



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 07:33 pm GMT

PDB ID : 6QNR  
Title : 70S ribosome elongation complex (EC) with experimentally assigned potassium ions  
Authors : Rozov, A.; Khusainov, I.; Yusupov, M.; Yusupova, G.  
Deposited on : 2019-02-11  
Resolution : 3.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

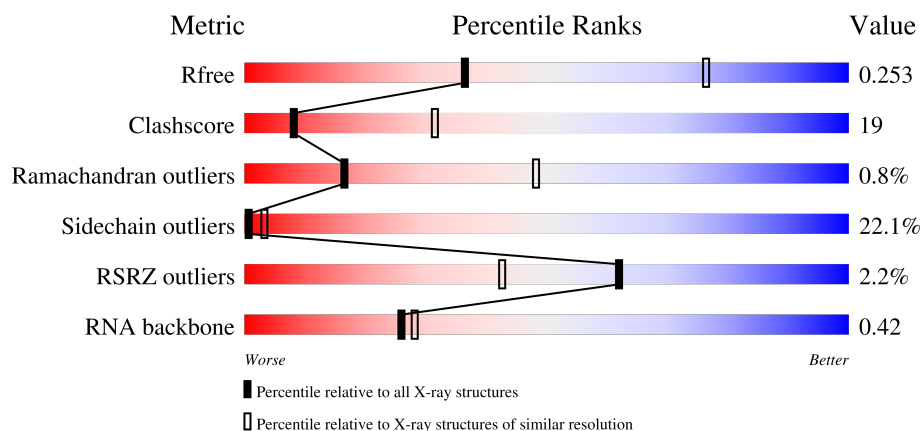
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



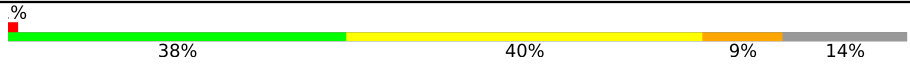


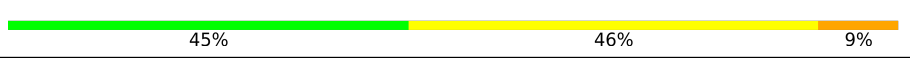
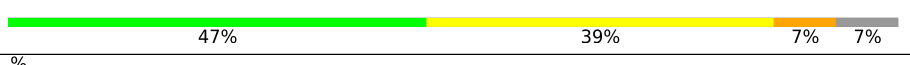
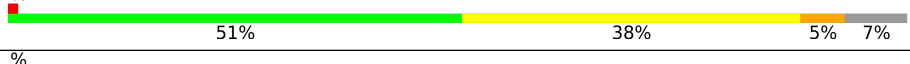
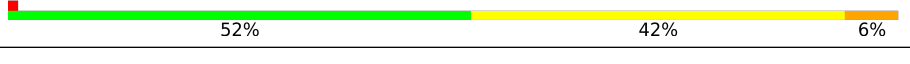
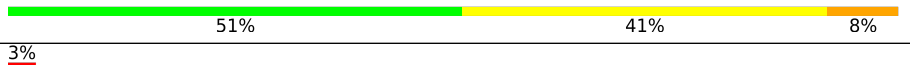
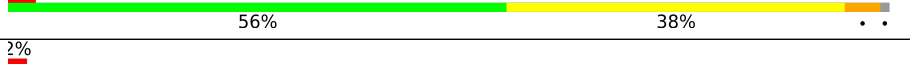


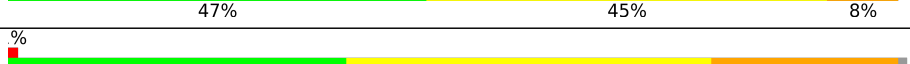
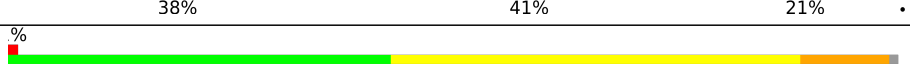
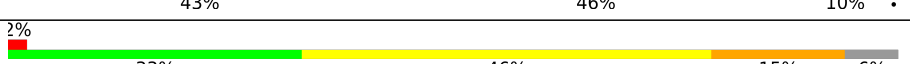
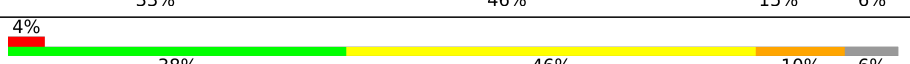



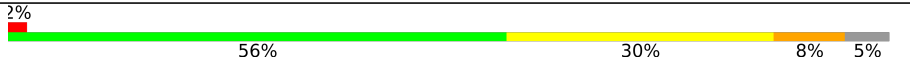

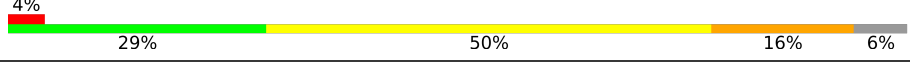
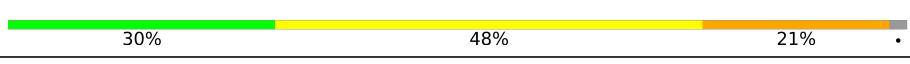



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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 of 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

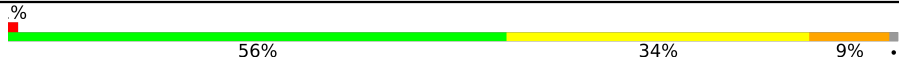
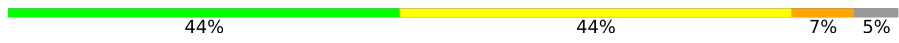



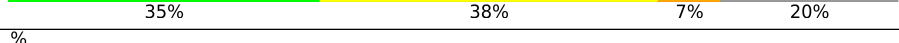
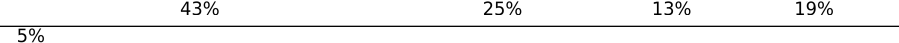
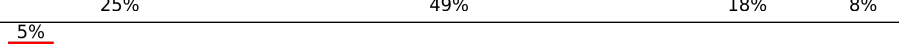
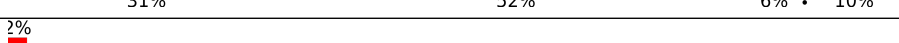
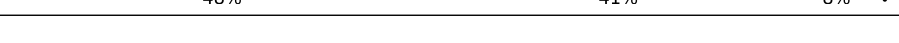
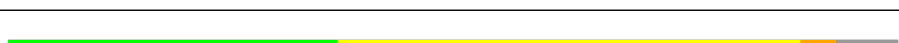
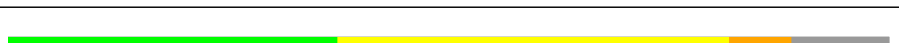
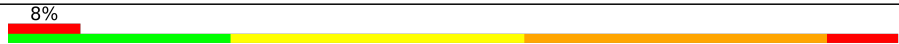


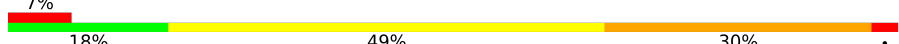


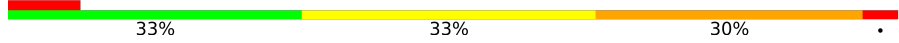
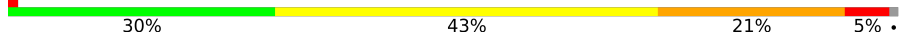


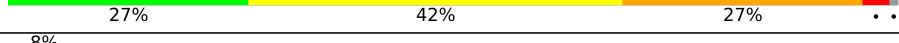


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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	76	
24	3K	76	
24	3L	76	
25	4K	60	
25	4L	60	
26	5K	76	
27	14	2917	
27	1H	2917	
28	16	122	
28	1J	122	
29	7I	229	

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Mol	Chain	Length	Quality of chain
29	79	229	
30	11	276	
30	19	276	
31	21	206	
31	29	206	
32	31	210	
32	39	210	
33	41	182	
33	49	182	
34	51	180	
34	59	180	
35	61	148	
35	69	148	
36	38	173	
37	15	140	
37	58	140	
38	25	122	
38	68	122	
39	35	150	
39	78	150	
40	45	141	
40	88	141	
41	55	118	
41	98	118	
42	65	112	

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Mol	Chain	Length	Quality of chain
42	A8	112	
43	75	146	
43	B8	146	
44	85	118	
44	C8	118	
45	95	101	
45	D8	101	
46	A5	113	
46	E8	113	
47	B5	96	
47	F8	96	
48	C5	110	
48	G8	110	
49	D5	206	
49	H8	206	
50	E5	85	
50	I8	85	
51	F5	98	
51	J8	98	
52	G5	72	
52	K8	72	
53	H5	60	
53	L8	60	
54	I5	71	
54	M8	71	

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Mol	Chain	Length	Quality of chain
55	J5	60	
55	N8	60	
56	K5	54	
56	O8	54	
57	L5	49	
57	P8	49	
58	M5	65	
58	Q8	65	
59	1L	76	
60	2L	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
62	MG	13	1709[A]	-	-	-	X
62	MG	13	1709[B]	-	-	-	X
62	MG	14	3175[A]	-	-	-	X
62	MG	14	3175[B]	-	-	-	X
62	MG	1G	1683[A]	-	-	-	X
62	MG	1G	1683[B]	-	-	-	X
62	MG	1H	3343[A]	-	-	-	X
62	MG	1H	3343[B]	-	-	-	X
63	SF4	3E	302	-	-	X	-

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 305753 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	1516	Total	C	N	O	P	0	0	0
			32589	14514	6024	10535	1516			
1	1G	1513	Total	C	N	O	P	0	0	0
			32526	14487	6018	10509	1512			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1004	636	195	173			
9	82	127	Total	C	N	O	0	0	0
			1004	636	195	173			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	125	Total	C	N	O	S	0	0	0
			977	615	196	164	2			
12	3A	125	Total	C	N	O	S	0	0	0
			977	615	196	164	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			
13	4A	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	71	Total	C	N	O	0	0	0
			584	373	116	95			
18	9A	70	Total	C	N	O	0	0	0
			573	367	112	94			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	AA	86	Total	C	N	O	S	0	0	0
			684	436	126	120	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	101	Total	C	N	O	S	0	0	0
			766	473	161	130	2			
20	BA	103	Total	C	N	O	S	0	0	0
			776	479	163	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	76	Total	C	N	O	P	S	0	0	0
			1628	731	290	530	75	2			

- Molecule 23 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	76	Total	C	N	O	P	S	0	0	0
			1635	735	291	532	75	2			

- Molecule 24 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			
24	3L	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	30	Total	C	N	O	P	0	0	0
			621	279	88	225	29			
25	4L	30	Total	C	N	O	P	0	0	0
			621	279	88	225	29			

- Molecule 26 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	5K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1H	2890	Total	C	N	O	P	0	0	0
			62245	27709	11634	20013	2889			
27	14	2876	Total	C	N	O	P	0	0	0
			61946	27576	11583	19912	2875			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
28	1J	121	Total	C	N	O	P	0	0	0
			2598	1156	481	840	121			

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	71	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			
29	79	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
30	19	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	21	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
31	29	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	39	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
33	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
34	59	173	Total	C	N	O	S	0	0	0
			1327	842	249	235	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
35	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 36 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	38	84	Total	C	N	O	0	0	0
			635	399	118	118			

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
37	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
38	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			
39	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	88	141	Total	C	N	O	S	0	5	0
			1150	732	218	193	7			
40	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
41	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	A8	112	Total	C	N	O	S	0	0	0
			889	561	177	150	1			
42	65	111	Total	C	N	O	S	0	0	0
			881	556	176	149				

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
44	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
45	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
46	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	F8	95	Total	C	N	O	S	0	0	0
			747	485	135	126	1			
47	B5	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	G8	109	Total	C	N	O	S	0	0	0
			825	528	153	139	5			
48	C5	107	Total	C	N	O	S	0	0	0
			776	494	147	130	5			



- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	H8	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			
49	D5	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	I8	84	Total	C	N	O	S	0	0	0
			661	410	140	110	1			
50	E5	84	Total	C	N	O	S	0	0	0
			657	407	139	110	1			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
51	F5	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	K8	72	Total	C	N	O	S	0	0	0
			598	372	120	104	2			
52	G5	71	Total	C	N	O	S	0	0	0
			590	367	119	103	1			

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	L8	59	Total	C	N	O	0	0	0
			468	298	90	80			
53	H5	59	Total	C	N	O	0	0	0
			468	298	90	80			

- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	71	Total	C	N	O	S	0	0	0
			580	364	108	103	5			
54	I5	71	Total	C	N	O	S	0	0	0
			580	364	108	103	5			

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	N8	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			
55	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
56	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 57 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	P8	49	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
57	L5	49	Total	C	N	O	S	0	0	0
			429	263	108	56	2			

- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	Q8	64	Total	C	N	O	S	0	0	0
			506	326	99	79	2			
58	M5	64	Total	C	N	O	S	0	0	0
			506	326	99	79	2			

- Molecule 59 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	1L	76	Total	C	N	O	P	S	0	0
			1627	730	290	531	75	1		

- Molecule 60 is a RNA chain called E. coli tRNAPhe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
60	2L	76	Total	C	N	O	P	S	0	0	0
			1635	735	291	532	75	2			

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	51	Total	K	0	0
			51	51		
61	5E	1	Total	K	0	0
			1	1		
61	4I	1	Total	K	0	0
			1	1		
61	BI	1	Total	K	0	0
			1	1		
61	1K	1	Total	K	0	0
			1	1		
61	2K	3	Total	K	0	0
			3	3		
61	1H	144	Total	K	0	1
			145	145		
61	16	3	Total	K	0	0
			3	3		
61	11	1	Total	K	0	0
			1	1		
61	21	1	Total	K	0	0
			1	1		
61	31	2	Total	K	0	0
			2	2		
61	41	1	Total	K	0	0
			1	1		
61	88	1	Total	K	0	0
			1	1		
61	1G	36	Total	K	0	0
			36	36		
61	32	1	Total	K	0	0
			1	1		
61	52	1	Total	K	0	0
			1	1		
61	2A	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	4A	1	Total 1	K 1	0	0
61	5A	1	Total 1	K 1	0	0
61	BA	1	Total 1	K 1	0	0
61	14	106	Total 106	K 106	0	0
61	1J	1	Total 1	K 1	0	0
61	19	1	Total 1	K 1	0	0
61	29	1	Total 1	K 1	0	0
61	39	2	Total 2	K 2	0	0
61	49	1	Total 1	K 1	0	0
61	45	1	Total 1	K 1	0	0

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	119	Total 120	Mg 120	0	1
62	3E	1	Total 1	Mg 1	0	0
62	6E	1	Total 1	Mg 1	0	0
62	7I	1	Total 1	Mg 1	0	0
62	2K	2	Total 2	Mg 2	0	0
62	1H	433	Total 439	Mg 439	0	6
62	16	12	Total 12	Mg 12	0	0
62	11	1	Total 1	Mg 1	0	0
62	21	2	Total 2	Mg 2	0	0

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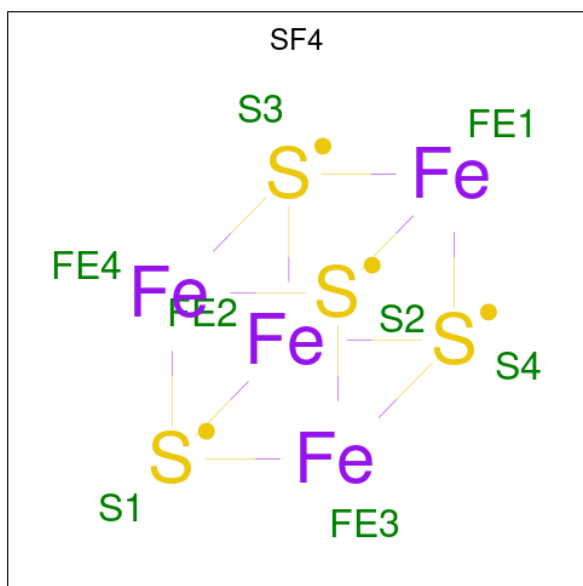
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	31	1	Total 1	Mg 1	0	0
62	41	1	Total 1	Mg 1	0	0
62	78	2	Total 2	Mg 2	0	0
62	C8	1	Total 1	Mg 1	0	0
62	F8	1	Total 1	Mg 1	0	0
62	I8	1	Total 1	Mg 1	0	0
62	J8	1	Total 1	Mg 1	0	0
62	L8	1	Total 1	Mg 1	0	0
62	N8	1	Total 1	Mg 1	0	0
62	O8	1	Total 1	Mg 1	0	0
62	P8	1	Total 1	Mg 1	0	0
62	Q8	1	Total 2	Mg 2	0	1
62	1G	100	Total 102	Mg 102	0	2
62	32	1	Total 1	Mg 1	0	0
62	42	1	Total 1	Mg 1	0	0
62	2L	3	Total 3	Mg 3	0	0
62	4L	1	Total 1	Mg 1	0	0
62	14	294	Total 295	Mg 295	0	1
62	1J	4	Total 4	Mg 4	0	0
62	29	2	Total 2	Mg 2	0	0
62	39	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	M5	2	Total	Mg	0	0
			2	2		

- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	3E	1	Total	Fe	S	0	0
			8	4	4		
63	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	5I	1	Total	Zn	0	0
			1	1		
64	5A	1	Total	Zn	0	0
			1	1		

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	13	233	Total	O	0	0
			233	233		
65	3E	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	4E	1	Total 1	O 1	0	0
65	3I	3	Total 3	O 3	0	0
65	4I	1	Total 1	O 1	0	0
65	5I	1	Total 1	O 1	0	0
65	7I	1	Total 1	O 1	0	0
65	BI	1	Total 1	O 1	0	0
65	1F	3	Total 3	O 3	0	0
65	2K	8	Total 8	O 8	0	0
65	3K	1	Total 1	O 1	0	0
65	4K	2	Total 2	O 2	0	0
65	1H	1009	Total 1009	O 1009	0	0
65	16	26	Total 26	O 26	0	0
65	11	11	Total 11	O 11	0	0
65	21	10	Total 10	O 10	0	0
65	31	10	Total 10	O 10	0	0
65	78	9	Total 9	O 9	0	0
65	88	1	Total 1	O 1	0	0
65	A8	2	Total 2	O 2	0	0
65	B8	2	Total 2	O 2	0	0
65	D8	1	Total 1	O 1	0	0
65	F8	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	I8	2	Total 2	O 2	0	0
65	L8	2	Total 2	O 2	0	0
65	P8	1	Total 1	O 1	0	0
65	Q8	1	Total 1	O 1	0	0
65	1G	194	Total 194	O 194	0	0
65	32	4	Total 4	O 4	0	0
65	82	1	Total 1	O 1	0	0
65	3A	2	Total 2	O 2	0	0
65	5A	1	Total 1	O 1	0	0
65	4L	4	Total 4	O 4	0	0
65	14	602	Total 602	O 602	0	0
65	1J	5	Total 5	O 5	0	0
65	19	12	Total 12	O 12	0	0
65	29	7	Total 7	O 7	0	0
65	39	2	Total 2	O 2	0	0
65	35	7	Total 7	O 7	0	0
65	75	2	Total 2	O 2	0	0
65	C5	1	Total 1	O 1	0	0
65	E5	1	Total 1	O 1	0	0
65	H5	2	Total 2	O 2	0	0
65	L5	1	Total 1	O 1	0	0

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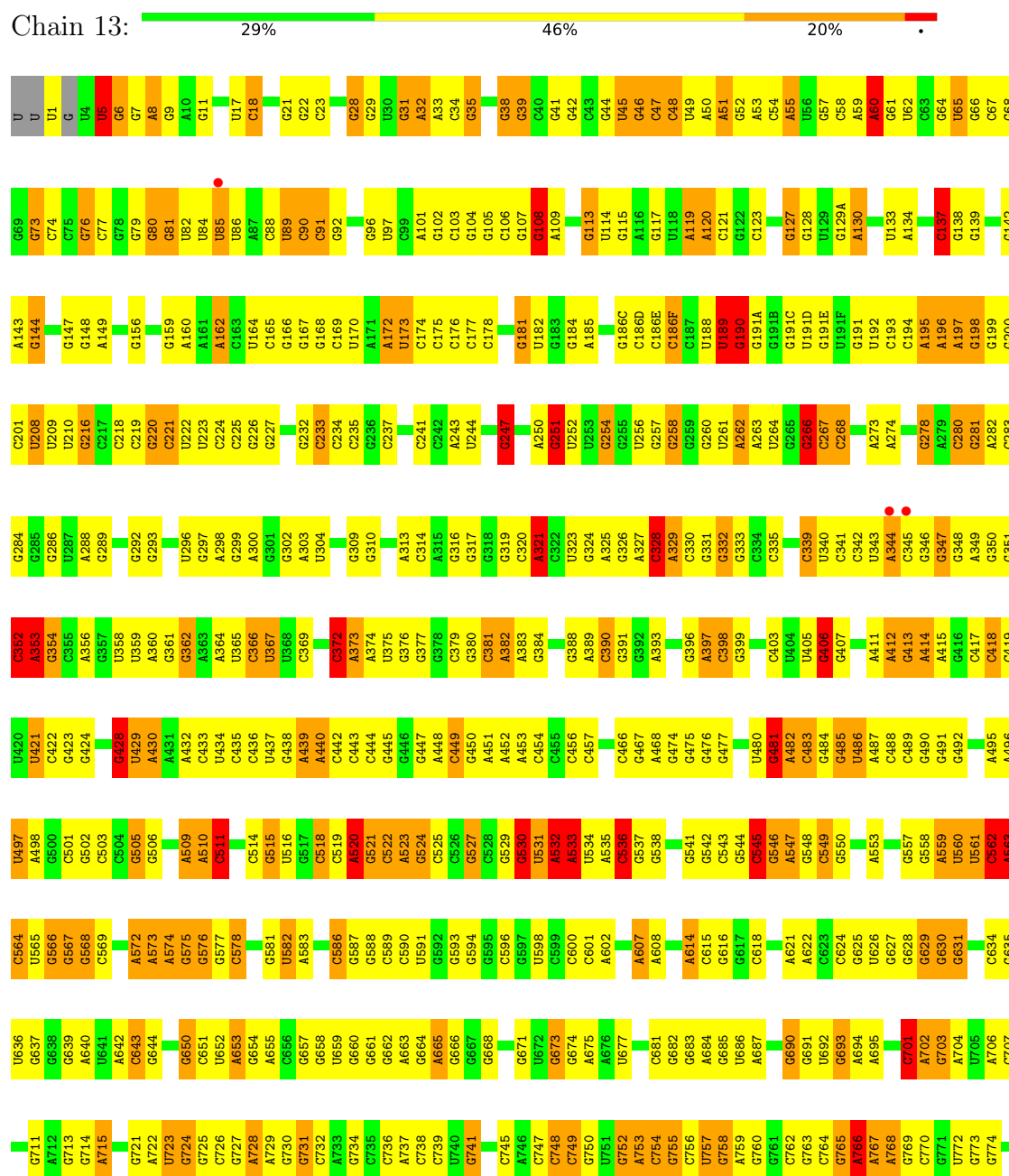
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	M5	6	Total	O	0	0
			6	6		

### 3 Residue-property plots

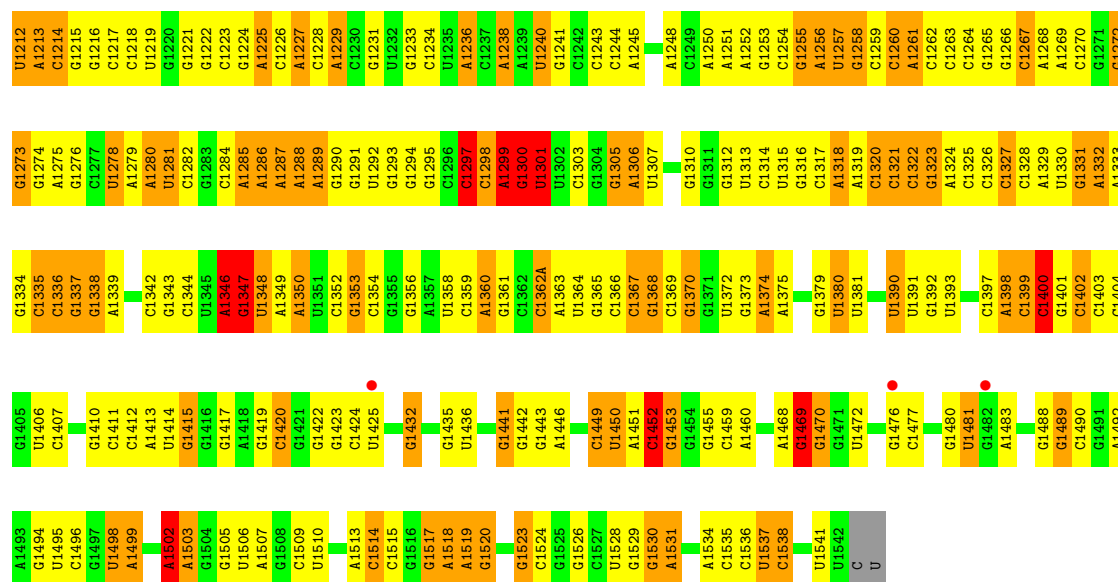
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

