



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2020 – 03:01 AM EDT

PDB ID : 6OSI  
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (near cognate)  
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2019-05-01  
Resolution : 4.14 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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



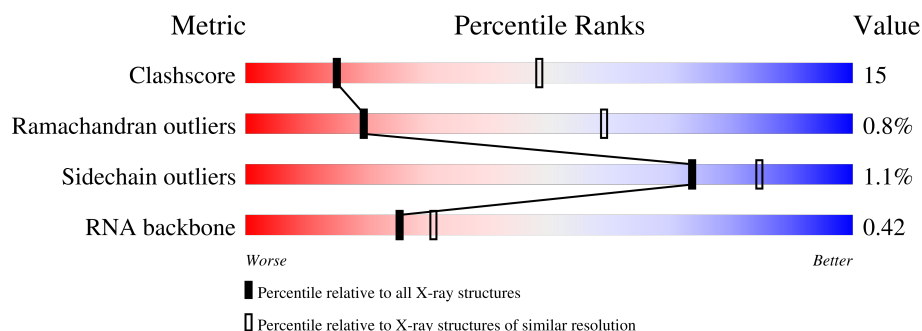
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.14 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	1041 (4.50-3.78)
Ramachandran outliers	138981	1036 (4.52-3.76)
Sidechain outliers	138945	1022 (4.52-3.76)
RNA backbone	3102	1049 (5.04-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .


























Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	
1	XA	1521	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	

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Mol	Chain	Length	Quality of chain
4	QD	209	
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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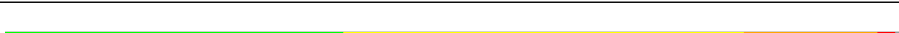













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Mol	Chain	Length	Quality of chain
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
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	 63% 30% 5% .
30	R6	54	 70% 22% . . .
30	Y6	54	 63% 28% 6% . .
31	R7	49	 61% 35% .
31	Y7	49	 82% 16% .
32	R8	65	 60% 32% 6% .
32	Y8	65	 63% 35% .
33	R9	37	 57% 38% 5%
33	Y9	37	 62% 35% .
34	RA	2905	 41% 42% 15% . .
34	YA	2905	 38% 45% 15% . .
35	RB	122	 55% 36% 6% . .
35	YB	122	 43% 45% 9% . .
36	RD	276	 76% 21% . .
36	YD	276	 79% 18% . .
37	RE	206	 73% 24% .
37	YE	206	 75% 24% .
38	RF	210	 75% 20% . .
38	YF	210	 73% 23% .
39	RG	182	 74% 25% . .
39	YG	182	 75% 24% .
40	RH	180	 62% 29% 6% .
40	YH	180	 77% 17% . . .
41	RI	148	 72% 24% . .

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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
55	MG	XA	1688	-	-	X	-
55	MG	YA	3192	-	-	X	-
56	SF4	QD	301	-	-	X	-



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291185 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	105	Total	C	N	O		0	0	0
			816	519	152	145				
9	XI	107	Total	C	N	O		0	0	0
			834	530	157	147				

- 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	115	Total	C	N	O	S	0	0	0
			921	569	190	160	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 tRNA(Pro).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			
22	XV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			

- 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	70	Total	Mg	0	0
			70	70		
55	YA	394	Total	Mg	0	0
			394	394		
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	2	Total	Mg	0	0
			2	2		
55	Y8	2	Total	Mg	0	0
			2	2		
55	XA	88	Total	Mg	0	0
			88	88		
55	R0	2	Total	Mg	0	0
			2	2		
55	QL	2	Total	Mg	0	0
			2	2		
55	YU	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

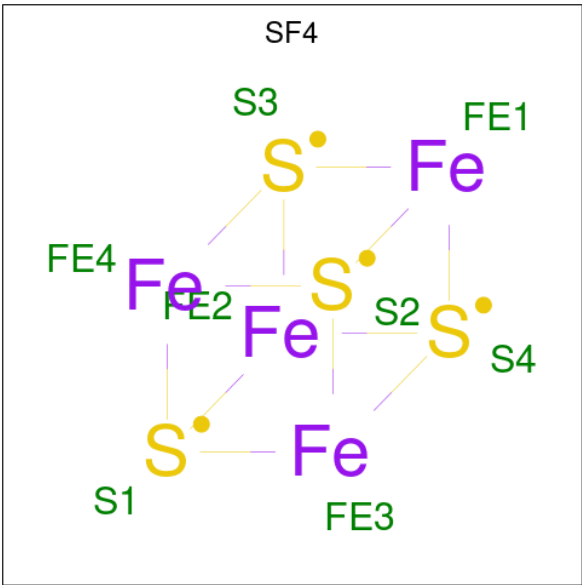


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QH	2	Total 2	Mg 2	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	R8	2	Total 2	Mg 2	0	0
55	YX	1	Total 1	Mg 1	0	0
55	RD	1	Total 1	Mg 1	0	0
55	XO	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	RA	432	Total 432	Mg 432	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YP	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0
55	YB	1	Total 1	Mg 1	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	QE	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	4	Total 4	Mg 4	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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		







A1534	C1535	U1472	G1334	G1274	C1214	G1143	G1079	G1013	G951	C811	C749	G685
C1536	A1473	A1397	C1335	A1275	G1215	G1144	A1080	A1014	U952	C812	G750	U656
U1537	G1474	A1398	C1336	C1276	C1216	C1145	G1081	A1015	G953	U884	U751	A657
C1538	G1475	C1399	G1337	G1277	G1217	A1146	U1086	A1016	G954	A814	G752	G688
U1541	C1476	C1400	G1338	U1278	C1218	C1147	U1086	G1017	U955	A815	A753	C689
U1540	C1477	C1401	C1339	U1279	U1219	U1148	U1086	G1023	U956	A816	G754	G690
U1542	C1478	C1402	A1340	A1280	G1220	G1149	G1087	G1024	U957	C817	G755	G691
C	C1479	C1403	U1341	G1281	G1221	U1150	G1088	U1025	A958	G819	C756	U692
U	C1480	C1404	C1342	C1282	C1222	A1151	G1089	U1026	A959	A919	U757	U693
	U1481	G1405	G1343	C1283	C1223	A1152	U1090	G1027	U960	U820	G758	A694
	G1482	U1406	G1344	G1224	G1224	C1153	U1092	C1027	U961	G821	A759	A695
	A1483	A1285	A1286	A1225	A1225	G1154	A1093	C1028A	G962	G822	G760	A696
	C1484	A1287	A1287	C1226	C1226	U1157	G1094	C1028B	G963	G823	G761	A697
	U1485	A1288	A1288	A1227	A1227	A1158	U1095	C1028C	U966	C824	C762	G698
	G1486	A1289	A1289	C1228	C1228	C1159	U1096	G1028D	G967	G825	G763	C699
	G1487	U1290	C1290	A1229	A1229	U1159	C1097	C1028E	U968	G826	G764	C700
		U1351	C1291	C1230	C1230	G1160	G1098	G1028F	U905	U827	G765	C701
	C1490	C1352	G1291	G1231	G1231	G1161	G1099	A1028G	G906	A828	A766	A702
	G1491	C1353	U1292	U1232	U1232	C1162	C1100	G1028H	A907	G829	A767	G703
	A1492	G1354	G1293	G1233	G1233	C1163	A1101	G1028I	A908	G830	A768	A704
	A1493	G1355	G1294	C1234	C1234	U1102	A1102	C1037	C972	U831	G769	U705
	G1494	G1356	U1295	U1235	U1235	A1169	C1103	C1038	G973	C912	C770	A706
		A1357	A1236	A1236	A1236	A1170	G1104	A1039	A974	A913	C771	C707
		U1358	C1237	C1237	C1237	G1175	A1105	U1040	G976	A914	C772	C708
	U1497	C1359	C1298	C1238	C1238	A1176	G1106	G1046	U982	U920	A715	A715
	A1498	A1360	A1299	A1239	A1239	A1177	C1107	G1047	A983	U921	A716	A716
	A1500	G1361	U1300	U1240	U1240	G1178	C1108	G1048	C984	G922	G717	A717
	C1501	C1362A	G1301	G1241	G1241	C1179	C1109	C1049	C985	U925	A718	G718
	A1502	C1362B	U1302	C1242	C1242	A1179	G1110	U1049	G986	G926	G719	C719
	A1503	A1363	C1303	C1243	C1243	A1180	A1111	C1050	A987	G927	G720	G720
	G1504	C1364	G1304	G1244	G1244	G1181	C1112	C1051	G988	G928	G721	G721
	G1505	C1365	G1305	A1245	A1245	G1182	C1113	U1052	G989	G929	A722	A722
	U1506	C1366	A1306	C1246	C1246	A1183	C1114	C1054	C990	C856	U723	U723
	G1507	C1367	U1307	U1247	U1247	G1184	C1115	A1055	U991	C930	G724	G724
	A1508	A1434	U1308	A1248	A1248	G1185	G1116	U1056	U992	G931	A725	A725
	C1509	C1369	G1309	C1249	C1249	G1186	C1117	C1060	C993	G861	C726	C726
	U1510	G1370	G1310	A1250	A1250	G1187	C1118	G1061	A994	C862	A727	A727
	G1511	G1371	G1311	A1251	A1251	A1188	C1119	U1062	C995	U863	A728	A728
	U1512	U1372	G1312	C1252	C1252	C1189	G1120	C1063	A996	A864	A729	A729
	A1513	G1373	U1313	G1253	G1253	G1190	U1121	G1064	C997	A865	G730	G730
	C1514	A1374	C1314	C1254	C1254	A1191	G1123	U1065	C998A	A937	G731	G731
	C1515	A1375	U1315	G1255	G1255	U1195	U1125	C1066	C998B	G938	C732	C732
	G1516	U1376	G1316	A1256	A1256	U1196	U1126	C1069	U999	G839	G736	G736
	G1517	A1377	C1317	U1257	U1257	G1197	G1127	U1070	A1000	U870	A737	A737
	A1518	C1378	A1318	G1258	G1258	U1198	C1128	G1071	G1001	U871	C738	C738
	A1519	U1379	C1319	C1259	C1259	U1199	C1129	C1072	G1003	A872	C739	C739
	G1520	U1380	C1320	C1260	C1260	U1200	C1129	G1073	A997	A873	U740	U740
	U1521	U1381	C1321	A1261	A1261	G1206	U1136	G1074	A1004	G944	G803	G803
	C1522	C1382	C1322	C1262	C1262	G1207	G1137	U1075	A1005	G945	U804	U804
	G1523	C1383	G1323	C1263	C1263	U1201	A1131	G1076	C1006	A946	G805	G805
	C1524	C1384	A1324	C1264	C1264	G1202	C1132	C1077	U999	G839	C806	C806
	G1525	C1388	C1325	G1265	G1265	C1203	G1133	U1078	A1000	U870	A807	A807
	C1527	C1389	C1326	G1266	G1266	A1204	G1134	U1079	G941	U871	C810	C810
	G1528	U1390	C1327	C1267	C1267	U1205	U1135	C1071	G942	A872		
	U1529	U1391	C1328	A1268	A1268	G1206	U1136	G1072	U943	A873		
	G1530	G1392	A1329	C1269	C1269	G1207	G1137	G1073	G944	G874		
	A1531	U1393	U1330	C1270	C1270	U1210	G1138	C1075	A945	C975		
	U1532	C1466	A1331	G1271	G1271	U1211	G1139	C1076	G947	C876		
	G1467	U1533	A1332	G1272	G1272	C1212	C1140	G1077	C948	G877		
		C1395	A1333	G1273	G1273	A1213	G1142	U1078	C949	C878		

