



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 08:36 pm BST

PDB ID : 6BUW
Title : Thermus thermophilus 70S complex containing 16S G299A ram mutation and empty A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-11
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)	:	2.11

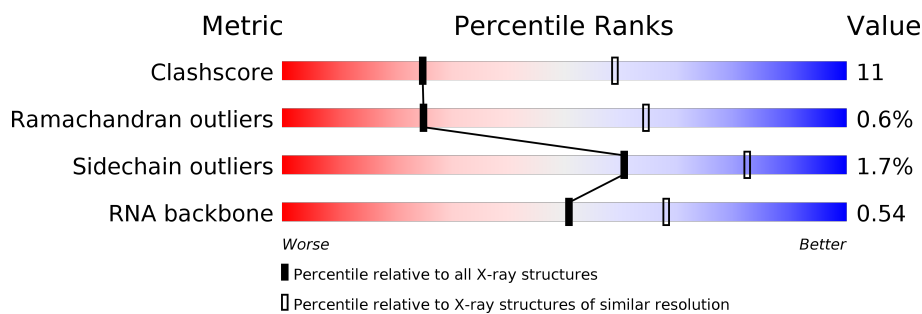
1 Overall quality at a glance

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)









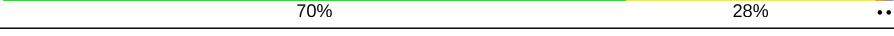


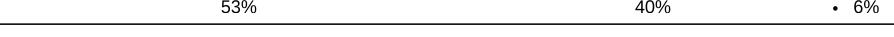

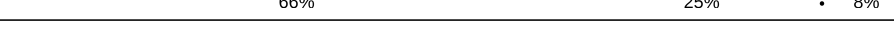


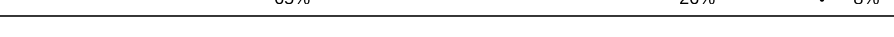

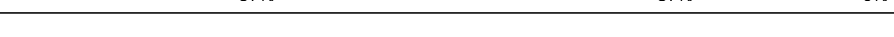
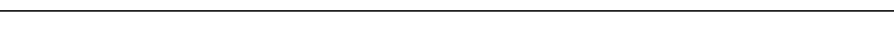

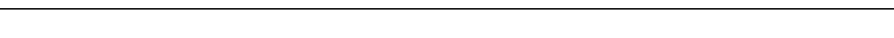
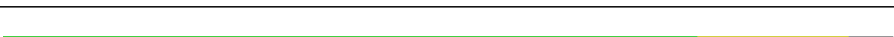


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1508	
1	XA	1508	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	
4	QD	209	


























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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	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	
16	XP	88	

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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	
28	RF	210	
28	YF	210	
29	RG	182	


























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Mol	Chain	Length	Quality of chain
29	YG	182	
30	RH	180	
30	YH	180	
31	RI	148	
31	YI	148	
32	RN	140	
32	YN	140	
33	RO	122	
33	YO	122	
34	RP	150	
34	YP	150	
35	RQ	141	
35	YQ	141	
36	RR	118	
36	YR	118	
37	RS	112	
37	YS	112	
38	RT	146	
38	YT	146	
39	RU	118	
39	YU	118	
40	RV	101	
40	YV	101	
41	RW	113	
41	YW	113	


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Mol	Chain	Length	Quality of chain
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	
53	R8	65	
53	Y8	65	
54	R9	37	

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Mol	Chain	Length	Quality of chain
54	Y9	37	 <div>62% 35%</div>

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	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291948 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
			32246	14353	5981	10413	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32248	14354	5984	10411	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	299	A	G	engineered mutation	GB 55771382
XA	299	A	G	engineered mutation	GB 55771382

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	119	Total	C	N	O	S	0	0	0
			946	585	195	164	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			

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	12	Total	C	N	O	P	0	0	0
			261	117	51	81	12			
23	XX	11	Total	C	N	O	P	0	0	0
			239	107	46	75	11			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R1	96	Total	C	N	O	S	0	0	0
			755	475	149	130	1			
46	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
49	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	180	Total	Mg	0	0
			180	180		
55	RP	3	Total	Mg	0	0
			3	3		
55	QX	2	Total	Mg	0	0
			2	2		
55	YA	515	Total	Mg	0	0
			515	515		
55	Y5	1	Total	Mg	0	0
			1	1		
55	RT	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	2	Total	Mg	0	0
			2	2		
55	XS	1	Total	Mg	0	0
			1	1		
55	YD	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QV	6	Total 6	Mg 6	0	0
55	RX	1	Total 1	Mg 1	0	0
55	Y8	1	Total 1	Mg 1	0	0
55	YO	1	Total 1	Mg 1	0	0
55	XA	171	Total 171	Mg 171	0	0
55	YY	1	Total 1	Mg 1	0	0
55	RQ	2	Total 2	Mg 2	0	0
55	R0	2	Total 2	Mg 2	0	0
55	QL	1	Total 1	Mg 1	0	0
55	YU	1	Total 1	Mg 1	0	0
55	RU	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	1	Total 1	Mg 1	0	0
55	YQ	3	Total 3	Mg 3	0	0
55	RY	1	Total 1	Mg 1	0	0
55	QC	1	Total 1	Mg 1	0	0
55	YX	2	Total 2	Mg 2	0	0
55	RD	1	Total 1	Mg 1	0	0
55	R1	2	Total 2	Mg 2	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	R5	1	Total 1	Mg 1	0	0
55	Y0	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	RA	493	Total 493	Mg 493	0	0
55	YP	3	Total 3	Mg 3	0	0
55	RE	4	Total 4	Mg 4	0	0
55	XL	1	Total 1	Mg 1	0	0
55	YB	10	Total 10	Mg 10	0	0
55	RW	1	Total 1	Mg 1	0	0
55	RI	1	Total 1	Mg 1	0	0
55	XV	8	Total 8	Mg 8	0	0
55	RB	10	Total 10	Mg 10	0	0
55	RF	1	Total 1	Mg 1	0	0
55	XM	1	Total 1	Mg 1	0	0
55	YE	4	Total 4	Mg 4	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	YY	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	RY	1	Total	Zn	0	0
			1	1		
57	Y4	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		

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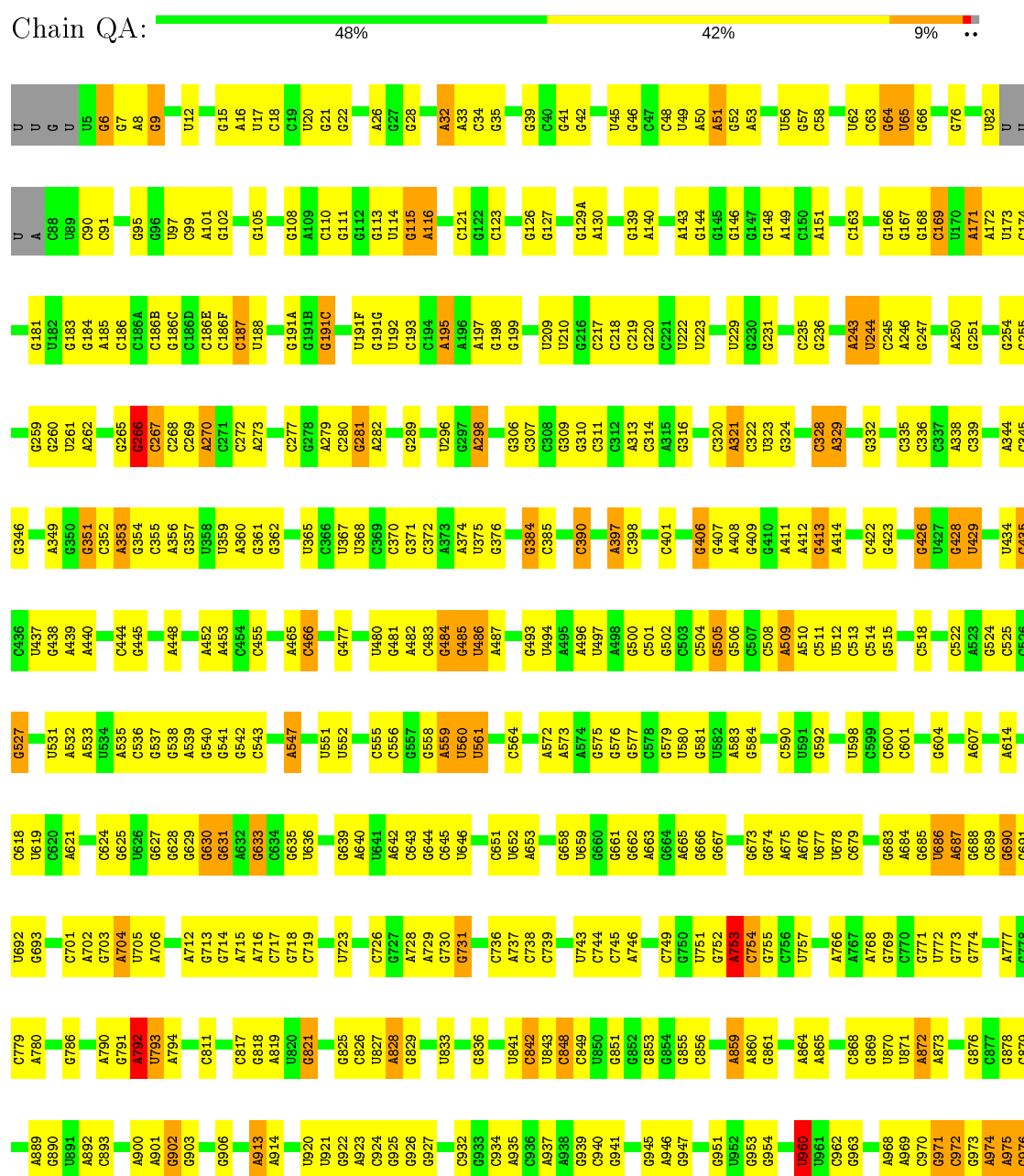
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R4	1	Total 1	Zn 1	0	0
57	R9	1	Total 1	Zn 1	0	0

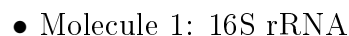
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

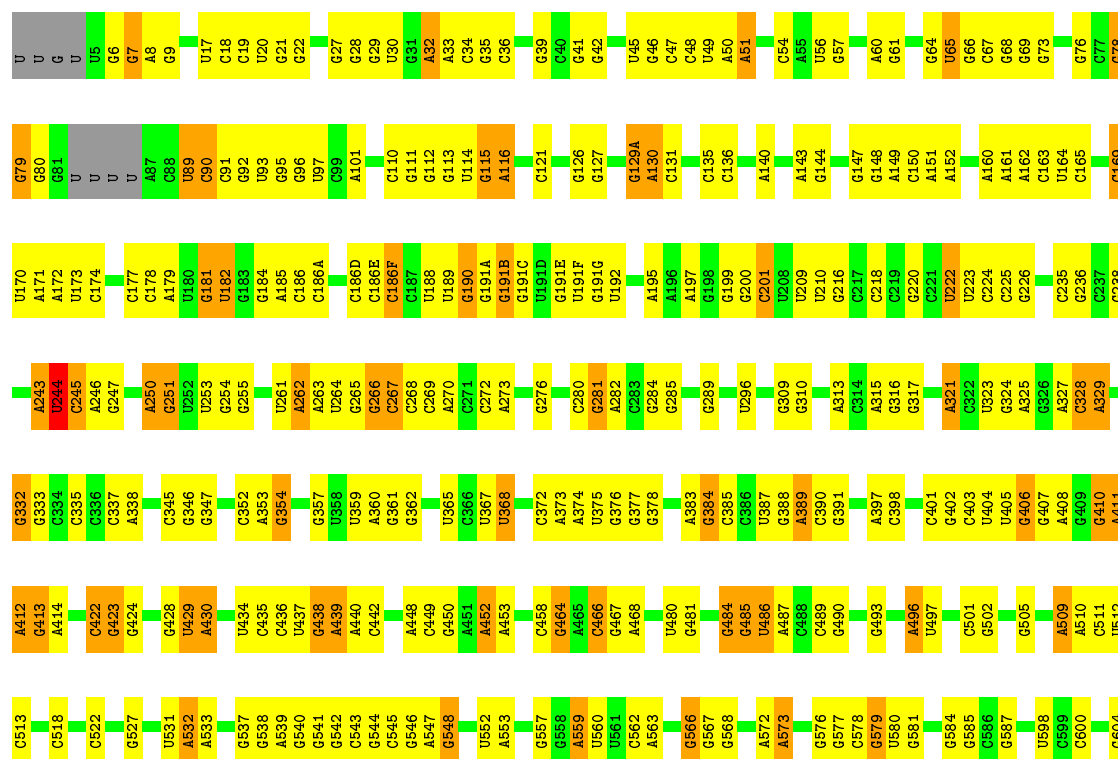
Note EDS failed to run properly.