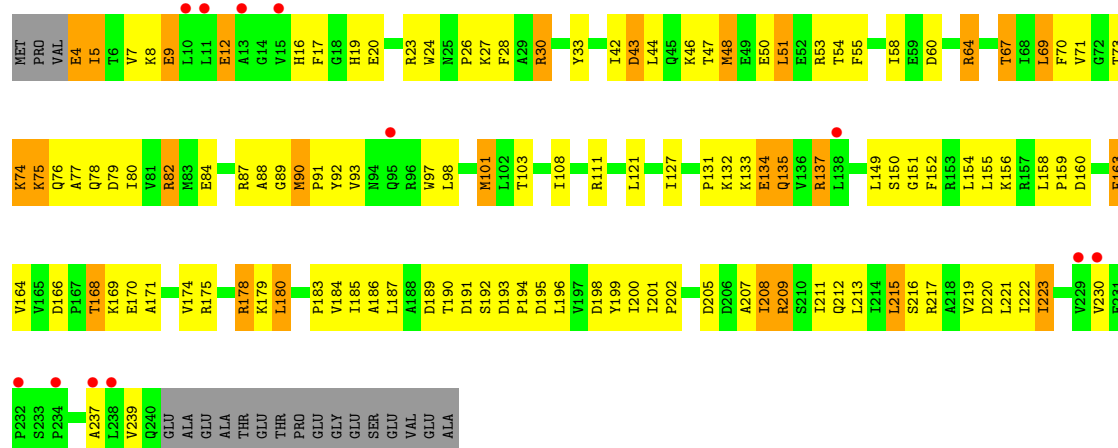
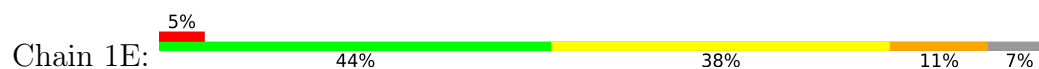




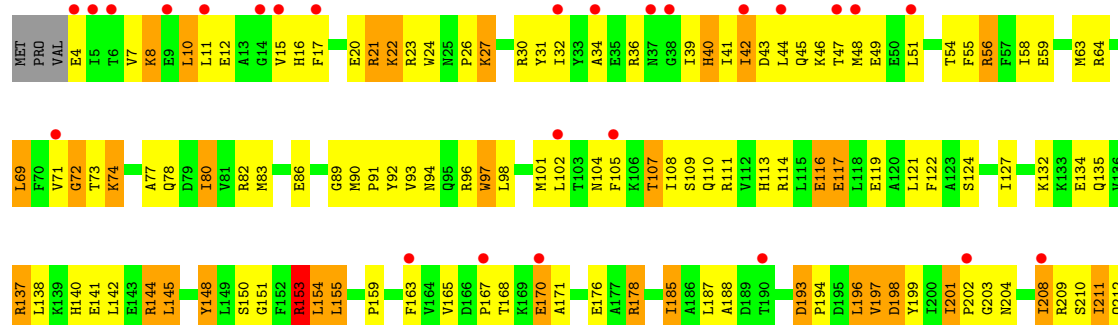
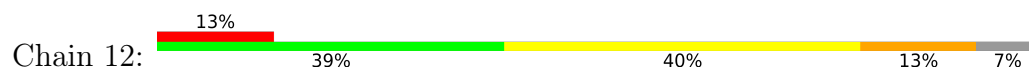




### • Molecule 2: 30S ribosomal protein S2

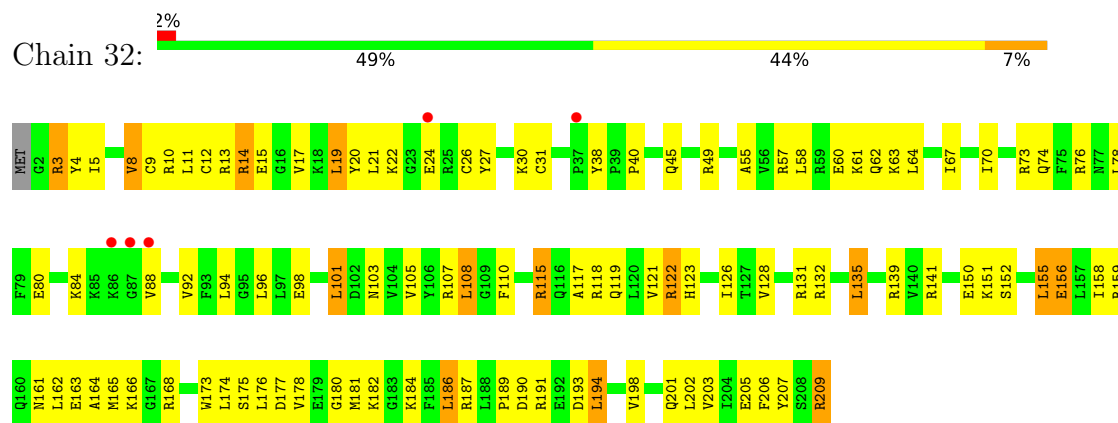


### • Molecule 2: 30S ribosomal protein S2

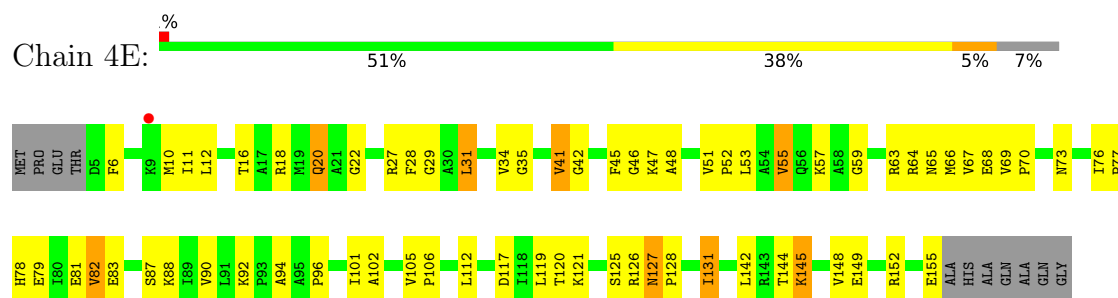




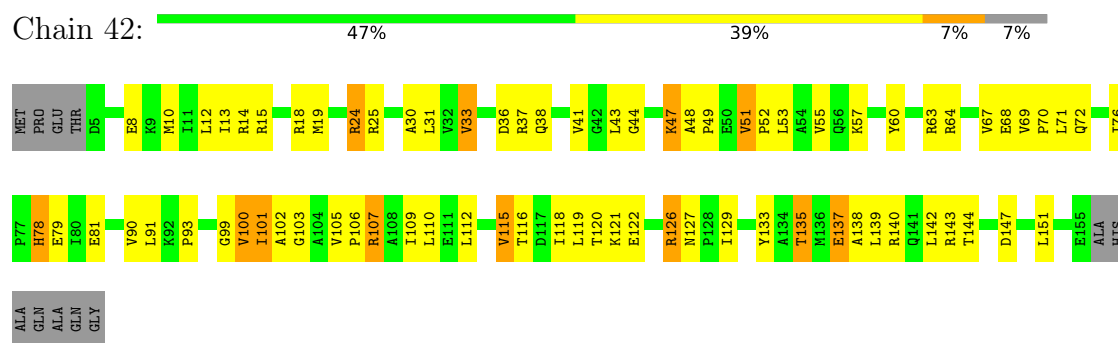
- Molecule 4: 30S ribosomal protein S4



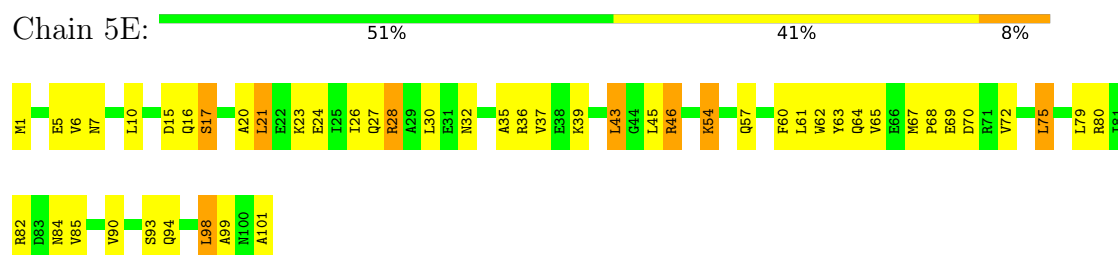
- Molecule 5: 30S ribosomal protein S5



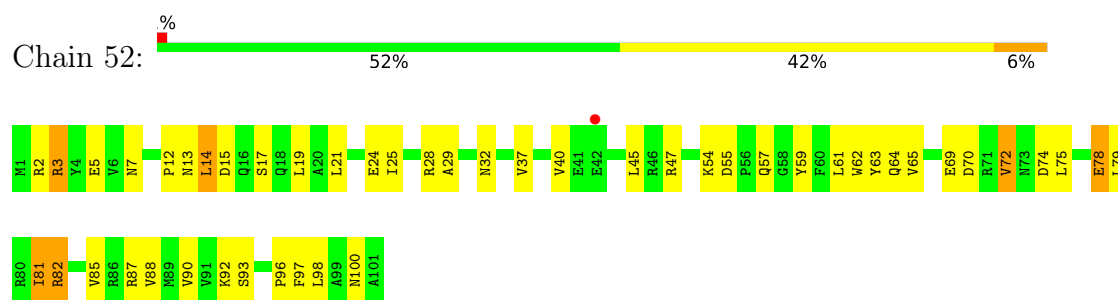
- Molecule 5: 30S ribosomal protein S5



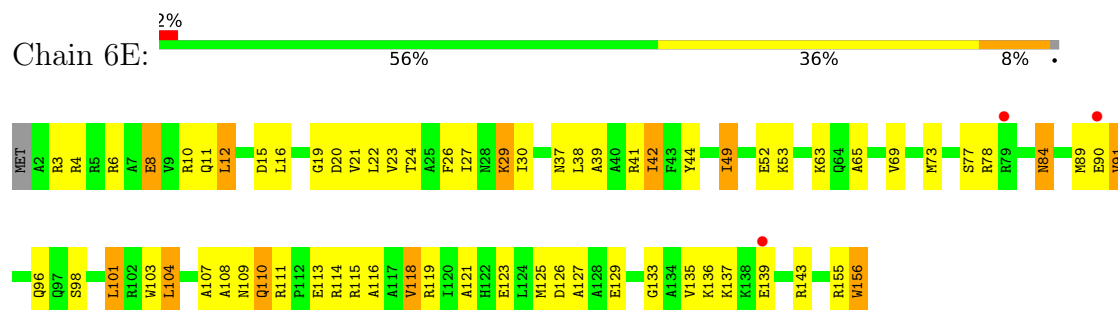
- Molecule 6: 30S ribosomal protein S6



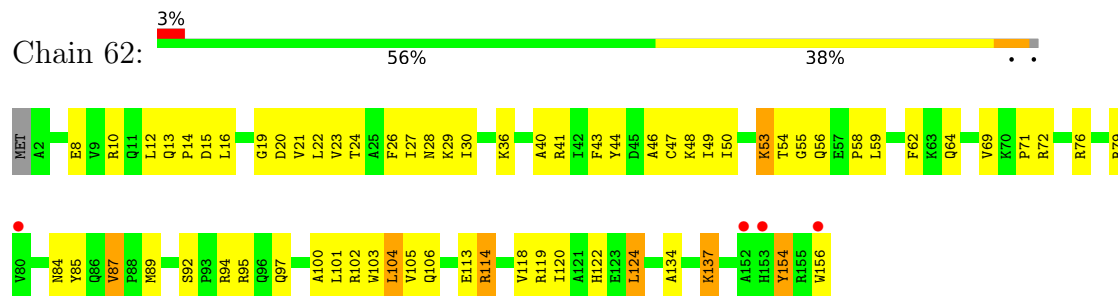
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



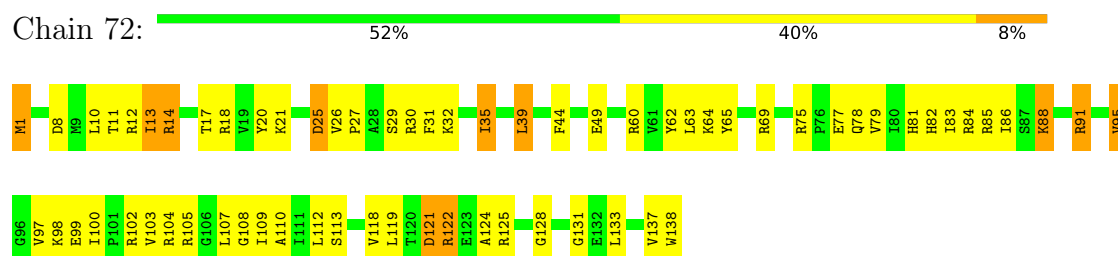
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

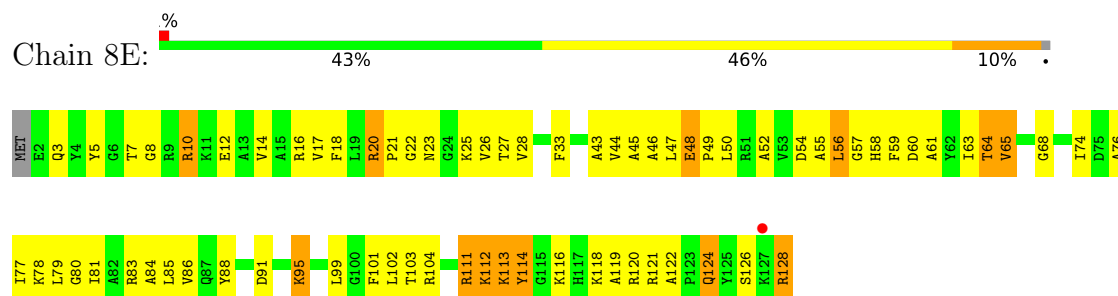


- Molecule 8: 30S ribosomal protein S8

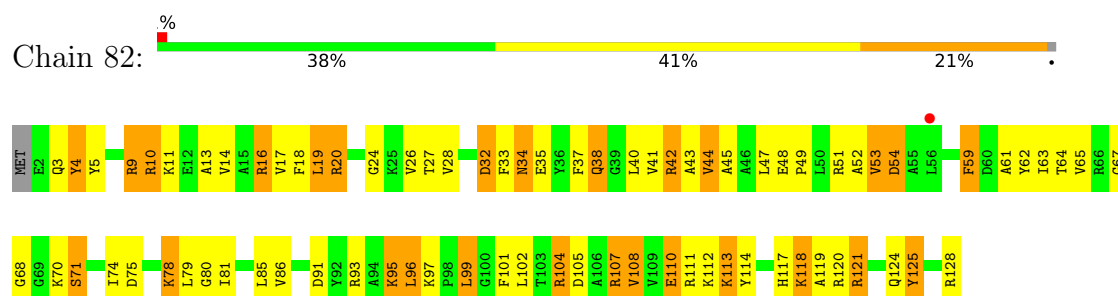




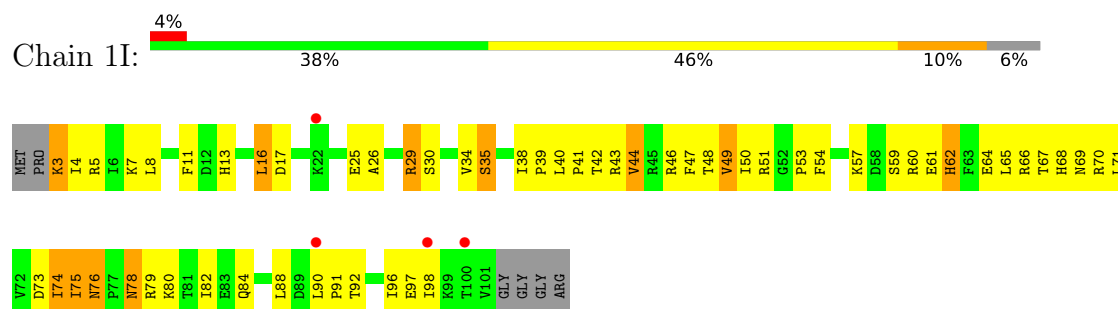
## • Molecule 9: 30S ribosomal protein S9



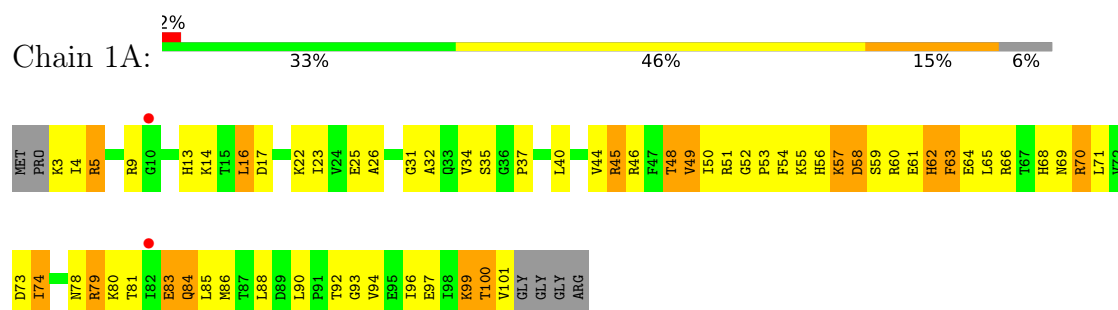
## • Molecule 9: 30S ribosomal protein S9



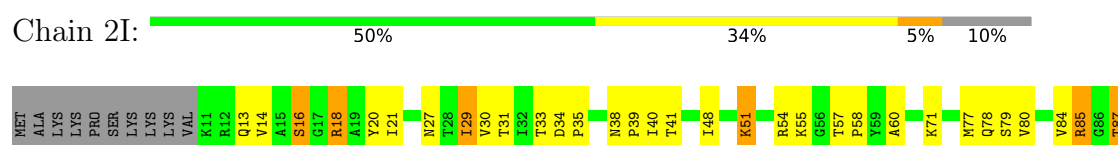
## • Molecule 10: 30S ribosomal protein S10



## • Molecule 10: 30S ribosomal protein S10



## • Molecule 11: 30S ribosomal protein S11





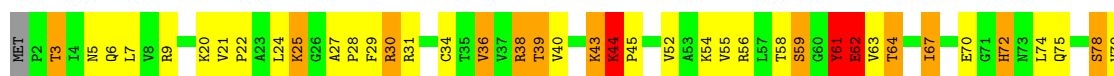
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

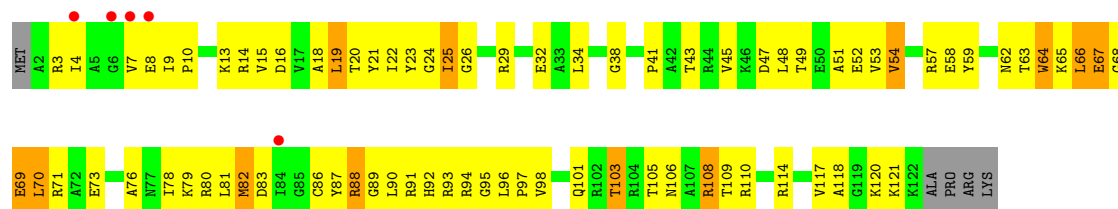


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13





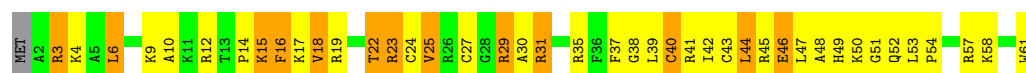
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I: 43% 46% 10%



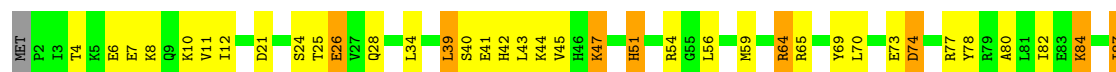
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A: 30% 48% 21%



- Molecule 15: 30S ribosomal protein S15

Chain 6I: 56% 34% 9%



- Molecule 15: 30S ribosomal protein S15

Chain 6A: 56% 38%



- Molecule 16: 30S ribosomal protein S16

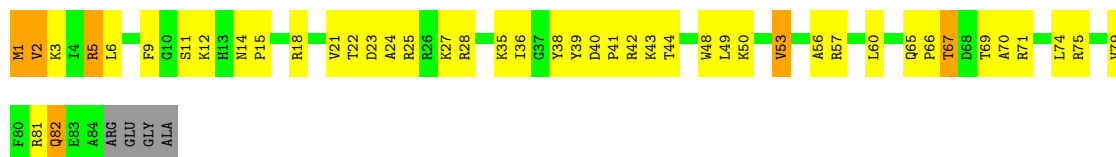
Chain 7I: 32% 51% 11% 6%





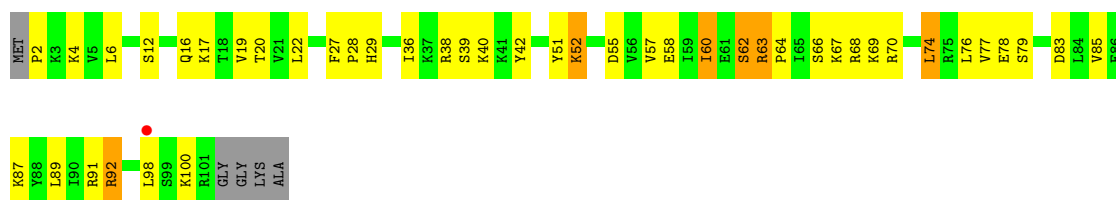
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 44% 44% 7% 5%



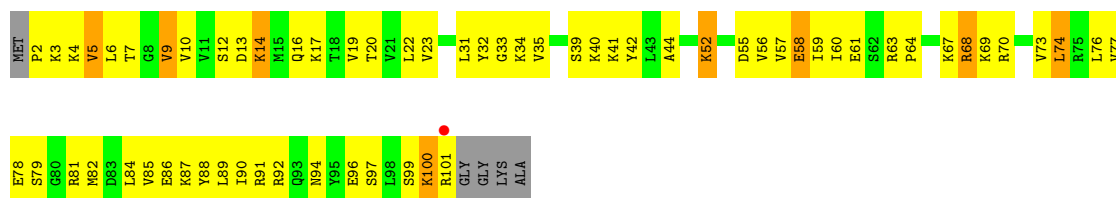
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 53% 36% 6% 5%



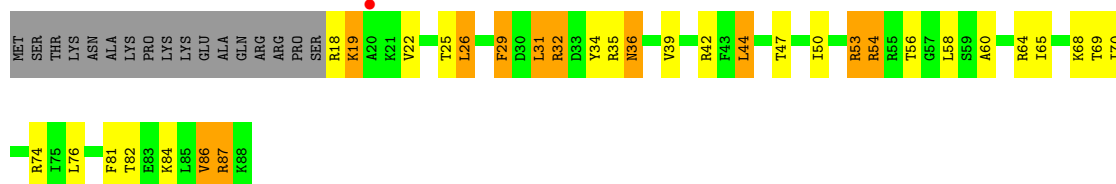
- Molecule 17: 30S ribosomal protein S17

Chain 8A: 34% 53% 8% 5%



- Molecule 18: 30S ribosomal protein S18

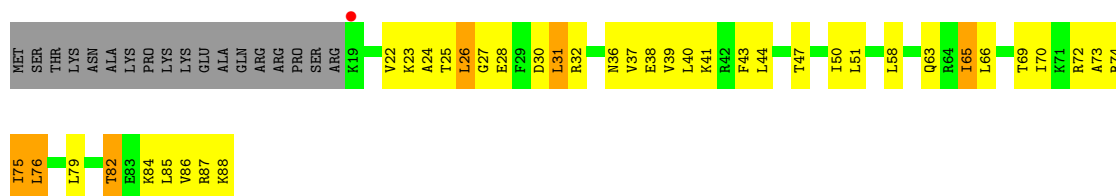
Chain 9I: 43% 25% 13% 19%



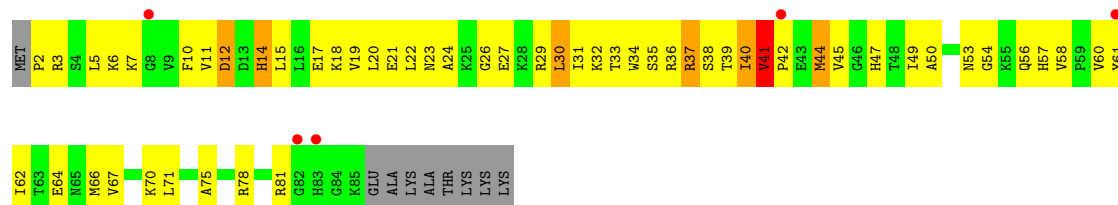
- Molecule 18: 30S ribosomal protein S18

