



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 05:13 am BST

PDB ID : 5J3C
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2016-03-30
Resolution : 3.04 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

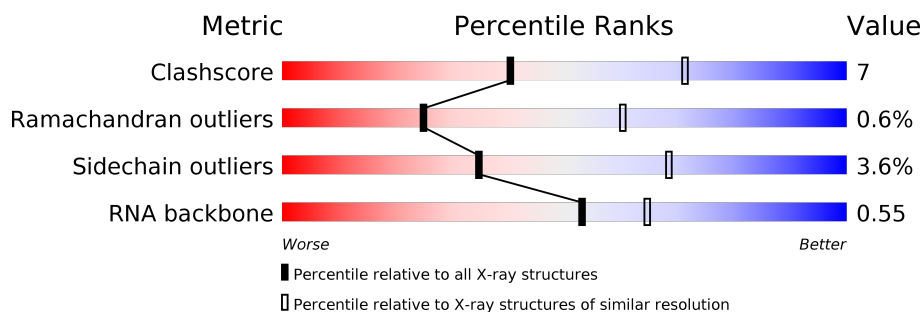
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RNA backbone	3102	1034 (3.30-2.78)















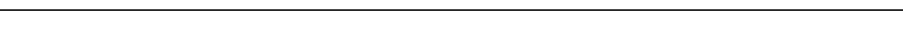




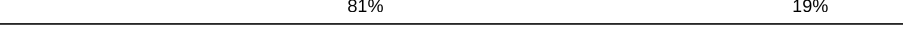





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	RA	2915	61% 31% 6% .
1	YA	2915	60% 31% 7% ..
2	RB	122	79% 16% ..
2	YB	122	77% 19% ..
3	RD	276	82% 17% .
3	YD	276	82% 16% .
4	RE	206	77% 20% ..


























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Mol	Chain	Length	Quality of chain
4	YE	206	 76% 21% ..
5	RF	210	 73% 21% . .
5	YF	210	 69% 27% ..
6	RG	182	 75% 25% .
6	YG	182	 71% 25% ..
7	RH	180	 82% 14% ..
7	YH	180	 68% 28% ..
8	RI	148	 80% 18% ..
8	YI	148	 80% 15% ..
9	RN	140	 81% 17% .
9	YN	140	 83% 14% .
10	RO	122	 76% 24%
10	YO	122	 81% 18% .
11	RP	150	 78% 19% ..
11	YP	150	 75% 21% ..
12	RQ	141	 81% 18% .
12	YQ	141	 77% 21% .
13	RR	118	 75% 22% .
13	YR	118	 81% 19%
14	RS	112	 80% 15% ..
14	YS	112	 81% 16% ..
15	RT	146	 66% 20% . 10%
15	YT	146	 71% 17% . 10%
16	RU	118	 81% 16% ..
16	YU	118	 83% 15% .


























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Mol	Chain	Length	Quality of chain
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	
28	R6	54	
28	Y6	54	
29	R7	49	

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Mol	Chain	Length	Quality of chain
29	Y7	49	
30	R8	65	
30	Y8	65	
31	R9	37	
31	Y9	37	
32	QA	1521	
32	XA	1521	
33	QB	256	
33	XB	256	
34	QC	239	
34	XC	239	
35	QD	209	
35	XD	209	
36	QE	162	
36	XE	162	
37	QF	101	
37	XF	101	
38	QG	156	
38	XG	156	
39	QH	138	
39	XH	138	
40	QI	128	
40	XI	128	
41	QJ	105	
41	XJ	105	




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Mol	Chain	Length	Quality of chain
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	
53	QV	77	
53	XV	77	
54	QX	25	

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Mol	Chain	Length	Quality of chain
54	XX	25	
55	QY	360	
55	XY	360	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 294929 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
1	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	RF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	YF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	RZ	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	YZ	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	Y3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	QI	127	Total	C	N	O		0	0	0
			986	625	193	168				
40	XI	126	Total	C	N	O		0	0	0
			966	613	186	167				

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QJ	97	Total	C	N	O		0	0	0
			719	446	142	131				
41	XJ	96	Total	C	N	O		0	0	0
			710	442	137	131				

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	XL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	XM	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	XO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QR	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	XR	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	QU	23	Total	C	N	O		0	0	0
			199	122	48	29				
52	XU	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 53 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
53	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 54 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	9	Total	C	N	O	P	0	0	0
			193	87	37	60	9			
54	XX	10	Total	C	N	O	P	0	0	0
			215	97	42	66	10			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	259	Total	C	N	O	S	0	0	0
			2014	1235	382	389	8			
55	XY	260	Total	C	N	O	S	0	0	0
			2022	1241	383	390	8			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	262	Total	Mg	0	0
			262	262		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	2	Total	Mg	0	0
			2	2		
56	R7	3	Total	Mg	0	0
			3	3		
56	YA	749	Total	Mg	0	0
			749	749		
56	Y5	2	Total	Mg	0	0
			2	2		
56	YR	1	Total	Mg	0	0
			1	1		
56	RT	3	Total	Mg	0	0
			3	3		
56	QD	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	2	Total 2	Mg 2	0	0
56	XE	2	Total 2	Mg 2	0	0
56	RG	4	Total 4	Mg 4	0	0
56	QI	1	Total 1	Mg 1	0	0
56	YD	9	Total 9	Mg 9	0	0
56	QV	6	Total 6	Mg 6	0	0
56	RX	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	187	Total 187	Mg 187	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	RQ	5	Total 5	Mg 5	0	0
56	R0	7	Total 7	Mg 7	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	RU	3	Total 3	Mg 3	0	0
56	QG	3	Total 3	Mg 3	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QH	1	Total 1	Mg 1	0	0
56	YG	2	Total 2	Mg 2	0	0
56	XY	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	RY	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	4	Total 4	Mg 4	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	4	Total 4	Mg 4	0	0
56	RD	15	Total 15	Mg 15	0	0
56	R1	5	Total 5	Mg 5	0	0
56	QO	1	Total 1	Mg 1	0	0
56	YT	3	Total 3	Mg 3	0	0
56	RV	3	Total 3	Mg 3	0	0
56	QF	1	Total 1	Mg 1	0	0
56	R5	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	RA	1032	Total 1032	Mg 1032	0	0
56	YF	2	Total 2	Mg 2	0	0
56	YP	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QB	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0
56	RS	1	Total 1	Mg 1	0	0
56	RE	7	Total 7	Mg 7	0	0
56	XL	1	Total 1	Mg 1	0	0
56	YB	20	Total 20	Mg 20	0	0
56	QT	1	Total 1	Mg 1	0	0
56	QN	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	2	Total 2	Mg 2	0	0
56	XV	4	Total 4	Mg 4	0	0
56	RB	22	Total 22	Mg 22	0	0
56	QJ	1	Total 1	Mg 1	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	2	Total 2	Mg 2	0	0
56	RF	11	Total 11	Mg 11	0	0
56	R3	2	Total 2	Mg 2	0	0
56	YE	6	Total 6	Mg 6	0	0

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

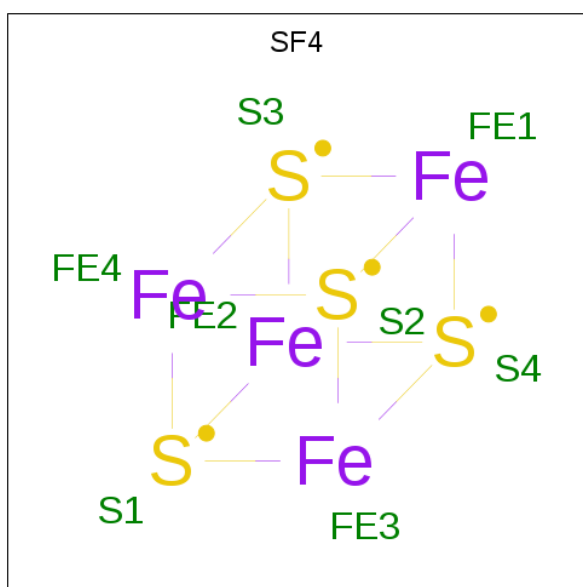
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total 1	Zn 1	0	0

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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



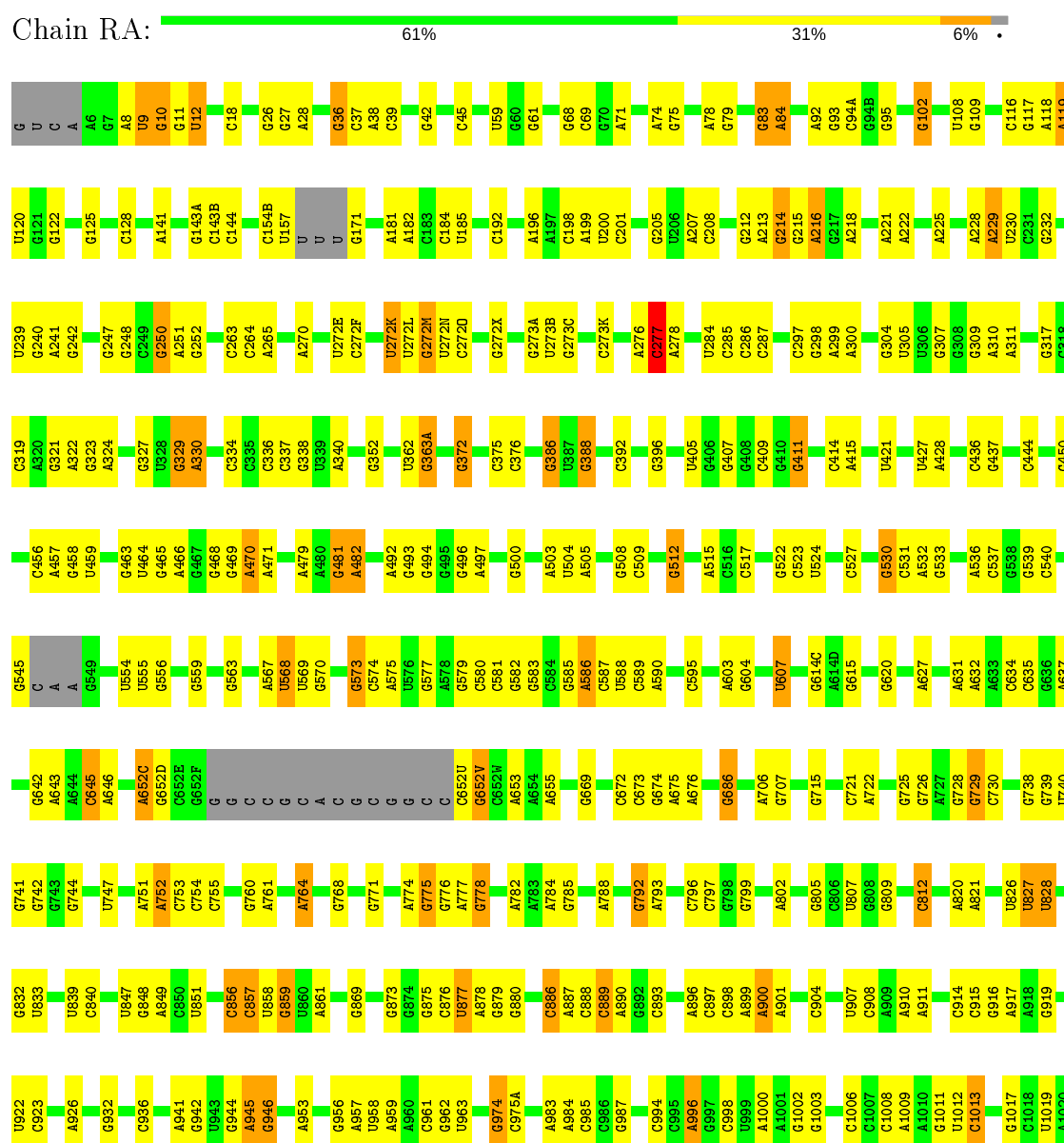
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots

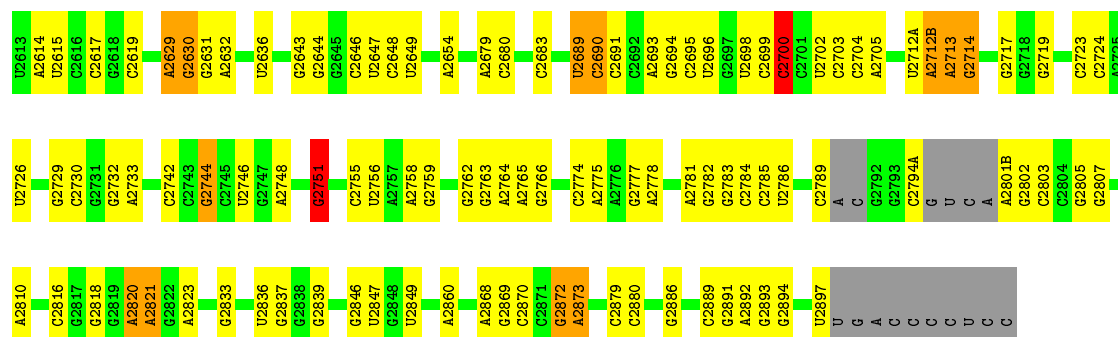
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 23S rRNA

