



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 10:03 am BST

PDB ID : 4WRO  
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the second position in the A-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-24  
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

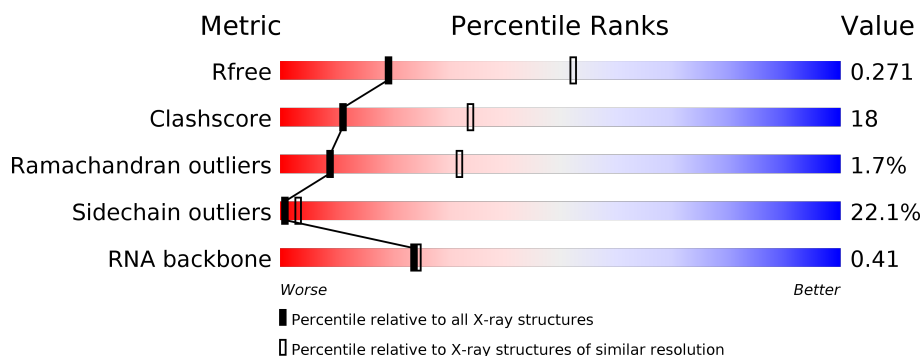
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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.



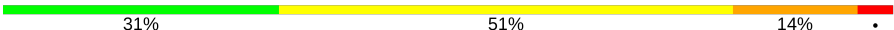


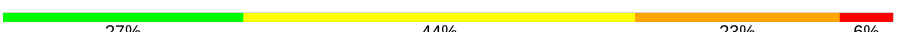
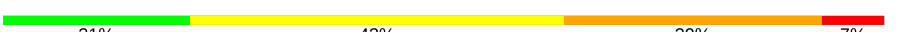
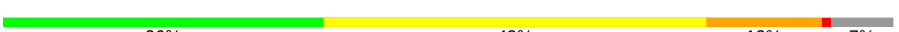
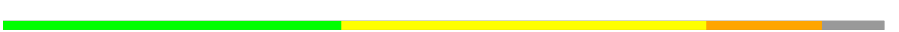







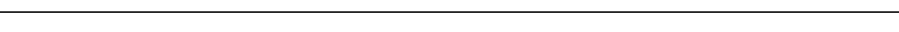

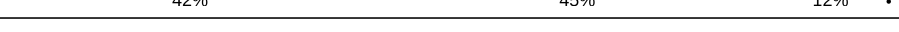

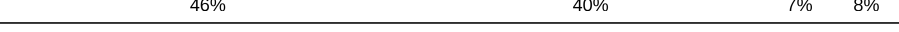





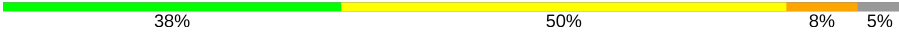
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	1L	76	
2	3K	76	
2	3L	76	
3	2K	77	



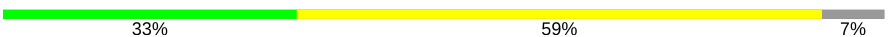

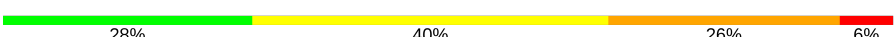
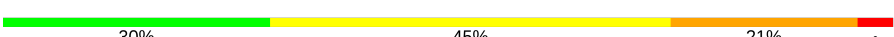


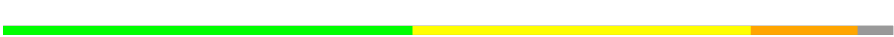

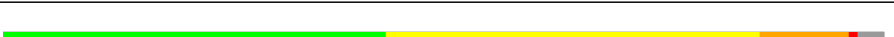


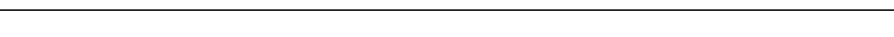











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Mol	Chain	Length	Quality of chain
3	2L	77	
4	4K	30	
4	4L	30	
5	14	2917	
5	1H	2917	
6	12	256	
6	1E	256	
7	22	239	
7	2E	239	
8	32	209	
8	3E	209	
9	4E	162	
10	5E	101	
11	6E	156	
12	7E	138	
13	8E	128	
14	1I	105	
15	2I	129	
16	3I	132	
17	4I	126	
18	5I	61	
19	6I	89	
20	7I	88	
21	8I	105	
22	9I	88	

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Mol	Chain	Length	Quality of chain
23	AI	93	
24	BI	106	
25	1F	27	
26	1K	76	
27	16	122	
27	1J	122	
28	11	276	
29	21	206	
30	31	210	
31	41	182	
32	51	180	
33	61	148	
34	58	140	
35	68	122	
36	78	150	
37	88	141	
38	98	118	
39	A8	112	
40	B8	146	
41	C8	118	
42	D8	101	
43	E8	113	
44	F8	96	
45	G8	110	
46	H8	206	

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Mol	Chain	Length	Quality of chain
47	I8	85	<div><div></div><div>46%36%11%6%</div></div>
48	J8	98	<div><div></div><div>52%36%10%</div></div>
49	K8	72	<div><div></div><div>31%44%13%6%7%</div></div>
50	L8	60	<div><div></div><div>47%37%12%5%</div></div>
51	M8	71	<div><div></div><div>32%46%13%7%</div></div>
52	N8	60	<div><div></div><div>50%33%12%</div></div>
53	O8	54	<div><div></div><div>19%37%26%17%</div></div>
54	P8	49	<div><div></div><div>53%35%8%</div></div>
55	Q8	65	<div><div></div><div>12%32%35%12%8%</div></div>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 260090 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

- Molecule 2 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	1L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

- Molecule 3 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			
3	2K	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

- Molecule 4 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4L	9	Total	C	N	O	P	0	0	0
			191	86	35	61	9			
4	4K	13	Total	C	N	O	P	0	0	0
			279	126	55	85	13			

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			
5	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
6	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
7	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
8	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2I	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 16 is a protein called 30S ribosomal protein S12.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3I	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4I	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AI	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- Molecule 25 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 26 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	1K	74	Total	C	N	O	P	S	0	0	0
			1587	712	286	514	73	2			

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1086	693	208	179	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	S	0	0	0
			881	556	176	149				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O		0	0	0
			452	288	88	76				

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	P8	1	Total Mg 1 1	0	0
56	13	149	Total Mg 149 149	0	0
56	1J	7	Total Mg 7 7	0	0
56	5I	1	Total Mg 1 1	0	0
56	16	13	Total Mg 13 13	0	0
56	21	2	Total Mg 2 2	0	0
56	2K	8	Total Mg 8 8	0	0
56	L8	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	I8	1	Total Mg 1 1	0	0
56	5E	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	J8	1	Total Mg 1 1	0	0
56	1L	1	Total Mg 1 1	0	0
56	1G	96	Total Mg 96 96	0	0
56	11	2	Total Mg 2 2	0	0
56	1H	537	Total Mg 537 537	0	0
56	88	2	Total Mg 2 2	0	0
56	14	421	Total Mg 421 421	0	0
56	3E	2	Total Mg 2 2	0	0
56	3L	3	Total Mg 3 3	0	0
56	1K	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	41	2	Total	Mg	0	0
			2	2		
56	2L	4	Total	Mg	0	0
			4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	1	Total	Zn	0	0
			1	1		
57	32	1	Total	Zn	0	0
			1	1		
57	3E	1	Total	Zn	0	0
			1	1		
57	1G	1	Total	Zn	0	0
			1	1		
57	G8	1	Total	Zn	0	0
			1	1		
57	5I	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	230	Total	O	0	0
			230	230		
58	2L	1	Total	O	0	0
			1	1		
58	4L	2	Total	O	0	0
			2	2		
58	14	863	Total	O	0	0
			863	863		
58	3E	1	Total	O	0	0
			1	1		
58	4E	3	Total	O	0	0
			3	3		
58	8E	2	Total	O	0	0
			2	2		
58	1I	1	Total	O	0	0
			1	1		
58	3I	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5I	1	Total 1	O 1	0	0
58	6I	1	Total 1	O 1	0	0
58	7I	1	Total 1	O 1	0	0
58	BI	1	Total 1	O 1	0	0
58	1K	6	Total 6	O 6	0	0
58	2K	8	Total 8	O 8	0	0
58	3K	1	Total 1	O 1	0	0
58	4K	4	Total 4	O 4	0	0
58	1H	1212	Total 1212	O 1212	0	0
58	1J	12	Total 12	O 12	0	0
58	16	21	Total 21	O 21	0	0
58	11	9	Total 9	O 9	0	0
58	21	3	Total 3	O 3	0	0
58	31	8	Total 8	O 8	0	0
58	58	3	Total 3	O 3	0	0
58	78	6	Total 6	O 6	0	0
58	98	1	Total 1	O 1	0	0
58	B8	1	Total 1	O 1	0	0
58	C8	3	Total 3	O 3	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	2	Total 2	O 2	0	0

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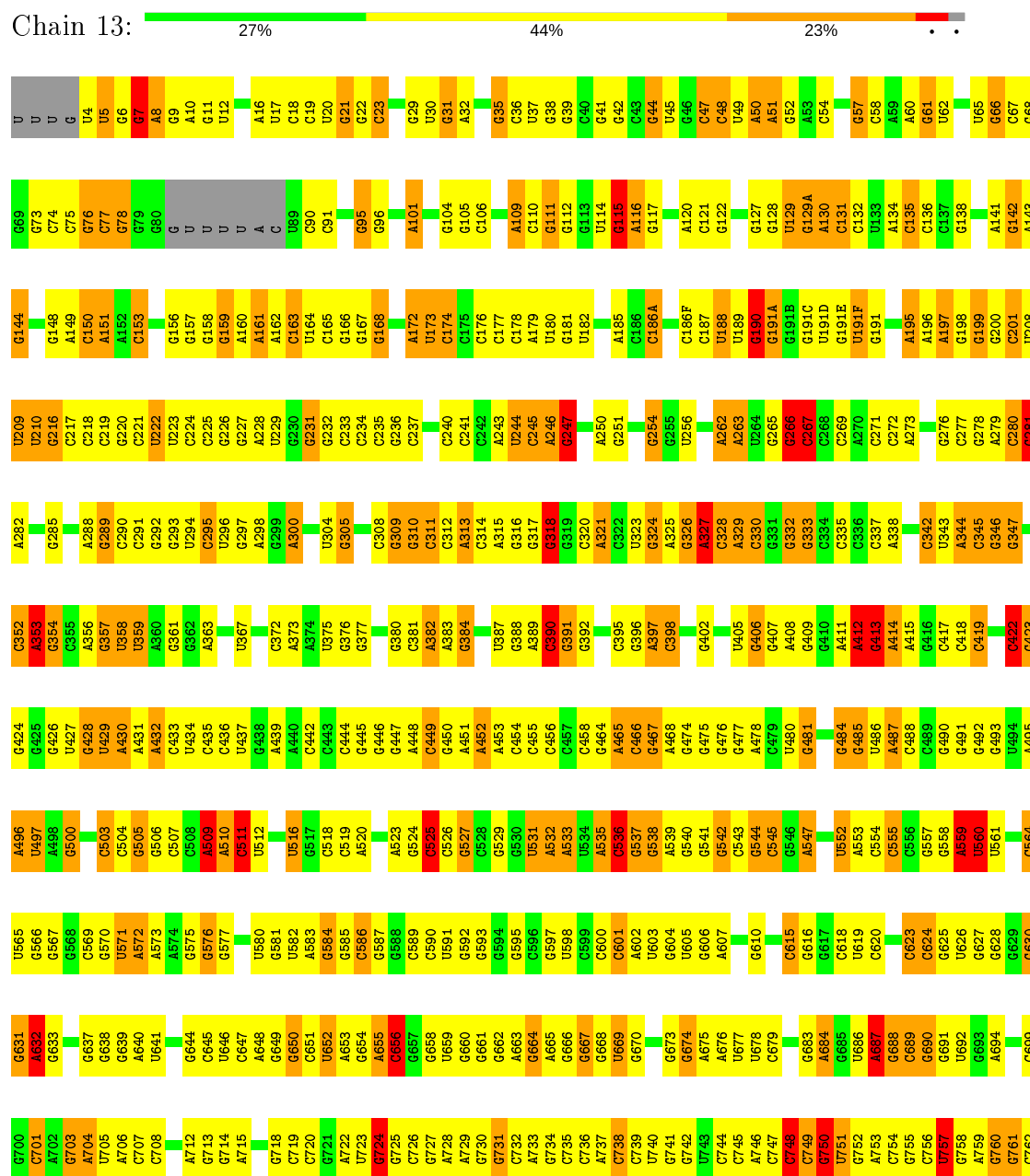
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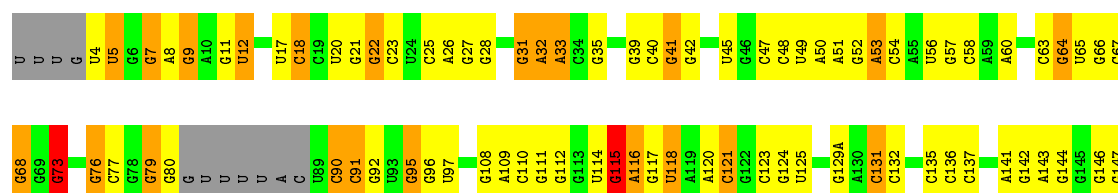
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	F8	2	Total 2	O 2	0	0
58	G8	3	Total 3	O 3	0	0
58	I8	5	Total 5	O 5	0	0
58	J8	1	Total 1	O 1	0	0
58	L8	1	Total 1	O 1	0	0
58	P8	4	Total 4	O 4	0	0
58	Q8	1	Total 1	O 1	0	0
58	1G	106	Total 106	O 106	0	0