Chain 9A: 35% 38% 7% 20%

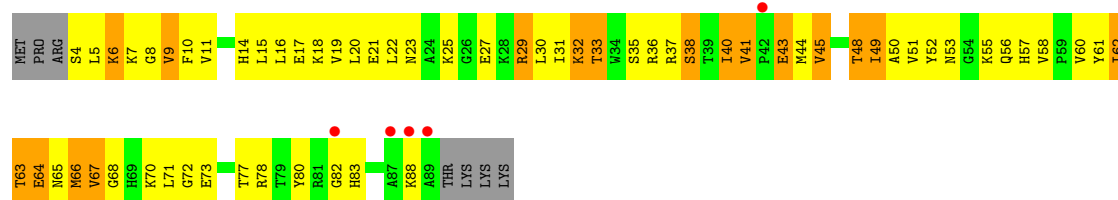




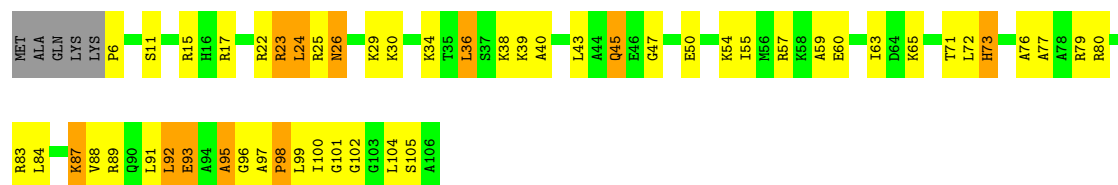
- Molecule 19: 30S ribosomal protein S19



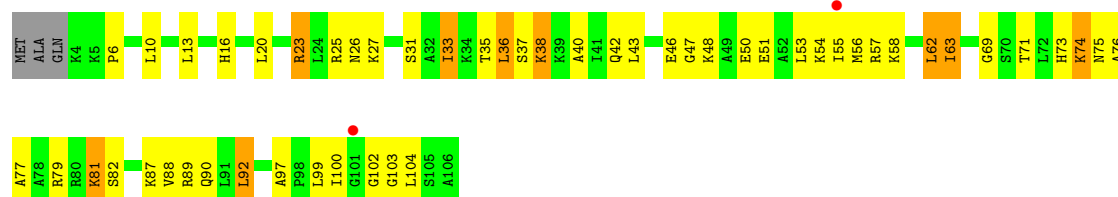
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

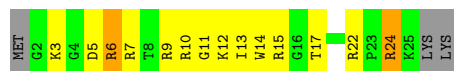


- Molecule 20: 30S ribosomal protein S20



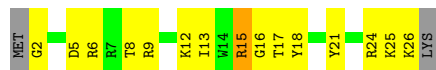
- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 




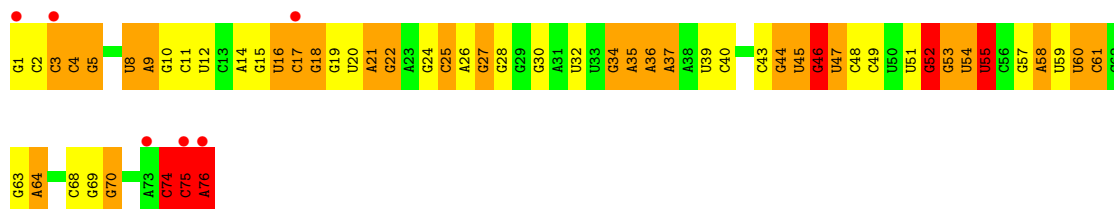
- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 



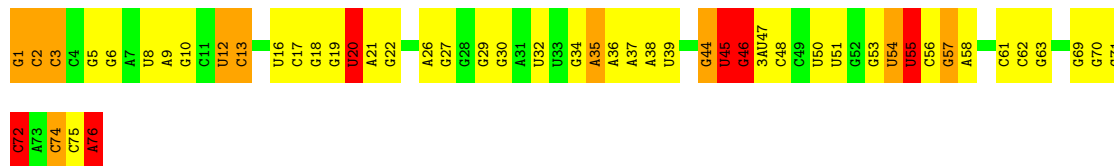
- Molecule 22: E. coli tRNAPhe

Chain 1K: 




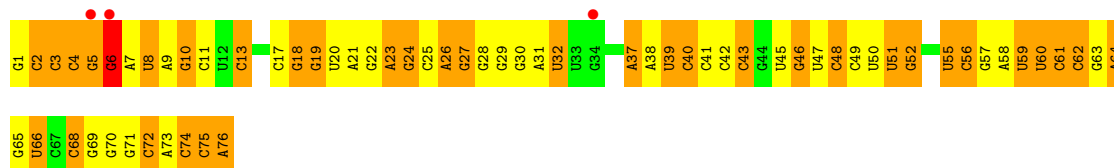
- Molecule 23: E. coli tRNAPhe

Chain 2K: 




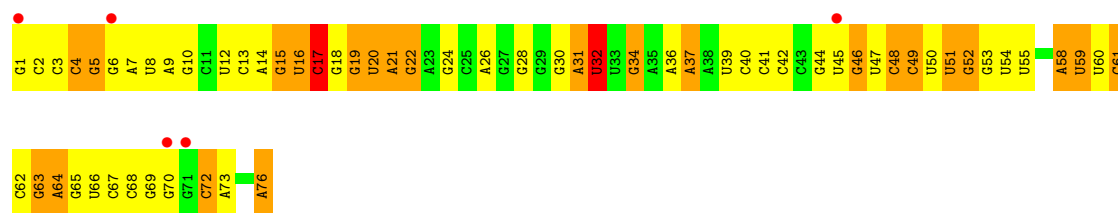
- Molecule 24: E. coli tRNAPhe

Chain 3K: 



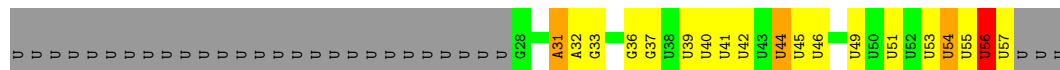
- Molecule 24: E. coli tRNAPhe

Chain 3L: 



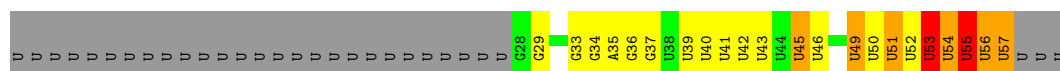
## ● Molecule 25: mRNA

Chain 4K: 18% 25% 5% 50%



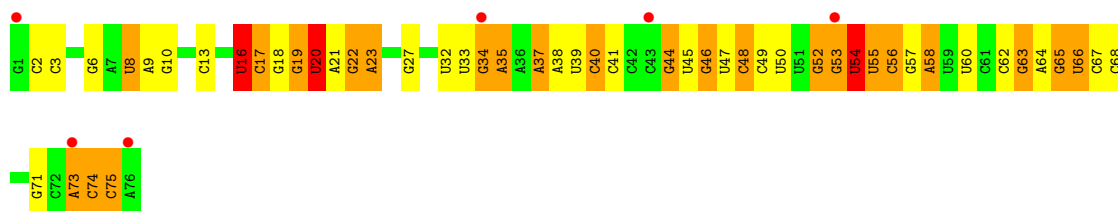
## ● Molecule 25: mRNA

Chain 4L: 13% 23% 10% 50%



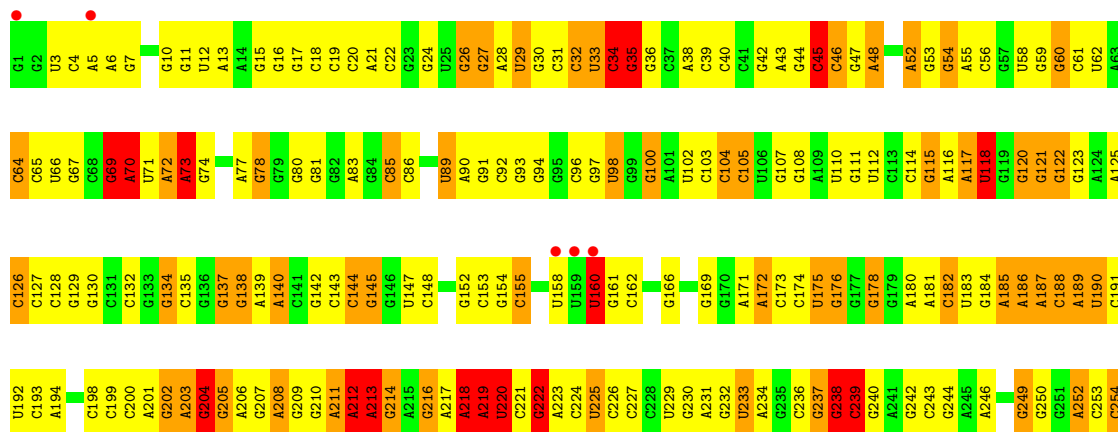
## ● Molecule 26: E. coli tRNAPhe

Chain 5K: 8% 33% 33% 30%



## ● Molecule 27: 23S ribosomal RNA

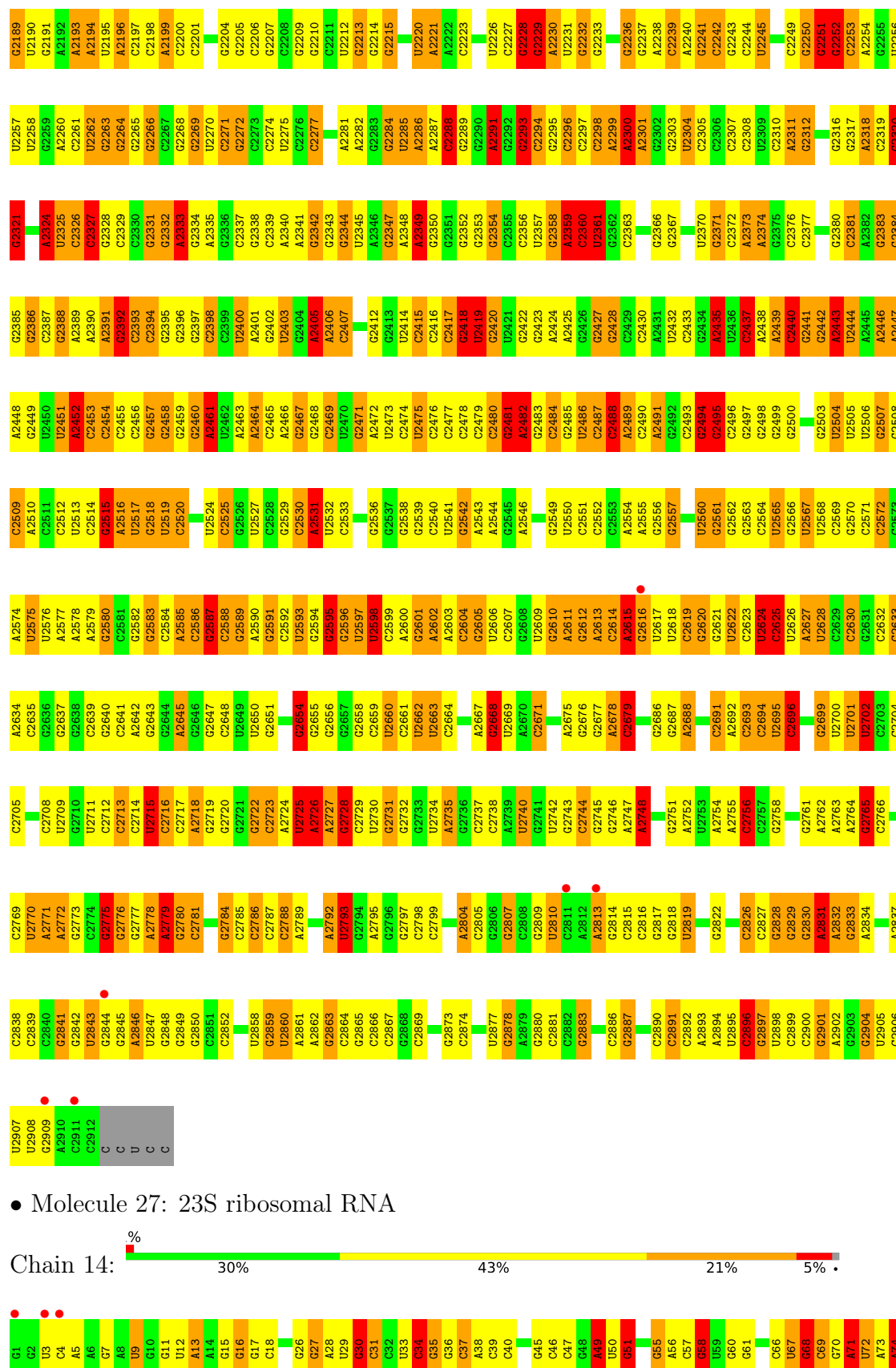
Chain 1H: 23% 43% 25% 7%



A1158	G1098	A1035	G901	A837	G777	G713	G653	C588	A528	G485	C397	U328	A255
G1159	G1099	G1036	G902	C838	C778	G714	U652	C589	A529	G486	C398	G329	G256
U1160	A1100	A1037	G903	C839	C779	U715	A653	U590	U530	G489	A399	G329	
G1161	A1101	C1038	C904	G840	C780	U716	G654	A591	A531	A470	G400	U330	U259
	G1102	C1039	C905	A841	C781	G717	G655	U592	Q532	C471	U401	U331	A260
G1168	G1103	G1040	U906	G842	A782	A718	G656	U593	A533	C472	G407	G332	A261
G1169	A1104	G1041	G907	C943	A783	C719	A657	G594	G473	G473		G334	A262
G1170	U1105	C1042	U908	C844	C784	C720	C660	A595	C536	A474	U412	A336	G265
A1043	A1043	G1043	A909	G845	C785	G721	C661	A596	C537	A475	U413	A337	G266
G1171	G1106	A1044	G908	G846	C786	G722	G662	U597	U537	A476	C413	U267	C267
G1172	U1107	G1044	A909	G847	C787	A723	G663	C598	G538	G477	C414	G340	G268
A1173	U1108	C1045	A911	G847	C787	G724	A663	A599	A539	C478	U415	G341	G269
A1174	G1109	U1046	G912	A848	U788	A725	G664	U600	A540	G479	U416	C341	G270
A1175	A1110	A1047	C913	G849	C789	A726	U665	G601	A541	C480	G417	G342	
A1176	C	A1048	G913	A850	C790	C726	U666	A602	C542	A481	A418	C343	C271
U1177	U	G1049	U916	G853	C791	G727	C667	A603	C543	A482	G419	C344	U272
G1178	U	G1050	G917	C854	C792	G728	G668	G604	C544	C483	A420	A345	U273
	A	C1051	A918	U855	A794	G730	G669	C605	U545	A484	C421	A346	G274
G1181	G	C1052	U919	G856	U795	C731	A670	G606	C546	U485	A422	A347	U275
G1182	A	C1053		G857	C796	G732	C671	G607	U547	U486	U423	G348	C276
G1183	A1117	C1054	G923	C857	C797	G733	C672	C608	G548	A487	G424	G349	C277
G1184	G1118	C1055	C924	U858	A798	A734	A672	G609	C549	C488	G425	G351	G278
G1185	A1119	A1056	U925	U859	A799	C735	G673	A610	U550	C489	G426	G352	
C1186	C1120	A1057	A926	C960	A799	G736	G674	A611	U551	C490	G427	U353	G283
U1187	G1121	G1058	G927	U861	A800	U736	G675	G612	A552	U491	G428	G354	G284
U1188	G1122	G994	G928	C862	C801		G676	U612	C553	C492	A429	A355	G285
U1189	C1123	G995	G929	C863	C802	C739	A679	C613	A554	C493	A430	A356	U286
A1190	A1124	G996	G930	G866	C803	C740	A680	A614	A555	A494	U431	A357	
G1191	U1125		G931	G867	C804	C741	A681	C615	A556	G494	U432	A358	U289
C1192	C1126	A999	C932	A868	U805	U742	G682	C616	C557	G495	C432	G359	G290
C1193	A1127	G1000	C933	A869	C806	G743	G683	G617	C558	G496	U433	G360	G291
C1194	U1128	C1001	C934	U870	G807	G744	G684	U618	A559	A497	G434	C361	
G1195	U1129	G1002	A935	U871	G808	C745	C	G619	U560	A498	G435	C362	G292
A1196	A1130	A1003	C936	G871	A809	C746	C	G620	C561	G500	C437	G363	
G1197	A1131	C937	C937	A872	U810	A747	C	U621	A562	G501	G438	U364	G298
G1198	U1070	A1004	A938	C873	G811	G748	C	G622	C563	U502	C439	A365	G299
C1199	G1071	A1006	G939	U874	A812	G749	C	G623	C564	G503	C440	G366	G300
C1200	G1072	C940	C940	U875	G813	G750	C	G624	A564	A504	C441	A367	A
G1201	U1073			U876	C814	U751	A	C625	C565	A505	C442	C368	C
A1202	A1074	A943	A943	A877	U815	G752	C	G626	C566	A506	A443	C369	A303
A1203	A1075	C944	C944	G878	G816	G753	G	A627	C567	A507	C444	G370	A304
G1204	G1076	C945	C945	G879	G817	A754	C	G628	C568	C508	C445	G371	C305
C1205	G1077	A946	A946	G880	G818	G755	C	C629	C569	G509	G446	G372	G306
U1206	G1078	A947	A947	U881	G819	G756	C	U630	C570	A510	C447	G373	
G1207	A1079	A948	A948	C882	C820	U757	C	U631	C571	C511	C448	G374	C311
C1208	U1080	C949	C949	A883	U821	G758	C697	A632	A572	C512	C449	G375	C312
G1209	G1081	C950	C950	G884	A822		C698	A633	A573	C513	U450	G376	C313
U1210	U1082	A956	A956	G885	G823	U762	C699	G634	A574	C514	A451	G377	A314
G1211	U1083	C1021	U952	C886	G824	G763	C700	C635	G575	C515	G452	G378	A315
U1212	G1084	G953	G953	U887	A825	A764	A701		G576	G517	G453	G379	G316
C1213	C1085	U954	U954	C888	G826	G765	A702	U639	C577	A518	C454	G380	G317
U1214		C955	C955		U827	A766	G703	G640	U578	G519	C455	G381	U318
G1215	G1089	A957	A957	G891	G828	C767	G704	A641	U579	G520	A456	G382	A319
U1216	C1090	G1026	G1026	C892	A829	C768	U705	G642	C580	G521	A457	G383	G320
G1217	G1091	A1027	A958	G893	A830	C769	C706		U581	G522	G458	G384	G321
U1218	A1092	C959	C959	U895	A832	A770	C707	G645	C582	G523	G459	G385	G322
G1219	A1093	U960	U960	U896	A833		G708	G646	C583	A524	C461	G386	G323
A1220	G1094	C961	C961	G896	G833	G773	C709	A647	C584	G525	U462	G387	A324
U1221	A1095	C962	C962	A897	C834	G774	G710	G648	U585	G526	C463	G388	A325
G1222	C1096	G963	G963	G897	U835	G775	G711	G649	U586	A527	C464	G389	G326
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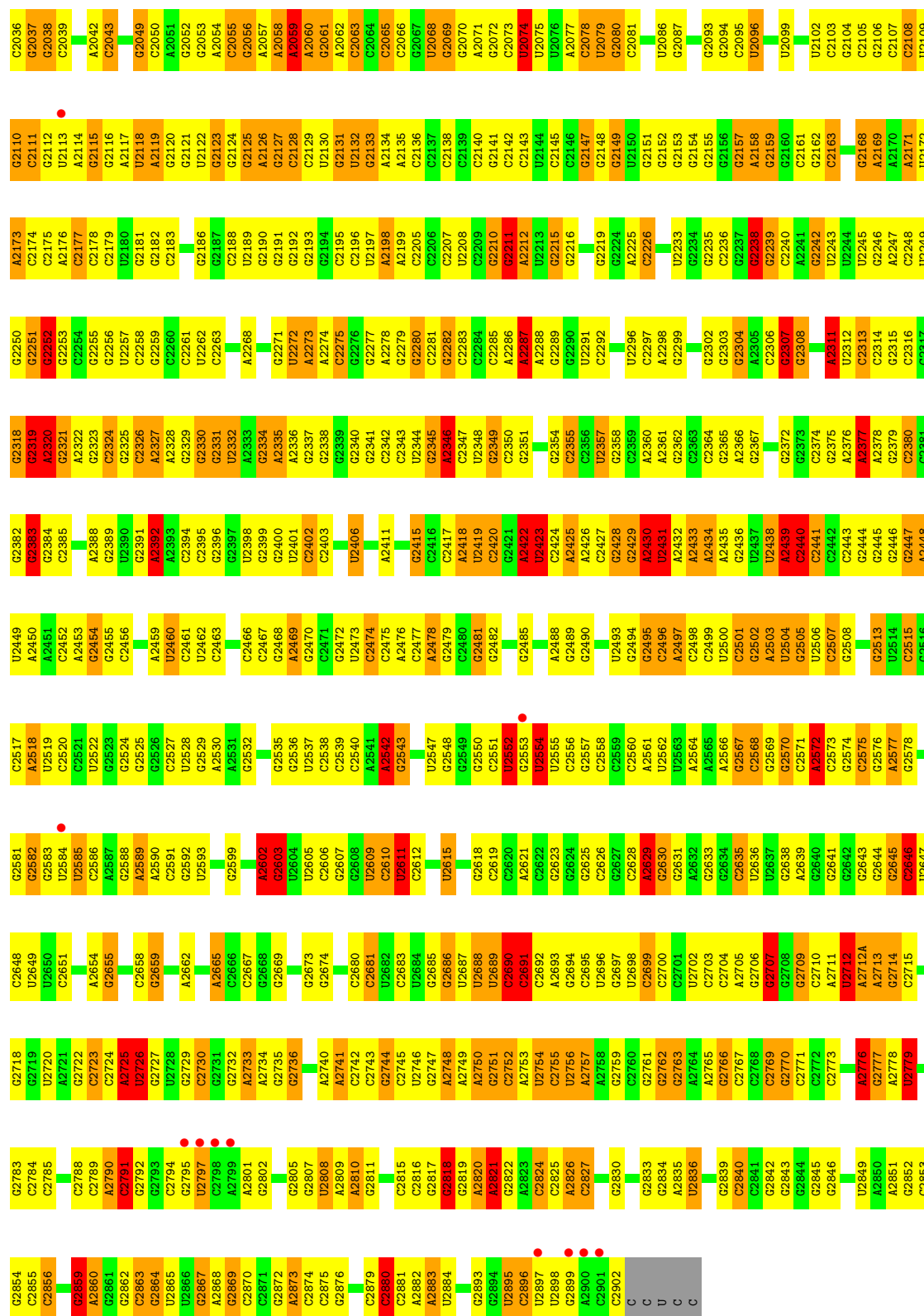


