



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2020 – 05:03 AM BST

PDB ID : 4Y4P
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome with rRNA modifications and bound to mRNA and A-, P- and E-site tRNAs at 2.5Å resolution
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.
Deposited on : 2015-02-10
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

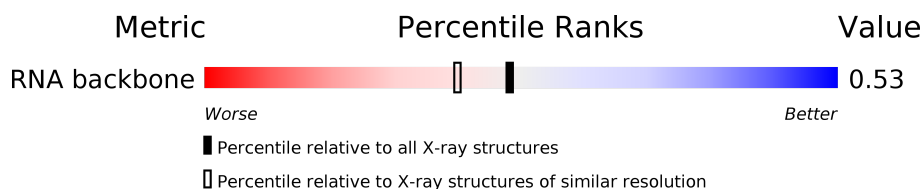
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

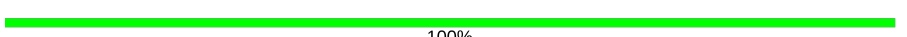
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
RNA backbone	3102	1008 (2.84-2.16)

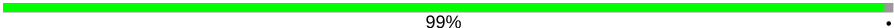
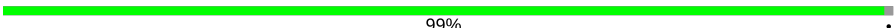

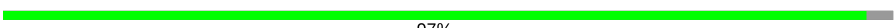











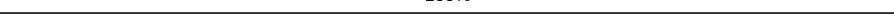
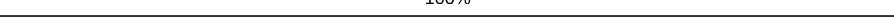
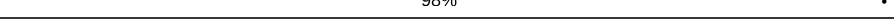
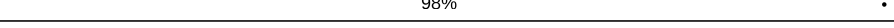


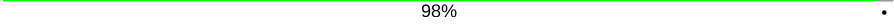
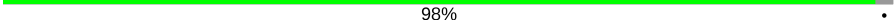
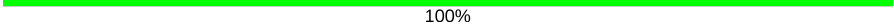
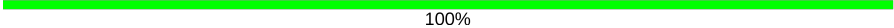
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1A	2915	 82% 16% ..
1	2A	2915	 77% 18% . .
2	1B	121	 89% 10% .
2	2B	121	 68% 31% ..
3	1D	276	 100%
3	2D	276	 100%
4	1E	206	 99% .
4	2E	206	 99% .
5	1F	210	 97% .
5	2F	210	 97% .

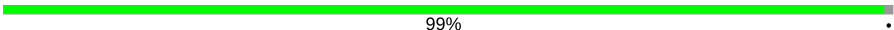

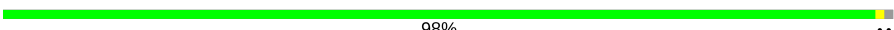
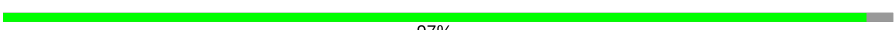











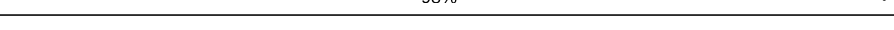
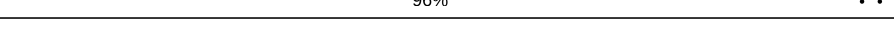
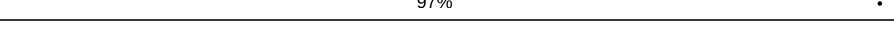
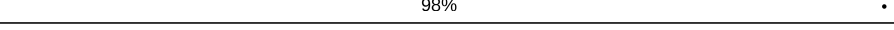
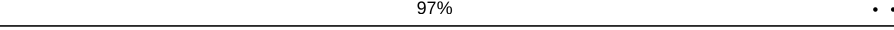
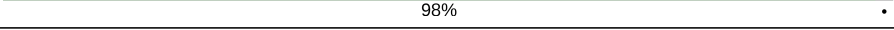
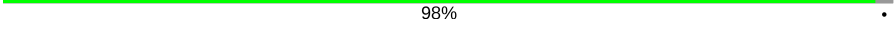
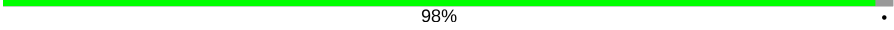
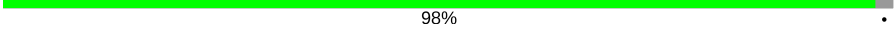
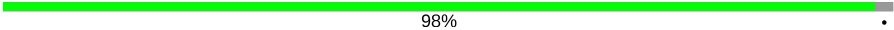
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Mol	Chain	Length	Quality of chain
6	1G	182	 99% .
6	2G	182	 99% .
7	1H	180	 97% .
7	2H	180	 97% .
8	1I	148	 99% .
8	2I	148	 99% .
9	1N	140	 100%
9	2N	140	 100%
10	1O	122	 100%
10	2O	122	 100%
11	1P	150	 99% .
11	2P	150	 99% .
12	1Q	141	 100%
12	2Q	141	 100%
13	1R	118	 100%
13	2R	118	 100%
14	1S	112	 98% .
14	2S	112	 98% .
15	1T	146	 89% . 10%
15	2T	146	 90% 10%
16	1U	118	 98% .
16	2U	118	 98% .
17	1V	101	 100%
17	2V	101	 100%
18	1W	113	 99% .
















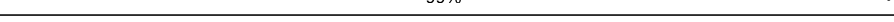
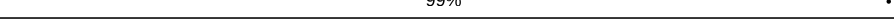
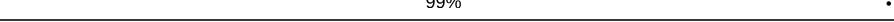
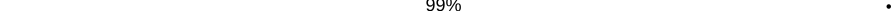
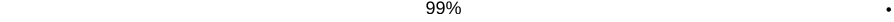
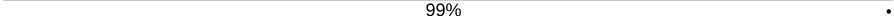




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Mol	Chain	Length	Quality of chain
18	2W	113	 99% .
19	1X	96	 99% .
19	2X	96	 98% ..
20	1Y	110	 97% .
20	2Y	110	 97% .
21	1Z	206	 75% 25%
21	2Z	206	 78% 22%
22	10	85	 96% ..
22	20	85	 98% .
23	11	98	 99% .
23	21	98	 99% .
24	12	72	 97% .
24	22	72	 97% .
25	13	60	 98% .
25	23	60	 98% .
26	14	71	 96% ..
26	24	71	 97% .
27	15	60	 98% .
27	25	60	 97% ..
28	16	54	 98% .
28	26	54	 98% .
29	17	49	 98% .
29	27	49	 98% .
30	18	65	 98% .
30	28	65	 98% .