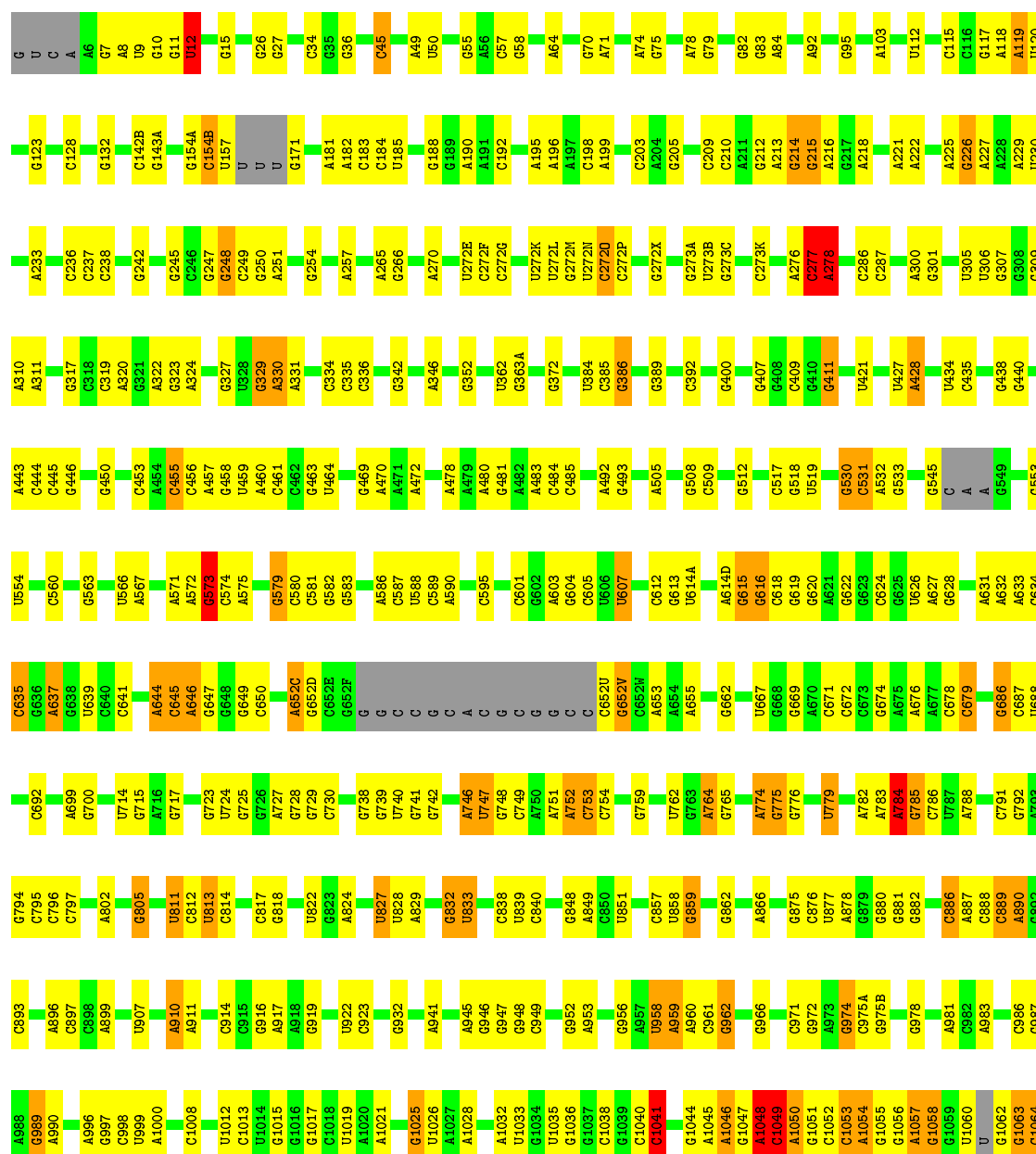


G2502	G2315	G2219	G2131	C2043	A1676	A	G1413	G1277	G1170	A1084	A1021
A2503	C2316	G2223	U2132	G2046	C1686	C1536	G1416	A1278	G1171	A1085	G1022
U2504	C2317	G2224	A1938	G1999	G1800	G1539	G1417	A1279	G	A1086	U1023
G2505	A2134	A2225	U1940	G1801	U1688	G1539	C1417	C1289	A	G1087	G1024
U2506	G2319	A2226	G1941	A1802	U1689	G1542	G1418	C1290	U	A1088	G1025
G2507	A2136	G2227	C1942	A1803	A1689	C1543	A1419	C1291	G	G1089	U1026
G2508	C2321	G2228	U1945	A1812	U1693	A1554	U1420	U1292	A	U1090	U1027
	A2322		G1958		U1696		G1421	C1293	C1178	A1091	A1028
G2512	G2325	U2232	C1958	A1815	G1696	A1554	G1422	C1293	C1179	C1092	A1029
G2513	C2326	U2233	G1959	G1816	G1697	C1557	G1423	U1300	C1180	G1093	G1030
G2516	C2327	G2234	A1960	G1817	A1698	A1558	G1424	A1301	U1094	U1094	U1033
G2517	A2328		C1961	U1818	G1699	A1566	G1425	C1306	A1095	A1095	U1034
A2518	A2422	G2238	C1962	U1818	U1700	A1567	G1426		U1096	A1096	U1035
U2519	G2334	G2239	G1963	G1826	A1701	A1568	A1427	G1309	U1098	U1098	G1037
C2520	A2335	G2240	G1964	C1827	G1702	A1569	G1428	U1205	C1092	G1099	G1038
	A2336	A2071	G1967	G1828	G1703	A1570	C1430	C1314	U1100	U1101	G1039
G2526	G2147		C1967	G1833	G1721		U1431		A1210	C1102	C1040
	G2148	U2074	G1968	U1833	G1722			C1320	G1212	A1103	C1041
G2529	C2342	U2075	A1969	U1834	U1722		A1445A	A1321	U1211	G1104	
A2430	U2150	U2076	A1970	G1835	U1739			U1322	G1212	U1105	C1043
U2537	G2151	U2077	A1971	U1835	G1740		A1449	U1322	G1219	G1106	
C2538	G2152	C2077	A1972	A1847	A1741		G1450A	U1323		G1107	A1045
G2539	G2153	C2078	A1972	A1848	G1758					U1108	A1046
C2540	G2154		G1975		G1746		G1455	U1341	G1223	G1109	G1047
A2541	G2155	G2087		U1864			A1584		C1224	A1111	C1049
A2542	G2156		U1991	G1865	G1750		A1587	C1351	G1225	G1112	
	A2157	G2094	G1992	C1866			A1588	U1352	G1226	G1113	C1053
G2549	G2158	C2095	U1993	A1876	G1756		C1589		G1117	A1054	G1055
C2550	G2159	U2096	G1993	A1877	U1757			G1356	G1238	G1056	
C2552	G2160	C2097	G1997	A1878	G1758		C1467	U1357	G1239	A1057	A1058
G2553	C2161	U2098	G1998	G1878			A1471	G1358	U1240	G1118	G1059
U2554	G2162	U2099	G1999		A1762		G1482	G1359	G1241	G1119	
U2555	G2163	C2103	G2000	C1895	G1763		A1490	A1365		C1123	U1060
U2563	U2167	C2105	A2001	G1899	G1764			G1248	U1249		U
A2564	G2168	G2106	G2002	A1900	G1769		C1493	G1250	G1251	A1127	G1062
G2565	A2171	C2107	C2006	G1903	A1773		A1494	G1252	A1128	G1063	C1064
A2566	U2172	C2108	A2014	G1906	U1776		A1495	G1253	U1130	U1065	U1066
G2567	A2173	U2109	A2015	G1907	U1777		A1507	A1254		A1067	A1068
C2568	C2174	G2110	A2015	C1908	U1778		C1504	U1255	U1133	G1069	A1070
	G2175	C2111	A2015	G1909	U1779		C1505	G1256	C1135	G1137	A1071
A2376	A2176	G2112	G2018	G1913	A1780		A1506	G1259	G1138	G1072	C1073
A2377	G2177	G2113	U2022	C1914	C1781		A1507	G1260	C1140	U1141	G1074
U2378	U2180	A2114	G2023	U1915	C1782		C1640		U1421A	C1075	C1075
G2379	G2181	G2115	G2026	U1916	A1783		A1508	G1263	A1142B	C1076	C1076
	G2186	A2117	C2026	A1917	A1784		C1509A	G1264	A1143	U1077	A1077
G2382	U2189	G2118	U2028	U1917	A1785		A1509B	G1385	A1268	U1078	C1079
G2383	G2190	G2119	G2029	A1918	A1786		A1509C	U1388	A1269	C1080	U1081
G2384	G2191	G2120	A2030	A1919			A1654			C1165	U1082
G2385	G2192	G2121	A2031	C1920	A1789		G1525	U1394	G1266	C1166	U1083
G2386	G2193	G2122	G2032	G1929	C1790		G1529	U1395	U1267		
	A2198	G2123	A2033	G1930	A1791		C1530	U1396	A1269	A1155	
G2387	G2206	A2126	G2035	U1934	U1794		G1531	C1404	G1270		
G2388	G2207	G2127	G2036	C1934	C1795		C1532	U1405	C1271	U165	
G2389	A2208	C2128	G2037	G1935	U1796		G1533	A1272	A1272		
G2390	U2218	U2130	G2037	A1936	C1797		U	A1412			

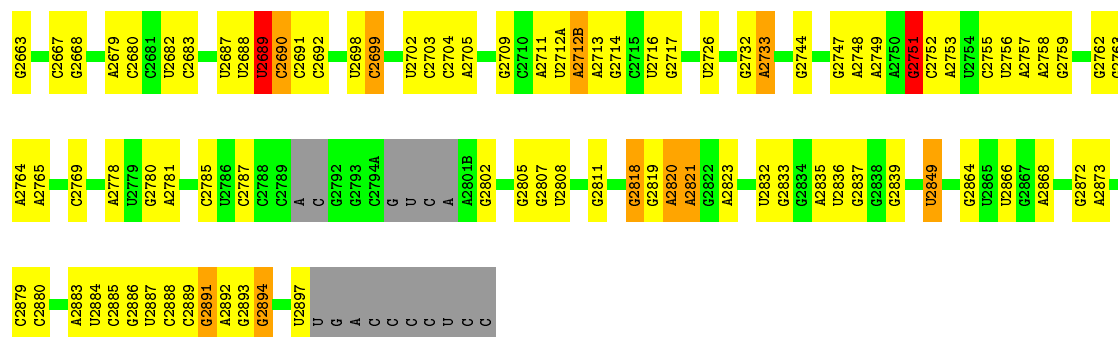


• Molecule 1: 23S rRNA

Chain YA: 60% 31% 7% ..



