

Chain QE:  74% 19% 7%



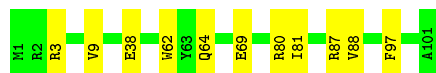
- Molecule 5: 30S ribosomal protein S5

Chain XE:  76% 17% 7%




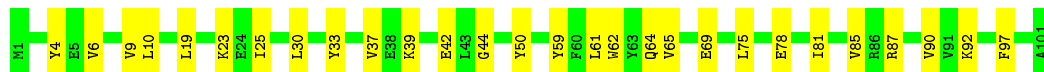
- Molecule 6: 30S ribosomal protein S6

Chain QF:  89% 11%



- Molecule 6: 30S ribosomal protein S6

Chain XF:  72% 28%



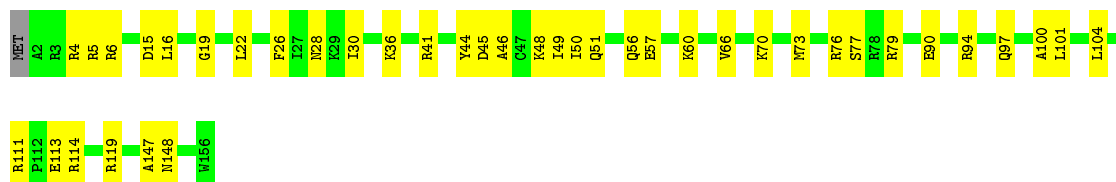
- Molecule 7: 30S ribosomal protein S7

Chain QG:  86% 13%



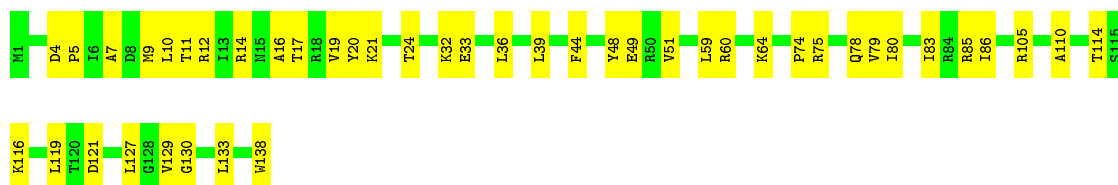
- Molecule 7: 30S ribosomal protein S7

Chain XG:  74% 26%



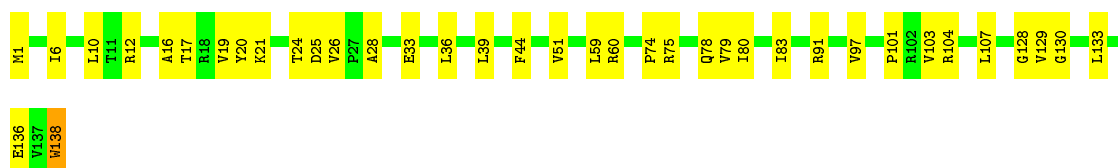
- Molecule 8: 30S ribosomal protein S8

Chain QH:  68% 32%



- Molecule 8: 30S ribosomal protein S8

Chain XH:  72% 27% .



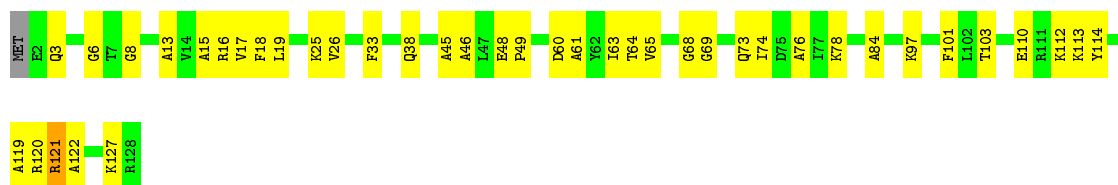
- Molecule 9: 30S ribosomal protein S9

Chain QI:  69% 30% ..



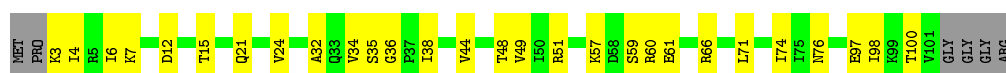
- Molecule 9: 30S ribosomal protein S9

Chain XI:  67% 31% ..



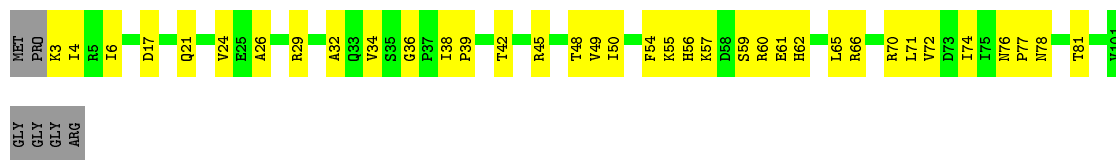
- Molecule 10: 30S ribosomal protein S10

Chain QJ:  68% 27% 6%



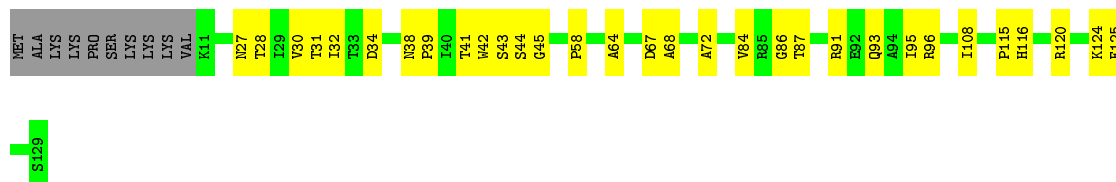
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 



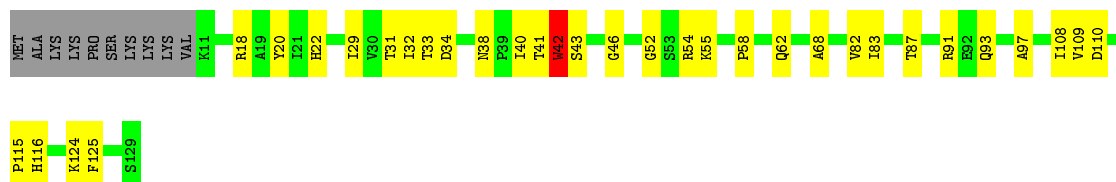
- Molecule 11: 30S ribosomal protein S11

Chain QK: 




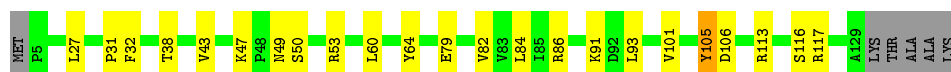
- Molecule 11: 30S ribosomal protein S11

Chain XK: 




- Molecule 12: 30S ribosomal protein S12

Chain QL: 



- Molecule 12: 30S ribosomal protein S12

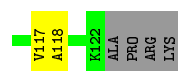
Chain XL: 



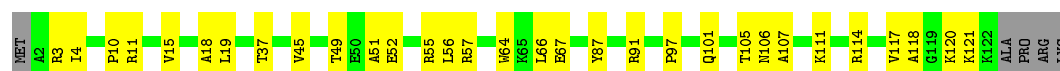
- Molecule 13: 30S ribosomal protein S13

Chain QM: 

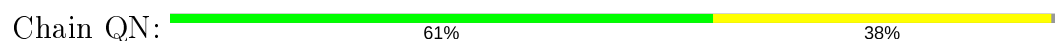




- Molecule 13: 30S ribosomal protein S13



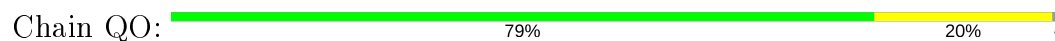
- Molecule 14: 30S ribosomal protein S14 type Z



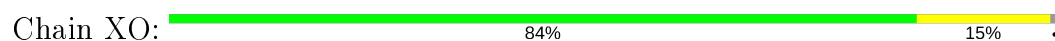
- Molecule 14: 30S ribosomal protein S14 type Z