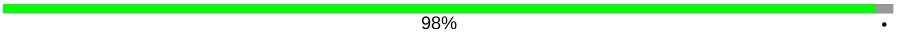
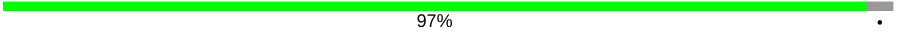
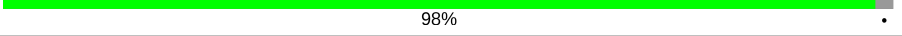
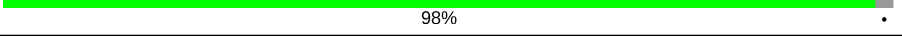
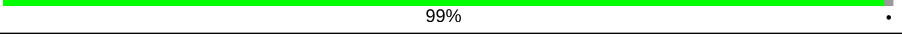
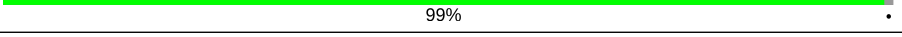
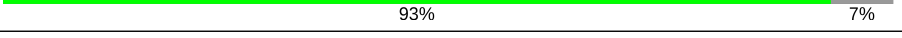
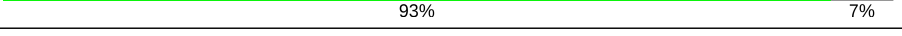
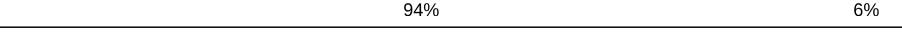
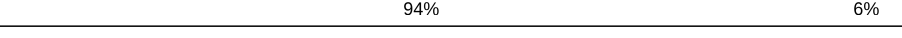
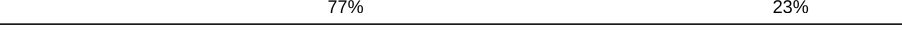

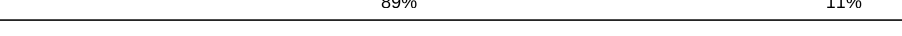


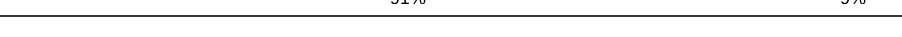

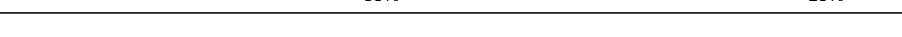
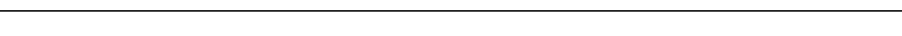

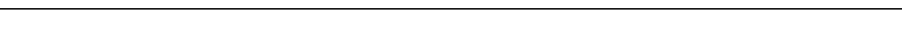
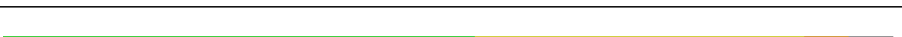


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Mol	Chain	Length	Quality of chain
31	19	37	 100%
31	29	37	 100%
32	1a	1521	 82% 16% ..
32	2a	1521	 81% 17% ..
33	1b	256	 90% 10%
33	2b	256	 90% 10%
34	1c	239	 86% 14%
34	2c	239	 86% 14%
35	1d	209	 100%
35	2d	209	 100%
36	1e	162	 91% 9%
36	2e	162	 91% 9%
37	1f	101	 99% .
37	2f	101	 99% .
38	1g	156	 99% .
38	2g	156	 99% .
39	1h	138	 99% .
39	2h	138	 99% .
40	1i	128	 99% .
40	2i	128	 99% .
41	1j	105	 92% 8%
41	2j	105	 90% . 9%
42	1k	129	 88% 12%
42	2k	129	 88% 12%
43	1l	132	 92% . 8%



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Mol	Chain	Length	Quality of chain
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	

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Mol	Chain	Length	Quality of chain
55	1x	77	 79% 19% .
55	2x	77	 69% 30% .

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 300910 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	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	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	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	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	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	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	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	1O	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	2O	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	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	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	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	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	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	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	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	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	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	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	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	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	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	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	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	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	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	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	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	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	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	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	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	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	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	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	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	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	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	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	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	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	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	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	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	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	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	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	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	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	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	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	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	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	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	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	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	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	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	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	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	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	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total 1592	C 713	N 285	O 518	P 74	S 2	0	0	0
54	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
54	2w	72	Total 1544	C 690	N 278	O 502	P 72	S 2	0	0	0
54	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	9	Total	Mg	0	0
			9	9		
56	17	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	3	Total	Mg	0	0
			3	3		
56	18	3	Total	Mg	0	0
			3	3		
56	2W	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	4	Total 4	Mg 4	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2a	244	Total 244	Mg 244	0	0
56	1E	11	Total 11	Mg 11	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1141	Total 1141	Mg 1141	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	6	Total 6	Mg 6	0	0
56	12	1	Total 1	Mg 1	0	0
56	1y	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2i	1	Total 1	Mg 1	0	0
56	1S	3	Total 3	Mg 3	0	0
56	25	4	Total 4	Mg 4	0	0
56	2T	3	Total 3	Mg 3	0	0
56	1D	12	Total 12	Mg 12	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	3	Total 3	Mg 3	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1a	229	Total 229	Mg 229	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	2	Total 2	Mg 2	0	0
56	1x	16	Total 16	Mg 16	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1s	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2U	4	Total 4	Mg 4	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	1	Total 1	Mg 1	0	0
56	11	3	Total 3	Mg 3	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	5	Total 5	Mg 5	0	0
56	2q	2	Total 2	Mg 2	0	0
56	1U	8	Total 8	Mg 8	0	0
56	2r	2	Total 2	Mg 2	0	0
56	1O	7	Total 7	Mg 7	0	0
56	27	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1F	8	Total	Mg	0	0
			8	8		
56	10	6	Total	Mg	0	0
			6	6		
56	2t	1	Total	Mg	0	0
			1	1		
56	1Q	6	Total	Mg	0	0
			6	6		
56	2A	909	Total	Mg	0	0
			909	909		
56	23	2	Total	Mg	0	0
			2	2		
56	2Z	1	Total	Mg	0	0
			1	1		
56	1B	37	Total	Mg	0	0
			37	37		
56	2y	7	Total	Mg	0	0
			7	7		
56	2w	8	Total	Mg	0	0
			8	8		

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1	Total	K	0	0
			1	1		
57	2A	1	Total	K	0	0
			1	1		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