G2557	C2441	A2335	C2261	C2161	U2096	A2001	G1826	G1702	C1598	U1497	U1396	C1270	G1135	U1065
A2561	G2447	A2342	U2262	G2165	U2099	G2002	A1829	G1703	C1599	G1500	U1397	G1271	G1136	U1066
A2564	A2448	C2343	C2263	G2166	C2103	G2003	U1834	C1710	U1602	A1507	C1404	U1272	U1141	A1067
A2565	G2455	U2344	U2265	U2167	G2104	G2012	U1835	C1719	A1608	A1508	U1405	A1278	U1142A	A1069
A2566	C2456	C2345	U2266	G2168	C2105	A2013	A1835	G1720	A1609	C1509A	U1406	G1278	A1142B	A1070
C2461	A2347	A2346	A2267	C2169	C2106	A2014	A1847	G1721	A1610	A1509B	C1407	G1283	A1143	G1071
C2462	A2347	C2347	A2268	A2171	C2107	A2018	A1848	G1722	C1611	U1514	C1408	G1285	G1151	C1072
C2463	A2347	A2173	A2269	A2172	C2108	G2019	A1854	U1739	C1617	G1515	A1412	G1286	G1152	A1073
C2350	A2173	A2173	A2173	A2173	C2109	A2020	A1854	G1740	A1618	U1514	C1412	G1287	G1153	G1074
C2355	A2176	A2176	A2176	A2176	C2110	A2021	C1866	G1741	C1625	G1520	G1416	U1292	A1155	C1076
C2358	A2273	A2273	A2273	A2273	C2111	G2023	A1876	A1741	U1602	U1514	C1417	G1293	A1156	U1078
C2359	A2274	A2274	A2274	A2274	C2112	U2028	A1877	G1756	C1636	G1526	G1418	G1296	G1157	C1080
A2360	A2275	A2275	A2275	A2275	U2113	G2029	G1878	A1762	C1637	U1420	U1419	G1296	G1164	U1081
A2361	A2277	A2277	A2277	A2277	G2115	A2030	A1889	G1763	C1638	C1530	U1421	U1300	U1165	U1082
A2364	A2278	A2278	A2278	A2278	G2116	A2031	A1890	G1764	U1639	C1531	G1422	U1300	C1166	U1083
A2364	A2279	A2279	A2279	A2279	A2117	A2032	A1890	G1769	C1640	C1532	G1423	A1302	U1167	A1084
A2364	A2280	A2280	A2280	A2280	U2118	A2033	G1899	G1773	C1642	U1533	A1427	G1303	G1171	A1085
A2364	A2281	A2281	A2281	A2281	C2120	G2034	A1900	A1773	G1645	A	C1428	G1303	G	A1086
A2364	A2282	A2282	A2282	A2282	G2121	G2035	A1900	A1773	C1646	U1536	G1429	A1308	A	G1087
A2364	A2283	A2283	A2283	A2283	U2122	G2036	A1900	A1773	C1646	G1539	U1431	G1309	U	A1088
A2364	A2284	A2284	A2284	A2284	G2123	C2043	A1906	G1776	C1646	U1539	U1431	G1309	G	U1090
A2364	A2285	A2285	A2285	A2285	A2126	U2047	A1912	A1780	C1647	U1539	U1431	G1309	A	A1088
A2364	A2286	A2286	A2286	A2286	G2127	U2047	A1913	C1781	C1648	U1539	U1431	G1309	U	A1088
A2364	A2287	A2287	A2287	A2287	C2128	U2047	A1914	C1782	C1649	U1539	U1431	G1309	G	A1088
A2364	A2288	A2288	A2288	A2288	G2129	C2055	G1929	A1786	C1650	U1539	U1431	G1309	A	A1088
A2364	A2289	A2289	A2289	A2289	U2130	G2056	G1930	A1786	C1651	U1539	U1431	G1309	A	A1088
A2364	A2290	A2290	A2290	A2290	C2131	A2060	U1932	A1791	A1654	U1539	U1431	G1309	A	A1088
A2364	A2291	A2291	A2291	A2291	U2132	G2061	A1932	A1791	C1657	U1539	U1431	G1309	A	A1088
A2364	A2292	A2292	A2292	A2292	C2133	A2062	C1933	U1794	C1657	U1539	U1431	G1309	A	A1088
A2364	A2293	A2293	A2293	A2293	G2134	G2063	G1935	C1795	C1658	U1539	U1431	G1309	A	A1088
A2364	A2294	A2294	A2294	A2294	A2135	C2064	A1935	U1796	C1658	U1539	U1431	G1309	A	A1088
A2364	A2295	A2295	A2295	A2295	C2136	C2065	A1937	C1797	A1664	U1539	U1431	G1309	A	A1088
A2364	A2296	A2296	A2296	A2296	C2137	C2066	A1938	U1798	A1668	U1539	U1431	G1309	A	A1088
A2364	A2297	A2297	A2297	A2297	G2138	G2067	U1939	C1799	A1669	U1539	U1431	G1309	A	A1088
A2364	A2298	A2298	A2298	A2298	C2139	U2068	U1955	C1800	C1670	U1539	U1431	G1309	A	A1088
A2364	A2299	A2299	A2299	A2299	G2140	G2069	U1955	G1801	U1671	U1539	U1431	G1309	A	A1088
A2364	A2300	A2300	A2300	A2300	C2141	G2070	U1955	A1802	C1672	U1539	U1431	G1309	A	A1088
A2364	A2301	A2301	A2301	A2301	C2142	A2071	U1955	A1803	U1673	U1539	U1431	G1309	A	A1088
A2364	A2302	A2302	A2302	A2302	G2143	G2072	C1962	U1806	G1674	U1539	U1431	G1309	A	A1088
A2364	A2303	A2303	A2303	A2303	U2144	C2073	U1963	C1807	C1675	U1539	U1431	G1309	A	A1088
A2364	A2304	A2304	A2304	A2304	C2145	U2074	C1965	G1807	C1683	U1539	U1431	G1309	A	A1088
A2364	A2305	A2305	A2305	A2305	G2146	U2075	C1965	C1807	C1683	U1539	U1431	G1309	A	A1088
A2364	A2306	A2306	A2306	A2306	C2147	U2076	C1967	G1811	C1684	U1539	U1431	G1309	A	A1088
A2364	A2307	A2307	A2307	A2307	U2150	A2077	U1967	A1812	U1688	U1539	U1431	G1309	A	A1088
A2364	A2308	A2308	A2308	A2308	G2151	C2078	A1970	G1813	U1688	U1539	U1431	G1309	A	A1088
A2364	A2309	A2309	A2309	A2309	U2152	U2079	A1971	A1814	C1584	U1539	U1431	G1309	A	A1088
A2364	A2310	A2310	A2310	A2310	G2153	G2080	A1972	A1815	C1584	U1539	U1431	G1309	A	A1088
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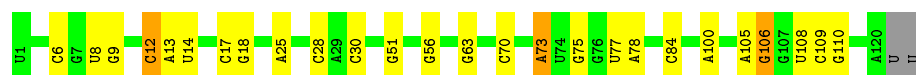
- Molecule 2: 5S rRNA

Chain RB: 79% 16%



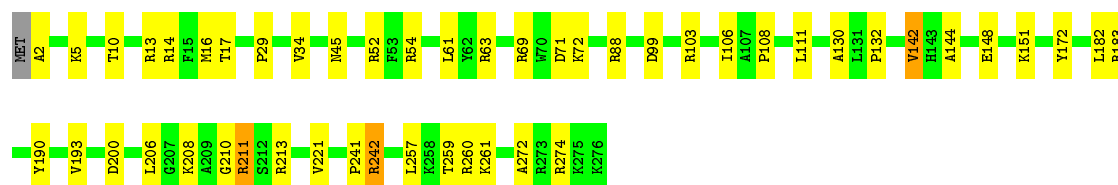
- Molecule 2: 5S rRNA

Chain YB: 77% 19%



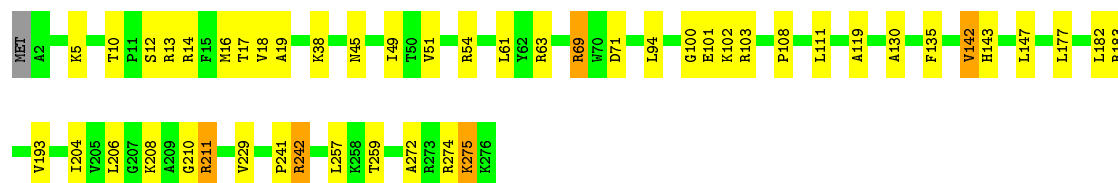
- Molecule 3: 50S ribosomal protein L2

Chain RD: 82% 17%



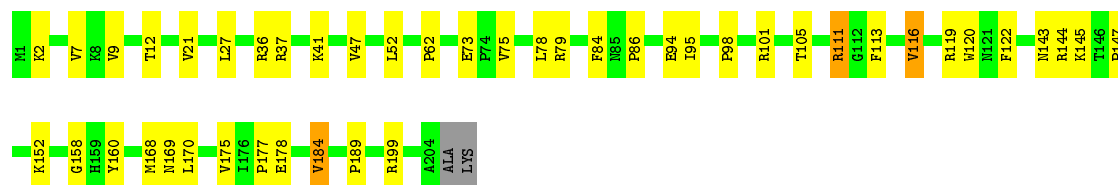
- Molecule 3: 50S ribosomal protein L2

Chain YD: 82% 16%



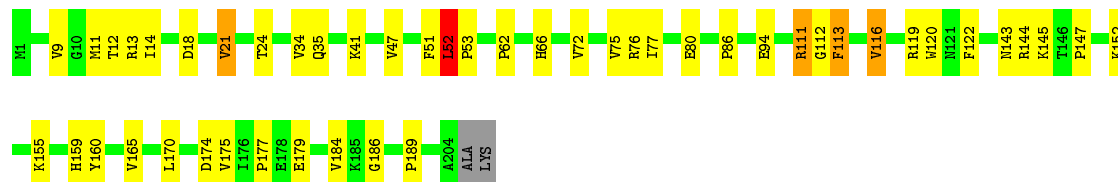
- Molecule 4: 50S ribosomal protein L3

Chain RE: 77% 20%



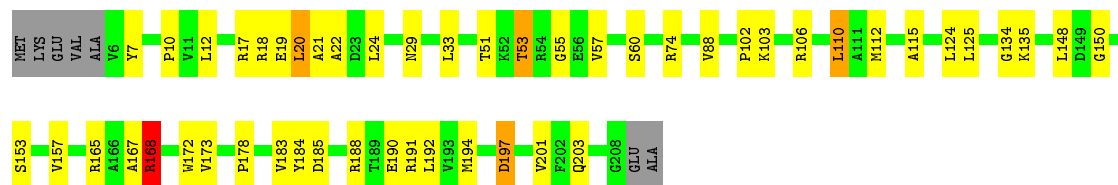
• Molecule 4: 50S ribosomal protein L3

Chain YE: 76% 21% ..



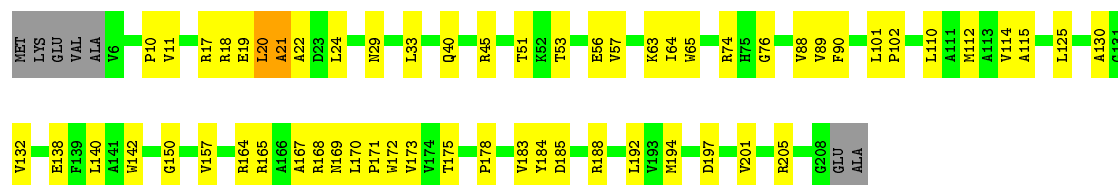
• Molecule 5: 50S ribosomal protein L4

Chain RF: 73% 21% ..



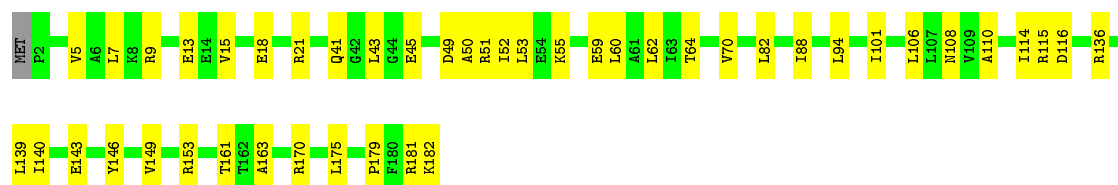
• Molecule 5: 50S ribosomal protein L4

Chain YF: 69% 27% ..



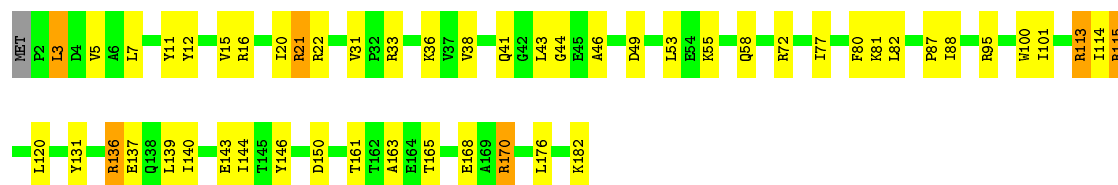
• Molecule 6: 50S ribosomal protein L5

Chain RG: 75% 25% .



• Molecule 6: 50S ribosomal protein L5

Chain YG: 71% 25% ..



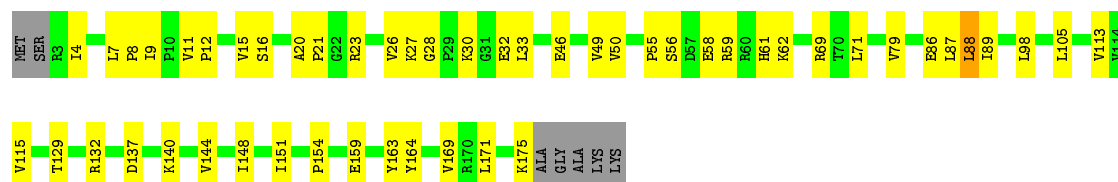
- Molecule 7: 50S ribosomal protein L6

Chain RH: 82% 14% ..



- Molecule 7: 50S ribosomal protein L6

Chain YH: 68% 28% ..



- Molecule 8: 50S ribosomal protein L9

Chain RI: 80% 18% ..



- Molecule 8: 50S ribosomal protein L9

Chain YI: 80% 15% ..



- Molecule 9: 50S ribosomal protein L13

Chain RN: 81% 17% .

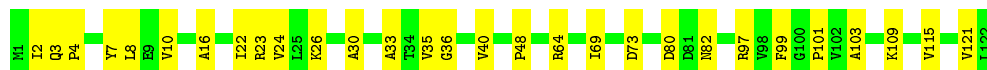
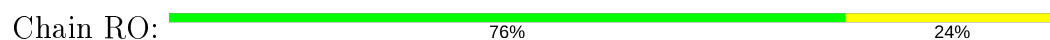


- Molecule 9: 50S ribosomal protein L13

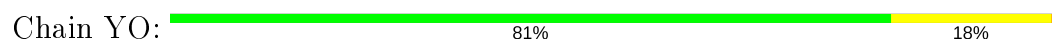
Chain YN: 83% 14% .



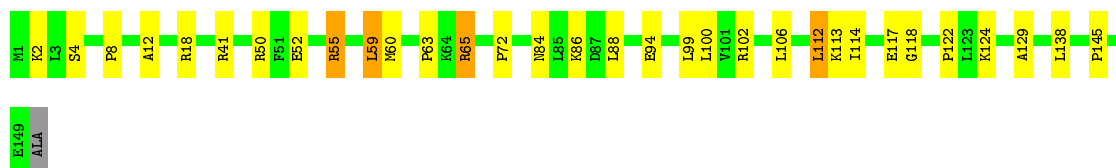
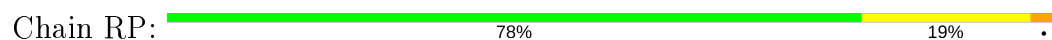
- Molecule 10: 50S ribosomal protein L14



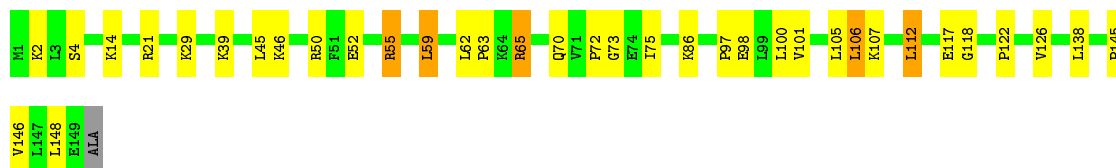
- Molecule 10: 50S ribosomal protein L14



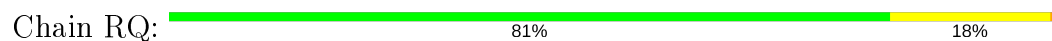
- Molecule 11: 50S ribosomal protein L15



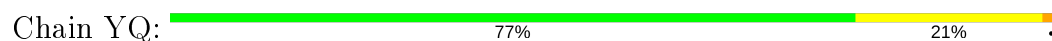
- Molecule 11: 50S ribosomal protein L15




- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16




- Molecule 13: 50S ribosomal protein L17

Chain RR:  75% 22% .