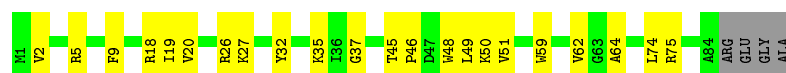
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

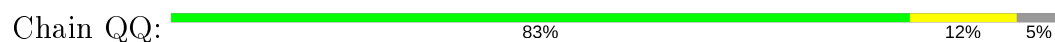


- Molecule 16: 30S ribosomal protein S16

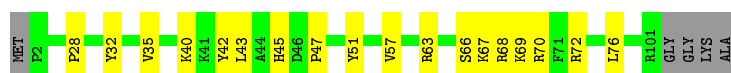
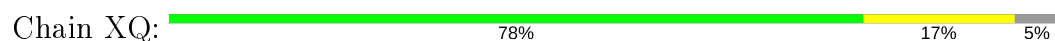




- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



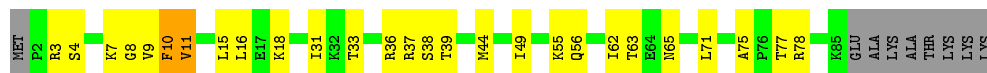
- Molecule 18: 30S ribosomal protein S18



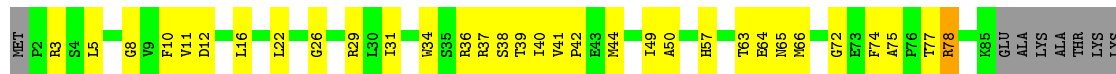
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

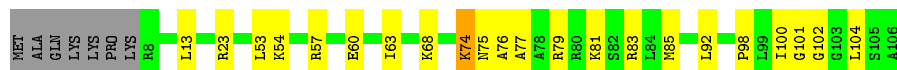


LYS

- Molecule 20: 30S ribosomal protein S20

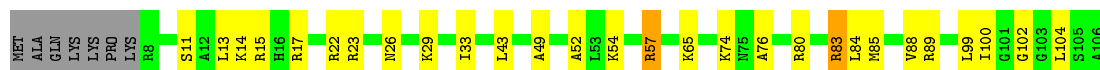


Chain QT:  73% 20% 7%



- Molecule 20: 30S ribosomal protein S20

Chain XT:  67% 25% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU:  67% 26% 7%



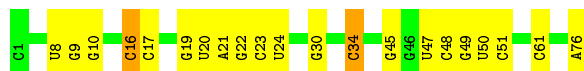
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  70% 22% 7%



- Molecule 22: P-site tRNAfMet

Chain QV:  73% 25% 2%



- Molecule 22: P-site tRNAfMet

Chain XV:  73% 27% 0%



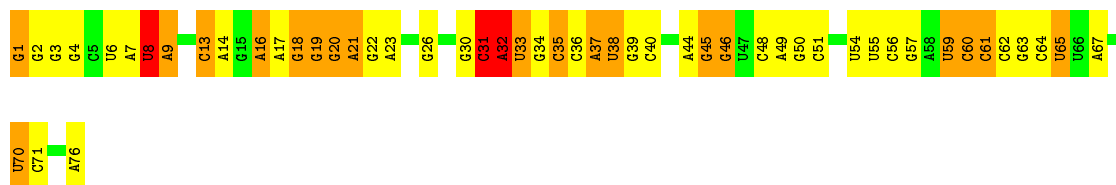
- Molecule 23: E-site tRNAAla(GGC)

Chain QW:  39% 47% 13%



- Molecule 23: E-site tRNAAla(GGC)

Chain XW: 



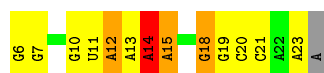
- Molecule 24: mRNA

Chain QX: 



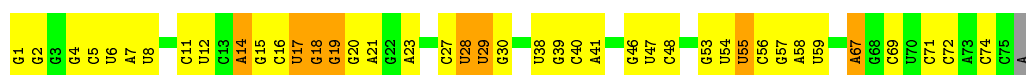
- Molecule 24: mRNA

Chain XX: 



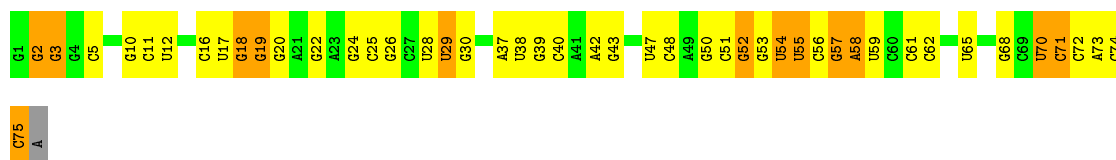
- Molecule 25: A-site tRNAAla(GGC)

Chain QY: 




- Molecule 25: A-site tRNAAla(GGC)

Chain XY: 



- Molecule 26: 50S ribosomal protein L27

Chain R0: 



- Molecule 26: 50S ribosomal protein L27

Chain Y0: 



- Molecule 27: 50S ribosomal protein L28

Chain R1:    .



- Molecule 27: 50S ribosomal protein L28

Chain Y1:    .



- Molecule 28: 50S ribosomal protein L29

Chain R2:    .



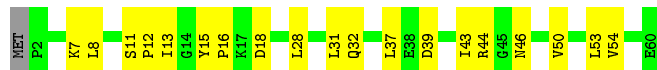
- Molecule 28: 50S ribosomal protein L29

Chain Y2:    .



- Molecule 29: 50S ribosomal protein L30

Chain R3:    .



- Molecule 29: 50S ribosomal protein L30

Chain Y3:    .



- Molecule 30: 50S ribosomal protein L31

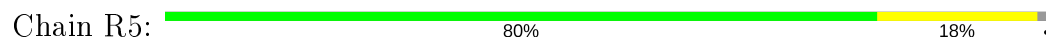
Chain R4:    .



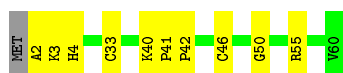
- Molecule 30: 50S ribosomal protein L31



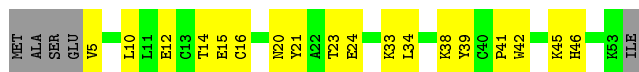
- Molecule 31: 50S ribosomal protein L32



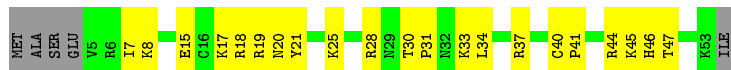
- Molecule 31: 50S ribosomal protein L32



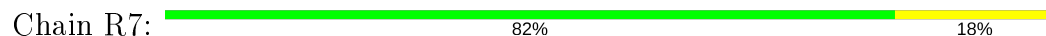
- Molecule 32: 50S ribosomal protein L33



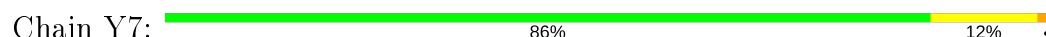
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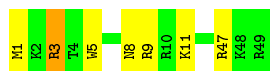


- Molecule 33: 50S ribosomal protein L34

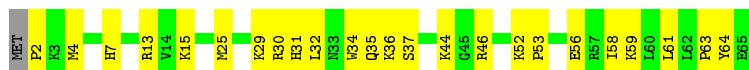


- Molecule 33: 50S ribosomal protein L34





- Molecule 34: 50S ribosomal protein L35



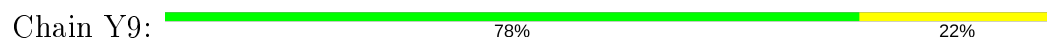
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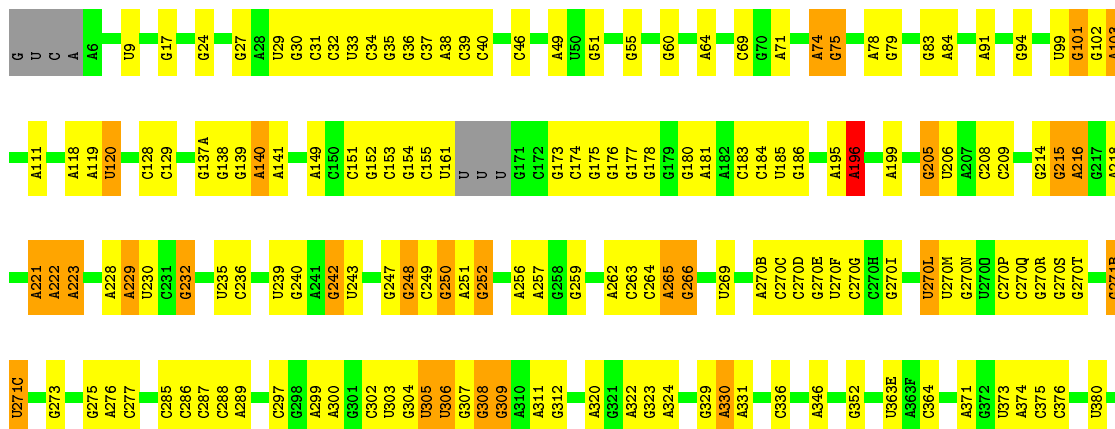
- Molecule 35: 50S ribosomal protein L36