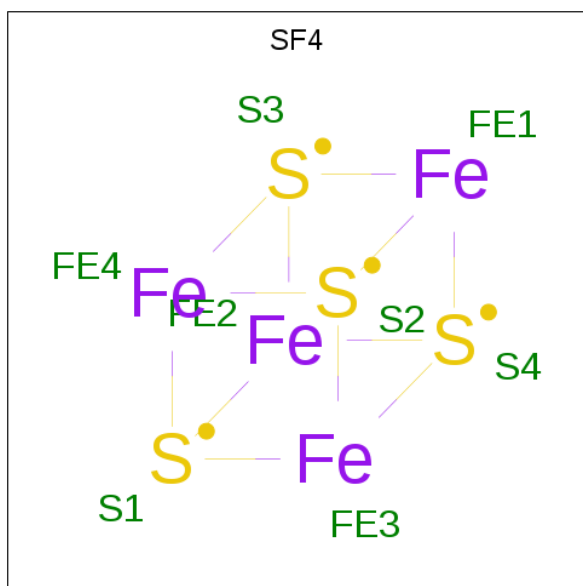
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	19	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2238	Total 2238	O 2238	0	0
60	1B	68	Total 68	O 68	0	0
60	1D	28	Total 28	O 28	0	0
60	1E	28	Total 28	O 28	0	0
60	1F	13	Total 13	O 13	0	0
60	1G	7	Total 7	O 7	0	0
60	1H	2	Total 2	O 2	0	0
60	1I	3	Total 3	O 3	0	0
60	1N	7	Total 7	O 7	0	0
60	1O	8	Total 8	O 8	0	0
60	1P	23	Total 23	O 23	0	0
60	1Q	14	Total 14	O 14	0	0
60	1R	14	Total 14	O 14	0	0
60	1S	5	Total 5	O 5	0	0
60	1T	8	Total 8	O 8	0	0
60	1U	11	Total 11	O 11	0	0
60	1V	9	Total 9	O 9	0	0
60	1W	6	Total 6	O 6	0	0
60	1X	8	Total 8	O 8	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	10	Total 10	O 10	0	0
60	12	4	Total 4	O 4	0	0
60	13	6	Total 6	O 6	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	3	Total 3	O 3	0	0
60	17	9	Total 9	O 9	0	0
60	18	13	Total 13	O 13	0	0
60	1a	438	Total 438	O 438	0	0
60	1b	1	Total 1	O 1	0	0
60	1d	1	Total 1	O 1	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1l	8	Total 8	O 8	0	0
60	1m	2	Total 2	O 2	0	0
60	1o	1	Total 1	O 1	0	0
60	1p	1	Total 1	O 1	0	0
60	1q	4	Total 4	O 4	0	0
60	1u	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1v	5	Total 5	O 5	0	0
60	1w	21	Total 21	O 21	0	0
60	1x	15	Total 15	O 15	0	0
60	1y	1	Total 1	O 1	0	0
60	2A	1389	Total 1389	O 1389	0	0
60	2B	26	Total 26	O 26	0	0
60	2D	28	Total 28	O 28	0	0
60	2E	16	Total 16	O 16	0	0
60	2F	16	Total 16	O 16	0	0
60	2H	1	Total 1	O 1	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	1	Total 1	O 1	0	0
60	2P	14	Total 14	O 14	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	2	Total 2	O 2	0	0
60	2T	6	Total 6	O 6	0	0
60	2U	2	Total 2	O 2	0	0
60	2V	2	Total 2	O 2	0	0
60	2W	2	Total 2	O 2	0	0
60	2X	5	Total 5	O 5	0	0
60	2Y	1	Total 1	O 1	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2Z	2	Total	O	0	0
			2	2		
60	20	7	Total	O	0	0
			7	7		
60	21	12	Total	O	0	0
			12	12		
60	22	1	Total	O	0	0
			1	1		
60	23	1	Total	O	0	0
			1	1		
60	25	4	Total	O	0	0
			4	4		
60	26	1	Total	O	0	0
			1	1		
60	27	4	Total	O	0	0
			4	4		
60	28	6	Total	O	0	0
			6	6		
60	29	1	Total	O	0	0
			1	1		
60	2a	377	Total	O	0	0
			377	377		
60	2d	1	Total	O	0	0
			1	1		
60	2e	2	Total	O	0	0
			2	2		
60	2g	1	Total	O	0	0
			1	1		
60	2i	1	Total	O	0	0
			1	1		
60	2j	4	Total	O	0	0
			4	4		
60	2l	5	Total	O	0	0
			5	5		
60	2o	1	Total	O	0	0
			1	1		
60	2p	2	Total	O	0	0
			2	2		
60	2q	1	Total	O	0	0
			1	1		
60	2r	1	Total	O	0	0
			1	1		

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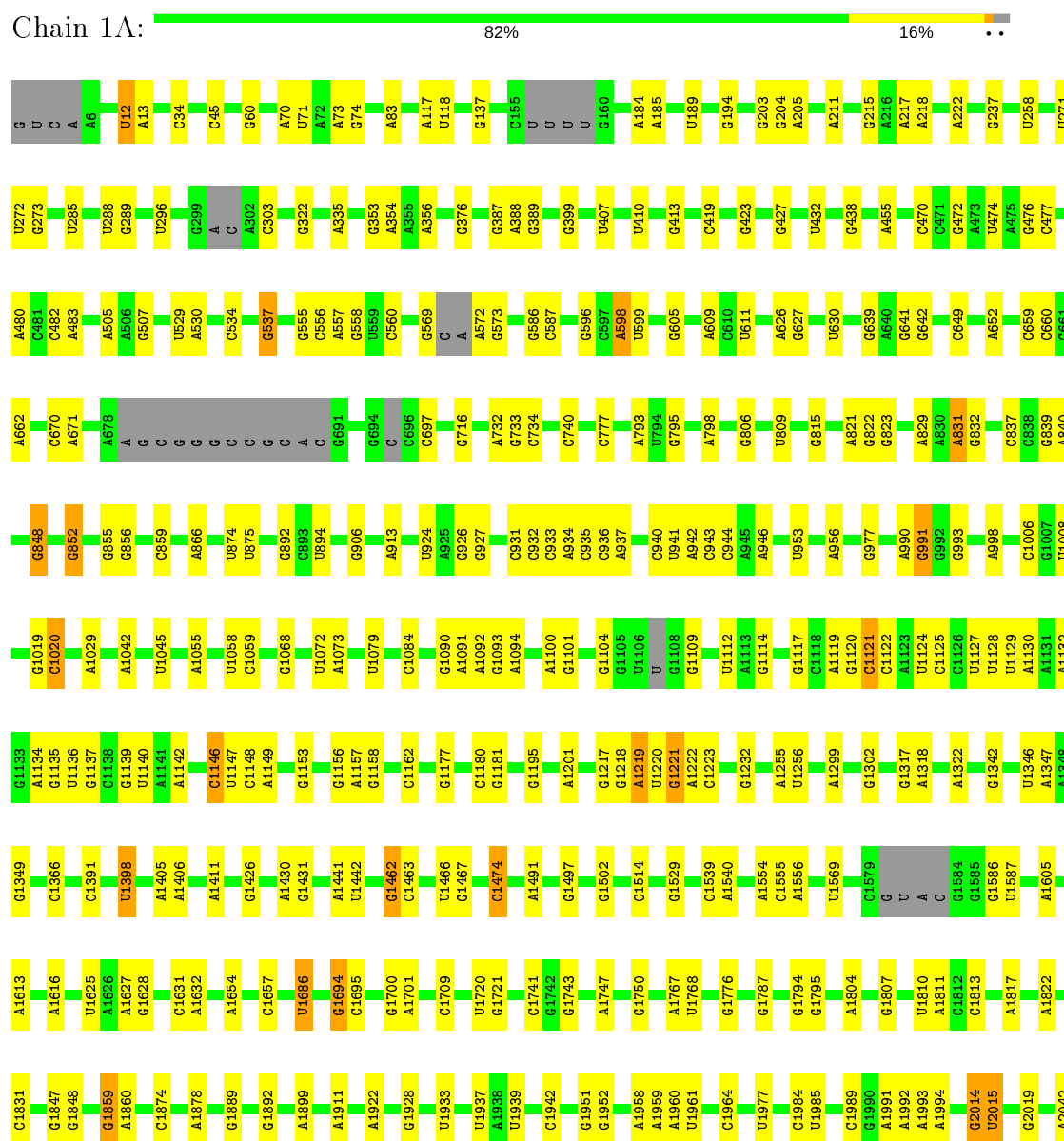
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2t	4	Total 4	O 4	0	0
60	2u	1	Total 1	O 1	0	0
60	2v	1	Total 1	O 1	0	0
60	2w	2	Total 2	O 2	0	0
60	2x	7	Total 7	O 7	0	0
60	2y	19	Total 19	O 19	0	0

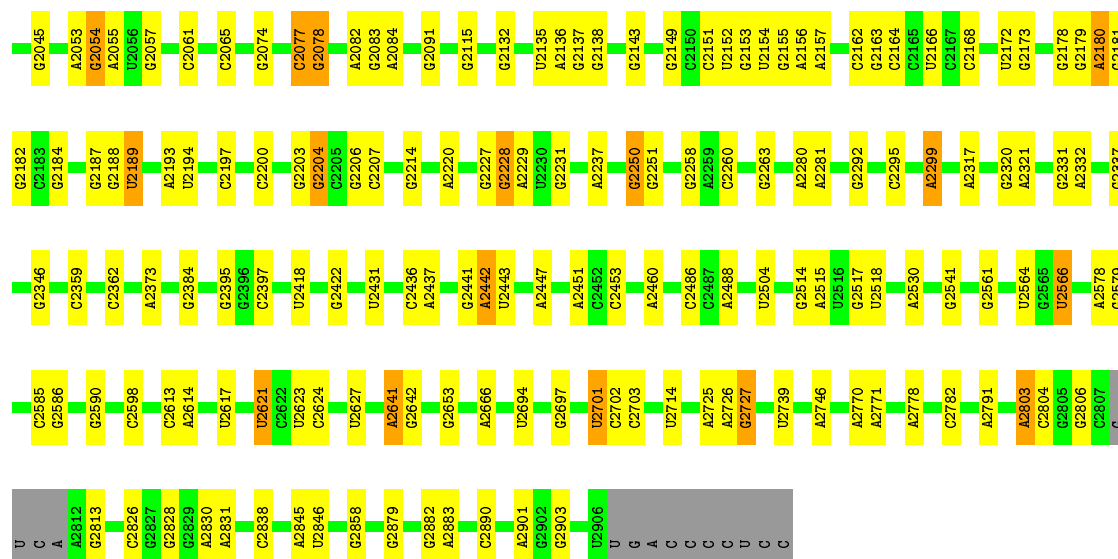
3 Residue-property plots

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

Note EDS failed to run properly.