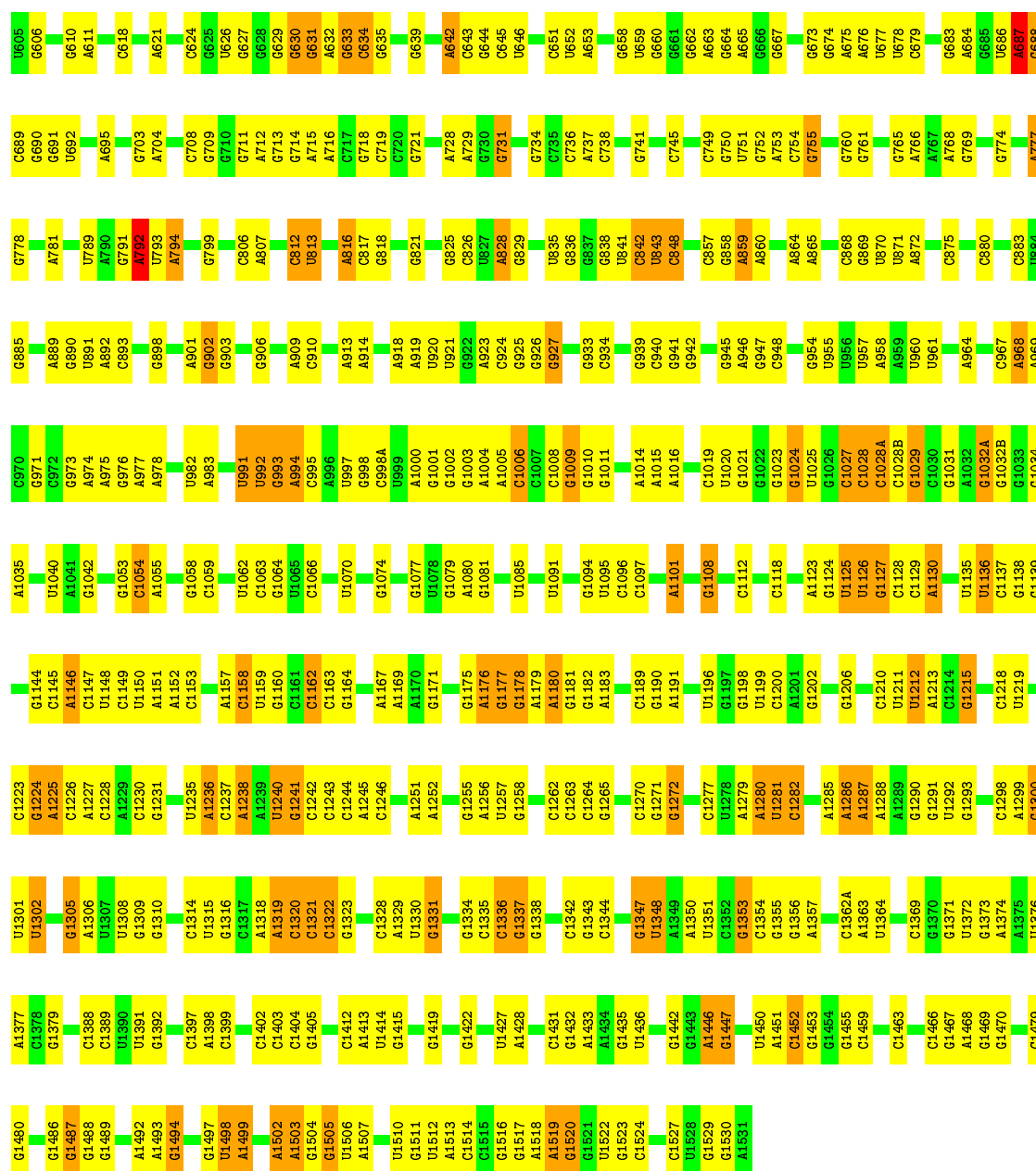
• Molecule 1: 16S rRNA



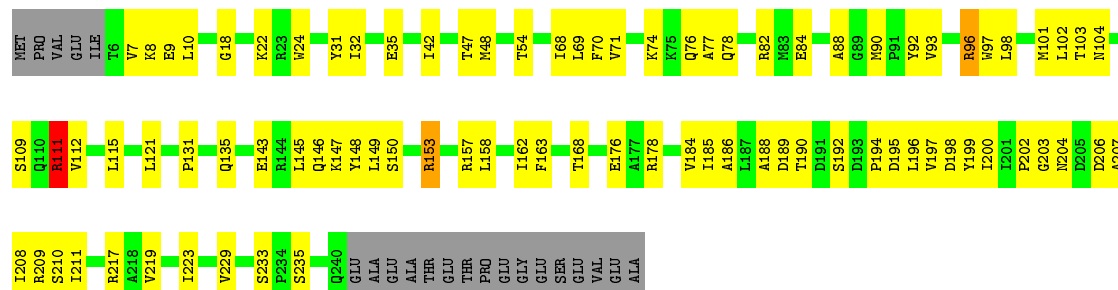


Chain XA: 

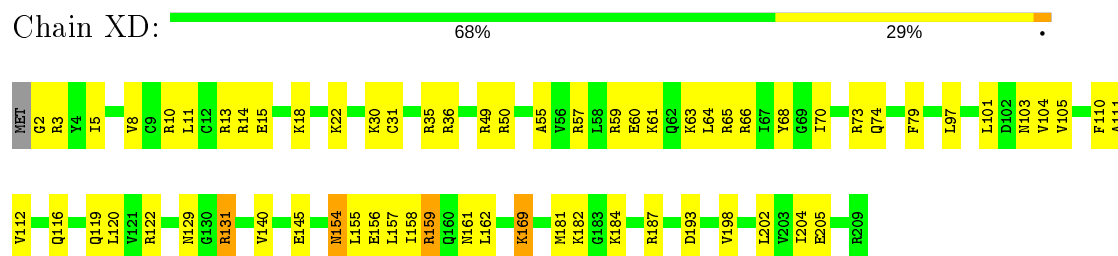




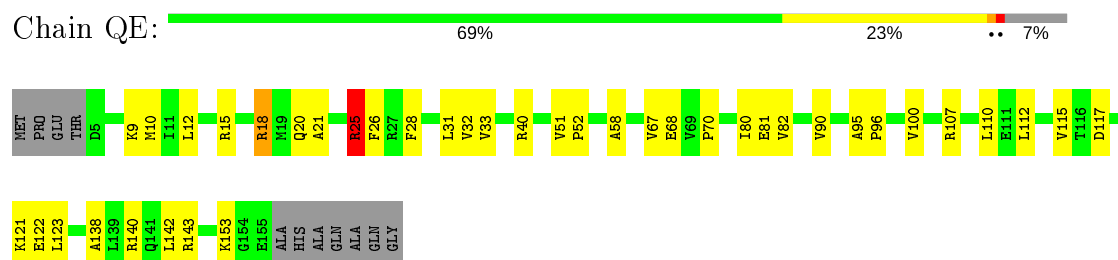
• Molecule 2: 30S ribosomal protein S2



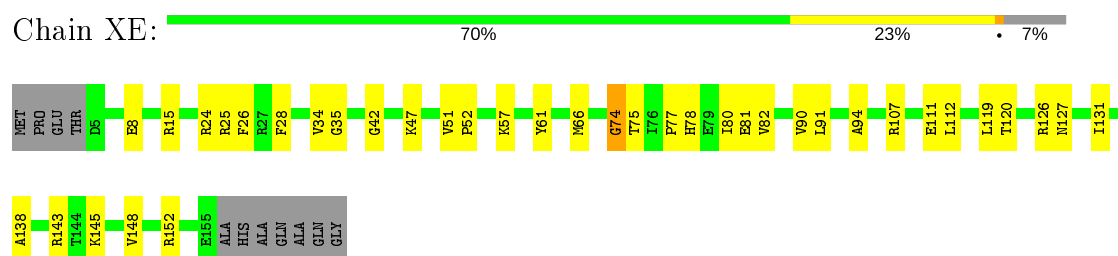
- Molecule 4: 30S ribosomal protein S4



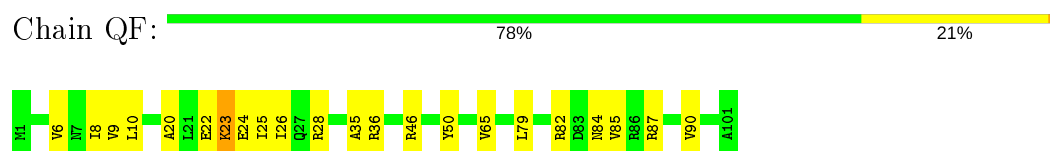
- Molecule 5: 30S ribosomal protein S5



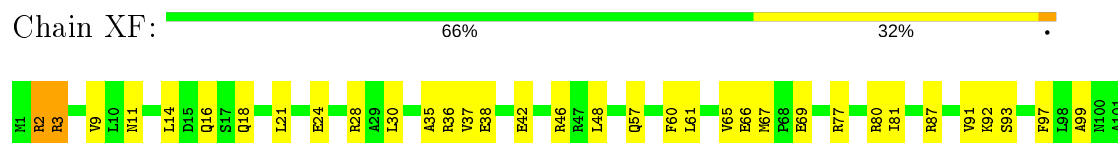
- Molecule 5: 30S ribosomal protein S5



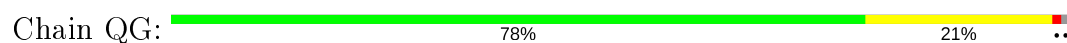
- Molecule 6: 30S ribosomal protein S6

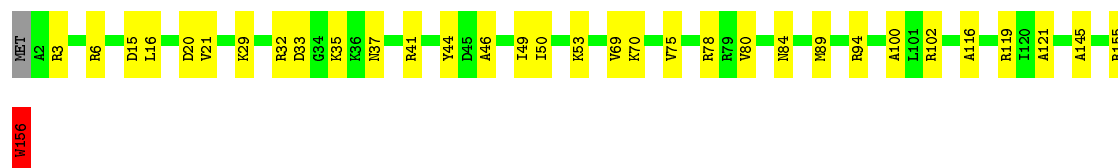


- Molecule 6: 30S ribosomal protein S6



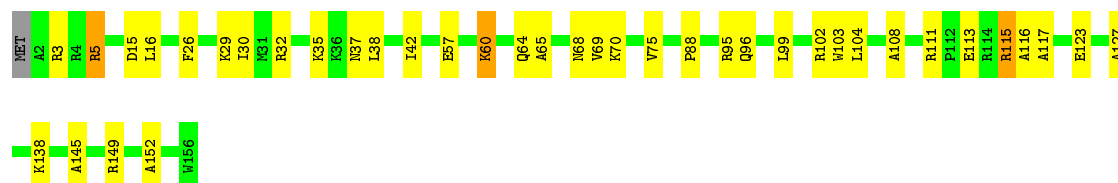
- Molecule 7: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S7

Chain XG: 74% 23% ..



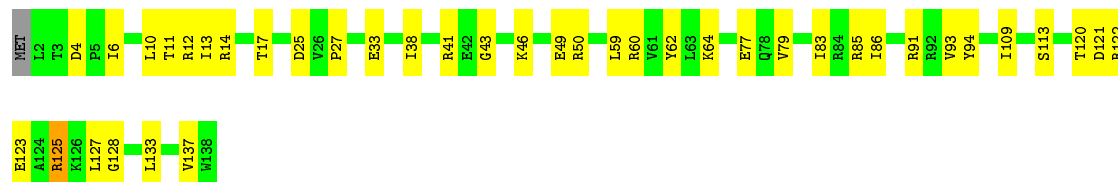
- Molecule 8: 30S ribosomal protein S8

Chain QH: 61% 38% .



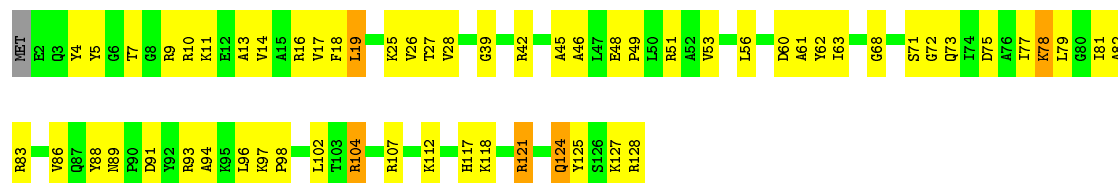
- Molecule 8: 30S ribosomal protein S8

Chain XH: 70% 28% ..



