



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2020 – 03:05 AM EDT

PDB ID : 6NWY
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (near-cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-07
Resolution : 3.50 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**
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) : 2.14.6

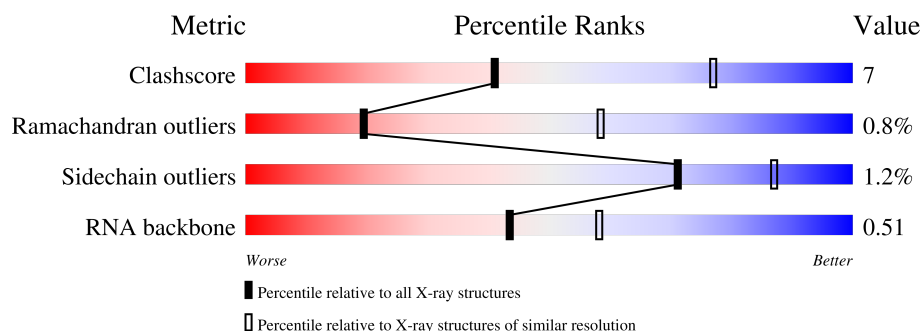
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)


























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	1521	52% 38% 9% ..
1	XA	1521	52% 38% 9% .
2	QB	256	66% 26% 8%
2	XB	256	68% 24% 8%
3	QC	239	65% 20% 14%
3	XC	239	71% 15% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	
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	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	


























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Mol	Chain	Length	Quality of chain
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	
28	R4	71	
28	Y4	71	

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Mol	Chain	Length	Quality of chain
29	R5	60	 68% 25% 5% .
29	Y5	60	 67% 27% . . .
30	R6	54	 72% 22% . . .
30	Y6	54	 65% 26% 6% . .
31	R7	49	 67% 29% .
31	Y7	49	 86% 12% .
32	R8	65	 69% 23% 6% .
32	Y8	65	 72% 26% .
33	R9	37	 70% 24% 5%
33	Y9	37	 68% 27% 5%
34	RA	2915	 53% 36% 9% . .
34	YA	2915	 53% 35% 10% . .
35	RB	122	 57% 37% . . .
35	YB	122	 53% 36% 7% . .
36	RD	276	 76% 21% . .
36	YD	276	 80% 18% . .
37	RE	206	 72% 25% .
37	YE	206	 75% 24%
38	RF	210	 75% 20% . .
38	YF	210	 73% 23% .
39	RG	182	 76% 23% . .
39	YG	182	 78% 21% .
40	RH	180	 64% 27% 6% .
40	YH	180	 77% 18% . . .
41	RI	148	 72% 23% . .

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Mol	Chain	Length	Quality of chain
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	
53	RY	110	
53	YY	110	

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Mol	Chain	Length	Quality of chain
54	RZ	206	
54	YZ	206	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	QD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 292039 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	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
1	XA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

- 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	96	Total	C	N	O	S	0	0	0
			777	487	153	136	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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	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 E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			
23	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
31	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

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

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
44	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
46	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
53	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	193	Total	C	N	O	S	0	0	0
			1529	973	270	283	3			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	87	Total	Mg	0	0
			87	87		
55	RP	1	Total	Mg	0	0
			1	1		
55	YA	439	Total	Mg	0	0
			439	439		
55	Y5	1	Total	Mg	0	0
			1	1		
55	YR	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	1	Total	Mg	0	0
			1	1		
55	Y1	1	Total	Mg	0	0
			1	1		
55	YD	1	Total	Mg	0	0
			1	1		
55	Y8	1	Total	Mg	0	0
			1	1		
55	XA	89	Total	Mg	0	0
			89	89		
55	RQ	1	Total	Mg	0	0
			1	1		
55	R0	2	Total	Mg	0	0
			2	2		
55	QL	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YU	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	2	Total 2	Mg 2	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0
55	YX	1	Total 1	Mg 1	0	0
55	RD	1	Total 1	Mg 1	0	0
55	R1	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	RA	429	Total 429	Mg 429	0	0
55	YF	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0
55	YB	8	Total 8	Mg 8	0	0
55	RB	11	Total 11	Mg 11	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	RF	2	Total 2	Mg 2	0	0
55	R3	1	Total 1	Mg 1	0	0
55	YE	2	Total 2	Mg 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

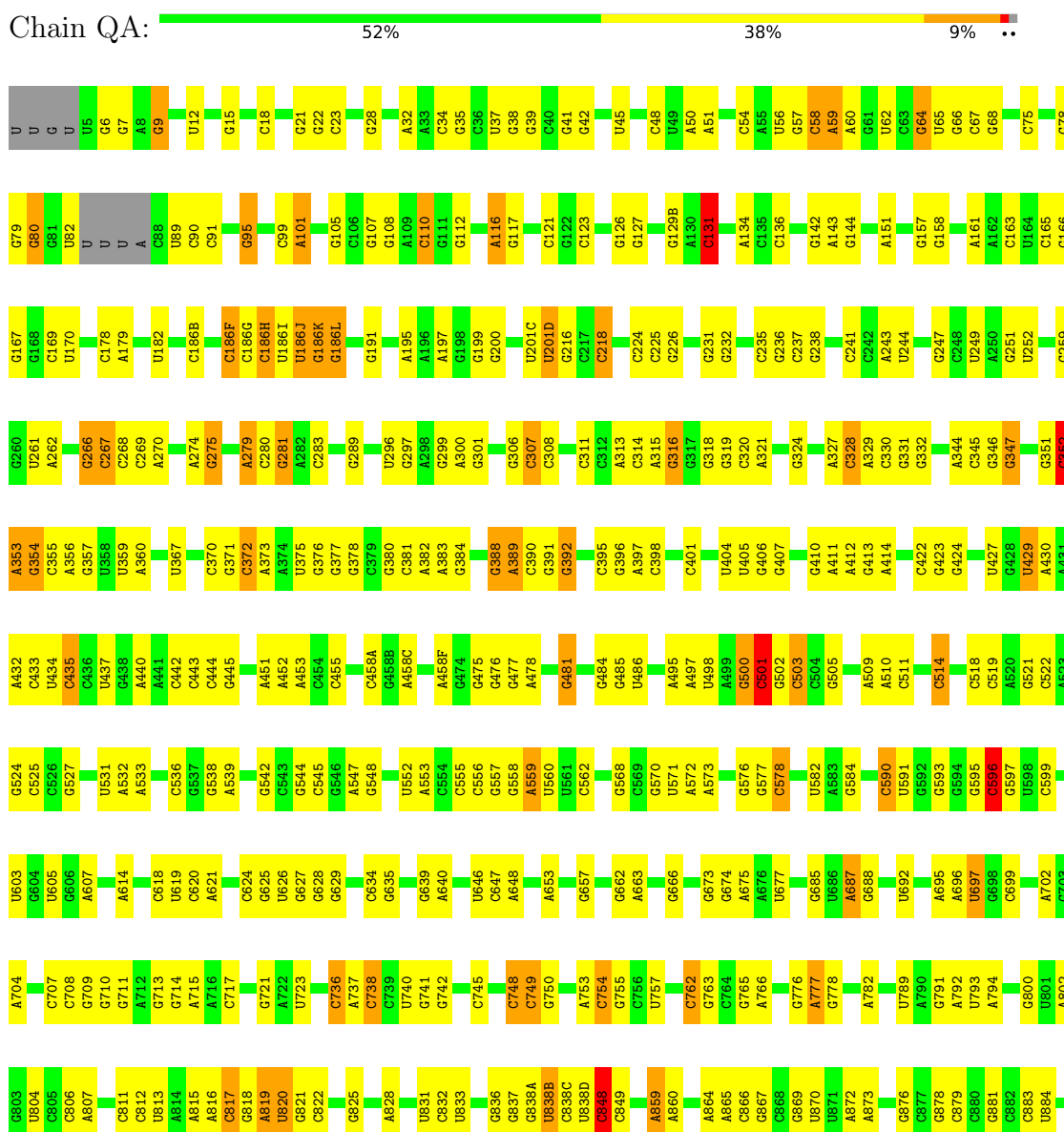
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0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

3 Residue-property plots [i](#)

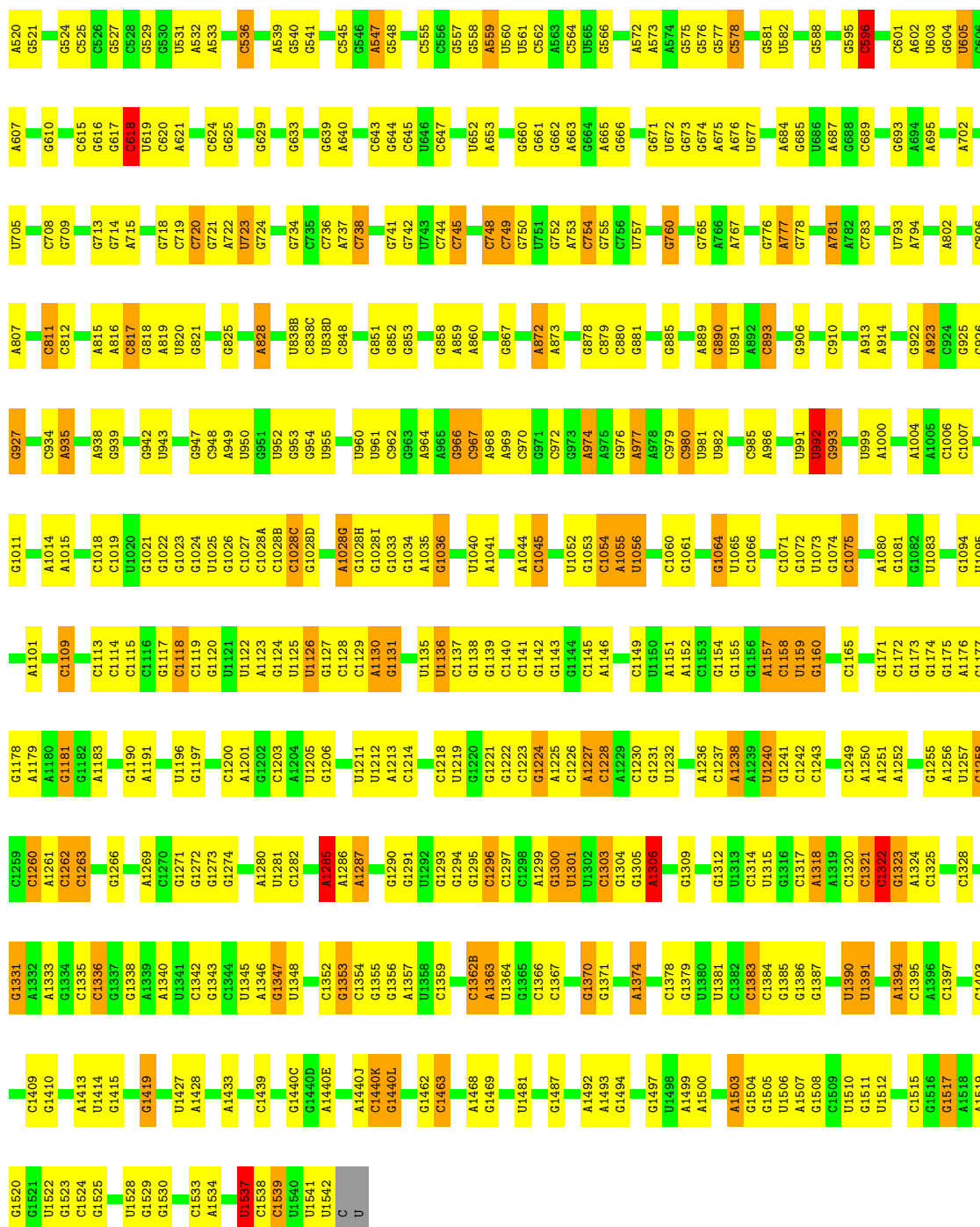
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