- Molecule 35: 50S ribosomal protein L36



- Molecule 36: 23S rRNA





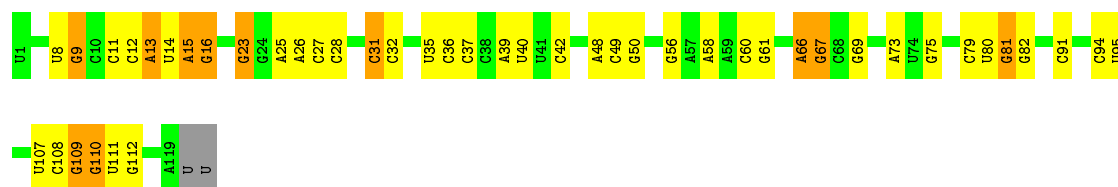


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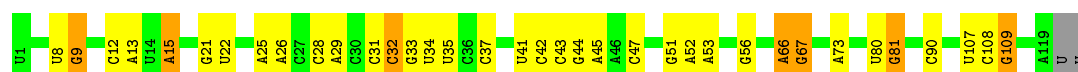
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C2982	C2871	C2670	C2671	A2565	G2448	A2376							

Chain RB: 



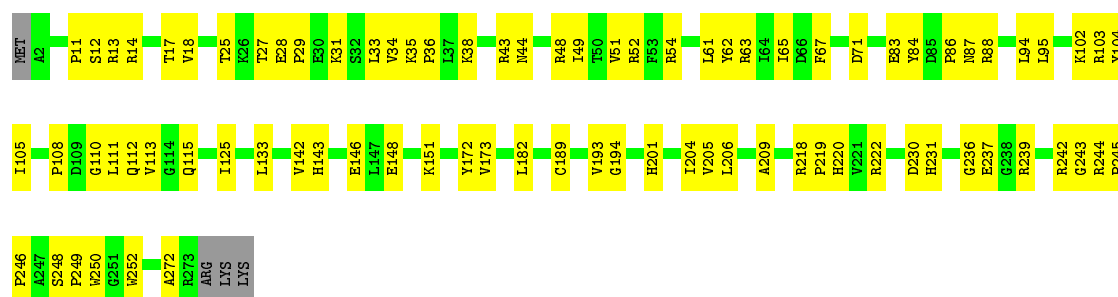
• Molecule 37: 5S rRNA

Chain YB: 




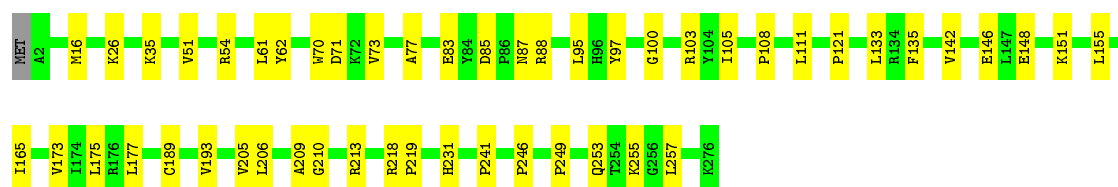
• Molecule 38: 50S ribosomal protein L2

Chain RD: 



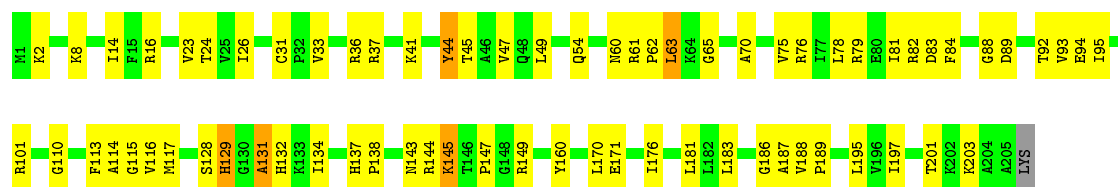
• Molecule 38: 50S ribosomal protein L2

Chain YD: 



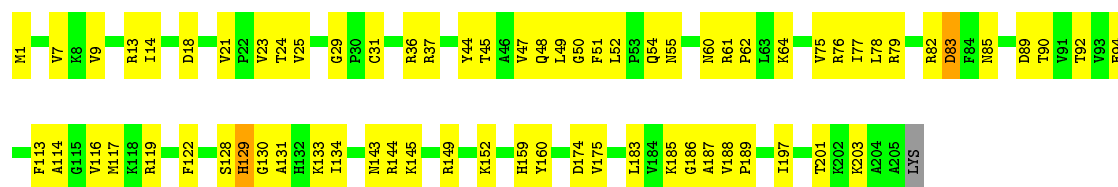
• Molecule 39: 50S ribosomal protein L3

Chain RE: 



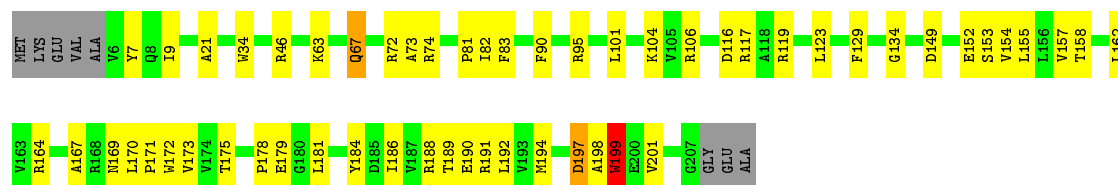
• Molecule 39: 50S ribosomal protein L3

Chain YE:  66% 33% .



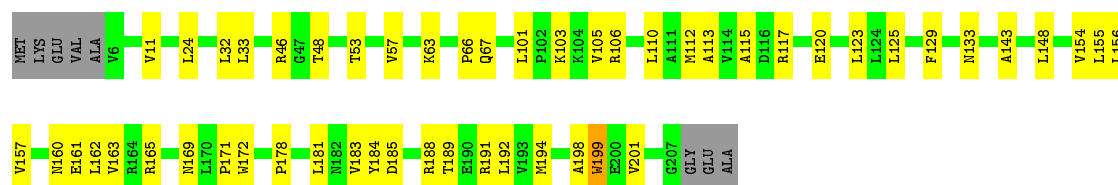
- Molecule 40: 50S ribosomal protein L4

Chain RF:  70% 25% . .



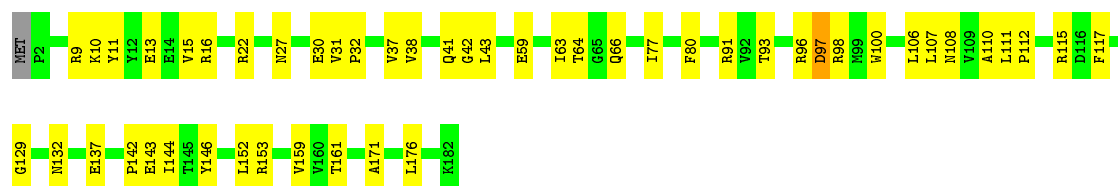
- Molecule 40: 50S ribosomal protein L4

Chain YF:  71% 24% .