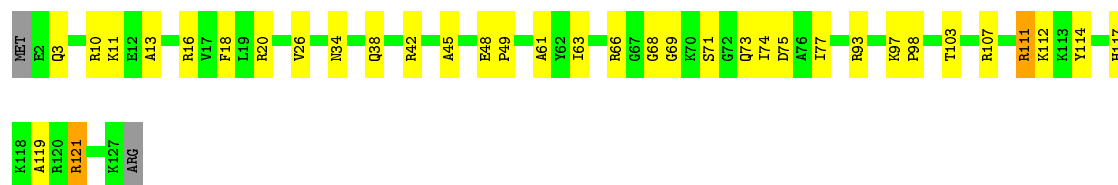
- Molecule 9: 30S ribosomal protein S9

Chain QI: 52% 43% . .

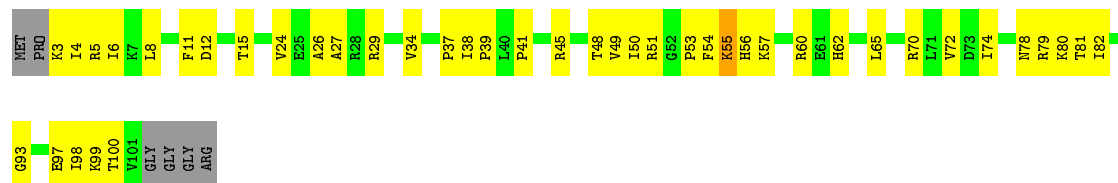


- Molecule 9: 30S ribosomal protein S9

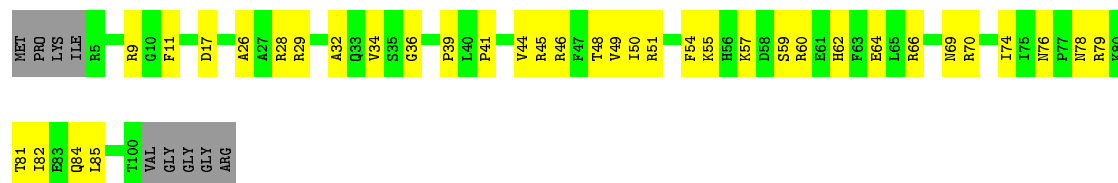
Chain XI: 71% 26% . .



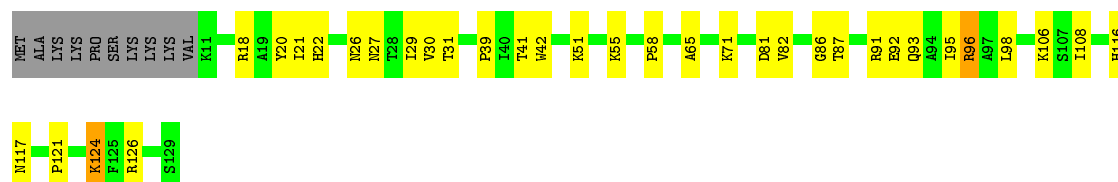
- Molecule 10: 30S ribosomal protein S10



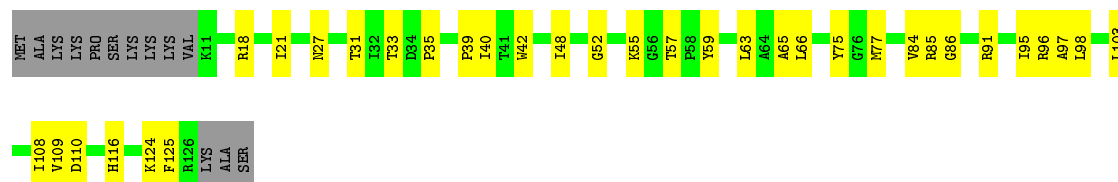
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

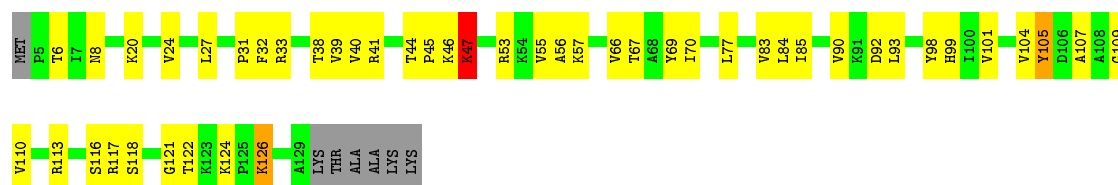


- Molecule 11: 30S ribosomal protein S11



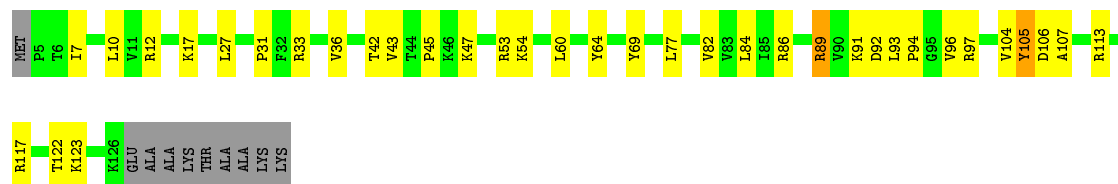
- Molecule 12: 30S ribosomal protein S12

Chain QL:  59% 33% 5%



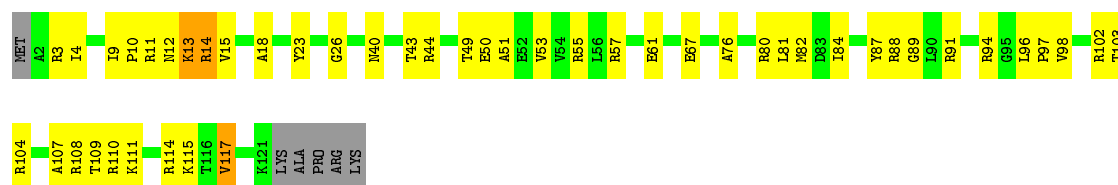
- Molecule 12: 30S ribosomal protein S12

Chain XL:  65% 26% 8%



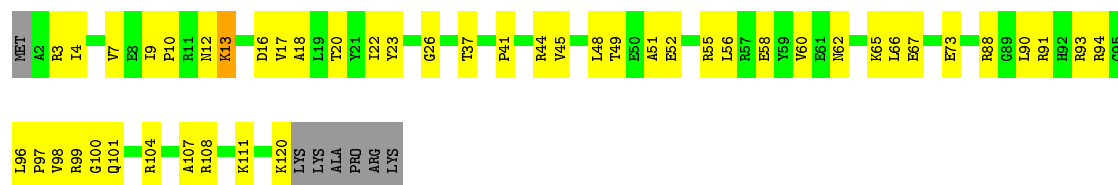
- Molecule 13: 30S ribosomal protein S13

Chain QM:  58% 35% 5%



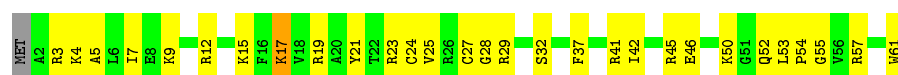
- Molecule 13: 30S ribosomal protein S13

Chain XM:  57% 37% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  51% 46% 2%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  66% 28% 5%



- Molecule 15: 30S ribosomal protein S15

Chain QQ: 74% 25% .



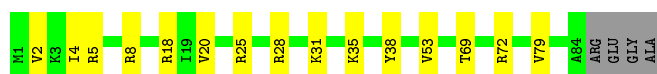
- Molecule 15: 30S ribosomal protein S15

Chain XO: 75% 22% .



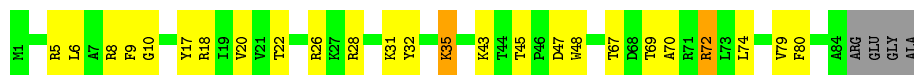
- Molecule 16: 30S ribosomal protein S16

Chain QP: 78% 17% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP: 67% 26% 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ: 73% 20% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 66% 29% 5%

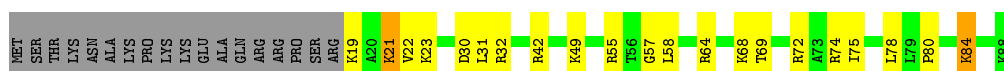


- Molecule 18: 30S ribosomal protein S18

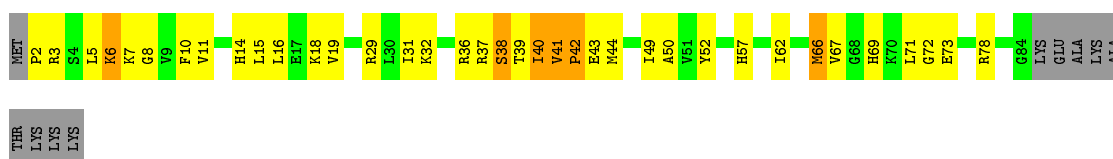
Chain QR: 52% 27% 20%



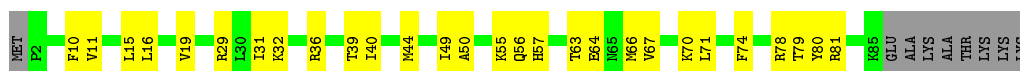
- Molecule 18: 30S ribosomal protein S18



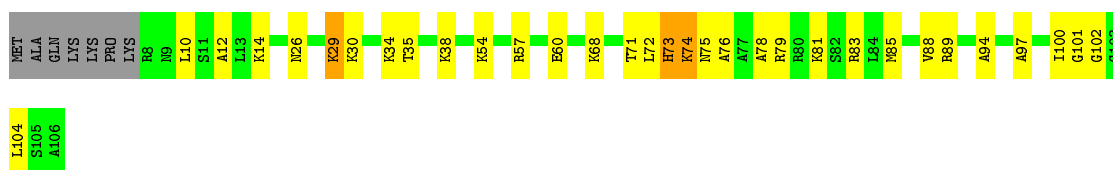
- Molecule 19: 30S ribosomal protein S19



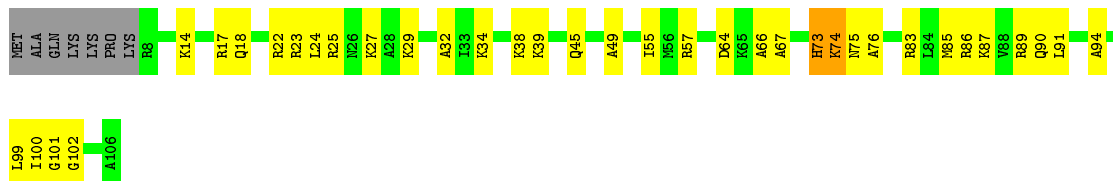
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx





- Molecule 21: 30S ribosomal protein Thx

Chain XU: 67% 22% 7%



- Molecule 22: P-site tRNA fMet

Chain QV: 55% 31% 14%



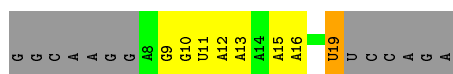
- Molecule 22: P-site tRNA fMet

Chain XV: 65% 26% 8%



- Molecule 23: messenger RNA

Chain QX: 16% 28% 52%



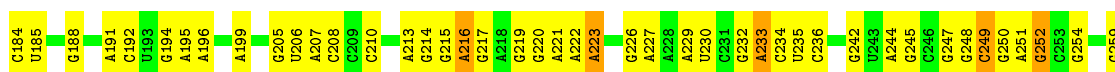
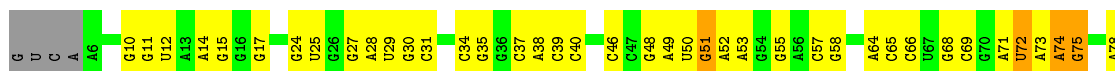
- Molecule 23: messenger RNA