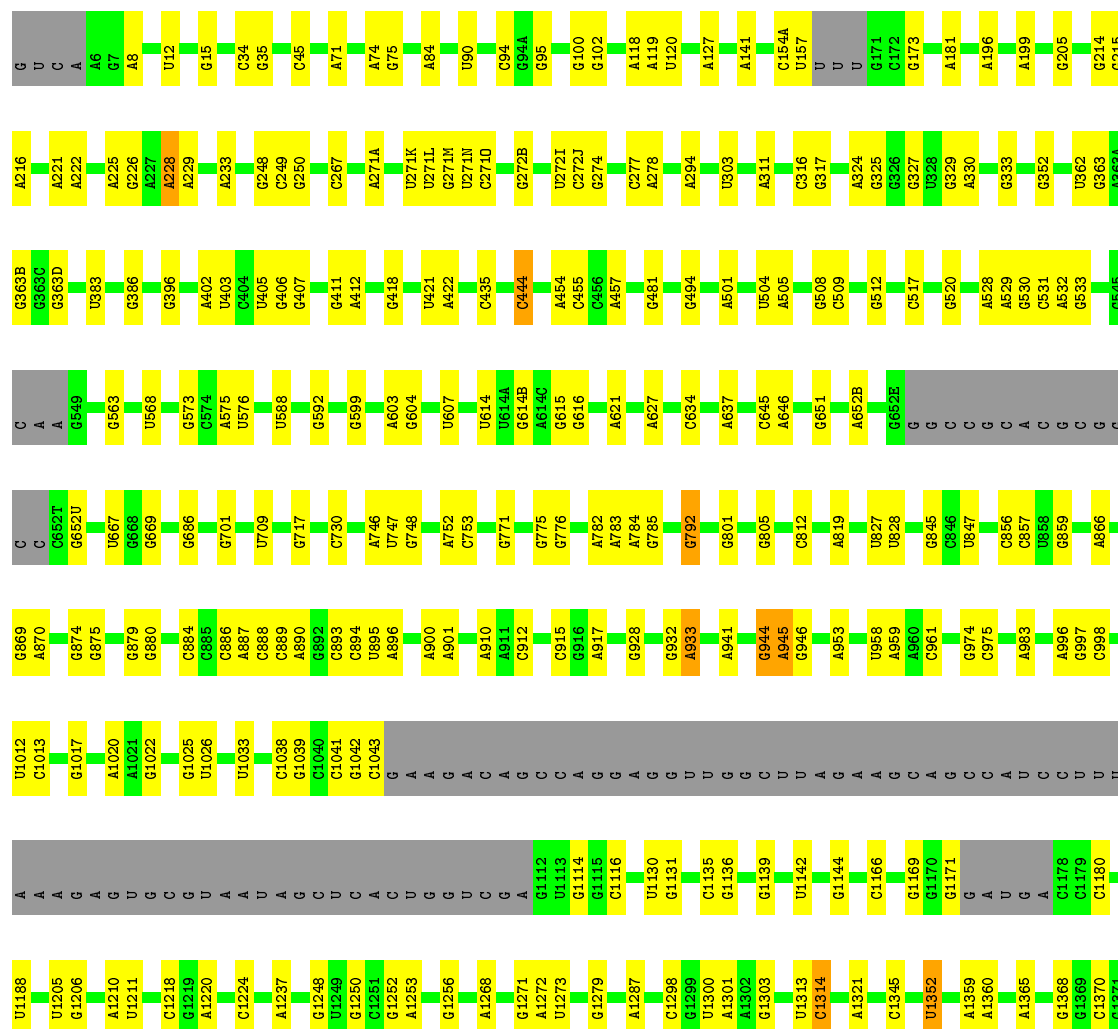
• Molecule 1: 23S Ribosomal RNA

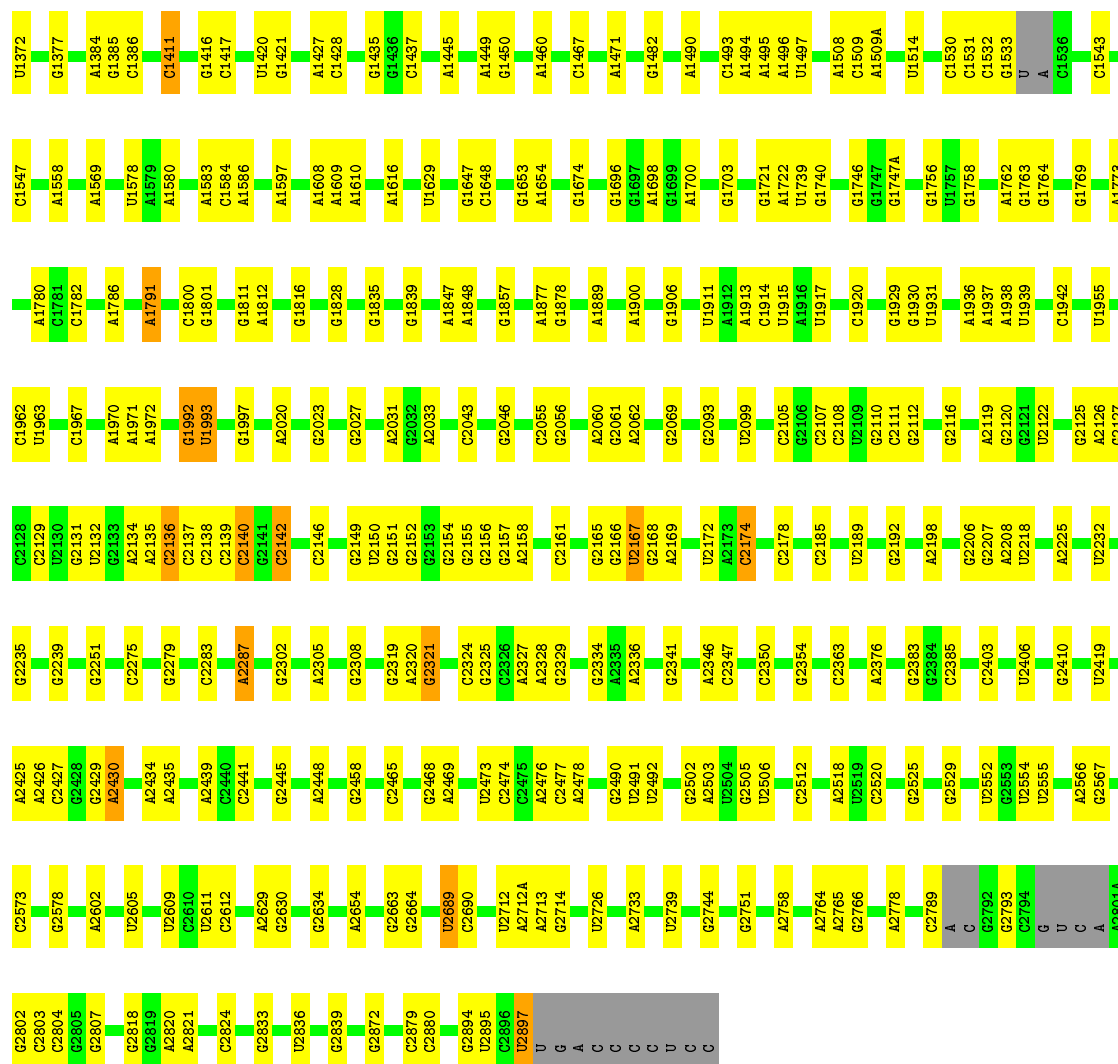




• Molecule 1: 23S Ribosomal RNA

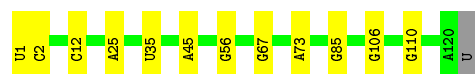
Chain 2A: 77% 18%





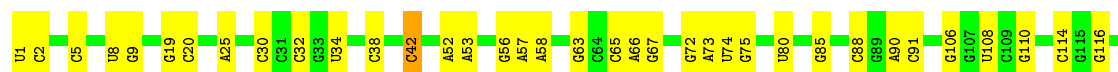
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 89% 10%



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 68% 31%



- Molecule 3: 50S ribosomal protein L2

Chain 1D:  100%



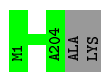
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  100%



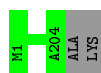
- Molecule 4: 50S ribosomal protein L3

Chain 1E:  99%



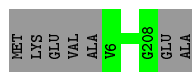
- Molecule 4: 50S ribosomal protein L3

Chain 2E:  99%



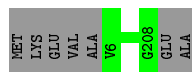
- Molecule 5: 50S ribosomal protein L4

Chain 1F:  97%



- Molecule 5: 50S ribosomal protein L4

Chain 2F:  97%



- Molecule 6: 50S ribosomal protein L5

Chain 1G:  99%



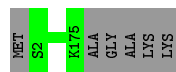
- Molecule 6: 50S ribosomal protein L5

Chain 2G:  99%



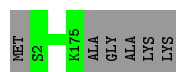
- Molecule 7: 50S ribosomal protein L6

Chain 1H:  97%



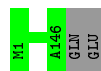
- Molecule 7: 50S ribosomal protein L6

Chain 2H:  97%



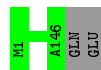
- Molecule 8: 50S ribosomal protein L9

Chain 1I:  99%



- Molecule 8: 50S ribosomal protein L9

Chain 2I:  99%



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: 50S ribosomal protein L13

Chain 2N:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 50S ribosomal protein L14

Chain 1O:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 50S ribosomal protein L14

Chain 2O:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L15

Chain 1P:  99%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  99%



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L17

Chain 1R:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L17

Chain 2R:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 50S ribosomal protein L18

Chain 1S:  98%



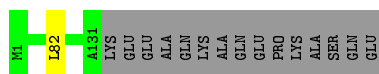
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  98%



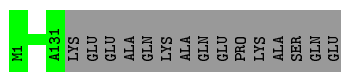
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  89%



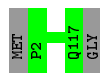
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  90%