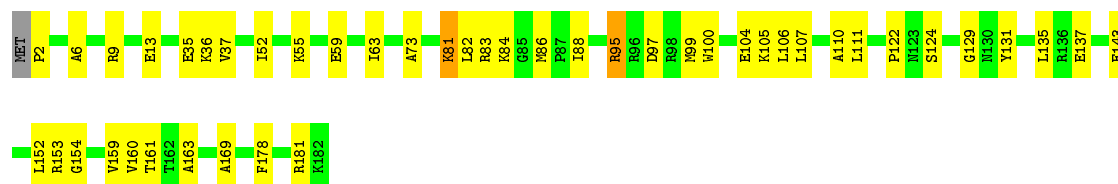
- Molecule 41: 50S ribosomal protein L5

Chain RG:  73% 26% . .



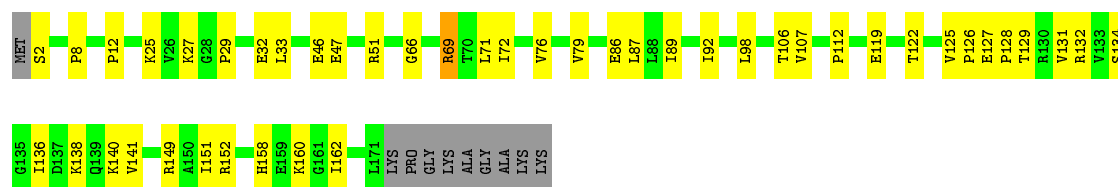
- Molecule 41: 50S ribosomal protein L5

Chain YG:  75% 24% . .



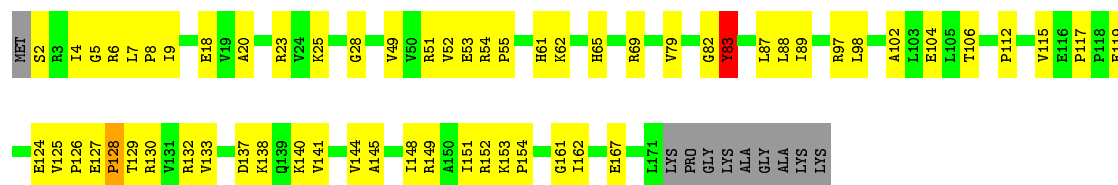
- Molecule 42: 50S ribosomal protein L6

Chain RH:  69% 24% 6%




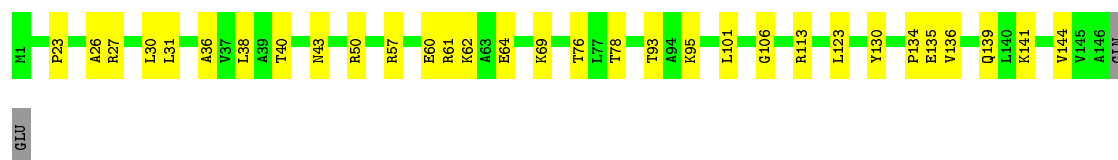
- Molecule 42: 50S ribosomal protein L6

Chain YH:  61% 33% 6%



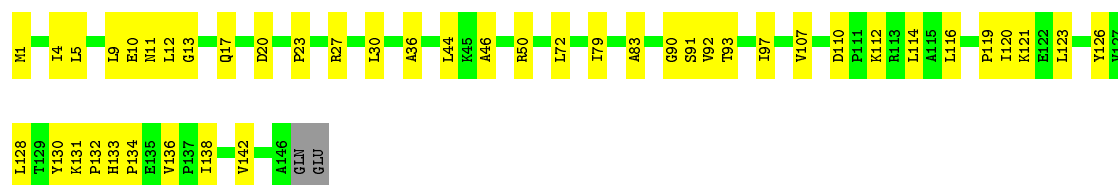
- Molecule 43: 50S ribosomal protein L9

Chain RI:  78% 21% 1%




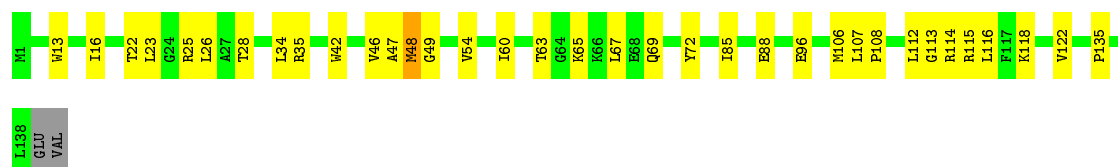
- Molecule 43: 50S ribosomal protein L9

Chain YI:  69% 30% 1%




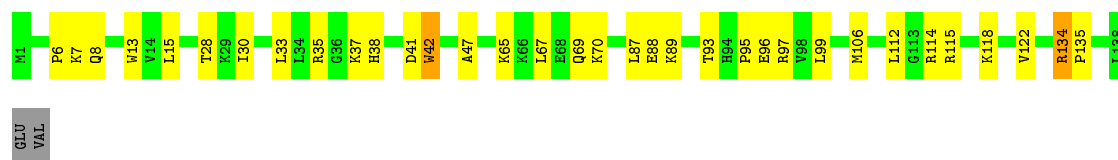
- Molecule 44: 50S ribosomal protein L13

Chain RN:  74% 24% 2%




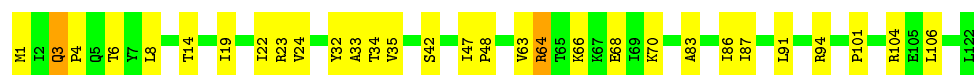
- Molecule 44: 50S ribosomal protein L13

Chain YN:  74% 23% ..




- Molecule 45: 50S ribosomal protein L14

Chain RO:  75% 23% .



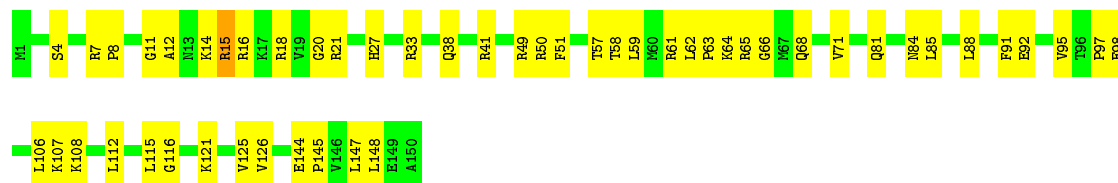
- Molecule 45: 50S ribosomal protein L14

Chain YO:  79% 21%



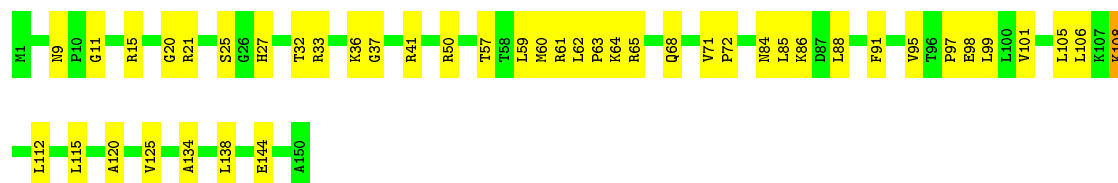
- Molecule 46: 50S ribosomal protein L15

Chain RP:  66% 33% .



- Molecule 46: 50S ribosomal protein L15

Chain YP:  71% 29% .