Chain XX: 12% 24% 8% 56%



- Molecule 24: 23S rRNA

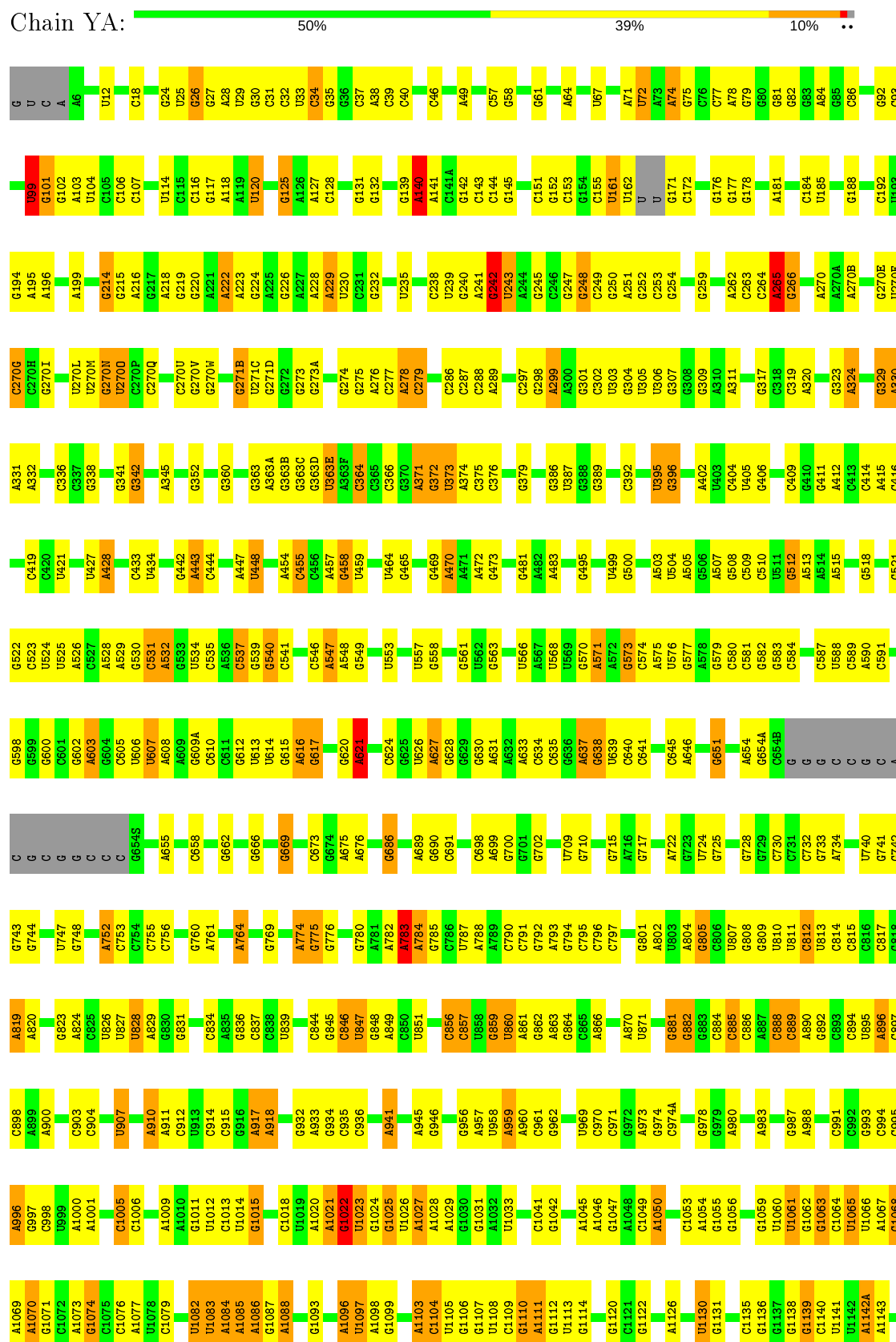
Chain RA: 51% 39% 8%



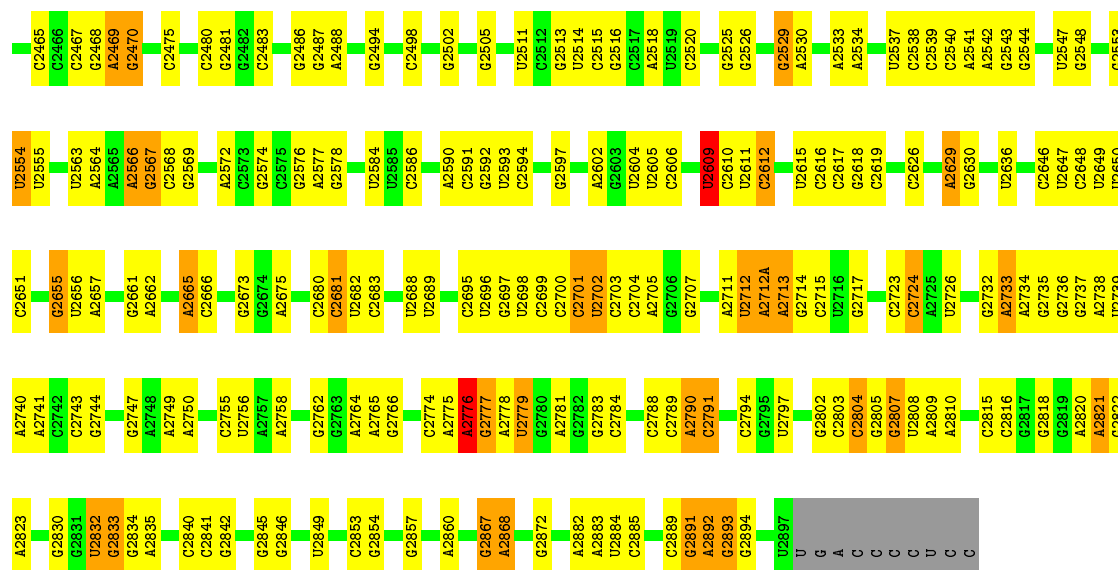


G2838	A2753	U2649	G2559	G2459	G2371	C2292	C2188	U2113	A2020	G1920	G1799	G1685	A1583	G1499
G2839	U2754	U2650	C2560	U2460	G2372	C2293	U2189	A2114	C2021	U1923	C1800	C1686	C1585	G1500
G2840	G2755	G2651	A2561	G2461	G2373	U2296	G2190	G2115	U2022	G1923	G1801	U1687	A1586	C1501
G2843	U2756	A2654	U2562	U2462	G2374	U2297	G2191	G2116	G2023	G1929	A1802	U1688	A1587	C1502
G2844	G2757	G2655	U2563	A2469	G2375	C2298	G2192	U2118	G2029	G1930	A1803	C1689	C1588	U1503
G2845	A2758	U2656	A2564	G2470	G2376	G2299	A2198	A2119	A2030	U1931	A1812	A1698	C1589	A1504
G2846	G2761	A2656	A2565	G2471	A2377	G2300	G2199	G2120	A2031	U1931	A1813	A1699	U1590	C1505
G2847	G2762	G2657	G2566	C2474	G2378	G2303	G2210	G2121	A2032	G1935	G1816	U1709	C1591	C1506
G2848	A2765	C2568	G2567	C2475	G2379	G2304	G2211	G2122	A2033	G1936	G1817	C1710	A1592	A1507
G2849	G2766	G2569	G2568	G2476	C2380	G2305	A2212	G2123	G2034	A1937	G1818	C1711	C1593	C1508
G2852	G2767	G2572	G2570	A2478	G2382	C2306	U2213	G2124	G2037	A1938	A1819	G1725	G1594	C1509
G2853	A2776	G2573	G2571	G2479	G2383	C2307	G2215	G2125	G2038	U1939	A1820	G1728	A1510	A1510
G2854	G2777	G2574	G2572	C2480	G2384	G2308	G2216	A2126	C2039	G1945	U1821	A1729	A1511	A1511
G2858	A2778	A2670	G2575	G2481	G2385	G2309	G2217	A2127	C2040	G1946	A1822	A1730	C1598	G1512
G2859	U2779	G2680	G2576	C2482	G2386	A2310	G2224	C2128	C2043	A1952	G1826	G1731	C1599	U1513
G2860	G2780	U2688	G2577	C2483	G2387	U2311	A2225	U2130	C2055	A1952	A1827	G1732	C1515	U1514
A2860	A2781	G2689	U2580	G2484	G2388	G2312	G2226	G2131	G2056	U1955	G1831	G1733	U1516	U1516
G2861	G2782	C2690	G2581	G2485	C2389	G2313	G2227	G2132	G2057	U1956	A1832	G1734	G1605	U1520
G2862	C2784	G2691	G2582	C2501	G2400	G2314	G2228	U2133	A2059	C1958	C1742	C1743	C1606	G1521
G2863	U2785	C2692	U2583	G2502	G2401	G2315	G2229	G2134	A2060	U1963	A1843	G1744	G1607	G1522
G2864	U2786	G2693	U2584	G2503	U2402	G2316	G2230	A2135	G2061	G1964	A1844	G1745	A1608	A1609
G2867	C2787	C2694	G2585	A2504	C2403	G2317	G2231	G2136	A2062	G1967	A1845	G1746	A1610	A1610
A2868	G2788	G2695	C2586	G2505	C2404	G2318	G2232	C2137	C2064	G1968	A1846	G1747	G1611	G1611
G2869	C2789	U2696	U2587	G2506	G2405	G2319	G2233	G2138	C2065	U1969	G1847	G1748	A1616	A1529
G2870	A2790	G2697	G2588	C2507	G2406	G2320	U2243	G2141	U2068	A1970	A1848	G1749	G1617	G1534
G2871	C2791	U2700	G2589	G2508	U2407	G2321	U2244	G2142	G2069	A1971	G1849	G1750	G1627	G1535
G2872	G2792	U2701	U2590	G2509	G2408	G2322	G2245	G2143	G2070	A1972	G1850	G1751	G1628	U1536
G2873	G2793	G2702	U2591	C2510	G2409	G2323	G2246	G2144	A2071	G1973	C1870	G1752	U1629	A1537
G2874	U2797	C2703	G2592	G2511	G2410	G2324	A2247	G2145	G1974	C1974	A1871	A1760	G1632	G1538
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C	A2868	G2772	C2656	U2588	A2496	G2390	A2324	G2215	G2151					
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● Molecule 24: 23S rRNA

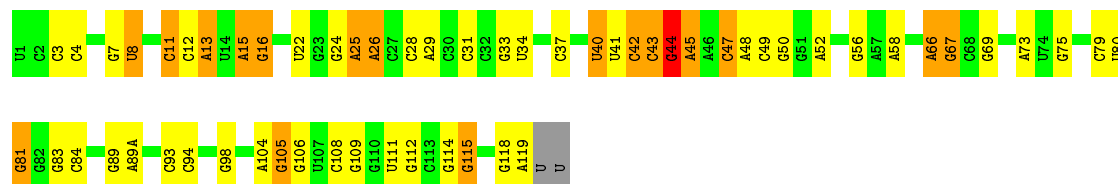


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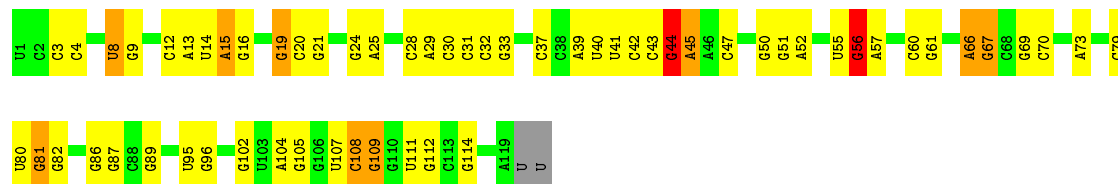
• Molecule 25: 5S rRNA

Chain RB: 51% 33% 14% ..



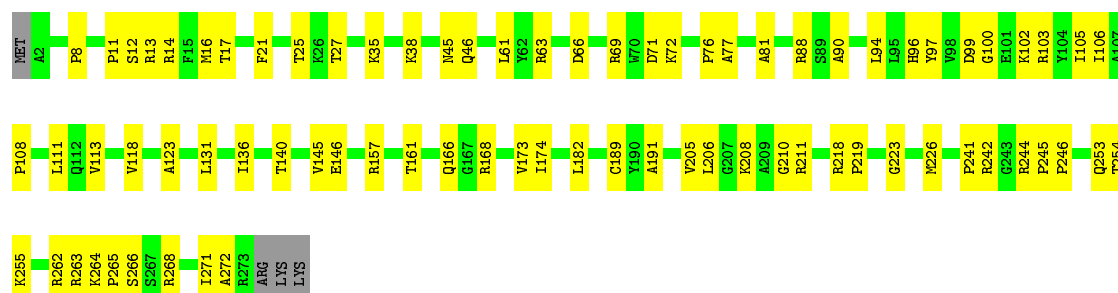
• Molecule 25: 5S rRNA

Chain YB: 49% 40% 7% ..