• Molecule 1: 16S rRNA







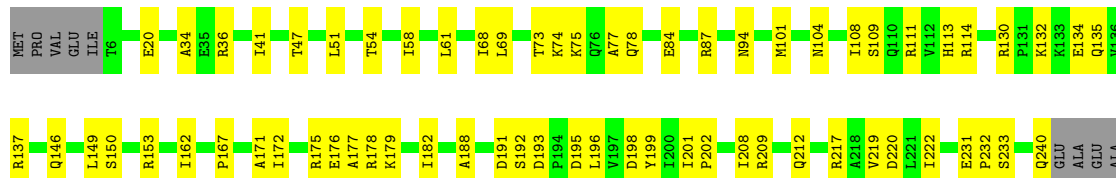
• Molecule 2: 30S ribosomal protein S2

Chain QB:

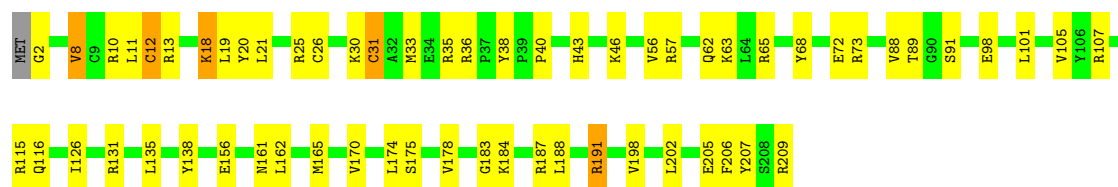
66%

26%


8%

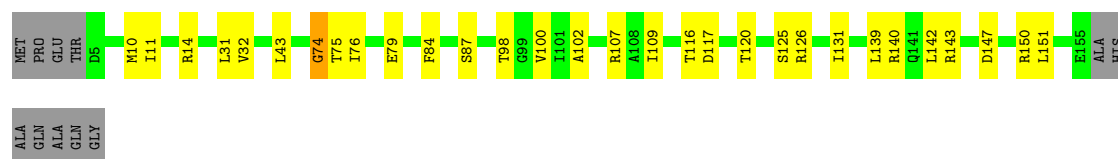


Chain XD:  70% 27% .



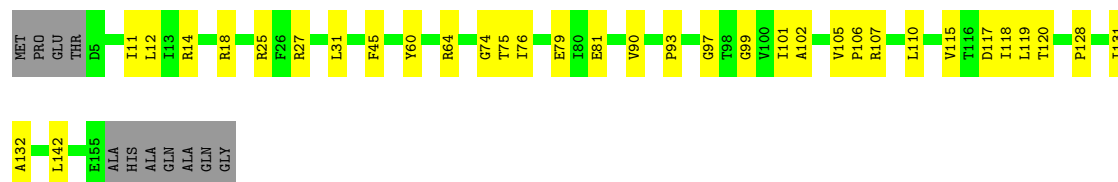
- Molecule 5: 30S ribosomal protein S5

Chain QE:  75% 18% 7% .




- Molecule 5: 30S ribosomal protein S5

Chain XE:  72% 21% 7% .




- Molecule 6: 30S ribosomal protein S6

Chain QF:  84% 16% .




- Molecule 6: 30S ribosomal protein S6

Chain XF:  82% 18% .

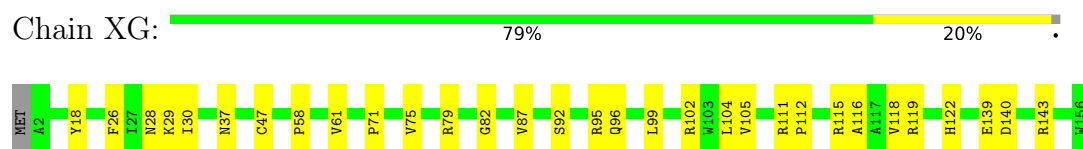


- Molecule 7: 30S ribosomal protein S7

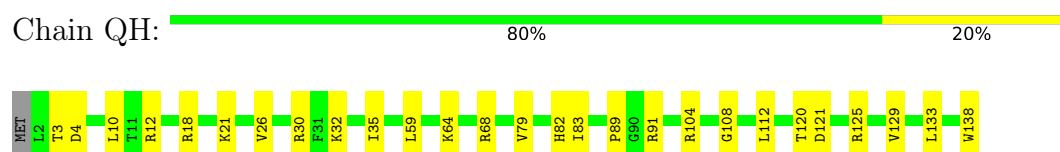
Chain QG:  81% 18% .



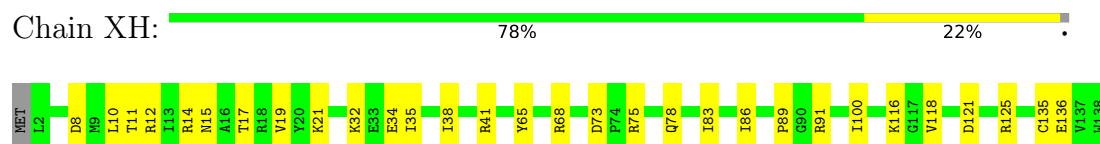
- Molecule 7: 30S ribosomal protein S7



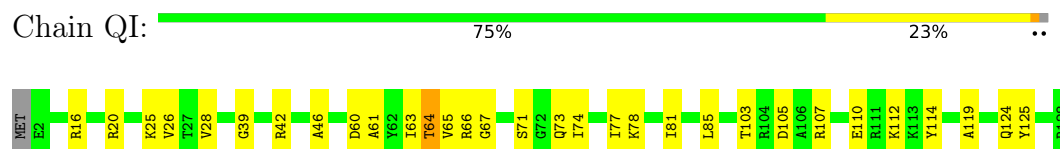
- Molecule 8: 30S ribosomal protein S8



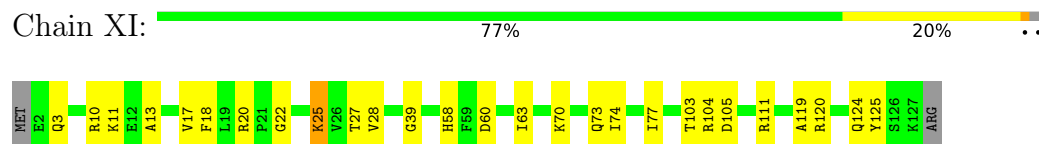
- Molecule 8: 30S ribosomal protein S8



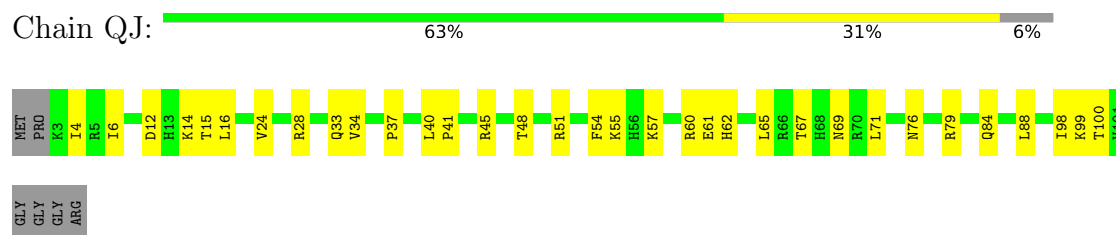
- Molecule 9: 30S ribosomal protein S9



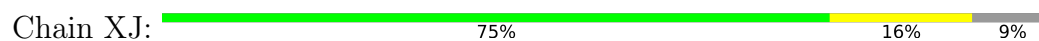
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

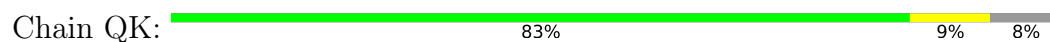


- Molecule 10: 30S ribosomal protein S10

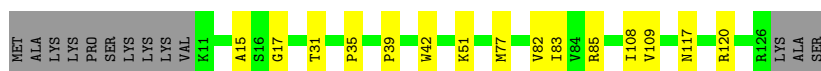
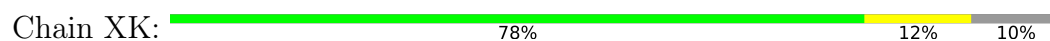




- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



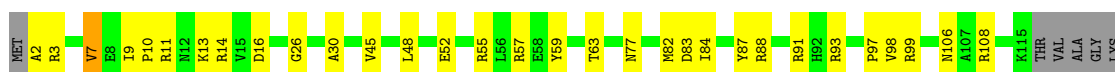
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



LYS
LYS
ALA
PRO
ARG
LYS

- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  70% 25% 5%

MET A2 R3 L6 K9 R12 T13 P14 K17 V18 R23 C24 G28 R35 C40 R41 I42 C43 L44 R45 P54 W61

- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  62% 31% 5%


MET A2 K9 R12 R19 R23 C24 C37 G28 R29 C40 R41 I42 C43 L44 E46 R45 L47 Q52 L53 P54 G55 V56 R57 K58 W61

- Molecule 15: 30S ribosomal protein S15

Chain QO:  89% 10% 1%


MET F2 T22 E26 Q27 V28 Q28 V29 L39 L56 R64 R72 I87 R88 G89

- Molecule 15: 30S ribosomal protein S15

Chain XO:  83% 15% 2%


MET F2 K10 Q13 E26 R35 L39 H53 L56 R64 R65 R68 R72 L81 R88 GLY

- Molecule 16: 30S ribosomal protein S16

Chain QP:  74% 22% 5%


H1 I4 R5 R8 M14 P15 H16 V21 R25 I33 G37 D40 K43 K50 V53 E54 R55 W59 V62 T69 R75 V79 A84 ARG GLU GLY ALA

- Molecule 16: 30S ribosomal protein S16

Chain XP:  76% 19% 5%

H1 I4 R5 L6 Y17 R18 I19 V20 V21 T22 D23 K27 K35 I36 G37 D40 W48 L49 K50 P66 R75 Q82 E83 A84 ARG GLU GLY ALA

- Molecule 17: 30S ribosomal protein S17

Chain QQ:  83% 12% 5%



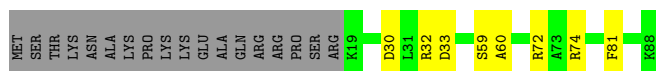
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 76% 19% 5%