### 3 Residue-property plots

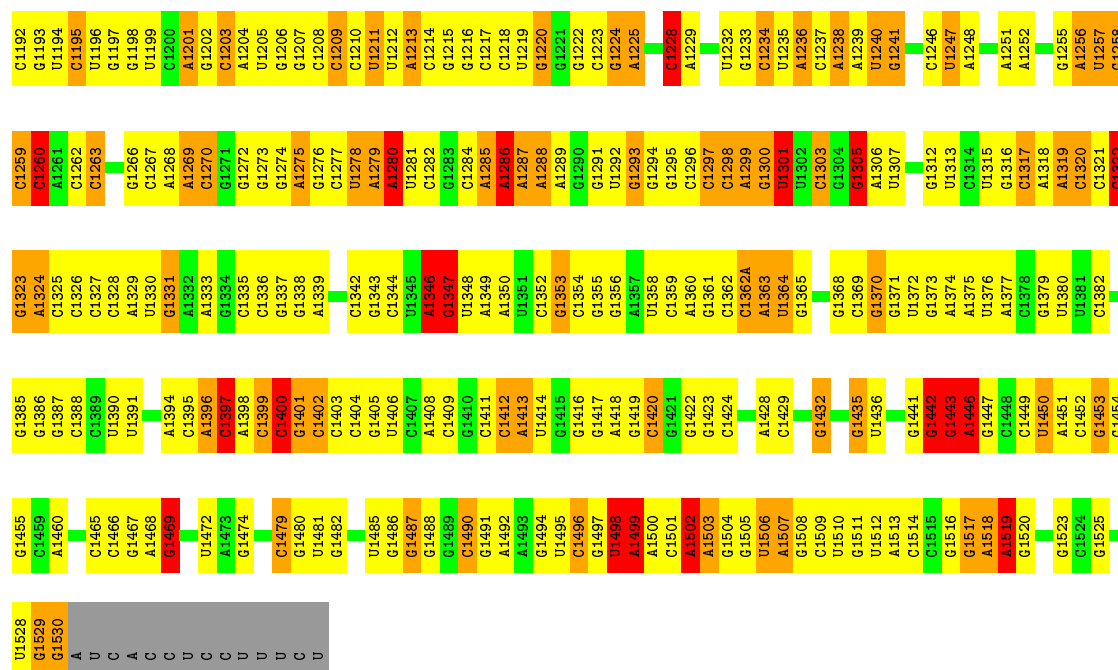
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: 16S ribosomal RNA

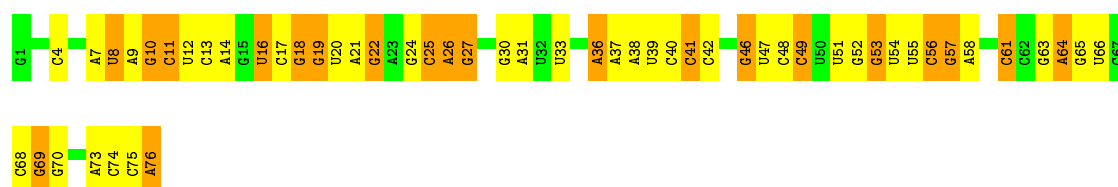




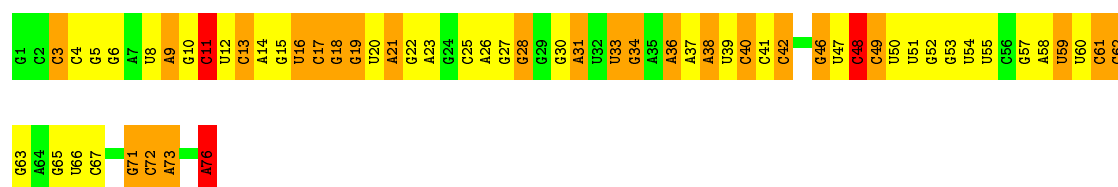
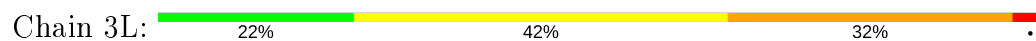
G1127	C995	C934	A865	A790	C720	U641	G576	C513	G438	A363	C290	G216	G148
C1128	G998	A935	C866	G791	G721	A642	G577	G517	A439	C366	C291	C217	A149
C1129	G998	C936	G867	A792	A722	A643	C578	G518	A440	C367	G297	C218	A150
A1130	C998A	A937	C868	A793	U723	C645	C579	C519	C442	U367	G298	U222	A151
C1132	U999	A938	G869	A794	G724	C646	U580	C520	C443	C368	G299	U223	C153
G1133	A1000	G939	A872	G800	G725	C647	G581	G521	C444	C369	G300	C224	C154
G1133	G1001	C940	A873	U801	G726	A648	U582	G522	C445	C370	G301	G227	C155
G1134	G1002	C941	C873	A802	G727	G649	A583	C523	G446	G371	G302	G228	G156
U1135	G1003	G942	C874	G803	A728	G650	G584	A523	G447	A373	A303	G230	G157
U1136	A1004	C943	C875	G804	A729	U652	G585	G524	A448	A374	U304	G231	G158
C1137	A1005	G944	C876	U805	G730	U653	G586	G525	C449	G372	G305	G232	G159
G1138	A1006	G945	C877	C805	G731	A653	G588	C526	G450	U375	G306	G233	A160
G1139	A1007	A846	C880	C806	G732	G654	C589	G527	G451	G376	G307	G234	C163
C1140	G1009	G947	G881	A807	A733	A655	C590	C528	A452	G377	G309	C235	C164
G1141	G1010	C948	C882	C810	G734	G660	U591	G529	A453	A382	G310	C236	G165
G1142	G1011	A949	C883	C811	C735	G661	G592	G530	C456	A383	C312	C237	G166
G1143	G1013	U950	U884	C812	A737	G662	G593	U531	C457	A384	C313	C238	G167
G1144	A1014	G951	G885	G813	A738	A663	C596	A532	C458	C385	A314	C239	G168
C1145	A1015	U952	G886	U813	C739	G664	C597	A533	G464	C386	C315	C240	G169
A1146	A1016	G953	G887	A814	C740	A665	U598	U534	G465	U387	A316	C241	
C1147	G1017	G954	G888	A816	U740	G666	C599	G535	C466	G390	G317	C242	
U1148	U1017	U955	A889	A817	G741	G667	C600	G537	G467	G391	G318	C243	
C1149	U1020	U956	G890	C818	G742	G668	C601	G538	G468	G392	G319	C244	
U1150	G1023	U957	U891	G819	U743	G669	A602	A539	A474	G393	G320	C245	
A1151	G1024	A958	A892	A820	C744	G670	U603	G540	G475	G394	C321	C246	
A1152	U1025	A959	C893	G821	C745	G671	G604	G541	G476	G395	A322	C247	
C1153	G1026	U960	G894	G822	C746	A675	U605	G542	G477	G396	A323	C248	
G1154	U1027	U961	G895	C823	C747	G676	G606	G543	A478	A397	U323	C249	
G1155	C1028	C962	C896	G750	U751	A677	A607	G544	C479	C398	G324	C250	
G1156	G1028A	G963	C997	G825	U752	U677	A608	G545	U480	G401	G325	C251	
A1157	C1028B	A964	G898	C826	C753	U678	A609	G546	U481	G402	G326	C252	
C1158	G1029	A965	C899	U827	G754	C879	G610	G547	A482	G403	A327	C253	
U1159	G1030	G966	G900	A828	G755	C880	G611	G548	G483	U405	G328	C254	
G1160	G1031	C967	A901	G829	C756	C881	A614	G549	G484	G406	G329	C255	
G1161	A1032	A968	G830	G830	U757	G682	G615	C515	G485	G407	G330	C256	
G1162	G1032A	A969	U831	U831	C758	G683	G616	G516	U486	A408	G331	C257	
C1163	G1032B	C970	C904	U832	U759	A684	G617	G517	U487	G409	G332	C258	
G1164	G1033	G971	G906	G836	G760	A687	C618	A553	C489	G410	C333	C259	
A1165	G1034	C972	A909	G837	G761	G688	U619	C555	G490	A411	C334	C260	
C1166	A1035	G973	C910	G838	A766	C889	C820	C556	G491	A412	U340	C261	
A1167	G1036	A974	U911	U841	A767	G690	A621	G557	G492	G413	C341	C262	
G1170	C1037	A975	U912	C842	A768	G691	A622	G558	U493	A414	C342	C263	
G1171	G1038	G976	C912	U843	C769	U692	C623	G559	A494	U421	C343	C264	
C1172	C1039	A977	A913	C848	C770	G693	C624	A560	U495	C422	C344	C265	
G1173	U1040	A978	A914	C849	G771	A694	U625	U561	A496	G423	G345	C266	
G1177	G1041	C979	A915	U850	U772	G695	U626	A562	A497	G424	G346	C267	
G1178	G1042	G980	G916	G851	C773	A696	G627	A563	G500	G425	G347	C268	
A1179	A1043	U981	G917	G852	U774	U697	G630	C564	C501	G426	G350	C269	
A1180	A1044	U982	A918	G853	G775	A702	G631	U565	C502	G427	G351	C270	
G1181	C1045	A983	A919	G854	A777	C708	A632	G567	C503	U429	C352	C271	
G1182	A1046	C984	U920	G855	G778	G709	G633	G568	C504	A430	A353	C272	
A1183	G1047	C985	U921	C856	C779	G710	C634	C569	G505	G507	G354	C273	
G1184	U1048	A986	C924	G858	A780	G711	G635	G570	G506	C433	U359	C274	
G1185	G1049	G987	G925	A859	C783	G712	U636	U571	C507	U434	A360	C275	
G1186	U1050	G988	G926	A860	C784	G713	G637	A572	C508	U435	A361	C276	
G1187	C1051	G989	G927	A861	C785	G714	G638	A573	C509	C436	G362	C277	
A1188	U1052	U991	G928	G862	U788	G715	G639	A574	A510	U437	G363	C278	
C1189	G1053	U992	G929	C863	U789	G716	A640	G575	A511				
G1190	U1054	G993	C932	U863									
A1191	A1055	A994	G933	A864									



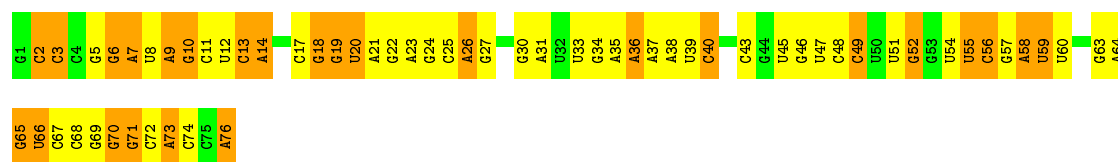
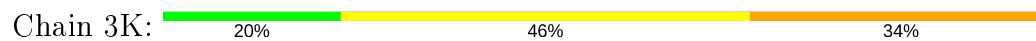
• Molecule 2: tRNA-Phe