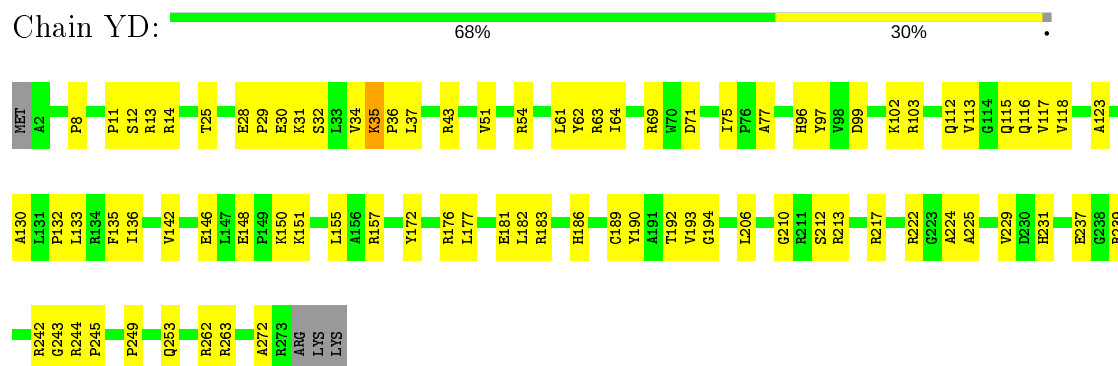


• Molecule 26: 50S ribosomal protein L2

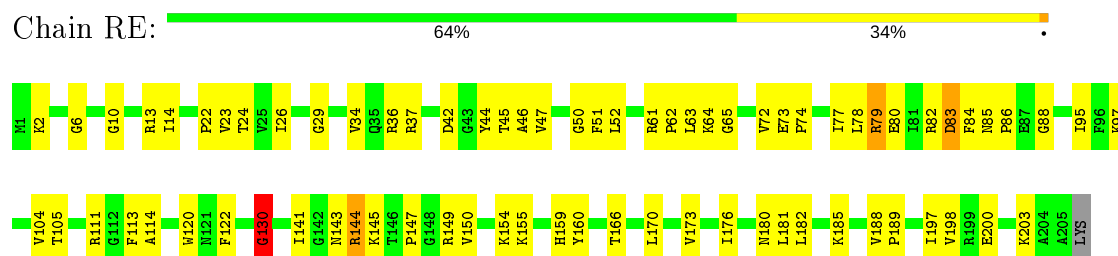
Chain RD: 70% 28% .



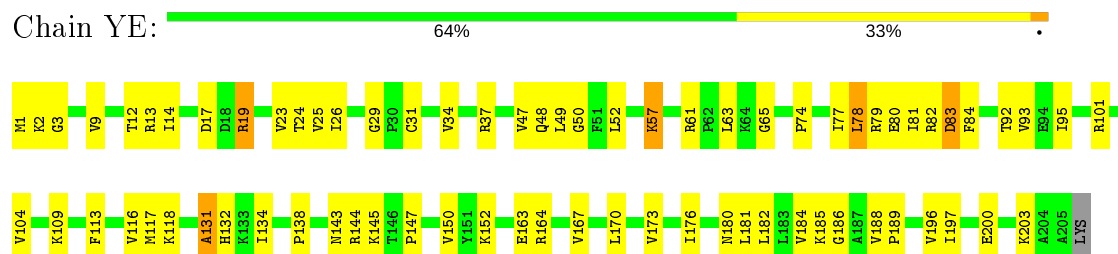
- Molecule 26: 50S ribosomal protein L2



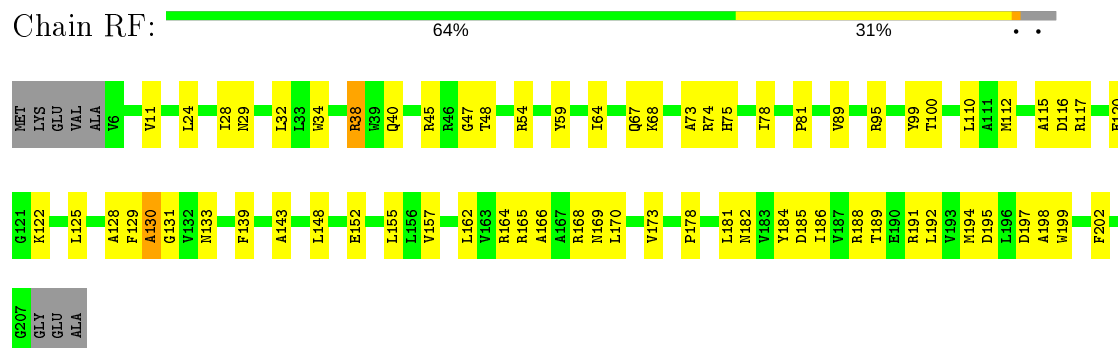
- Molecule 27: 50S ribosomal protein L3



- Molecule 27: 50S ribosomal protein L3

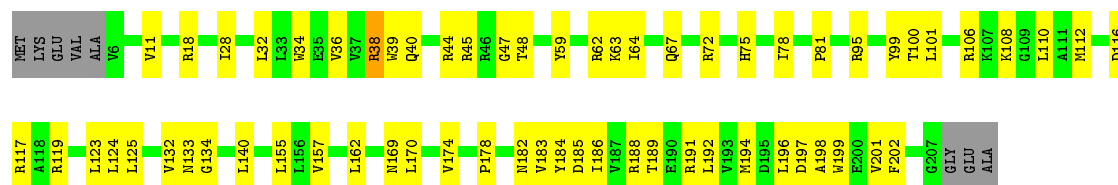


- Molecule 28: 50S ribosomal protein L4

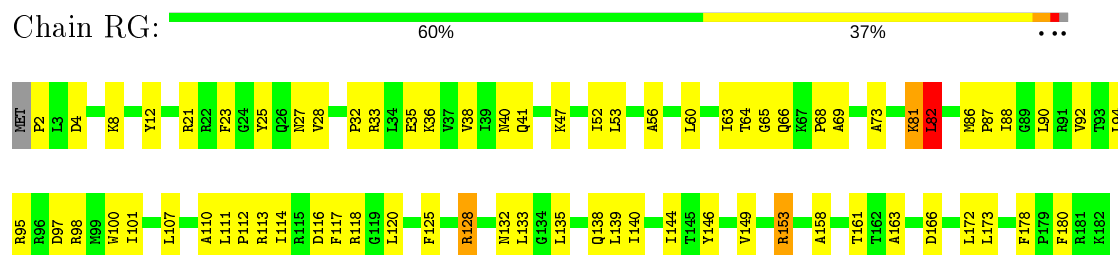


- Molecule 28: 50S ribosomal protein L4

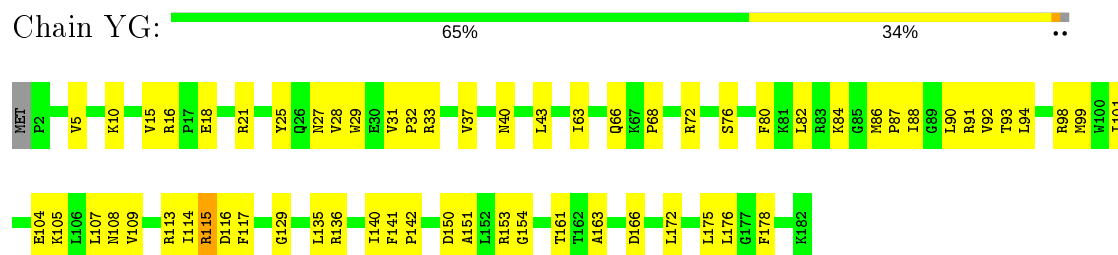




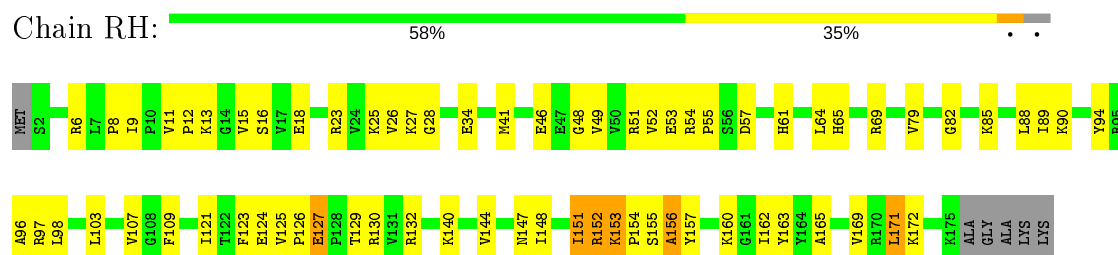
• Molecule 29: 50S ribosomal protein L5



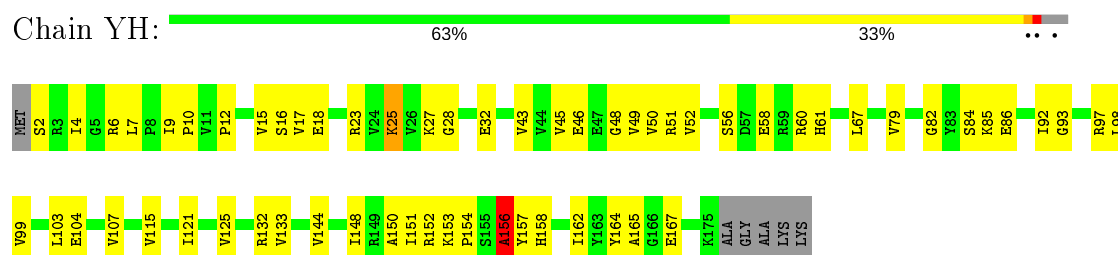
• Molecule 29: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L6

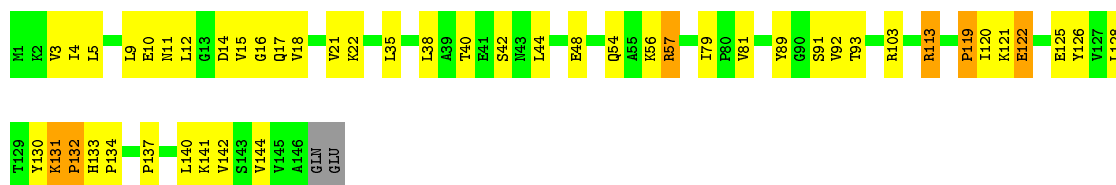


• Molecule 30: 50S ribosomal protein L6



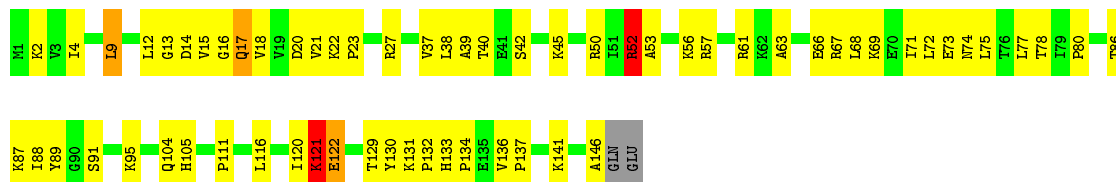
• Molecule 31: 50S ribosomal protein L9





- Molecule 31: 50S ribosomal protein L9

Chain YI: 56% 39% ..



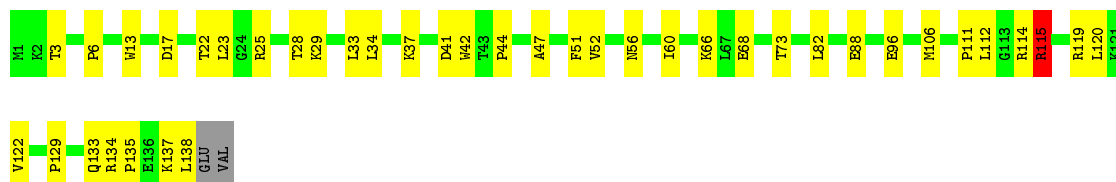
- Molecule 32: 50S ribosomal protein L13

Chain RN: 79% 20% .



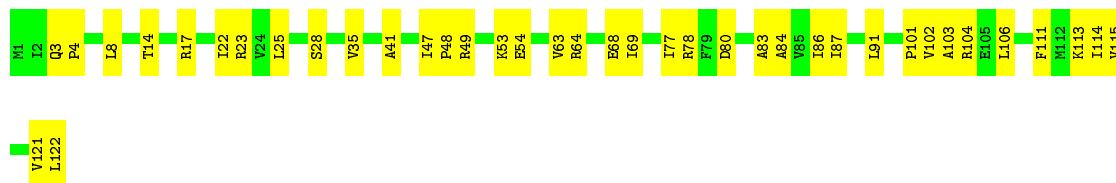
- Molecule 32: 50S ribosomal protein L13

Chain YN: 70% 28% ..



- Molecule 33: 50S ribosomal protein L14

Chain RO: 68% 32%



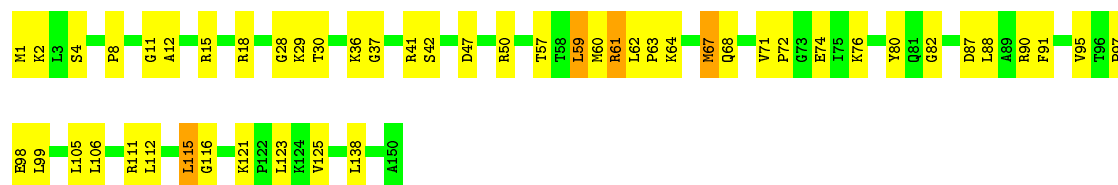
- Molecule 33: 50S ribosomal protein L14

Chain YO: 79% 21%



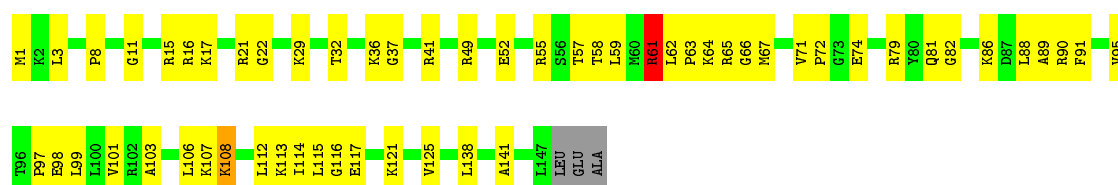
- Molecule 34: 50S ribosomal protein L15

Chain RP:  67% 31% .