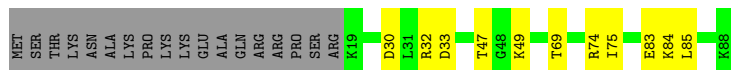
- Molecule 18: 30S ribosomal protein S18

Chain QR: 70% 9% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR: 67% 13% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS: 73% 15% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS: 68% 23% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 70% 22% 7%



- Molecule 20: 30S ribosomal protein S20

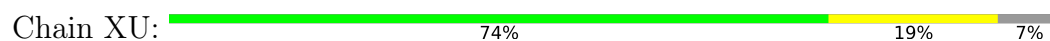
Chain XT: 69% 21% 7%



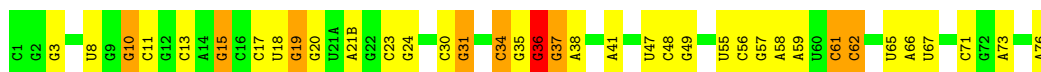
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



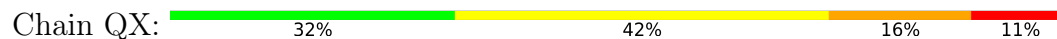
- Molecule 22: E-site tRNA-Pro



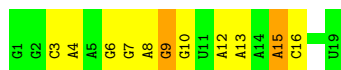
- Molecule 22: E-site tRNA-Pro



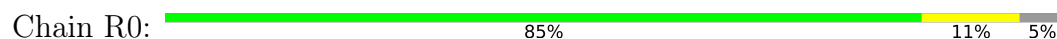
- Molecule 23: mRNA

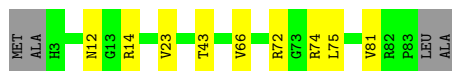


- Molecule 23: mRNA



- Molecule 24: 50S ribosomal protein L27





- Molecule 24: 50S ribosomal protein L27

Chain Y0: 80% 16% .



- Molecule 25: 50S ribosomal protein L28

Chain R1: 80% 17% .



- Molecule 25: 50S ribosomal protein L28

Chain Y1: 83% 12% 5%



- Molecule 26: 50S ribosomal protein L29

Chain R2: 82% 14% .



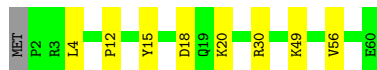
- Molecule 26: 50S ribosomal protein L29

Chain Y2: 82% 13% 6%



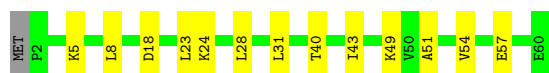
- Molecule 27: 50S ribosomal protein L30

Chain R3: 85% 13% .

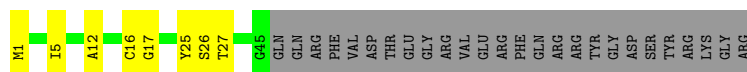


- Molecule 27: 50S ribosomal protein L30

Chain Y3: 77% 22% .



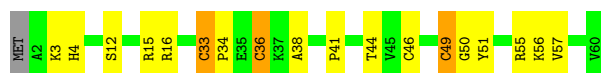
- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33

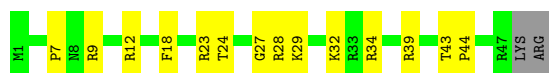


- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L34

Chain Y7: 86% 12%



- Molecule 32: 50S ribosomal protein L35

Chain R8: 69% 23% 6%



- Molecule 32: 50S ribosomal protein L35

Chain Y8: 72% 26%



- Molecule 33: 50S ribosomal protein L36

Chain R9: 70% 24% 5%



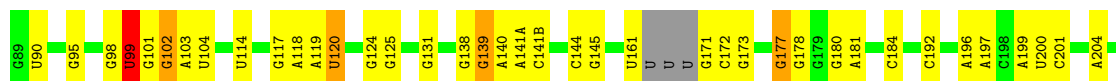
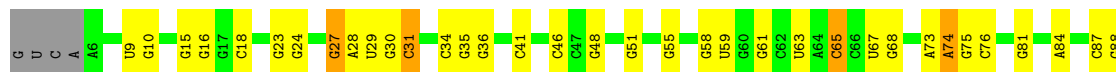
- Molecule 33: 50S ribosomal protein L36