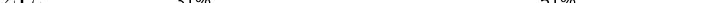
• Molecule 2: tRNA-Phe

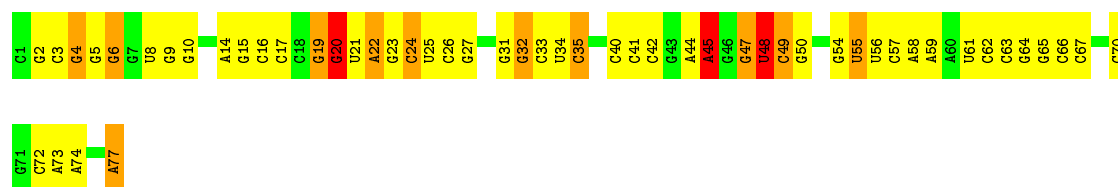


• Molecule 2: tRNA-Phe



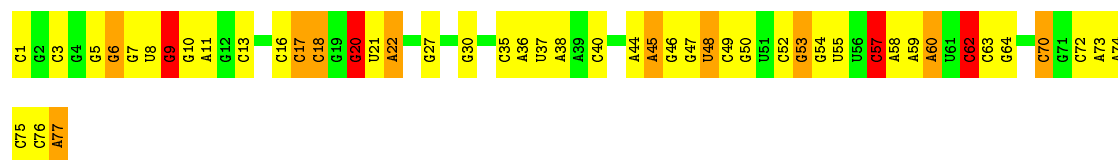
• Molecule 3: tRNA-fMet

Chain 2L:  31% 51% 14% 4%



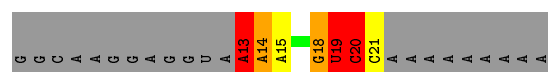
- Molecule 3: tRNA-fMet

Chain 2K: 

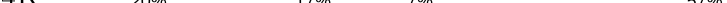


- Molecule 4: RNA (30-MER)

Chain 4L:  7% 7% 7% 10% 70%

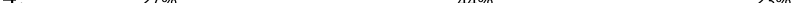


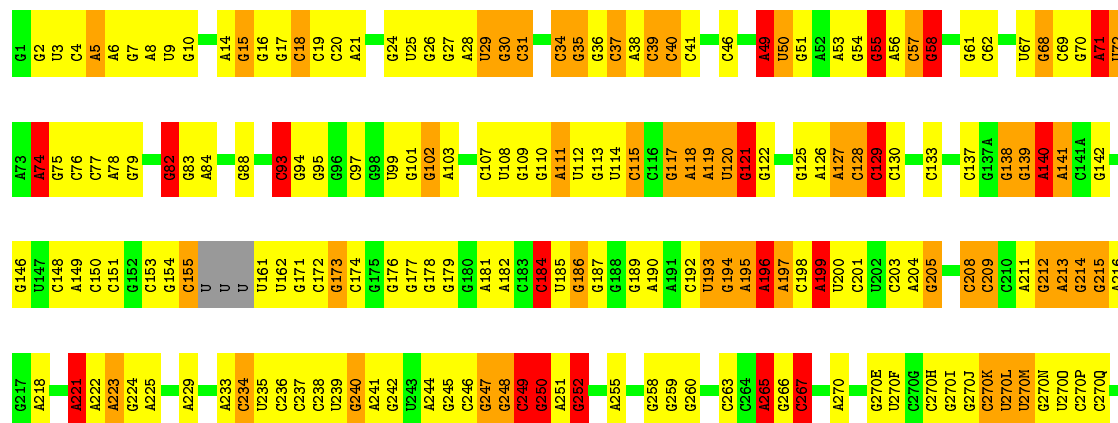
- Molecule 4: RNA (30-MER)

Chain 4K:  20% 17% 7% 57%



- Molecule 5: 23S ribosomal RNA

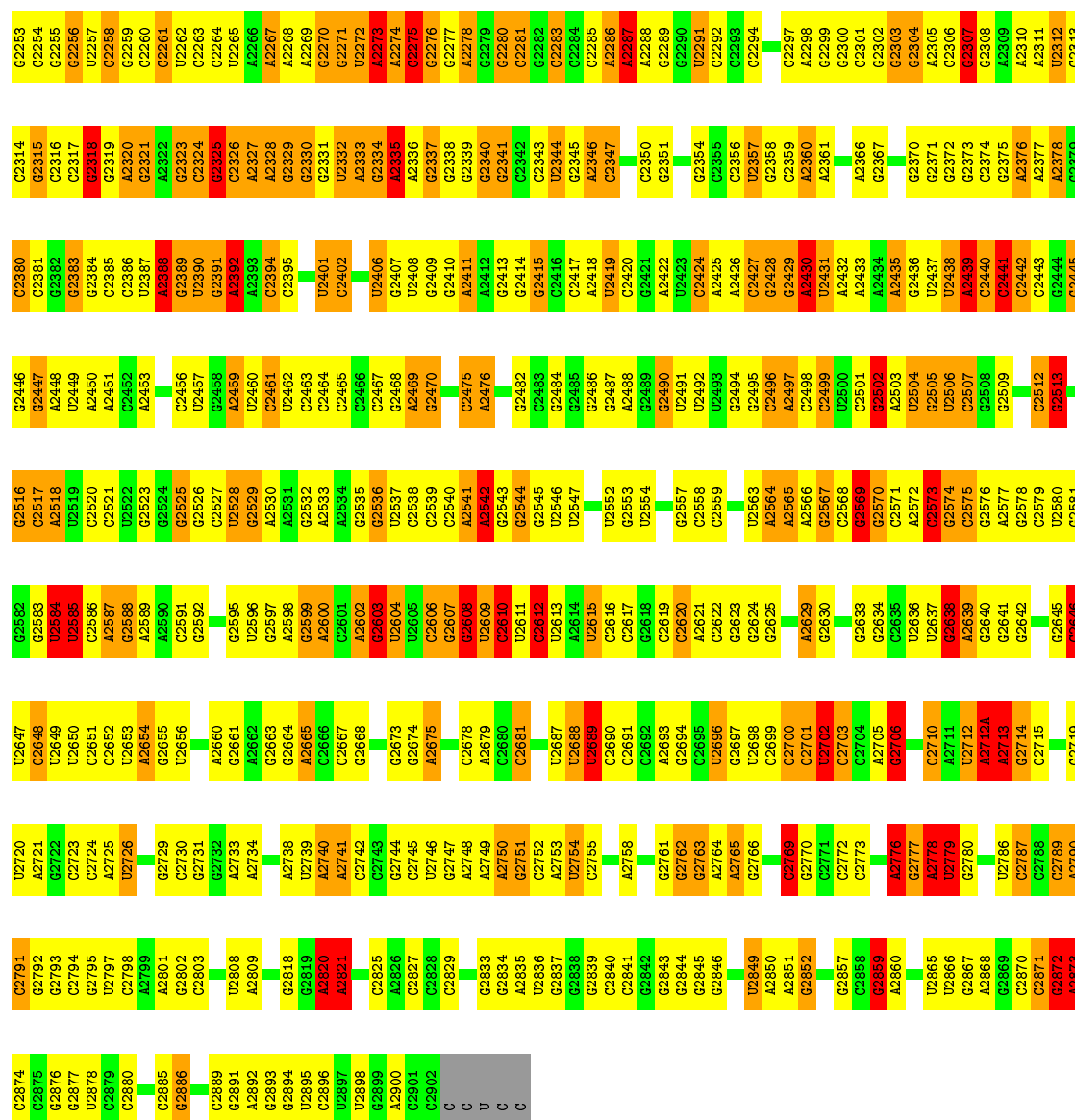
Chain 14:  27% 44% 23% 6%





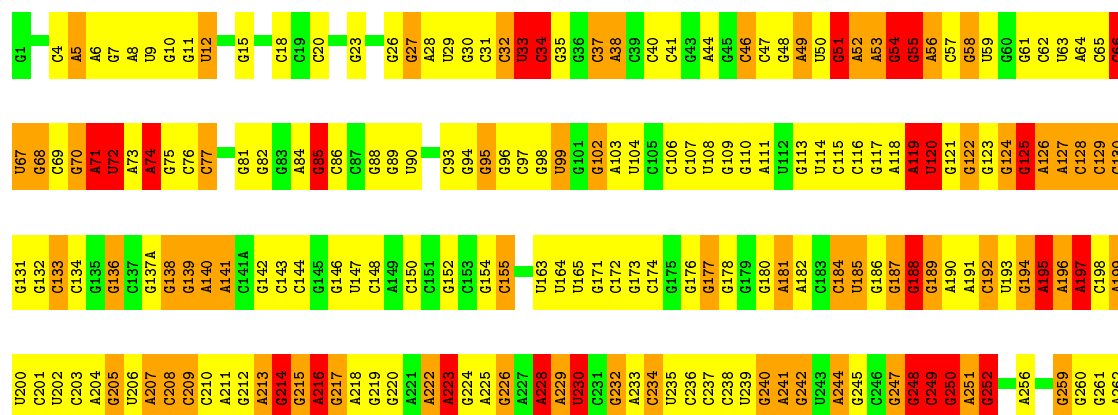


C2174	G1331	G1296	G1355	G1416	G1479	G1555	G1620	U1680	G1770	U1833	U1935	G1979	C2043	G2112	C2174
C2175	G1292	G1297	G1356	G1417	G1480	C1556	U1621	G1681	C1771	C1838	A1916	G1980	C2044	U2113	C2175
C2177	G1293	G1298	U1357	G1418	G1483	C1557	G1624	G1682	A1772	G1839	A1917	A1981	C2045	A2114	A2176
G2182	G1294	G1299	G1358	G1419	G1484	G1559	G1625	G1686	A1773	G1840	A1918	G1982	G2046	G2115	C2177
C2183	G1295	U1300	A1360	G1420	G1485	G1560	G1626	G1687	U1774	C1844	G1920	G1983	G2047	G2116	G2182
C2184	G1296	A1301	G1361	G1422	G1486	G1561	G1627	G1688	U1775	C1845	G1921	G1984	C2048	U2117	C2183
G2185	A1297	A1302	C1362	G1423	G1487	A1566	G1628	U1689	U1776	C1846	G1922	A1986	C2049	U2118	G2184
G2186	U1240	A1303	G1363	G1424	G1488	A1567	U1629	G1690	U1777	A1847	C1923	G1987	A2051	A2119	G2185
A1241	G1303	C1304	G1364	G1425	G1489	C1568	G1630	A1691	U1778	A1848	U1925	G1988	C2052	G2120	C2186
G1244	G1305	C1305	A1365	G1426	A1490	A1569	C1630A	G1692	U1779	G1949	C1926	G1989	G2053	U2121	G2187
A1247	G1306	C1306	A1366	A1427	G1491	A1570	G1631	U1693	G1781	G1850	A1927	G1990	C2054	U2122	G2188
A1247	A1307	A1307	A1367	G1428	G1492	A1571	G1632	U1694	C1782	U1851	A1928	G1991	C2055	G2123	C2189
A1247	A1308	A1308	G1368	G1429	C1493	A1572	G1633	C1694	A1783	C1852	G1929	G1992	A2057	G2124	U2189
G1249	G1309	G1309	G1369	G1430	A1494	C1573	A1634	G1695	A1784	A1853	G1930	U1993	G2058	G2125	G2190
U1249	G1310	G1310	C1370	A1431	A1495	C1574	G1635	G1696	U1785	C1853	G1931	G1994	A2059	A2126	G2191
G1250	G1311	G1311	G1371	G1432	A1496	C1575	G1636	G1697	A1786	G1854	G1932	G1995	G2060	G2127	G2192
G1251	U1312	U1312	U1372	U1433	A1497	C1576	G1637	G1698	A1787	G1855	G1933	G1996	A2061	C2128	G2193
G1252	U1313	U1313	A1373	A1434	C1498	C1577	G1638	G1699	C1788	G1856	G1934	G1997	A2062	C2129	A2198
A1253	G1314	G1314	G1374	G1435	C1504	U1578	G1639	U1701	U1789	G1857	G1935	G1998	C2063	U2130	A2199
G1257	G1315	G1315	G1375	G1436	C1505	A1580	U1640	A1702	A1789	G1858	A1936	G2000	C2064	G2131	A2199
G1258	A1316	A1316	C1376	U1438	C1506	G1581	G1641	G1703	C1790	G1859	A1937	A2001	C2065	U2132	C2206
G1259	G1317	G1317	G1377	U1439	A1507	C1582	G1642	G1704	C1791	G1860	U1938	G2002	C2066	A2134	C2207
G1260	G1318	G1318	A1378	G1440	A1508	C1583	G1643	U1709	U1794	U1864	U1940	A2005	G2067	A2135	G2210
G1261	G1319	G1319	A1379	G1441	C1509	C1585	G1644	C1710	C1795	U1864	C1941	C2006	U2068	G2136	G2211
G1262	C1320	C1320	G1380	G1442	A1510	C1586	G1645	G1716	U1796	A1871	C1942	C2007	C2069	C2137	A2212
G1263	A1321	A1321	G1381	G1443	C1511	A1587	G1646	U1717	U1797	A1872	G1943	G2008	A2070	G2140	G2213
G1264	G1322	G1322	G1382	G1444	G1512	C1588	G1647	G1718	U1798	A1873	U1944	G2009	A2071	G2141	G2214
G1265	G1323	G1323	C1383	G1445	C1513	C1589	G1648	G1719	G1799	G1878	U1945	G2010	A2072	G2142	G2215
G1266	G1324	G1324	A1384	U1446A	G1514	C1590	G1649	G1720	C1800	C1882	U1946	G2011	C2073	G2143	G2216
G1267	G1325	G1325	G1385	G1446	U1515	U1591	G1650	G1721	G1801	G1883	G1947	G2012	U2074	G2144	G2217
G1268	U1326	U1326	C1386	G1446	C1516	C1592	G1651	G1722	A1802	A1884	G1948	A2013	U2075	U2145	G2218
G1269	C1327	C1327	C1387	G1447	U1517	C1593	A1652	U1723	A1803	A1885	G1949	A2014	U2076	C2146	G2219
G1270	G1328	G1328	G1388	G1448	C1518	G1594	G1653	G1724	C1804	C1886	G1950	U2015	A2077	G2147	A2225
G1271	A1329	A1329	G1389	G1449	G1519	C1595	A1654	A1729	U1805	C1887	U1951	U2016	C2078	G2148	C2226
G1272	C1330	C1330	U1390	G1449A	G1520	A1596	C1655	G1730	G1806	G1888	A1952	G2017	U2079	G2149	A2227
G1273	A1331	A1331	U1391	C1450	G1521	A1597	C1656	G1731	U1807	A1889	G1953	G2018	C2081	U2150	G2228
G1274	G1332	G1332	A1392	C1451	G1522	C1598	C1657	C1734	U1808	A1890	G1954	A2019	C2082	U2151	C2231
G1275	C1333	C1333	U1393	A1463	G1523	C1599	U1659	C1742	A1809	C1894	A1960	U2020	G2087	G2152	U2232
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G1293	A1353	A1353	G1413	G1478	A1554	C1618	U1678	G1769	C1832	C1914	A1978	G2040	C2111	U2172	G2252