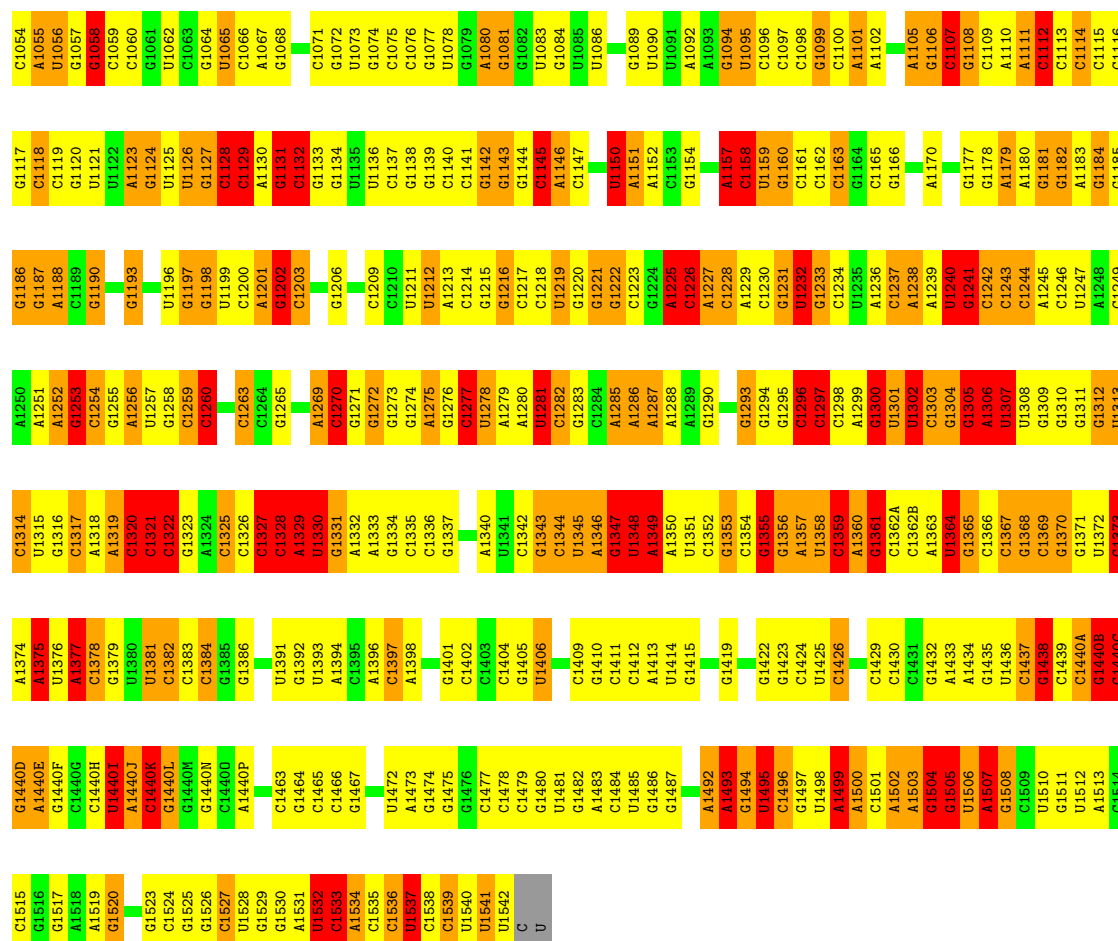
• Molecule 1: 16S rRNA

Chain XA:  28% 44% 21% 7%



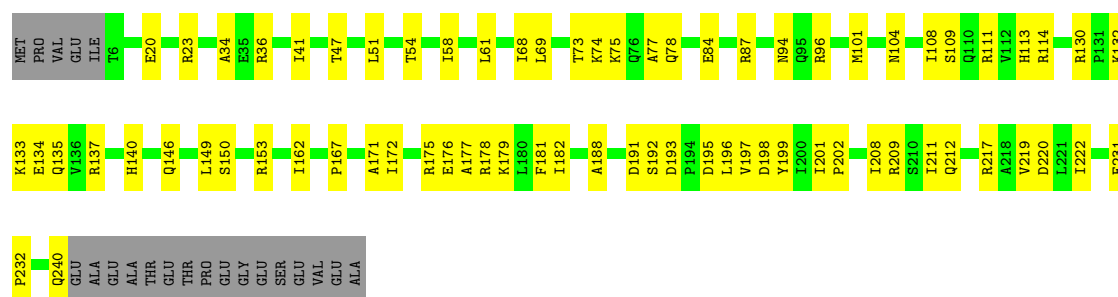
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U	C68C	C355	C283	A356	G428	A520	C590	G657	G720	G786	C856	U921	C984
G	G68H	C200	G288	A356	G428	G521	U591	G658	G721	G787	C857	G922	C985
U	G68J	C201A	A289	A364	U429	C522	G592	G661	A722	U788	G858	G926	A986
U	G68K	U201B	G288	A364	C435	A523	G593	G662	U723	U789	A859	G927	G987
G6	G68L	U201C	C290	U365	C436	G524	G594	A663	G724	A790	A860		G988
G7	U68M	U201D	C291	C366	C436	C525	G595	A664	G725	G791	G861	C930	G989
G9	U68N	G216	C292	C367	U367	C526	C596	G665	U726	A792	G862	C931	C990
	U68O	C217	C293	U368	A440	G527	G597	A666	G727	U793	U983	G932	U991
		C218	G294	U369	C440	C528	U598	G667	A728	A794	G863	G933	U992
		C219	G295	C369	C443	C529	C599	G668	U729	G795	A865	G934	G993
		G215	U296	C370	C443	G530	C600	G669	G730	G796	C866	G934	A994
		G215	G297	C371	C444	G531	C601	U669	G731	G797	G867	A935	C995
		G215	G298	C372	G445	U531	A602	G670	G732	U798	G868	C936	A996
		G215	G299	A373	G446	A532		G671	G732	G799	G869	A937	U997
		G215	A300	A374	G447	A533							
		G215	G301	U375	C447								
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		G215	G302	G518									
		G215	G302	G519									
		G215	G302	G520									
		G215	G302	G521									
		G215</											