Chain Y9: 68% 27% 5%



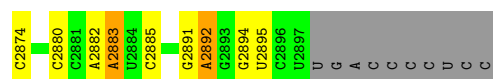
- Molecule 34: 23S rRNA

Chain RA: 53% 36% 9%



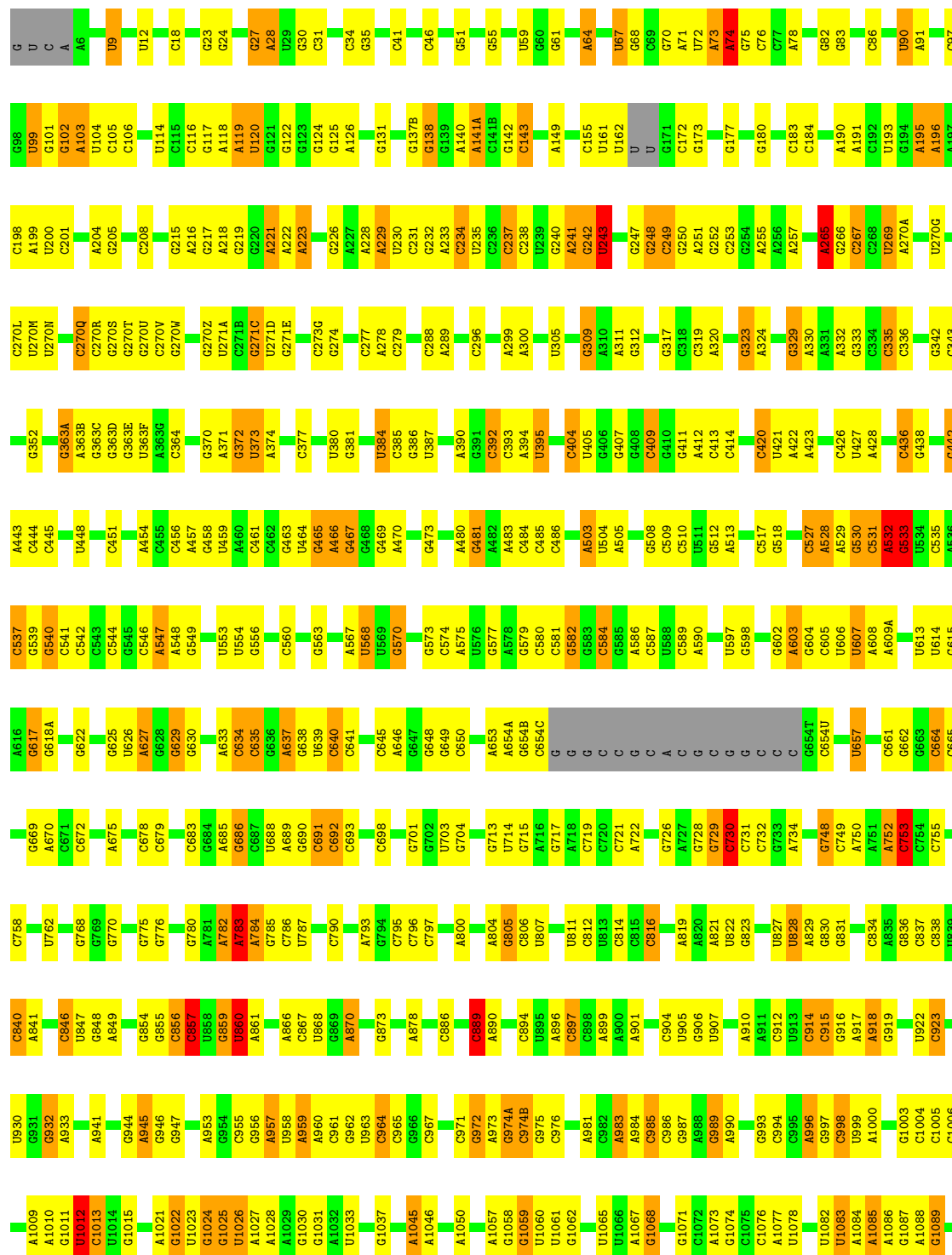
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G1407	C1407	A1308	G1225	G1136	G1058	A983	C904	G809	G707	G650	A571	A501	U380	G275	C209
C1411	C1411	G1310	G1226	G1137	G1062	A984	U907	G810	G715	G651	A572	A502	U381	G276	A221
G1416	G1417	U1312	A1227	G1138	G1063	C985	A910	U810	G717	G652	A573	A503	U382	G277	A222
G1418	G1419	U1313	G1139	G1064	G1065	C986	A911	U811	G717	G653	A574	A504	U383	A278	A223
A1419	U1420	G1314	G1140	U1141	U1066	C987	A912	U812	G721	G654	A575	A505	U384	G288	A224
U1421	G1422	U1315	G1141	U1067	U1068	A990	C913	G816	A722	G655	A576	A506	U385	G289	A225
G1423	G1424	U1316	G1142	U1069	C914	C991	U915	G817	A723	G656	A577	A507	U386	G290	A226
G1425	G1426	U1317	G1143	U1070	C915	C992	C916	G818	A724	G657	A578	A508	U387	G291	A227
G1427	G1428	G1325	G1144	U1071	C916	C993	G916	G819	A725	G658	A579	A509	U388	G292	A228
U1429	G1430	U1329	G1145	U1072	C917	C994	A917	G820	A726	G659	A580	A510	U389	G293	A229
C1437	C1437	U1330	G1146	U1073	C918	C995	A918	G821	A727	G660	A581	A511	U390	G294	A230
G1441	G1442	U1331	G1147	U1074	C919	C996	U919	G822	A728	G661	A582	A512	U391	G295	A231
A1444B	C1445	U1332	G1148	U1075	C920	C997	U920	G823	A729	G662	A583	A513	U392	G296	A232
C1445	C1446	U1333	G1149	U1076	C921	C998	C922	G824	A730	G663	A584	A514	U393	G297	A233
G1449A	G1449B	U1334	G1150	U1077	C923	C999	C924	G825	A731	G664	A585	A515	U394	G298	A234
U1454	G1455	U1335	G1151	U1078	C925	C1000	A926	G826	A732	G665	A586	A516	U395	G299	A235
G1461	C1462	U1336	G1152	U1079	C926	C1001	G927	G827	A733	G666	A587	A517	U396	G300	A236
C1467	C1468	U1337	G1153	U1080	C927	C1002	G928	G828	A734	G667	A588	A518	U397	G301	A237
A1471	C1474	U1338	G1154	U1081	C928	C1003	G929	G829	A735	G668	A589	A519	U398	G302	A238
U1482	G1483	U1339	G1155	U1082	C929	C1004	G930	G830	A736	G669	A590	A520	U399	G303	A239
G1484	G1485	U1340	G1156	U1083	C930	C1005	G931	G831	A737	G670	A591	A521	U400	G304	A240
C1493	A1494	U1341	G1157	U1084	C931	C1006	G932	G832	A738	G671	A592	A522	U401	G305	A241
A1495	A1496	U1342	G1158	U1085	C932	C1007	G933	G833	A739	G672	A593	A523	U402	G306	A242
U1497	C1498	U1343	G1159	U1086	C933	C1008	G934	G834	A740	G673	A594	A524	U403	G307	A243
G270E	G270F	U1344	G1160	U1087	C934	C1009	G935	G835	A741	G674	A595	A525	U404	G308	A244
G270G	G270H	U1345	G1161	U1088	C935	C1010	G936	G836	A742	G675	A596	A526	U405	G309	A245
G270I	G270J	U1346	G1162	U1089	C936	C1011	G937	G837	A743	G676	A597	A527	U406	G310	A246
G270K	G270L	U1347	G1163	U1090	C937	C1012	G938	G838	A744	G677	A598	A528	U407	G311	A247
G270M	G270N	U1348	G1164	U1091	C938	C1013	G939	G839	A745	G678	A599	A529	U408	G312	A248
G270O	G270P	U1349	G1165	U1092	C939	C1014	G940	G840	A746	G679	A600	A530	U409	G313	A249
G270Q	G270R	U1350	G1166	U1093	C940	C1015	G941	G841	A747	G680	A601	A531	U410	G314	A250
G270S	G270T	U1351	G1167	U1094	C941	C1016	G942	G842	A748	G681	A602	A532	U411	G315	A251
G270U	G270V	U1352	G1168	U1095	C942	C1017	G943	G843	A749	G682	A603	A533	U412	G316	A252
G270W	G270X	U1353	G1169	U1096	C943	C1018	G944	G844	A750	G683	A604	A534	U413	G317	A253
G270Y	G271A	U1354	G1170	U1097	C944	C1019	G945	G845	A751	G684	A605	A535	U414	G318	A254
G271B	G271C	U1355	G1171	U1098	C945	C1020	G946	G846	A752	G685	A606	A536	U415	G319	A255
G271D	G271E	U1356	G1172	U1099	C946	C1021	G947	G847	A753	G686	A607	A537	U416	G320	A256
G271F	G271G	U1357	G1173	U1100	C947	C1022	G948	G848	A754	G687	A608	A538	U417	G321	A257
G271H	G271I	U1358	G1174	U1101	C948	C1023	G949	G849	A755	G688	A609	A539	U418	G322	A258
G271J	G271K	U1359	G1175	U1102	C949	C1024	G950	G850	A756	G689	A610	A540	U419	G323	A259
G271L	G271M	U1360	G1176	U1103	C950	C1025	G951	G851	A757	G690	A611	A541	U420	G324	A260
G271N	G271O	U1361	G1177	U1104	C951	C1026	G952	G852	A758	G691	A612	A542	U421	G325	A261
G271P	G271Q	U1362	G1178	U1105	C952	C1027	G953	G853	A759	G692	A613	A543	U422	G326	A262
G271R	G271S	U1363	G1179	U1106	C953	C1028	G954	G854	A760	G693	A614	A544	U423	G327	A263
G271T	G271U	U1364	G1180	U1107	C954	C1029	G955	G855	A761	G694	A615	A545	U424	G328	A264
G271V	G271W	U1365	G1181	U1108	C955	C1030	G956	G856	A762	G695	A616	A546	U425	G329	A265
G271X	G271Y	U1366	G1182	U1109	C956	C1031	G957	G857	A763	G696	A617	A547	U426	G330	A266
G272A	G272B	U1367	G1183	U1110	C957	C1032	G958	G858	A764	G697	A618	A548	U427	G331	A267
G272C	G272D	U1368	G1184	U1111	C958	C1033	G959	G859	A765	G698	A619	A549	U428	G332	A268
G272E	G272F	U1369	G1185	U1112	C959	C1034	G960	G860	A766	G699	A620	A550	U429	G333	A269
G272G	G272H	U1370	G1186	U1113	C960	C1035	G961	G861	A767	G700	A621	A551	U430	G334	A270
G272I	G272J	U1371	G1187	U1114	C961	C1036	G962	G862	A768	G701	A622	A552	U431	G335	A271
G272K	G272L	U1372	G1188	U1115	C962	C1037	G963	G863	A769	G702	A623	A553	U432	G336	A272
G272M	G272N	U1373	G1189	U1116	C963	C1038	G964	G864	A770	G703	A624	A554	U433	G337	A273
G272O	G272P	U1374	G1190	U1117	C964	C1039	G965	G865	A771	G704	A625	A555	U434	G338	A274
G272Q	G272R	U1375	G1191	U1118	C965	C1040	G966	G866	A772	G705	A626	A556	U435	G339	A275
G272S	G272T	U1376	G1192	U1119	C966	C1041	G967	G867	A773	G706	A627	A557	U436	G340	A276
G272U	G272V	U1377	G1193	U1120	C967	C1042	G968	G868	A774	G707	A628	A558	U437	G341	A277
G272W	G272X	U1378	G1194	U1121	C968	C1043	G969	G869	A775	G708	A629	A559	U438	G342	A278
G272Y	G273A	U1379	G1195	U1122	C969	C1044	G970	G870	A776	G709	A630	A560	U439	G343	A279
G273B	G273C	U1380	G1196	U1123	C970	C1045	G971	G871	A777	G710	A631	A561	U440	G344	A280
G273D	G273E	U1381	G1197	U1124	C971	C1046	G972	G872	A778	G711	A632	A562	U441	G345	A281
G273F	G273G	U1382	G1198	U1125	C972	C1047	G973	G873	A779	G712	A633	A563	U442	G346	A282
G273H	G273I	U1383	G1199	U1126	C973	C1048	G974	G874	A780	G713	A634	A564	U443	G347	A283
G273J	G273K	U1384	G1200	U1127	C974	C1049	G975	G875	A781	G714	A635	A565	U444	G348	A284
G273L	G273M	U1385	G1201	U1128	C975	C1050	G976	G876	A782	G715	A636	A566	U445	G349	A285
G273N	G273O	U1386	G1202	U1129	C976	C1051	G977	G877	A783	G716	A637	A567	U446	G350	A286
G273P	G273Q	U1387	G1203	U1130	C977	C1052	G978	G878	A784	G717	A638	A568	U447	G351	A287
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G273T	G273U	U1389	G1205	U1132	C979	C1054	G980	G880	A786	G719	A640	A570	U449	G353	A289
G273V	G273W	U1390	G1206	U1133	C980	C1055	G981	G881	A787	G720	A641	A571	U450	G354	A290
G273X	G273Y	U1391	G1207	U1134	C981	C1056	G982	G882	A788	G721	A642	A572	U451	G355	A291
G274A	G274B	U1392	G1208	U1135	C982	C1057	G983	G883	A789	G722	A643	A573	U452	G356	A292
G274C	G274D	U1393	G1209	U1136	C983	C1058	G984	G884	A790	G723	A644	A574	U453	G357	A293
G274E	G274F	U1394	G1210	U1137	C984	C1059	G985	G885	A791	G724	A645	A575	U454	G358	A294
G274G	G274H	U1395	G1211	U1138	C985	C1060	G986	G886	A792	G725	A646	A576	U455	G359	A295
G274I	G274J	U1396	G1212	U1139	C986	C1061	G987	G887	A793	G726	A647	A577	U456	G360	A296
G274K	G274L	U1397	G1213	U1140	C987	C1062	G988	G888	A794	G727	A648	A578	U457	G361	A297
G274M	G274N	U1398	G1214	U1141	C988	C1063	G989	G889	A795	G728	A649	A579	U458	G362	A298
G274O	G274P	U1399	G1215	U1142	C989	C1064	G990	G890	A796	G729	A650	A580	U459	G363	A299
G274Q	G274R	U1400	G1216	U1143	C990	C1065	G991	G891	A797	G730	A651	A581	U460	G364	A300
G274S	G274T	U1401	G1217	U1144	C991	C1066	G992	G892	A798	G731	A652	A582	U461	G365	A301
G274U	G274V	U1402	G1218	U1145	C992	C1067	G993	G893	A799	G732	A653	A583	U462	G366	A302
G274W	G274X	U1403	G1219	U1146	C993	C1068	G994	G894	A800	G733	A654	A584	U463	G367	A303
G274Y	G275A	U1404	G1220	U1147	C994	C1069	G995	G895	G801	G734	A655	A585	U464	G368	A304
G275B	G275C	U1405	G1221												



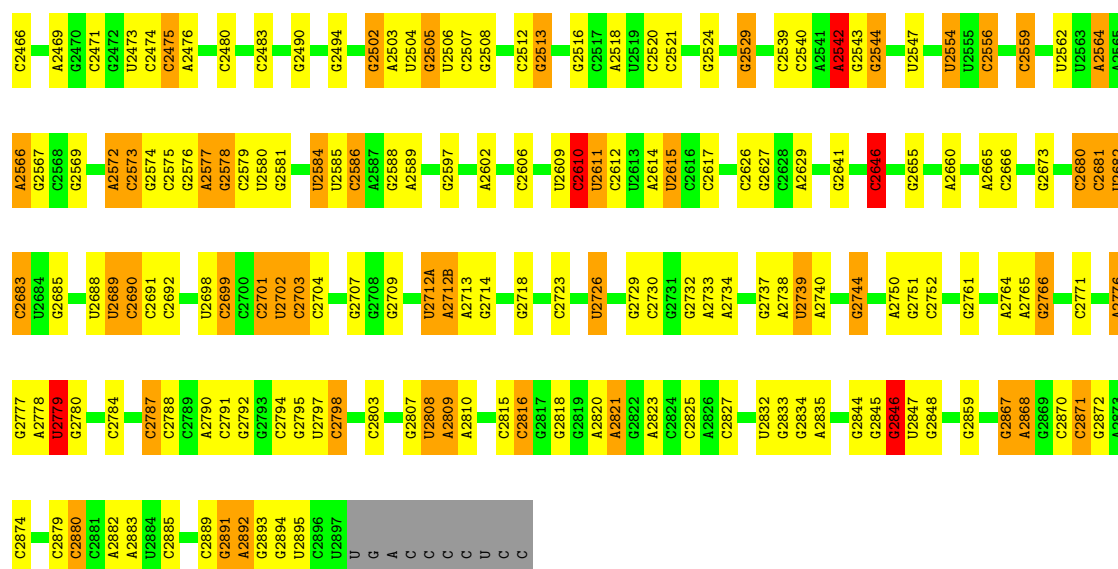


• Molecule 34: 23S rRNA

Chain YA: 53% 35% 10% ..