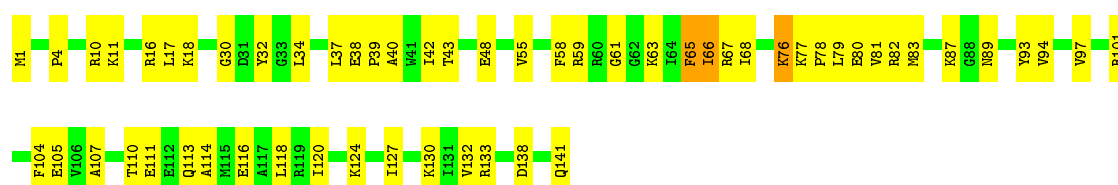
- Molecule 34: 50S ribosomal protein L15

Chain YP:  60% 37% ..



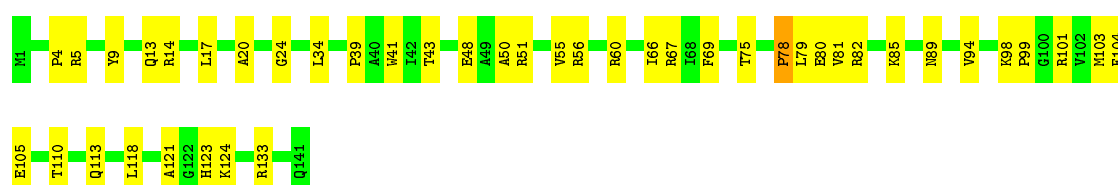
- Molecule 35: 50S ribosomal protein L16

Chain RQ:  60% 38% .



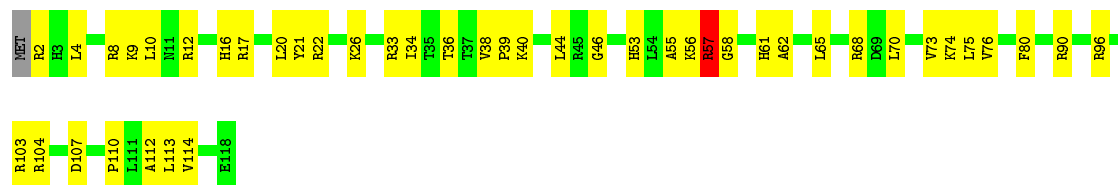
- Molecule 35: 50S ribosomal protein L16

Chain YQ:  70% 30% .

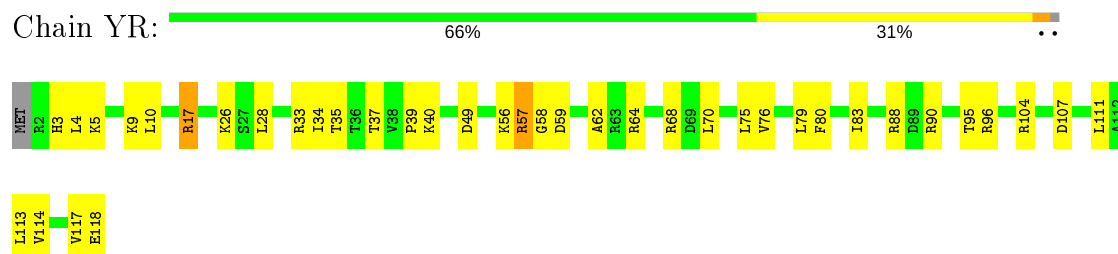


- Molecule 36: 50S ribosomal protein L17

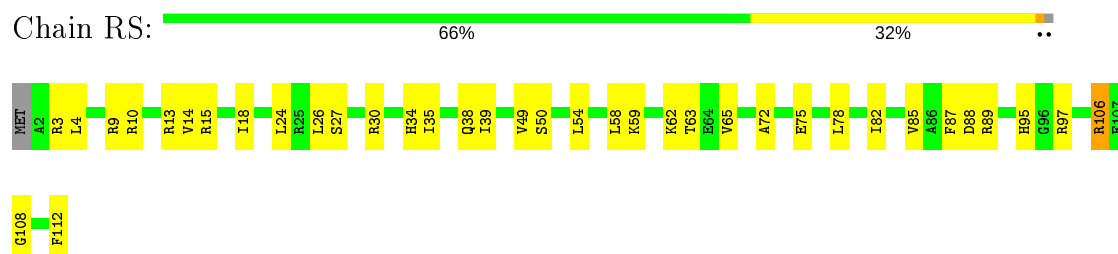
Chain RR:  62% 36% ..



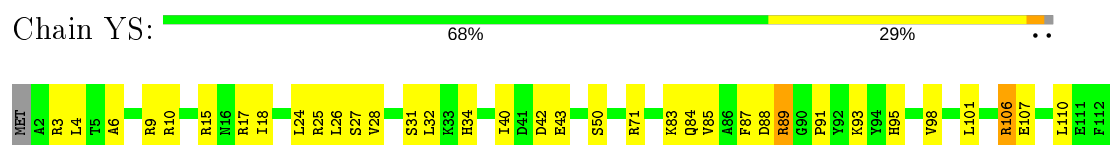
- Molecule 36: 50S ribosomal protein L17



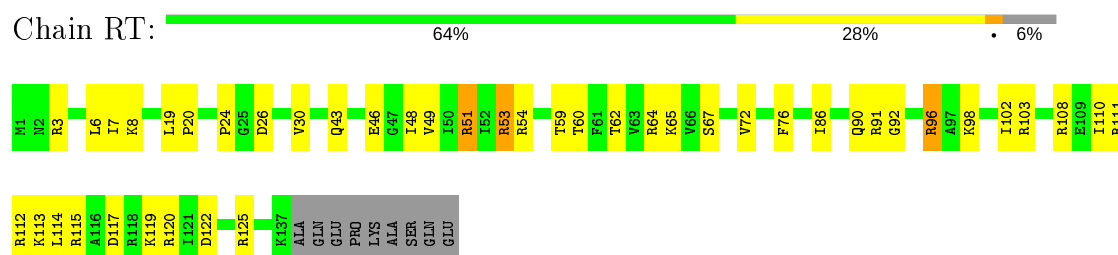
- Molecule 37: 50S ribosomal protein L18



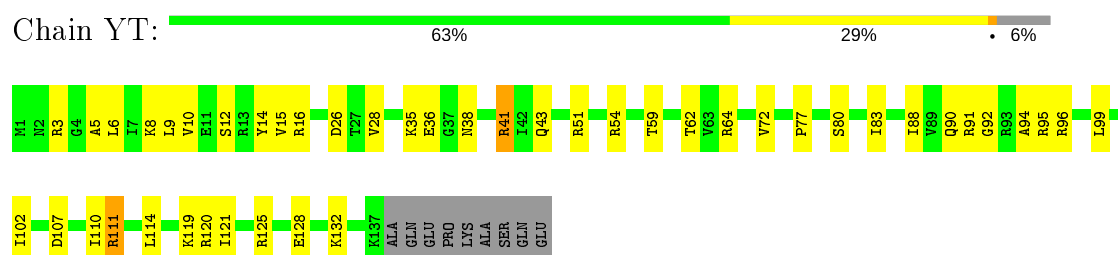
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L19



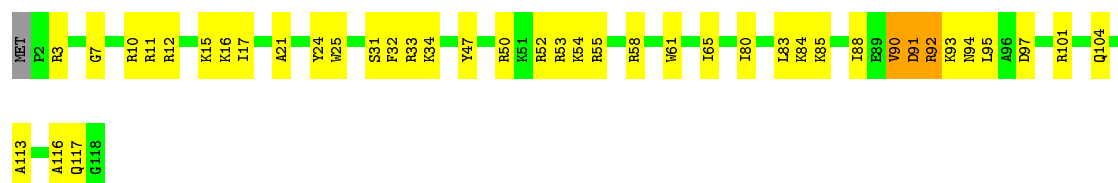
- Molecule 39: 50S ribosomal protein L20

Chain RU:  70% 25% ..



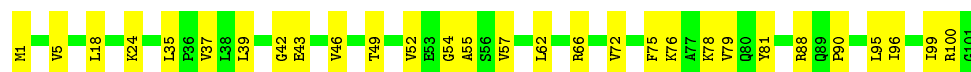
- Molecule 39: 50S ribosomal protein L20

Chain YU:  64% 32% ..




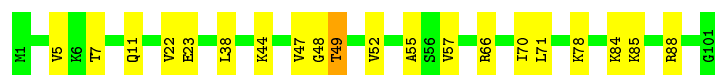
- Molecule 40: 50S ribosomal protein L21

Chain RV:  71% 29%



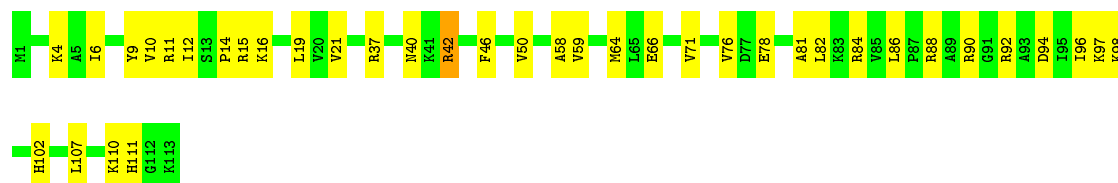
- Molecule 40: 50S ribosomal protein L21

Chain YV:  80% 19% .




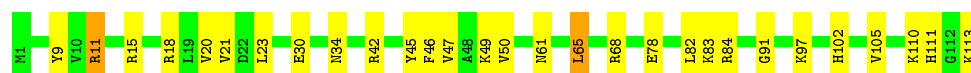
- Molecule 41: 50S ribosomal protein L22

Chain RW:  66% 33% .



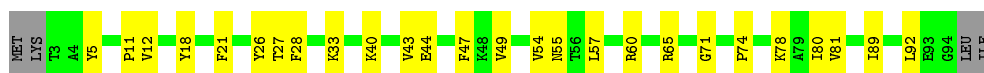
- Molecule 41: 50S ribosomal protein L22

Chain YW:  74% 24% .



- Molecule 42: 50S ribosomal protein L23

Chain RX:  69% 27% .



- Molecule 42: 50S ribosomal protein L23

Chain YX: 76% 20% .



- Molecule 43: 50S ribosomal protein L24

Chain RY: 79% 18% .



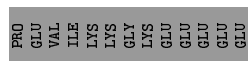
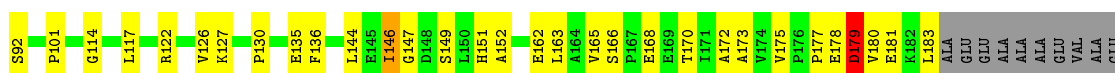
- Molecule 43: 50S ribosomal protein L24

Chain YY: 64% 33% . .



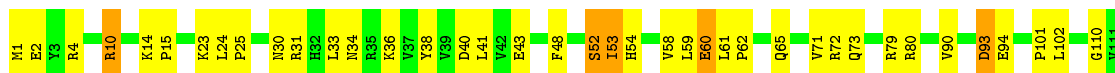
- Molecule 44: 50S ribosomal protein L25

Chain RZ: 55% 31% . 11%



- Molecule 44: 50S ribosomal protein L25

Chain YZ: 58% 27% . 11%



- Molecule 45: 50S ribosomal protein L27

Chain R0: 



- Molecule 45: 50S ribosomal protein L27

Chain Y0: 



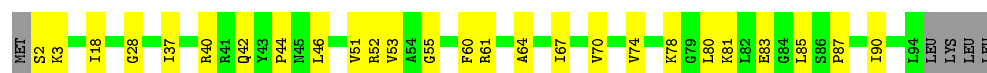
- Molecule 46: 50S ribosomal protein L28

Chain R1: 



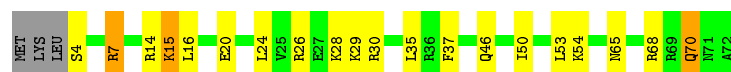
- Molecule 46: 50S ribosomal protein L28

Chain Y1: 



- Molecule 47: 50S ribosomal protein L29

Chain R2: 



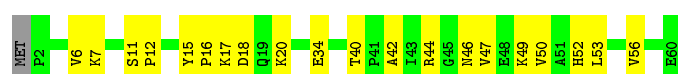
- Molecule 47: 50S ribosomal protein L29

Chain Y2: 



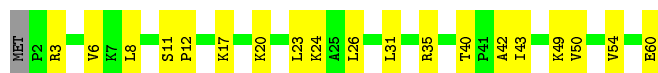
- Molecule 48: 50S ribosomal protein L30

Chain R3: 



- Molecule 48: 50S ribosomal protein L30

Chain Y3:  67% 32% .