• Molecule 5: 23S ribosomal RNA

Chain 1H: 21% 42% 29% 7%



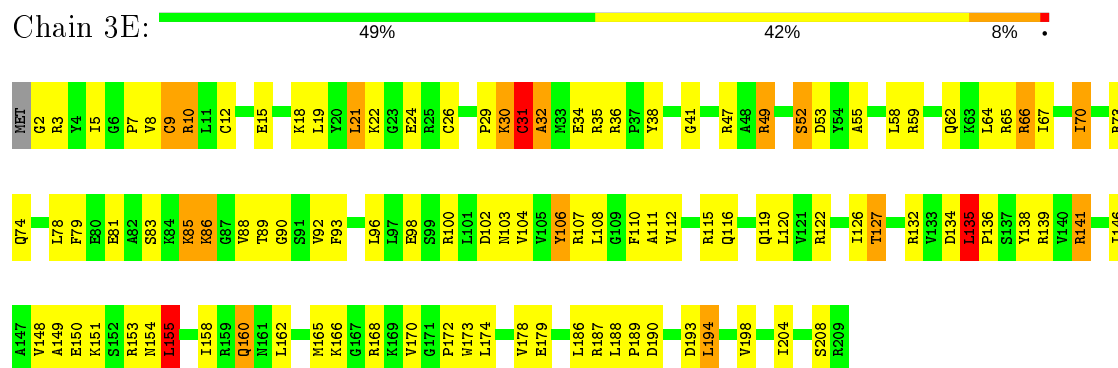
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G1110	G1039	C977	G853	G853	A793	C733	C672	A632	A572	U504		G307	G267	
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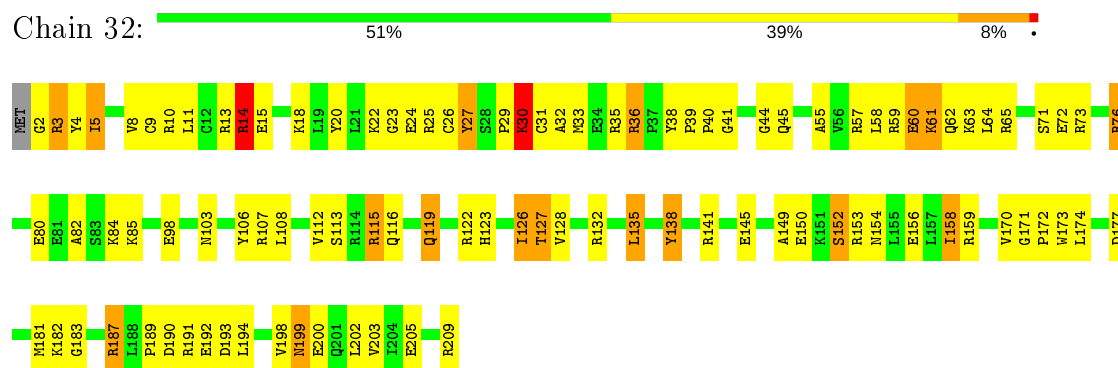




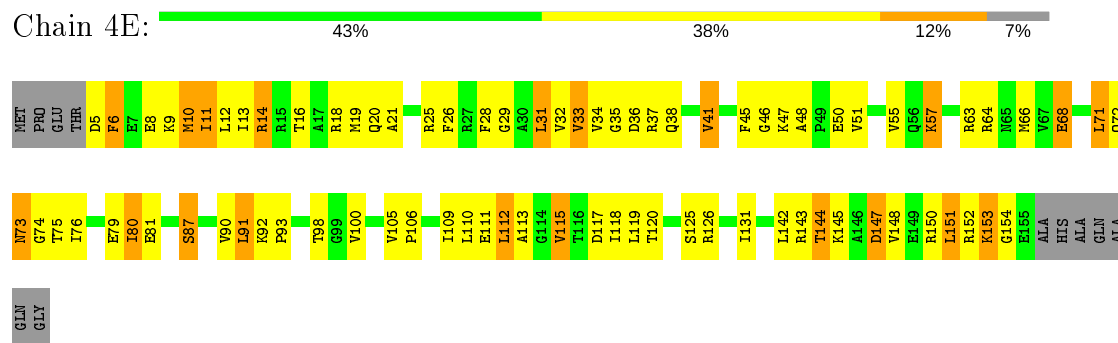
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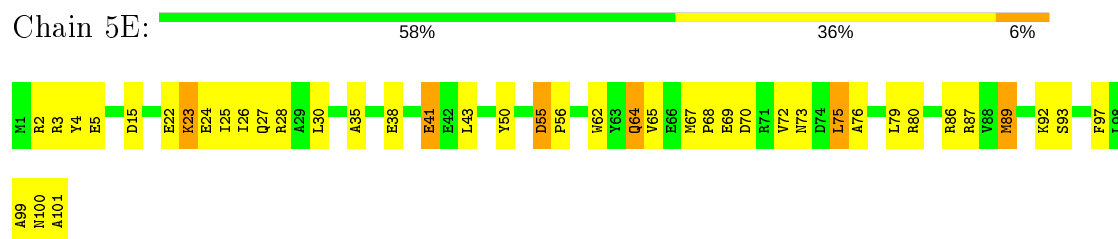
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- Molecule 9: 30S ribosomal protein S5

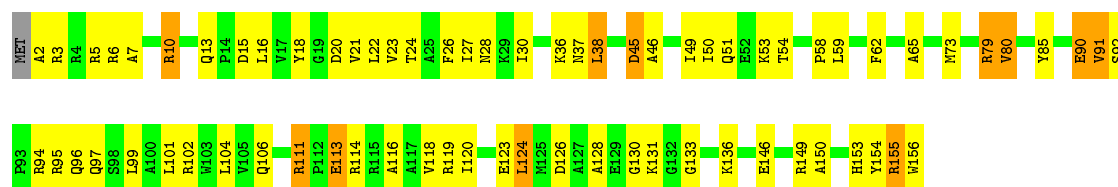


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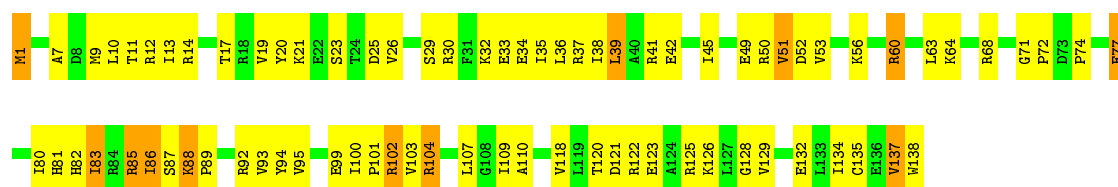
- Molecule 11: 30S ribosomal protein S7

Chain 6E: 



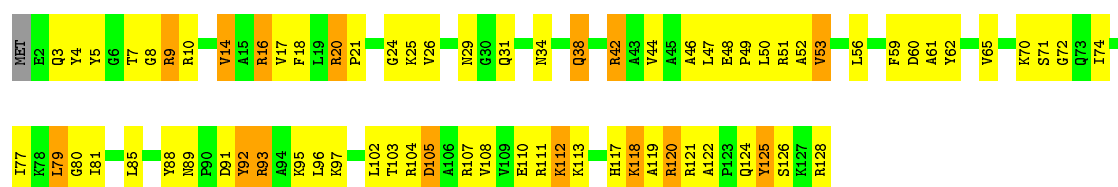
- Molecule 12: 30S ribosomal protein S8

Chain 7E: 



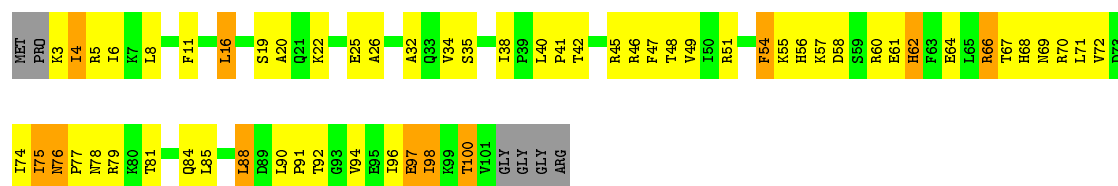
- Molecule 13: 30S ribosomal protein S9

Chain 8E: 



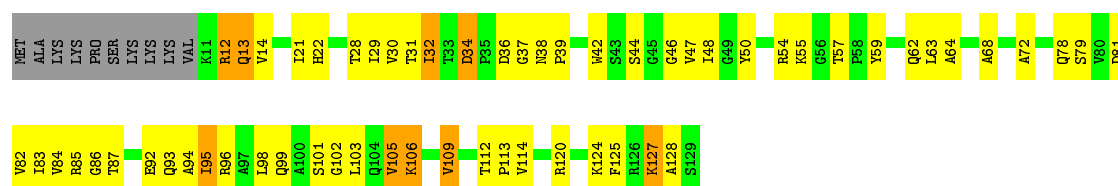
- Molecule 14: 30S ribosomal protein S10

Chain 1I: 



- Molecule 15: 30S ribosomal protein S11

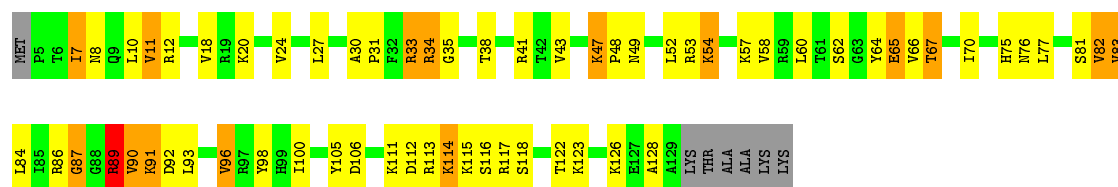
Chain 2I: 