- Molecule 13: 50S ribosomal protein L17

Chain YR:  81% 19%




- Molecule 14: 50S ribosomal protein L18

Chain RS:  80% 15% . .



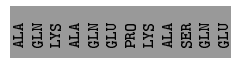
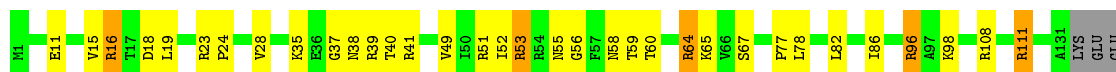
- Molecule 14: 50S ribosomal protein L18

Chain YS:  81% 16% . .



- Molecule 15: 50S ribosomal protein L19

Chain RT:  66% 20% 10%




- Molecule 15: 50S ribosomal protein L19

Chain YT:  71% 17% 10%



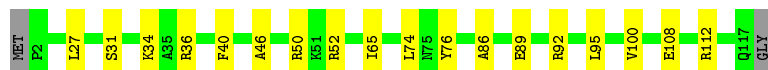
- Molecule 16: 50S ribosomal protein L20

Chain RU:  81% 16% . .



- Molecule 16: 50S ribosomal protein L20

Chain YU: 83% 15% .



- Molecule 17: 50S ribosomal protein L21

Chain RV: 83% 15% .



- Molecule 17: 50S ribosomal protein L21

Chain YV: 79% 19% ..



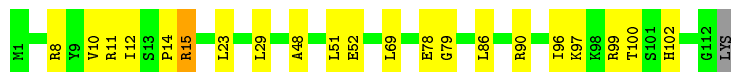
- Molecule 18: 50S ribosomal protein L22

Chain RW: 84% 14% ..



- Molecule 18: 50S ribosomal protein L22

Chain YW: 81% 18% ..



- Molecule 19: 50S ribosomal protein L23

Chain RX: 76% 23% .

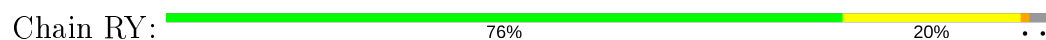


- Molecule 19: 50S ribosomal protein L23

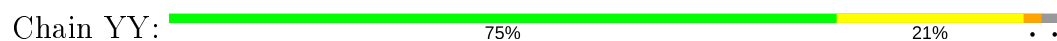
Chain YX: 88% 11% .



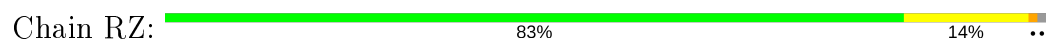
- Molecule 20: 50S ribosomal protein L24



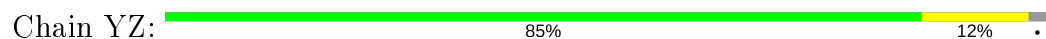
- Molecule 20: 50S ribosomal protein L24



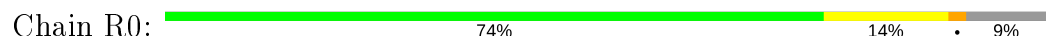
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



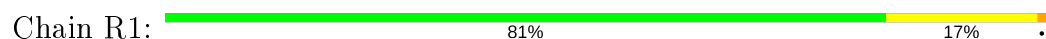
- Molecule 22: 50S ribosomal protein L27

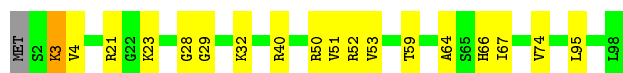


- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28





- Molecule 23: 50S ribosomal protein L28

Chain Y1: 76% 21% ..



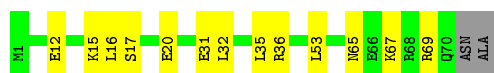
- Molecule 24: 50S ribosomal protein L29

Chain R2: 75% 22% .



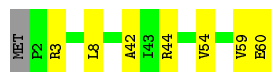
- Molecule 24: 50S ribosomal protein L29

Chain Y2: 79% 18% .



- Molecule 25: 50S ribosomal protein L30

Chain R3: 87% 12% .



- Molecule 25: 50S ribosomal protein L30

Chain Y3: 78% 18% ..



- Molecule 26: 50S ribosomal protein L31

Chain R4: 58% 35% ...



- Molecule 26: 50S ribosomal protein L31

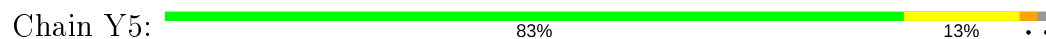
Chain Y4: 63% 30% ...



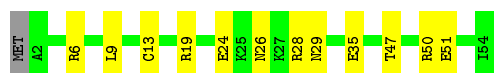
- Molecule 27: 50S ribosomal protein L32



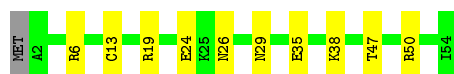
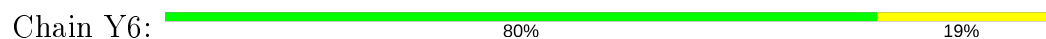
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

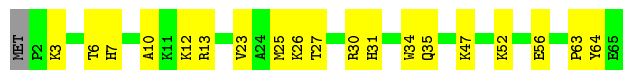


- Molecule 30: 50S ribosomal protein L35





- Molecule 30: 50S ribosomal protein L35



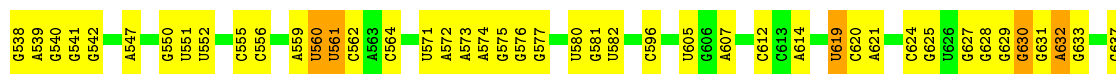
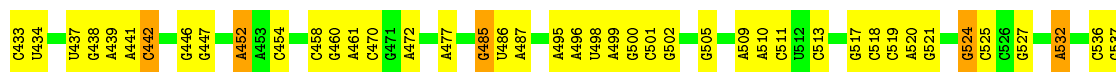
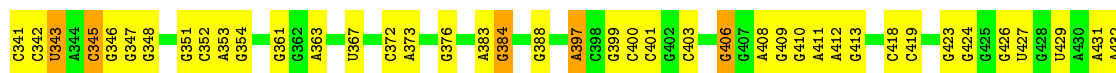
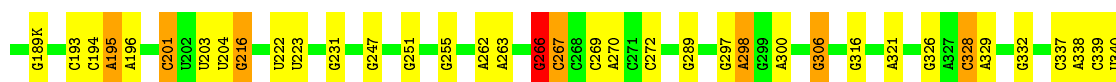
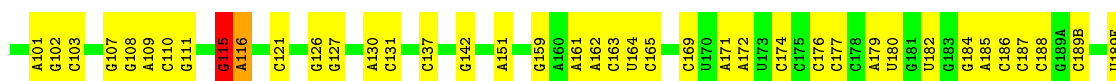
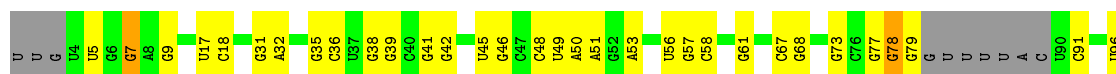
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

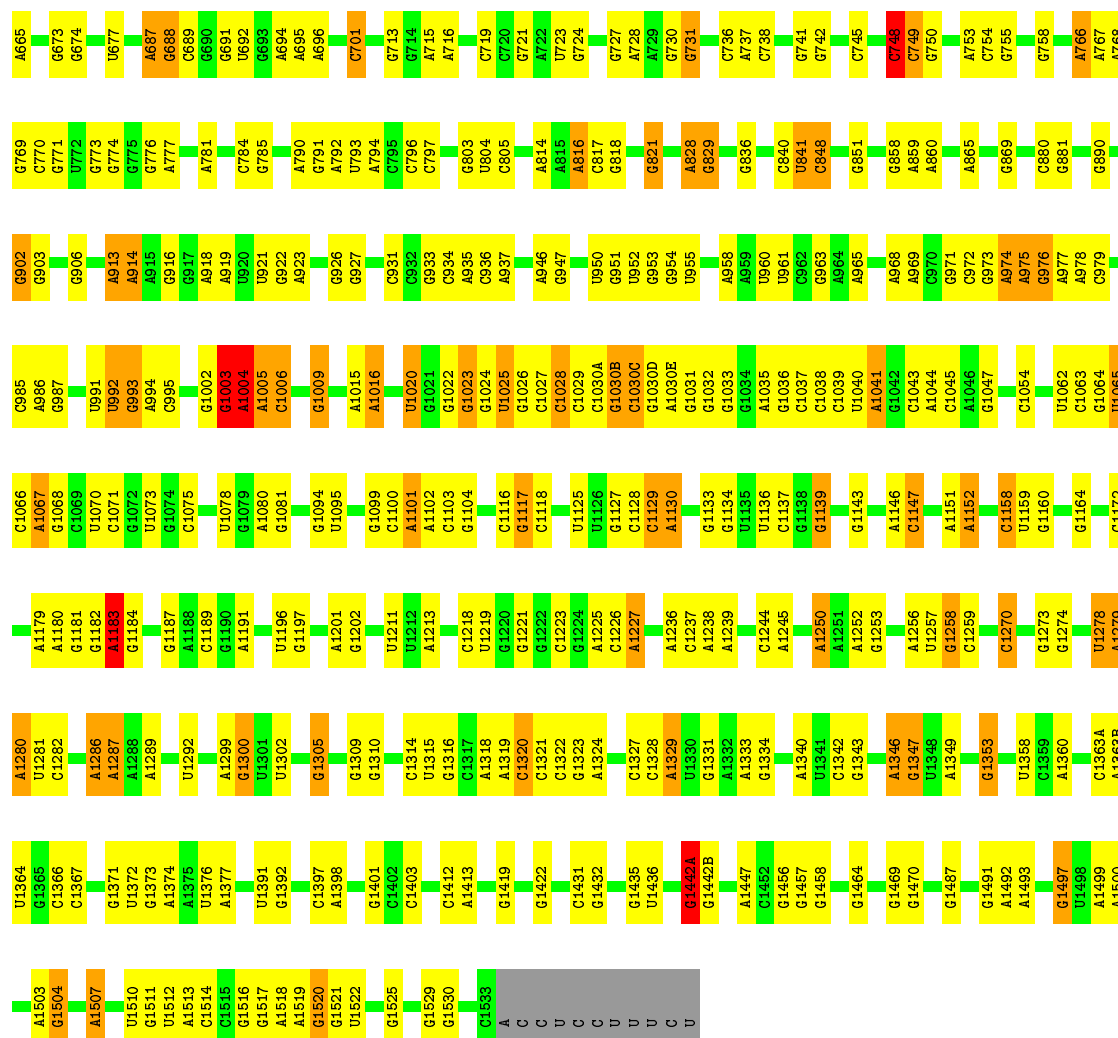


- Molecule 32: 16S rRNA



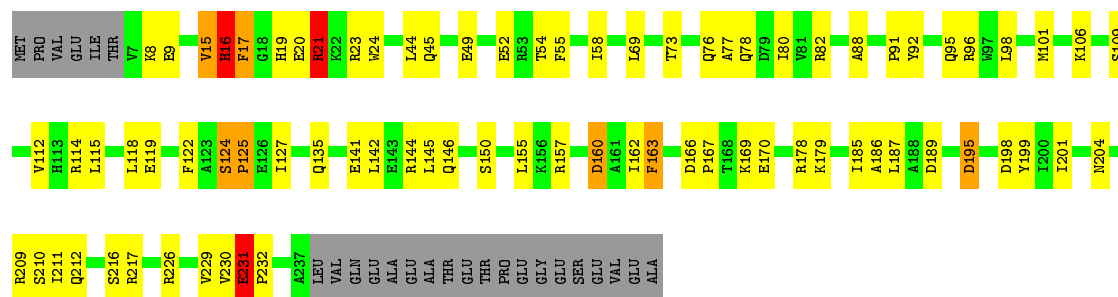


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C548	C452	C352		C110	U5
C549	A482	A353		G111	G6
U652	C457	C354	G251		G7
C556	C458	C355	G255	U114	A8
		A356	U256	G115	G9
A559	C470	U359	G257	A116	
U660	G473	A360	G258	C121	U17
U661	G474	G361		G122	C18
C564	G475	U367	A262	C123	C19
					U20
A572	A482	G371	G265	G126	G21
A573	C483	C372	G267	C131	C25
A574	G484	A373	C268	C132	A26
G575	G485	G376	A270	G142	G31
U496	U495			G143	A32
G576	G486	G380	A273		G35
G577	A487			G148	C36
				A149	
G581	G490	A383	A279	C150	G39
U582	U494	G384	G281	C40	C40
A583	U495	C390	G284	A151	G41
G584	A496	G391		C163	G42
C596	U498		G289	U164	
G597		G396		C165	C47
U598	C501	A397	G292	C174	C48
C599	C502	C398	G293	U49	U49
C600	C503			A50	A50
C601	C504	C401	A298	C176	A51
A602	G505	G402		C177	
		C403			G57
U605	A509	U404	G302	U182	C58
	A510	U405		C58	A59
G625	C511	G406	C311	C186	A60
	U512	G407	C312	C187	G61
G630	C513	A408	A313	C188	
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G633	A632	G410	A315	U189F	U65
		A411	G316	G66	
A642	G524	A412		U189L	C67
	C525	G413	A321	G189M	G68
	C526			U190	G69
U646	G527	G424	G324		
				A195	G78
A653	G530	U427	A327	A196	G79
G657	A532	G428	C328	A197	G80
G658	A533	U429			U
U659			G332	C201	U
G660	C536	C435		U202	U84
G661	G537	C436	U340	U203	A88
G662	G538	U437	U343	G216	A88
A663	C539	G438	U344	U204	C89
G664	A540	A439	A344	C217	
		U441	C245	C219	A403