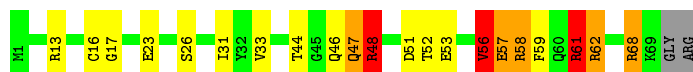
- Molecule 49: 50S ribosomal protein L31

Chain R4:  58% 30% . 6% .



- Molecule 49: 50S ribosomal protein L31

Chain Y4:  68% 18% 7% . .



- Molecule 50: 50S ribosomal protein L32

Chain R5:  73% 22% . .



- Molecule 50: 50S ribosomal protein L32

Chain Y5:  73% 25% .




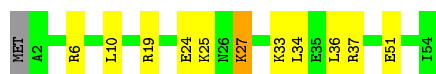
- Molecule 51: 50S ribosomal protein L33

Chain R6:  61% 35% . .



- Molecule 51: 50S ribosomal protein L33

Chain Y6:  78% 19% . .



- Molecule 52: 50S ribosomal protein L34

Chain R7:  59% 37% .



- Molecule 52: 50S ribosomal protein L34

Chain Y7:  69% 29% .



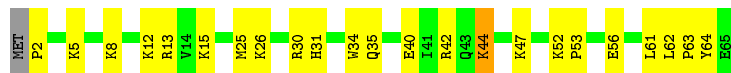
- Molecule 53: 50S ribosomal protein L35

Chain R8:  55% 37% . . .




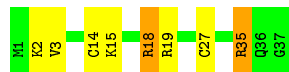
- Molecule 53: 50S ribosomal protein L35

Chain Y8:  63% 34% . .



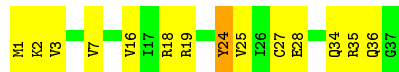
- Molecule 54: 50S ribosomal protein L36

Chain R9:  78% 16% 5%



- Molecule 54: 50S ribosomal protein L36

Chain Y9:  62% 35% .



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	210.24Å 449.36Å 618.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.99 – 3.50	Depositor
% Data completeness (in resolution range)	97.9 (121.99-3.50)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.207 , 0.250	Depositor
Wilson B-factor (Å ²)	86.9	Xtriage
Anisotropy	0.138	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291948	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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, 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	0.31	0/36097	0.87	27/56339 (0.0%)
1	XA	0.33	0/36100	0.90	26/56344 (0.0%)
2	QB	0.26	0/1942	0.55	2/2619 (0.1%)
2	XB	0.26	0/1950	0.51	0/2630
3	QC	0.26	0/1629	0.52	0/2195
3	XC	0.26	0/1629	0.51	0/2195
4	QD	0.28	0/1733	0.52	0/2318
4	XD	0.33	1/1733 (0.1%)	0.71	2/2318 (0.1%)
5	QE	0.29	0/1171	0.55	1/1576 (0.1%)
5	XE	0.26	0/1171	0.51	0/1576
6	QF	0.25	0/856	0.51	0/1154
6	XF	0.25	0/856	0.50	0/1154
7	QG	0.27	0/1276	0.50	1/1709 (0.1%)
7	XG	0.25	0/1276	0.47	0/1709
8	QH	0.26	0/1128	0.48	0/1517
8	XH	0.26	0/1128	0.49	0/1517
9	QI	0.31	0/1029	0.59	0/1379
9	XI	0.30	0/1017	0.52	0/1365
10	QJ	0.27	0/814	0.54	0/1095
10	XJ	0.26	0/790	0.53	0/1063
11	QK	0.25	0/900	0.50	0/1213
11	XK	0.25	0/879	0.46	0/1187
12	QL	0.27	0/991	0.53	0/1327
12	XL	0.26	0/972	0.54	0/1301
13	QM	0.25	0/965	0.52	0/1292
13	XM	0.27	0/956	0.55	0/1281
14	QN	0.27	0/501	0.54	0/664
14	XN	0.26	0/501	0.54	0/664
15	QO	0.25	0/745	0.48	0/992
15	XO	0.25	0/740	0.47	0/987
16	QP	0.26	0/721	0.47	0/970
16	XP	0.26	0/721	0.51	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.26	0/847	0.48	0/1131
17	XQ	0.25	0/847	0.53	0/1131
18	QR	0.25	0/579	0.49	0/768
18	XR	0.25	0/579	0.51	0/768
19	QS	0.27	0/680	0.64	0/915
19	XS	0.25	0/689	0.56	0/926
20	QT	0.27	0/765	0.57	0/1007
20	XT	0.27	0/765	0.55	0/1007
21	QU	0.23	0/221	0.49	0/288
21	XU	0.38	0/221	0.56	1/288 (0.3%)
22	QV	0.40	1/1836 (0.1%)	0.91	0/2859
22	XV	0.41	1/1836 (0.1%)	0.89	1/2859 (0.0%)
23	QX	0.23	0/293	0.69	0/455
23	XX	0.24	0/268	0.68	0/416
24	RA	0.38	0/69521	0.92	54/108529 (0.0%)
24	YA	0.41	0/69543	0.96	70/108563 (0.1%)
25	RB	0.32	0/2878	0.91	3/4490 (0.1%)
25	YB	0.36	0/2878	0.97	6/4490 (0.1%)
26	RD	0.29	0/2165	0.54	0/2919
26	YD	0.28	0/2165	0.52	0/2919
27	RE	0.28	0/1601	0.59	0/2160
27	YE	0.34	1/1601 (0.1%)	0.60	1/2160 (0.0%)
28	RF	0.29	0/1620	0.50	0/2194
28	YF	0.28	0/1620	0.51	0/2194
29	RG	0.28	0/1499	0.65	1/2016 (0.0%)
29	YG	0.26	0/1499	0.53	0/2016
30	RH	0.27	0/1362	0.58	1/1841 (0.1%)
30	YH	0.29	0/1362	0.55	0/1841
31	RI	0.28	0/1151	0.64	0/1558
31	YI	0.31	0/1151	0.68	2/1558 (0.1%)
32	RN	0.27	0/1131	0.52	0/1525
32	YN	0.27	0/1131	0.53	0/1525
33	RO	0.27	0/943	0.49	0/1269
33	YO	0.26	0/943	0.52	0/1269
34	RP	0.52	1/1162 (0.1%)	0.68	2/1544 (0.1%)
34	YP	0.29	0/1139	0.67	4/1514 (0.3%)
35	RQ	0.28	0/1143	0.59	1/1527 (0.1%)
35	YQ	0.27	0/1143	0.54	0/1527
36	RR	0.28	0/974	0.52	0/1302
36	YR	0.29	0/974	0.56	0/1302
37	RS	0.28	0/892	0.54	0/1187
37	YS	0.28	0/892	0.53	0/1187
38	RT	0.27	0/1155	0.51	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.28	0/1155	0.56	0/1542
39	RU	0.28	0/982	0.52	0/1306
39	YU	0.28	0/982	0.50	0/1306
40	RV	0.27	0/790	0.55	0/1057
40	YV	0.29	0/790	0.60	0/1057
41	RW	0.27	0/911	0.50	0/1220
41	YW	0.26	0/911	0.56	1/1220 (0.1%)
42	RX	0.27	0/739	0.47	0/993
42	YX	0.28	0/739	0.51	0/993
43	RY	0.27	0/831	0.48	0/1108
43	YY	0.29	0/831	0.57	2/1108 (0.2%)
44	RZ	0.28	0/1493	0.65	1/2026 (0.0%)
44	YZ	0.27	0/1493	0.61	1/2026 (0.0%)
45	R0	0.27	0/652	0.47	0/867
45	Y0	0.31	0/657	0.51	0/874
46	R1	0.29	0/761	0.53	0/1008
46	Y1	0.27	0/736	0.52	0/978
47	R2	0.27	0/583	0.51	0/771
47	Y2	0.26	0/583	0.48	0/771
48	R3	0.25	0/474	0.46	0/635
48	Y3	0.25	0/474	0.47	0/635
49	R4	0.28	0/578	0.60	0/776
49	Y4	0.27	0/578	0.60	0/776
50	R5	0.25	0/473	0.45	0/639
50	Y5	0.37	0/473	0.52	0/639
51	R6	0.23	0/460	0.47	0/613
51	Y6	0.43	1/460 (0.2%)	0.63	1/613 (0.2%)
52	R7	0.24	0/417	0.51	0/550
52	Y7	0.25	0/426	0.45	0/561
53	R8	0.30	0/525	0.65	1/691 (0.1%)
53	Y8	0.29	0/525	0.62	0/691
54	R9	0.24	0/310	0.48	0/407
54	Y9	0.26	0/310	0.50	0/407
All	All	0.35	6/315683 (0.0%)	0.84	213/471970 (0.0%)

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
2	XB	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	QC	0	1
4	QD	0	1
5	QE	0	2
5	XE	0	2
7	QG	0	1
7	XG	0	1
9	QI	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
18	QR	0	1
18	XR	0	1
19	QS	0	5
20	QT	0	3
20	XT	0	3
26	YD	0	2
27	RE	0	3
27	YE	0	2
29	RG	0	4
29	YG	0	1
30	RH	0	7
30	YH	0	9
31	RI	0	7
31	YI	0	4
32	RN	0	2
32	YN	0	2
33	YO	0	1
34	RP	0	1
34	YP	0	2
35	RQ	0	3
35	YQ	0	2
36	RR	0	1
38	RT	0	1
38	YT	0	2
39	RU	0	1
39	YU	0	1
40	RV	0	2
40	YV	0	2
44	RZ	0	5
44	YZ	0	4
46	R1	0	1
46	Y1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	R2	0	2
47	Y2	0	1
49	R4	0	4
49	Y4	0	3
53	R8	0	3
53	Y8	0	1
54	Y9	0	1
All	All	0	116

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	RP	68	GLN	CG-CD	-11.33	1.25	1.51
22	XV	1	C	OP3-P	-10.64	1.48	1.61
22	QV	1	C	OP3-P	-10.59	1.48	1.61
27	YE	109	LYS	C-N	6.64	1.45	1.33
51	Y6	27	LYS	CD-CE	6.39	1.67	1.51

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	XD	159	ARG	NE-CZ-NH2	-18.27	111.16	120.30
4	XD	159	ARG	NE-CZ-NH1	14.35	127.48	120.30
29	RG	21	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	XA	792	A	O4'-C1'-N9	8.90	115.32	108.20
1	XA	1158	C	C2-N1-C1'	8.42	128.06	118.80