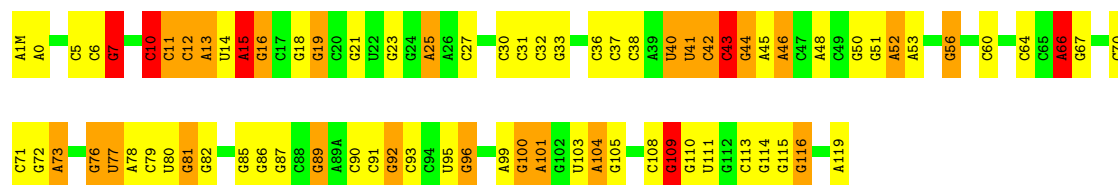
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C1225	C1226	A1288	G1356	C1421	G1482	C1553	A1617	A1679	U1741	U1807	G1867	A1935	A2001	G2061	U2125
		G1290	G1357	C1422	G1493	A1554	A1618	G1680	C1742	U1808	C1868	A1936	C2002	C2062	C2126
G1229		G1291	G1360	C1423	G1484	A1555	A1619	G1681	G1743	U1809	C1869	C1937	G2003	C2063	C2127
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			G1379	A1443		C1508	G1640	U1700	G1764	C1828	G1889	U1958	C2022	A2083	A2148
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						G1522	G1654	G1714		A1842	C1904	U1974	A2036	U2097	C2163
			G1395	C1458		A1592	A1655	G1715	G1782	G1843	C1905	A1975	A2037	U2098	G2164
			A1396	A1459		C1524	A1656	A1716	C1783	U1844	G1906	A1976	A2038	U2099	
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			U1398	G1461		C1526	C1658	C1718	G1785	G1846	A1908	U1978	U2040		C2169
			U1399	U1462		G1527	C1659	U1719	G1786	A1847	A1909	U1979	G2041		C2170
			A1400	G1463		C1528	G1660	C1720	A1787	G1848	C1910		A2042	C2104	C2171
			U1401	C1464		U1529	A1661	U1721	G1788	G1849	G1911	C1980	A2043	A2105	G2172
			G1402	G1465		G1530	C1662	G1722	U1789	U1850	A1912		C2044	G2106	U2173
			U1403	A1466		G1531	A1663	C1723		A1851	A1913		U2045	C2107	G2174
			G1404	U1467		A1533	C1664	A1724	A1792	U1852		C1984	G2046	C2108	G2175
			A1405	G1468		A1601	A1665	A1725	C1793	A1853	U1921	U1986	G2047	G2109	G2176
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			A1407	G1470		G1534	G1667	U1727	G1795	G1855	G1923	C1988	C2049	G2111	G2178
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			G1409	G1472		A1541	G1669	G1729		A1857	A1924	C1990	U2051	G2113	G2180
			U1410	A1473		A1542	G1670		U1798	G1858	C1925	G1991	G2052	U2114	A2181
			G1411	G1474		G1544	G1671	C1733	U1799	G1859	C1926	A1992	A2053	U2115	C2182
			A1412	C1475		U1544	G1672	C1734	U1800	G1860	G1927	A1993	G2054	C2116	C2183
			U1413	G1476		A1610	G1673	G1735	U1801	A1861	C1928	A1994	G2055	C2117	C2184
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			U1418	U1478		C1548	G1675	A1737	C1803	G1863	G1930		U2057	U2121	C2186
			G1419	C1479		A1614	U1676	C1738	G1804	U1965	C1931		G2058	U2122	C2187
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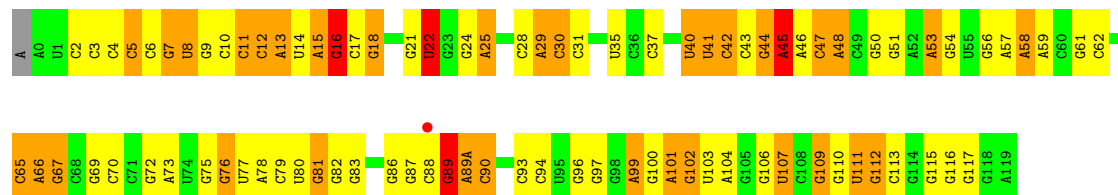
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G1975	A1911	C1764	G1673	C1612	A1545	U1482	G1416	G1346	G1279	A1210	A142A
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C1982	U1915		A1677	A1614	A1548	G1486	G1421	C1350	G1284	G1216	G1149
C1983	A1916	C1771	G1678	A1615	C1549	A1486	G1422	C1351	G1285	A1220	A1080
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A1985	A1773	A1773	U1680	A1618	G1552	U1489	G1424	A1353	A1287		
	G1920		G1681	G1619	A1553	U1490	G1425	A1354			
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C1990	C1924	U1779	U1688	G1624	C1557	A1494	G1429	G1358	U1294	G1224	A1085
U1991	C1925	A1780	A1689	G1625	A1558	A1495	C1430	A1359	G1295	C1225	A1086
G1992	U1926	C1781		G1626	G1559	A1496	U1431	A1360	G1296	G1226	G1087
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C1994	A1928	A1783	U1693	G1628	A1562	C1498	U1433	C1362	C1298	G1228	G1089
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A2001	G1935	C1790	A1700	A1634	A1571	C1506	G1440	C1370	C1305	U1249	A
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C2000	C1941	C1795	C1708	U1639	C1578	A1511	C1445		G1309	G1244	U
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C2014	C1946	G1801	G1725	C1646	A1583	G1519	C1451	A1384	G1315	G1252	C1109
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A2016	G1948	A1803	U1727	C1648	A1586	U1520	U1454	C1386	G1319	A1253	G1111
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A2020	C1952	C1887	G1731	U1590	G1591	G1525	G1459	A1392	C1258	C1258	C
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C2024	U1956	G1816	C1741	C1657	G1595	A1529	G1464	A1396	U1263	U1263	U
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A2031	C1967	A1824	C1754	A1665	A1603	C1537	A1472	C1407	C1270	C1270	U
C2032	G1968	G1825	A1755	G1666	C1604	G1538	G1473	G1408	G1198	G1198	C
A2033	A1969	A1826	G1756	C1667	C1605	U1539	C1474	C1409	A1272	A1272	U
U2034	G1904	C1827	U1757	A1668	G1606	G1540	G1475	U1341	U1273	U1273	C
C2035	A1971	C1828	C1759	A1669	C1607	U1541	C1476	A1412	A1274	A1274	A

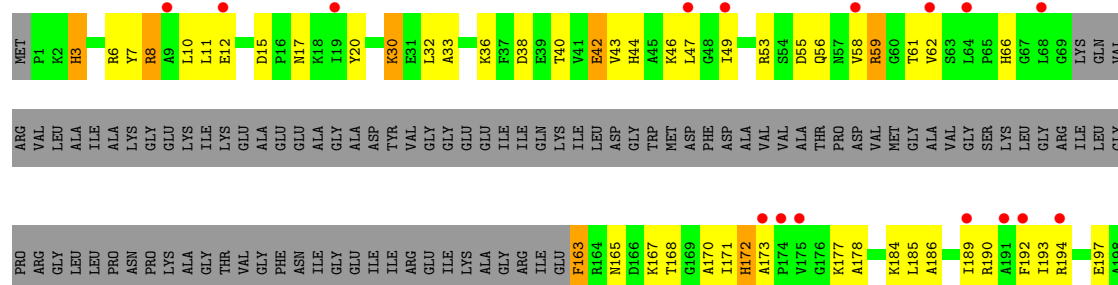
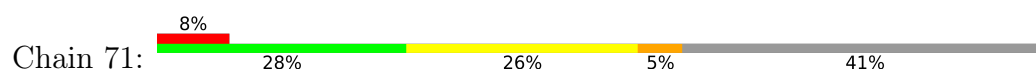




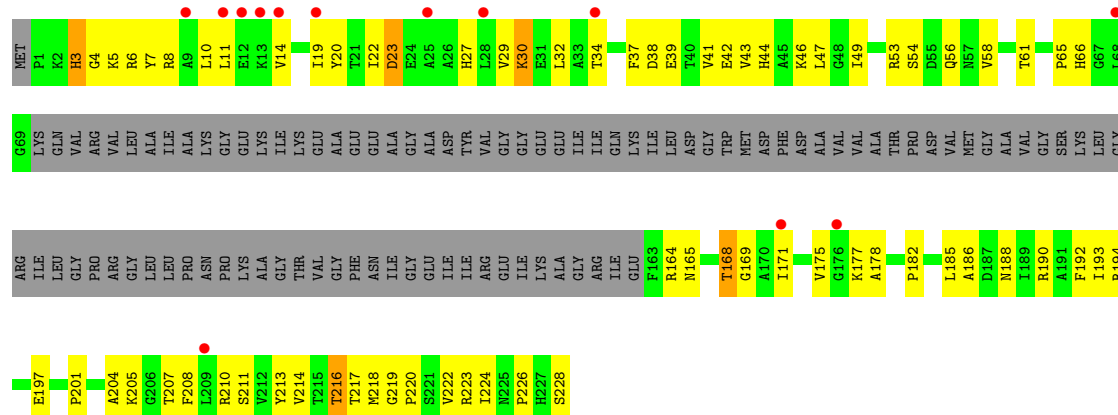
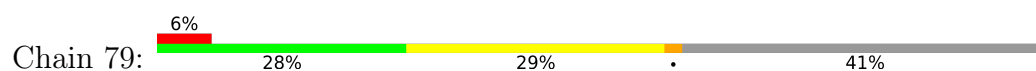
• Molecule 28: 5S ribosomal RNA



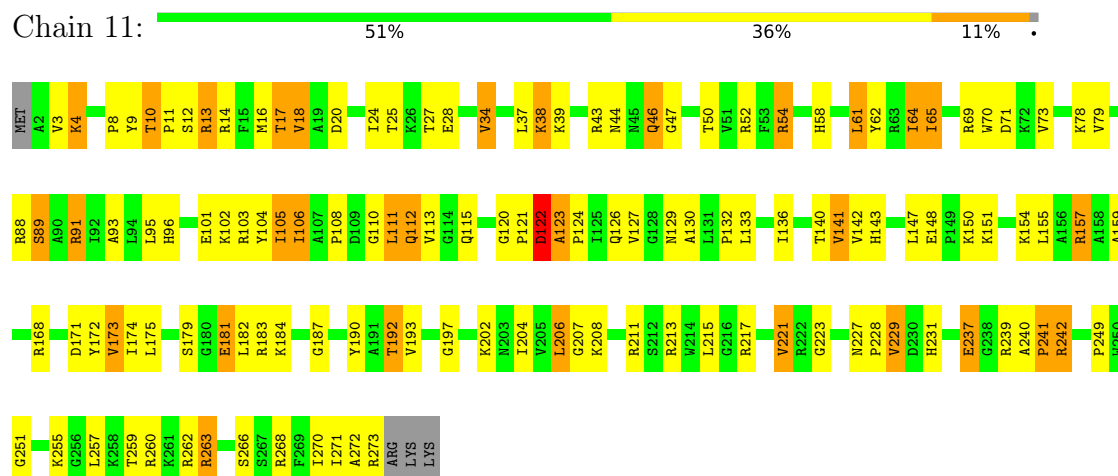
• Molecule 29: 50S ribosomal protein L1



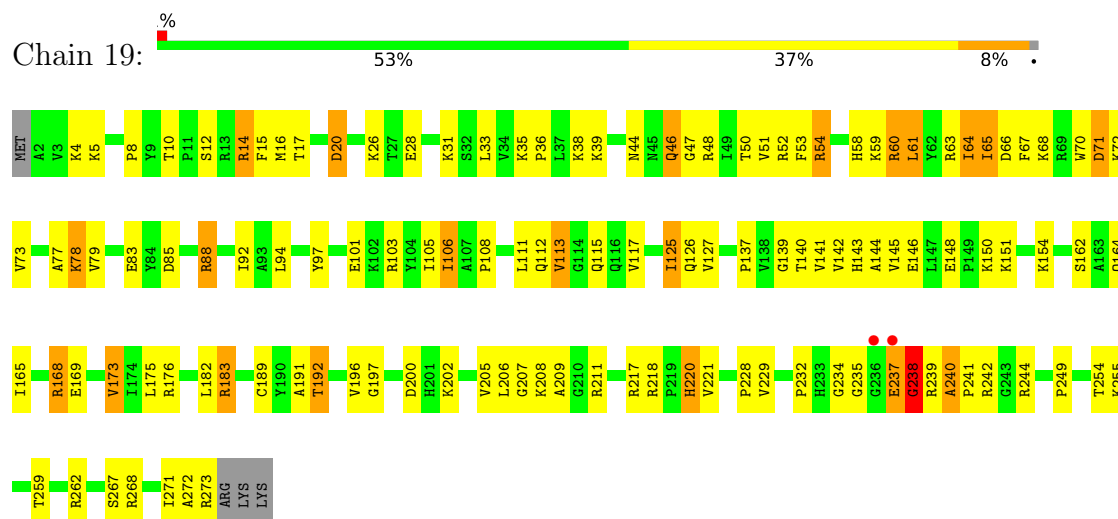
• Molecule 29: 50S ribosomal protein L1



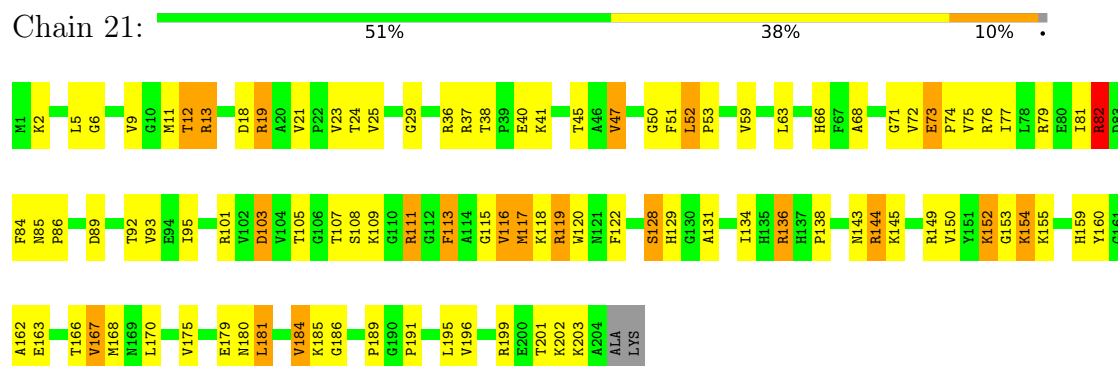
- Molecule 30: 50S ribosomal protein L2



- Molecule 30: 50S ribosomal protein L2

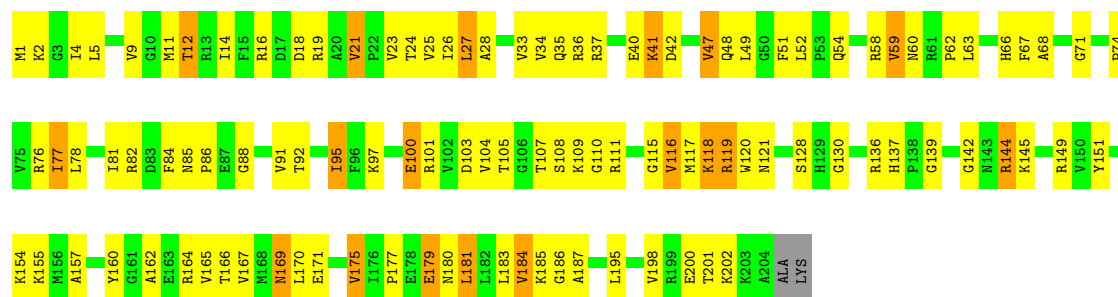


- Molecule 31: 50S ribosomal protein L3



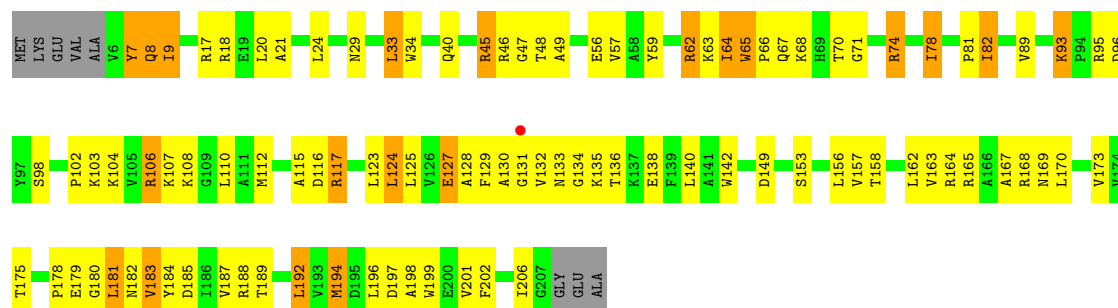
- Molecule 31: 50S ribosomal protein L3





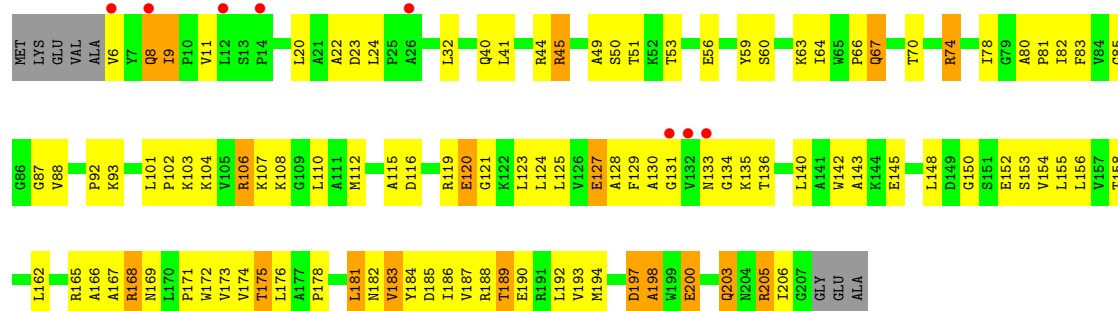
• Molecule 32: 50S ribosomal protein L4

Chain 31: 49% 38% 10% .



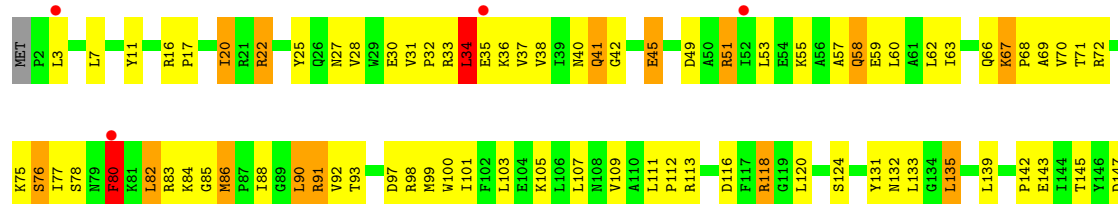
• Molecule 32: 50S ribosomal protein L4

Chain 39: 4% 46% 42% 9% .

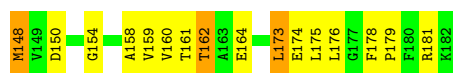


• Molecule 33: 50S ribosomal protein L5

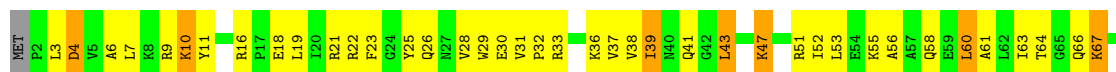
Chain 41: 2% 47% 42% 9% ..



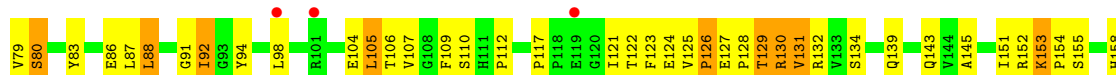
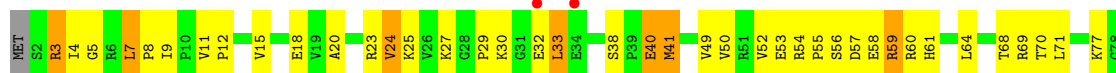




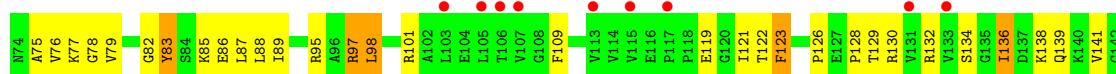
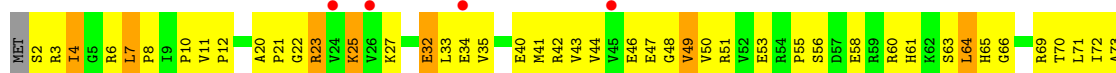
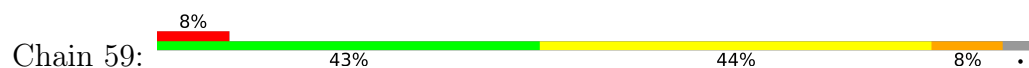
• Molecule 33: 50S ribosomal protein L5



• Molecule 34: 50S ribosomal protein L6



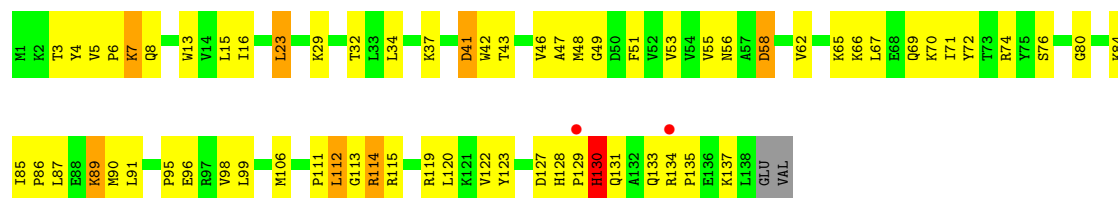
• Molecule 34: 50S ribosomal protein L6



• Molecule 35: 50S ribosomal protein L9

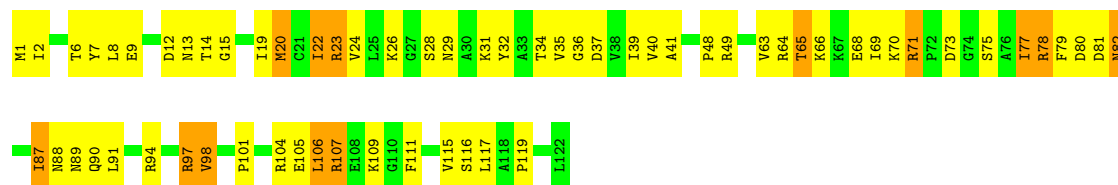






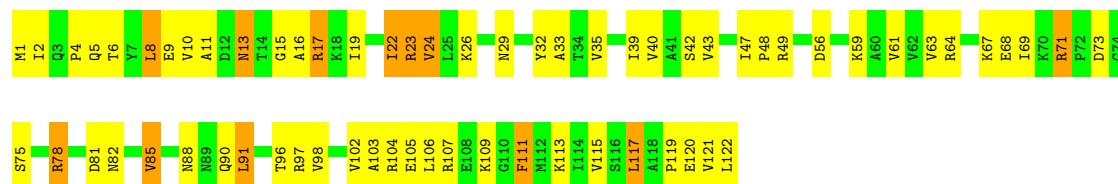
• Molecule 38: 50S ribosomal protein L14

Chain 68: 48% 42% 11%



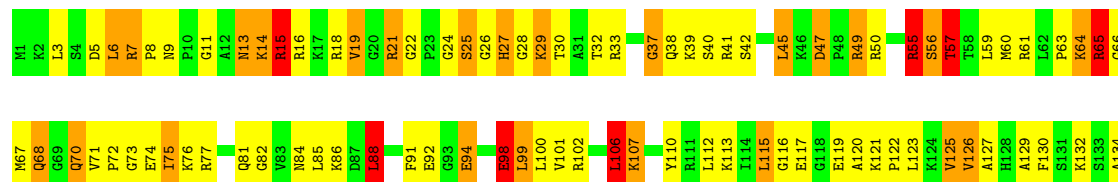
• Molecule 38: 50S ribosomal protein L14

Chain 25: 47% 43% 10%



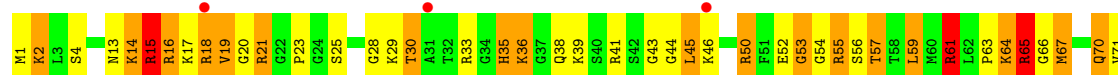
• Molecule 39: 50S ribosomal protein L15

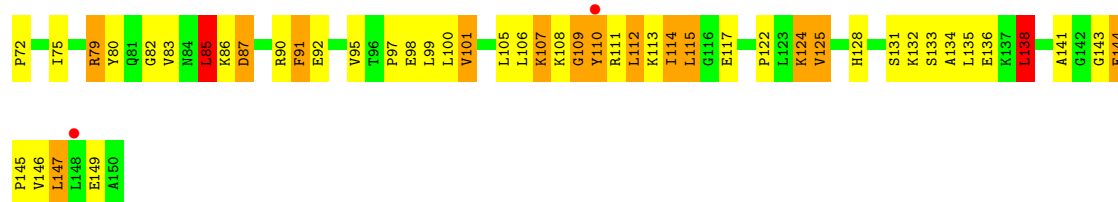
Chain 78: 35% 41% 19% 5%



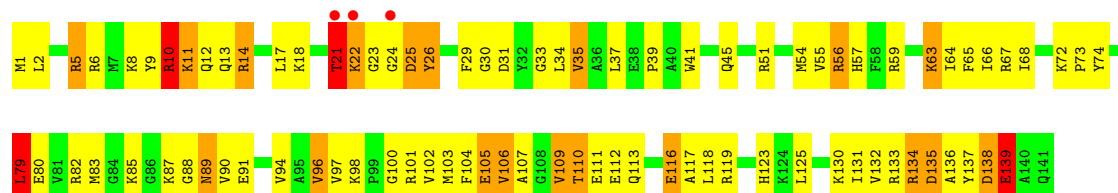
• Molecule 39: 50S ribosomal protein L15