• Molecule 2: 30S ribosomal protein S2

Chain QB: 64% 28% 8%

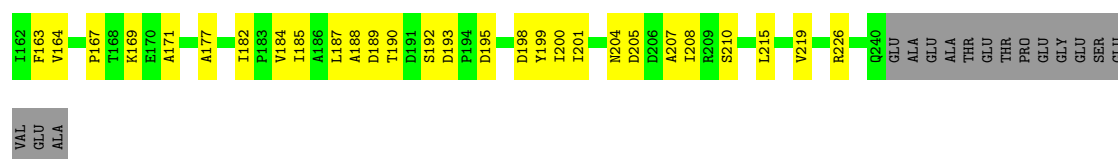


• Molecule 2: 30S ribosomal protein S2

Chain XB: 69% 23% 8%

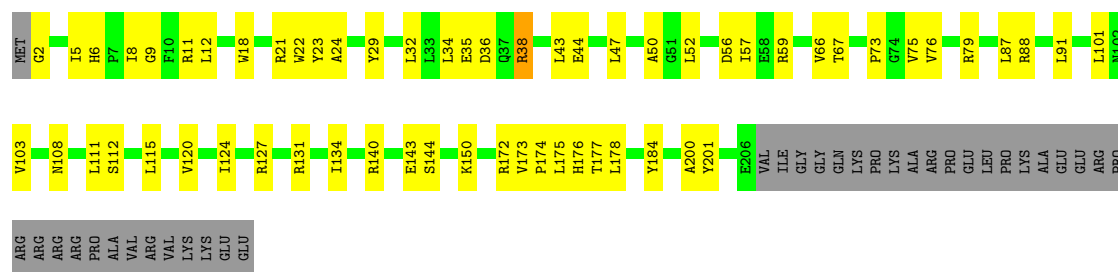






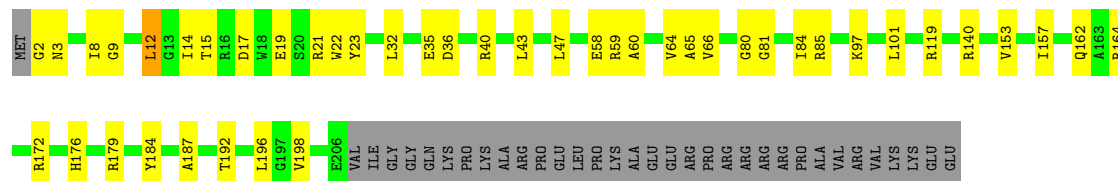
- Molecule 3: 30S ribosomal protein S3

Chain QC: 61% 25% 14%



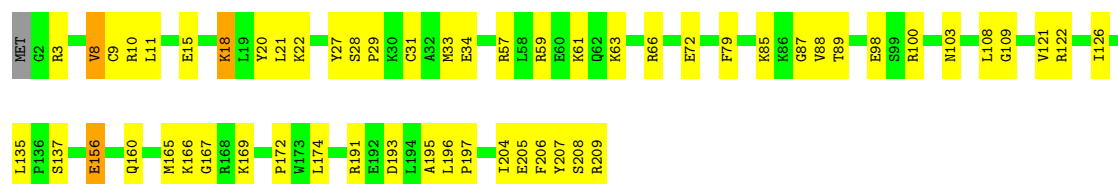
- Molecule 3: 30S ribosomal protein S3

Chain XC: 67% 18% 14%



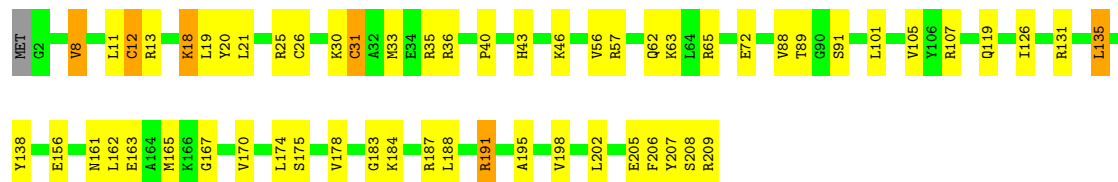
- Molecule 4: 30S ribosomal protein S4

Chain QD: 73% 25% 2%



- Molecule 4: 30S ribosomal protein S4

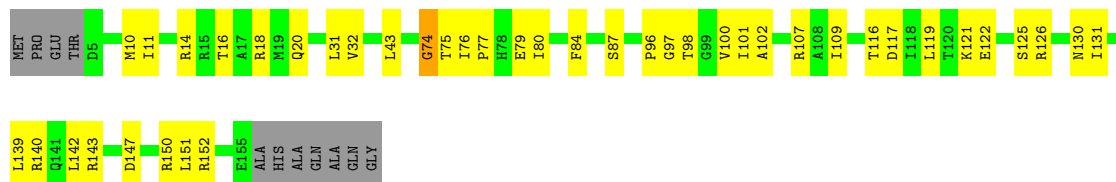
Chain XD: 72% 25% 3%



- Molecule 5: 30S ribosomal protein S5

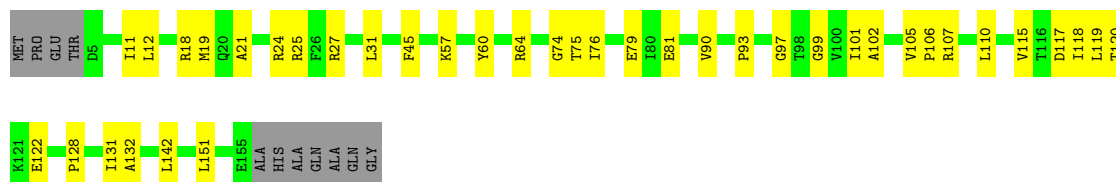


Chain QE:  67% 25% 7%




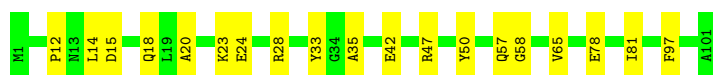
- Molecule 5: 30S ribosomal protein S5

Chain XE:  69% 24% 7%



- Molecule 6: 30S ribosomal protein S6

Chain QF:  81% 19%




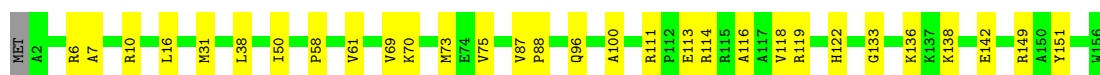
- Molecule 6: 30S ribosomal protein S6

Chain XF:  64% 36%




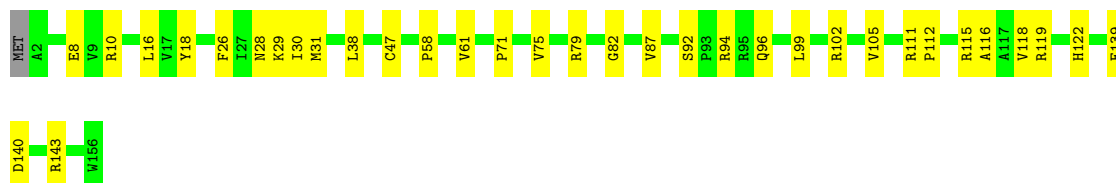
- Molecule 7: 30S ribosomal protein S7

Chain QG:  80% 19%



- Molecule 7: 30S ribosomal protein S7

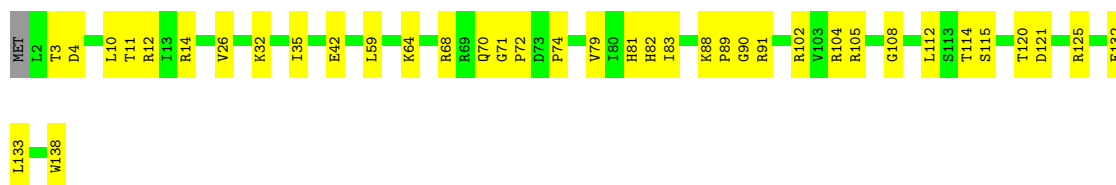
Chain XG:  78% 22%






- Molecule 8: 30S ribosomal protein S8

Chain QH:  72% 28%



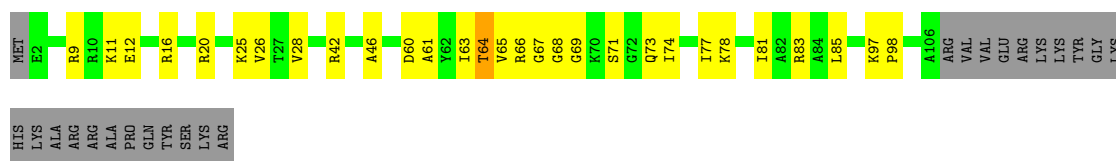
- Molecule 8: 30S ribosomal protein S8

Chain XH:  76% 23%



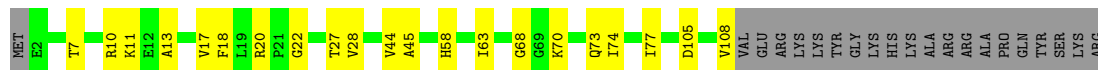
- Molecule 9: 30S ribosomal protein S9

Chain QI:  59% 22% 18%



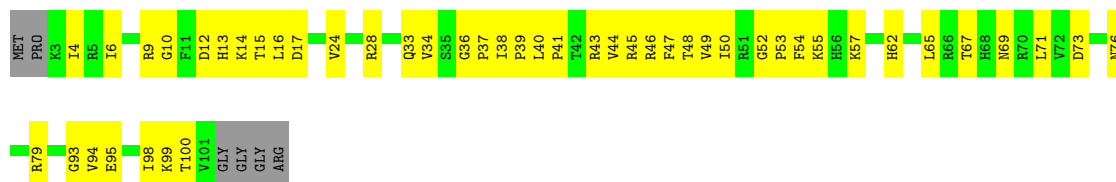
- Molecule 9: 30S ribosomal protein S9

Chain XI:  67% 16% 16%



- Molecule 10: 30S ribosomal protein S10

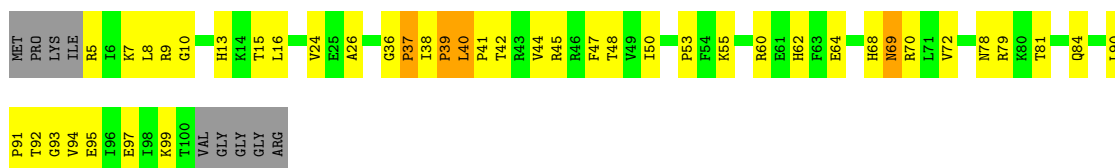
Chain QJ:  50% 45% 6%



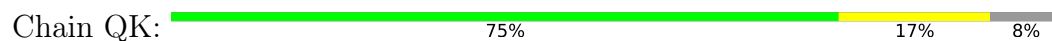
- Molecule 10: 30S ribosomal protein S10

Chain XJ:  50% 37% 9%





- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



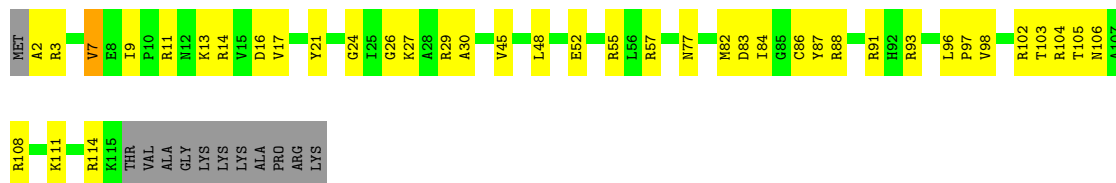
- Molecule 13: 30S ribosomal protein S13





- Molecule 13: 30S ribosomal protein S13

Chain XM:  59% 31% 10%



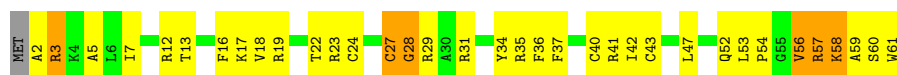
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  43% 51% 5%




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  41% 48% 10%




- Molecule 15: 30S ribosomal protein S15

Chain QO:  74% 25% 1%



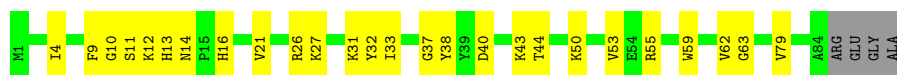
- Molecule 15: 30S ribosomal protein S15

Chain XO:  79% 19% 2%



- Molecule 16: 30S ribosomal protein S16

Chain QP:  66% 30% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP:  72% 24% 5%





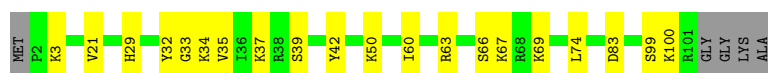
- Molecule 17: 30S ribosomal protein S17

Chain QQ: 77% 18% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 76% 19% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR: 68% 11% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR: 52% 27% 20%



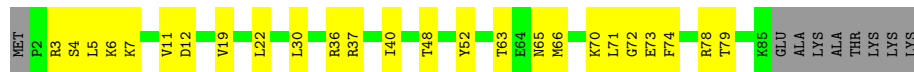
- Molecule 19: 30S ribosomal protein S19

Chain QS: 57% 31% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS: 63% 27% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 68% 24% 7%





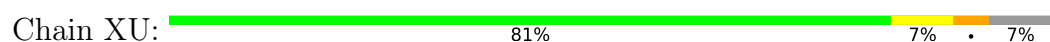
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA(Pro)



- Molecule 22: tRNA(Pro)



- Molecule 23: mRNA



- Molecule 23: mRNA







- Molecule 24: 50S ribosomal protein L27

Chain R0: 81% 13% 5%



- Molecule 24: 50S ribosomal protein L27

Chain Y0: 81% 15% 5%



- Molecule 25: 50S ribosomal protein L28

Chain R1: 77% 20% 3%



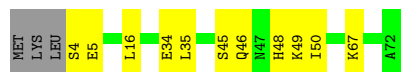
- Molecule 25: 50S ribosomal protein L28

Chain Y1: 82% 13% 5%



- Molecule 26: 50S ribosomal protein L29

Chain R2: 81% 15% 4%



- Molecule 26: 50S ribosomal protein L29

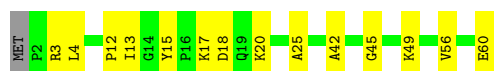
Chain Y2: 81% 14% 6%



- Molecule 27: 50S ribosomal protein L30

Chain R3: 75% 23% 2%





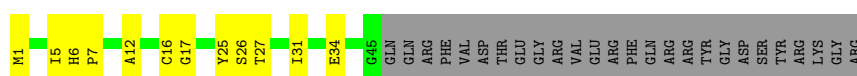
- Molecule 27: 50S ribosomal protein L30

Chain Y3: 73% 25% .