- Molecule 16: 30S ribosomal protein S12

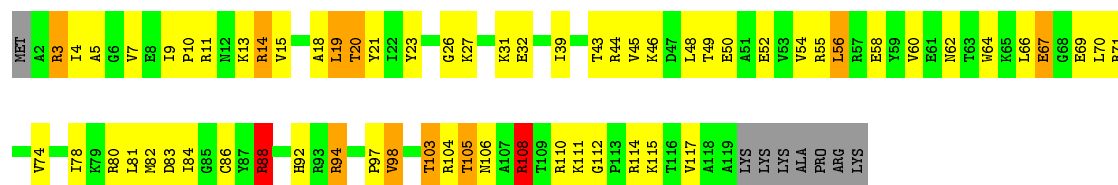


Chain 3I: 



- Molecule 17: 30S ribosomal protein S13

Chain 4I: 



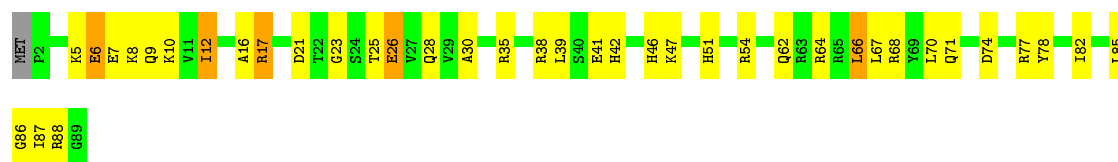
- Molecule 18: 30S ribosomal protein S14 type Z

Chain 5I: 



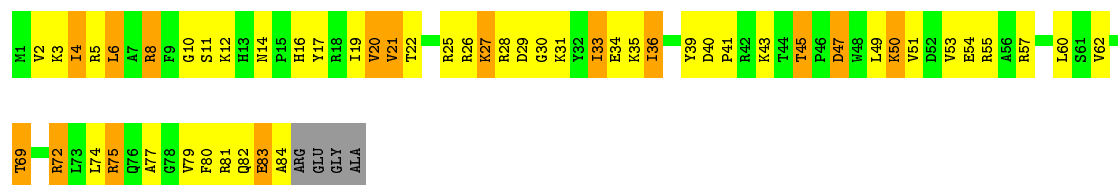
- Molecule 19: 30S ribosomal protein S15

Chain 6I: 



- Molecule 20: 30S ribosomal protein S16

Chain 7I: 



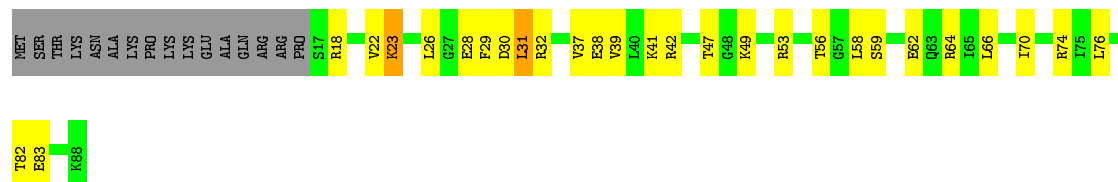
- Molecule 21: 30S ribosomal protein S17

Chain 8I: 



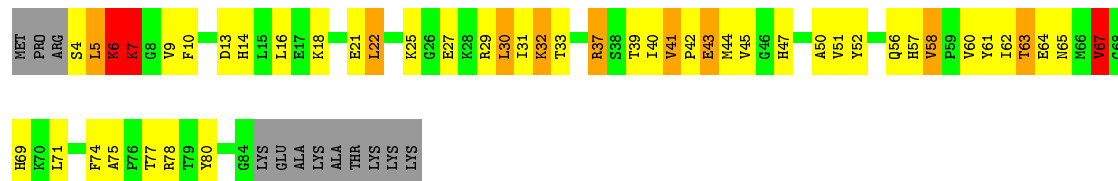
- Molecule 22: 30S ribosomal protein S18

Chain 9I: 50% 30% 18%



- Molecule 23: 30S ribosomal protein S19

Chain AI: 35% 39% 10% 13%



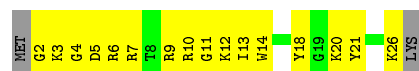
- Molecule 24: 30S ribosomal protein S20

Chain BI: 49% 33% 11% 7%



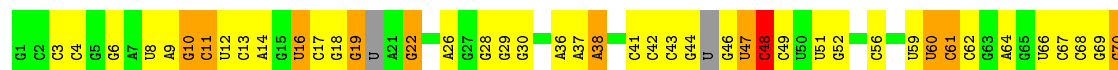
- Molecule 25: 30S ribosomal protein Thx

Chain 1F: 33% 59% 7%



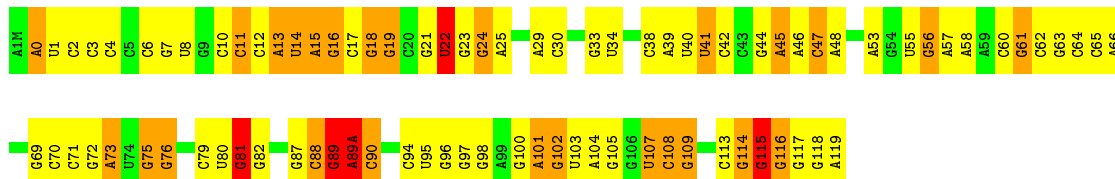
- Molecule 26: tRNA-Phe

Chain 1K: 33% 46% 16% 5%

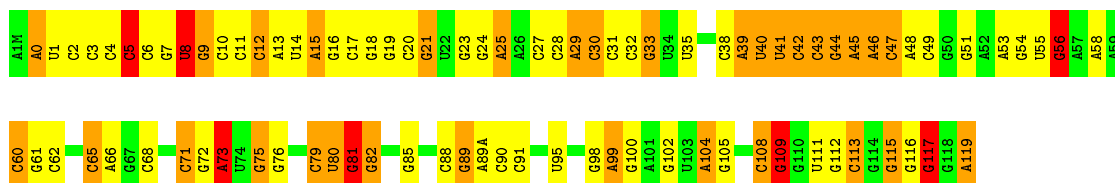




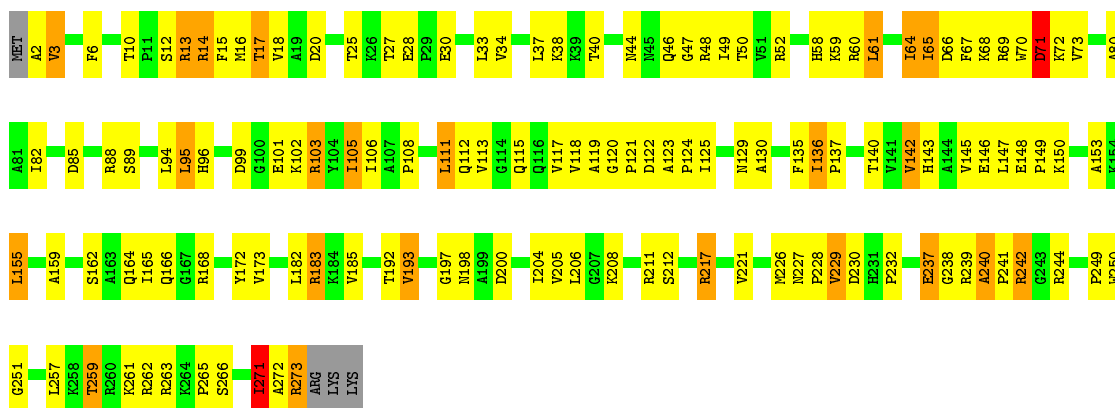
• Molecule 27: 5S ribosomal RNA



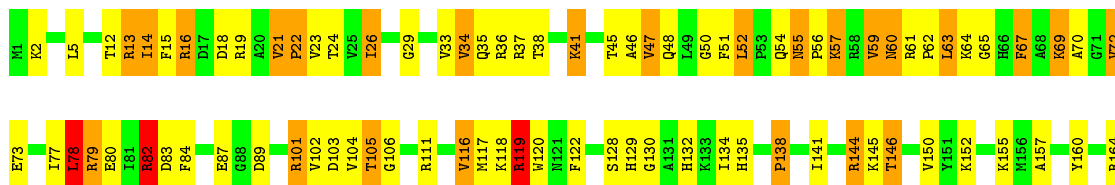
• Molecule 27: 5S ribosomal RNA



• Molecule 28: 50S ribosomal protein L2



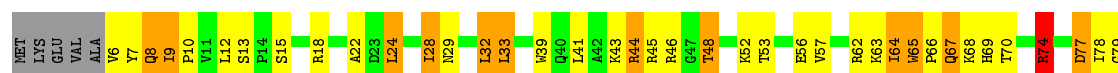
• Molecule 29: 50S ribosomal protein L3





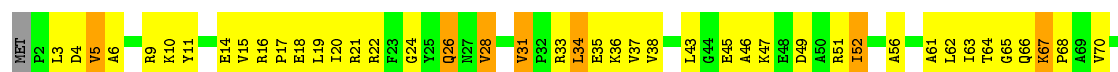
- Molecule 30: 50S ribosomal protein L4

Chain 31: 46% 38% 12%



- Molecule 31: 50S ribosomal protein L5

Chain 41: 42% 47% 11%



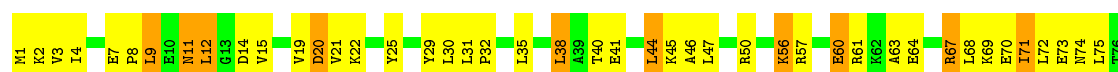
- Molecule 32: 50S ribosomal protein L6

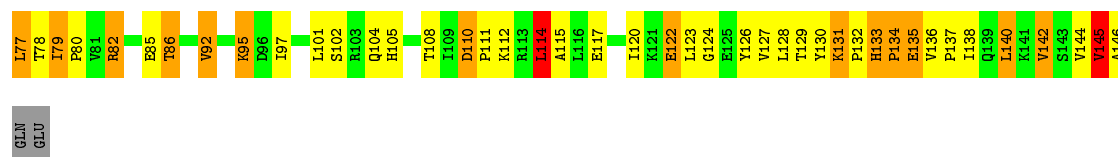
Chain 51: 43% 42% 10%



- Molecule 33: 50S ribosomal protein L9

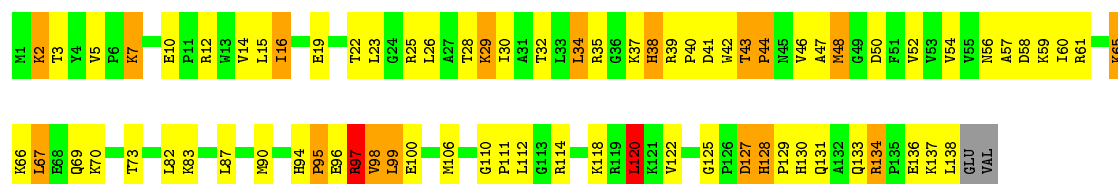
Chain 61: 40% 41% 16%





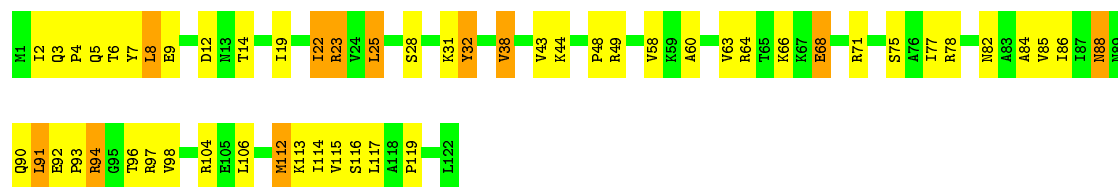
- Molecule 34: 50S ribosomal protein L13

Chain 58: 44% 41% 12% ..