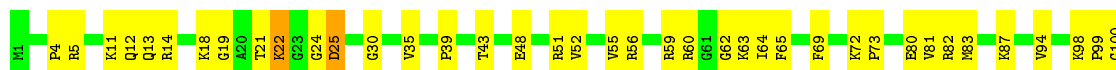
- Molecule 47: 50S ribosomal protein L16

Chain RQ:  64% 36%

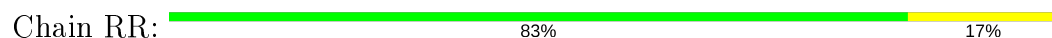




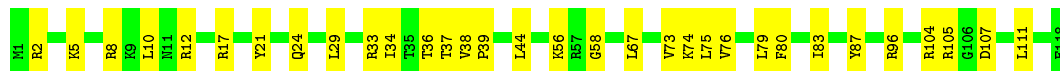
- Molecule 47: 50S ribosomal protein L16



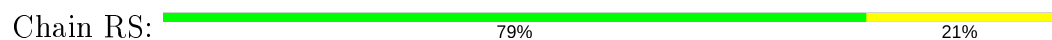
- Molecule 48: 50S ribosomal protein L17



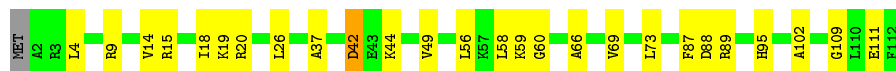
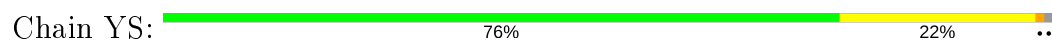
- Molecule 48: 50S ribosomal protein L17



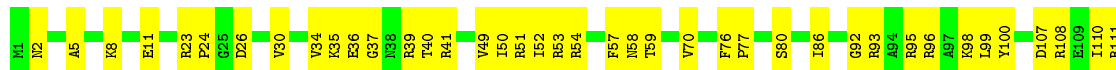
- Molecule 49: 50S ribosomal protein L18



- Molecule 49: 50S ribosomal protein L18



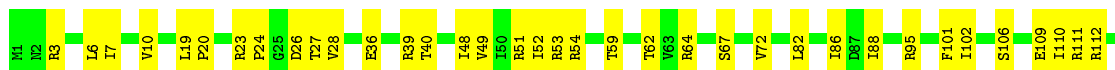
- Molecule 50: 50S ribosomal protein L19





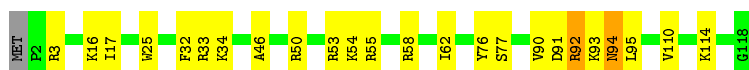
- Molecule 50: 50S ribosomal protein L19

Chain YT: 63% 31% 6%



- Molecule 51: 50S ribosomal protein L20

Chain RU: 79% 19% ..



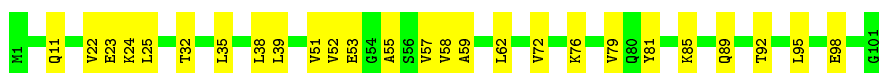
- Molecule 51: 50S ribosomal protein L20

Chain YU: 75% 24% .



- Molecule 52: 50S ribosomal protein L21

Chain RV: 74% 26%



- Molecule 52: 50S ribosomal protein L21

Chain YV: 74% 26%




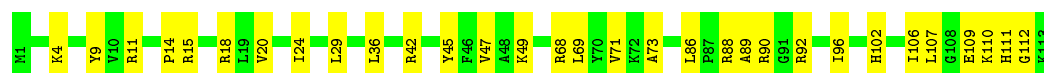
- Molecule 53: 50S ribosomal protein L22

Chain RW: 78% 22%




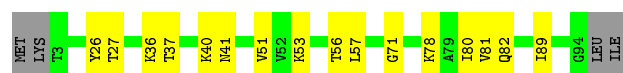
- Molecule 53: 50S ribosomal protein L22

Chain YW: 




- Molecule 54: 50S ribosomal protein L23

Chain RX: 



- Molecule 54: 50S ribosomal protein L23

Chain YX: 



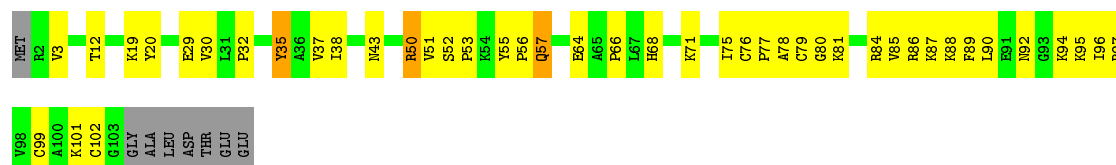
- Molecule 55: 50S ribosomal protein L24

Chain RY: 



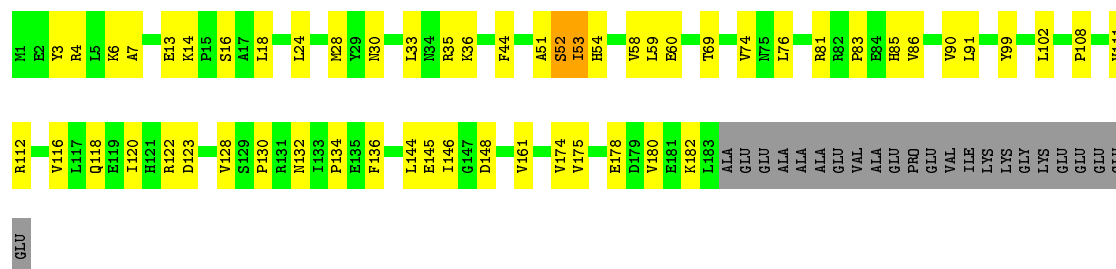
- Molecule 55: 50S ribosomal protein L24

Chain YY: 



- Molecule 56: 50S ribosomal protein L25

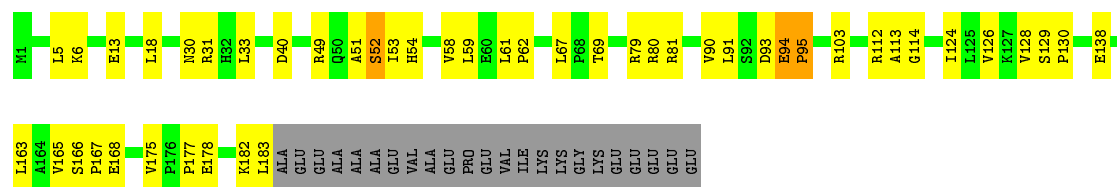
Chain RZ: 



- Molecule 56: 50S ribosomal protein L25



Chain YZ:



## 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, $\alpha$ , $\beta$ , $\gamma$	211.26Å 452.33Å 626.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20	Depositor
% Data completeness (in resolution range)	91.2 (44.53-3.20)	Depositor
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.195 , 0.232	Depositor
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.170	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.27	0/36098	0.78	21/56341 (0.0%)
1	XA	0.27	0/36101	0.77	11/56346 (0.0%)
2	QB	0.26	0/1959	0.48	0/2642
2	XB	0.27	0/1959	0.50	0/2642
3	QC	0.29	0/1629	0.49	0/2195
3	XC	0.30	0/1629	0.50	0/2195
4	QD	0.25	0/1704	0.46	0/2284
4	XD	0.33	1/1704 (0.1%)	0.49	0/2284
5	QE	0.25	0/1171	0.50	0/1576
5	XE	0.26	0/1171	0.50	0/1576
6	QF	0.24	0/856	0.46	0/1154
6	XF	0.26	0/856	0.50	0/1154
7	QG	0.27	0/1276	0.44	0/1709
7	XG	0.26	0/1276	0.48	0/1709
8	QH	0.26	0/1136	0.50	0/1527
8	XH	1.43	8/1136 (0.7%)	1.25	11/1527 (0.7%)
9	QI	0.27	0/1029	0.49	0/1379
9	XI	0.26	0/1029	0.48	0/1379
10	QJ	0.24	0/814	0.45	0/1095
10	XJ	0.24	0/814	0.47	0/1095
11	QK	0.30	0/900	0.50	0/1213
11	XK	2.12	11/900 (1.2%)	1.08	10/1213 (0.8%)
12	QL	0.25	0/991	0.53	0/1327
12	XL	0.26	0/991	0.55	0/1327
13	QM	0.24	0/974	0.55	0/1303
13	XM	0.24	0/974	0.56	0/1303
14	QN	0.28	0/501	0.49	0/664
14	XN	0.29	0/501	0.57	0/664
15	QO	0.23	0/745	0.43	0/992
15	XO	0.24	0/745	0.45	0/992
16	QP	0.28	0/721	0.51	0/970
16	XP	0.44	1/721 (0.1%)	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.24	0/847	0.44	0/1131
17	XQ	0.24	0/847	0.46	0/1131
18	QR	0.24	0/579	0.47	0/768
18	XR	0.25	0/579	0.49	0/768
19	QS	0.30	0/689	0.53	0/926
19	XS	0.29	0/689	0.53	0/926
20	QT	0.23	0/765	0.44	0/1007
20	XT	0.29	0/765	0.53	0/1007
21	QU	0.24	0/221	0.51	0/288
21	XU	0.22	0/221	0.47	0/288
22	QV	0.25	0/1832	0.78	1/2855 (0.0%)
22	XV	0.26	0/1832	0.77	0/2855
23	QW	0.32	1/1819 (0.1%)	0.82	0/2833
23	XW	0.42	3/1819 (0.2%)	0.89	2/2833 (0.1%)
24	QX	0.22	0/468	0.72	0/729
24	XX	0.27	0/443	0.88	2/690 (0.3%)
25	QY	0.17	0/1791	0.74	0/2791
25	XY	0.20	0/1791	0.73	0/2791
26	R0	0.25	0/657	0.54	0/874
26	Y0	0.26	0/657	0.50	0/874
27	R1	0.27	0/770	0.48	0/1022
27	Y1	0.27	0/770	0.50	0/1022
28	R2	0.24	0/583	0.46	0/771
28	Y2	0.26	0/583	0.54	0/771
29	R3	0.23	0/474	0.44	0/635
29	Y3	0.25	0/474	0.47	0/635
30	R4	0.28	0/594	0.62	1/795 (0.1%)
30	Y4	0.25	0/594	0.54	0/795
31	R5	0.26	0/473	0.49	0/639
31	Y5	0.28	0/473	0.54	0/639
32	R6	0.27	0/431	0.57	0/575
32	Y6	0.26	0/431	0.62	0/575
33	R7	0.27	0/438	0.53	0/575
33	Y7	0.32	0/438	0.61	0/575
34	R8	0.38	0/525	0.63	0/691
34	Y8	0.28	0/525	0.51	0/691
35	R9	0.21	0/310	0.40	0/407
35	Y9	0.21	0/310	0.44	0/407
36	RA	0.31	1/69521 (0.0%)	0.79	37/108529 (0.0%)
36	YA	0.35	1/69543 (0.0%)	0.81	34/108563 (0.0%)
37	RB	0.28	0/2878	0.76	2/4490 (0.0%)
37	YB	0.30	0/2878	0.83	5/4490 (0.1%)
38	RD	0.35	1/2165 (0.0%)	0.56	1/2919 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YD	0.31	0/2195	0.52	0/2955
39	RE	0.26	0/1601	0.58	0/2160
39	YE	0.27	0/1601	0.60	0/2160
40	RF	1.28	9/1620 (0.6%)	0.74	7/2194 (0.3%)
40	YF	2.62	13/1620 (0.8%)	1.04	13/2194 (0.6%)
41	RG	0.24	0/1499	0.49	0/2016
41	YG	0.25	0/1499	0.55	0/2016
42	RH	0.24	0/1332	0.49	0/1802
42	YH	0.27	0/1332	0.60	2/1802 (0.1%)
43	RI	0.24	0/1151	0.49	0/1558
43	YI	0.25	0/1151	0.58	0/1558
44	RN	0.29	0/1131	0.52	0/1525
44	YN	2.01	10/1131 (0.9%)	1.39	15/1525 (1.0%)
45	RO	0.28	0/943	0.52	0/1269
45	YO	0.27	0/943	0.51	0/1269
46	RP	0.27	0/1162	0.59	0/1544
46	YP	0.28	0/1162	0.62	0/1544
47	RQ	0.26	0/1143	0.54	0/1527
47	YQ	0.28	0/1143	0.57	0/1527
48	RR	0.25	0/982	0.51	0/1312
48	YR	0.26	0/982	0.54	0/1312
49	RS	0.25	0/892	0.53	0/1187
49	YS	0.26	0/892	0.55	0/1187
50	RT	0.25	0/1155	0.53	0/1542
50	YT	0.26	0/1155	0.58	0/1542
51	RU	0.27	0/982	0.47	0/1306
51	YU	0.26	0/982	0.49	0/1306
52	RV	0.26	0/790	0.53	0/1057
52	YV	0.28	0/790	0.55	0/1057
53	RW	0.25	0/911	0.50	0/1220
53	YW	0.26	0/911	0.53	0/1220
54	RX	0.30	0/739	0.49	0/993
54	YX	0.28	0/739	0.49	0/993
55	RY	0.26	0/798	0.54	0/1064
55	YY	0.27	0/798	0.58	0/1064
56	RZ	0.24	0/1493	0.51	0/2026
56	YZ	0.25	0/1493	0.56	0/2026
All	All	0.40	60/323346 (0.0%)	0.74	175/483882 (0.0%)

The worst 5 of 60 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	YF	199	TRP	CD2-CE3	58.05	2.27	1.40
40	YF	199	TRP	CE2-CZ2	48.67	2.22	1.39
40	YF	199	TRP	CD2-CE2	36.57	1.85	1.41
11	XK	42	TRP	CE3-CZ3	36.22	2.00	1.38
40	YF	199	TRP	CG-CD1	35.50	1.86	1.36

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	YF	199	TRP	CD1-CG-CD2	-22.65	88.18	106.30
44	YN	42	TRP	CE2-CD2-CG	-21.78	89.88	107.30
44	YN	42	TRP	NE1-CE2-CD2	20.45	127.75	107.30
8	XH	138	TRP	CG-CD2-CE3	-18.67	117.10	133.90
8	XH	138	TRP	CB-CG-CD2	18.35	150.46	126.60