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  98%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  98%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L21

Chain 2V:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L22

Chain 1W:  99%



- Molecule 18: 50S ribosomal protein L22

Chain 2W: 99% .



- Molecule 19: 50S ribosomal protein L23

Chain 1X: 99% .



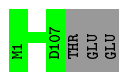
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 98% ..



- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 97% .



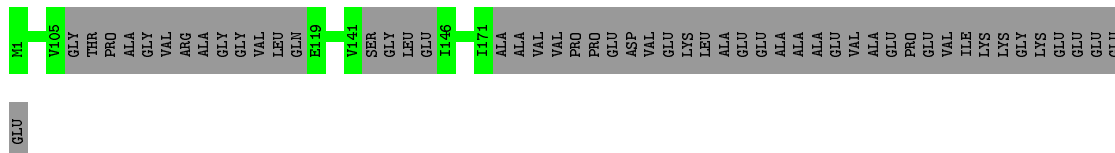
- Molecule 20: 50S ribosomal protein L24

Chain 2Y: 97% .




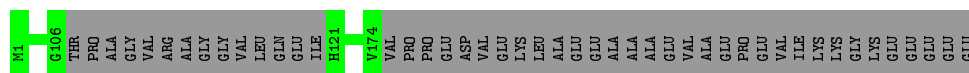
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 75% 25%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  78% 22%



- Molecule 22: 50S ribosomal protein L27

Chain 10:  96% ..



- Molecule 22: 50S ribosomal protein L27

Chain 20:  98% .



- Molecule 23: 50S ribosomal protein L28

Chain 11:  99% .



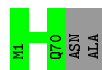
- Molecule 23: 50S ribosomal protein L28

Chain 21:  99% .



- Molecule 24: 50S ribosomal protein L29

Chain 12:  97% .



- Molecule 24: 50S ribosomal protein L29

Chain 22:  97% .



- Molecule 25: 50S ribosomal protein L30

Chain 13:  98% .



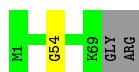
- Molecule 25: 50S ribosomal protein L30

Chain 23:  98% .



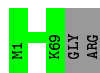
- Molecule 26: 50S ribosomal protein L31

Chain 14:  96% . .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  97% .



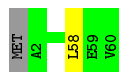
- Molecule 27: 50S ribosomal protein L32

Chain 15:  98% .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  97% . .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain 26:  98% .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  98% .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  98% .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  98% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  98% .



- Molecule 31: 50S ribosomal protein L36

Chain 19:  100%


There are no outlier residues recorded for this chain.

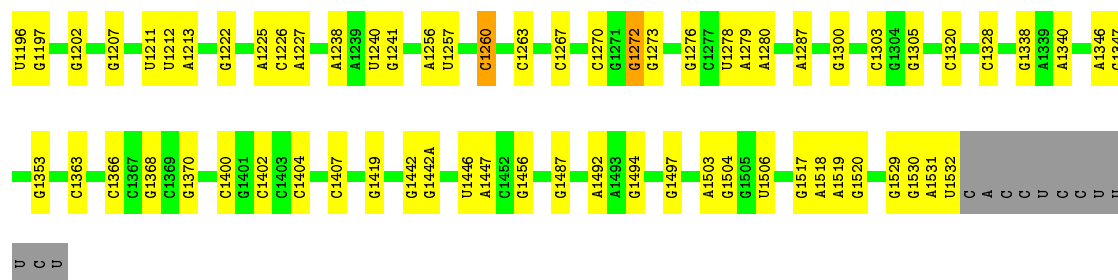
- Molecule 31: 50S ribosomal protein L36

Chain 29:  100%

There are no outlier residues recorded for this chain.

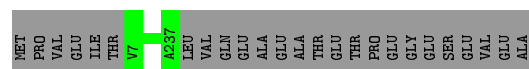
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  82% 16% ..