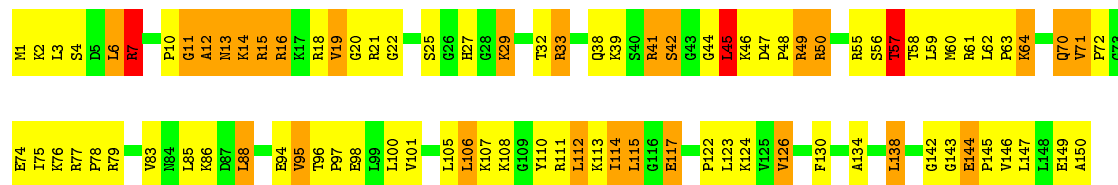
- Molecule 35: 50S ribosomal protein L14

Chain 68: 56% 35% 9%



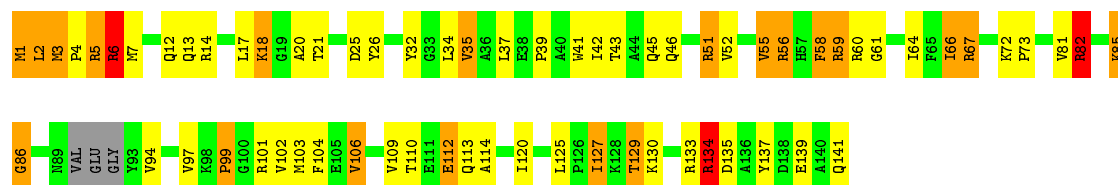
- Molecule 36: 50S ribosomal protein L15

Chain 78: 40% 40% 18% .



- Molecule 37: 50S ribosomal protein L16

Chain 88: 50% 31% 14% ..

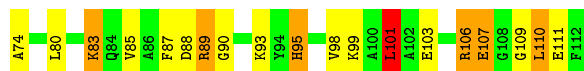


- Molecule 38: 50S ribosomal protein L17

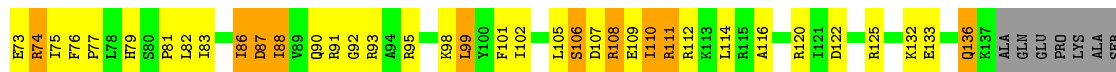
Chain 98: 37% 48% 14% .



- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19

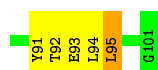
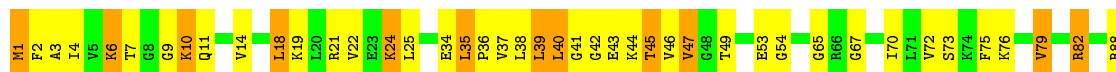


GLN  
GLU

- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21



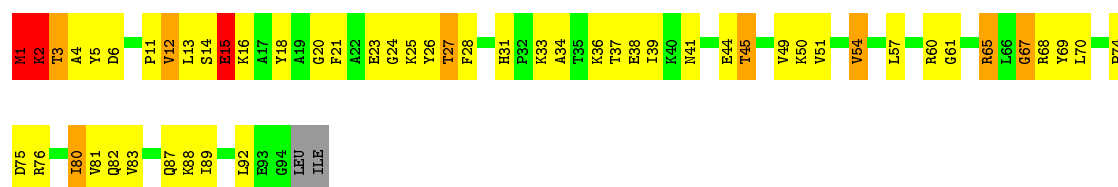
- Molecule 43: 50S ribosomal protein L22

Chain E8: 



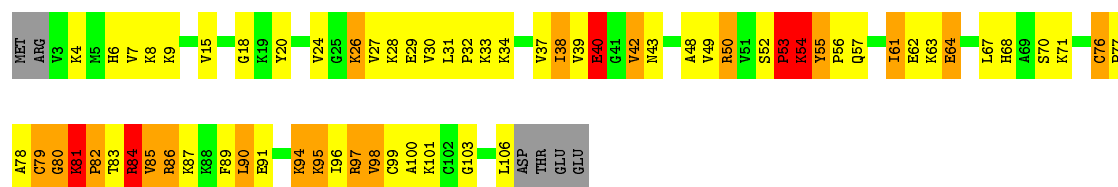
- Molecule 44: 50S ribosomal protein L23

Chain F8: 



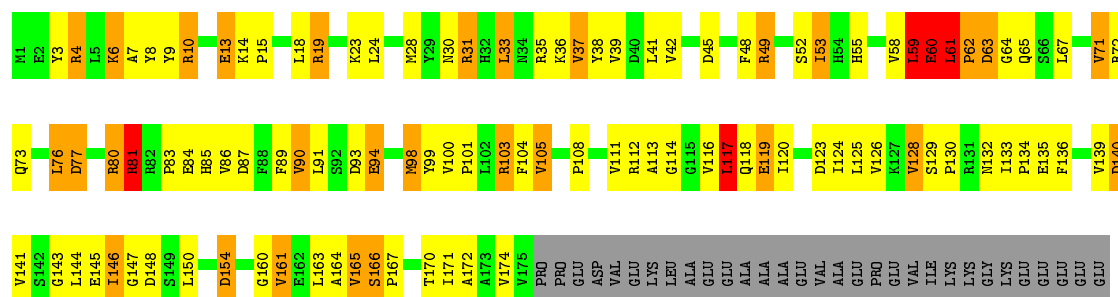
- Molecule 45: 50S ribosomal protein L24

Chain G8: 



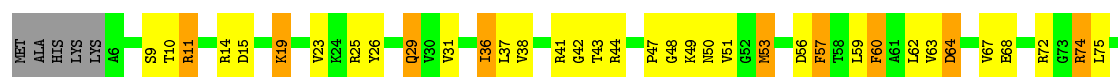
- Molecule 46: 50S ribosomal protein L25

Chain H8: 



- Molecule 47: 50S ribosomal protein L27

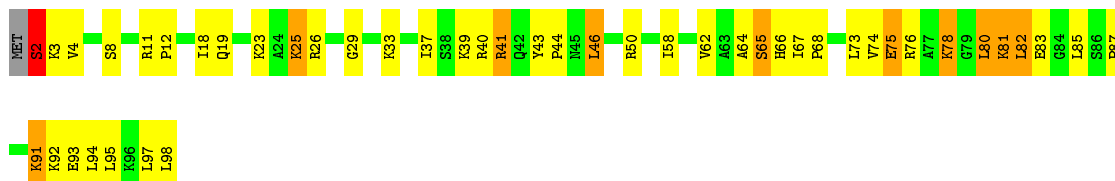
Chain I8: 





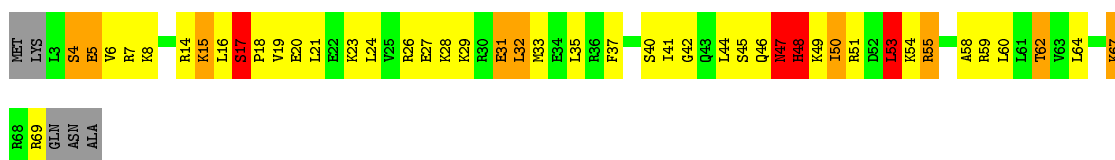
- Molecule 48: 50S ribosomal protein L28

Chain J8: 52% 36% 10% ..



- Molecule 49: 50S ribosomal protein L29

Chain K8: 31% 44% 13% 6% 7%



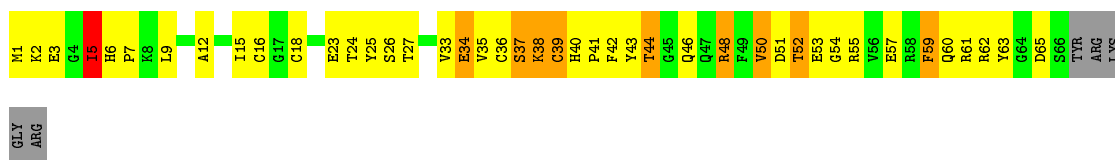
- Molecule 50: 50S ribosomal protein L30

Chain L8: 47% 37% 12% 5%



- Molecule 51: 50S ribosomal protein L31

Chain M8: 32% 46% 13% 7%



- Molecule 52: 50S ribosomal protein L32

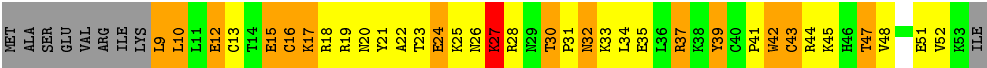
Chain N8: 50% 33% 12% ..



- Molecule 53: 50S ribosomal protein L33

Chain O8: 19% 37% 26% 17%

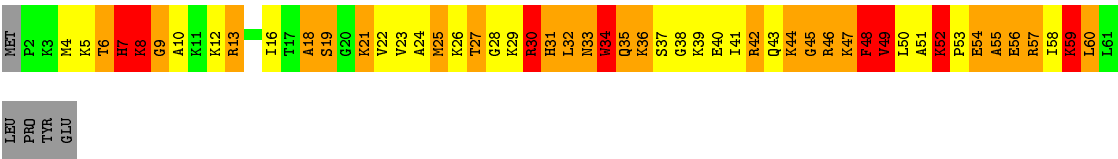
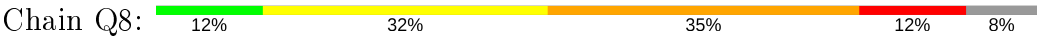




● Molecule 54: 50S ribosomal protein L34



● Molecule 55: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.40 Å   447.70 Å   619.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	151.96 – 3.05 254.70 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.96-3.05) 92.8 (254.70-3.05)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.193   ,   0.231 0.248   ,   0.271	Depositor DCC
$R_{free}$ test set	2000 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.4	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	260090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, ZN, MIA, MG, H2U, 4SU, 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	13	0.87	14/36028 (0.0%)	1.59	679/56231 (1.2%)
1	1G	0.75	2/36025 (0.0%)	1.44	481/56227 (0.9%)
2	1L	0.51	1/1625 (0.1%)	1.02	1/2531 (0.0%)
2	3K	0.57	0/1625	1.17	11/2531 (0.4%)
2	3L	0.63	0/1625	1.20	16/2531 (0.6%)
3	2K	1.02	2/1721 (0.1%)	1.69	42/2682 (1.6%)
3	2L	0.78	1/1721 (0.1%)	1.49	23/2682 (0.9%)
4	4K	1.03	0/313	1.37	4/485 (0.8%)
4	4L	1.26	0/213	1.79	4/329 (1.2%)
5	14	0.99	84/70167 (0.1%)	1.74	2119/109541 (1.9%)
5	1H	1.24	280/70233 (0.4%)	2.01	3566/109643 (3.3%)
6	12	0.40	0/1959	0.68	2/2642 (0.1%)
6	1E	0.48	0/1959	0.74	0/2642
7	22	0.45	0/1636	0.67	1/2205 (0.0%)
7	2E	0.58	0/1629	0.74	0/2195
8	32	0.53	0/1732	0.76	1/2318 (0.0%)
8	3E	0.65	2/1732 (0.1%)	0.80	3/2318 (0.1%)
9	4E	0.62	0/1171	0.81	0/1576
10	5E	0.61	0/855	0.78	0/1154
11	6E	0.56	0/1275	0.70	0/1709
12	7E	0.59	0/1135	0.79	0/1527
13	8E	0.52	0/1028	0.75	1/1379 (0.1%)
14	1I	0.54	0/814	0.75	0/1095
15	2I	0.64	0/899	0.85	1/1213 (0.1%)
16	3I	0.79	0/991	1.03	4/1327 (0.3%)
17	4I	0.59	0/948	0.84	2/1272 (0.2%)
18	5I	0.83	1/500 (0.2%)	0.85	1/664 (0.2%)
19	6I	0.62	0/744	0.84	0/992
20	7I	0.56	0/721	0.77	0/970
21	8I	0.60	0/847	0.77	0/1131
22	9I	0.58	0/595	0.79	0/790
23	AI	0.60	0/661	0.84	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
24	BI	0.47	0/764	0.73	1/1007 (0.1%)
25	1F	0.52	0/221	0.81	0/288
26	1K	0.56	0/1602	1.16	9/2493 (0.4%)
27	16	0.97	2/2928 (0.1%)	1.87	95/4568 (2.1%)
27	1J	0.80	1/2928 (0.0%)	1.48	31/4568 (0.7%)
28	11	0.96	3/2165 (0.1%)	1.09	6/2919 (0.2%)
29	21	0.78	0/1601	0.99	3/2160 (0.1%)
30	31	0.88	1/1620 (0.1%)	1.02	6/2194 (0.3%)
31	41	0.65	0/1498	0.86	1/2016 (0.0%)
32	51	0.68	0/1362	0.92	3/1841 (0.2%)
33	61	0.59	0/1151	0.83	0/1558
34	58	0.69	0/1131	0.88	1/1525 (0.1%)
35	68	0.75	0/942	0.85	1/1269 (0.1%)
36	78	0.82	0/1161	1.14	3/1544 (0.2%)
37	88	0.94	0/1106	1.13	4/1478 (0.3%)
38	98	0.66	0/981	1.00	1/1312 (0.1%)
39	A8	0.74	0/891	1.05	6/1187 (0.5%)
40	B8	0.77	0/1155	0.92	0/1542
41	C8	0.82	0/981	0.93	1/1306 (0.1%)
42	D8	0.69	0/789	0.93	2/1057 (0.2%)
43	E8	0.77	0/910	0.98	2/1220 (0.2%)
44	F8	1.00	2/756 (0.3%)	1.04	4/1014 (0.4%)
45	G8	0.83	0/804	1.11	6/1073 (0.6%)
46	H8	0.54	0/1427	0.84	1/1935 (0.1%)
47	I8	0.86	0/634	1.01	0/847
48	J8	0.84	0/769	1.03	4/1022 (0.4%)
49	K8	0.99	2/565 (0.4%)	1.16	4/748 (0.5%)
50	L8	0.70	0/457	0.99	1/613 (0.2%)
51	M8	0.58	0/545	0.84	0/733
52	N8	0.69	0/467	0.98	1/632 (0.2%)
53	O8	0.81	1/396 (0.3%)	0.97	0/529
54	P8	0.98	0/399	1.12	1/526 (0.2%)
55	Q8	1.30	3/486 (0.6%)	1.71	9/638 (1.4%)
All	All	0.96	402/280719 (0.1%)	1.64	7169/426784 (1.7%)