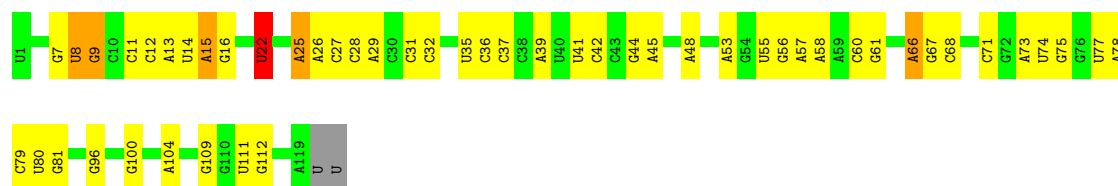


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G2383	G2212	A2212	C2129	A2059	A1970	G1872	U1780	C1672	G1568	A1274	A1378	A1275	G1186	U1094
G2384	G2213	U2213	U2130	A2059	A1971	G1878	A1780	U1673	A1569	A1471	A1379	A1275	G1187	A1095
G2385	G2215	G2215	G2131	G2061	A1972	C1881	C1782	C1675	C1575	G1473	A1379	A1286	U1188	U1097
G2386	G2219	G2219	G2133	A2062	C1979	C1882	A1783	C1675	U1578	C1474	C1383	A1286	G1193	A1098
U2387	G2307	G2224	A2134	C2063	G1980	G1883	A1786	C1675	U1578	A1477	C1385	C1289	A1194	A1099
G2387	G2308	A2224	C2136	C2064	A1981	A1884	A1786	C1682	A1585	G1478	G1385	C1290	G1195	C1100
G2388	A2225	G2226	C2137	C2065	C1982	C1887	A1788	C1685	A1586	G1479	C1392	C1196	C1196	U1101
A2392	A2311	G2230	C2140	U2068	G1983	C1887	A1789	C1686	A1586	G1480	A1393	G1293	G1203	A1103
A2393	U2312	G2233	G2141	G2069	G1989	A1889	A1790	C1686	A1585	U1482	A1394	C1295	A1204	A1104
G2394	G2314	G2234	G2142	G2070	G1990	A1890	A1791	C1686	C1598	G1483	A1395	G1297	U1205	U1105
G2395	G2315	G2235	C2145	A2071	G1991	C1891	G1792	C1686	C1599	G1484	C1398	C1298	G1206	G1110
C2402	G2316	G2236	C2145	U2074	G1992	C1892	G1793	A1689	C1600	G1485	C1399	G1299	A1210	A1111
C2403	G2317	G2236	G2148	U2075	G1993	C1893	C1793	A1689	C1600	G1485	C1399	G1299	A1210	A1111
C2404	G2318	G2237	G2149	U2076	G1994	C1894	C1793	A1689	C1600	G1485	C1399	G1299	A1210	A1111
U2405	G2319	G2237	G2149	U2076	G1995	G1899	G1799	C1694	C1607	A1490	C1402	U1300	U1211	U1113
U2406	A2320	G2238	U2150	C2081	G1996	G1899	C1800	C1695	A1608	C1493	C1403	C1306	G1215	C1121
G2410	G2321	G2239	G2151	G2081	A2005	A1900	A1802	A1698	A1608	C1493	C1404	C1307	G1216	G1122
A2411	G2325	G2243	G2152	A2082	C2006	A1901	A1803	A1699	A1610	U1497	U1405	A1308	G1217	G1126
G2415	G2326	U2244	G2153	G2083	C2007	C1905	C1804	A1701	C1611	U1499	U1407	G1309	G1218	A1126
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G2417	G2328	G2246	G2155	G2087	G2009	A1913	C1806	U1709	A1616	C1506	C1409	U1313	A1220	G1131
G2418	A2329	G2247	G2156	G2087	G2010	U1914	A1809	G1725	A1617	A1507	G1410	C1314	G1224	C1135
G2419	G2330	U2249	A2158	U2089	U2011	U1914	A1809	G1725	A1618	A1508	G1411	C1318	G1224	G1136
U2420	G2331	G2250	G2159	U2092	G2012	U1915	A1812	G1728	G1619	C1509	G1416	C1318	G1226	G1136
A2421	G2334	G2253	C2161	G2093	A2015	A1918	A1813	A1729	G1620	A1510	C1417	G1325	A1227	G1139
A2422	A2335	C2254	G2162	G2094	A2019	A1919	G1814	U1730	U1621	A1511	G1418	U1326	G1228	C1140
U2423	G2340	G2260	G2163	C2095	A2019	A1920	A1815	A1731	G1622	A1512	U1419	C1327	U1411	U1411
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G2428	G2345	A2267	G2168	U2089	C2025	G1935	A1820	C1741	C1640	U1519	A1427	A1331	G1236	C1145
G2429	A2346	A2268	A2169	C2026	C2026	G1936	A1824	C1742	C1640	U1520	C1428	A1332	G1237	C1146
A2430	G2347	A2269	A2169	C2026	C2026	A1936	A1824	G1743	C1644	G1526	C1430	C1333	G1238	C1147
A2435	U2348	C2103	U2172	G2102	A2030	A1937	G1828	G1750	G1645	G1533	C1432	G1338	G1244	G1151
A2439	G2349	A2273	A2173	G2104	A2031	A1938	A1829	G1750	G1646	C1533	U1431	G1339	G1245	C1152
C2440	G2350	A2274	G2173	C2105	C2032	U1939	C1830	G1753	G1647	G1534	U1433	U1340	A1246	C1153
C2441	G2351	C2275	A2176	G2106	A2033	U1939	C1830	G1754	C1648	U1535	U1434	U1341	A1246	G1154
C2442	G2352	C2275	A2176	C2107	A2033	C1947	U1833	A1755	C1648	A1536	G1435	A1342	G1250	G1157
G2446	G2353	G2108	G2182	U2109	C2036	C1947	U1833	G1756	G1651	C1537	G1437	G1343	G1251	C1158
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G2448	G2355	G2110	G2182	U2109	C2036	G1950	G1839	U1757	A1652	G1538	C1437	G1343	G1251	C1158
G2449	G2356	G2111	C2185	C2111	C2039	A1953	C1844	G1758	G1653	A1543	A1444B	A1349	A1253	U1165
G2453	G2357	G2112	G2186	G2112	C2040	G1954	C1844	G1763	A1654	A1544	A1444B	A1349	A1253	U1165
G2454	G2358	G2113	G2187	G2113	C2041	C1955	A1847	G1764	A1655	C1544	C1445	U1352	A1254	C1166
G2455	G2359	A2042	C2043	G2114	A2042	U1955	A1847	G1765	C1657	A1545A	C1445	U1352	A1254	C1166
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U2458	G2372	U2118	G2193	U2118	U2047	U1963	A1854	U1768	A1654	A1554	G1455	C1362	G1264	A1174
U2459	G2373	A2119	G2194	A2119	G2048	G1964	A1858	G1769	A1655	A1554	G1455	C1362	G1264	A1174
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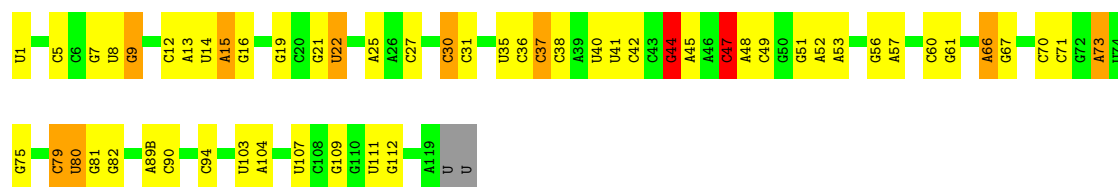
• Molecule 35: 5S rRNA

Chain RB: 57% 37% ..



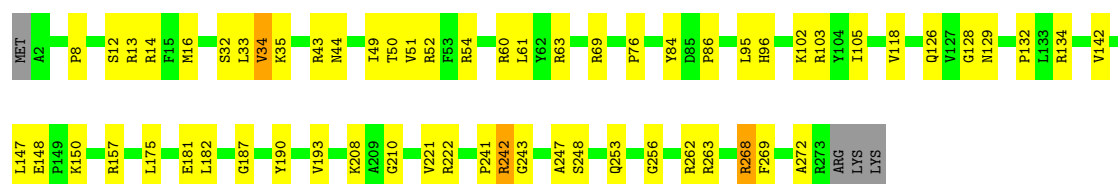
• Molecule 35: 5S rRNA

Chain YB: 53% 36% 7% ..



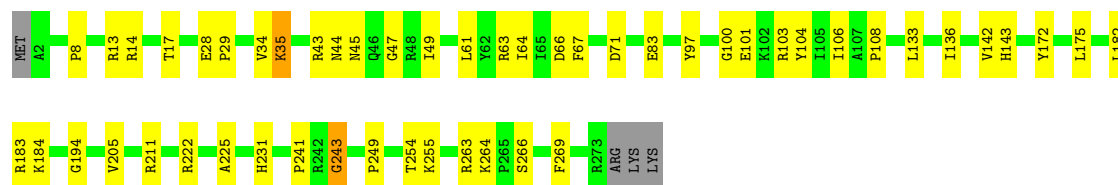
• Molecule 36: 50S ribosomal protein L2

Chain RD: 76% 21% ..