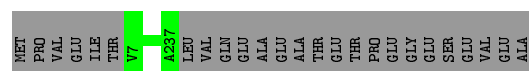
- Molecule 33: 30S ribosomal protein S2

Chain 1b: 90% 10%



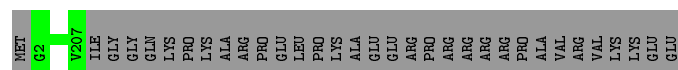
- Molecule 33: 30S ribosomal protein S2

Chain 2b: 90% 10%



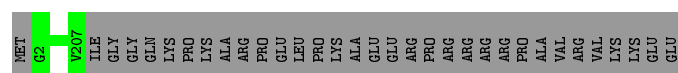
- Molecule 34: 30S ribosomal protein S3

Chain 1c: 86% 14%



- Molecule 34: 30S ribosomal protein S3

Chain 2c: 86% 14%



- Molecule 35: 30S ribosomal protein S4

Chain 1d: 100%



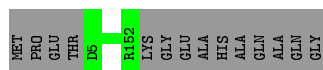
- Molecule 35: 30S ribosomal protein S4

Chain 2d: 100%



- Molecule 36: 30S ribosomal protein S5

Chain 1e: 91% 9%



- Molecule 36: 30S ribosomal protein S5

Chain 2e: 91% 9%



- Molecule 37: 30S ribosomal protein S6

Chain 1f: 99% .



- Molecule 37: 30S ribosomal protein S6

Chain 2f: 99% .



- Molecule 38: 30S ribosomal protein S7

Chain 1g: 99% .



- Molecule 38: 30S ribosomal protein S7

Chain 2g: 99% .



- Molecule 39: 30S ribosomal protein S8

Chain 1h: 99% .



- Molecule 39: 30S ribosomal protein S8

Chain 2h: 99%



- Molecule 40: 30S ribosomal protein S9

Chain 1i: 99%



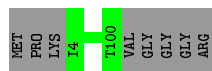
- Molecule 40: 30S ribosomal protein S9

Chain 2i: 99%



- Molecule 41: 30S ribosomal protein S10

Chain 1j: 92% 8%



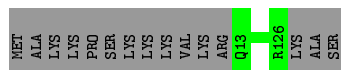
- Molecule 41: 30S ribosomal protein S10

Chain 2j: 90% 9%



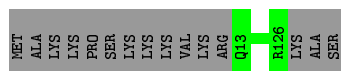
- Molecule 42: 30S ribosomal protein S11

Chain 1k: 88% 12%



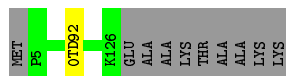
- Molecule 42: 30S ribosomal protein S11

Chain 2k: 88% 12%



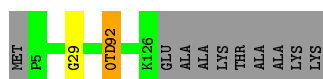
- Molecule 43: 30S ribosomal protein S12

Chain 1l: 92% 8%



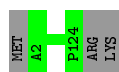
- Molecule 43: 30S ribosomal protein S12

Chain 2l: 91% 8%



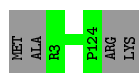
- Molecule 44: 30S ribosomal protein S13

Chain 1m: 98%



- Molecule 44: 30S ribosomal protein S13

Chain 2m: 97%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n: 98%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n: 98%



- Molecule 46: 30S ribosomal protein S15

Chain 1o: 99%



- Molecule 46: 30S ribosomal protein S15

Chain 2o: 99%



- Molecule 47: 30S ribosomal protein S16

Chain 1p: 93% 7%



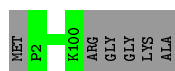
- Molecule 47: 30S ribosomal protein S16

Chain 2p: 93% 7%



- Molecule 48: 30S ribosomal protein S17

Chain 1q: 94% 6%



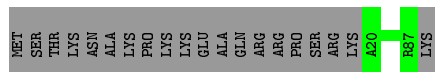
- Molecule 48: 30S ribosomal protein S17

Chain 2q: 94% 6%



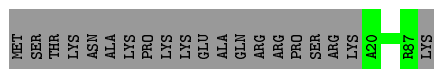
- Molecule 49: 30S ribosomal protein S18

Chain 1r: 77% 23%

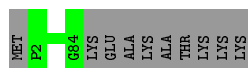


- Molecule 49: 30S ribosomal protein S18

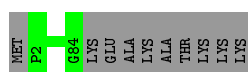
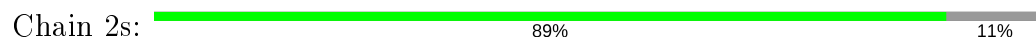
Chain 2r: 77% 23%



- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19



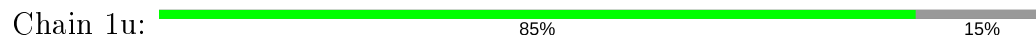
- Molecule 51: 30S ribosomal protein S20



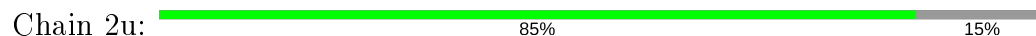
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA

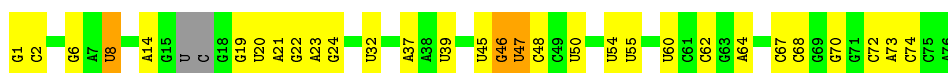




- Molecule 53: mRNA



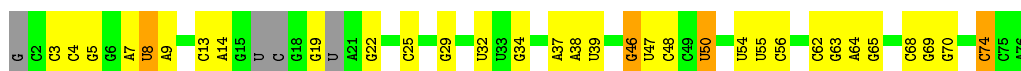
- Molecule 54: A-site and E-site tRNAs



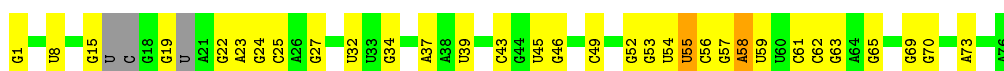
- Molecule 54: A-site and E-site tRNAs



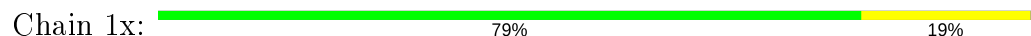
- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA