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
6	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	1E	0	3
8	32	0	2
8	3E	0	1
13	8E	0	1
16	3I	0	1
17	4I	0	1
20	7I	0	1
23	AI	0	2
28	11	0	1
29	21	0	3
30	31	0	2
31	41	0	2
33	61	0	4
36	78	0	3
37	88	0	1
38	98	0	1
39	A8	0	1
40	B8	0	1
41	C8	0	1
45	G8	0	4
46	H8	0	2
47	I8	0	2
48	J8	0	1
49	K8	0	2
51	M8	0	1
52	N8	0	2
53	O8	0	3
55	Q8	0	8
All	All	0	58

The worst 5 of 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1H	2430	A	N9-C4	-15.74	1.28	1.37
5	1H	774	A	N9-C4	-13.11	1.29	1.37
5	1H	1786	A	N9-C4	-13.10	1.29	1.37
18	5I	27	CYS	CB-SG	-12.07	1.61	1.82
5	14	783	A	N9-C4	-11.82	1.30	1.37

The worst 5 of 7169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1H	1899	G	N3-C4-N9	-27.85	109.29	126.00
5	1H	1786	A	C2-N3-C4	-22.12	99.54	110.60
5	1H	917	A	N1-C2-N3	21.20	139.90	129.30
5	1H	1332	G	N3-C4-N9	-21.08	113.35	126.00
5	1H	1899	G	N3-C4-C5	21.00	139.10	128.60

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1E	15	VAL	Peptide
6	1E	169	LYS	Peptide
6	1E	237	ALA	Peptide
8	3E	31	CYS	Peptide
13	8E	110	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32185	0	16244	835	0
1	1G	32182	0	16243	773	1
2	1L	1627	0	842	40	0
2	3K	1627	0	842	51	0
2	3L	1627	0	842	53	0
3	2K	1645	0	845	23	0
3	2L	1645	0	845	38	0
4	4K	279	0	142	6	0
4	4L	191	0	98	8	0
5	14	62647	0	31582	1217	0
5	1H	62707	0	31606	1584	1
6	12	1924	0	1975	116	0
6	1E	1924	0	1975	112	0
7	22	1612	0	1677	87	0
7	2E	1605	0	1668	48	0
8	32	1702	0	1763	87	0
8	3E	1702	0	1763	82	0
9	4E	1155	0	1213	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	5E	842	0	857	29	0
11	6E	1256	0	1296	51	0
12	7E	1115	0	1177	61	0
13	8E	1009	0	1037	60	0
14	1I	801	0	849	56	0
15	2I	884	0	904	39	0
16	3I	975	0	1062	47	0
17	4I	938	0	997	54	0
18	5I	491	0	529	28	0
19	6I	733	0	771	32	0
20	7I	705	0	725	50	0
21	8I	834	0	904	58	0
22	9I	590	0	662	25	0
23	AI	647	0	665	50	0
24	BI	762	0	861	35	0
25	1F	217	0	234	19	0
26	1K	1587	0	822	25	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	81	0
28	11	2115	0	2195	102	0
29	21	1568	0	1634	92	0
30	31	1585	0	1632	93	0
31	41	1473	0	1535	99	0
32	51	1336	0	1418	73	0
33	61	1136	0	1223	66	0
34	58	1104	0	1180	60	0
35	68	932	0	996	42	0
36	78	1144	0	1228	96	0
37	88	1086	0	1129	57	0
38	98	967	0	1033	61	0
39	A8	881	0	943	61	0
40	B8	1141	0	1202	70	0
41	C8	963	0	1022	68	0
42	D8	778	0	852	39	0
43	E8	899	0	964	30	0
44	F8	742	0	803	46	0
45	G8	791	0	881	61	0
46	H8	1397	0	1430	78	0
47	I8	626	0	642	38	0
48	J8	762	0	848	37	0
49	K8	563	0	612	30	0
50	L8	452	0	503	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M8	533	0	526	38	0
52	N8	453	0	475	29	0
53	O8	389	0	404	35	0
54	P8	391	0	432	17	0
55	Q8	480	0	549	106	0
56	11	2	0	0	0	0
56	13	149	0	0	0	0
56	14	421	0	0	0	0
56	16	13	0	0	0	0
56	1G	96	0	0	0	0
56	1H	537	0	0	0	0
56	1J	7	0	0	0	0
56	1K	2	0	0	0	0
56	1L	1	0	0	0	0
56	21	2	0	0	0	0
56	2K	8	0	0	0	0
56	2L	4	0	0	0	0
56	3E	2	0	0	0	0
56	3I	1	0	0	0	0
56	3L	3	0	0	0	0
56	41	2	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	88	2	0	0	0	0
56	I8	1	0	0	0	0
56	J8	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	14	1	0	0	0	0
57	1G	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5I	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	3	0
58	13	230	0	0	36	0
58	14	863	0	0	119	0
58	16	21	0	0	3	0
58	1G	106	0	0	22	0
58	1H	1212	0	0	257	0
58	1I	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1J	12	0	0	4	0
58	1K	6	0	0	0	0
58	2I	3	0	0	2	0
58	2K	8	0	0	1	0
58	2L	1	0	0	0	0
58	3I	8	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3K	1	0	0	0	0
58	4E	3	0	0	0	0
58	4K	4	0	0	0	0
58	4L	2	0	0	0	0
58	58	3	0	0	0	0
58	5I	1	0	0	0	0
58	6I	1	0	0	0	0
58	78	6	0	0	0	0
58	7I	1	0	0	0	0
58	8E	2	0	0	0	0
58	98	1	0	0	1	0
58	B8	1	0	0	0	0
58	BI	1	0	0	0	0
58	C8	3	0	0	2	0
58	D8	1	0	0	0	0
58	E8	2	0	0	0	0
58	F8	2	0	0	0	0
58	G8	3	0	0	0	0
58	I8	5	0	0	1	0
58	J8	1	0	0	0	0
58	L8	1	0	0	1	0
58	P8	4	0	0	0	0
58	Q8	1	0	0	0	0
All	All	260090	0	157464	7103	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 18.

The worst 5 of 7103 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)
5:1H:567:A:OP1	58:1H:3610:HOH:O	1.72	1.07
5:1H:2714:G:OP2	58:1H:3679:HOH:O	1.74	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:987:G:OP2	58:1H:4091:HOH:O	1.74	1.03
36:78:19:VAL:HG12	36:78:21:ARG:H	1.24	1.02
5:1H:945:A:OP1	58:1H:4240:HOH:O	1.80	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.11	0.09

## 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	
6	12	235/256 (92%)	196 (83%)	35 (15%)	4 (2%)	9	32
6	1E	235/256 (92%)	199 (85%)	33 (14%)	3 (1%)	12	38
7	22	204/239 (85%)	185 (91%)	19 (9%)	0	100	100
7	2E	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
8	32	206/209 (99%)	181 (88%)	23 (11%)	2 (1%)	15	45
8	3E	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	15	45
9	4E	149/162 (92%)	138 (93%)	10 (7%)	1 (1%)	22	52
10	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
11	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
12	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	52
13	8E	125/128 (98%)	105 (84%)	20 (16%)	0	100	100
14	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
15	2I	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	17	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3I	123/132 (93%)	103 (84%)	20 (16%)	0	100	100
17	4I	116/126 (92%)	97 (84%)	18 (16%)	1 (1%)	17	47
18	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	17
19	6I	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
20	7I	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
21	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
22	9I	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	4	20
23	AI	79/93 (85%)	66 (84%)	9 (11%)	4 (5%)	2	10
24	BI	97/106 (92%)	80 (82%)	17 (18%)	0	100	100
25	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	270/276 (98%)	252 (93%)	15 (6%)	3 (1%)	14	42
29	21	203/206 (98%)	164 (81%)	29 (14%)	10 (5%)	2	11
30	31	200/210 (95%)	182 (91%)	16 (8%)	2 (1%)	15	45
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	9	32
32	51	172/180 (96%)	143 (83%)	22 (13%)	7 (4%)	3	14
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	7	26
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	4	20
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	78	148/150 (99%)	116 (78%)	27 (18%)	5 (3%)	3	17
37	88	134/141 (95%)	110 (82%)	20 (15%)	4 (3%)	4	19
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	47
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	47
40	B8	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	22	52
41	C8	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5	22
42	D8	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	45
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	25
45	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	1	8
46	H8	173/206 (84%)	141 (82%)	24 (14%)	8 (5%)	2	12
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	12	38
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	K8	65/72 (90%)	57 (88%)	6 (9%)	2 (3%)	4	19
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	8	30
51	M8	64/71 (90%)	40 (62%)	22 (34%)	2 (3%)	4	19
52	N8	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	3	16
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	12
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	Q8	58/65 (89%)	33 (57%)	19 (33%)	6 (10%)	0	2
All	All	6312/6731 (94%)	5477 (87%)	730 (12%)	105 (2%)	9	32

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
32	51	169	VAL
36	78	57	THR
45	G8	54	LYS
49	K8	48	HIS

### 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	
6	12	205/220 (93%)	155 (76%)	50 (24%)	0	2
6	1E	205/220 (93%)	157 (77%)	48 (23%)	1	2
7	22	160/188 (85%)	130 (81%)	30 (19%)	1	5
7	2E	159/188 (85%)	131 (82%)	28 (18%)	2	7
8	32	180/181 (99%)	149 (83%)	31 (17%)	2	7
8	3E	180/181 (99%)	143 (79%)	37 (21%)	1	4
9	4E	116/123 (94%)	87 (75%)	29 (25%)	0	1
10	5E	90/90 (100%)	79 (88%)	11 (12%)	5	17
11	6E	126/127 (99%)	101 (80%)	25 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7E	119/119 (100%)	98 (82%)	21 (18%)	2	7
13	8E	98/99 (99%)	74 (76%)	24 (24%)	0	2
14	1I	89/92 (97%)	71 (80%)	18 (20%)	1	4
15	2I	90/99 (91%)	76 (84%)	14 (16%)	2	10
16	3I	104/109 (95%)	83 (80%)	21 (20%)	1	4
17	4I	94/101 (93%)	70 (74%)	24 (26%)	0	1
18	5I	49/50 (98%)	41 (84%)	8 (16%)	2	9
19	6I	79/80 (99%)	67 (85%)	12 (15%)	3	10
20	7I	72/74 (97%)	54 (75%)	18 (25%)	0	1
21	8I	95/97 (98%)	79 (83%)	16 (17%)	2	8
22	9I	63/77 (82%)	58 (92%)	5 (8%)	12	36
23	AI	70/80 (88%)	50 (71%)	20 (29%)	0	1
24	BI	76/82 (93%)	60 (79%)	16 (21%)	1	4
25	1F	20/22 (91%)	19 (95%)	1 (5%)	24	54
28	1I	214/218 (98%)	169 (79%)	45 (21%)	1	4
29	2I	165/166 (99%)	125 (76%)	40 (24%)	0	2
30	3I	161/166 (97%)	127 (79%)	34 (21%)	1	4
31	4I	155/156 (99%)	125 (81%)	30 (19%)	1	5
32	5I	145/148 (98%)	110 (76%)	35 (24%)	0	2
33	6I	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	58	117/119 (98%)	92 (79%)	25 (21%)	1	3
35	68	100/100 (100%)	85 (85%)	15 (15%)	3	11
36	78	116/116 (100%)	82 (71%)	34 (29%)	0	0
37	88	104/111 (94%)	75 (72%)	29 (28%)	0	1
38	98	101/101 (100%)	72 (71%)	29 (29%)	0	1
39	A8	87/88 (99%)	68 (78%)	19 (22%)	1	3
40	B8	120/127 (94%)	93 (78%)	27 (22%)	1	3
41	C8	93/94 (99%)	76 (82%)	17 (18%)	1	6
42	D8	82/82 (100%)	63 (77%)	19 (23%)	1	2
43	E8	92/92 (100%)	71 (77%)	21 (23%)	1	3
44	F8	76/78 (97%)	61 (80%)	15 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	G8	85/91 (93%)	56 (66%)	29 (34%)	0	0
46	H8	154/179 (86%)	114 (74%)	40 (26%)	0	1
47	I8	61/67 (91%)	47 (77%)	14 (23%)	1	2
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	4
49	K8	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	L8	49/52 (94%)	40 (82%)	9 (18%)	1	6
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	N8	51/52 (98%)	37 (72%)	14 (28%)	0	1
53	O8	44/52 (85%)	31 (70%)	13 (30%)	0	0
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	9
55	Q8	50/55 (91%)	31 (62%)	19 (38%)	0	0
All	All	5324/5588 (95%)	4147 (78%)	1177 (22%)	1	3