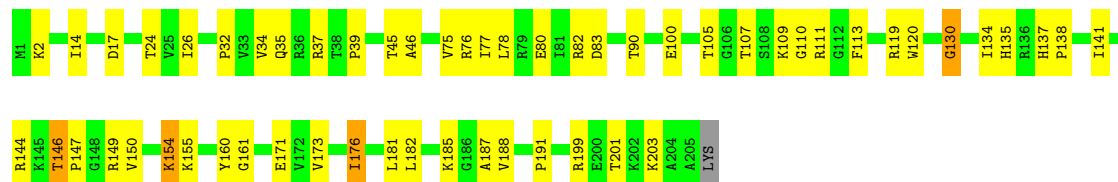
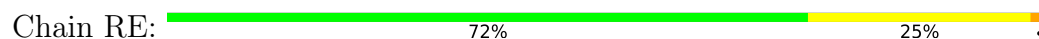


• Molecule 36: 50S ribosomal protein L2

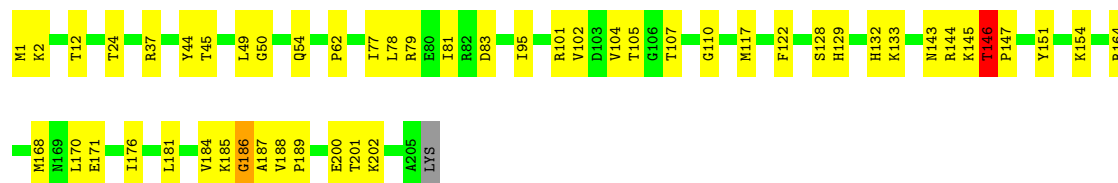
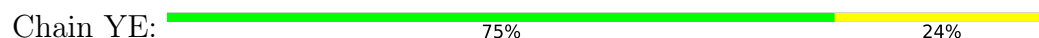
Chain YD: 80% 18% ..



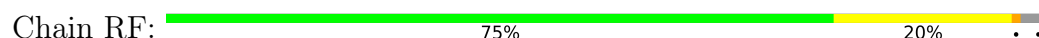
- Molecule 37: 50S ribosomal protein L3



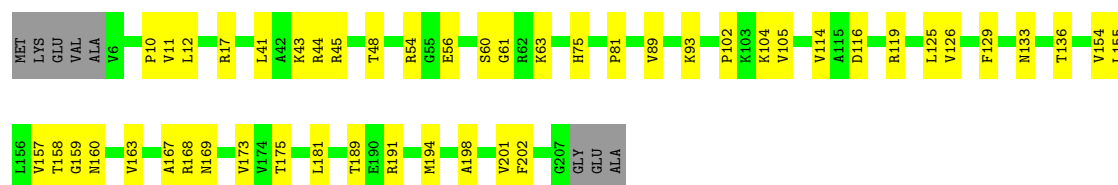
- Molecule 37: 50S ribosomal protein L3



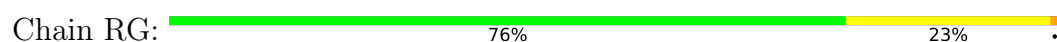
- Molecule 38: 50S ribosomal protein L4

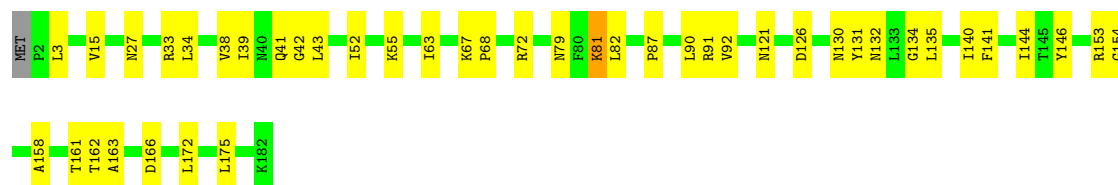


- Molecule 38: 50S ribosomal protein L4



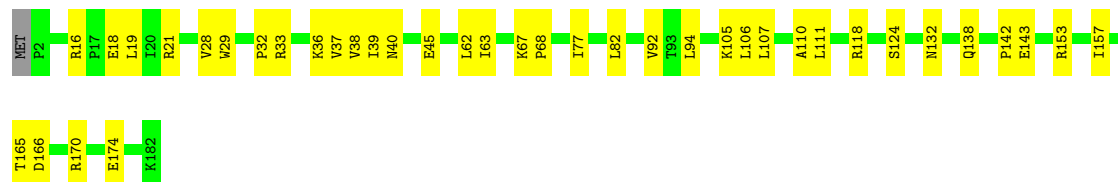
- Molecule 39: 50S ribosomal protein L5





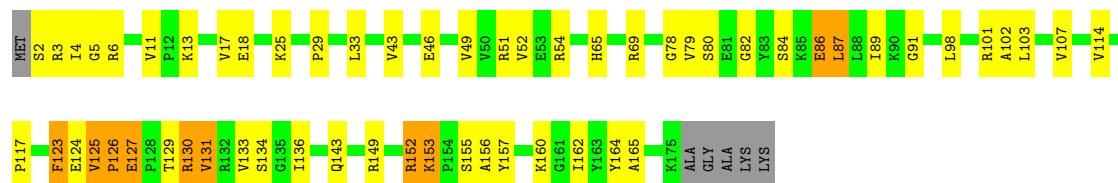
- Molecule 39: 50S ribosomal protein L5

Chain YG: 78% 21% .



- Molecule 40: 50S ribosomal protein L6

Chain RH: 64% 27% 6% .



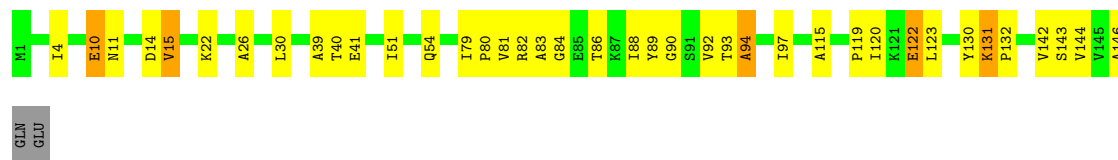
- Molecule 40: 50S ribosomal protein L6

Chain YH: 77% 18% . . .



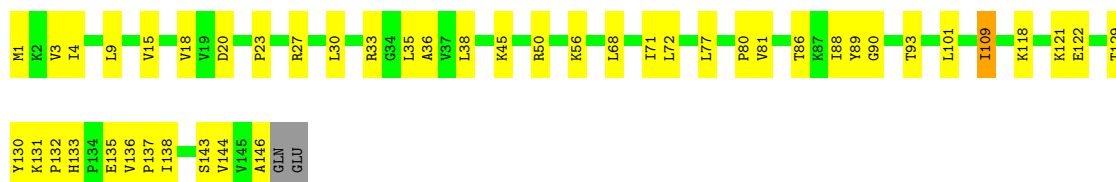
- Molecule 41: 50S ribosomal protein L9

Chain RI: 72% 23% . .



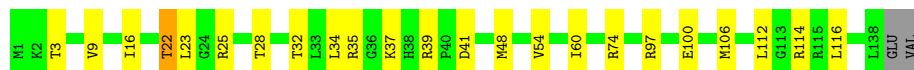
- Molecule 41: 50S ribosomal protein L9

Chain YI: 68% 30% . .



- Molecule 42: 50S ribosomal protein L13

Chain RN: 82% 16% ..



- Molecule 42: 50S ribosomal protein L13

Chain YN: 79% 20% .



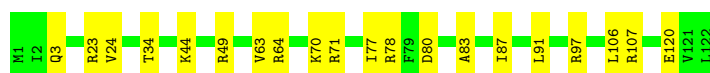
- Molecule 43: 50S ribosomal protein L14

Chain RO: 75% 25%



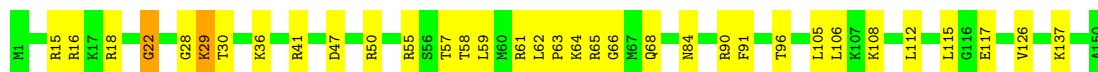
- Molecule 43: 50S ribosomal protein L14

Chain YO: 84% 16%



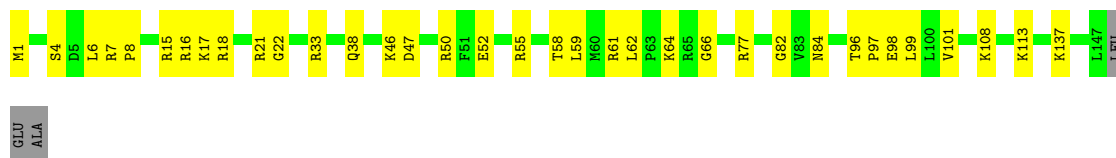
- Molecule 44: 50S ribosomal protein L15

Chain RP: 77% 21% .




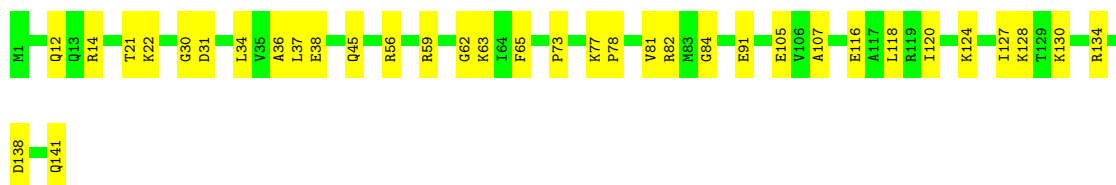
- Molecule 44: 50S ribosomal protein L15

Chain YP: 75% 23% .



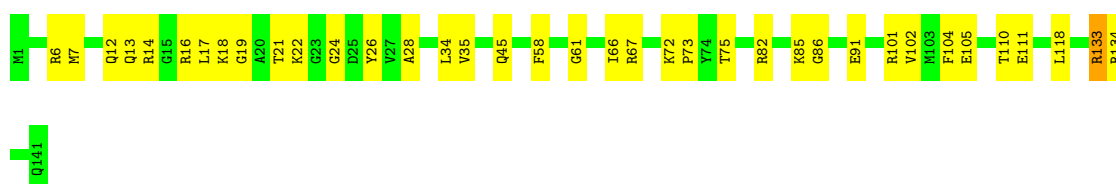
- Molecule 45: 50S ribosomal protein L16

Chain RQ:  75% 25%



- Molecule 45: 50S ribosomal protein L16

Chain YQ:  74% 26%




- Molecule 46: 50S ribosomal protein L17

Chain RR:  69% 28%




- Molecule 46: 50S ribosomal protein L17

Chain YR:  75% 24%




- Molecule 47: 50S ribosomal protein L18

Chain RS:  75% 24%




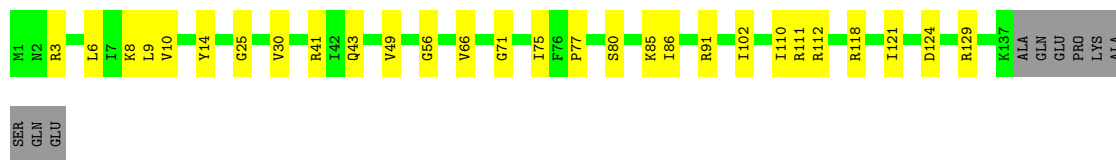
- Molecule 47: 50S ribosomal protein L18

Chain YS:  79% 18%



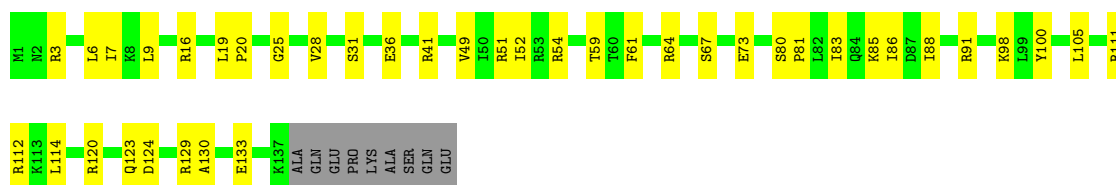
- Molecule 48: 50S ribosomal protein L19

Chain RT:  75% 19% 6%




- Molecule 48: 50S ribosomal protein L19

Chain YT:  66% 27% 6%




- Molecule 49: 50S ribosomal protein L20

Chain RU:  77% 19% ..