Chain 35: 3% 39% 36% 21%

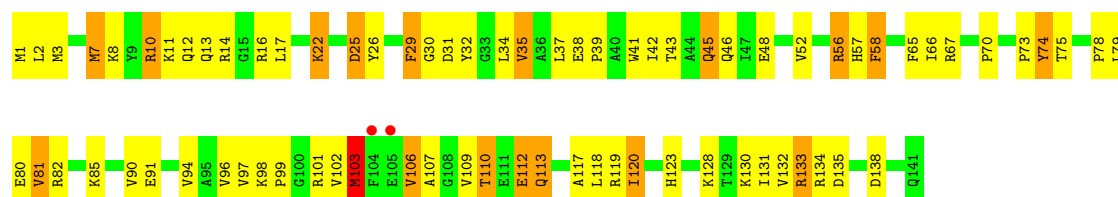




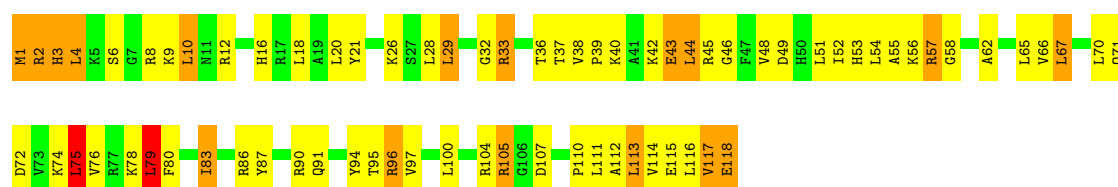
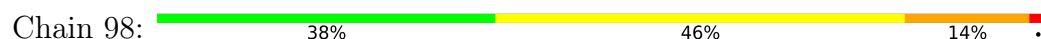
• Molecule 40: 50S ribosomal protein L16



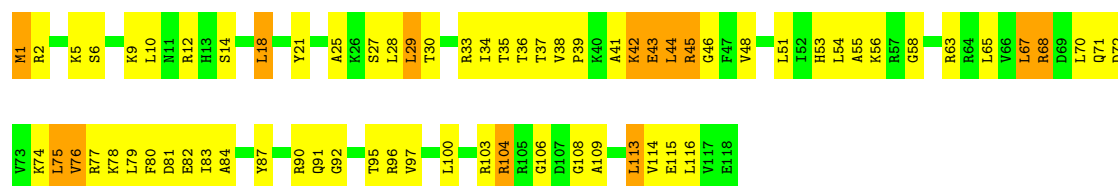
• Molecule 40: 50S ribosomal protein L16



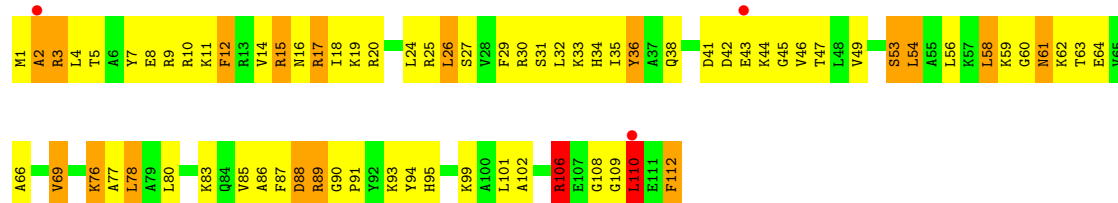
• Molecule 41: 50S ribosomal protein L17



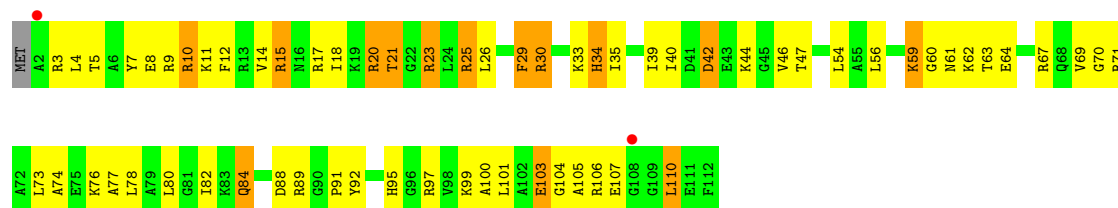
• Molecule 41: 50S ribosomal protein L17



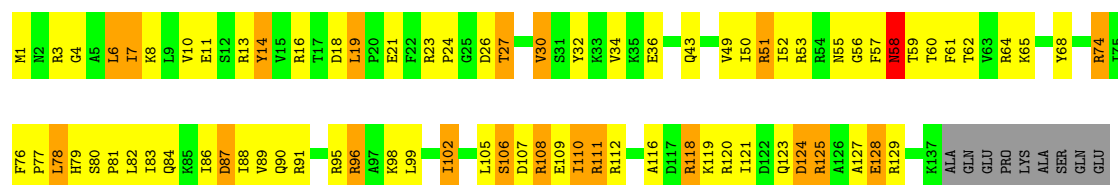
• Molecule 42: 50S ribosomal protein L18



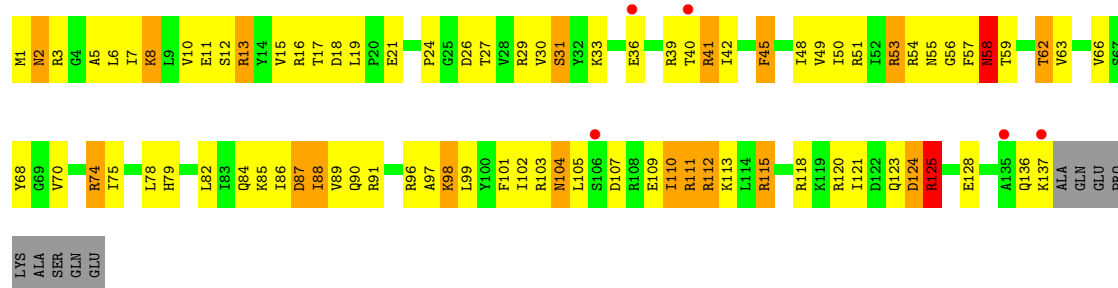
• Molecule 42: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L19



• Molecule 43: 50S ribosomal protein L19

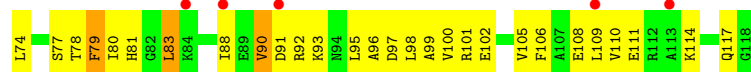
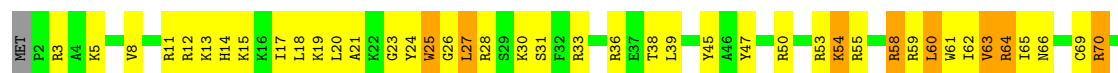


• Molecule 44: 50S ribosomal protein L20

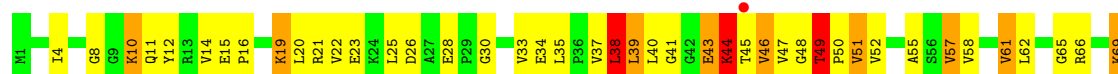




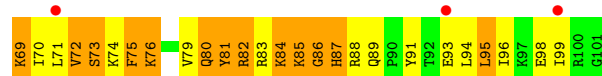
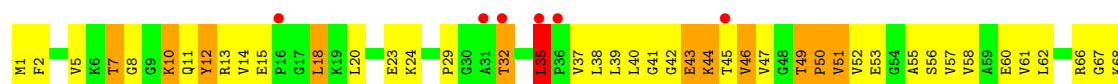
- Molecule 44: 50S ribosomal protein L20



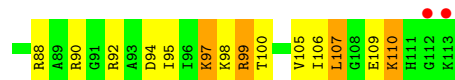
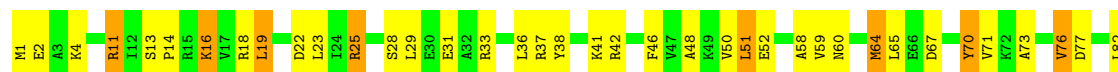
- Molecule 45: 50S ribosomal protein L21



- Molecule 45: 50S ribosomal protein L21

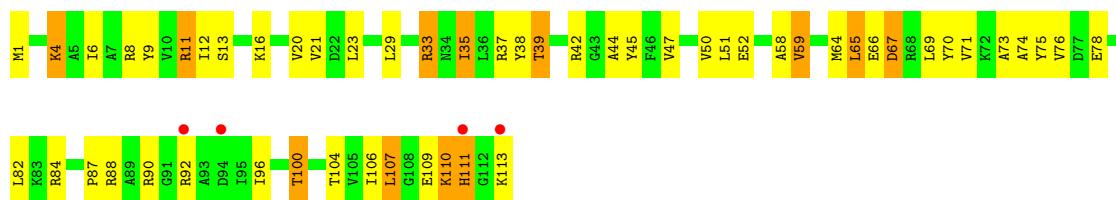


- Molecule 46: 50S ribosomal protein L22



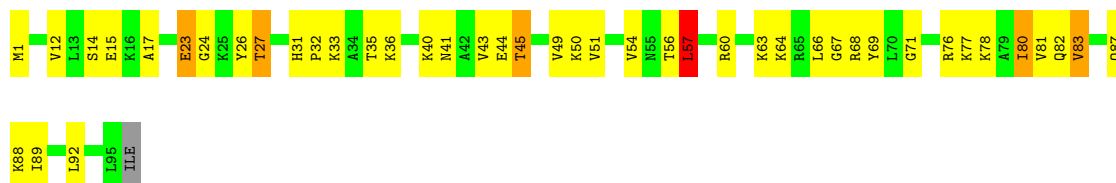
- Molecule 46: 50S ribosomal protein L22





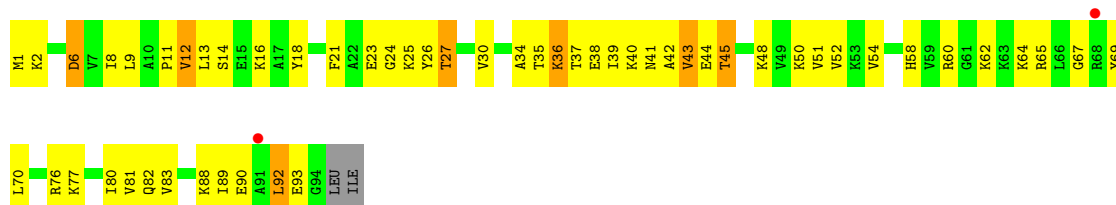
• Molecule 47: 50S ribosomal protein L23

Chain F8: 53% 40% 5% ..



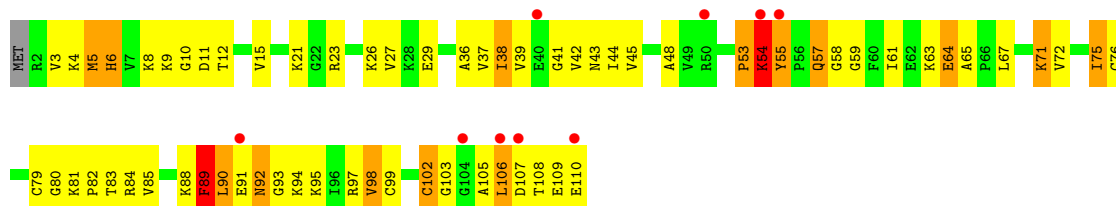
• Molecule 47: 50S ribosomal protein L23

Chain B5: 2% 42% 49% 7% ..



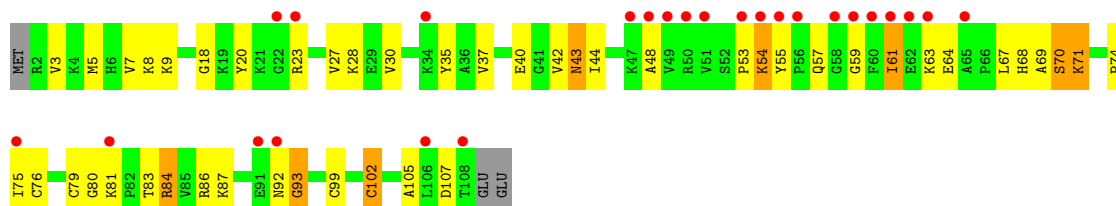
• Molecule 48: 50S ribosomal protein L24

Chain G8: 8% 39% 45% 13% ..



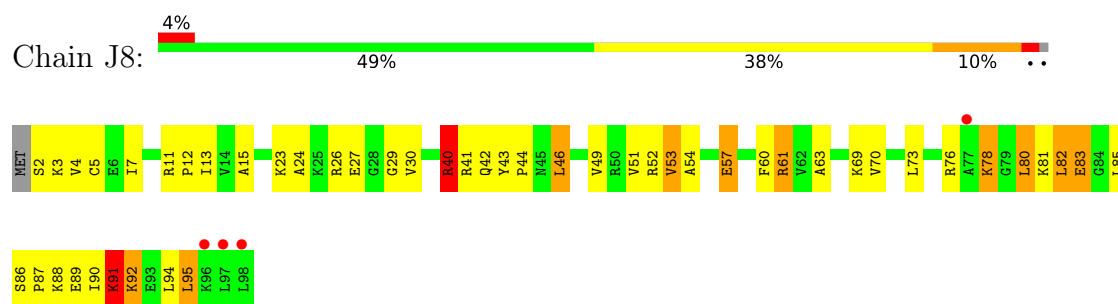
• Molecule 48: 50S ribosomal protein L24

Chain C5: 23% 55% 35% 7% ..

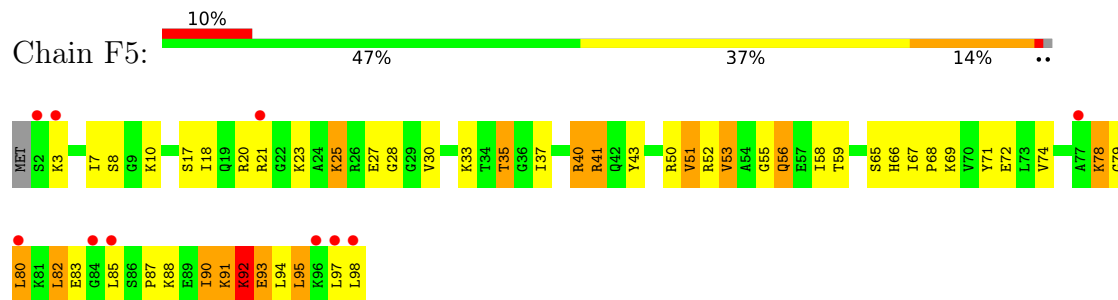


WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

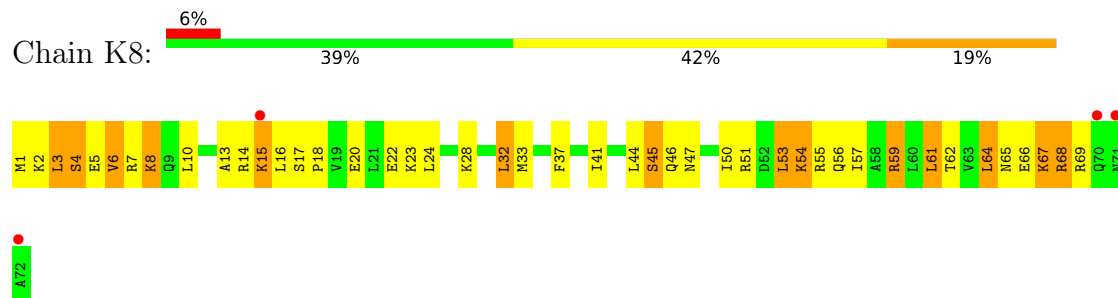




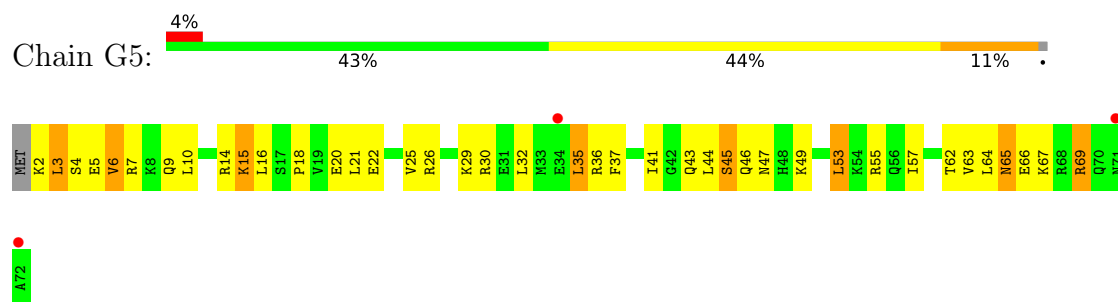
- Molecule 51: 50S ribosomal protein L28



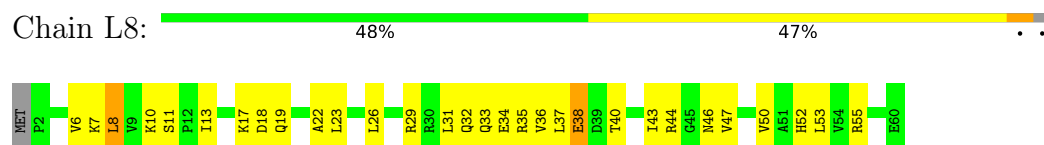
- Molecule 52: 50S ribosomal protein L29



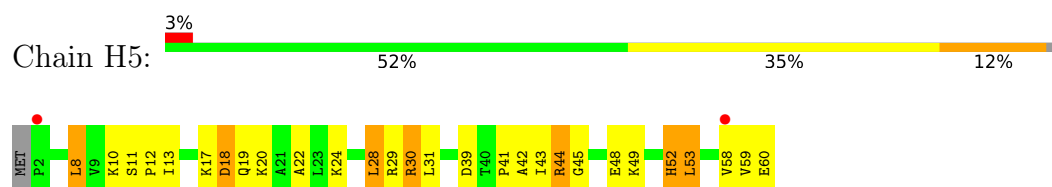
- Molecule 52: 50S ribosomal protein L29



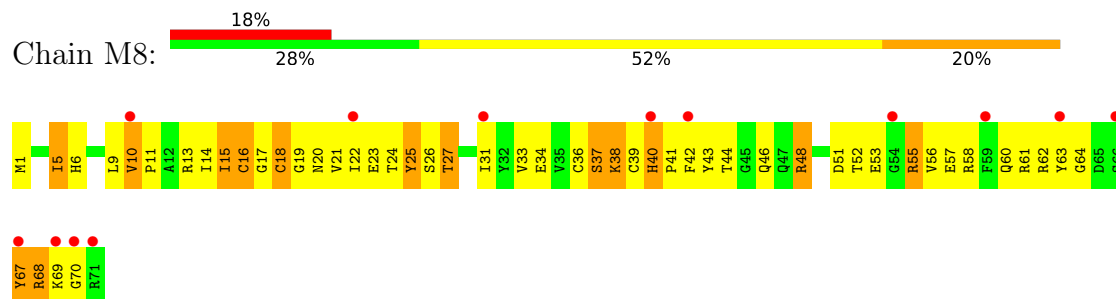
- Molecule 53: 50S ribosomal protein L30



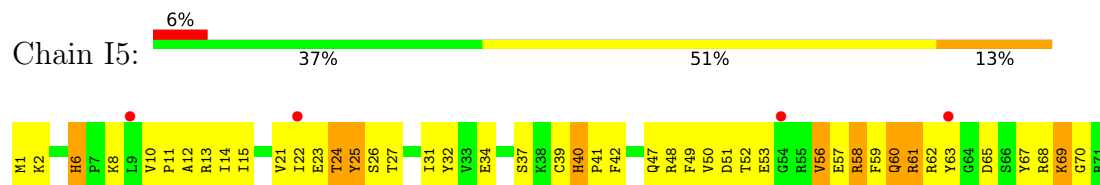
- Molecule 53: 50S ribosomal protein L30



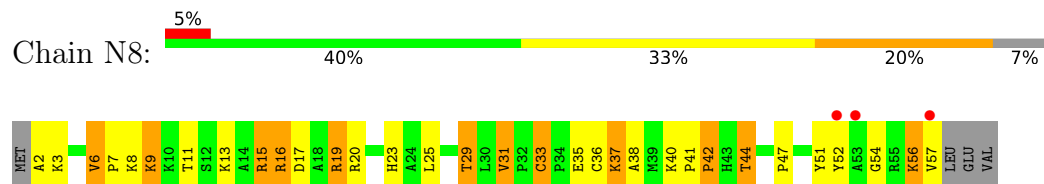
- Molecule 54: 50S ribosomal protein L31



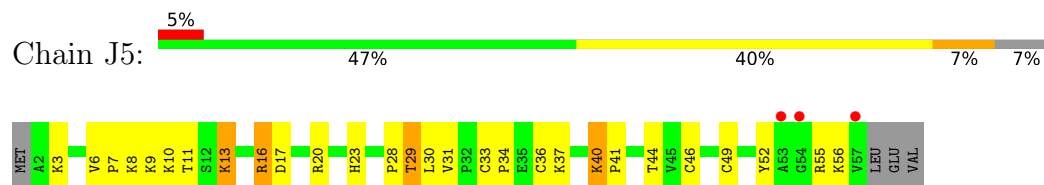
- Molecule 54: 50S ribosomal protein L31



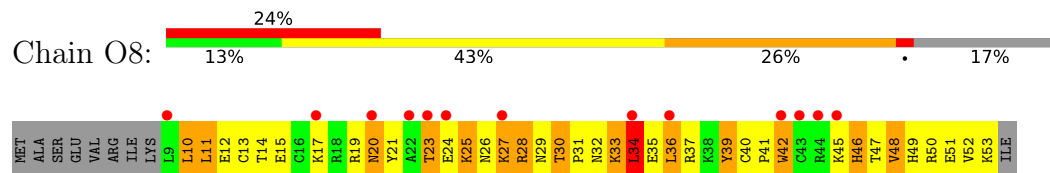
- Molecule 55: 50S ribosomal protein L32



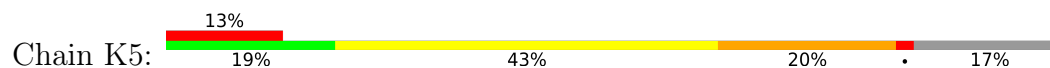
- Molecule 55: 50S ribosomal protein L32

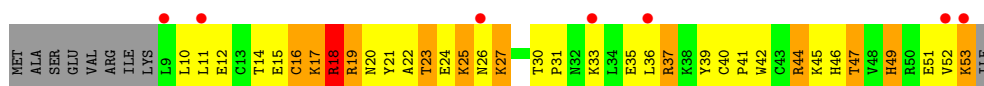


- Molecule 56: 50S ribosomal protein L33



- Molecule 56: 50S ribosomal protein L33





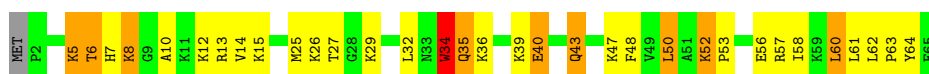
- Molecule 57: 50S ribosomal protein L34



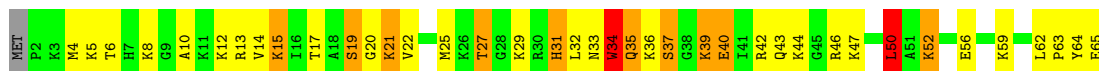
- Molecule 57: 50S ribosomal protein L34



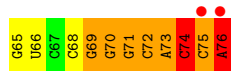
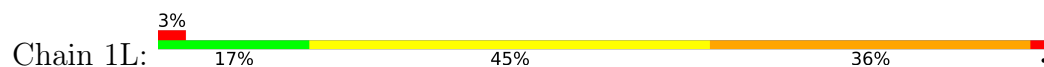
- Molecule 58: 50S ribosomal protein L35