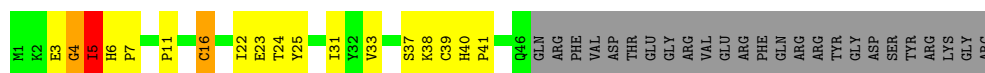
- Molecule 28: 50S ribosomal protein L31

Chain R4: 46% 17% 37%



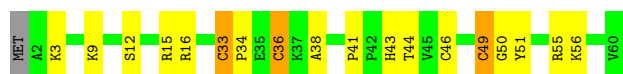
- Molecule 28: 50S ribosomal protein L31

Chain Y4: 39% 21% 35%



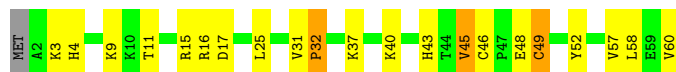
- Molecule 29: 50S ribosomal protein L32

Chain R5: 68% 25% 5%



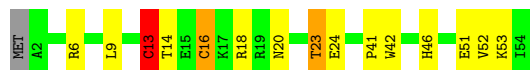
- Molecule 29: 50S ribosomal protein L32

Chain Y5: 63% 30% 5%



- Molecule 30: 50S ribosomal protein L33

Chain R6: 70% 22% . . .



- Molecule 30: 50S ribosomal protein L33

Chain Y6: 63% 28% 6% . . .

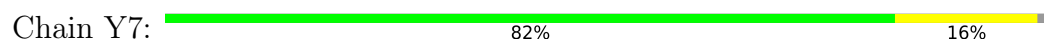




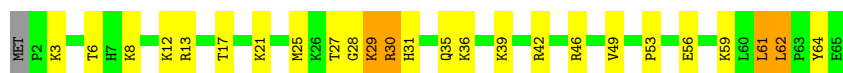
- Molecule 31: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L34



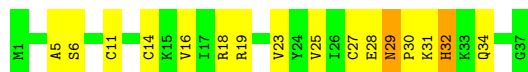
- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36



- Molecule 34: 23S rRNA



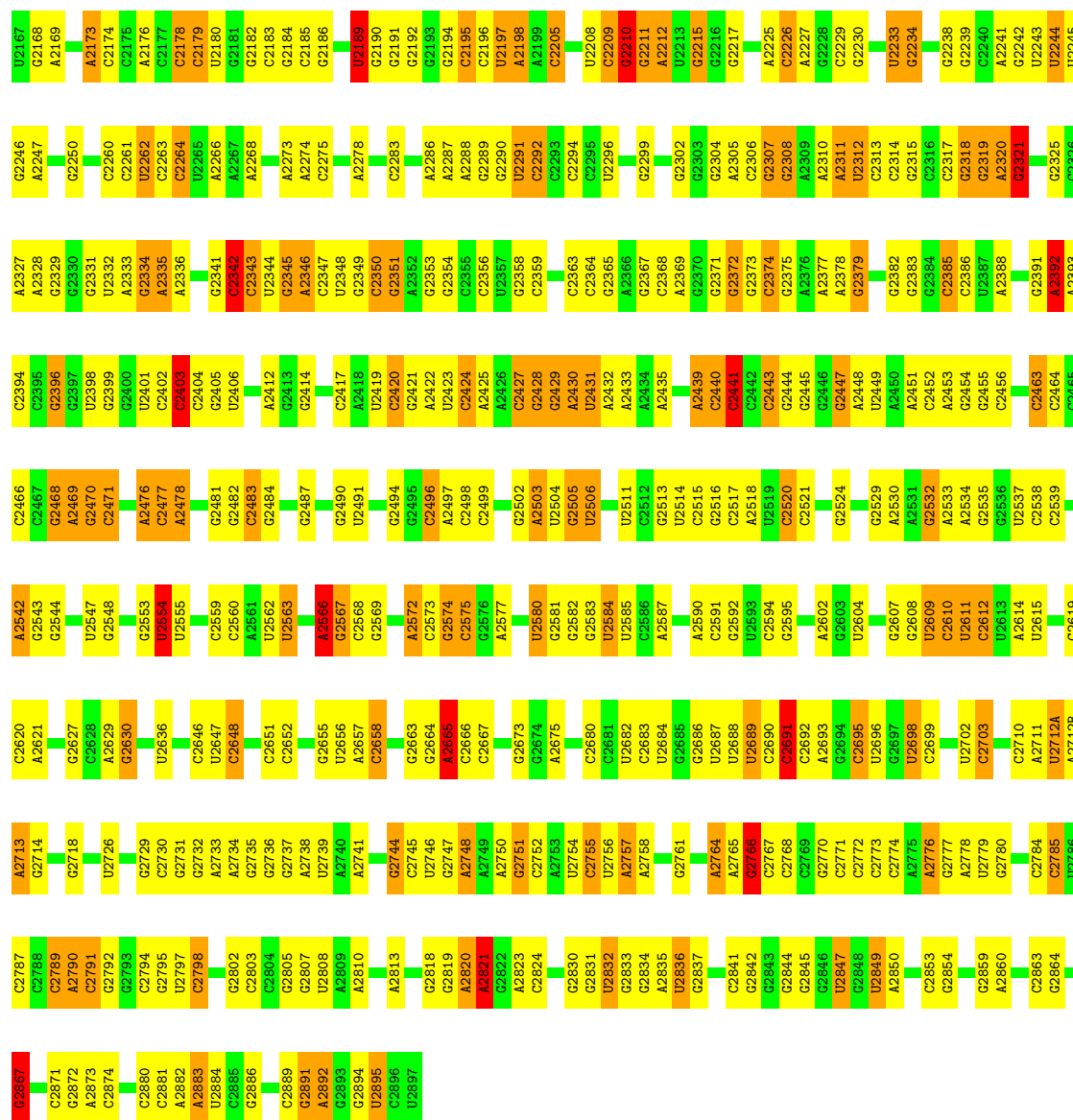


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U1019	G944	U860	G792	G713	C595	G521	C	G370	C254	C	G81	C
A1020	A945	G	G	U714	C596	G522	C451	G371	A255	A	G82	A
A1021	G946	A863	C795	G715	U597	G523	G452	G372	G189	G	G83	G
G1022	C949	G864	C796	A716	C598	U524	C453	U373	A256	G	G84	G
U1023	G950	G865	C797	G717	G599	U525	A454	A374	A257	G	G85	G
G1024	C867	A866	C798	C721	G602	A526	C455	C375	G258	G	G86	G
U1025	U877	U867	G799	A722	A603	C527	C456	C376	G259	G	G87	G
U1026	G869	U868	A800	G	A604	A528	A457	G	G260	G	G88	G
C955	G873	G805	A804	G725	C605	A529	G458	G379	A196	G	G89	G
A1028	G806	G806	G805	G726	G606	A530	U459	U380	A197	G	G90	G
A1029	C806	C806	C806	G727	C531	A532	A460	G381	C198	G	G91	G
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A990	G	G	G	G765	G636	G570	G500	G417	G232	G	G154	G
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C994	G	G	G	C923	G640	A575	G	G421	G235	G	G152	G
C995	G	G	G	G776	C641	U576	U504	G422	G236	G	G153	G
A996	G	G	G	A777	G642	U577	A505	G423	C237	G	G154	G
G997	G	G	G	G778	A643	A578	G	G424	C238	G	C155	G
C998	G	G	G	U779	G644	G579	G508	G425	G239	G	U161	G
U999	G	G	G	G780	C645	C580	C509	G426	C280	G	U	G
A1000	G	G	G	A781	A646	C581	U511	G427	G281	G	U	G
C1005	G	G	G	G782	G651	C582	G	G428	A282	G	U	G
C1008	G	G	G	A783	C652	G583	U512	G429	G283	G	G171	G
G1074	G	G	G	G784	A653	G584	A513	G430	U284	G	C172	G
C1075	G	G	G	G785	G654	A586	A514	G431	G285	G	G173	G
A1076	G	G	G	C786	A654A	C589	A515	G432	C286	G	G177	G
U1082	G	G	G	U787	G654B	C590	C516	G433	G287	G	G178	G
U1083	G	G	G	A788	C654C	A590	C517	G434	C288	G	G179	G
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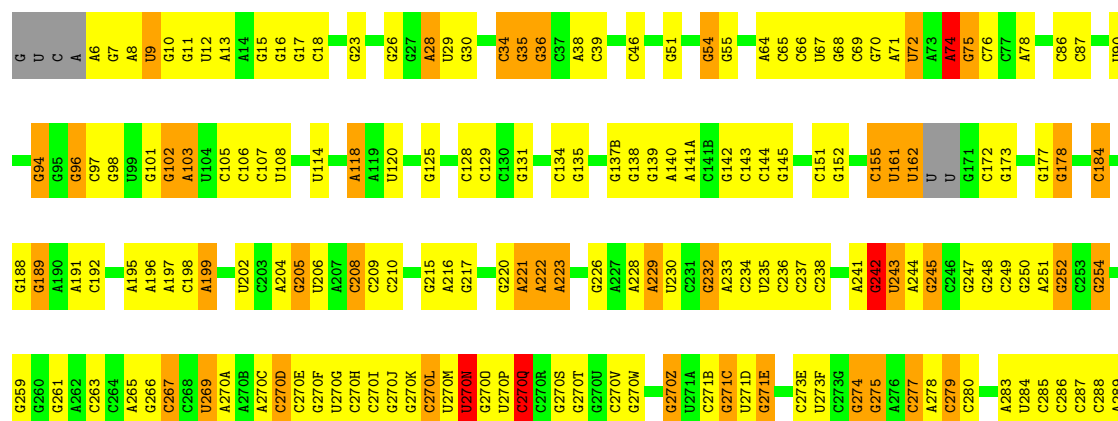
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





• Molecule 34: 23S rRNA

Chain YA: 38% 45% 15% ..