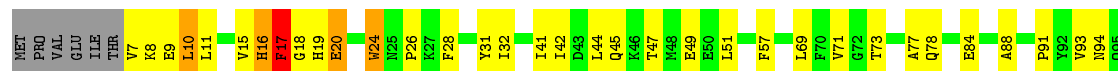
• Molecule 33: 30S ribosomal protein S2

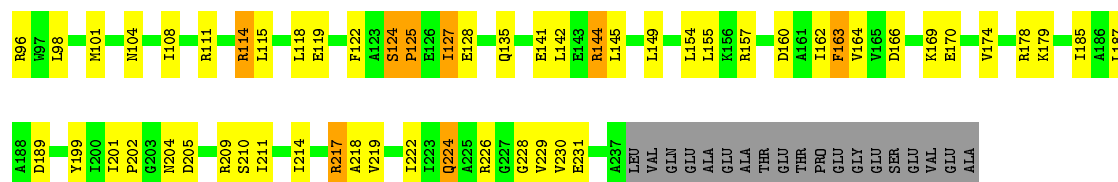
Chain QB:



• Molecule 33: 30S ribosomal protein S2

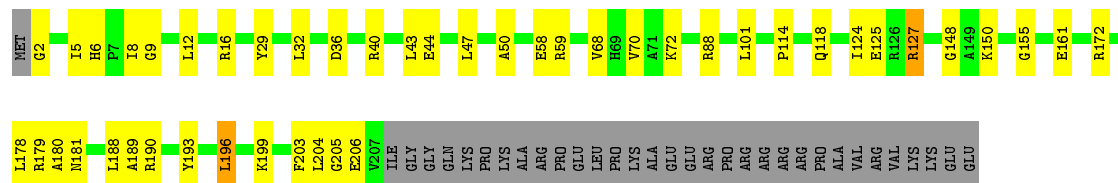
Chain XB:





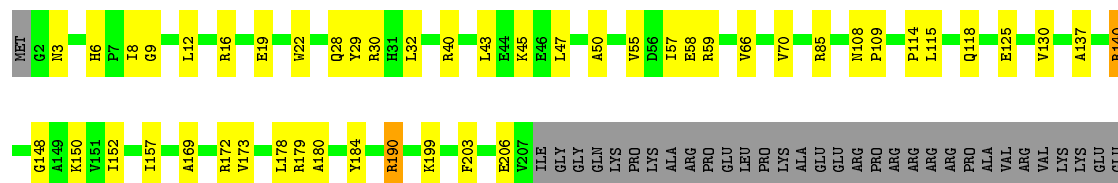
• Molecule 34: 30S ribosomal protein S3

Chain QC:



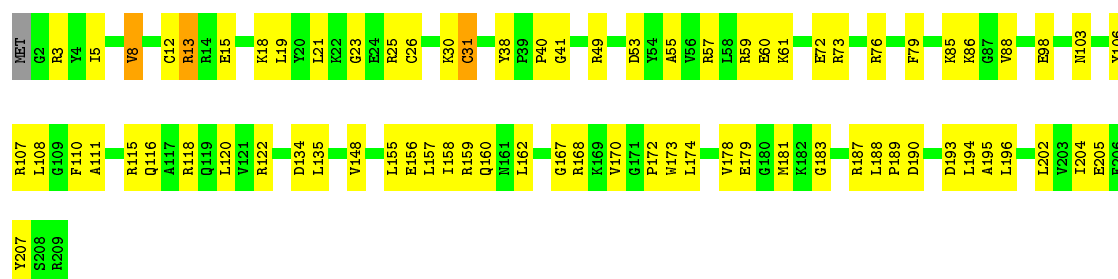
• Molecule 34: 30S ribosomal protein S3

Chain XC:



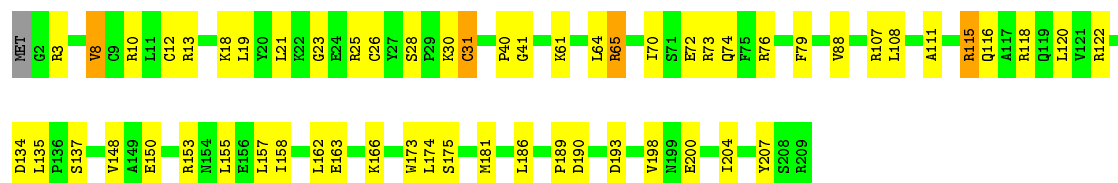
• Molecule 35: 30S ribosomal protein S4

Chain QD:

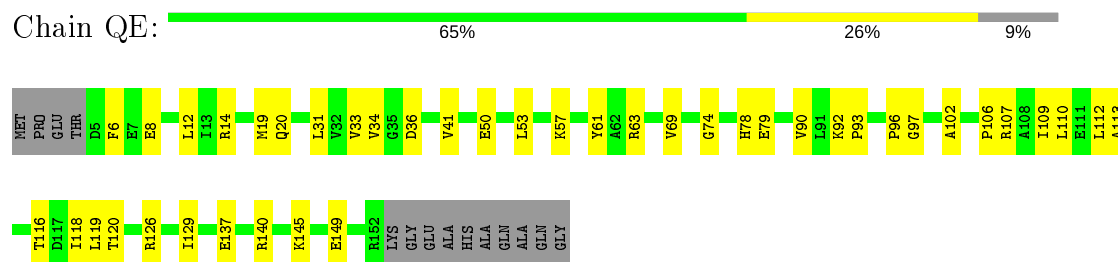


• Molecule 35: 30S ribosomal protein S4

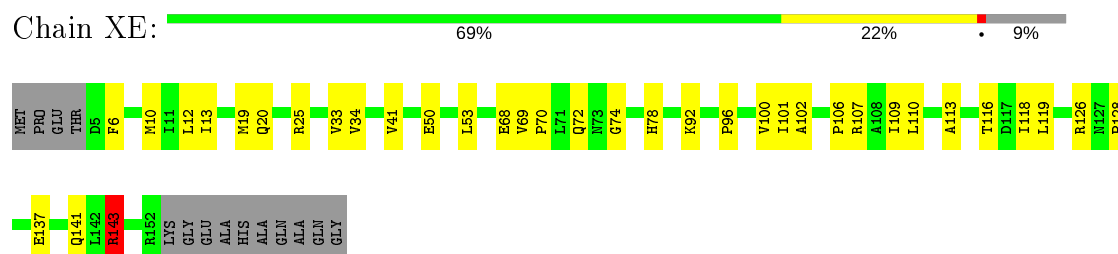
Chain XD:



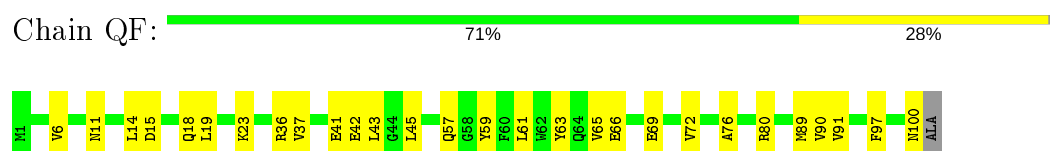
- Molecule 36: 30S ribosomal protein S5



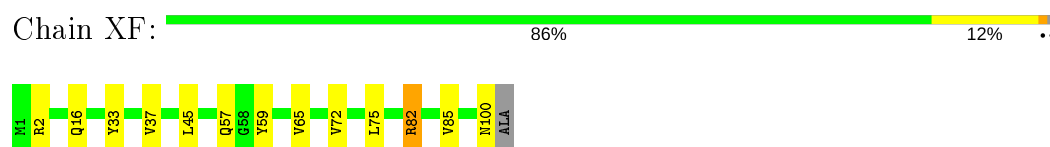
- Molecule 36: 30S ribosomal protein S5



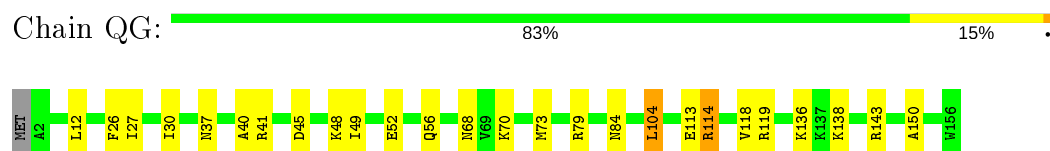
- Molecule 37: 30S ribosomal protein S6



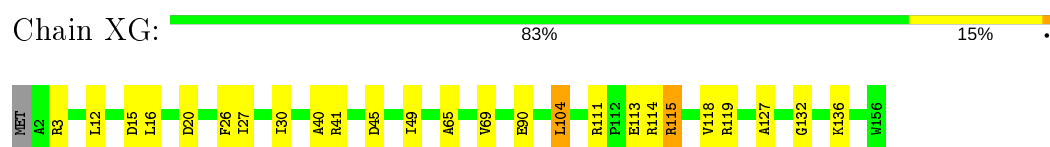
- Molecule 37: 30S ribosomal protein S6



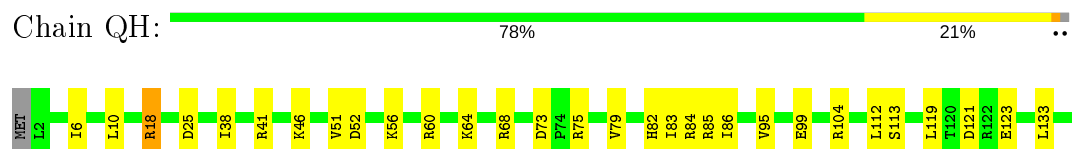
- Molecule 38: 30S ribosomal protein S7



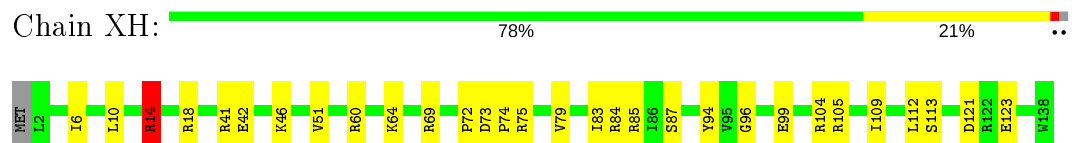
- Molecule 38: 30S ribosomal protein S7



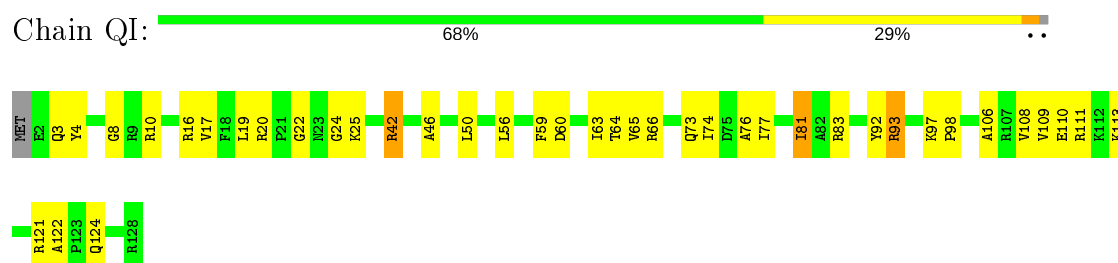
- Molecule 39: 30S ribosomal protein S8



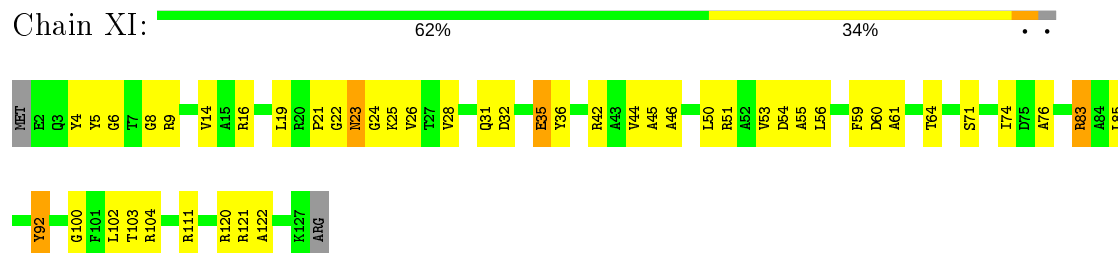
- Molecule 39: 30S ribosomal protein S8



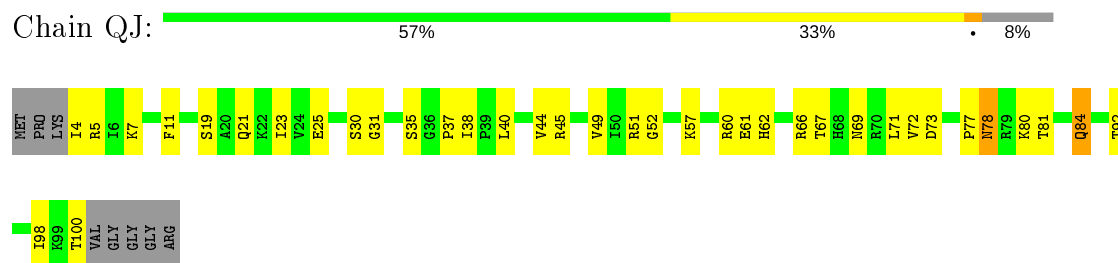
- Molecule 40: 30S ribosomal protein S9



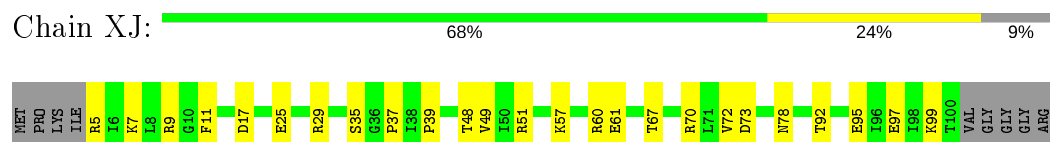
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10