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: E. coli tRNAPhe



- Molecule 60: E. coli tRNAPhe



C74  
C75  
A76

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.46Å 446.20Å 623.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	223.10 – 3.10 223.10 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (223.10-3.10) 99.7 (223.10-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.196 , 0.253 0.196 , 0.253	Depositor DCC
$R_{free}$ test set	31126 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 65.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	305753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: 3AU, 0TD, OMU, MA6, MG, 5MC, M2G, K, 7MG, 2MG, ZN, 4OC, 5MU, H2U, OMG, UR3, 4SU, MIA, OMC, SF4, 2MA, 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	0.79	8/36175 (0.0%)	1.40	445/56452 (0.8%)
1	1G	0.69	1/36106 (0.0%)	1.30	264/56346 (0.5%)
2	12	0.36	0/1959	0.61	1/2642 (0.0%)
2	1E	0.38	0/1959	0.59	1/2642 (0.0%)
3	22	0.37	0/1636	0.60	0/2205
3	2E	0.44	0/1629	0.61	0/2195
4	32	0.48	0/1732	0.62	1/2318 (0.0%)
4	3E	0.49	0/1732	0.64	0/2318
5	42	0.46	0/1171	0.64	0/1576
5	4E	0.54	1/1171 (0.1%)	0.64	0/1576
6	52	0.47	0/855	0.65	0/1154
6	5E	0.49	0/855	0.62	0/1154
7	62	0.43	0/1275	0.54	0/1709
7	6E	0.47	0/1275	0.57	0/1709
8	72	0.39	0/1135	0.62	0/1527
8	7E	0.49	0/1135	0.67	0/1527
9	82	0.36	0/1022	0.56	0/1371
9	8E	0.44	0/1022	0.58	0/1371
10	1A	0.41	0/814	0.63	0/1095
10	1I	0.43	0/814	0.64	0/1095
11	2A	0.42	0/888	0.58	0/1198
11	2I	0.48	0/879	0.62	0/1187
12	3A	0.50	0/982	0.71	1/1313 (0.1%)
12	3I	0.61	0/982	0.80	1/1313 (0.1%)
13	4A	0.38	0/974	0.59	0/1303
13	4I	0.44	0/956	0.65	0/1281
14	5A	0.43	0/500	0.65	0/664
14	5I	0.51	0/500	0.66	0/664
15	6A	0.44	0/744	0.56	0/992
15	6I	0.49	0/744	0.65	0/992
16	7A	0.50	0/721	0.63	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	7I	0.43	0/716	0.66	0/963
17	8A	0.46	0/847	0.62	0/1131
17	8I	0.49	0/847	0.65	0/1131
18	9A	0.47	0/578	0.72	0/768
18	9I	0.48	0/589	0.73	0/782
19	AA	0.38	0/698	0.60	0/938
19	AI	0.44	0/689	0.71	0/926
20	BA	0.43	0/778	0.62	1/1028 (0.1%)
20	BI	0.38	0/768	0.61	1/1014 (0.1%)
21	1B	0.36	0/221	0.52	0/288
21	1F	0.37	0/212	0.57	0/277
22	1K	0.60	1/1647 (0.1%)	1.23	10/2565 (0.4%)
23	2K	0.90	0/1580	1.61	29/2459 (1.2%)
24	3K	0.53	1/1739 (0.1%)	1.20	10/2708 (0.4%)
24	3L	0.52	0/1739	1.17	12/2708 (0.4%)
25	4K	0.63	0/689	1.18	4/1069 (0.4%)
25	4L	0.59	0/689	1.25	9/1069 (0.8%)
26	5K	0.47	0/1629	1.05	1/2538 (0.0%)
27	14	0.87	47/69120 (0.1%)	1.52	1139/107900 (1.1%)
27	1H	1.18	189/69453 (0.3%)	1.87	2698/108417 (2.5%)
28	16	0.90	1/2928 (0.0%)	1.60	59/4568 (1.3%)
28	1J	0.65	0/2906	1.29	15/4533 (0.3%)
29	7I	0.27	0/1072	0.51	0/1447
29	79	0.30	0/1072	0.51	0/1447
30	11	0.75	2/2165 (0.1%)	0.95	4/2919 (0.1%)
30	19	0.64	1/2165 (0.0%)	0.81	3/2919 (0.1%)
31	21	0.65	0/1592	0.77	2/2149 (0.1%)
31	29	0.46	0/1592	0.66	0/2149
32	31	0.75	1/1620 (0.1%)	0.84	0/2194
32	39	0.53	0/1620	0.72	1/2194 (0.0%)
33	41	0.51	0/1498	0.71	1/2016 (0.0%)
33	49	0.38	0/1498	0.61	1/2016 (0.0%)
34	51	0.49	0/1362	0.69	0/1841
34	59	0.32	0/1353	0.56	0/1830
35	61	0.47	0/1146	0.80	5/1551 (0.3%)
35	69	0.45	0/1151	0.64	0/1558
36	38	0.36	0/636	0.75	2/847 (0.2%)
37	15	0.41	0/1131	0.63	0/1525
37	58	0.65	0/1131	0.84	1/1525 (0.1%)
38	25	0.54	0/942	0.72	2/1269 (0.2%)
38	68	0.66	0/942	0.78	0/1269
39	35	0.54	0/1161	0.92	5/1544 (0.3%)
39	78	0.65	0/1161	0.99	2/1544 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	45	0.49	0/1142	0.66	0/1527
40	88	0.69	0/1171	0.85	3/1565 (0.2%)
41	55	0.47	0/981	0.69	0/1312
41	98	0.56	0/981	0.88	2/1312 (0.2%)
42	65	0.47	0/891	0.71	0/1187
42	A8	0.57	0/899	0.89	2/1197 (0.2%)
43	75	0.47	0/1155	0.63	0/1542
43	B8	0.63	0/1155	0.77	1/1542 (0.1%)
44	85	0.48	0/981	0.65	0/1306
44	C8	0.67	0/981	0.85	1/1306 (0.1%)
45	95	0.50	0/789	0.76	1/1057 (0.1%)
45	D8	0.61	0/789	0.84	3/1057 (0.3%)
46	A5	0.55	0/910	0.66	0/1220
46	E8	0.68	0/910	0.84	2/1220 (0.2%)
47	B5	0.60	0/756	0.71	1/1014 (0.1%)
47	F8	0.76	1/761 (0.1%)	0.88	3/1021 (0.3%)
48	C5	0.49	0/788	0.77	0/1059
48	G8	0.58	0/838	0.77	1/1121 (0.1%)
49	D5	0.35	0/1435	0.59	0/1947
49	H8	0.48	0/1460	0.68	1/1982 (0.1%)
50	E5	0.49	0/666	0.69	0/888
50	I8	0.75	1/670 (0.1%)	0.88	0/892
51	F5	0.55	0/769	0.76	0/1022
51	J8	0.69	0/769	0.89	1/1022 (0.1%)
52	G5	0.53	0/592	0.66	0/784
52	K8	0.65	0/600	0.73	0/794
53	H5	0.40	0/473	0.61	0/635
53	L8	0.58	0/473	0.79	0/635
54	I5	0.39	0/593	0.64	0/795
54	M8	0.46	0/593	0.66	0/795
55	J5	0.52	0/448	0.76	0/606
55	N8	0.56	0/448	0.81	1/606 (0.2%)
56	K5	0.45	0/396	0.76	0/529
56	O8	0.64	0/396	0.80	1/529 (0.2%)
57	L5	0.59	0/437	0.75	0/575
57	P8	0.76	0/427	0.99	2/564 (0.4%)
58	M5	0.52	0/514	0.79	1/679 (0.1%)
58	Q8	0.66	0/514	0.86	1/679 (0.1%)
59	1L	0.43	0/1717	1.06	3/2674 (0.1%)
60	2L	0.67	0/1602	1.28	8/2493 (0.3%)
All	All	0.83	255/326284 (0.1%)	1.39	4770/488082 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if



the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	2
3	22	0	1
3	2E	0	1
5	4E	0	1
9	82	0	1
12	3A	0	2
12	3I	0	3
13	4A	0	1
13	4I	0	1
14	5I	0	1
19	AA	0	2
19	AI	0	1
20	BI	0	1
30	11	0	1
30	19	0	2
32	31	0	3
32	39	0	2
33	41	0	2
34	51	0	2
34	59	0	1
35	61	0	4
36	38	0	3
37	58	0	2
39	35	0	4
39	78	0	10
40	45	0	2
40	88	0	2
41	55	0	1
41	98	0	1
42	A8	0	2
43	75	0	3
43	B8	0	1
44	85	0	1
44	C8	0	2
45	95	0	3
45	D8	0	3
46	E8	0	1
48	C5	0	5
48	G8	0	4
49	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	H8	0	3
50	E5	0	1
50	I8	0	1
51	F5	0	2
51	J8	0	1
52	G5	0	1
52	K8	0	1
54	M8	0	1
56	K5	0	3
56	O8	0	1
58	M5	0	3
58	Q8	0	1
All	All	0	105

The worst 5 of 255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1H	831	A	N9-C4	-14.30	1.29	1.37
27	1H	1818	A	N9-C4	-12.52	1.30	1.37
27	1H	822	A	N9-C4	-12.46	1.30	1.37
27	1H	1189	A	N9-C4	-11.38	1.31	1.37
27	1H	70	A	N9-C4	-11.34	1.31	1.37

The worst 5 of 4770 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1H	2150	G	O5'-P-OP2	-30.77	73.78	110.70
27	1H	2150	G	OP1-P-OP2	-27.63	78.15	119.60
27	1H	991	A	N1-C6-N6	23.99	133.00	118.60
27	1H	991	A	C6-C5-N7	-22.83	116.32	132.30
27	1H	1922	G	N3-C4-N9	-22.27	112.64	126.00

There are no chirality outliers.

5 of 105 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2E	11	ARG	Peptide
12	3I	101	VAL	Peptide
12	3I	115	SER	Peptide
12	3I	44	LYS	Peptide
5	4E	20	GLN	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	32589	0	16470	898	0
1	1G	32526	0	16442	922	0
2	12	1924	0	1975	99	0
2	1E	1924	0	1975	96	0
3	22	1612	0	1677	92	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1762	71	0
4	3E	1702	0	1764	89	0
5	42	1155	0	1212	55	0
5	4E	1155	0	1213	40	0
6	52	842	0	857	33	0
6	5E	842	0	857	33	0
7	62	1256	0	1296	48	0
7	6E	1256	0	1296	54	0
8	72	1115	0	1177	49	0
8	7E	1115	0	1177	53	0
9	82	1004	0	1032	80	0
9	8E	1004	0	1032	55	0
10	1A	801	0	849	59	0
10	1I	801	0	849	47	0
11	2A	873	0	894	38	0
11	2I	864	0	881	32	0
12	3A	977	0	1064	49	0
12	3I	977	0	1061	40	0
13	4A	964	0	1034	61	0
13	4I	946	0	1008	75	0
14	5A	491	0	530	50	0
14	5I	491	0	529	33	0
15	6A	733	0	771	26	0
15	6I	733	0	771	28	0
16	7A	705	0	725	37	0
16	7I	700	0	720	57	0
17	8A	834	0	904	53	0
17	8I	834	0	904	36	0
18	9A	573	0	644	30	0
18	9I	584	0	657	31	0
19	AA	684	0	707	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	674	0	699	32	0
20	BA	776	0	856	48	0
20	BI	766	0	854	44	0
21	1B	217	0	234	12	0
21	1F	208	0	221	14	0
22	1K	1628	0	839	53	0
23	2K	1635	0	850	32	0
24	3K	1626	0	832	68	0
24	3L	1626	0	834	48	0
25	4K	621	0	311	15	0
25	4L	621	0	311	20	0
26	5K	1627	0	840	34	1
27	14	61946	0	31226	1510	0
27	1H	62245	0	31354	1477	1
28	16	2617	0	1327	63	0
28	1J	2598	0	1316	81	0
29	71	1049	0	1071	61	0
29	79	1049	0	1071	59	0
30	11	2115	0	2195	106	0
30	19	2115	0	2195	94	0
31	21	1559	0	1618	78	0
31	29	1559	0	1618	92	0
32	31	1585	0	1632	89	0
32	39	1585	0	1632	85	0
33	41	1473	0	1535	75	0
33	49	1473	0	1535	75	0
34	51	1336	0	1418	69	0
34	59	1327	0	1405	71	0
35	61	1131	0	1218	72	0
35	69	1136	0	1223	60	0
36	38	635	0	677	26	0
37	15	1104	0	1180	46	0
37	58	1104	0	1180	58	0
38	25	932	0	996	50	0
38	68	932	0	996	46	0
39	35	1144	0	1228	80	0
39	78	1144	0	1228	111	0
40	45	1121	0	1179	71	0
40	88	1150	0	1209	87	0
41	55	967	0	1033	62	0
41	98	967	0	1033	63	0
42	65	881	0	943	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	A8	889	0	955	63	0
43	75	1141	0	1202	67	0
43	B8	1141	0	1202	64	0
44	85	963	0	1022	65	0
44	C8	963	0	1022	55	0
45	95	778	0	852	65	0
45	D8	778	0	852	39	0
46	A5	899	0	964	34	0
46	E8	899	0	964	37	0
47	B5	742	0	803	39	0
47	F8	747	0	805	33	0
48	C5	776	0	820	29	0
48	G8	825	0	898	39	0
49	D5	1404	0	1437	75	0
49	H8	1428	0	1454	72	0
50	E5	657	0	677	40	0
50	I8	661	0	688	36	0
51	F5	762	0	848	37	0
51	J8	762	0	848	42	0
52	G5	590	0	643	35	0
52	K8	598	0	655	35	0
53	H5	468	0	518	31	0
53	L8	468	0	518	16	0
54	I5	580	0	577	41	0
54	M8	580	0	577	50	0
55	J5	434	0	454	25	0
55	N8	434	0	454	29	0
56	K5	389	0	404	31	0
56	O8	389	0	404	33	0
57	L5	429	0	480	17	0
57	P8	419	0	458	17	0
58	M5	506	0	567	50	0
58	Q8	506	0	567	34	0
59	1L	1627	0	836	63	0
60	2L	1635	0	847	34	0
61	11	1	0	0	0	0
61	13	51	0	0	0	0
61	14	106	0	0	0	0
61	16	3	0	0	0	0
61	19	1	0	0	0	0
61	1G	36	0	0	0	0
61	1H	145	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1J	1	0	0	0	0
61	1K	1	0	0	0	0
61	2I	1	0	0	0	0
61	29	1	0	0	0	0
61	2A	1	0	0	0	0
61	2K	3	0	0	0	0
61	3I	2	0	0	0	0
61	32	1	0	0	0	0
61	39	2	0	0	0	0
61	4I	1	0	0	0	0
61	45	1	0	0	0	0
61	49	1	0	0	0	0
61	4A	1	0	0	0	0
61	4I	1	0	0	0	0
61	52	1	0	0	0	0
61	5A	1	0	0	0	0
61	5E	1	0	0	0	0
61	88	1	0	0	0	0
61	BA	1	0	0	0	0
61	BI	1	0	0	0	0
62	1I	1	0	0	0	0
62	13	120	0	0	0	0
62	14	295	0	0	0	0
62	16	12	0	0	0	0
62	1G	102	0	0	0	0
62	1H	439	0	0	0	0
62	1J	4	0	0	0	0
62	2I	2	0	0	0	0
62	29	2	0	0	0	0
62	2K	2	0	0	0	0
62	2L	3	0	0	0	0
62	3I	1	0	0	0	0
62	32	1	0	0	0	0
62	39	1	0	0	0	0
62	3E	1	0	0	0	0
62	4I	1	0	0	0	0
62	42	1	0	0	0	0
62	4L	1	0	0	0	0
62	6E	1	0	0	0	0
62	78	2	0	0	0	0
62	7I	1	0	0	0	0
62	C8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	F8	1	0	0	0	0
62	I8	1	0	0	0	0
62	J8	1	0	0	0	0
62	L8	1	0	0	0	0
62	M5	2	0	0	0	0
62	N8	1	0	0	0	0
62	O8	1	0	0	0	0
62	P8	1	0	0	0	0
62	Q8	2	0	0	0	0
63	32	8	0	0	1	0
63	3E	8	0	0	3	0
64	5A	1	0	0	0	0
64	5I	1	0	0	0	0
65	11	11	0	0	1	0
65	13	233	0	0	31	0
65	14	602	0	0	66	0
65	16	26	0	0	4	0
65	19	12	0	0	2	0
65	1F	3	0	0	0	0
65	1G	194	0	0	21	0
65	1H	1009	0	0	134	0
65	1J	5	0	0	1	0
65	21	10	0	0	0	0
65	29	7	0	0	0	0
65	2K	8	0	0	1	0
65	31	10	0	0	0	0
65	32	4	0	0	1	0
65	35	7	0	0	1	0
65	39	2	0	0	0	0
65	3A	2	0	0	0	0
65	3E	2	0	0	0	0
65	3I	3	0	0	0	0
65	3K	1	0	0	0	0
65	4E	1	0	0	0	0
65	4I	1	0	0	0	0
65	4K	2	0	0	0	0
65	4L	4	0	0	0	0
65	5A	1	0	0	0	0
65	5I	1	0	0	0	0
65	75	2	0	0	1	0
65	78	9	0	0	1	0
65	7I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	82	1	0	0	0	0
65	88	1	0	0	0	0
65	A8	2	0	0	1	0
65	B8	2	0	0	0	0
65	BI	1	0	0	0	0
65	C5	1	0	0	0	0
65	D8	1	0	0	0	0
65	E5	1	0	0	0	0
65	F8	1	0	0	0	0
65	H5	2	0	0	0	0
65	I8	2	0	0	0	0
65	L5	1	0	0	0	0
65	L8	2	0	0	0	0
65	M5	6	0	0	1	0
65	P8	1	0	0	0	0
65	Q8	1	0	0	0	0
All	All	305753	0	204808	9273	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 19.

The worst 5 of 9273 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)
27:14:1780:A:OP1	65:14:3511:HOH:O	1.75	1.02
27:14:676:A:H8	27:14:2069:G:H21	1.08	1.02
27:1H:1066:U:HO2'	27:1H:1068:A:H2	1.07	1.00
27:14:249:C:OP1	65:14:3512:HOH:O	1.80	1.00
1:13:1422:G:H5''	38:68:48:PRO:HB3	1.43	0.99

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)
26:5K:75:C:O2'	27:1H:100:G:O6[1_455]	1.97	0.23



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	188 (80%)	45 (19%)	2 (1%)	14	45
2	1E	235/256 (92%)	176 (75%)	58 (25%)	1 (0%)	30	63
3	22	204/239 (85%)	166 (81%)	38 (19%)	0	100	100
3	2E	203/239 (85%)	167 (82%)	36 (18%)	0	100	100
4	32	206/209 (99%)	180 (87%)	26 (13%)	0	100	100
4	3E	206/209 (99%)	176 (85%)	30 (15%)	0	100	100
5	42	149/162 (92%)	131 (88%)	18 (12%)	0	100	100
5	4E	149/162 (92%)	131 (88%)	18 (12%)	0	100	100
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
7	62	153/156 (98%)	127 (83%)	25 (16%)	1 (1%)	19	51
7	6E	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	72	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	7E	136/138 (99%)	115 (85%)	21 (15%)	0	100	100
9	82	125/128 (98%)	102 (82%)	22 (18%)	1 (1%)	16	48
9	8E	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	48
10	1A	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
10	1I	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
11	2A	115/129 (89%)	104 (90%)	11 (10%)	0	100	100
11	2I	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
12	3A	122/132 (92%)	93 (76%)	24 (20%)	5 (4%)	2	13
12	3I	122/132 (92%)	100 (82%)	22 (18%)	0	100	100
13	4A	119/126 (94%)	88 (74%)	31 (26%)	0	100	100
13	4I	117/126 (93%)	94 (80%)	22 (19%)	1 (1%)	14	45
14	5A	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	73 (85%)	13 (15%)	0	100	100
16	7A	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
16	7I	81/88 (92%)	71 (88%)	10 (12%)	0	100	100
17	8A	98/105 (93%)	87 (89%)	11 (11%)	0	100	100
17	8I	98/105 (93%)	82 (84%)	16 (16%)	0	100	100
18	9A	68/88 (77%)	52 (76%)	16 (24%)	0	100	100
18	9I	69/88 (78%)	57 (83%)	12 (17%)	0	100	100
19	AA	84/93 (90%)	56 (67%)	28 (33%)	0	100	100
19	AI	82/93 (88%)	65 (79%)	16 (20%)	1 (1%)	11	38
20	BA	101/106 (95%)	80 (79%)	20 (20%)	1 (1%)	13	42
20	BI	99/106 (93%)	81 (82%)	17 (17%)	1 (1%)	13	42
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
29	7I	131/229 (57%)	111 (85%)	20 (15%)	0	100	100
29	79	131/229 (57%)	115 (88%)	16 (12%)	0	100	100
30	11	270/276 (98%)	234 (87%)	31 (12%)	5 (2%)	6	27
30	19	270/276 (98%)	237 (88%)	29 (11%)	4 (2%)	8	33
31	21	202/206 (98%)	185 (92%)	16 (8%)	1 (0%)	25	58
31	29	202/206 (98%)	171 (85%)	31 (15%)	0	100	100
32	31	200/210 (95%)	177 (88%)	20 (10%)	3 (2%)	8	33
32	39	200/210 (95%)	168 (84%)	30 (15%)	2 (1%)	13	42
33	41	179/182 (98%)	145 (81%)	34 (19%)	0	100	100
33	49	179/182 (98%)	149 (83%)	30 (17%)	0	100	100
34	51	172/180 (96%)	133 (77%)	37 (22%)	2 (1%)	11	38
34	59	171/180 (95%)	122 (71%)	48 (28%)	1 (1%)	22	53
35	61	143/148 (97%)	105 (73%)	34 (24%)	4 (3%)	4	20
35	69	144/148 (97%)	109 (76%)	35 (24%)	0	100	100
36	38	74/173 (43%)	43 (58%)	29 (39%)	2 (3%)	4	21
37	15	136/140 (97%)	113 (83%)	22 (16%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	58	136/140 (97%)	108 (79%)	25 (18%)	3 (2%)	5	24
38	25	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
38	68	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	48
39	35	148/150 (99%)	104 (70%)	38 (26%)	6 (4%)	2	13
39	78	148/150 (99%)	113 (76%)	29 (20%)	6 (4%)	2	13
40	45	139/141 (99%)	105 (76%)	32 (23%)	2 (1%)	9	34
40	88	144/141 (102%)	109 (76%)	30 (21%)	5 (4%)	3	16
41	55	116/118 (98%)	98 (84%)	17 (15%)	1 (1%)	14	45
41	98	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
42	65	109/112 (97%)	82 (75%)	27 (25%)	0	100	100
42	A8	110/112 (98%)	86 (78%)	22 (20%)	2 (2%)	7	29
43	75	135/146 (92%)	112 (83%)	23 (17%)	0	100	100
43	B8	135/146 (92%)	117 (87%)	18 (13%)	0	100	100
44	85	115/118 (98%)	97 (84%)	18 (16%)	0	100	100
44	C8	115/118 (98%)	98 (85%)	15 (13%)	2 (2%)	7	30
45	95	99/101 (98%)	70 (71%)	26 (26%)	3 (3%)	3	19
45	D8	99/101 (98%)	82 (83%)	15 (15%)	2 (2%)	6	26
46	A5	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
46	E8	111/113 (98%)	97 (87%)	14 (13%)	0	100	100
47	B5	92/96 (96%)	78 (85%)	14 (15%)	0	100	100
47	F8	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
48	C5	105/110 (96%)	76 (72%)	27 (26%)	2 (2%)	6	27
48	G8	107/110 (97%)	80 (75%)	22 (21%)	5 (5%)	2	12
49	D5	174/206 (84%)	125 (72%)	47 (27%)	2 (1%)	12	39
49	H8	177/206 (86%)	127 (72%)	48 (27%)	2 (1%)	12	39
50	E5	82/85 (96%)	70 (85%)	12 (15%)	0	100	100
50	I8	82/85 (96%)	72 (88%)	10 (12%)	0	100	100
51	F5	95/98 (97%)	78 (82%)	16 (17%)	1 (1%)	12	39
51	J8	95/98 (97%)	74 (78%)	20 (21%)	1 (1%)	12	39
52	G5	69/72 (96%)	60 (87%)	8 (12%)	1 (1%)	9	34
52	K8	70/72 (97%)	61 (87%)	8 (11%)	1 (1%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	H5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
53	L8	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
54	I5	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	3	20
54	M8	69/71 (97%)	38 (55%)	28 (41%)	3 (4%)	2	13
55	J5	54/60 (90%)	45 (83%)	8 (15%)	1 (2%)	6	27
55	N8	54/60 (90%)	44 (82%)	9 (17%)	1 (2%)	6	27
56	K5	43/54 (80%)	22 (51%)	21 (49%)	0	100	100
56	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	12
57	L5	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
57	P8	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
58	M5	62/65 (95%)	52 (84%)	10 (16%)	0	100	100
58	Q8	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
All	All	11746/12685 (93%)	9634 (82%)	2013 (17%)	99 (1%)	16	48