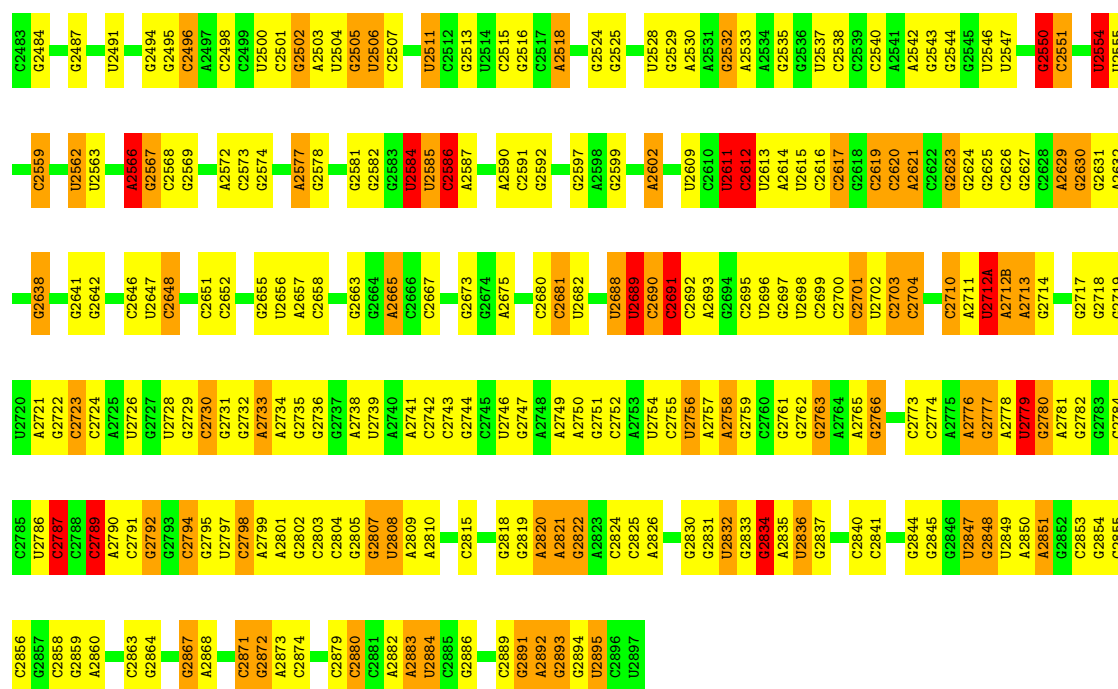






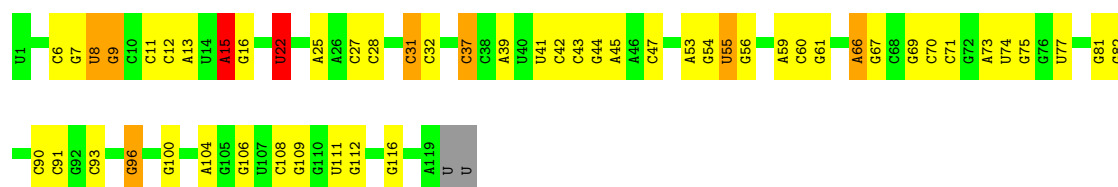
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C2424	G2354	C2285	A2198	C2138	A2077	G2011	G1930	C1839	G1756	C1658	A1571	C1502	C1428	A1360
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A2433	C2363	G2293	U2213	G2147	C2087	G2023	U1944	G1857	U1775	C1667	A1580	G1511	C1446	C1370
A2434	C2364	C2294	G2215	G2148	G2088	G2024	U1945	G1858	U1776	C1670	G1581	G1512	C1447	G1371
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G2436	A2366	G2296	A2226	U2150	U2090	G2026	C1947	G1860	U1778	C1672	A1583	C1514	G1449	U1372
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U2457	A2392	G2322	A2247	A2171	C2111	G2049	A1970	A1900	A1802	U1709	A1617	C1544	G1475	G1400
G2458	A2393	A2322	G2248	C2172	G2112	C2050	A1971	G1903	A1803	C1710	G1618	A1545A	A1476	A1401
A2459	C2394	G2323	G2249	U2173	U2113	A2051	A1981	G1904	A1812	C1711	G1633	C1546	A1477	C1402
U2460	G2395	C2324	G2250	C2174	A2114	G2052	C1982	G1907	G1813	G1718	A1634	C1547	G1478	C1403
C2461	G2396	G2325	G2251	C2175	G2115	G2053	A1982	C1908	G1816	G1725	C1638	C1548	G1479	C1404
U2462	G2397	G2252	A2176	A2176	G2116	C2054	C1983	C1909	G1817	C1726	U1639	C1549	G1480	C1405
G2463	U2400	C2261	C2328	C2179	U2118	C2055	G1989	C1908	U1818	G1728	C1640	A1554	U1482	U1406
C2464	C2401	U2262	G2329	U2180	A2119	G2056	C1990	C1909	U1819	A1729	A1541	G1555	G1483	C1407
C2465	C2402	C2263	G2330	G2181	G2120	A2059	U1991	C1910	A1820	U1730	G1644	C1556	G1484	C1408
G2466	C2403	C2264	G2331	C2182	G2121	G2060	U1992	A1913	U1820	G1731	C1645	C1557	A1486	C1409
A2469	U2406	U2265	A2335	G2183	U2122	A2061	C1993	C1914	A1825	A1732	G1646	A1558	G1487	G1410
G2470	G2407	A2266	G2336	C2184	G2123	A2062	U1994	U1915	G1826	G1733	C1647	G1559	A1490	C1411
C2471	U2408	A2267	G2337	G2185	G2124	C2063	C1994	U1918	C1827	C1734	G1648	G1560	A1491	U1415
G2472	G2409	A2268	G2338	G2186	G2125	C2064	U1995	A1919	G1828	G1735	C1649	G1561	A1492	G1416
U2473	G2410	G2271	G2339	G2187	A2126	C2065	C1996	C1920	A1829	C1741	G1650	G1562	A1493	C1417
C2474	G2411	G2272	C2341	C2188	G2127	C2066	C1999	A1918	G1830	C1742	G1651	G1563	C1494	A1418
G2475	G2412	U2273	C2342	C2189	C2128	C2067	C1999	A1919	C1831	G1743	A1652	C1564	A1495	C1419
A2476	G2413	C2274	C2343	U2193	G2129	A2069	G2001	A1918	U1834	G1750	G1653	A1565	U1496	A1497
C2477	G2414	A2274	U2344	G2190	C2129	G2069	A2001	C1920	G1835		A1654	C1567	C1498	U1420
G2478	G2415	C2275	G2345	C2191	U2130	G2070	G2002	U1923						
A2479	C2417	A2276	A2346	G2192	U2131	A2071	G2003	C1924						
C2480	U2418	A2277	G2347	G2193	U2132	G2072	G2004	C1925						
G2481	C2419	A2278	G2348	G2194	G2133	C2073		U1926						
G2482	C2420	G2279	U2348											





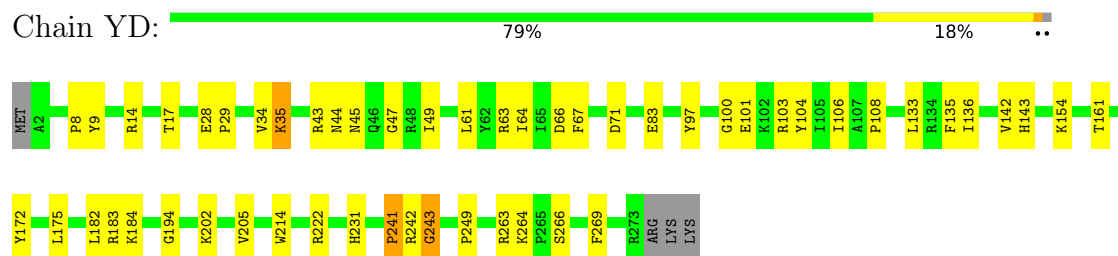
• Molecule 35: 5S rRNA

Chain RB: 55% 36% 6% ..