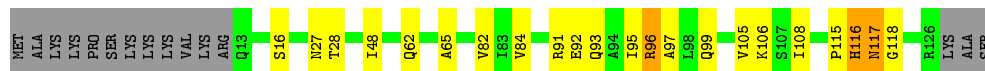
- Molecule 42: 30S ribosomal protein S11

Chain QK:  72% 16% 12%




- Molecule 42: 30S ribosomal protein S11

Chain XK:  71% 15% 12%



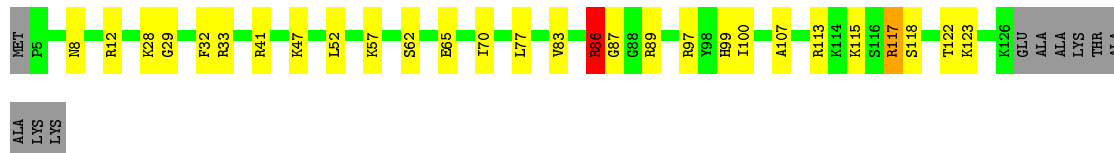
- Molecule 43: 30S ribosomal protein S12

Chain QL:  77% 15% 8%



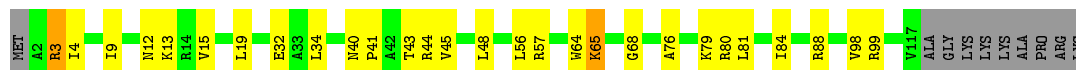
- Molecule 43: 30S ribosomal protein S12

Chain XL:  71% 20% 8%



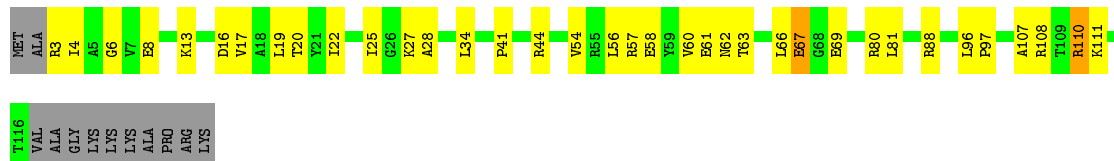
- Molecule 44: 30S ribosomal protein S13

Chain QM:  70% 21% 8%




- Molecule 44: 30S ribosomal protein S13

Chain XM:  62% 27% 10%




- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:  77% 20% ..




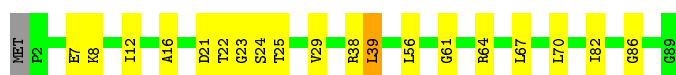
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN:  77% 20% ..




- Molecule 46: 30S ribosomal protein S15

Chain QO:  78% 20% ..



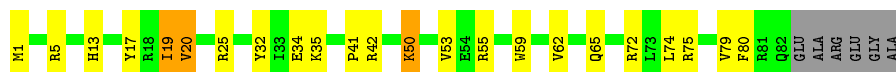
- Molecule 46: 30S ribosomal protein S15

Chain XO:  79% 19% ..



- Molecule 47: 30S ribosomal protein S16

Chain QP:  67% 23% • 7%




- Molecule 47: 30S ribosomal protein S16

Chain XP:  63% 27% • 7%




- Molecule 48: 30S ribosomal protein S17

Chain QQ:  84% 10% • 6%



- Molecule 48: 30S ribosomal protein S17

Chain XQ:  83% 11% 6%



- Molecule 49: 30S ribosomal protein S18

Chain QR:  64% 13% 23%



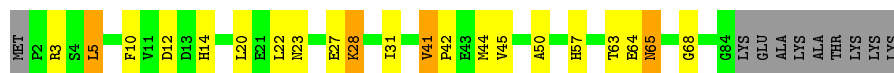
- Molecule 49: 30S ribosomal protein S18

Chain XR:  64% 13% 23%



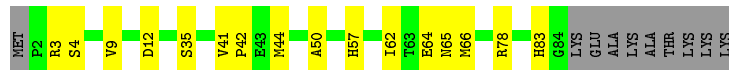
- Molecule 50: 30S ribosomal protein S19

Chain QS:  67% 18% 11%



- Molecule 50: 30S ribosomal protein S19

Chain XS:  72% 17% 11%




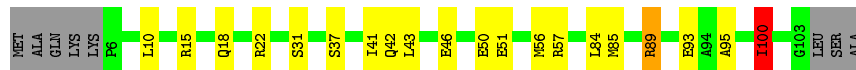
- Molecule 51: 30S ribosomal protein S20

Chain QT:  68% 21% 9%



- Molecule 51: 30S ribosomal protein S20

Chain XT:  74% 17% 8%




- Molecule 52: 30S ribosomal protein Thx

Chain QU:  70% 15% 15%



- Molecule 52: 30S ribosomal protein Thx

Chain XU:  74% 11% 15%



- Molecule 53: P-site tRNA fMet

Chain QV:  62% 32% 5%



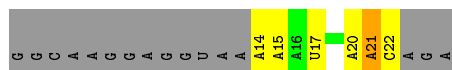
- Molecule 53: P-site tRNA fMet

Chain XV:  64% 26% 9%



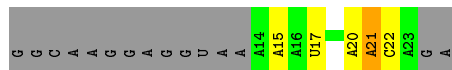
- Molecule 54: messenger RNA

Chain QX:  12% 20% 64%



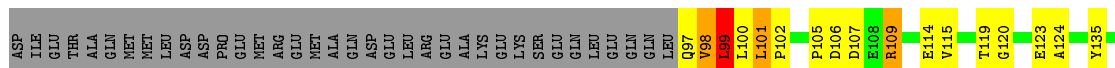
- Molecule 54: messenger RNA

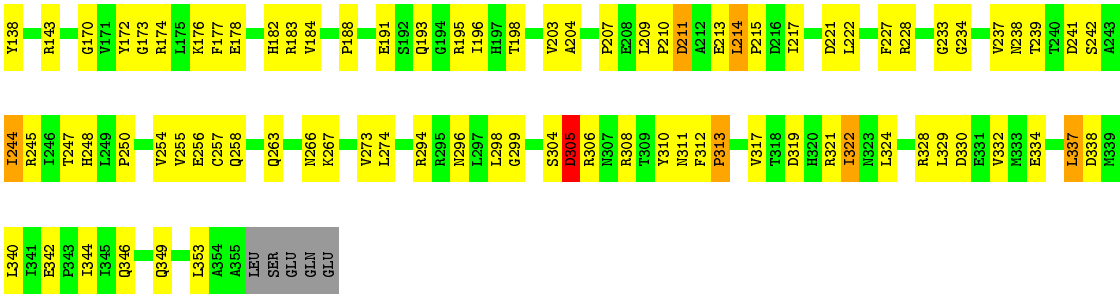
Chain XX:  20% 16% 60%



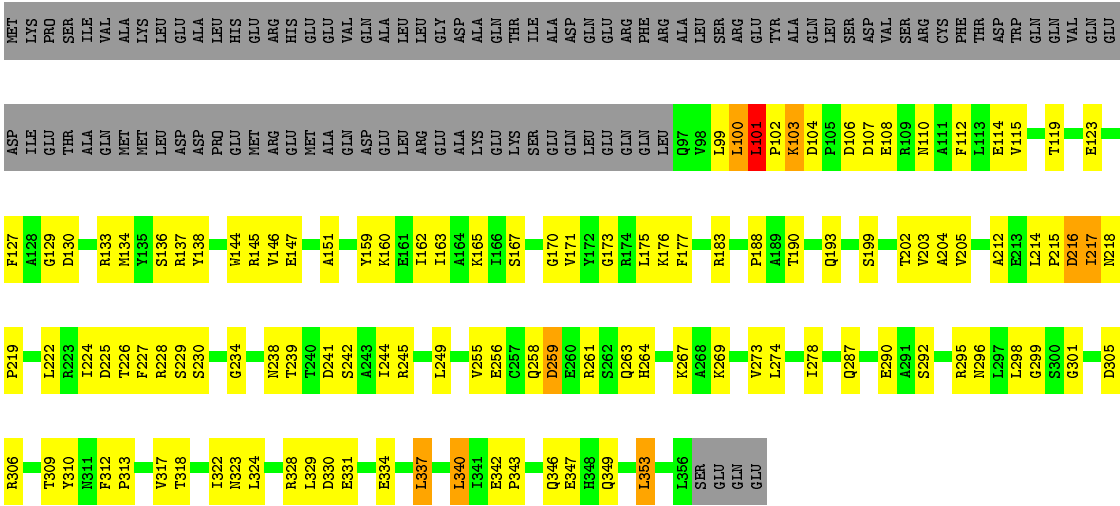
- Molecule 55: Peptide chain release factor 1

Chain QY:  44% 25% 28%





• Molecule 55: Peptide chain release factor 1



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	209.51Å 450.89Å 622.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.04	Depositor
% Data completeness (in resolution range)	99.3 (49.86-3.04)	Depositor
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.07Å)	Xtriage
Refinement program	PHENIX, PHENIX	Depositor
R, R_{free}	0.246 , 0.279	Depositor
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.225	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294929	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: 5MU, ZN, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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	RA	0.43	0/68901	1.00	55/107544 (0.1%)
1	YA	0.51	1/68901 (0.0%)	1.10	180/107544 (0.2%)
2	RB	0.35	0/2876	0.90	0/4486
2	YB	0.43	0/2878	1.00	1/4490 (0.0%)
3	RD	0.38	0/2181	0.64	1/2940 (0.0%)
3	YD	0.40	0/2186	0.66	1/2944 (0.0%)
4	RE	0.37	0/1592	0.60	0/2149
4	YE	0.38	0/1592	0.65	1/2149 (0.0%)
5	RF	0.36	0/1619	0.61	2/2193 (0.1%)
5	YF	0.42	0/1615	0.61	0/2188
6	RG	0.29	0/1451	0.54	0/1961
6	YG	0.34	0/1449	0.57	0/1957
7	RH	0.31	0/1356	0.54	1/1834 (0.1%)
7	YH	0.35	0/1350	0.57	1/1826 (0.1%)
8	RI	0.29	0/1109	0.57	0/1512
8	YI	0.34	0/1091	0.60	1/1490 (0.1%)
9	RN	0.36	0/1148	0.56	0/1547
9	YN	0.35	0/1144	0.55	0/1543
10	RO	0.34	0/943	0.58	0/1269
10	YO	0.42	1/943 (0.1%)	0.61	0/1269
11	RP	0.35	0/1152	0.60	0/1533
11	YP	0.41	0/1152	0.66	0/1533
12	RQ	0.35	0/1143	0.62	0/1527
12	YQ	0.40	0/1143	0.66	0/1527
13	RR	0.34	0/982	0.62	0/1312
13	YR	0.34	0/982	0.62	0/1312
14	RS	0.35	0/887	0.59	0/1180
14	YS	0.37	0/880	0.62	0/1172
15	RT	0.36	0/1105	0.67	1/1477 (0.1%)
15	YT	0.35	0/1097	0.63	1/1468 (0.1%)
16	RU	0.32	0/977	0.55	0/1301
16	YU	0.37	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RV	0.35	0/786	0.57	0/1053
17	YV	0.37	0/782	0.61	0/1049
18	RW	0.35	0/897	0.57	0/1205
18	YW	0.37	0/897	0.57	0/1205
19	RX	0.39	0/764	0.59	0/1025
19	YX	0.39	0/764	0.61	0/1025
20	RY	0.34	0/823	0.64	0/1099
20	YY	0.39	0/823	0.63	0/1100
21	RZ	0.33	0/1620	0.55	0/2200
21	YZ	0.35	0/1590	0.59	0/2162
22	R0	0.39	0/616	0.70	1/821 (0.1%)
22	Y0	0.42	0/616	0.77	2/821 (0.2%)
23	R1	0.37	0/761	0.59	0/1013
23	Y1	0.38	0/766	0.64	0/1018
24	R2	0.29	0/590	0.50	0/781
24	Y2	0.35	0/594	0.54	0/785
25	R3	0.35	0/474	0.59	0/635
25	Y3	0.36	0/469	0.58	0/630
26	R4	0.37	0/559	0.70	0/754
26	Y4	0.40	0/549	0.70	1/741 (0.1%)
27	R5	0.44	0/473	0.64	0/639
27	Y5	0.41	0/469	0.60	0/635
28	R6	0.30	0/460	0.54	0/613
28	Y6	0.30	0/456	0.53	0/608
29	R7	0.40	0/426	0.67	0/561
29	Y7	0.42	0/426	0.69	0/561
30	R8	0.38	0/525	0.61	0/691
30	Y8	0.39	0/525	0.61	0/691
31	R9	0.32	0/310	0.68	0/407
31	Y9	0.33	0/310	0.68	0/407
32	QA	0.34	0/35795	0.88	12/55864 (0.0%)
32	XA	0.36	1/35890 (0.0%)	0.90	29/56012 (0.1%)
33	QB	0.34	0/1876	0.59	0/2533
33	XB	0.34	0/1860	0.60	1/2518 (0.0%)
34	QC	0.30	0/1582	0.53	0/2137
34	XC	0.36	1/1566 (0.1%)	0.61	0/2119
35	QD	0.33	0/1695	0.59	1/2274 (0.0%)
35	XD	0.32	0/1698	0.57	0/2277
36	QE	0.34	0/1149	0.55	0/1548
36	XE	0.32	0/1149	0.57	1/1548 (0.1%)
37	QF	0.31	0/827	0.55	0/1120
37	XF	0.33	0/829	0.64	1/1123 (0.1%)
38	QG	0.31	0/1254	0.46	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XG	0.31	0/1248	0.51	0/1676
39	QH	0.30	0/1118	0.53	0/1506
39	XH	0.32	0/1108	0.58	1/1494 (0.1%)
40	QI	0.32	0/1005	0.60	1/1351 (0.1%)
40	XI	0.31	0/985	0.54	0/1329
41	QJ	0.28	0/732	0.51	0/993
41	XJ	0.29	0/723	0.52	0/984
42	QK	0.30	0/849	0.55	0/1150
42	XK	0.30	0/848	0.57	0/1149
43	QL	0.39	0/937	0.61	0/1260
43	XL	0.36	0/937	0.67	0/1260
44	QM	0.30	0/924	0.57	0/1242
44	XM	0.31	0/905	0.55	0/1217
45	QN	0.34	0/501	0.59	1/664 (0.2%)
45	XN	0.35	0/501	0.58	0/664
46	QO	0.32	0/739	0.52	0/985
46	XO	0.35	0/739	0.56	0/985
47	QP	0.32	0/697	0.54	0/939
47	XP	0.30	0/693	0.57	0/935
48	QQ	0.33	0/836	0.55	0/1117
48	XQ	0.32	0/836	0.54	0/1117
49	QR	0.31	0/560	0.54	0/746
49	XR	0.32	0/560	0.59	0/746
50	QS	0.29	0/663	0.58	1/895 (0.1%)
50	XS	0.27	0/660	0.54	0/893
51	QT	0.31	0/734	0.51	0/969
51	XT	0.29	0/736	0.47	0/976
52	QU	0.30	0/203	0.58	0/266
52	XU	0.31	0/203	0.70	0/266
53	QV	0.34	0/1832	0.92	0/2855
53	XV	0.42	1/1836 (0.1%)	0.91	2/2859 (0.1%)
54	QX	0.39	0/216	0.83	0/334
54	XX	0.46	0/241	0.92	0/373
55	QY	0.36	0/2046	0.65	1/2759 (0.0%)
55	XY	0.40	0/2054	0.69	2/2770 (0.1%)
All	All	0.41	5/316497 (0.0%)	0.90	304/472893 (0.1%)