- Molecule 49: 50S ribosomal protein L20

Chain YU:  79% 19% ..




- Molecule 50: 50S ribosomal protein L21

Chain RV:  78% 22%




- Molecule 50: 50S ribosomal protein L21

Chain YV:  79% 21%

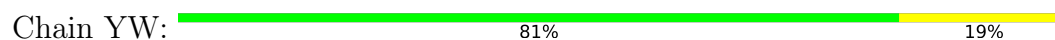


- Molecule 51: 50S ribosomal protein L22

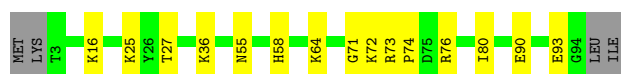
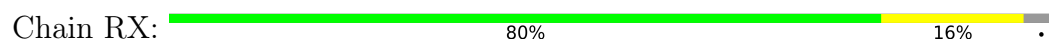
Chain RW:  79% 21%



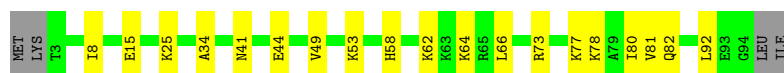
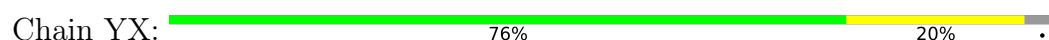
- Molecule 51: 50S ribosomal protein L22



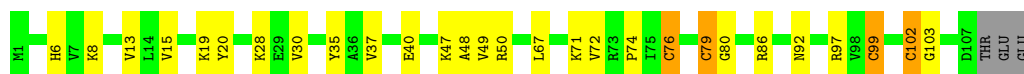
- Molecule 52: 50S ribosomal protein L23



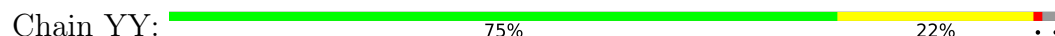
- Molecule 52: 50S ribosomal protein L23



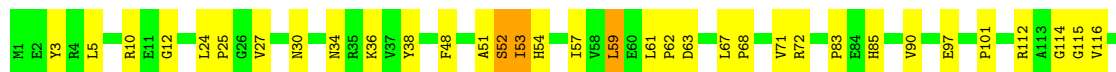
- Molecule 53: 50S ribosomal protein L24



- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



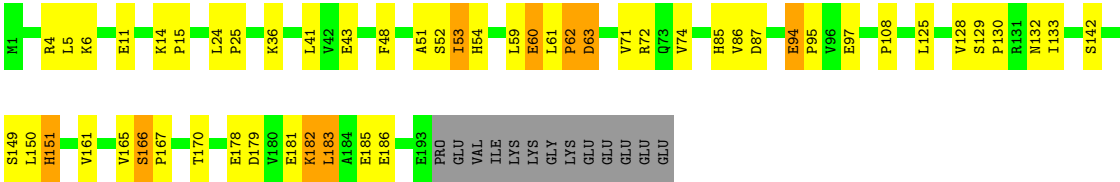
- Molecule 54: 50S ribosomal protein L25

Chain YZ:

68%

21%

• 6%



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	210.74Å 450.26Å 626.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.50	Depositor
% Data completeness (in resolution range)	97.6 (49.94-3.50)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.240 , 0.258	Depositor
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.423	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: MG, ZN, 1MG, 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	0.69	1/36343 (0.0%)	1.14	198/56720 (0.3%)
1	XA	0.77	0/36435	1.15	194/56865 (0.3%)
2	QB	0.35	0/1942	0.67	0/2619
2	XB	0.37	0/1950	0.64	1/2630 (0.0%)
3	QC	0.36	0/1629	0.66	0/2195
3	XC	0.37	0/1629	0.61	0/2195
4	QD	0.45	1/1733 (0.1%)	0.65	0/2318
4	XD	0.52	2/1733 (0.1%)	0.70	2/2318 (0.1%)
5	QE	0.37	0/1171	0.67	0/1576
5	XE	0.43	0/1171	0.62	0/1576
6	QF	0.39	0/856	0.68	0/1154
6	XF	0.41	0/856	0.62	0/1154
7	QG	0.35	0/1276	0.63	1/1709 (0.1%)
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1128	0.62	0/1517
8	XH	0.42	0/1128	0.66	0/1517
9	QI	0.42	0/1029	0.74	0/1379
9	XI	0.36	0/1017	0.70	0/1365
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.34	0/790	0.59	0/1063
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/879	0.59	0/1187
12	QL	0.41	0/991	0.70	1/1327 (0.1%)
12	XL	0.45	0/972	0.77	2/1301 (0.2%)
13	QM	0.35	0/965	0.78	0/1292
13	XM	0.37	0/924	0.66	0/1238
14	QN	0.67	1/501 (0.2%)	0.84	3/664 (0.5%)
14	XN	0.68	1/501 (0.2%)	0.88	2/664 (0.3%)
15	QO	0.38	0/745	0.57	0/992
15	XO	0.40	0/740	0.56	0/987
16	QP	0.40	0/721	0.64	0/970
16	XP	0.38	0/721	0.66	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.39	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.37	0/579	0.56	0/768
18	XR	0.39	0/579	0.58	0/768
19	QS	0.35	0/680	0.72	1/915 (0.1%)
19	XS	0.36	0/689	0.70	0/926
20	QT	0.77	2/765 (0.3%)	1.14	8/1007 (0.8%)
20	XT	0.37	0/765	0.75	2/1007 (0.2%)
21	QU	0.34	0/221	0.58	0/288
21	XU	0.32	0/221	0.54	0/288
22	QV	0.70	2/1813 (0.1%)	1.39	32/2825 (1.1%)
22	XV	0.66	0/1813	1.20	13/2825 (0.5%)
23	QX	0.99	1/459 (0.2%)	2.11	25/715 (3.5%)
23	XX	0.63	0/459	1.26	1/715 (0.1%)
24	R0	0.40	0/652	0.63	0/867
24	Y0	0.59	0/657	0.60	0/874
25	R1	0.54	0/753	0.68	0/1000
25	Y1	0.59	0/736	0.73	0/978
26	R2	0.37	0/583	0.62	0/771
26	Y2	0.47	0/577	0.62	0/764
27	R3	0.39	0/474	0.59	0/635
27	Y3	0.62	0/474	0.59	0/635
28	R4	0.33	0/357	0.60	0/483
28	Y4	1.56	2/366 (0.5%)	1.47	8/495 (1.6%)
29	R5	0.88	3/473 (0.6%)	0.79	2/639 (0.3%)
29	Y5	0.94	2/473 (0.4%)	0.77	1/639 (0.2%)
30	R6	0.96	3/460 (0.7%)	0.78	2/613 (0.3%)
30	Y6	1.33	6/460 (1.3%)	1.01	3/613 (0.5%)
31	R7	0.53	0/417	0.62	0/550
31	Y7	0.63	0/426	0.66	0/561
32	R8	0.43	0/525	0.88	3/691 (0.4%)
32	Y8	0.59	0/525	0.84	0/691
33	R9	0.62	1/310 (0.3%)	0.72	1/407 (0.2%)
33	Y9	0.63	0/310	0.73	0/407
34	RA	0.91	2/69520 (0.0%)	1.22	576/108527 (0.5%)
34	YA	1.27	23/69543 (0.0%)	1.33	807/108563 (0.7%)
35	RB	0.71	0/2878	1.14	18/4490 (0.4%)
35	YB	1.08	0/2878	1.32	38/4490 (0.8%)
36	RD	0.52	0/2165	0.71	3/2919 (0.1%)
36	YD	0.64	0/2165	0.74	4/2919 (0.1%)
37	RE	0.50	0/1601	0.83	3/2160 (0.1%)
37	YE	0.66	0/1601	0.84	3/2160 (0.1%)
38	RF	0.49	0/1620	0.70	1/2194 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.67	0/1620	0.65	1/2194 (0.0%)
39	RG	0.40	0/1499	0.69	0/2016
39	YG	0.43	0/1499	0.68	0/2016
40	RH	0.39	0/1362	0.83	5/1841 (0.3%)
40	YH	0.58	0/1362	0.82	4/1841 (0.2%)
41	RI	0.48	2/1151 (0.2%)	0.86	6/1558 (0.4%)
41	YI	0.45	1/1151 (0.1%)	0.79	0/1558
42	RN	0.45	0/1131	0.68	1/1525 (0.1%)
42	YN	0.63	0/1131	0.70	2/1525 (0.1%)
43	RO	0.51	0/943	0.65	0/1269
43	YO	0.60	0/943	0.63	0/1269
44	RP	0.44	0/1162	0.76	1/1544 (0.1%)
44	YP	0.54	0/1139	0.83	1/1514 (0.1%)
45	RQ	0.45	0/1143	0.73	0/1527
45	YQ	0.61	0/1143	0.77	2/1527 (0.1%)
46	RR	0.48	0/974	0.68	0/1302
46	YR	0.57	0/974	0.70	0/1302
47	RS	0.39	0/892	0.66	0/1187
47	YS	0.52	0/892	0.67	0/1187
48	RT	0.43	0/1155	0.69	0/1542
48	YT	0.54	0/1155	0.72	1/1542 (0.1%)
49	RU	0.49	0/982	0.62	0/1306
49	YU	0.70	0/982	0.61	0/1306
50	RV	0.47	0/790	0.74	1/1057 (0.1%)
50	YV	0.63	0/790	0.76	1/1057 (0.1%)
51	RW	0.52	0/911	0.63	0/1220
51	YW	0.68	0/911	0.64	0/1220
52	RX	0.52	0/739	0.60	0/993
52	YX	0.66	0/739	0.68	0/993
53	RY	0.72	4/831 (0.5%)	0.66	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	2/1108 (0.2%)
54	RZ	0.43	0/1493	0.89	6/2026 (0.3%)
54	YZ	0.51	0/1561	0.85	5/2119 (0.2%)
All	All	0.87	61/316163 (0.0%)	1.12	2000/472822 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y4	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	1	7