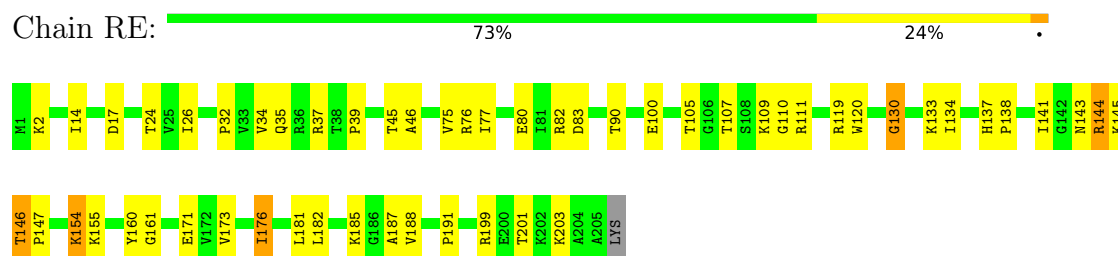




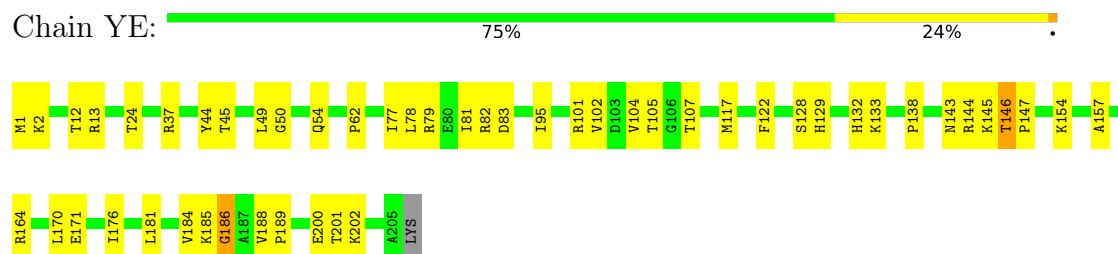
- Molecule 36: 50S ribosomal protein L2



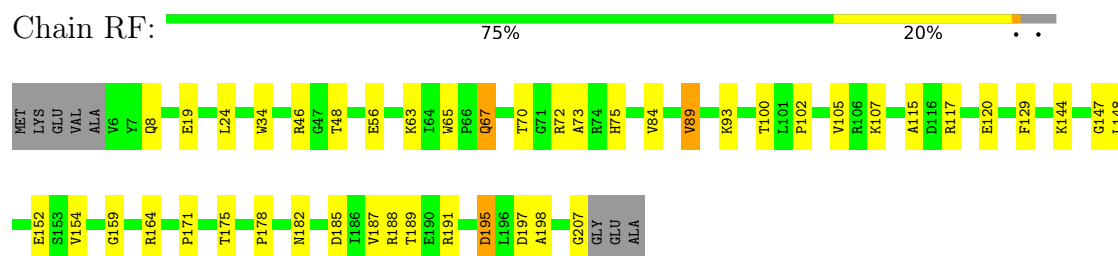
- Molecule 37: 50S ribosomal protein L3



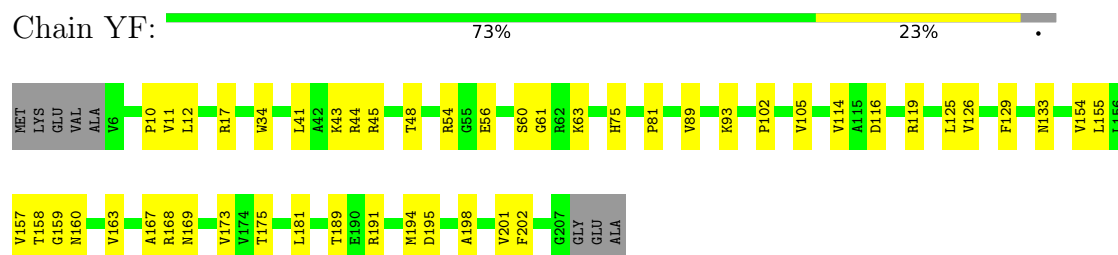
- Molecule 37: 50S ribosomal protein L3



- Molecule 38: 50S ribosomal protein L4

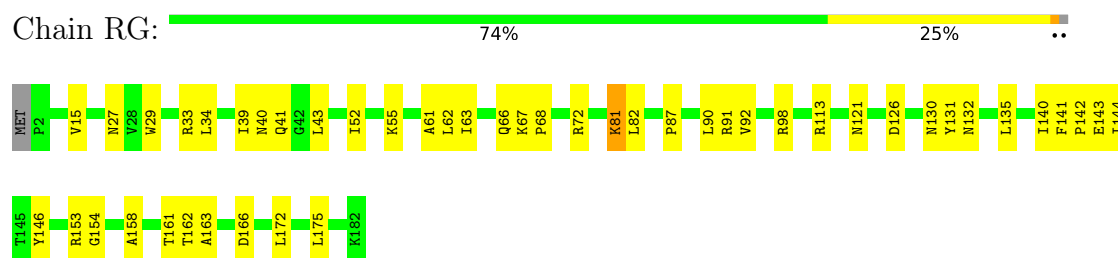


- Molecule 38: 50S ribosomal protein L4

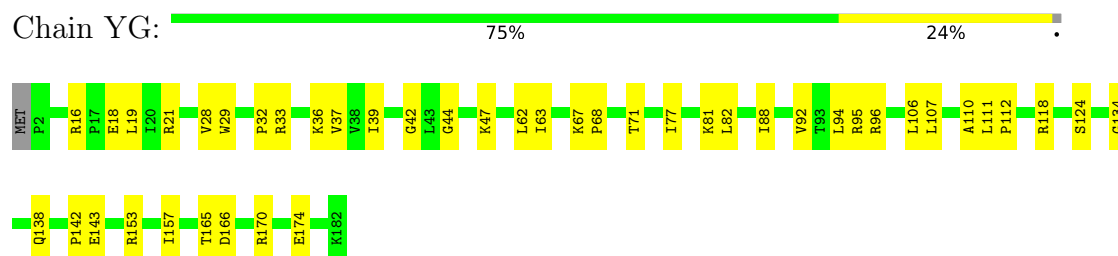




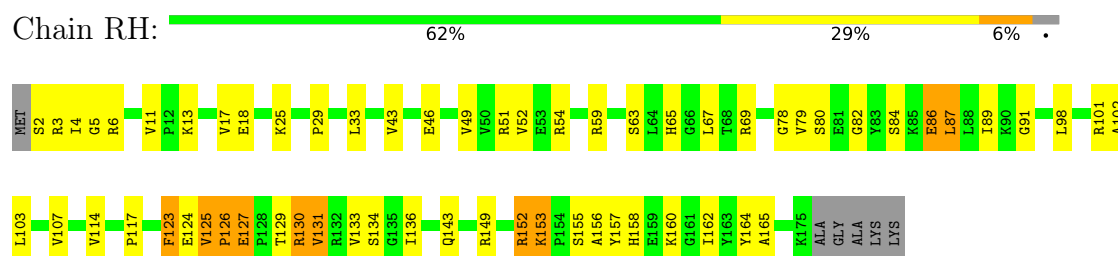
- Molecule 39: 50S ribosomal protein L5



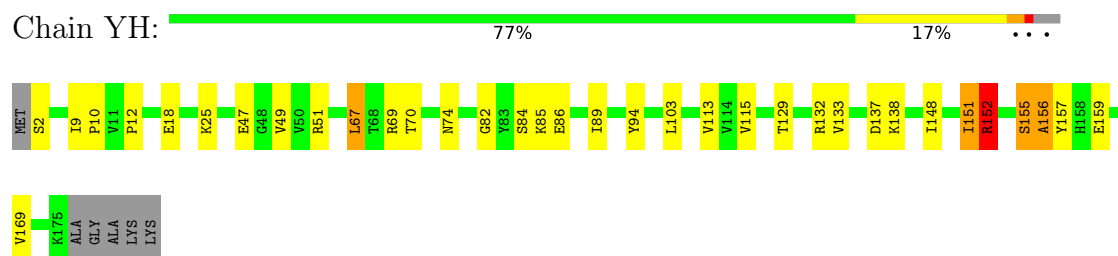
- Molecule 39: 50S ribosomal protein L5



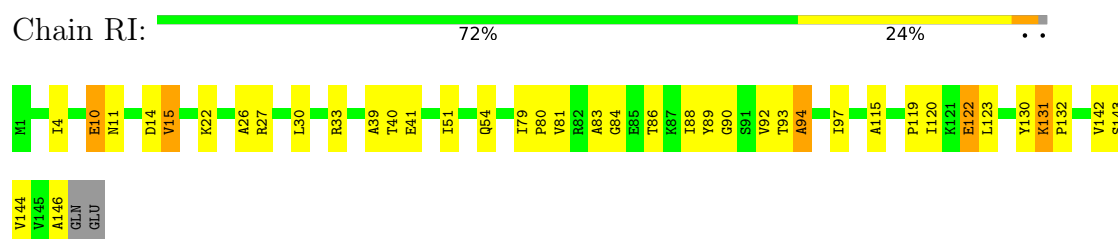
- Molecule 40: 50S ribosomal protein L6



- Molecule 40: 50S ribosomal protein L6

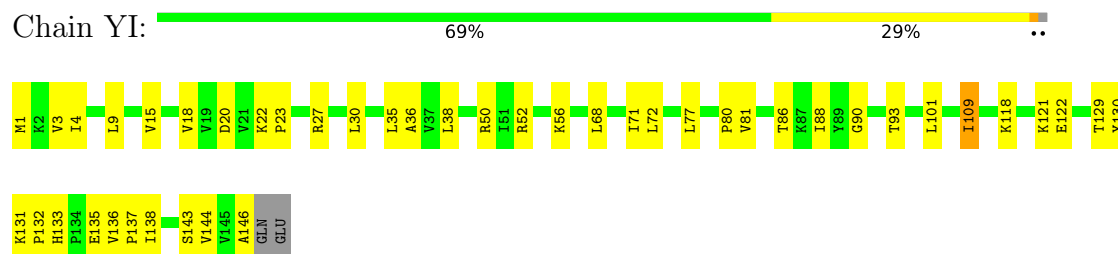


- Molecule 41: 50S ribosomal protein L9

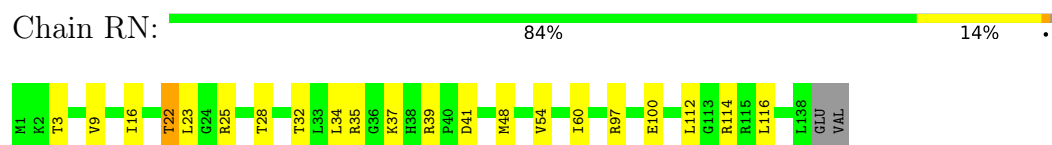




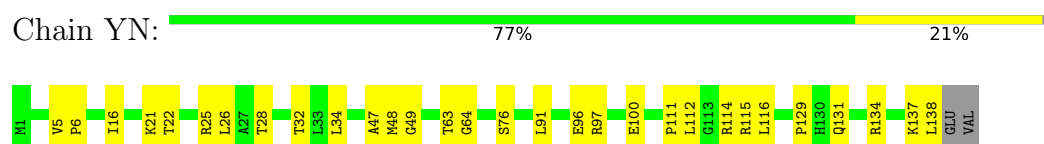
- Molecule 41: 50S ribosomal protein L9



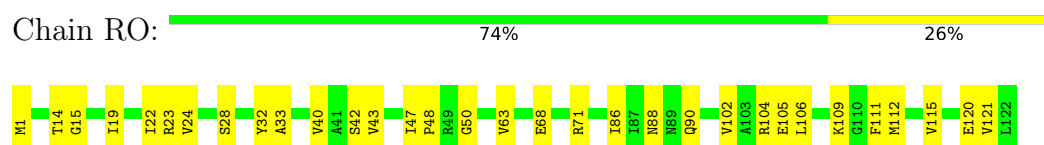
- Molecule 42: 50S ribosomal protein L13



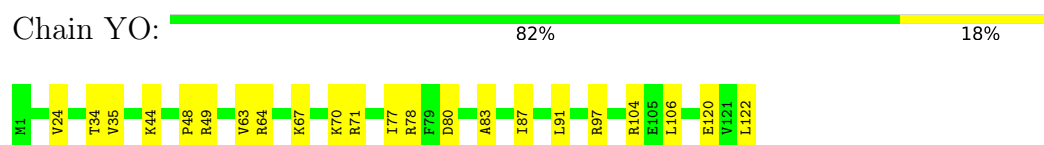
- Molecule 42: 50S ribosomal protein L13