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	209.70Å 450.05Å 624.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.01 – 2.50	Depositor
% Data completeness (in resolution range)	97.8 (122.01-2.50)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.281	Depositor
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.174	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	300910	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, M2G, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, 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	1A	0.61	0/69009	1.05	129/107712 (0.1%)
1	2A	0.52	1/67293 (0.0%)	1.03	84/105034 (0.1%)
2	1B	0.51	1/2882 (0.0%)	0.87	0/4494
2	2B	0.59	1/2879 (0.0%)	1.01	4/4487 (0.1%)
3	1D	0.44	0/2186	0.61	0/2944
3	2D	0.38	0/2186	0.61	0/2944
4	1E	0.43	0/1592	0.61	0/2149
4	2E	0.37	0/1592	0.59	0/2149
5	1F	0.40	0/1619	0.58	0/2193
5	2F	0.37	0/1615	0.58	0/2188
6	1G	0.34	0/1448	0.54	0/1957
6	2G	0.36	0/1453	0.58	0/1963
7	1H	0.36	0/1356	0.55	0/1834
7	2H	0.33	0/1356	0.55	0/1834
8	1I	0.31	0/1112	0.55	0/1514
8	2I	0.30	0/1079	0.54	0/1475
9	1N	0.39	0/1144	0.57	0/1543
9	2N	0.36	0/1144	0.58	0/1543
10	1O	0.42	0/943	0.58	0/1269
10	2O	0.35	0/943	0.54	0/1269
11	1P	0.39	0/1152	0.60	0/1533
11	2P	0.36	0/1152	0.62	0/1533
12	1Q	0.41	0/1143	0.57	0/1527
12	2Q	0.37	0/1143	0.60	0/1527
13	1R	0.43	0/982	0.63	0/1312
13	2R	0.38	0/982	0.60	0/1312
14	1S	0.34	0/883	0.56	0/1176
14	2S	0.38	0/880	0.59	0/1172
15	1T	0.39	0/1105	0.61	1/1477 (0.1%)
15	2T	0.36	0/1097	0.59	0/1468
16	1U	0.46	0/977	0.62	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.39	0/977	0.60	0/1301
17	1V	0.45	0/782	0.62	0/1049
17	2V	0.35	0/782	0.59	0/1049
18	1W	0.45	0/897	0.66	0/1205
18	2W	0.39	0/897	0.58	0/1205
19	1X	0.44	0/764	0.61	0/1025
19	2X	0.40	0/764	0.63	1/1025 (0.1%)
20	1Y	0.39	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.56	0/1095
21	1Z	0.35	0/1267	0.59	0/1717
21	2Z	0.31	0/1299	0.53	0/1763
22	10	0.43	0/662	0.66	1/881 (0.1%)
22	20	0.33	0/662	0.56	0/881
23	11	0.39	0/762	0.58	0/1014
23	21	0.35	0/762	0.57	0/1014
24	12	0.35	0/590	0.56	0/781
24	22	0.33	0/590	0.51	0/781
25	13	0.41	0/474	0.60	0/635
25	23	0.33	0/469	0.57	0/630
26	14	0.35	0/565	0.69	1/761 (0.1%)
26	24	0.37	0/545	0.64	0/737
27	15	0.42	0/469	0.64	0/635
27	25	0.38	0/469	0.60	1/635 (0.2%)
28	16	0.44	0/460	0.56	0/613
28	26	0.35	0/456	0.51	0/608
29	17	0.44	0/426	0.70	0/561
29	27	0.42	0/426	0.66	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.39	0/525	0.60	0/691
31	19	0.42	0/310	0.60	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.43	0/35795	0.92	40/55864 (0.1%)
32	2a	0.45	3/35886 (0.0%)	0.98	62/56005 (0.1%)
33	1b	0.31	0/1881	0.59	0/2542
33	2b	0.34	0/1860	0.57	0/2518
34	1c	0.28	0/1572	0.49	0/2126
34	2c	0.34	0/1566	0.55	0/2119
35	1d	0.31	0/1685	0.54	0/2262
35	2d	0.31	0/1704	0.52	0/2284
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.34	0/1149	0.61	0/1548
37	1f	0.32	0/823	0.53	0/1115
37	2f	0.32	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.52	0/1679
38	2g	0.31	0/1254	0.54	0/1683
39	1h	0.30	0/1108	0.54	0/1494
39	2h	0.30	0/1108	0.55	0/1494
40	1i	0.31	0/1002	0.59	0/1346
40	2i	0.32	0/997	0.56	0/1343
41	1j	0.30	0/722	0.54	0/982
41	2j	0.34	0/727	0.59	1/988 (0.1%)
42	1k	0.30	0/844	0.55	0/1145
42	2k	0.31	0/848	0.52	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.32	0/937	0.59	1/1260 (0.1%)
44	1m	0.32	0/969	0.57	0/1302
44	2m	0.31	0/961	0.57	0/1291
45	1n	0.33	0/501	0.51	0/664
45	2n	0.31	0/501	0.53	0/664
46	1o	0.30	0/739	0.49	0/985
46	2o	0.30	0/739	0.51	0/985
47	1p	0.31	0/697	0.54	0/939
47	2p	0.31	0/693	0.53	0/935
48	1q	0.33	0/836	0.55	0/1117
48	2q	0.31	0/836	0.52	0/1117
49	1r	0.32	0/560	0.53	0/746
49	2r	0.30	0/560	0.51	0/746
50	1s	0.29	0/667	0.58	0/900
50	2s	0.38	0/661	0.66	0/893
51	1t	0.28	0/730	0.53	0/965
51	2t	0.30	0/729	0.54	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.34	0/203	0.50	0/266
53	1v	0.46	0/310	0.93	0/480
53	2v	0.60	0/310	0.91	0/480
54	1w	0.57	1/1606 (0.1%)	1.10	3/2497 (0.1%)
54	1y	0.56	1/1606 (0.1%)	1.13	9/2497 (0.4%)
54	2w	0.53	0/1556	1.12	2/2418 (0.1%)
54	2y	0.59	1/1583 (0.1%)	1.17	4/2459 (0.2%)
55	1x	0.57	3/1725 (0.2%)	1.16	16/2689 (0.6%)
55	2x	0.49	0/1725	1.06	8/2689 (0.3%)
All	All	0.49	12/316686 (0.0%)	0.92	368/474113 (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
43	2l	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.21	1.48	1.61
2	1B	1	U	OP3-P	-10.20	1.49	1.61
54	1y	1	G	OP3-P	-10.20	1.49	1.61
2	2B	1	U	OP3-P	-9.87	1.49	1.61
54	1w	1	G	OP3-P	-9.63	1.49	1.61

The worst 5 of 368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.29	132.27	118.90
32	2a	1272	G	N3-C2-N2	21.80	135.16	119.90
32	2a	1272	G	C5-C6-O6	20.59	140.96	128.60
32	2a	1272	G	N1-C2-N2	-18.95	99.14	116.20
32	2a	1263	C	C2-N3-C4	15.04	127.42	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	2l	92	0TD	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2859/2915 (98%)	414 (14%)	0
1	2A	2788/2915 (95%)	510 (18%)	0
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	27 (39%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	8 (10%)	0
55	2x	75/77 (97%)	16 (21%)	0
All	All	9329/9620 (96%)	1590 (17%)	0

5 of 1590 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	60	G

There are no RNA pucker outliers to report.