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.70	1.04	1.54
28	Y4	4	GLY	N-CA	-18.70	1.18	1.46
30	R6	16	CYS	CB-SG	14.24	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82
20	QT	74	LYS	CA-CB	-13.71	1.23	1.53

The worst 5 of 2000 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	74	LYS	N-CA-CB	21.28	148.91	110.60
23	QX	17	C	C6-N1-C2	-19.01	112.70	120.30
22	QV	35	G	C8-N9-C4	-16.76	99.70	106.40
28	Y4	5	ILE	CB-CA-C	16.14	143.88	111.60
34	YA	2453	A	N1-C2-N3	-15.63	121.48	129.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	Y4	5	ILE	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
28	Y4	5	ILE	Mainchain
37	YE	146	THR	Peptide

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	32469	0	16393	389	0
1	XA	32551	0	16433	382	1
2	QB	1907	0	1958	40	0
2	XB	1915	0	1968	37	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	22	0
4	QD	1703	0	1763	55	0
4	XD	1703	0	1763	47	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	9	0
6	XF	843	0	857	11	0
7	QG	1257	0	1296	21	0
7	XG	1257	0	1296	23	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	23	0
9	QI	1010	0	1037	22	0
9	XI	998	0	1024	21	0
10	QJ	801	0	849	22	0
10	XJ	777	0	816	13	0
11	QK	885	0	904	7	0
11	XK	864	0	881	11	0
12	QL	975	0	1062	23	0
12	XL	956	0	1046	14	0
13	QM	955	0	1021	27	0
13	XM	914	0	971	23	0
14	QN	492	0	532	18	0
14	XN	492	0	531	16	0
15	QO	734	0	771	5	0
15	XO	729	0	768	10	0
16	QP	705	0	725	13	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	5	0
18	XR	574	0	644	11	0
19	QS	665	0	686	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	16	0
20	QT	763	0	861	17	0
20	XT	763	0	861	17	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1647	0	834	23	0
22	XV	1647	0	834	18	0
23	QX	409	0	209	13	0
23	XX	409	0	209	6	0
24	R0	643	0	667	6	0
24	Y0	648	0	672	14	0
25	R1	746	0	826	21	0
25	Y1	729	0	802	7	0
26	R2	581	0	629	7	0
26	Y2	575	0	624	5	0
27	R3	469	0	518	6	0
27	Y3	469	0	518	10	0
28	R4	348	0	354	6	0
28	Y4	357	0	362	12	0
29	R5	459	0	477	23	0
29	Y5	459	0	476	17	0
30	R6	453	0	474	7	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	9	0
31	Y7	418	0	467	7	0
32	R8	517	0	582	19	0
32	Y8	517	0	582	16	0
33	R9	307	0	335	9	0
33	Y9	307	0	336	17	0
34	RA	62070	0	31284	607	0
34	YA	62091	0	31294	489	0
35	RB	2573	0	1306	26	0
35	YB	2573	0	1306	24	0
36	RD	2115	0	2195	50	0
36	YD	2115	0	2195	39	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	34	0
38	RF	1585	0	1632	30	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	32	0
39	YG	1474	0	1535	24	0
40	RH	1336	0	1418	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	21	0
41	RI	1136	0	1223	32	1
41	YI	1136	0	1223	25	0
42	RN	1104	0	1180	14	0
42	YN	1104	0	1180	15	0
43	RO	933	0	996	21	0
43	YO	933	0	996	14	0
44	RP	1145	0	1228	27	0
44	YP	1122	0	1206	28	0
45	RQ	1122	0	1179	23	0
45	YQ	1122	0	1179	25	0
46	RR	960	0	1021	31	0
46	YR	960	0	1021	19	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	17	0
48	YT	1141	0	1202	27	0
49	RU	964	0	1022	25	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	14	0
50	YV	779	0	852	12	0
51	RW	900	0	964	17	0
51	YW	900	0	964	16	0
52	RX	725	0	778	9	0
52	YX	725	0	778	14	0
53	RY	818	0	911	24	0
53	YY	818	0	910	21	0
54	RZ	1461	0	1493	32	0
54	YZ	1529	0	1551	29	0
55	QA	87	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	1	0	0	0	0
55	R0	2	0	0	0	0
55	R1	1	0	0	0	0
55	R3	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	429	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	89	0	0	0	0
55	XE	1	0	0	0	0
55	Y1	1	0	0	0	0
55	Y2	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	439	0	0	0	0
55	YB	8	0	0	0	0
55	YD	1	0	0	0	0
55	YE	2	0	0	0	0
55	YF	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	1	0
All	All	292039	0	197760	3309	1

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 7.

The worst 5 of 3309 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)
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:98:LEU:CD2	40:RH:125:VAL:HG11	1.44	1.45
29:Y5:32:PRO:CA	29:Y5:32:PRO:N	1.69	1.44
30:R6:16:CYS:CB	30:R6:16:CYS:SG	2.06	1.44
14:QN:24:CYS:SG	14:QN:40:CYS:CB	2.14	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.70	0.50

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	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	72
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	68
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	68
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	22	61
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	61
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	13 (10%)	1 (1%)	19	58
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	54
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	19	58
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	9	42
13	XM	112/126 (89%)	101 (90%)	10 (9%)	1 (1%)	17	56
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
14	XN	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	28
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	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	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	30
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	4	30
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	13 (30%)	3 (7%)	1	13
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	41
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	4	29
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	22	61
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	34	72
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	34
37	YE	203/206 (98%)	163 (80%)	38 (19%)	2 (1%)	15	54
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	54
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	68
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	64
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	9	42
40	YH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	4	31
41	RI	144/148 (97%)	115 (80%)	23 (16%)	6 (4%)	3	23
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	5	32
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	61
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	22	61
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	7	39
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	22	61
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	22	61
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	61
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	17	56
47	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	17	56
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	5	33
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	54
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	6	37
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	3	26
All	All	11414/12128 (94%)	10111 (89%)	1217 (11%)	86 (1%)	19	58

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR

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	203/220 (92%)	200 (98%)	3 (2%)	65	84
2	XB	204/220 (93%)	203 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	86
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	86
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	94
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	88
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	91
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	79
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	79
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	88
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	99 (96%)	4 (4%)	32	64
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	46 (94%)	3 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	86
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	58
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	47	75
25	Y1	78/83 (94%)	77 (99%)	1 (1%)	69	86
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	83
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	39 (95%)	2 (5%)	25	59
29	R5	51/52 (98%)	50 (98%)	1 (2%)	55	79
29	Y5	51/52 (98%)	47 (92%)	4 (8%)	12	42
30	R6	51/52 (98%)	48 (94%)	3 (6%)	19	53
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	53
36	RD	214/218 (98%)	212 (99%)	2 (1%)	78	90
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49	76
37	YE	165/166 (99%)	162 (98%)	3 (2%)	59	81
38	RF	161/166 (97%)	158 (98%)	3 (2%)	57	80
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	155 (100%)	0	100	100
39	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21	54
40	YH	145/148 (98%)	142 (98%)	3 (2%)	53	79
41	RI	122/124 (98%)	122 (100%)	0	100	100
41	YI	122/124 (98%)	118 (97%)	4 (3%)	38	68
42	RN	117/119 (98%)	116 (99%)	1 (1%)	78	90
42	YN	117/119 (98%)	115 (98%)	2 (2%)	60	82
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	97 (97%)	3 (3%)	41	71
44	RP	116/116 (100%)	115 (99%)	1 (1%)	78	90
44	YP	114/116 (98%)	114 (100%)	0	100	100
45	RQ	111/111 (100%)	111 (100%)	0	100	100
45	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	90
46	RR	100/101 (99%)	98 (98%)	2 (2%)	55	79
46	YR	100/101 (99%)	99 (99%)	1 (1%)	76	88
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47	75
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60	82
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	30	63
52	YX	74/78 (95%)	72 (97%)	2 (3%)	44	73
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	71	87
All	All	9648/10066 (96%)	9536 (99%)	112 (1%)	71	87

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	XB	21	ARG
12	XL	89	ARG
49	YU	92	ARG
3	XC	162	GLN
6	XF	80	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	RR	16	HIS
47	RS	38	GLN
37	YE	132	HIS
39	RG	79	ASN
11	XK	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	309 (20%)	9 (0%)
1	XA	1514/1521 (99%)	322 (21%)	10 (0%)
22	QV	76/77 (98%)	17 (22%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QX	18/19 (94%)	4 (22%)	1 (5%)
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2915 (98%)	617 (21%)	40 (1%)
34	YA	2880/2915 (98%)	634 (22%)	44 (1%)
35	RB	119/122 (97%)	21 (17%)	1 (0%)
35	YB	119/122 (97%)	25 (21%)	1 (0%)
All	All	9207/9308 (98%)	1975 (21%)	109 (1%)

5 of 1975 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	38	G
1	QA	39	G

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	RA	2712(A)	U
1	XA	1504	G
34	YA	2439	A
34	RA	2776	A
1	XA	328	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	1MG	XV	37	22	18,26,27	1.40	3 (16%)	19,39,42	1.97	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	1MG	QV	37	22	18,26,27	2.26	4 (22%)	19,39,42	2.47	3 (15%)

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
22	1MG	XV	37	22	-	2/3/25/26	0/3/3/3
22	1MG	QV	37	22	-	2/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C6-C5	6.87	1.52	1.41
22	XV	37	1MG	C6-C5	4.58	1.48	1.41
22	QV	37	1MG	C5-C4	3.99	1.51	1.40
22	QV	37	1MG	C2-N3	2.72	1.38	1.34
22	QV	37	1MG	C6-N1	2.70	1.42	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	37	1MG	C2-N3-C4	8.22	124.75	115.36
22	XV	37	1MG	C2-N3-C4	6.46	122.73	115.36
22	QV	37	1MG	C1'-N9-C4	5.07	135.56	126.64
22	XV	37	1MG	C6-C5-C4	-3.44	117.75	119.96
22	QV	37	1MG	C4-C5-N7	-3.16	106.10	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	37	1MG	O4'-C4'-C5'-O5'
22	XV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	XV	37	1MG	2	0
22	QV	37	1MG	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1110 ligands modelled in this entry, 1108 are monoatomic - leaving 2 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	$\# Z > 2$
56	SF4	QD	301	4	0,12,12	0.00	-	-		
56	SF4	XD	301	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	RI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RI	82:ARG	C	83:ALA	N	1.18

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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