5 of 1177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	41	84	LYS
36	78	13	ASN
6	12	76	GLN
32	51	10	PRO
33	61	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
23	AI	56	GLN
29	21	135	HIS
47	I8	29	GLN
15	2I	93	GLN
44	F8	31	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	353 (23%)	38 (2%)
1	1G	1495/1522 (98%)	374 (25%)	37 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1L	74/76 (97%)	32 (43%)	3 (4%)
2	3K	74/76 (97%)	36 (48%)	5 (6%)
2	3L	74/76 (97%)	32 (43%)	1 (1%)
26	1K	70/76 (92%)	32 (45%)	2 (2%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
3	2K	76/77 (98%)	15 (19%)	2 (2%)
3	2L	76/77 (98%)	17 (22%)	3 (3%)
4	4K	12/30 (40%)	2 (16%)	0
4	4L	9/30 (30%)	4 (44%)	2 (22%)
5	14	2908/2917 (99%)	754 (25%)	46 (1%)
5	1H	2911/2917 (99%)	685 (23%)	62 (2%)
All	All	9516/9640 (98%)	2393 (25%)	207 (2%)

5 of 2393 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	9	G

5 of 207 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1K	10	G
5	1H	685	A
1	1G	812	C
3	2K	48	U
5	1H	196	A

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

41 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
2	PSU	3L	55	2	17,21,22	0.97	1 (5%)	20,30,33	3.23	5 (25%)
26	PSU	1K	32	26,56	17,21,22	1.12	2 (11%)	20,30,33	3.25	5 (25%)
2	7MG	3K	46	2	22,26,27	3.45	6 (27%)	28,39,42	2.48	11 (39%)
3	H2U	2K	21	3	18,21,22	2.80	3 (16%)	21,30,33	1.82	4 (19%)
2	H2U	3L	16	2	18,21,22	2.16	4 (22%)	21,30,33	1.97	4 (19%)
26	H2U	1K	16	26	18,21,22	2.52	3 (16%)	21,30,33	1.81	5 (23%)
2	7MG	3L	46	2	22,26,27	3.59	6 (27%)	28,39,42	2.42	10 (35%)
2	H2U	3K	16	2	18,21,22	2.21	4 (22%)	21,30,33	1.99	5 (23%)
2	H2U	3L	20	2	18,21,22	2.23	4 (22%)	21,30,33	1.79	5 (23%)
2	7MG	1L	46	2	22,26,27	3.49	6 (27%)	28,39,42	2.45	11 (39%)
26	MIA	1K	37	26	24,31,32	2.47	3 (12%)	26,44,47	2.67	6 (23%)
2	MIA	3L	37	2	24,31,32	2.84	4 (16%)	26,44,47	3.85	10 (38%)
3	4SU	2L	8	3	14,21,22	3.66	2 (14%)	15,30,33	1.05	2 (13%)
2	MIA	1L	37	2	24,31,32	2.43	4 (16%)	26,44,47	2.55	9 (34%)
3	PSU	2L	56	3	17,21,22	1.29	1 (5%)	20,30,33	3.28	5 (25%)
3	7MG	2K	47	3	22,26,27	3.36	7 (31%)	28,39,42	2.47	10 (35%)
2	4SU	1L	8	2	14,21,22	3.24	2 (14%)	15,30,33	1.55	2 (13%)
3	OMC	2K	33	3	15,22,23	2.33	4 (26%)	17,31,34	1.54	3 (17%)
2	MIA	3K	37	2	24,31,32	2.56	4 (16%)	26,44,47	4.00	10 (38%)
2	H2U	1L	16	2	18,21,22	2.27	4 (22%)	21,30,33	2.06	5 (23%)
2	PSU	3K	55	2	17,21,22	1.14	3 (17%)	20,30,33	3.16	7 (35%)
3	4SU	2K	8	3	14,21,22	3.47	2 (14%)	15,30,33	1.10	2 (13%)
3	H2U	2L	21	3	18,21,22	2.12	3 (16%)	21,30,33	1.63	4 (19%)
2	4SU	3K	8	2	14,21,22	3.43	2 (14%)	15,30,33	1.23	2 (13%)
2	PSU	3K	39	2	17,21,22	1.15	1 (5%)	20,30,33	3.51	7 (35%)
2	PSU	3L	39	2	17,21,22	1.18	1 (5%)	20,30,33	3.35	4 (20%)
26	4SU	1K	8	26	14,21,22	3.23	2 (14%)	15,30,33	1.27	2 (13%)
3	7MG	2L	47	3	22,26,27	3.35	7 (31%)	28,39,42	2.54	11 (39%)
2	H2U	1L	20	2	18,21,22	2.16	3 (16%)	21,30,33	2.20	5 (23%)
3	OMC	2L	33	3	15,22,23	2.19	4 (26%)	17,31,34	1.49	2 (11%)
2	4SU	3L	8	2	14,21,22	3.41	2 (14%)	15,30,33	1.60	2 (13%)
3	PSU	2K	56	3	17,21,22	1.30	2 (11%)	20,30,33	3.18	6 (30%)
2	PSU	1L	39	2	17,21,22	1.12	1 (5%)	20,30,33	3.43	5 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	7MG	1K	46	26	22,26,27	3.46	7 (31%)	28,39,42	2.53	11 (39%)
2	PSU	1L	55	2	17,21,22	1.30	2 (11%)	20,30,33	3.71	5 (25%)
2	PSU	3L	32	2	17,21,22	1.20	1 (5%)	20,30,33	3.55	6 (30%)
2	PSU	3K	32	2	17,21,22	1.14	1 (5%)	20,30,33	3.28	6 (30%)
26	PSU	1K	55	26	17,21,22	1.10	1 (5%)	20,30,33	3.51	6 (30%)
2	PSU	1L	32	2	17,21,22	1.23	2 (11%)	20,30,33	3.93	7 (35%)
26	PSU	1K	39	26	17,21,22	0.97	1 (5%)	20,30,33	3.26	6 (30%)
2	H2U	3K	20	2	18,21,22	2.19	4 (22%)	21,30,33	2.07	5 (23%)

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
2	PSU	3L	55	2	-	0/7/25/26	0/2/2/2
26	PSU	1K	32	26,56	-	0/7/25/26	0/2/2/2
2	7MG	3K	46	2	-	2/7/37/38	0/3/3/3
3	H2U	2K	21	3	-	3/7/38/39	0/2/2/2
2	H2U	3L	16	2	-	3/7/38/39	0/2/2/2
26	H2U	1K	16	26	-	3/7/38/39	0/2/2/2
2	7MG	3L	46	2	-	2/7/37/38	0/3/3/3
2	H2U	3K	16	2	-	0/7/38/39	0/2/2/2
2	H2U	3L	20	2	-	6/7/38/39	0/2/2/2
2	7MG	1L	46	2	-	5/7/37/38	0/3/3/3
26	MIA	1K	37	26	-	7/11/33/34	0/3/3/3
2	MIA	3L	37	2	-	8/11/33/34	0/3/3/3
3	4SU	2L	8	3	-	0/5/25/26	0/2/2/2
2	MIA	1L	37	2	-	6/11/33/34	0/3/3/3
3	PSU	2L	56	3	-	0/7/25/26	0/2/2/2
3	7MG	2K	47	3	-	6/7/37/38	0/3/3/3
2	4SU	1L	8	2	-	4/5/25/26	0/2/2/2
3	OMC	2K	33	3	-	0/7/27/28	0/2/2/2
2	MIA	3K	37	2	-	6/11/33/34	0/3/3/3
2	H2U	1L	16	2	-	5/7/38/39	0/2/2/2
2	PSU	3K	55	2	-	2/7/25/26	0/2/2/2
3	4SU	2K	8	3	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H2U	2L	21	3	-	4/7/38/39	0/2/2/2
2	4SU	3K	8	2	-	1/5/25/26	0/2/2/2
2	PSU	3K	39	2	-	0/7/25/26	0/2/2/2
2	PSU	3L	39	2	-	2/7/25/26	0/2/2/2
26	4SU	1K	8	26	-	0/5/25/26	0/2/2/2
3	7MG	2L	47	3	-	4/7/37/38	0/3/3/3
2	H2U	1L	20	2	-	4/7/38/39	0/2/2/2
3	OMC	2L	33	3	-	1/7/27/28	0/2/2/2
2	4SU	3L	8	2	-	3/5/25/26	0/2/2/2
3	PSU	2K	56	3	-	0/7/25/26	0/2/2/2
2	PSU	1L	39	2	-	0/7/25/26	0/2/2/2
26	7MG	1K	46	26	-	2/7/37/38	0/3/3/3
2	PSU	1L	55	2	-	0/7/25/26	0/2/2/2
2	PSU	3L	32	2	-	0/7/25/26	0/2/2/2
2	PSU	3K	32	2	-	0/7/25/26	0/2/2/2
26	PSU	1K	55	26	-	0/7/25/26	0/2/2/2
2	PSU	1L	32	2	-	2/7/25/26	0/2/2/2
26	PSU	1K	39	26	-	0/7/25/26	0/2/2/2
2	H2U	3K	20	2	-	0/7/38/39	0/2/2/2

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3L	46	7MG	C4-N3	11.24	1.48	1.34
2	1L	46	7MG	C4-N3	11.14	1.48	1.34
26	1K	46	7MG	C4-N3	11.05	1.48	1.34
2	3K	46	7MG	C4-N3	11.02	1.48	1.34
3	2L	8	4SU	C5-C4	10.78	1.50	1.38

The worst 5 of 238 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3K	37	MIA	C11-S10-C2	14.91	113.40	102.27
2	3L	37	MIA	C11-S10-C2	14.37	113.00	102.27
2	1L	32	PSU	N1-C2-N3	-12.60	118.41	128.43
2	1L	55	PSU	N1-C2-N3	-12.21	118.73	128.43
2	3L	32	PSU	N1-C2-N3	-12.08	118.83	128.43

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3K	46	7MG	C3'-C4'-C5'-O5'
2	3L	16	H2U	O4'-C4'-C5'-O5'
2	3L	16	H2U	C3'-C4'-C5'-O5'
26	1K	16	H2U	C4'-C5'-O5'-P
2	3L	20	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3L	55	PSU	1	0
2	3L	16	H2U	1	0
26	1K	16	H2U	1	0
2	3L	46	7MG	2	0
2	3L	20	H2U	4	0
2	1L	46	7MG	2	0
26	1K	37	MIA	1	0
2	3L	37	MIA	2	0
3	2L	8	4SU	2	0
2	1L	37	MIA	1	0
3	2L	56	PSU	2	0
3	2K	47	7MG	5	0
2	1L	8	4SU	4	0
2	3K	37	MIA	4	0
2	1L	16	H2U	1	0
2	3K	55	PSU	3	0
3	2K	8	4SU	1	0
2	3K	39	PSU	1	0
26	1K	8	4SU	1	0
3	2L	47	7MG	2	0
3	2L	33	OMC	3	0
2	3L	8	4SU	2	0
2	1L	39	PSU	3	0
26	1K	46	7MG	1	0
2	1L	55	PSU	1	0
2	3K	20	H2U	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1265 ligands modelled in this entry, 1265 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.