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

84 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
54	7MG	1w	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.87	8 (28%)
32	5MC	2a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.32	3 (15%)
1	2MU	2A	2552	1,56	14,22,24	0.99	0	14,31,36	1.04	1 (7%)
1	4OC	1A	1942	1	15,22,24	0.66	0	17,31,35	1.41	1 (5%)
1	2MA	1A	2515	1,56	17,25,26	1.45	2 (11%)	19,37,40	2.08	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.12	1 (6%)	16,32,35	1.75	2 (12%)
43	0TD	1l	92	43	4,9,10	4.08	3 (75%)	3,11,13	5.57	2 (66%)
32	2MG	2a	1207	32	19,26,27	1.28	2 (10%)	21,38,41	2.23	7 (33%)
55	5MC	1x	32	55	15,22,23	1.32	1 (6%)	19,32,35	1.44	3 (15%)
1	2MA	2A	2503	1,56	17,25,26	1.25	2 (11%)	19,37,40	1.86	3 (15%)
54	PSU	1w	39	54	17,21,22	1.52	2 (11%)	20,30,33	3.16	5 (25%)
1	PSU	2A	2605	1	17,21,22	1.35	2 (11%)	20,30,33	2.90	6 (30%)
32	PSU	2a	516	32	17,21,22	1.44	2 (11%)	20,30,33	3.25	7 (35%)
54	PSU	2w	39	54	17,21,22	1.46	2 (11%)	20,30,33	3.30	6 (30%)
1	PSU	1A	2617	1,56	17,21,22	1.91	5 (29%)	20,30,33	3.10	6 (30%)
32	MA6	1a	1519	32	19,26,27	1.10	1 (5%)	18,38,41	1.58	4 (22%)
54	MIA	1y	37	54	18,24,32	1.13	2 (11%)	18,35,47	1.32	2 (11%)
32	5MC	1a	1404	32	15,22,23	1.31	1 (6%)	19,32,35	1.39	3 (15%)
1	5MC	1A	1964	1,56	15,22,23	1.28	1 (6%)	19,32,35	1.49	3 (15%)
32	7MG	1a	527	32,56	22,26,27	1.78	4 (18%)	28,39,42	2.59	9 (32%)
1	5MU	1A	1937	1	15,22,23	1.05	1 (6%)	16,32,35	1.72	2 (12%)
32	4OC	1a	1402	32	16,23,24	0.73	0	17,32,35	1.63	1 (5%)
1	OMG	1A	2263	1,55,56	18,26,27	1.17	2 (11%)	20,38,41	2.29	6 (30%)
1	OMG	2A	2251	1,55,56	18,26,27	1.24	2 (11%)	20,38,41	2.13	6 (30%)
54	5MU	1w	54	54	15,22,23	1.13	1 (6%)	16,32,35	1.84	2 (12%)
1	2MU	1A	2564	1,56	14,22,24	0.85	1 (7%)	14,31,36	0.61	0
54	MIA	2y	37	54	18,24,32	1.10	2 (11%)	18,35,47	1.31	3 (16%)
54	PSU	2w	55	54,56	17,21,22	1.38	2 (11%)	20,30,33	3.38	6 (30%)
54	5MU	2y	54	54	15,22,23	1.09	1 (6%)	16,32,35	2.05	1 (6%)
32	7MG	2a	527	32,56	22,26,27	1.82	4 (18%)	28,39,42	2.66	9 (32%)
54	4SU	2w	8	54	14,21,22	1.29	1 (7%)	15,30,33	1.20	2 (13%)
1	5MC	1A	1984	1,56	15,22,23	1.26	1 (6%)	19,32,35	1.35	2 (10%)
32	5MC	1a	1400	32	15,22,23	1.31	1 (6%)	19,32,35	1.46	4 (21%)
1	5MC	2A	1962	1,56	15,22,23	1.24	1 (6%)	19,32,35	1.48	3 (15%)
54	5MU	2w	54	54	15,22,23	1.10	1 (6%)	16,32,35	2.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1961	1,56	15,22,23	1.02	2 (13%)	16,32,35	1.71	2 (12%)
54	PSU	2y	39	54	17,21,22	1.59	2 (11%)	20,30,33	3.35	6 (30%)
54	PSU	1y	55	54	17,21,22	1.61	3 (17%)	20,30,33	3.11	7 (35%)
32	MA6	2a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.79	4 (22%)
54	PSU	1y	39	54	17,21,22	1.48	2 (11%)	20,30,33	3.21	5 (25%)
1	5MU	2A	1939	1,56	15,22,23	1.19	2 (13%)	16,32,35	1.72	2 (12%)
32	5MC	2a	967	32	15,22,23	1.49	1 (6%)	19,32,35	1.24	2 (10%)
32	UR3	1a	1498	32	14,22,23	0.80	1 (7%)	15,32,35	0.82	1 (6%)
55	5MU	1x	54	55,56	15,22,23	1.12	1 (6%)	16,32,35	2.05	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.37	3 (15%)
32	5MC	1a	967	32	15,22,23	1.32	1 (6%)	19,32,35	1.38	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	3 (15%)
1	5MC	2A	1942	1	15,22,23	1.19	1 (6%)	19,32,35	1.53	4 (21%)
54	4SU	1y	8	54	14,21,22	1.23	1 (7%)	15,30,33	1.73	2 (13%)
54	PSU	1w	32	54,56	17,21,22	1.55	2 (11%)	20,30,33	3.17	6 (30%)
54	7MG	2y	46	54	22,26,27	1.94	4 (18%)	28,39,42	3.21	12 (42%)
54	7MG	1y	46	54	22,26,27	1.81	3 (13%)	28,39,42	2.89	9 (32%)
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.22	7 (33%)
54	MIA	2w	37	54	20,27,32	1.73	3 (15%)	22,39,47	1.88	7 (31%)
1	PSU	2A	1917	1	17,21,22	1.60	2 (11%)	20,30,33	3.22	6 (30%)
54	5MU	1y	54	54	15,22,23	1.14	2 (13%)	16,32,35	1.96	2 (12%)
54	4SU	1w	8	54	14,21,22	1.25	1 (7%)	15,30,33	1.56	2 (13%)
54	PSU	2y	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.36	7 (35%)
54	PSU	2w	32	54	17,21,22	1.59	2 (11%)	20,30,33	3.11	6 (30%)
32	PSU	1a	516	32	17,21,22	1.45	3 (17%)	20,30,33	3.18	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.91	1 (5%)	18,38,41	1.73	6 (33%)
55	PSU	2x	55	55	17,21,22	1.54	2 (11%)	20,30,33	3.17	6 (30%)
54	PSU	1y	32	54	17,21,22	1.43	2 (11%)	20,30,33	3.26	6 (30%)
1	PSU	1A	1933	1	17,21,22	1.50	3 (17%)	20,30,33	3.01	5 (25%)
1	4OC	2A	1920	1	15,22,24	0.69	0	17,31,35	1.50	2 (11%)
1	PSU	2A	1911	1	17,21,22	1.50	2 (11%)	20,30,33	3.32	6 (30%)
32	M2G	2a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.18	6 (27%)
54	4SU	2y	8	54	14,21,22	1.37	1 (7%)	15,30,33	1.49	2 (13%)
55	4SU	2x	8	55	14,21,22	1.27	2 (14%)	15,30,33	2.44	2 (13%)
32	4OC	2a	1402	32,56	16,23,24	0.61	0	17,32,35	1.50	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	7MG	2w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.54	7 (25%)
32	UR3	2a	1498	32	14,22,23	0.74	0	15,32,35	0.80	0
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.60	9 (34%)
55	PSU	1x	55	55,56	17,21,22	1.60	3 (17%)	20,30,33	3.17	6 (30%)
55	5MC	2x	32	55	15,22,23	1.22	1 (6%)	19,32,35	1.41	2 (10%)
54	PSU	1w	55	54	17,21,22	1.42	2 (11%)	20,30,33	3.42	6 (30%)
55	4SU	1x	8	55	14,21,22	1.34	2 (14%)	15,30,33	3.01	2 (13%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.74	5 (27%)
1	PSU	1A	1939	1	17,21,22	1.70	4 (23%)	20,30,33	3.15	6 (30%)
54	PSU	2y	32	54	17,21,22	1.43	3 (17%)	20,30,33	3.14	6 (30%)
55	5MU	2x	54	55	15,22,23	1.14	1 (6%)	16,32,35	1.75	2 (12%)
32	5MC	2a	1407	32	15,22,23	1.31	1 (6%)	19,32,35	1.33	2 (10%)
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.18	7 (31%)
43	0TD	2l	92	43	4,9,10	3.64	1 (25%)	3,11,13	2.91	1 (33%)

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
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
1	4OC	1A	1942	1	-	0/7/27/30	0/2/2/2
1	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1964	1,56	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	5/9/29/30	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
54	PSU	2w	55	54,56	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	1/5/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	2/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/5/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
54	4SU	1y	8	54	-	5/5/25/26	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	4SU	2y	8	54	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/5/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	7MG	2w	46	54	-	5/7/37/38	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
43	2l	92	0TD	CB-SB	-7.05	1.67	1.84
43	1l	92	0TD	CB-SB	-7.02	1.67	1.84
54	1w	37	MIA	C2-S10	-6.78	1.70	1.75
54	2w	37	MIA	C2-S10	-6.02	1.70	1.75

The worst 5 of 351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N3-C4-N9	10.36	140.22	126.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	C2-N3-C4	10.10	129.79	115.15
54	2y	55	PSU	N1-C2-N3	-9.57	120.82	128.43
54	2w	39	PSU	N1-C2-N3	-9.35	121.00	128.43
54	1y	46	7MG	N3-C4-N9	9.26	138.80	126.91

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1402	4OC	N3-C4-N4-CM4
32	1a	1402	4OC	C5-C4-N4-CM4
54	2y	37	MIA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2853 ligands modelled in this entry, 2851 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	$\# Z > 2$
59	SF4	2d	501	35	0,12,12	0.00	-	-		
59	SF4	1d	501	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
59	SF4	2d	501	35	-	-	0/6/5/5
59	SF4	1d	501	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.