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	16278	512	0
1	XA	32249	0	16278	480	0
2	QB	1924	0	1975	31	0
2	XB	1924	0	1975	54	0
3	QC	1605	0	1668	44	0
3	XC	1605	0	1668	39	0
4	QD	1674	0	1716	33	0
4	XD	1674	0	1718	38	0
5	QE	1155	0	1213	23	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	24	0
7	QG	1257	0	1296	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	32	0
8	QH	1116	0	1177	34	0
8	XH	1116	0	1177	30	0
9	QI	1010	0	1037	28	0
9	XI	1010	0	1037	29	0
10	QJ	801	0	849	24	0
10	XJ	801	0	849	33	0
11	QK	885	0	904	37	0
11	XK	885	0	904	39	0
12	QL	975	0	1062	21	0
12	XL	975	0	1062	23	0
13	QM	964	0	1034	27	0
13	XM	964	0	1034	23	0
14	QN	492	0	532	23	0
14	XN	492	0	529	20	0
15	QO	734	0	771	14	0
15	XO	734	0	771	10	0
16	QP	705	0	725	16	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	10	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	12	0
18	XR	574	0	644	12	0
19	QS	674	0	699	30	0
19	XS	674	0	699	26	0
20	QT	763	0	861	16	0
20	XT	763	0	861	23	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1640	0	837	9	0
22	XV	1640	0	837	8	0
23	QW	1627	0	823	21	0
23	XW	1627	0	823	39	0
24	QX	416	0	208	4	0
24	XX	394	0	197	9	0
25	QY	1603	0	811	23	0
25	XY	1603	0	811	24	0
26	R0	648	0	672	10	0
26	Y0	648	0	672	19	0
27	R1	763	0	848	15	0
27	Y1	763	0	848	18	0
28	R2	581	0	629	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Y2	581	0	629	7	0
29	R3	469	0	518	11	0
29	Y3	469	0	518	11	0
30	R4	581	0	577	24	0
30	Y4	581	0	577	19	0
31	R5	459	0	480	22	0
31	Y5	459	0	480	8	0
32	R6	424	0	450	20	0
32	Y6	424	0	450	17	0
33	R7	430	0	480	10	0
33	Y7	430	0	480	19	0
34	R8	517	0	582	36	0
34	Y8	517	0	582	27	0
35	R9	307	0	338	7	0
35	Y9	307	0	338	7	0
36	RA	62071	0	31289	870	0
36	YA	62091	0	31301	797	0
37	RB	2573	0	1306	33	0
37	YB	2573	0	1306	22	0
38	RD	2115	0	2195	69	0
38	YD	2145	0	2234	35	0
39	RE	1568	0	1633	54	0
39	YE	1568	0	1634	55	0
40	RF	1585	0	1632	42	0
40	YF	1585	0	1632	43	0
41	RG	1474	0	1535	36	0
41	YG	1474	0	1535	32	0
42	RH	1307	0	1382	30	0
42	YH	1307	0	1381	44	0
43	RI	1136	0	1223	18	0
43	YI	1136	0	1223	31	0
44	RN	1104	0	1180	25	0
44	YN	1104	0	1180	29	0
45	RO	933	0	996	24	0
45	YO	933	0	996	20	0
46	RP	1145	0	1227	52	0
46	YP	1145	0	1227	53	0
47	RQ	1122	0	1179	45	0
47	YQ	1122	0	1179	41	0
48	RR	968	0	1033	19	0
48	YR	968	0	1033	23	0
49	RS	882	0	943	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	YS	882	0	943	22	0
50	RT	1141	0	1202	32	0
50	YT	1141	0	1202	35	0
51	RU	964	0	1022	26	0
51	YU	964	0	1022	33	0
52	RV	779	0	852	18	0
52	YV	779	0	852	22	0
53	RW	900	0	964	18	0
53	YW	900	0	964	21	0
54	RX	725	0	778	11	0
54	YX	725	0	778	10	0
55	RY	785	0	878	28	0
55	YY	785	0	878	32	0
56	RZ	1461	0	1493	44	0
56	YZ	1461	0	1493	42	0
57	QA	124	0	0	0	0
57	QD	1	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QK	2	0	0	0	0
57	QL	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	6	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	R9	1	0	0	0	0
57	RA	378	0	0	0	0
57	RB	4	0	0	0	0
57	RD	2	0	0	0	0
57	RE	8	0	0	0	0
57	RF	2	0	0	0	0
57	RG	1	0	0	0	0
57	RI	1	0	0	0	0
57	RP	3	0	0	0	0
57	RR	2	0	0	0	0
57	RT	2	0	0	0	0
57	XA	123	0	0	0	0
57	XB	2	0	0	0	0
57	XD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	2	0	0	0	0
57	XM	1	0	0	0	0
57	XV	7	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	3	0	0	0	0
57	Y2	3	0	0	0	0
57	Y3	1	0	0	0	0
57	Y4	2	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	457	0	0	0	0
57	YB	8	0	0	0	0
57	YD	4	0	0	0	0
57	YE	6	0	0	0	0
57	YF	5	0	0	0	0
57	YG	2	0	0	0	0
57	YH	5	0	0	0	0
57	YI	1	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	7	0	0	0	0
57	YQ	4	0	0	0	0
57	YR	2	0	0	0	0
57	YT	2	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	YX	2	0	0	0	0
57	YY	5	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	2	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	QN	1	0	0	0	0
60	XN	1	0	0	0	0
61	QY	22	0	12	1	0
62	QA	1	0	0	0	0
62	QX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	298675	0	201403	4630	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 9.

The worst 5 of 4630 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)
40:YF:199:TRP:CH2	40:YF:199:TRP:CZ3	1.78	1.69
8:XH:138:TRP:CZ3	8:XH:138:TRP:CE3	1.75	1.64
40:YF:199:TRP:CG	40:YF:199:TRP:CD1	1.86	1.62
44:YN:42:TRP:CE2	44:YN:42:TRP:CZ2	1.86	1.62
40:YF:199:TRP:CE2	40:YF:199:TRP:CD2	1.85	1.61

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	212 (90%)	21 (9%)	2 (1%)	17	56
2	XB	235/256 (92%)	208 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
3	XC	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	QD	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
4	XD	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	XE	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	146 (95%)	7 (5%)	0	100	100
8	QH	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
8	XH	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	19	58
9	XI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
10	QJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
10	XJ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
11	XK	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
12	QL	123/131 (94%)	110 (89%)	13 (11%)	0	100	100
12	XL	123/131 (94%)	114 (93%)	9 (7%)	0	100	100
13	QM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
13	XM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	QP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	82/93 (88%)	73 (89%)	7 (8%)	2 (2%)	6	34
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
20	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	10 (10%)	1 (1%)	14	51
27	Y1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	14	51
28	R2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
28	Y2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
29	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
30	R4	69/71 (97%)	41 (59%)	25 (36%)	3 (4%)	2	20
30	Y4	69/71 (97%)	45 (65%)	21 (30%)	3 (4%)	2	20
31	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	Y5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
32	R6	47/54 (87%)	30 (64%)	17 (36%)	0	100	100
32	Y6	47/54 (87%)	35 (74%)	12 (26%)	0	100	100
33	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
34	R8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	9	43
34	Y8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
35	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
38	RD	270/276 (98%)	245 (91%)	24 (9%)	1 (0%)	34	69
38	YD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
39	RE	203/206 (98%)	170 (84%)	28 (14%)	5 (2%)	5	32
39	YE	203/206 (98%)	166 (82%)	35 (17%)	2 (1%)	15	54
40	RF	200/210 (95%)	185 (92%)	12 (6%)	3 (2%)	10	44
40	YF	200/210 (95%)	187 (94%)	13 (6%)	0	100	100
41	RG	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	64
41	YG	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	25	64
42	RH	168/180 (93%)	157 (94%)	11 (6%)	0	100	100
42	YH	168/180 (93%)	143 (85%)	22 (13%)	3 (2%)	8	41
43	RI	144/148 (97%)	132 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YI	144/148 (97%)	121 (84%)	23 (16%)	0	100	100
44	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	61
44	YN	136/140 (97%)	125 (92%)	11 (8%)	0	100	100
45	RO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	58
45	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
46	RP	148/150 (99%)	131 (88%)	16 (11%)	1 (1%)	22	61
46	YP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	22	61
47	RQ	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
47	YQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6	35
48	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	YR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
49	RS	109/112 (97%)	96 (88%)	13 (12%)	0	100	100
49	YS	109/112 (97%)	92 (84%)	17 (16%)	0	100	100
50	RT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	YT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
51	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	56
51	YU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	56
52	RV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
52	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
53	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
53	YW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
54	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
54	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
55	RY	100/110 (91%)	75 (75%)	24 (24%)	1 (1%)	15	54
55	YY	100/110 (91%)	76 (76%)	22 (22%)	2 (2%)	7	38
56	RZ	181/206 (88%)	155 (86%)	24 (13%)	2 (1%)	14	51
56	YZ	181/206 (88%)	147 (81%)	29 (16%)	5 (3%)	5	29
All	All	11473/12126 (95%)	10363 (90%)	1058 (9%)	52 (0%)	29	67

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	RN	22	THR

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Mol	Chain	Res	Type
51	RU	92	ARG
30	Y4	24	THR
42	YH	128	PRO
47	YQ	105	GLU