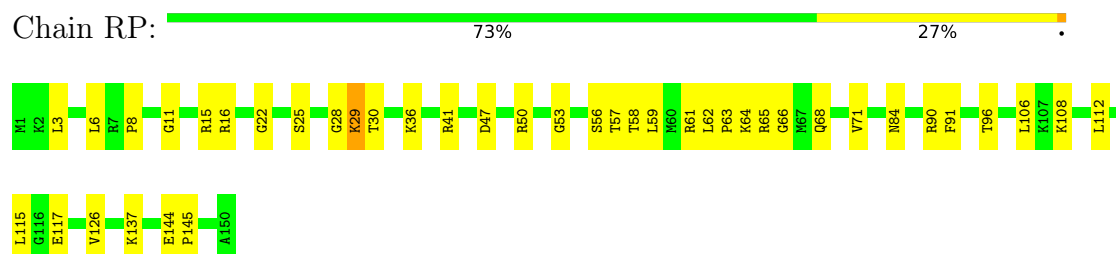
- Molecule 43: 50S ribosomal protein L14



- Molecule 43: 50S ribosomal protein L14

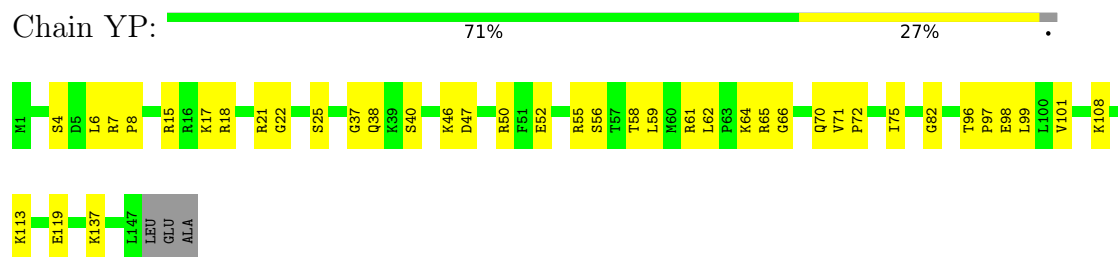


- Molecule 44: 50S ribosomal protein L15

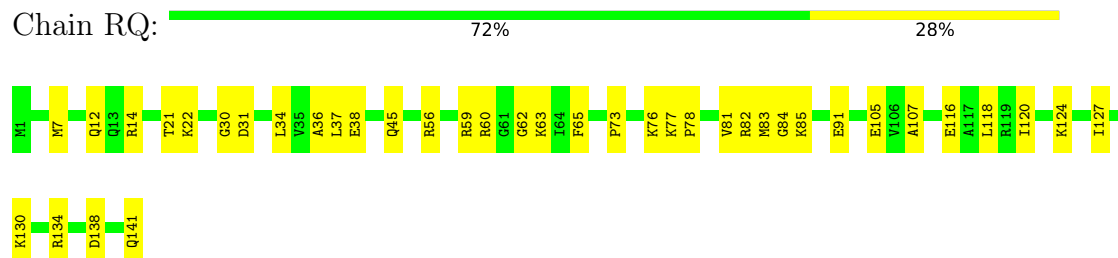


- Molecule 44: 50S ribosomal protein L15

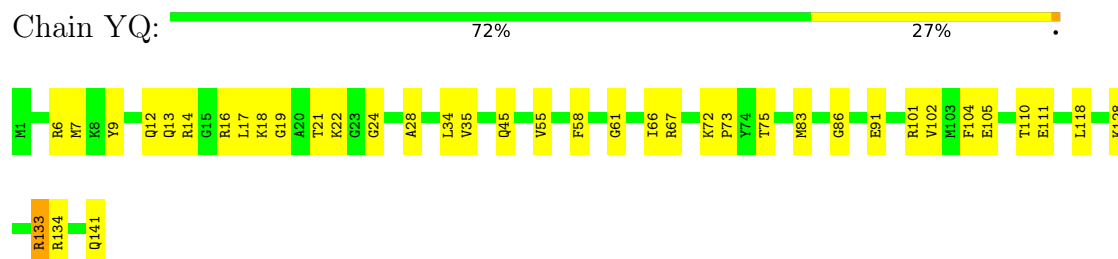




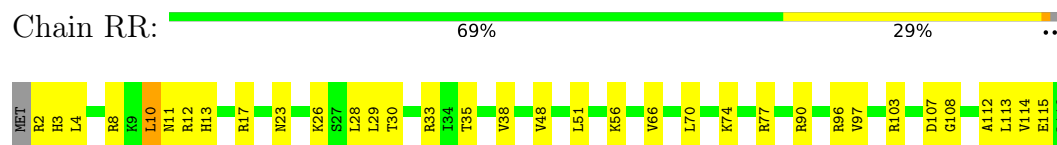
- Molecule 45: 50S ribosomal protein L16



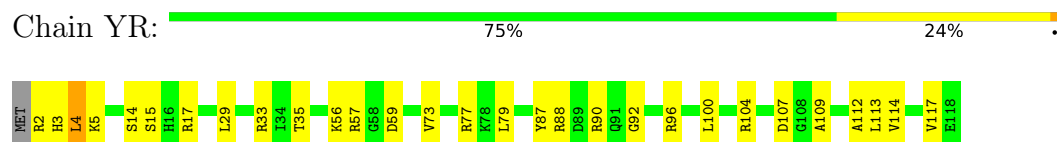
- Molecule 45: 50S ribosomal protein L16



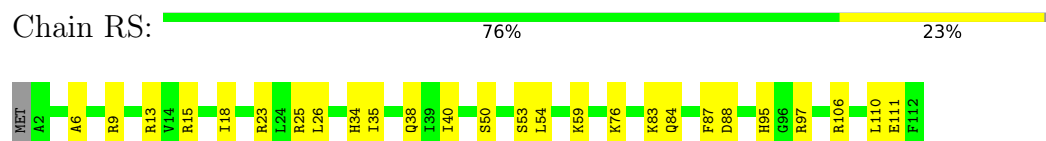
- Molecule 46: 50S ribosomal protein L17



- Molecule 46: 50S ribosomal protein L17




- Molecule 47: 50S ribosomal protein L18

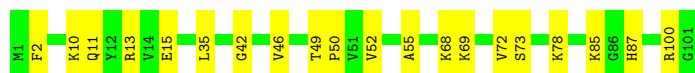





- Molecule 50: 50S ribosomal protein L21



Chain YV:  80% 20%




- Molecule 51: 50S ribosomal protein L22

Chain RW:  78% 22%




- Molecule 51: 50S ribosomal protein L22

Chain YW:  78% 22%




- Molecule 52: 50S ribosomal protein L23

Chain RX:  81% 15% .




- Molecule 52: 50S ribosomal protein L23

Chain YX:  80% 16% .




- Molecule 53: 50S ribosomal protein L24

Chain RY:  75% 19% . .



- Molecule 53: 50S ribosomal protein L24

Chain YY:  76% 20% . .



- Molecule 54: 50S ribosomal protein L25



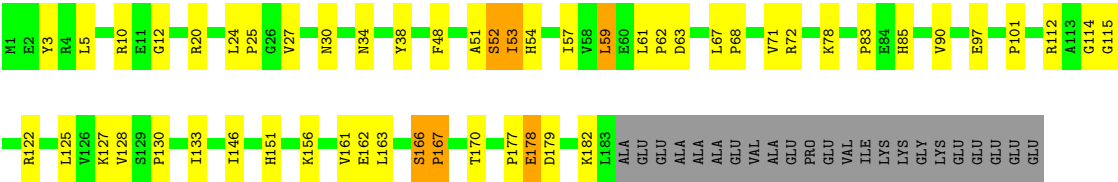
Chain RZ: 

63%

23%

•

11%



• Molecule 54: 50S ribosomal protein L25

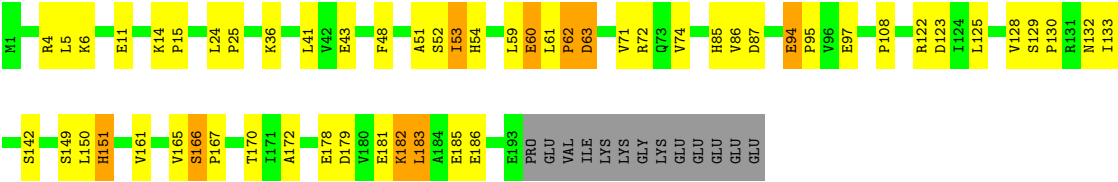
Chain YZ: 

67%

23%

•

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, $\alpha$ , $\beta$ , $\gamma$	210.09Å 450.32Å 622.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 4.14	Depositor
% Data completeness (in resolution range)	98.5 (49.85-4.14)	Depositor
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.248 , 0.294	Depositor
Wilson B-factor (Å <sup>2</sup> )	171.1	Xtriage
Anisotropy	0.389	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/36343	1.10	485/56720 (0.9%)
1	XA	0.44	28/36435 (0.1%)	1.31	648/56865 (1.1%)
2	QB	0.36	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	0.61	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	0/831	0.74	0/1120
9	XI	0.36	0/849	0.72	0/1144
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.68	1/790 (0.1%)	0.80	1/1063 (0.1%)
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	0.76	2/1301 (0.2%)
13	QM	0.35	0/931	0.75	0/1248
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	0.69	1/501 (0.2%)	0.89	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	0.38	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.38	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	0.52	0/221	0.61	0/288
22	QV	0.28	0/1621	0.84	5/2523 (0.2%)
22	XV	0.44	0/1621	1.24	15/2523 (0.6%)
23	QX	0.41	0/459	1.04	0/715
23	XX	0.60	0/459	1.31	2/715 (0.3%)
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	0.74	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	9/495 (1.8%)
29	R5	0.87	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	0.95	3/460 (0.7%)	0.81	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	4/691 (0.6%)
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	0.64	0/310	0.73	0/407
34	RA	0.26	0/69520	1.00	605/108527 (0.6%)
34	YA	0.29	2/69543 (0.0%)	1.02	662/108563 (0.6%)
35	RB	0.57	0/2878	1.40	38/4490 (0.8%)
35	YB	0.72	0/2878	1.67	85/4490 (1.9%)
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	0.85	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	0.41	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	0.68	1/1362 (0.1%)	0.86	6/1841 (0.3%)
41	RI	0.45	1/1151 (0.1%)	0.81	3/1558 (0.2%)
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	0.71	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	0.40	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	0.62	0/1306
50	RV	0.48	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%)	0.67	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	1/1108 (0.1%)
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	0.40	63/315379 (0.0%)	1.01	2644/471694 (0.6%)