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
14	RS	0	1
33	QB	0	1
43	XL	0	1
55	QY	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	1	C	OP3-P	-10.47	1.48	1.61
32	XA	68	G	O3'-P	-6.54	1.53	1.61
34	XC	173	VAL	C-N	6.47	1.46	1.34
10	YO	21	CYS	CB-SG	-5.52	1.72	1.81
1	YA	1046	A	N3-C4	-5.10	1.31	1.34

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	277	C	N1-C2-O2	17.75	129.55	118.90
1	YA	210	C	C6-N1-C2	12.43	125.27	120.30
1	YA	277	C	N3-C2-O2	-11.59	113.79	121.90
1	YA	277	C	N3-C4-N4	-11.48	109.96	118.00
1	YA	277	C	C5-C4-N4	10.97	127.88	120.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
55	QY	305	ASP	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61758	0	31144	585	0
1	YA	61758	0	31147	606	1
2	RB	2572	0	1305	11	0
2	YB	2573	0	1306	12	0
3	RD	2131	0	2207	49	0
3	YD	2136	0	2218	49	0
4	RE	1559	0	1618	34	0
4	YE	1559	0	1618	40	0
5	RF	1584	0	1625	37	0
5	YF	1580	0	1619	46	0
6	RG	1426	0	1445	30	0
6	YG	1424	0	1441	38	0
7	RH	1330	0	1407	20	0
7	YH	1324	0	1402	33	0
8	RI	1094	0	1127	22	0
8	YI	1076	0	1093	14	0
9	RN	1121	0	1195	16	0
9	YN	1117	0	1184	16	0
10	RO	933	0	996	17	0
10	YO	933	0	996	14	0
11	RP	1135	0	1212	22	0
11	YP	1135	0	1212	32	0
12	RQ	1122	0	1179	20	0
12	YQ	1122	0	1179	20	0
13	RR	968	0	1033	21	0
13	YR	968	0	1033	13	0
14	RS	877	0	938	12	0
14	YS	870	0	923	13	0
15	RT	1091	0	1151	25	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	18	0
17	RV	775	0	841	13	0
17	YV	771	0	830	13	0
18	RW	886	0	940	12	0
18	YW	886	0	940	12	0
19	RX	750	0	814	16	0
19	YX	750	0	814	6	0
20	RY	810	0	894	15	0
20	YY	810	0	891	17	0
21	RZ	1587	0	1598	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YZ	1557	0	1564	24	0
22	R0	608	0	622	12	0
22	Y0	608	0	622	15	0
23	R1	754	0	823	10	0
23	Y1	759	0	837	18	0
24	R2	588	0	643	11	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	5	0
25	Y3	464	0	514	6	0
26	R4	546	0	523	27	0
26	Y4	536	0	516	26	0
27	R5	459	0	477	12	0
27	Y5	455	0	467	5	0
28	R6	453	0	475	7	0
28	Y6	449	0	471	7	0
29	R7	418	0	467	11	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	17	0
30	Y8	517	0	582	19	0
31	R9	307	0	336	14	0
31	Y9	307	0	336	11	0
32	QA	32246	0	16294	307	0
32	XA	32331	0	16338	343	0
33	QB	1842	0	1862	54	0
33	XB	1825	0	1828	62	0
34	QC	1558	0	1557	33	0
34	XC	1542	0	1517	32	0
35	QD	1665	0	1690	60	0
35	XD	1668	0	1706	44	0
36	QE	1133	0	1191	28	0
36	XE	1133	0	1191	25	0
37	QF	814	0	808	20	0
37	XF	816	0	807	8	0
38	QG	1235	0	1249	18	0
38	XG	1229	0	1238	15	0
39	QH	1098	0	1143	20	0
39	XH	1088	0	1126	21	0
40	QI	986	0	990	28	0
40	XI	966	0	953	35	0
41	QJ	719	0	672	27	0
41	XJ	710	0	661	20	0
42	QK	834	0	838	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	XK	833	0	836	13	0
43	QL	932	0	981	18	0
43	XL	932	0	981	26	0
44	QM	914	0	954	23	0
44	XM	895	0	920	24	0
45	QN	492	0	529	11	0
45	XN	492	0	529	14	0
46	QO	728	0	760	12	0
46	XO	728	0	760	13	0
47	QP	681	0	697	19	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	8	0
48	XQ	823	0	891	9	0
49	QR	555	0	618	11	0
49	XR	555	0	618	9	0
50	QS	648	0	658	17	0
50	XS	645	0	635	19	0
51	QT	732	0	809	15	0
51	XT	733	0	795	13	0
52	QU	199	0	208	3	0
52	XU	199	0	208	1	0
53	QV	1640	0	837	15	0
53	XV	1644	0	836	15	0
54	QX	193	0	98	5	0
54	XX	215	0	108	2	0
55	QY	2014	0	1980	73	0
55	XY	2022	0	1991	85	0
56	QA	262	0	0	0	0
56	QB	1	0	0	0	0
56	QD	2	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	1	0	0	0	0
56	QI	1	0	0	0	0
56	QJ	1	0	0	0	0
56	QL	2	0	0	0	0
56	QN	1	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QV	6	0	0	0	0
56	R0	7	0	0	0	0
56	R1	5	0	0	0	0
56	R3	2	0	0	0	0
56	R5	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	1032	0	0	0	0
56	RB	22	0	0	0	0
56	RD	15	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	0	0	0	0
56	RG	4	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	5	0	0	0	0
56	RR	4	0	0	0	0
56	RS	1	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	3	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	187	0	0	0	0
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	2	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	749	0	0	0	0
56	YB	20	0	0	0	0
56	YD	9	0	0	0	0
56	YE	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YF	2	0	0	0	0
56	YG	2	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	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
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	294929	0	198658	3416	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3416 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)
1:RA:2552:2MU:C4	1:RA:2552:2MU:C5	1.74	1.65
1:YA:2552:2MU:C5	1:YA:2552:2MU:C4	1.75	1.56
32:XA:1003:G:H2'	32:XA:1004:A:H4'	1.40	1.03
1:YA:2131:G:H5''	1:YA:2132:U:H5'	1.46	0.98
26:Y4:59:PHE:HA	26:Y4:61:ARG:H	1.26	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.02	0.18

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	
3	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	65
4	YE	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	RF	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	YF	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	65
6	RG	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	47
6	YG	179/182 (98%)	169 (94%)	9 (5%)	1 (1%)	25	60
7	RH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
8	RI	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	22	57
8	YI	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
9	RN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	YN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	YR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	52
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	49
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	0	1 (1%)	14	47
20	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	14	47
23	Y1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	47
24	R2	68/72 (94%)	68 (100%)	0	0	100	100
24	Y2	68/72 (94%)	68 (100%)	0	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	4
26	Y4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	4	21
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	204 (89%)	17 (7%)	8 (4%)	3	18
33	XB	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	6	28
34	QC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	65
35	QD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
38	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	9	37
41	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	20
41	XJ	94/105 (90%)	83 (88%)	10 (11%)	1 (1%)	14	47
42	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	52
43	QL	119/132 (90%)	118 (99%)	1 (1%)	0	100	100
43	XL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	8 (7%)	1 (1%)	17	52
44	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	66 (100%)	0	0	100	100
50	QS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	90 (96%)	3 (3%)	1 (1%)	14	47
51	XT	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	7	30
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	QY	257/360 (71%)	218 (85%)	21 (8%)	18 (7%)	1	5
55	XY	258/360 (72%)	215 (83%)	30 (12%)	13 (5%)	2	11
All	All	11955/12848 (93%)	11397 (95%)	481 (4%)	77 (1%)	25	60

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	47	GLN
26	R4	49	PHE
33	QB	16	HIS
55	QY	98	VAL
55	QY	210	PRO

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	
3	RD	214/218 (98%)	210 (98%)	4 (2%)	57	82
3	YD	215/218 (99%)	209 (97%)	6 (3%)	43	75
4	RE	164/166 (99%)	157 (96%)	7 (4%)	29	63
4	YE	164/166 (99%)	157 (96%)	7 (4%)	29	63
5	RF	160/166 (96%)	151 (94%)	9 (6%)	21	54
5	YF	159/166 (96%)	153 (96%)	6 (4%)	33	67
6	RG	144/156 (92%)	139 (96%)	5 (4%)	36	69
6	YG	142/156 (91%)	134 (94%)	8 (6%)	21	54
7	RH	144/148 (97%)	141 (98%)	3 (2%)	53	80
7	YH	143/148 (97%)	138 (96%)	5 (4%)	36	69
8	RI	111/124 (90%)	106 (96%)	5 (4%)	27	62
8	YI	108/124 (87%)	99 (92%)	9 (8%)	11	37
9	RN	119/119 (100%)	113 (95%)	6 (5%)	24	58
9	YN	118/119 (99%)	111 (94%)	7 (6%)	19	51
10	RO	100/100 (100%)	99 (99%)	1 (1%)	76	91
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	110 (96%)	5 (4%)	29	63
11	YP	115/116 (99%)	109 (95%)	6 (5%)	23	57
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
12	YQ	111/111 (100%)	107 (96%)	4 (4%)	35	68
13	RR	101/101 (100%)	95 (94%)	6 (6%)	19	51
13	YR	101/101 (100%)	95 (94%)	6 (6%)	19	51
14	RS	87/88 (99%)	84 (97%)	3 (3%)	37	70
14	YS	85/88 (97%)	82 (96%)	3 (4%)	36	69
15	RT	115/127 (91%)	110 (96%)	5 (4%)	29	63
15	YT	113/127 (89%)	109 (96%)	4 (4%)	36	69
16	RU	93/94 (99%)	91 (98%)	2 (2%)	52	79
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	RV	81/82 (99%)	77 (95%)	4 (5%)	25	59
17	YV	80/82 (98%)	76 (95%)	4 (5%)	24	58
18	RW	90/92 (98%)	86 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	YW	90/92 (98%)	86 (96%)	4 (4%)	28	63
19	RX	77/78 (99%)	76 (99%)	1 (1%)	69	88
19	YX	77/78 (99%)	76 (99%)	1 (1%)	69	88
20	RY	86/91 (94%)	85 (99%)	1 (1%)	71	89
20	YY	86/91 (94%)	84 (98%)	2 (2%)	50	78
21	RZ	169/179 (94%)	165 (98%)	4 (2%)	49	78
21	YZ	165/179 (92%)	163 (99%)	2 (1%)	71	89
22	R0	61/67 (91%)	59 (97%)	2 (3%)	38	71
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	79/83 (95%)	76 (96%)	3 (4%)	33	67
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	25	59
24	R2	65/67 (97%)	65 (100%)	0	100	100
24	Y2	66/67 (98%)	66 (100%)	0	100	100
25	R3	51/52 (98%)	48 (94%)	3 (6%)	19	51
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	19	51
26	R4	58/63 (92%)	56 (97%)	2 (3%)	37	70
26	Y4	54/63 (86%)	50 (93%)	4 (7%)	13	42
27	R5	51/52 (98%)	48 (94%)	3 (6%)	19	51
27	Y5	50/52 (96%)	47 (94%)	3 (6%)	19	51
28	R6	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	81
29	R7	41/42 (98%)	39 (95%)	2 (5%)	25	59
29	Y7	41/42 (98%)	39 (95%)	2 (5%)	25	59
30	R8	54/55 (98%)	51 (94%)	3 (6%)	21	54
30	Y8	54/55 (98%)	51 (94%)	3 (6%)	21	54
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	177 (93%)	14 (7%)	14	42
33	XB	187/220 (85%)	173 (92%)	14 (8%)	13	41
34	QC	144/188 (77%)	138 (96%)	6 (4%)	30	64
34	XC	140/188 (74%)	133 (95%)	7 (5%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	QD	171/181 (94%)	166 (97%)	5 (3%)	42	74
35	XD	172/181 (95%)	163 (95%)	9 (5%)	23	57
36	QE	114/123 (93%)	112 (98%)	2 (2%)	59	83
36	XE	114/123 (93%)	110 (96%)	4 (4%)	36	69
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	71	89
38	QG	120/127 (94%)	115 (96%)	5 (4%)	30	64
38	XG	119/127 (94%)	116 (98%)	3 (2%)	47	77
39	QH	116/119 (98%)	112 (97%)	4 (3%)	37	70
39	XH	114/119 (96%)	111 (97%)	3 (3%)	46	76
40	QI	91/99 (92%)	85 (93%)	6 (7%)	16	47
40	XI	88/99 (89%)	83 (94%)	5 (6%)	20	53
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	65	86
41	XJ	68/92 (74%)	68 (100%)	0	100	100
42	QK	83/99 (84%)	80 (96%)	3 (4%)	35	68
42	XK	83/99 (84%)	80 (96%)	3 (4%)	35	68
43	QL	96/108 (89%)	96 (100%)	0	100	100
43	XL	96/108 (89%)	92 (96%)	4 (4%)	30	64
44	QM	90/101 (89%)	88 (98%)	2 (2%)	52	79
44	XM	87/101 (86%)	84 (97%)	3 (3%)	37	70
45	QN	49/50 (98%)	45 (92%)	4 (8%)	11	37
45	XN	49/50 (98%)	48 (98%)	1 (2%)	55	81
46	QO	78/80 (98%)	77 (99%)	1 (1%)	69	88
46	XO	78/80 (98%)	76 (97%)	2 (3%)	46	76
47	QP	69/74 (93%)	66 (96%)	3 (4%)	29	63
47	XP	68/74 (92%)	64 (94%)	4 (6%)	19	51
48	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	90
48	XQ	94/97 (97%)	92 (98%)	2 (2%)	53	80
49	QR	59/77 (77%)	57 (97%)	2 (3%)	37	70
49	XR	59/77 (77%)	58 (98%)	1 (2%)	60	84
50	QS	68/80 (85%)	65 (96%)	3 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	67 (94%)	4 (6%)	21	54
51	XT	70/82 (85%)	67 (96%)	3 (4%)	29	63
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	21	54
55	QY	210/300 (70%)	206 (98%)	4 (2%)	57	82
55	XY	211/300 (70%)	202 (96%)	9 (4%)	29	63
All	All	9784/10664 (92%)	9432 (96%)	352 (4%)	35	68