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	61	134	PRO
37	58	137	LYS
40	88	22[A]	LYS
40	88	22[B]	LYS
2	12	154	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	156 (76%)	49 (24%)	0	2
2	1E	205/220 (93%)	162 (79%)	43 (21%)	1	4
3	22	160/188 (85%)	124 (78%)	36 (22%)	1	3
3	2E	159/188 (85%)	122 (77%)	37 (23%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	146 (81%)	34 (19%)	1	5
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	4
5	42	116/123 (94%)	96 (83%)	20 (17%)	1	7
5	4E	116/123 (94%)	95 (82%)	21 (18%)	1	6
6	52	90/90 (100%)	76 (84%)	14 (16%)	2	9
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	9
7	62	126/127 (99%)	105 (83%)	21 (17%)	2	7
7	6E	126/127 (99%)	99 (79%)	27 (21%)	1	4
8	72	119/119 (100%)	98 (82%)	21 (18%)	1	7
8	7E	119/119 (100%)	101 (85%)	18 (15%)	2	10
9	82	97/99 (98%)	67 (69%)	30 (31%)	0	0
9	8E	97/99 (98%)	73 (75%)	24 (25%)	0	2
10	1A	89/92 (97%)	69 (78%)	20 (22%)	1	3
10	1I	89/92 (97%)	68 (76%)	21 (24%)	0	2
11	2A	89/99 (90%)	69 (78%)	20 (22%)	1	3
11	2I	88/99 (89%)	74 (84%)	14 (16%)	2	9
12	3A	103/108 (95%)	77 (75%)	26 (25%)	0	1
12	3I	103/108 (95%)	83 (81%)	20 (19%)	1	5
13	4A	97/101 (96%)	77 (79%)	20 (21%)	1	4
13	4I	95/101 (94%)	70 (74%)	25 (26%)	0	1
14	5A	49/50 (98%)	35 (71%)	14 (29%)	0	1
14	5I	49/50 (98%)	37 (76%)	12 (24%)	0	2
15	6A	79/80 (99%)	73 (92%)	6 (8%)	11	36
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	5
16	7A	72/74 (97%)	59 (82%)	13 (18%)	1	6
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	5
17	8A	95/97 (98%)	80 (84%)	15 (16%)	2	9
17	8I	95/97 (98%)	83 (87%)	12 (13%)	3	15
18	9A	61/77 (79%)	47 (77%)	14 (23%)	0	3
18	9I	62/77 (80%)	47 (76%)	15 (24%)	0	2
19	AA	73/80 (91%)	50 (68%)	23 (32%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	73/80 (91%)	52 (71%)	21 (29%)	0	1
20	BA	75/82 (92%)	65 (87%)	10 (13%)	3	13
20	BI	75/82 (92%)	63 (84%)	12 (16%)	2	9
21	1B	20/22 (91%)	17 (85%)	3 (15%)	2	10
21	1F	19/22 (86%)	17 (90%)	2 (10%)	5	22
29	71	111/181 (61%)	95 (86%)	16 (14%)	2	11
29	79	111/181 (61%)	97 (87%)	14 (13%)	3	15
30	11	214/218 (98%)	171 (80%)	43 (20%)	1	4
30	19	214/218 (98%)	172 (80%)	42 (20%)	1	5
31	21	164/166 (99%)	133 (81%)	31 (19%)	1	5
31	29	164/166 (99%)	132 (80%)	32 (20%)	1	5
32	31	161/166 (97%)	130 (81%)	31 (19%)	1	5
32	39	161/166 (97%)	130 (81%)	31 (19%)	1	5
33	41	155/156 (99%)	119 (77%)	36 (23%)	0	2
33	49	155/156 (99%)	114 (74%)	41 (26%)	0	1
34	51	145/148 (98%)	113 (78%)	32 (22%)	1	3
34	59	144/148 (97%)	115 (80%)	29 (20%)	1	4
35	61	122/124 (98%)	86 (70%)	36 (30%)	0	0
35	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
36	38	66/135 (49%)	39 (59%)	27 (41%)	0	0
37	15	117/119 (98%)	94 (80%)	23 (20%)	1	5
37	58	117/119 (98%)	83 (71%)	34 (29%)	0	1
38	25	100/100 (100%)	79 (79%)	21 (21%)	1	4
38	68	100/100 (100%)	76 (76%)	24 (24%)	0	2
39	35	116/116 (100%)	71 (61%)	45 (39%)	0	0
39	78	116/116 (100%)	83 (72%)	33 (28%)	0	1
40	45	111/111 (100%)	88 (79%)	23 (21%)	1	4
40	88	113/111 (102%)	88 (78%)	25 (22%)	1	3
41	55	101/101 (100%)	80 (79%)	21 (21%)	1	4
41	98	101/101 (100%)	74 (73%)	27 (27%)	0	1
42	65	87/88 (99%)	68 (78%)	19 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	A8	88/88 (100%)	62 (70%)	26 (30%)	0	0
43	75	120/127 (94%)	88 (73%)	32 (27%)	0	1
43	B8	120/127 (94%)	87 (72%)	33 (28%)	0	1
44	85	93/94 (99%)	73 (78%)	20 (22%)	1	4
44	C8	93/94 (99%)	69 (74%)	24 (26%)	0	1
45	95	82/82 (100%)	54 (66%)	28 (34%)	0	0
45	D8	82/82 (100%)	56 (68%)	26 (32%)	0	0
46	A5	92/92 (100%)	70 (76%)	22 (24%)	0	2
46	E8	92/92 (100%)	75 (82%)	17 (18%)	1	6
47	B5	76/78 (97%)	58 (76%)	18 (24%)	0	2
47	F8	76/78 (97%)	63 (83%)	13 (17%)	1	7
48	C5	78/91 (86%)	62 (80%)	16 (20%)	1	4
48	G8	88/91 (97%)	64 (73%)	24 (27%)	0	1
49	D5	155/179 (87%)	122 (79%)	33 (21%)	1	4
49	H8	158/179 (88%)	122 (77%)	36 (23%)	0	3
50	E5	65/67 (97%)	50 (77%)	15 (23%)	0	3
50	I8	66/67 (98%)	52 (79%)	14 (21%)	1	4
51	F5	82/83 (99%)	63 (77%)	19 (23%)	0	2
51	J8	82/83 (99%)	64 (78%)	18 (22%)	1	3
52	G5	64/67 (96%)	52 (81%)	12 (19%)	1	5
52	K8	65/67 (97%)	45 (69%)	20 (31%)	0	0
53	H5	51/52 (98%)	41 (80%)	10 (20%)	1	5
53	L8	51/52 (98%)	42 (82%)	9 (18%)	1	7
54	I5	63/63 (100%)	49 (78%)	14 (22%)	1	3
54	M8	63/63 (100%)	47 (75%)	16 (25%)	0	1
55	J5	48/52 (92%)	40 (83%)	8 (17%)	2	7
55	N8	48/52 (92%)	35 (73%)	13 (27%)	0	1
56	K5	44/52 (85%)	31 (70%)	13 (30%)	0	0
56	O8	44/52 (85%)	27 (61%)	17 (39%)	0	0
57	L5	42/42 (100%)	33 (79%)	9 (21%)	1	4
57	P8	40/42 (95%)	32 (80%)	8 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	M5	52/55 (94%)	42 (81%)	10 (19%)	1	5
58	Q8	52/55 (94%)	41 (79%)	11 (21%)	1	4
All	All	9889/10493 (94%)	7700 (78%)	2189 (22%)	1	3

5 of 2189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	45	22	LYS
42	65	101	LEU
40	45	10	ARG
50	E5	7	LEU
41	98	6	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
7	62	97	GLN
52	G5	46	GLN
32	39	169	ASN
56	K5	49	HIS
50	E5	35	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1511/1522 (99%)	364 (24%)	51 (3%)
1	1G	1509/1522 (99%)	385 (25%)	48 (3%)
22	1K	74/76 (97%)	38 (51%)	0
23	2K	73/76 (96%)	20 (27%)	2 (2%)
24	3K	74/76 (97%)	39 (52%)	3 (4%)
24	3L	74/76 (97%)	37 (50%)	1 (1%)
25	4K	29/60 (48%)	8 (27%)	2 (6%)
25	4L	29/60 (48%)	12 (41%)	2 (6%)
26	5K	74/76 (97%)	35 (47%)	5 (6%)
27	14	2871/2917 (98%)	785 (27%)	65 (2%)
27	1H	2884/2917 (98%)	724 (25%)	77 (2%)
28	16	121/122 (99%)	27 (22%)	1 (0%)
28	1J	120/122 (98%)	39 (32%)	4 (3%)
59	1L	74/76 (97%)	35 (47%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
60	2L	73/76 (96%)	23 (31%)	0
All	All	9590/9774 (98%)	2571 (26%)	262 (2%)

5 of 2571 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G
1	13	28	G

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	14	1762	A
27	14	2032	G
28	1J	66	A
27	1H	1256	A
27	1H	1156	C

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

92 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
60	5MU	2L	54	60	19,22,23	3.81	5 (26%)	28,32,35	3.10	10 (35%)
22	MIA	1K	37	22	24,31,32	2.23	3 (12%)	26,44,47	3.01	8 (30%)
23	H2U	2K	16	23	18,21,22	1.88	4 (22%)	21,30,33	1.90	5 (23%)
24	PSU	3K	32	24	18,21,22	1.03	1 (5%)	22,30,33	1.61	4 (18%)
1	5MC	13	1407	1	18,22,23	3.34	7 (38%)	26,32,35	1.12	2 (7%)
27	5MU	14	1939	27,61	19,22,23	3.79	5 (26%)	28,32,35	3.43	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	PSU	1H	1940	27	18,21,22	0.93	1 (5%)	22,30,33	1.58	4 (18%)
1	UR3	1G	1498	1	19,22,23	2.64	6 (31%)	26,32,35	1.72	4 (15%)
59	MIA	1L	37	59	24,31,32	2.29	3 (12%)	26,44,47	3.02	9 (34%)
24	MIA	3K	37	24,25	24,31,32	2.51	4 (16%)	26,44,47	3.26	11 (42%)
27	PSU	1H	1934	27	18,21,22	1.11	2 (11%)	22,30,33	1.77	6 (27%)
27	OMU	1H	2565	27,62	19,22,23	2.11	6 (31%)	26,31,34	2.36	9 (34%)
1	7MG	1G	527	61,1	22,26,27	3.06	6 (27%)	29,39,42	2.86	10 (34%)
27	5MU	14	1915	27	19,22,23	3.95	5 (26%)	28,32,35	3.43	9 (32%)
59	5MU	1L	54	59	19,22,23	3.86	5 (26%)	28,32,35	3.21	8 (28%)
1	5MC	13	967	1	18,22,23	3.70	7 (38%)	26,32,35	1.09	1 (3%)
1	5MC	1G	1400	1	18,22,23	3.78	7 (38%)	26,32,35	1.47	5 (19%)
26	5MU	5K	54	26	19,22,23	3.98	5 (26%)	28,32,35	3.12	9 (32%)
27	PSU	14	1911	27	18,21,22	1.10	1 (5%)	22,30,33	1.51	4 (18%)
26	H2U	5K	16	26	18,21,22	2.15	4 (22%)	21,30,33	1.97	5 (23%)
27	PSU	14	2605	27	18,21,22	1.32	3 (16%)	22,30,33	2.05	7 (31%)
27	5MU	1H	1962	27,61	19,22,23	3.37	5 (26%)	28,32,35	4.32	9 (32%)
1	2MG	13	1207	61,1	18,26,27	2.46	7 (38%)	16,38,41	1.69	3 (18%)
1	MA6	13	1518	1	18,26,27	0.93	0	19,38,41	2.68	2 (10%)
1	MA6	13	1519	1	18,26,27	0.94	1 (5%)	19,38,41	3.16	3 (15%)
1	5MC	13	1400	1	18,22,23	3.62	7 (38%)	26,32,35	1.11	2 (7%)
22	4SU	1K	8	22	18,21,22	1.77	3 (16%)	26,30,33	2.30	6 (23%)
26	4SU	5K	8	26	18,21,22	1.73	3 (16%)	26,30,33	2.42	5 (19%)
60	H2U	2L	16	60	18,21,22	2.10	4 (22%)	21,30,33	1.94	5 (23%)
22	PSU	1K	55	22	18,21,22	1.13	1 (5%)	22,30,33	1.84	6 (27%)
23	PSU	2K	39	23	18,21,22	1.32	2 (11%)	22,30,33	1.88	5 (22%)
26	PSU	5K	55	26	18,21,22	1.13	1 (5%)	22,30,33	1.61	4 (18%)
27	OMG	1H	2264	27,61,23	18,26,27	5.00	8 (44%)	19,38,41	3.70	8 (42%)
1	M2G	1G	966	1	20,27,28	3.80	7 (35%)	22,40,43	1.30	4 (18%)
22	7MG	1K	46	22	22,26,27	3.09	6 (27%)	29,39,42	2.81	10 (34%)
23	4SU	2K	8	23	18,21,22	1.74	4 (22%)	26,30,33	2.44	6 (23%)
24	PSU	3L	32	24	18,21,22	1.14	1 (5%)	22,30,33	1.73	4 (18%)
27	OMC	1H	1943	27,61	19,22,23	1.73	3 (15%)	26,31,34	1.31	4 (15%)
1	4OC	1G	1402	62,1	20,23,24	2.62	7 (35%)	26,32,35	1.58	4 (15%)
59	PSU	1L	32	59	18,21,22	0.99	1 (5%)	22,30,33	1.43	3 (13%)
27	5MC	1H	1965	27	18,22,23	3.32	7 (38%)	26,32,35	1.47	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	13	516	62,1	18,21,22	0.91	1 (5%)	22,30,33	1.55	4 (18%)
27	5MC	1H	1985	27,61	18,22,23	3.68	6 (33%)	26,32,35	1.44	3 (11%)
27	5MC	14	1942	27	18,22,23	3.76	7 (38%)	26,32,35	1.32	5 (19%)
1	5MC	1G	1407	1	18,22,23	3.42	7 (38%)	26,32,35	1.21	3 (11%)
23	3AU	2K	47	23	24,28,29	2.94	7 (29%)	33,40,43	1.71	8 (24%)
12	0TD	3A	89	12	7,9,10	1.40	1 (14%)	6,11,13	1.74	2 (33%)
26	PSU	5K	32	26	18,21,22	1.12	1 (5%)	22,30,33	1.68	3 (13%)
27	5MC	14	1962	27,61	18,22,23	3.42	7 (38%)	26,32,35	1.29	3 (11%)
1	4OC	13	1402	62,1	20,23,24	2.86	8 (40%)	26,32,35	1.45	4 (15%)
12	0TD	3I	89	12	7,9,10	1.32	0	6,11,13	3.46	3 (50%)
1	UR3	13	1498	1	19,22,23	2.72	6 (31%)	26,32,35	1.93	6 (23%)
22	5MU	1K	54	22	19,22,23	3.86	5 (26%)	28,32,35	3.20	9 (32%)
27	5MU	1H	1938	27	19,22,23	4.22	5 (26%)	28,32,35	3.87	10 (35%)
60	4SU	2L	8	60	18,21,22	1.77	3 (16%)	26,30,33	2.20	6 (23%)
1	7MG	13	527	61,1	22,26,27	2.99	8 (36%)	29,39,42	2.75	9 (31%)
1	5MC	13	1404	1	18,22,23	3.19	7 (38%)	26,32,35	1.22	1 (3%)
22	PSU	1K	32	22,61	18,21,22	1.08	1 (5%)	22,30,33	1.22	2 (9%)
1	5MC	1G	967	1	18,22,23	3.57	7 (38%)	26,32,35	1.16	2 (7%)
1	PSU	1G	516	62,1	18,21,22	1.16	1 (5%)	22,30,33	1.45	2 (9%)
23	H2U	2K	20	23	18,21,22	2.11	4 (22%)	21,30,33	1.98	4 (19%)
60	3AU	2L	47	60	24,28,29	2.80	8 (33%)	33,40,43	1.90	8 (24%)
27	2MA	1H	2516	27,61	19,25,26	2.67	6 (31%)	21,37,40	2.22	6 (28%)
60	PSU	2L	55	60	18,21,22	1.33	2 (11%)	22,30,33	1.69	4 (18%)
26	MIA	5K	37	26	24,31,32	2.56	4 (16%)	26,44,47	3.34	11 (42%)
1	2MG	1G	1207	1	18,26,27	2.59	7 (38%)	16,38,41	1.33	3 (18%)
22	PSU	1K	39	22	18,21,22	1.04	1 (5%)	22,30,33	2.00	4 (18%)
1	MA6	1G	1518	1	18,26,27	1.12	2 (11%)	19,38,41	2.49	2 (10%)
27	2MA	14	2503	27,61,62	19,25,26	2.78	4 (21%)	21,37,40	1.81	3 (14%)
59	PSU	1L	39	59	18,21,22	1.13	3 (16%)	22,30,33	2.02	7 (31%)
1	MA6	1G	1519	1	18,26,27	1.05	2 (11%)	19,38,41	2.80	2 (10%)
23	5MU	2K	54	23	19,22,23	3.74	5 (26%)	28,32,35	3.26	7 (25%)
26	PSU	5K	39	26	18,21,22	1.20	1 (5%)	22,30,33	1.75	5 (22%)
23	PSU	2K	32	23	18,21,22	1.07	2 (11%)	22,30,33	1.84	4 (18%)
27	OMU	14	2552	27,62	19,22,23	2.43	6 (31%)	26,31,34	1.91	6 (23%)
26	H2U	5K	20	26,28	18,21,22	2.32	4 (22%)	21,30,33	1.88	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	PSU	2L	32	60	18,21,22	1.02	1 (5%)	22,30,33	2.00	5 (22%)
23	7MG	2K	46	23	22,26,27	3.02	6 (27%)	29,39,42	2.76	10 (34%)
60	PSU	2L	39	60	18,21,22	1.16	1 (5%)	22,30,33	1.65	4 (18%)
1	5MC	1G	1404	1	18,22,23	3.44	7 (38%)	26,32,35	1.51	3 (11%)
27	PSU	14	1917	27	18,21,22	1.11	2 (11%)	22,30,33	1.65	5 (22%)
27	OMG	14	2251	27,60,61	18,26,27	5.21	8 (44%)	19,38,41	3.84	6 (31%)
23	MIA	2K	37	23	24,31,32	2.37	4 (16%)	26,44,47	2.56	10 (38%)
23	PSU	2K	55	23	18,21,22	1.24	1 (5%)	22,30,33	1.64	3 (13%)
24	MIA	3L	37	24	24,31,32	2.55	4 (16%)	26,44,47	3.40	11 (42%)
24	PSU	3K	39	24	18,21,22	1.15	1 (5%)	22,30,33	1.61	4 (18%)
60	MIA	2L	37	60	24,31,32	2.30	3 (12%)	26,44,47	2.80	8 (30%)
60	7MG	2L	46	60	22,26,27	3.24	5 (22%)	29,39,42	2.76	11 (37%)
24	PSU	3L	39	24	18,21,22	1.15	1 (5%)	22,30,33	1.61	3 (13%)
27	OMC	14	1920	27	19,22,23	1.75	3 (15%)	26,31,34	1.08	1 (3%)
1	M2G	13	966	1	20,27,28	3.39	7 (35%)	22,40,43	1.53	6 (27%)
27	PSU	1H	2618	27	18,21,22	1.29	3 (16%)	22,30,33	1.88	6 (27%)

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
60	5MU	2L	54	60	–	2/7/25/26	0/2/2/2
22	MIA	1K	37	22	–	4/11/33/34	0/3/3/3
23	H2U	2K	16	23	–	0/7/38/39	0/2/2/2
24	PSU	3K	32	24	–	2/7/25/26	0/2/2/2
1	5MC	13	1407	1	–	0/7/25/26	0/2/2/2
27	5MU	14	1939	27,61	–	0/7/25/26	0/2/2/2
27	PSU	1H	1940	27	–	0/7/25/26	0/2/2/2
1	UR3	1G	1498	1	–	0/7/25/26	0/2/2/2
59	MIA	1L	37	59	–	2/11/33/34	0/3/3/3
24	MIA	3K	37	24,25	–	8/11/33/34	0/3/3/3
27	PSU	1H	1934	27	–	0/7/25/26	0/2/2/2
27	OMU	1H	2565	27,62	–	0/9/27/28	0/2/2/2
1	7MG	1G	527	61,1	–	2/7/37/38	0/3/3/3
27	5MU	14	1915	27	–	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	5MU	1L	54	59	-	0/7/25/26	0/2/2/2
1	5MC	13	967	1	-	0/7/25/26	0/2/2/2
1	5MC	1G	1400	1	-	2/7/25/26	0/2/2/2
26	5MU	5K	54	26	-	2/7/25/26	0/2/2/2
27	PSU	14	1911	27	-	0/7/25/26	0/2/2/2
26	H2U	5K	16	26	-	3/7/38/39	0/2/2/2
27	PSU	14	2605	27	-	0/7/25/26	0/2/2/2
27	5MU	1H	1962	27,61	-	2/7/25/26	0/2/2/2
1	2MG	13	1207	61,1	-	0/5/27/28	0/3/3/3
1	MA6	13	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	13	1519	1	-	3/7/29/30	0/3/3/3
1	5MC	13	1400	1	-	0/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	1/7/25/26	0/2/2/2
26	4SU	5K	8	26	-	2/7/25/26	0/2/2/2
60	H2U	2L	16	60	-	0/7/38/39	0/2/2/2
22	PSU	1K	55	22	-	4/7/25/26	0/2/2/2
23	PSU	2K	39	23	-	0/7/25/26	0/2/2/2
26	PSU	5K	55	26	-	2/7/25/26	0/2/2/2
27	OMG	1H	2264	27,61,23	-	0/5/27/28	0/3/3/3
1	M2G	1G	966	1	-	0/7/29/30	0/3/3/3
22	7MG	1K	46	22	-	2/7/37/38	0/3/3/3
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
24	PSU	3L	32	24	-	6/7/25/26	0/2/2/2
27	OMC	1H	1943	27,61	-	0/9/27/28	0/2/2/2
1	4OC	1G	1402	62,1	-	2/9/29/30	0/2/2/2
59	PSU	1L	32	59	-	0/7/25/26	0/2/2/2
27	5MC	1H	1965	27	-	0/7/25/26	0/2/2/2
1	PSU	13	516	62,1	-	0/7/25/26	0/2/2/2
27	5MC	1H	1985	27,61	-	0/7/25/26	0/2/2/2
27	5MC	14	1942	27	-	0/7/25/26	0/2/2/2
1	5MC	1G	1407	1	-	0/7/25/26	0/2/2/2
23	3AU	2K	47	23	-	7/16/34/35	0/2/2/2
12	0TD	3A	89	12	-	4/7/12/14	-
26	PSU	5K	32	26	-	0/7/25/26	0/2/2/2
27	5MC	14	1962	27,61	-	2/7/25/26	0/2/2/2
1	4OC	13	1402	62,1	-	2/9/29/30	0/2/2/2
12	0TD	3I	89	12	-	3/7/12/14	-
1	UR3	13	1498	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
27	5MU	1H	1938	27	-	3/7/25/26	0/2/2/2
60	4SU	2L	8	60	-	2/7/25/26	0/2/2/2
1	7MG	13	527	61,1	-	2/7/37/38	0/3/3/3
1	5MC	13	1404	1	-	0/7/25/26	0/2/2/2
22	PSU	1K	32	22,61	-	0/7/25/26	0/2/2/2
1	5MC	1G	967	1	-	0/7/25/26	0/2/2/2
1	PSU	1G	516	62,1	-	0/7/25/26	0/2/2/2
23	H2U	2K	20	23	-	5/7/38/39	0/2/2/2
60	3AU	2L	47	60	-	7/16/34/35	0/2/2/2
27	2MA	1H	2516	27,61	-	1/3/25/26	0/3/3/3
60	PSU	2L	55	60	-	0/7/25/26	0/2/2/2
26	MIA	5K	37	26	-	6/11/33/34	0/3/3/3
1	2MG	1G	1207	1	-	2/5/27/28	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
1	MA6	1G	1518	1	-	5/7/29/30	0/3/3/3
27	2MA	14	2503	27,61,62	-	1/3/25/26	0/3/3/3
59	PSU	1L	39	59	-	0/7/25/26	0/2/2/2
1	MA6	1G	1519	1	-	2/7/29/30	0/3/3/3
23	5MU	2K	54	23	-	0/7/25/26	0/2/2/2
26	PSU	5K	39	26	-	1/7/25/26	0/2/2/2
23	PSU	2K	32	23	-	0/7/25/26	0/2/2/2
27	OMU	14	2552	27,62	-	4/9/27/28	0/2/2/2
26	H2U	5K	20	26,28	-	5/7/38/39	0/2/2/2
60	PSU	2L	32	60	-	0/7/25/26	0/2/2/2
23	7MG	2K	46	23	-	0/7/37/38	0/3/3/3
60	PSU	2L	39	60	-	0/7/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/7/25/26	0/2/2/2
27	PSU	14	1917	27	-	0/7/25/26	0/2/2/2
27	OMG	14	2251	27,60,61	-	0/5/27/28	0/3/3/3
23	MIA	2K	37	23	-	3/11/33/34	0/3/3/3
23	PSU	2K	55	23	-	2/7/25/26	0/2/2/2
24	MIA	3L	37	24	-	4/11/33/34	0/3/3/3
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
60	MIA	2L	37	60	-	4/11/33/34	0/3/3/3
60	7MG	2L	46	60	-	2/7/37/38	0/3/3/3
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
27	OMC	14	1920	27	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M2G	13	966	1	-	0/7/29/30	0/3/3/3
27	PSU	1H	2618	27	-	0/7/25/26	0/2/2/2

The worst 5 of 374 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	14	2251	OMG	C8-N7	-14.81	1.09	1.35
27	1H	1938	5MU	C2-N1	14.31	1.61	1.38
27	1H	2264	OMG	C8-N7	-13.83	1.11	1.35
26	5K	54	5MU	C2-N1	12.92	1.59	1.38
27	14	1915	5MU	C2-N1	12.72	1.58	1.38