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
1	XA	1	16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y4	1	1
34	RA	0	1
34	YA	0	6
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	2	30

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.62	1.05	1.54
28	Y4	4	GLY	N-CA	-18.71	1.18	1.46
1	XA	309	G	C3'-C2'	-15.74	1.35	1.52
30	R6	16	CYS	CB-SG	14.21	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82

The worst 5 of 2644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	617	G	C4-N9-C1'	38.95	177.13	126.50
1	XA	617	G	C8-N9-C1'	-38.89	76.44	127.00
1	XA	1505	G	C8-N9-C1'	-27.87	90.77	127.00
1	XA	625	G	C8-N9-C1'	-27.83	90.82	127.00
1	XA	1505	G	C4-N9-C1'	27.65	162.44	126.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	XA	617	G	C2'
28	Y4	5	ILE	CA

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	RA	1649	G	Sidechain
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
1	XA	308	C	Sidechain



## 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	16385	1571	0
1	XA	32551	0	16418	1288	0
2	QB	1907	0	1958	99	0
2	XB	1915	0	1965	40	0
3	QC	1605	0	1667	135	0
3	XC	1605	0	1668	92	18
4	QD	1703	0	1762	108	0
4	XD	1703	0	1763	57	7
5	QE	1155	0	1213	76	0
5	XE	1155	0	1213	33	0
6	QF	843	0	857	10	5
6	XF	843	0	855	89	0
7	QG	1257	0	1296	53	18
7	XG	1257	0	1295	62	0
8	QH	1108	0	1165	52	0
8	XH	1108	0	1165	26	0
9	QI	816	0	822	51	6
9	XI	834	0	847	22	0
10	QJ	801	0	843	199	0
10	XJ	777	0	816	114	6
11	QK	885	0	904	35	0
11	XK	864	0	880	70	0
12	QL	975	0	1062	46	0
12	XL	956	0	1046	30	0
13	QM	921	0	974	137	0
13	XM	914	0	966	128	0
14	QN	492	0	528	288	0
14	XN	492	0	521	172	0
15	QO	734	0	770	57	0
15	XO	729	0	767	44	0
16	QP	705	0	725	71	0
16	XP	705	0	725	16	0
17	QQ	834	0	904	43	0
17	XQ	834	0	902	23	0
18	QR	574	0	644	8	0
18	XR	574	0	643	102	0
19	QS	665	0	678	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	695	110	0
20	QT	763	0	861	26	0
20	XT	763	0	861	40	0
21	QU	217	0	223	44	0
21	XU	217	0	234	10	0
22	QV	1452	0	736	3	0
22	XV	1452	0	736	16	0
23	QX	409	0	209	5	0
23	XX	409	0	209	23	0
24	R0	643	0	667	12	0
24	Y0	648	0	672	11	0
25	R1	746	0	826	26	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	6	1
26	Y2	575	0	624	6	0
27	R3	469	0	518	13	2
27	Y3	469	0	518	12	0
28	R4	348	0	354	25	0
28	Y4	357	0	362	9	0
29	R5	459	0	477	20	0
29	Y5	459	0	476	25	1
30	R6	453	0	474	11	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	12	0
31	Y7	418	0	467	18	0
32	R8	517	0	582	31	0
32	Y8	517	0	582	27	0
33	R9	307	0	335	24	0
33	Y9	307	0	336	19	0
34	RA	62070	0	31282	990	0
34	YA	62091	0	31289	1253	1
35	RB	2573	0	1306	21	0
35	YB	2573	0	1306	13	0
36	RD	2115	0	2195	53	2
36	YD	2115	0	2195	64	0
37	RE	1568	0	1634	34	0
37	YE	1568	0	1633	33	0
38	RF	1585	0	1632	33	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	49	0
39	YG	1474	0	1535	27	0
40	RH	1336	0	1418	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	25	0
41	RI	1136	0	1223	41	0
41	YI	1136	0	1223	30	0
42	RN	1104	0	1180	13	0
42	YN	1104	0	1180	17	0
43	RO	933	0	996	23	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	37	0
44	YP	1122	0	1206	44	2
45	RQ	1122	0	1179	41	0
45	YQ	1122	0	1179	33	0
46	RR	960	0	1021	22	0
46	YR	960	0	1021	24	0
47	RS	882	0	943	19	0
47	YS	882	0	943	16	0
48	RT	1141	0	1202	19	0
48	YT	1141	0	1202	29	0
49	RU	964	0	1022	38	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	17	0
50	YV	779	0	852	11	1
51	RW	900	0	964	20	0
51	YW	900	0	964	19	0
52	RX	725	0	778	11	0
52	YX	725	0	778	9	0
53	RY	818	0	911	25	0
53	YY	818	0	910	19	0
54	RZ	1461	0	1493	36	0
54	YZ	1529	0	1551	33	0
55	QA	70	0	0	0	0
55	QE	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	2	0	0	0	0
55	R0	2	0	0	0	0
55	R3	1	0	0	0	0
55	R8	2	0	0	0	0
55	RA	432	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
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	XA	88	0	0	2	0
55	XE	1	0	0	0	0
55	XO	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	2	0	0	0	0
55	YA	394	0	0	3	0
55	YB	1	0	0	0	0
55	YD	2	0	0	0	0
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YP	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	291185	0	197033	6993	35

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 15.

The worst 5 of 6993 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)
10:QJ:47:PHE:CZ	14:QN:36:PHE:HB3	1.21	1.72
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:980:C:C1'	14:QN:19:ARG:HG2	1.23	1.68
1:QA:1049:U:C5	14:QN:3:ARG:HB3	1.26	1.66
1:XA:1190:G:H5'	3:XC:176:HIS:CE1	1.30	1.64

The worst 5 of 35 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)
7:QG:149:ARG:NE	3:XC:81:GLY:O[4_555]	0.51	1.69
7:QG:149:ARG:NH1	3:XC:85:ARG:N[4_555]	1.02	1.18
7:QG:149:ARG:NH1	3:XC:85:ARG:CA[4_555]	1.16	1.04
7:QG:149:ARG:CZ	3:XC:85:ARG:N[4_555]	1.35	0.85
7:QG:149:ARG:NH1	3:XC:85:ARG:CB[4_555]	1.52	0.68

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	71
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	67
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	103/128 (80%)	91 (88%)	12 (12%)	0	100	100
9	XI	105/128 (82%)	97 (92%)	8 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	53
10	XJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	7	38
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	59
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	113/126 (90%)	96 (85%)	16 (14%)	1 (1%)	17	55
13	XM	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	17	55
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	43
14	XN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	29
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%)	91 (93%)	7 (7%)	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	31
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	4	31
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	51
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%)	12 (27%)	4 (9%)	1	12
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	30
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	71
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	35
37	YE	203/206 (98%)	162 (80%)	39 (19%)	2 (1%)	15	53
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	53
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	67
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	43
40	YH	172/180 (96%)	147 (86%)	21 (12%)	4 (2%)	6	37
41	RI	144/148 (97%)	114 (79%)	24 (17%)	6 (4%)	3	25
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
43	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	7	40
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	55
47	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	17	55
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	34
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	53
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	53
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	28
All	All	11368/12128 (94%)	10080 (89%)	1202 (11%)	86 (1%)	19	59

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN

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Mol	Chain	Res	Type
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	79
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	82
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	82
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	92
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	84
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	88
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	84
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	89
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	79/99 (80%)	77 (98%)	2 (2%)	47	68
9	XI	81/99 (82%)	80 (99%)	1 (1%)	71	83
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	84 (98%)	2 (2%)	50	70
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	84
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	84
12	QL	104/109 (95%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	100 (97%)	3 (3%)	42	64
13	QM	93/101 (92%)	93 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	73
14	XN	49/50 (98%)	47 (96%)	2 (4%)	30	56
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	68
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	71
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	82
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	51
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	51
24	R0	65/67 (97%)	64 (98%)	1 (2%)	65	79
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	47	68
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	79
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%)	40 (98%)	1 (2%)	49	68
29	R5	51/52 (98%)	50 (98%)	1 (2%)	55	73
29	Y5	51/52 (98%)	48 (94%)	3 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R6	51/52 (98%)	49 (96%)	2 (4%)	32	57
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	57
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
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%)	33 (97%)	1 (3%)	42	64
36	RD	214/218 (98%)	212 (99%)	2 (1%)	78	88
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49	68
37	YE	165/166 (99%)	163 (99%)	2 (1%)	71	83
38	RF	161/166 (97%)	158 (98%)	3 (2%)	57	74
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	92
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21	49
40	YH	145/148 (98%)	143 (99%)	2 (1%)	67	80
41	RI	122/124 (98%)	121 (99%)	1 (1%)	81	89
41	YI	122/124 (98%)	118 (97%)	4 (3%)	38	61
42	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88
42	YN	117/119 (98%)	115 (98%)	2 (2%)	60	78
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	98 (98%)	2 (2%)	55	73
44	RP	116/116 (100%)	115 (99%)	1 (1%)	78	88
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	88
46	RR	100/101 (99%)	99 (99%)	1 (1%)	76	86
46	YR	100/101 (99%)	99 (99%)	1 (1%)	76	86
47	RS	87/88 (99%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	YS	87/88 (99%)	85 (98%)	2 (2%)	50	70
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47	68
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60	78
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52	70
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	49	68
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73	84
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	30	56
52	YX	74/78 (95%)	72 (97%)	2 (3%)	44	66
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	73	84
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	71	83
All	All	9610/10066 (96%)	9507 (99%)	103 (1%)	73	84

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	RX	16	LYS
10	XJ	69	ASN
49	YU	94	ASN
52	RX	27	THR
4	XD	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
42	RN	101	HIS
3	XC	176	HIS
29	Y5	22	HIS
52	RX	41	ASN
4	XD	116	GLN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	531 (35%)	14 (0%)
1	XA	1514/1521 (99%)	469 (30%)	27 (1%)
22	QV	66/77 (85%)	15 (22%)	1 (1%)
22	XV	66/77 (85%)	16 (24%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	0
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2905 (99%)	706 (24%)	40 (1%)
34	YA	2880/2905 (99%)	754 (26%)	40 (1%)
35	RB	119/122 (97%)	20 (16%)	1 (0%)
35	YB	119/122 (97%)	23 (19%)	1 (0%)
All	All	9187/9288 (98%)	2544 (27%)	125 (1%)

5 of 2544 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	8	A
1	QA	9	G
1	QA	15	G

5 of 125 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	115	G
1	XA	1253	G
34	YA	1992	G
1	XA	309	G
1	XA	635	G

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 1038 ligands modelled in this entry, 1036 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

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 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.