### 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%)	204 (100%)	1 (0%)	88	95
2	XB	205/220 (93%)	203 (99%)	2 (1%)	76	90
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	171 (99%)	2 (1%)	71	88
4	XD	173/181 (96%)	172 (99%)	1 (1%)	86	94
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	81	93
8	QH	119/119 (100%)	118 (99%)	1 (1%)	81	93
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	72
9	XI	98/99 (99%)	97 (99%)	1 (1%)	76	90
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	90/99 (91%)	89 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76	90
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	96 (99%)	1 (1%)	76	90
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	86
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	86
17	QQ	95/97 (98%)	95 (100%)	0	100	100
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%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	70 (96%)	3 (4%)	30	66
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	87
20	XT	76/82 (93%)	74 (97%)	2 (3%)	46	76
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%)	63 (97%)	2 (3%)	40	72
26	Y0	65/67 (97%)	64 (98%)	1 (2%)	65	85
27	R1	82/83 (99%)	82 (100%)	0	100	100
27	Y1	82/83 (99%)	82 (100%)	0	100	100
28	R2	64/67 (96%)	63 (98%)	1 (2%)	62	84
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%)	63 (100%)	0	100	100
31	R5	51/52 (98%)	50 (98%)	1 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Y5	51/52 (98%)	51 (100%)	0	100	100
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%)	41 (98%)	1 (2%)	49	77
34	R8	54/55 (98%)	52 (96%)	2 (4%)	34	68
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	34 (100%)	0	100	100
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	214 (100%)	0	100	100
38	YD	217/218 (100%)	217 (100%)	0	100	100
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%)	155 (100%)	0	100	100
41	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
42	RH	142/148 (96%)	141 (99%)	1 (1%)	84	94
42	YH	142/148 (96%)	142 (100%)	0	100	100
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%)	116 (99%)	1 (1%)	78	91
45	RO	100/100 (100%)	99 (99%)	1 (1%)	76	90
45	YO	100/100 (100%)	100 (100%)	0	100	100
46	RP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	YP	116/116 (100%)	116 (100%)	0	100	100
47	RQ	111/111 (100%)	111 (100%)	0	100	100
47	YQ	111/111 (100%)	111 (100%)	0	100	100
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	RS	87/88 (99%)	87 (100%)	0	100	100
49	YS	87/88 (99%)	86 (99%)	1 (1%)	73	88
50	RT	120/127 (94%)	118 (98%)	2 (2%)	60	83
50	YT	120/127 (94%)	120 (100%)	0	100	100
51	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
51	YU	93/94 (99%)	93 (100%)	0	100	100
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	82 (100%)	0	100	100
53	RW	92/92 (100%)	92 (100%)	0	100	100
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	74 (100%)	0	100	100
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%)	83 (98%)	2 (2%)	49	77
56	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
56	YZ	162/179 (90%)	162 (100%)	0	100	100
All	All	9691/10064 (96%)	9636 (99%)	55 (1%)	86	94

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	RI	113	ARG
51	RU	94	ASN
41	YG	95	ARG
44	RN	48	MET
46	RP	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
46	RP	81	GLN
47	RQ	123	HIS
7	XG	51	GLN
44	RN	130	HIS
53	RW	62	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	262 (17%)	31 (2%)
1	XA	1498/1522 (98%)	257 (17%)	30 (2%)
22	QV	76/77 (98%)	11 (14%)	0
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	25 (33%)	2 (2%)
23	XW	75/76 (98%)	33 (44%)	7 (9%)
24	QX	18/19 (94%)	9 (50%)	1 (5%)
24	XX	17/19 (89%)	7 (41%)	1 (5%)
25	QY	74/76 (97%)	22 (29%)	0
25	XY	74/76 (97%)	31 (41%)	1 (1%)
36	RA	2879/2915 (98%)	542 (18%)	44 (1%)
36	YA	2880/2915 (98%)	541 (18%)	45 (1%)
37	RB	119/122 (97%)	18 (15%)	2 (1%)
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1789 (18%)	165 (1%)

5 of 1789 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 165 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	RA	2566	A
1	XA	485	G
36	YA	2126	A
36	RA	2712	U
1	XA	243	A

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

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 1222 ligands modelled in this entry, 1217 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	QA	1711	-	45,45,45	0.54	0	64,67,67	0.95	2 (3%)
59	SF4	XD	501	4	0,12,12	0.00	-	-		
59	SF4	QD	501	4	0,12,12	0.00	-	-		
58	PAR	XA	1717	-	45,45,45	0.53	0	64,67,67	0.86	1 (1%)

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	QD	501	4	-	-	0/6/5/5
59	SF4	XD	501	4	-	-	0/6/5/5
58	PAR	QA	1711	-	-	3/18/94/94	0/4/4/4
58	PAR	XA	1717	-	-	2/18/94/94	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1711	PAR	C13-O52-C52	-2.82	110.99	117.96
58	XA	1717	PAR	C13-O52-C52	-2.71	111.26	117.96
58	QA	1711	PAR	O52-C13-C23	2.56	113.28	107.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

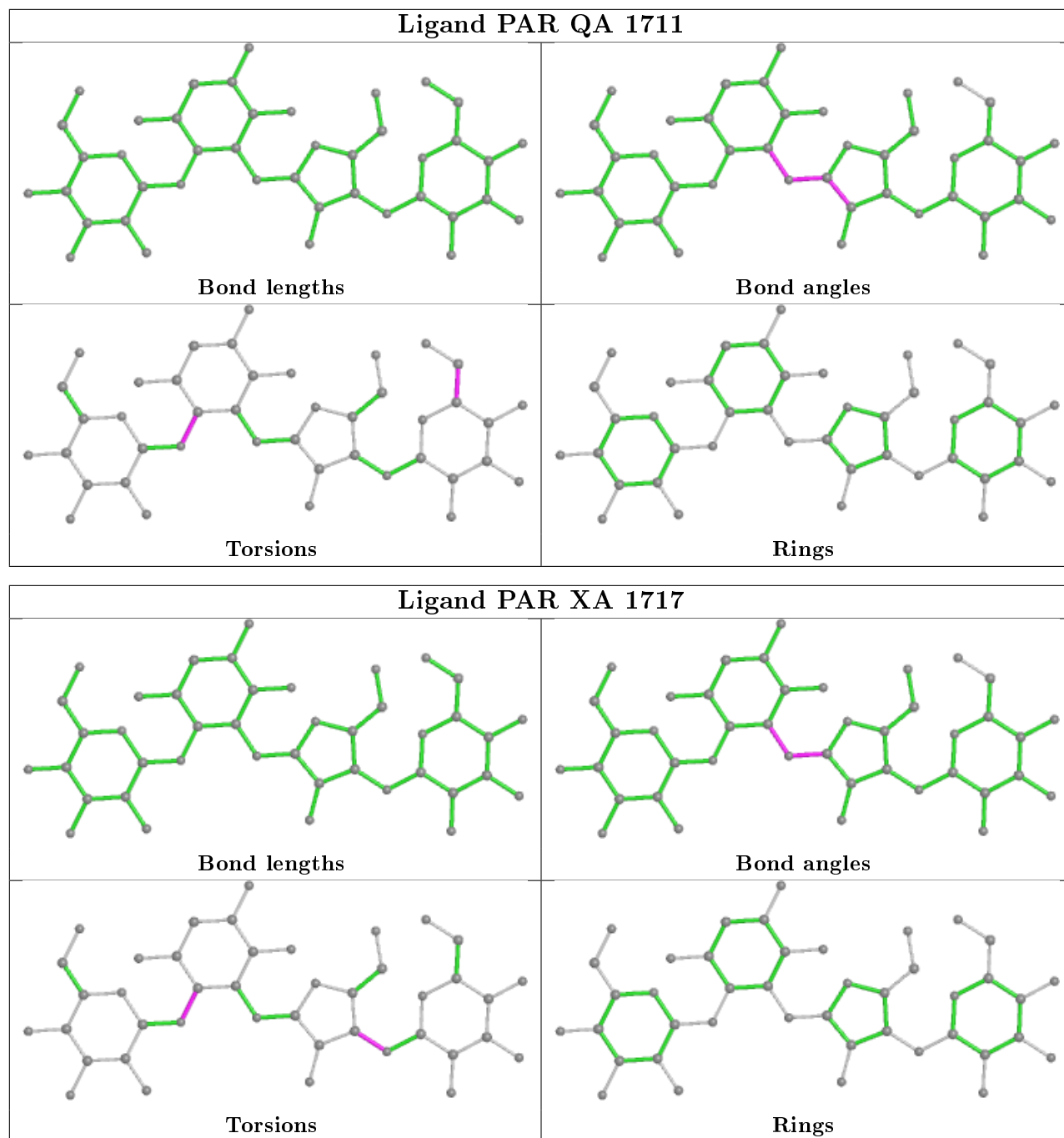
Mol	Chain	Res	Type	Atoms
58	QA	1711	PAR	O54-C54-C64-N64
58	XA	1717	PAR	C23-C33-O33-C14
58	QA	1711	PAR	C52-C42-O11-C11
58	XA	1717	PAR	C52-C42-O11-C11
58	QA	1711	PAR	C44-C54-C64-N64

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1711	PAR	1	0
58	XA	1717	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.