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	QS	65	ASN
7	YH	33	LEU
43	XL	117	ARG
51	QT	100	ILE
4	YE	111	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
50	QS	65	ASN
6	YG	79	ASN
33	XB	78	GLN
33	QB	95	GLN
20	YY	6	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	494 (17%)	22 (0%)
1	YA	2855/2915 (97%)	484 (16%)	24 (0%)
2	RB	119/122 (97%)	14 (11%)	0
2	YB	119/122 (97%)	13 (10%)	0
32	QA	1494/1521 (98%)	257 (17%)	15 (1%)
32	XA	1498/1521 (98%)	234 (15%)	16 (1%)
53	QV	76/77 (98%)	16 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	XV	76/77 (98%)	16 (21%)	1 (1%)
54	QX	8/25 (32%)	4 (50%)	0
54	XX	9/25 (36%)	4 (44%)	0
All	All	9109/9320 (97%)	1536 (16%)	78 (0%)

5 of 1536 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	12	U
1	RA	36	G
1	RA	45	C
1	RA	59	U

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	QA	1285	A
1	YA	827	U
32	XA	1065	U
32	QA	1442(A)	G
1	YA	277	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	2MU	YA	2552	1,56	14,22,24	7.85	8 (57%)	14,31,36	1.53	1 (7%)
32	2MG	XA	1207	32	19,26,27	4.84	6 (31%)	21,38,41	3.83	5 (23%)
32	PSU	QA	516	32,56	17,21,22	1.06	2 (11%)	20,30,33	3.46	6 (30%)
1	2MA	YA	2503	1,56	17,25,26	3.92	6 (35%)	19,37,40	4.02	6 (31%)
1	5MU	RA	1939	1	15,22,23	2.63	4 (26%)	16,32,35	3.42	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	QA	1498	32	14,22,23	3.15	3 (21%)	15,32,35	0.89	1 (6%)
32	7MG	QA	527	32,56	22,26,27	5.44	11 (50%)	28,39,42	3.07	10 (35%)
32	MA6	XA	1519	32	19,26,27	1.44	2 (10%)	18,38,41	4.11	2 (11%)
32	5MC	QA	967	32	15,22,23	3.63	5 (33%)	19,32,35	2.35	4 (21%)
32	5MC	XA	1400	32	15,22,23	3.64	6 (40%)	19,32,35	2.51	4 (21%)
32	PSU	XA	516	32	17,21,22	1.09	2 (11%)	20,30,33	3.47	6 (30%)
32	2MG	QA	1207	32	19,26,27	5.03	6 (31%)	21,38,41	4.01	7 (33%)
1	5MU	YA	1915	1	15,22,23	2.73	4 (26%)	16,32,35	3.02	2 (12%)
32	5MC	QA	1404	32	15,22,23	3.63	5 (33%)	19,32,35	2.34	4 (21%)
1	5MC	YA	1962	1,56	15,22,23	3.41	5 (33%)	19,32,35	2.02	2 (10%)
32	4OC	QA	1402	32	16,23,24	3.51	6 (37%)	17,32,35	1.46	2 (11%)
32	7MG	XA	527	32,56	22,26,27	5.39	11 (50%)	28,39,42	2.94	9 (32%)
1	2MU	RA	2552	1,56	14,22,24	7.66	8 (57%)	14,31,36	1.38	1 (7%)
32	5MC	XA	967	32	15,22,23	3.57	5 (33%)	19,32,35	2.45	4 (21%)
1	5MC	RA	1942	1,56	15,22,23	3.46	5 (33%)	19,32,35	2.25	4 (21%)
1	5MU	YA	1939	1,56	15,22,23	2.61	4 (26%)	16,32,35	3.39	2 (12%)
32	5MC	QA	1407	32	15,22,23	3.49	5 (33%)	19,32,35	2.32	4 (21%)
1	5MU	RA	1915	1	15,22,23	2.78	4 (26%)	16,32,35	2.92	2 (12%)
32	M2G	XA	966	32	20,27,28	3.75	6 (30%)	22,40,43	2.70	5 (22%)
1	PSU	YA	1917	1	17,21,22	1.01	1 (5%)	20,30,33	3.19	6 (30%)
32	UR3	XA	1498	32,56	14,22,23	3.05	3 (21%)	15,32,35	0.78	0
1	2MA	RA	2503	1,56	17,25,26	4.14	6 (35%)	19,37,40	4.12	6 (31%)
1	PSU	RA	2605	1	17,21,22	0.97	1 (5%)	20,30,33	3.13	6 (30%)
32	5MC	XA	1407	32	15,22,23	3.53	5 (33%)	19,32,35	2.68	4 (21%)
1	5MC	YA	1942	1	15,22,23	3.40	5 (33%)	19,32,35	2.25	4 (21%)
1	4OC	RA	1920	1	15,22,24	3.83	6 (40%)	17,31,35	2.61	4 (23%)
43	0TD	XL	92	43	4,9,10	1.11	0	3,11,13	3.02	2 (66%)
32	4OC	XA	1402	32	16,23,24	3.43	6 (37%)	17,32,35	2.69	2 (11%)
32	5MC	XA	1404	32	15,22,23	3.56	5 (33%)	19,32,35	2.25	3 (15%)
1	PSU	RA	1917	1	17,21,22	1.09	3 (17%)	20,30,33	3.47	6 (30%)
1	OMG	RA	2251	1,56,53	18,26,27	3.70	7 (38%)	20,38,41	3.84	6 (30%)
32	MA6	QA	1519	32	19,26,27	1.28	3 (15%)	18,38,41	3.53	2 (11%)
1	4OC	YA	1920	1	15,22,24	3.65	6 (40%)	17,31,35	2.49	4 (23%)
1	PSU	YA	2605	1	17,21,22	1.02	2 (11%)	20,30,33	3.56	6 (30%)
1	PSU	YA	1911	1	17,21,22	1.05	2 (11%)	20,30,33	3.39	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	QA	1518	32	19,26,27	1.27	2 (10%)	18,38,41	3.29	2 (11%)
1	OMG	YA	2251	1,56,53	18,26,27	3.73	7 (38%)	20,38,41	3.90	8 (40%)
32	M2G	QA	966	32	20,27,28	3.93	6 (30%)	22,40,43	2.83	5 (22%)
1	5MC	RA	1962	1,56	15,22,23	3.44	5 (33%)	19,32,35	2.07	3 (15%)
43	0TD	QL	92	43	4,9,10	1.28	0	3,11,13	3.67	2 (66%)
1	PSU	RA	1911	1	17,21,22	0.94	2 (11%)	20,30,33	3.28	6 (30%)
32	MA6	XA	1518	32	19,26,27	1.16	2 (10%)	18,38,41	3.42	2 (11%)
32	5MC	QA	1400	32	15,22,23	3.59	6 (40%)	19,32,35	2.22	4 (21%)

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
1	2MU	YA	2552	1,56	-	0/7/27/28	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	QA	516	32,56	-	0/7/25/26	0/2/2/2
1	2MA	YA	2503	1,56	-	2/3/25/26	0/3/3/3
1	5MU	RA	1939	1	-	3/5/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/5/25/26	0/2/2/2
32	7MG	QA	527	32,56	-	2/7/37/38	0/3/3/3
32	MA6	XA	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	QA	967	32	-	0/5/25/26	0/2/2/2
32	5MC	XA	1400	32	-	2/5/25/26	0/2/2/2
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	2MG	QA	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	YA	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	QA	1404	32	-	0/5/25/26	0/2/2/2
1	5MC	YA	1962	1,56	-	2/5/25/26	0/2/2/2
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
32	7MG	XA	527	32,56	-	2/7/37/38	0/3/3/3
1	2MU	RA	2552	1,56	-	0/7/27/28	0/2/2/2
32	5MC	XA	967	32	-	0/5/25/26	0/2/2/2
1	5MC	RA	1942	1,56	-	0/5/25/26	0/2/2/2
1	5MU	YA	1939	1,56	-	0/5/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	RA	1915	1	-	0/5/25/26	0/2/2/2
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	XA	1498	32,56	-	0/5/25/26	0/2/2/2
1	2MA	RA	2503	1,56	-	1/3/25/26	0/3/3/3
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/5/25/26	0/2/2/2
1	4OC	RA	1920	1	-	0/7/27/30	0/2/2/2
43	0TD	XL	92	43	-	2/3/12/14	-
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	XA	1404	32	-	0/5/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	RA	2251	1,56,53	-	0/5/27/28	0/3/3/3
32	MA6	QA	1519	32	-	3/7/29/30	0/3/3/3
1	4OC	YA	1920	1	-	1/7/27/30	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
1	OMG	YA	2251	1,56,53	-	0/5/27/28	0/3/3/3
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
1	5MC	RA	1962	1,56	-	2/5/25/26	0/2/2/2
43	0TD	QL	92	43	-	1/3/12/14	-
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	XA	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	QA	1400	32	-	2/5/25/26	0/2/2/2

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	C6-N1	21.02	1.61	1.35
1	RA	2552	2MU	C6-N1	20.03	1.60	1.35
32	QA	1207	2MG	C2-N2	16.24	1.47	1.34
32	XA	1207	2MG	C2-N2	15.36	1.47	1.34
32	QA	527	7MG	C4-N3	13.28	1.51	1.34

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	1519	MA6	N1-C6-N6	-16.79	99.39	117.06
1	RA	2503	2MA	C2-N3-C4	14.48	127.28	115.52
32	QA	1519	MA6	N1-C6-N6	-13.43	102.92	117.06
32	XA	1518	MA6	N1-C6-N6	-13.13	103.24	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2503	2MA	C2-N3-C4	13.11	126.17	115.52

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	RA	1939	5MU	O4'-C1'-N1-C6
32	QA	527	7MG	C3'-C4'-C5'-O5'
32	XA	1519	MA6	O4'-C4'-C5'-O5'
1	YA	1962	5MC	O4'-C1'-N1-C6
1	YA	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	2552	2MU	3	0
32	XA	1519	MA6	4	0
1	YA	1962	5MC	2	0
32	QA	1402	4OC	1	0
1	RA	2552	2MU	3	0
1	RA	1942	5MC	1	0
1	YA	1939	5MU	1	0
1	RA	2503	2MA	2	0
1	RA	1920	4OC	1	0
1	RA	1917	PSU	1	0
1	RA	2251	OMG	1	0
32	QA	1519	MA6	2	0
32	QA	1518	MA6	1	0
1	YA	2251	OMG	1	0
1	RA	1962	5MC	1	0
32	XA	1518	MA6	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2450 ligands modelled in this entry, 2448 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	$\# Z > 2$
58	SF4	XD	301	35	0,12,12	0.00	-	-		
58	SF4	QD	302	35	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
58	SF4	XD	301	35	-	-	0/6/5/5
58	SF4	QD	302	35	-	-	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.

No monomer is involved in short contacts.

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.