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	QC	143	GLU	Peptide
4	QD	33	MET	Peptide
5	QE	10	MET	Peptide
5	QE	25	ARG	Peptide
7	QG	155	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16278	582	0
1	XA	32248	0	16279	542	2
2	QB	1907	0	1958	59	0
2	XB	1915	0	1969	56	0
3	QC	1605	0	1668	59	0
3	XC	1605	0	1668	47	0
4	QD	1703	0	1766	63	0
4	XD	1703	0	1767	50	1
5	QE	1155	0	1213	25	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	15	0
6	XF	843	0	857	28	0
7	QG	1257	0	1296	23	0
7	XG	1257	0	1296	27	0
8	QH	1108	0	1165	44	0
8	XH	1108	0	1165	37	0
9	QI	1010	0	1037	57	0
9	XI	998	0	1024	32	0
10	QJ	801	0	849	42	0
10	XJ	777	0	816	38	0
11	QK	885	0	904	26	0
11	XK	864	0	881	28	0
12	QL	975	0	1062	33	0
12	XL	956	0	1046	25	0
13	QM	955	0	1021	43	0
13	XM	946	0	1007	36	0
14	QN	492	0	529	27	0
14	XN	492	0	529	16	0
15	QO	734	0	771	18	0
15	XO	729	0	768	12	0
16	QP	705	0	725	12	0
16	XP	705	0	725	25	0
17	QQ	834	0	904	21	0
17	XQ	834	0	904	25	0
18	QR	574	0	644	16	0
18	XR	574	0	644	19	0
19	QS	665	0	686	40	0
19	XS	674	0	699	24	0
20	QT	763	0	861	23	0
20	XT	763	0	861	25	0
21	QU	217	0	234	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XU	217	0	234	6	0
22	QV	1644	0	836	23	0
22	XV	1644	0	836	15	0
23	QX	261	0	130	2	0
23	XX	239	0	119	3	0
24	RA	62071	0	31291	862	2
24	YA	62091	0	31301	958	0
25	RB	2573	0	1306	44	0
25	YB	2573	0	1306	45	0
26	RD	2115	0	2195	56	0
26	YD	2115	0	2195	75	0
27	RE	1568	0	1634	52	0
27	YE	1568	0	1634	65	0
28	RF	1585	0	1632	54	0
28	YF	1585	0	1632	44	0
29	RG	1474	0	1535	58	0
29	YG	1474	0	1535	51	0
30	RH	1336	0	1418	41	0
30	YH	1336	0	1418	38	0
31	RI	1136	0	1223	26	2
31	YI	1136	0	1223	43	0
32	RN	1104	0	1180	17	0
32	YN	1104	0	1180	30	0
33	RO	933	0	996	26	0
33	YO	933	0	996	17	0
34	RP	1145	0	1228	43	0
34	YP	1122	0	1206	56	0
35	RQ	1122	0	1179	51	0
35	YQ	1122	0	1179	32	0
36	RR	960	0	1021	38	0
36	YR	960	0	1021	29	0
37	RS	882	0	943	31	0
37	YS	882	0	943	32	0
38	RT	1141	0	1202	37	0
38	YT	1141	0	1202	41	0
39	RU	964	0	1022	33	0
39	YU	964	0	1022	39	0
40	RV	779	0	852	24	0
40	YV	779	0	852	17	1
41	RW	900	0	964	26	0
41	YW	900	0	964	21	0
42	RX	725	0	778	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YX	725	0	778	14	0
43	RY	818	0	911	12	0
43	YY	818	0	912	26	0
44	RZ	1461	0	1493	55	0
44	YZ	1461	0	1493	46	0
45	R0	643	0	667	18	0
45	Y0	648	0	672	23	0
46	R1	755	0	836	16	0
46	Y1	729	0	802	20	0
47	R2	581	0	629	13	0
47	Y2	581	0	629	12	1
48	R3	469	0	518	13	0
48	Y3	469	0	518	14	0
49	R4	565	0	560	31	0
49	Y4	565	0	559	20	0
50	R5	459	0	476	17	0
50	Y5	459	0	478	11	1
51	R6	453	0	475	16	0
51	Y6	453	0	474	11	0
52	R7	409	0	454	14	0
52	Y7	418	0	467	10	0
53	R8	517	0	582	25	0
53	Y8	517	0	582	24	0
54	R9	307	0	336	6	0
54	Y9	307	0	335	13	0
55	QA	180	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QL	1	0	0	0	0
55	QV	6	0	0	0	0
55	QX	2	0	0	0	0
55	R0	2	0	0	0	0
55	R1	2	0	0	0	0
55	R5	1	0	0	0	0
55	RA	493	0	0	0	0
55	RB	10	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	1	0	0	0	0
55	RI	1	0	0	0	0
55	RN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RO	1	0	0	0	0
55	RP	3	0	0	0	0
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RU	1	0	0	0	0
55	RW	1	0	0	0	0
55	RX	1	0	0	0	0
55	RY	1	0	0	0	0
55	XA	171	0	0	0	0
55	XE	2	0	0	0	0
55	XL	1	0	0	0	0
55	XM	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	XV	8	0	0	0	0
55	Y0	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	515	0	0	0	0
55	YB	10	0	0	0	0
55	YD	2	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	3	0	0	0	0
55	YQ	3	0	0	0	0
55	YU	1	0	0	0	0
55	YX	2	0	0	0	0
55	YY	1	0	0	0	0
56	QD	8	0	0	1	0
56	XD	8	0	0	2	0
57	QN	1	0	0	0	0
57	R4	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	Y4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YY	1	0	0	0	0
All	All	291948	0	197745	5207	5

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 11.

The worst 5 of 5207 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)
24:RA:2285:C:OP2	51:R6:6:ARG:NH2	1.85	1.08
24:RA:2068:U:H3	24:RA:2430:A:H2	1.11	0.99
24:RA:676:A:H8	24:RA:2069:G:H21	1.04	0.98
10:QJ:4:ILE:HG22	10:QJ:74:ILE:HG12	1.46	0.96
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.31	0.93

All (5) 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)
24:RA:2217:G:OP1	4:XD:159:ARG:NH2[4_555]	2.08	0.12
31:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	2.11	0.09
40:YV:49:THR:OG1	50:Y5:60:VAL:O[4_445]	2.12	0.08
24:RA:310:A:OP2	47:Y2:71:ASN:ND2[3_555]	2.14	0.06
31:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.17	0.03

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%)	197 (84%)	35 (15%)	1 (0%)	34	72
2	XB	234/256 (91%)	203 (87%)	31 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QC	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	29	68
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	29	68
4	QD	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	68
4	XD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	15	54
5	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	22	61
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
7	XG	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	54
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
12	QL	123/132 (93%)	109 (89%)	12 (10%)	2 (2%)	9	43
12	XL	120/132 (91%)	104 (87%)	14 (12%)	2 (2%)	9	42
13	QM	118/126 (94%)	102 (86%)	14 (12%)	2 (2%)	9	42
13	XM	117/126 (93%)	104 (89%)	12 (10%)	1 (1%)	17	56
14	QN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	42
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	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%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	13	50
19	XS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
20	QT	97/106 (92%)	83 (86%)	11 (11%)	3 (3%)	4	30
20	XT	97/106 (92%)	86 (89%)	9 (9%)	2 (2%)	7	38
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	RD	270/276 (98%)	251 (93%)	19 (7%)	0	100	100
26	YD	270/276 (98%)	244 (90%)	25 (9%)	1 (0%)	34	72
27	RE	203/206 (98%)	169 (83%)	31 (15%)	3 (2%)	10	45
27	YE	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	29	68
28	RF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	68
28	YF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
29	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	25	64
29	YG	179/182 (98%)	157 (88%)	22 (12%)	0	100	100
30	RH	172/180 (96%)	151 (88%)	21 (12%)	0	100	100
30	YH	172/180 (96%)	145 (84%)	25 (14%)	2 (1%)	13	50
31	RI	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	7	38
31	YI	144/148 (97%)	123 (85%)	18 (12%)	3 (2%)	7	38
32	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
32	YN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
33	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	RP	148/150 (99%)	123 (83%)	25 (17%)	0	100	100
34	YP	145/150 (97%)	111 (77%)	34 (23%)	0	100	100
35	RQ	139/141 (99%)	115 (83%)	22 (16%)	2 (1%)	11	46
35	YQ	139/141 (99%)	118 (85%)	19 (14%)	2 (1%)	11	46
36	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56
36	YR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56
37	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
37	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	RT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
38	YT	135/146 (92%)	115 (85%)	20 (15%)	0	100	100
39	RU	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	27
39	YU	115/118 (98%)	104 (90%)	8 (7%)	3 (3%)	5	33
40	RV	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
40	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
41	RW	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
41	YW	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
42	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
43	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
44	RZ	181/206 (88%)	147 (81%)	30 (17%)	4 (2%)	6	37
44	YZ	181/206 (88%)	145 (80%)	32 (18%)	4 (2%)	6	37
45	R0	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
45	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
46	R1	92/98 (94%)	79 (86%)	13 (14%)	0	100	100
46	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
47	R2	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	10	45
47	Y2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
48	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	51 (76%)	11 (16%)	5 (8%)	1	11
49	Y4	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	15
50	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	Y6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	46 (100%)	0	0	100	100
53	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
54	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
54	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11456/12128 (94%)	10265 (90%)	1120 (10%)	71 (1%)	25	64

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QC	12	LEU
20	QT	74	LYS
39	RU	91	ASP
39	RU	92	ARG
44	RZ	53	ILE

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%)	199 (98%)	5 (2%)	47	75
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	94
3	XC	159/188 (85%)	158 (99%)	1 (1%)	86	94
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	88
4	XD	180/181 (99%)	173 (96%)	7 (4%)	32	64
5	QE	116/123 (94%)	113 (97%)	3 (3%)	46	74
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	90
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	78
6	XF	90/90 (100%)	87 (97%)	3 (3%)	38	68
7	QG	126/127 (99%)	124 (98%)	2 (2%)	62	83
7	XG	126/127 (99%)	122 (97%)	4 (3%)	39	69
8	QH	118/119 (99%)	116 (98%)	2 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91
9	QI	98/99 (99%)	94 (96%)	4 (4%)	30	63
9	XI	97/99 (98%)	94 (97%)	3 (3%)	40	70
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	88
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	88 (98%)	2 (2%)	52	78
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	98 (94%)	6 (6%)	20	53
12	XL	103/109 (94%)	101 (98%)	2 (2%)	57	80
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76	88
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	45 (92%)	4 (8%)	11	40
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	86
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	85
16	XP	72/74 (97%)	70 (97%)	2 (3%)	43	72
17	QQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
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%)	60 (98%)	1 (2%)	62	83
19	QS	72/80 (90%)	70 (97%)	2 (3%)	43	72
19	XS	73/80 (91%)	72 (99%)	1 (1%)	67	85
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
26	RD	214/218 (98%)	214 (100%)	0	100	100
26	YD	214/218 (98%)	212 (99%)	2 (1%)	78	90
27	RE	165/166 (99%)	163 (99%)	2 (1%)	71	87
27	YE	165/166 (99%)	163 (99%)	2 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
28	YF	161/166 (97%)	158 (98%)	3 (2%)	57	80
29	RG	155/156 (99%)	153 (99%)	2 (1%)	69	86
29	YG	155/156 (99%)	153 (99%)	2 (1%)	69	86
30	RH	145/148 (98%)	142 (98%)	3 (2%)	53	79
30	YH	145/148 (98%)	143 (99%)	2 (1%)	67	85
31	RI	122/124 (98%)	118 (97%)	4 (3%)	38	68
31	YI	122/124 (98%)	120 (98%)	2 (2%)	62	83
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	90
33	RO	100/100 (100%)	99 (99%)	1 (1%)	76	88
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	114 (98%)	2 (2%)	60	82
34	YP	114/116 (98%)	111 (97%)	3 (3%)	46	74
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	78	90
35	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	81
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	88
36	YR	100/101 (99%)	97 (97%)	3 (3%)	41	71
37	RS	87/88 (99%)	86 (99%)	1 (1%)	73	88
37	YS	87/88 (99%)	85 (98%)	2 (2%)	50	77
38	RT	120/127 (94%)	116 (97%)	4 (3%)	38	68
38	YT	120/127 (94%)	119 (99%)	1 (1%)	81	91
39	RU	93/94 (99%)	91 (98%)	2 (2%)	52	78
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	89 (97%)	3 (3%)	38	68
41	YW	92/92 (100%)	90 (98%)	2 (2%)	52	78
42	RX	74/78 (95%)	73 (99%)	1 (1%)	67	85
42	YX	74/78 (95%)	73 (99%)	1 (1%)	67	85
43	RY	88/91 (97%)	86 (98%)	2 (2%)	50	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	159 (98%)	3 (2%)	57	80
44	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	87
45	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84
45	Y0	65/67 (97%)	63 (97%)	2 (3%)	40	70
46	R1	81/83 (98%)	79 (98%)	2 (2%)	47	75
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	60 (94%)	4 (6%)	18	51
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	59 (95%)	3 (5%)	25	60
49	Y4	62/63 (98%)	58 (94%)	4 (6%)	17	50
50	R5	51/52 (98%)	48 (94%)	3 (6%)	19	53
50	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	79
51	R6	51/52 (98%)	50 (98%)	1 (2%)	55	79
51	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	52 (96%)	2 (4%)	34	65
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	57	80
54	R9	34/34 (100%)	32 (94%)	2 (6%)	19	53
54	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	71
All	All	9690/10066 (96%)	9524 (98%)	166 (2%)	60	82

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	R2	68	ARG
3	XC	85	ARG
44	YZ	10	ARG
49	R4	58	ARG
53	R8	44	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
47	R2	65	ASN
51	R6	26	ASN
20	XT	90	GLN
36	RR	53	HIS
31	YI	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	263 (17%)	30 (2%)
1	XA	1498/1508 (99%)	286 (19%)	27 (1%)
22	QV	76/77 (98%)	18 (23%)	2 (2%)
22	XV	76/77 (98%)	16 (21%)	3 (3%)
23	QX	11/25 (44%)	7 (63%)	0
23	XX	10/25 (40%)	6 (60%)	0
24	RA	2879/2915 (98%)	577 (20%)	33 (1%)
24	YA	2880/2915 (98%)	570 (19%)	36 (1%)
25	RB	119/122 (97%)	24 (20%)	1 (0%)
25	YB	119/122 (97%)	23 (19%)	1 (0%)
All	All	9166/9294 (98%)	1790 (19%)	133 (1%)

5 of 1790 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	RA	2439	A
1	XA	266	G
24	YA	1694	C
24	RA	2566	A
1	XA	78	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1464 ligands modelled in this entry, 1462 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	-	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	-	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	1	0
56	XD	301	SF4	2	0

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.