The worst 5 of 499 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1H	1962	5MU	C5-C4-N3	13.97	127.23	115.31
1	13	1519	MA6	N1-C6-N6	-12.51	103.89	117.06
27	1H	1938	5MU	C5-C4-N3	12.45	125.94	115.31
24	3L	37	MIA	C11-S10-C2	11.84	111.11	102.27
26	5K	37	MIA	C11-S10-C2	11.46	110.83	102.27

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	13	527	7MG	O4'-C4'-C5'-O5'
1	13	527	7MG	C3'-C4'-C5'-O5'
1	1G	1207	2MG	O4'-C4'-C5'-O5'
1	1G	1207	2MG	C3'-C4'-C5'-O5'
1	13	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

55 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2L	54	5MU	4	0
22	1K	37	MIA	1	0
27	14	1939	5MU	3	0
27	1H	1940	PSU	1	0
1	1G	1498	UR3	3	0
59	1L	37	MIA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3K	37	MIA	2	0
27	1H	2565	OMU	3	0
27	14	1915	5MU	1	0
1	13	967	5MC	1	0
1	1G	1400	5MC	1	0
26	5K	54	5MU	1	0
27	14	1911	PSU	1	0
26	5K	16	H2U	4	0
27	1H	1962	5MU	1	0
1	13	1207	2MG	1	0
1	13	1518	MA6	2	0
1	13	1519	MA6	2	0
1	13	1400	5MC	1	0
22	1K	55	PSU	4	0
26	5K	55	PSU	1	0
27	1H	2264	OMG	1	0
22	1K	46	7MG	4	0
24	3L	32	PSU	1	0
27	1H	1943	OMC	2	0
1	1G	1402	4OC	2	0
27	1H	1985	5MC	1	0
27	14	1942	5MC	1	0
12	3A	89	0TD	3	0
27	14	1962	5MC	2	0
1	13	1402	4OC	1	0
1	13	1498	UR3	4	0
22	1K	54	5MU	1	0
27	1H	1938	5MU	1	0
60	2L	8	4SU	2	0
1	1G	967	5MC	2	0
1	1G	516	PSU	1	0
23	2K	20	H2U	1	0
27	1H	2516	2MA	3	0
26	5K	37	MIA	1	0
1	1G	1207	2MG	3	0
1	1G	1518	MA6	2	0
27	14	2503	2MA	2	0
59	1L	39	PSU	1	0
1	1G	1519	MA6	4	0
23	2K	54	5MU	2	0
27	14	2552	OMU	4	0
26	5K	20	H2U	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2L	32	PSU	1	0
23	2K	46	7MG	1	0
27	14	2251	OMG	2	0
23	2K	55	PSU	1	0
24	3L	37	MIA	2	0
24	3K	39	PSU	1	0
1	13	966	M2G	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1376 ligands modelled in this entry, 1374 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	$\# Z  > 2$
63	SF4	3E	302	4	0,12,12	-	-	-		
63	SF4	32	303	4	0,12,12	-	-	-		

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
63	SF4	3E	302	4	-	-	0/6/5/5
63	SF4	32	303	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	3E	302	SF4	3	0
63	32	303	SF4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1504/1522 (98%)	-0.40	5 (0%) 90 81	28, 69, 150, 240	0
1	1G	1501/1522 (98%)	-0.34	7 (0%) 87 75	38, 81, 144, 248	0
2	12	237/256 (92%)	1.04	34 (14%) 7 4	85, 134, 165, 184	0
2	1E	237/256 (92%)	0.51	12 (5%) 34 20	67, 105, 146, 160	0
3	22	206/239 (86%)	0.35	2 (0%) 79 64	81, 109, 137, 144	0
3	2E	205/239 (85%)	0.25	4 (1%) 64 45	62, 81, 122, 145	0
4	32	208/209 (99%)	0.12	5 (2%) 59 41	58, 74, 95, 120	0
4	3E	208/209 (99%)	0.24	0 100 100	58, 77, 99, 108	0
5	42	151/162 (93%)	0.15	0 100 100	67, 84, 102, 133	0
5	4E	151/162 (93%)	0.01	1 (0%) 84 70	50, 67, 90, 113	0
6	52	101/101 (100%)	0.15	1 (0%) 79 64	53, 74, 90, 111	0
6	5E	101/101 (100%)	0.02	0 100 100	50, 73, 89, 106	0
7	62	155/156 (99%)	0.16	4 (2%) 57 38	78, 93, 131, 152	0
7	6E	155/156 (99%)	0.05	3 (1%) 66 47	66, 85, 109, 117	0
8	72	138/138 (100%)	-0.08	0 100 100	64, 85, 96, 105	0
8	7E	138/138 (100%)	-0.12	0 100 100	55, 72, 85, 97	0
9	82	127/128 (99%)	0.18	1 (0%) 82 68	78, 115, 132, 137	0
9	8E	127/128 (99%)	0.16	1 (0%) 82 68	57, 102, 119, 123	0
10	1A	99/105 (94%)	0.53	2 (2%) 64 45	86, 123, 142, 144	0
10	1I	99/105 (94%)	0.64	4 (4%) 43 25	52, 105, 131, 135	0
11	2A	117/129 (90%)	-0.02	1 (0%) 81 66	50, 77, 104, 140	0
11	2I	116/129 (89%)	-0.20	0 100 100	42, 69, 94, 119	0
12	3A	124/132 (93%)	-0.07	0 100 100	49, 69, 95, 149	0
12	3I	124/132 (93%)	-0.24	2 (1%) 70 52	37, 47, 77, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	121/126 (96%)	0.29	5 (4%) 42 24	81, 118, 131, 141	0
13	4I	119/126 (94%)	0.36	5 (4%) 41 24	57, 92, 109, 118	0
14	5A	60/61 (98%)	0.02	0 100 100	83, 97, 121, 126	0
14	5I	60/61 (98%)	-0.19	0 100 100	61, 71, 85, 99	0
15	6A	88/89 (98%)	-0.26	0 100 100	53, 75, 94, 100	0
15	6I	88/89 (98%)	-0.14	1 (1%) 77 61	44, 66, 90, 98	0
16	7A	84/88 (95%)	0.01	0 100 100	59, 68, 86, 124	0
16	7I	83/88 (94%)	0.09	1 (1%) 76 60	63, 76, 99, 127	0
17	8A	100/105 (95%)	-0.14	1 (1%) 79 64	57, 77, 94, 110	0
17	8I	100/105 (95%)	-0.24	1 (1%) 79 64	53, 69, 81, 87	0
18	9A	70/88 (79%)	0.08	1 (1%) 73 56	60, 75, 104, 126	0
18	9I	71/88 (80%)	-0.00	1 (1%) 73 56	54, 69, 110, 127	0
19	AA	86/93 (92%)	0.58	5 (5%) 30 18	105, 131, 158, 170	0
19	AI	84/93 (90%)	0.56	5 (5%) 29 17	72, 96, 114, 119	0
20	BA	103/106 (97%)	0.02	2 (1%) 66 47	65, 84, 109, 116	0
20	BI	101/106 (95%)	-0.17	0 100 100	65, 83, 111, 123	0
21	1B	25/27 (92%)	-0.04	0 100 100	94, 109, 123, 127	0
21	1F	24/27 (88%)	-0.09	0 100 100	74, 85, 99, 110	0
22	1K	69/76 (90%)	0.52	6 (8%) 17 10	51, 163, 204, 219	0
23	2K	66/76 (86%)	-0.53	0 100 100	33, 59, 81, 131	0
24	3K	73/76 (96%)	0.73	3 (4%) 42 24	35, 200, 222, 230	0
24	3L	73/76 (96%)	0.71	5 (6%) 25 14	49, 197, 229, 238	0
25	4K	30/60 (50%)	0.29	0 100 100	43, 130, 219, 232	0
25	4L	30/60 (50%)	0.24	0 100 100	61, 148, 218, 223	0
26	5K	68/76 (89%)	0.94	6 (8%) 17 10	80, 154, 180, 197	0
27	14	2865/2917 (98%)	-0.38	22 (0%) 82 68	27, 59, 194, 252	0
27	1H	2879/2917 (98%)	-0.64	27 (0%) 81 66	13, 37, 171, 243	0
28	16	122/122 (100%)	-0.79	0 100 100	37, 55, 74, 146	0
28	1J	121/122 (99%)	-0.27	1 (0%) 82 68	65, 90, 118, 175	0
29	71	135/229 (58%)	1.07	18 (13%) 8 5	113, 202, 228, 236	0
29	79	135/229 (58%)	0.99	13 (9%) 15 9	131, 194, 215, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	11	272/276 (98%)	-0.51	0 100 100	14, 32, 47, 68	0
30	19	272/276 (98%)	-0.28	2 (0%) 84 70	25, 45, 61, 73	0
31	21	204/206 (99%)	-0.44	0 100 100	16, 46, 74, 97	0
31	29	204/206 (99%)	-0.08	0 100 100	38, 72, 98, 111	0
32	31	202/210 (96%)	-0.39	1 (0%) 87 75	13, 42, 72, 99	0
32	39	202/210 (96%)	0.32	8 (3%) 43 25	30, 64, 95, 109	0
33	41	181/182 (99%)	0.08	4 (2%) 62 42	50, 66, 95, 111	0
33	49	181/182 (99%)	0.20	1 (0%) 85 72	82, 99, 124, 132	0
34	51	174/180 (96%)	0.32	6 (3%) 48 28	53, 76, 96, 117	0
34	59	173/180 (96%)	0.81	15 (8%) 17 10	135, 183, 220, 240	0
35	61	145/148 (97%)	0.51	7 (4%) 36 21	43, 96, 112, 126	0
35	69	146/148 (98%)	0.58	9 (6%) 28 17	52, 93, 116, 129	0
36	38	84/173 (48%)	1.46	20 (23%) 2 1	116, 159, 172, 180	0
37	15	138/140 (98%)	0.22	2 (1%) 73 56	51, 84, 109, 119	0
37	58	138/140 (98%)	-0.08	5 (3%) 46 27	29, 46, 80, 92	0
38	25	122/122 (100%)	-0.03	0 100 100	43, 65, 83, 95	0
38	68	122/122 (100%)	-0.56	0 100 100	21, 40, 54, 64	0
39	35	150/150 (100%)	0.30	5 (3%) 49 30	35, 77, 106, 122	0
39	78	150/150 (100%)	-0.20	2 (1%) 74 58	19, 46, 81, 121	0
40	45	141/141 (100%)	0.03	2 (1%) 73 56	47, 85, 114, 163	0
40	88	141/141 (100%)	-0.16	3 (2%) 63 44	25, 44, 67, 91	5 (3%)
41	55	118/118 (100%)	-0.37	0 100 100	38, 57, 78, 93	0
41	98	118/118 (100%)	-0.46	0 100 100	24, 42, 61, 73	0
42	65	111/112 (99%)	0.39	2 (1%) 67 49	63, 89, 122, 132	0
42	A8	112/112 (100%)	-0.01	3 (2%) 56 36	41, 55, 75, 94	0
43	75	137/146 (93%)	0.25	5 (3%) 46 27	57, 73, 145, 164	0
43	B8	137/146 (93%)	-0.27	0 100 100	32, 53, 104, 138	0
44	85	117/118 (99%)	0.32	5 (4%) 40 24	41, 78, 120, 134	0
44	C8	117/118 (99%)	-0.35	3 (2%) 57 38	20, 36, 63, 93	0
45	95	101/101 (100%)	0.92	9 (8%) 17 10	41, 94, 109, 125	0
45	D8	101/101 (100%)	-0.01	2 (1%) 64 45	23, 57, 73, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	A5	113/113 (100%)	0.10	4 (3%) 47 28	37, 50, 93, 124	0
46	E8	113/113 (100%)	-0.31	2 (1%) 67 49	25, 35, 63, 104	0
47	B5	94/96 (97%)	-0.03	2 (2%) 63 44	40, 58, 79, 106	0
47	F8	95/96 (98%)	-0.36	0 100 100	23, 36, 54, 74	0
48	C5	107/110 (97%)	1.27	25 (23%) 2 1	61, 81, 130, 140	0
48	G8	109/110 (99%)	0.46	9 (8%) 19 10	44, 71, 118, 137	0
49	D5	176/206 (85%)	0.48	1 (0%) 85 72	89, 130, 206, 210	0
49	H8	179/206 (86%)	0.57	11 (6%) 28 17	47, 85, 160, 171	0
50	E5	84/85 (98%)	-0.08	2 (2%) 59 41	44, 65, 88, 110	0
50	I8	84/85 (98%)	-0.32	0 100 100	21, 38, 63, 81	0
51	F5	97/98 (98%)	0.36	10 (10%) 13 8	37, 57, 98, 111	0
51	J8	97/98 (98%)	-0.12	4 (4%) 42 24	20, 41, 88, 114	0
52	G5	71/72 (98%)	0.29	3 (4%) 41 24	49, 69, 96, 122	0
52	K8	72/72 (100%)	-0.00	4 (5%) 31 19	30, 47, 64, 82	0
53	H5	59/60 (98%)	0.21	2 (3%) 48 28	57, 76, 119, 122	0
53	L8	59/60 (98%)	-0.43	0 100 100	30, 44, 74, 93	0
54	I5	71/71 (100%)	0.73	4 (5%) 31 19	104, 142, 169, 174	0
54	M8	71/71 (100%)	1.17	13 (18%) 4 2	72, 115, 152, 158	0
55	J5	56/60 (93%)	0.29	3 (5%) 32 19	35, 63, 121, 129	0
55	N8	56/60 (93%)	-0.03	3 (5%) 32 19	18, 47, 108, 114	0
56	K5	45/54 (83%)	1.32	7 (15%) 6 3	103, 136, 163, 169	0
56	O8	45/54 (83%)	1.33	13 (28%) 1 1	73, 103, 134, 144	0
57	L5	49/49 (100%)	-0.31	1 (2%) 64 45	28, 35, 77, 88	0
57	P8	49/49 (100%)	-0.65	0 100 100	15, 20, 50, 71	0
58	M5	64/65 (98%)	-0.17	0 100 100	41, 51, 76, 94	0
58	Q8	64/65 (98%)	-0.62	0 100 100	21, 31, 41, 62	0
59	1L	72/76 (94%)	0.08	2 (2%) 55 35	80, 196, 235, 239	0
60	2L	67/76 (88%)	-0.48	0 100 100	52, 82, 113, 145	0
All	All	21491/22459 (95%)	-0.11	464 (2%) 62 42	13, 69, 169, 252	5 (0%)

The worst 5 of 464 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	14	2797	U	6.5
32	39	133	ASN	6.4
45	95	36	PRO	6.1
27	14	2900	A	5.1
48	C5	61	ILE	5.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	4SU	1K	8	20/21	0.61	0.12	181,183,191,193	0
26	H2U	5K	20	20/21	0.66	0.14	119,139,156,163	0
26	H2U	5K	16	20/21	0.67	0.15	121,137,151,153	0
24	PSU	3L	32	20/21	0.71	0.14	116,119,126,129	0
26	PSU	5K	55	20/21	0.71	0.11	115,127,149,152	0
59	5MU	1L	54	21/22	0.71	0.10	139,160,167,169	0
60	H2U	2L	16	20/21	0.72	0.10	100,112,131,139	0
26	PSU	5K	39	20/21	0.73	0.14	116,146,158,158	0
22	7MG	1K	46	24/25	0.74	0.11	180,185,193,198	0
26	PSU	5K	32	20/21	0.75	0.14	152,165,171,173	0
60	3AU	2L	47	27/28	0.76	0.11	95,125,138,141	0
60	5MU	2L	54	21/22	0.76	0.12	75,85,99,108	0
26	4SU	5K	8	20/21	0.77	0.13	147,151,156,157	0
22	PSU	1K	55	20/21	0.77	0.10	123,134,149,150	0
60	7MG	2L	46	24/25	0.81	0.09	89,104,121,126	0
26	5MU	5K	54	21/22	0.81	0.12	129,137,141,145	0
24	PSU	3K	32	20/21	0.81	0.13	111,117,123,125	0
23	H2U	2K	16	20/21	0.82	0.10	67,90,114,126	0
23	H2U	2K	20	20/21	0.82	0.11	88,97,110,111	0
24	PSU	3K	39	20/21	0.82	0.15	100,112,118,119	0
60	PSU	2L	55	20/21	0.83	0.08	77,82,88,89	0
22	5MU	1K	54	21/22	0.84	0.11	94,115,123,126	0
24	MIA	3K	37	29/30	0.84	0.16	95,112,116,117	0
23	PSU	2K	55	20/21	0.85	0.11	60,67,80,86	0
1	2MG	1G	1207	24/25	0.85	0.09	91,101,104,108	0
59	PSU	1L	32	20/21	0.85	0.09	96,104,118,121	0
23	3AU	2K	47	27/28	0.86	0.12	62,95,113,114	0
24	PSU	3L	39	20/21	0.88	0.10	97,111,120,122	0
12	0TD	3I	89	10/11	0.89	0.11	44,46,56,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MIA	3L	37	29/30	0.90	0.15	81,113,120,124	0
26	MIA	5K	37	29/30	0.90	0.14	89,114,142,145	0
23	7MG	2K	46	24/25	0.90	0.10	56,62,98,99	0
27	PSU	1H	1940	20/21	0.91	0.14	35,44,54,54	0
12	0TD	3A	89	10/11	0.91	0.09	65,69,72,77	0
59	PSU	1L	39	20/21	0.91	0.07	77,98,110,110	0
27	5MU	14	1915	21/22	0.91	0.10	63,72,80,88	0
60	4SU	2L	8	20/21	0.91	0.08	70,83,90,90	0
59	MIA	1L	37	29/30	0.92	0.08	68,80,95,96	0
22	PSU	1K	32	20/21	0.92	0.08	65,70,79,85	0
1	5MC	1G	1407	21/22	0.92	0.14	43,49,53,60	0
1	5MC	13	1400	21/22	0.93	0.14	38,45,51,56	0
23	5MU	2K	54	21/22	0.93	0.07	64,68,76,78	0
1	5MC	1G	1404	21/22	0.93	0.11	44,49,55,59	0
27	PSU	14	1911	20/21	0.93	0.08	51,59,64,64	0
60	PSU	2L	32	20/21	0.93	0.10	68,73,80,80	0
60	PSU	2L	39	20/21	0.93	0.07	59,68,72,72	0
1	7MG	13	527	24/25	0.93	0.10	42,50,56,63	0
1	7MG	1G	527	24/25	0.93	0.10	60,65,70,73	0
1	PSU	1G	516	20/21	0.93	0.07	71,76,78,79	0
22	PSU	1K	39	20/21	0.93	0.09	50,67,75,75	0
27	5MC	14	1942	21/22	0.94	0.11	47,57,61,71	0
27	5MC	14	1962	21/22	0.94	0.12	38,45,53,58	0
27	OMG	14	2251	24/25	0.94	0.09	35,40,44,46	0
60	MIA	2L	37	29/30	0.94	0.08	64,69,80,85	0
27	OMU	14	2552	21/22	0.94	0.12	37,42,47,58	0
1	5MC	13	1407	21/22	0.94	0.13	29,32,37,40	0
1	M2G	1G	966	25/26	0.94	0.09	59,67,76,77	0
27	PSU	1H	1934	20/21	0.94	0.10	36,42,47,51	0
27	PSU	14	1917	20/21	0.94	0.07	53,60,67,70	0
1	5MC	13	967	21/22	0.95	0.09	43,50,56,59	0
1	5MC	1G	967	21/22	0.95	0.07	61,68,76,86	0
27	OMU	1H	2565	21/22	0.95	0.10	19,22,26,36	0
1	M2G	13	966	25/26	0.95	0.11	40,46,57,61	0
27	PSU	14	2605	20/21	0.95	0.14	29,33,41,51	0
1	UR3	13	1498	21/22	0.95	0.13	29,33,42,43	0
1	UR3	1G	1498	21/22	0.95	0.10	40,49,53,55	0
23	PSU	2K	32	20/21	0.95	0.07	45,50,57,58	0
27	5MU	1H	1938	21/22	0.95	0.07	45,48,54,64	0
1	MA6	1G	1519	24/25	0.95	0.14	44,54,57,58	0
1	PSU	13	516	20/21	0.95	0.07	50,55,58,60	0
1	5MC	1G	1400	21/22	0.95	0.08	52,64,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	OMC	1H	1943	21/22	0.95	0.10	34,37,43,46	0
27	OMC	14	1920	21/22	0.95	0.07	54,60,62,64	0
27	5MU	1H	1962	21/22	0.95	0.10	20,23,30,41	0
27	5MC	1H	1965	21/22	0.95	0.11	27,33,36,42	0
1	4OC	1G	1402	22/23	0.95	0.07	46,57,61,71	0
27	5MC	1H	1985	21/22	0.95	0.09	24,30,34,37	0
1	MA6	1G	1518	24/25	0.96	0.10	52,57,60,62	0
1	MA6	13	1519	24/25	0.96	0.13	28,31,33,33	0
27	5MU	14	1939	21/22	0.96	0.10	34,40,44,51	0
23	PSU	2K	39	20/21	0.96	0.09	39,48,57,59	0
1	5MC	13	1404	21/22	0.96	0.12	26,29,41,43	0
1	4OC	13	1402	22/23	0.96	0.12	29,37,42,46	0
23	4SU	2K	8	20/21	0.96	0.07	42,48,57,62	0
1	2MG	13	1207	24/25	0.96	0.07	57,64,68,69	0
27	OMG	1H	2264	24/25	0.97	0.07	19,23,25,26	0
1	MA6	13	1518	24/25	0.97	0.13	27,32,35,38	0
27	2MA	1H	2516	23/24	0.97	0.08	13,17,24,26	0
27	2MA	14	2503	23/24	0.97	0.08	28,32,36,41	0
22	MIA	1K	37	29/30	0.97	0.09	43,49,58,62	0
23	MIA	2K	37	29/30	0.97	0.07	41,47,63,67	0
27	PSU	1H	2618	20/21	0.97	0.09	17,19,24,24	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3343[A]	1/1	-0.05	0.61	55,55,55,55	1
62	MG	1H	3343[B]	1/1	-0.05	0.61	68,68,68,68	1
62	MG	1G	1674	1/1	0.46	0.30	122,122,122,122	0
62	MG	1G	1683[A]	1/1	0.55	0.42	51,51,51,51	1
62	MG	1G	1683[B]	1/1	0.55	0.42	45,45,45,45	1
61	K	14	3053	1/1	0.56	0.19	102,102,102,102	0
62	MG	13	1709[B]	1/1	0.59	0.44	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	13	1709[A]	1/1	0.59	0.44	40,40,40,40	1
62	MG	14	3175[A]	1/1	0.59	0.44	39,39,39,39	1
62	MG	14	3175[B]	1/1	0.59	0.44	36,36,36,36	1
62	MG	14	3260	1/1	0.62	0.33	84,84,84,84	0
61	K	49	201	1/1	0.65	0.13	108,108,108,108	0
61	K	13	1611	1/1	0.70	0.19	114,114,114,114	0
61	K	1H	3040[B]	1/1	0.71	0.26	43,43,43,43	1
62	MG	13	1674	1/1	0.71	0.21	75,75,75,75	0
61	K	32	301	1/1	0.71	0.15	104,104,104,104	0
61	K	1H	3040[A]	1/1	0.71	0.26	46,46,46,46	1
61	K	1H	3142	1/1	0.72	0.17	78,78,78,78	0
62	MG	13	1698	1/1	0.72	0.29	84,84,84,84	0
61	K	14	3012	1/1	0.72	0.18	117,117,117,117	0
61	K	1G	1601	1/1	0.73	0.22	115,115,115,115	0
62	MG	1G	1690	1/1	0.74	0.32	74,74,74,74	0
61	K	14	3004	1/1	0.74	0.12	81,81,81,81	0
62	MG	1G	1661	1/1	0.75	0.31	79,79,79,79	0
62	MG	13	1721	1/1	0.76	0.20	99,99,99,99	0
62	MG	14	3136	1/1	0.76	0.23	59,59,59,59	0
61	K	14	3067	1/1	0.76	0.17	70,70,70,70	0
61	K	13	1620	1/1	0.76	0.12	87,87,87,87	0
62	MG	16	210	1/1	0.76	0.23	62,62,62,62	0
62	MG	14	3257	1/1	0.77	0.32	65,65,65,65	0
62	MG	14	3249	1/1	0.77	0.19	62,62,62,62	0
62	MG	1H	3363	1/1	0.78	0.14	56,56,56,56	0
61	K	BI	201	1/1	0.78	0.13	108,108,108,108	0
61	K	13	1648	1/1	0.78	0.10	71,71,71,71	0
62	MG	14	3124	1/1	0.78	0.13	58,58,58,58	0
62	MG	13	1684	1/1	0.78	0.28	73,73,73,73	0
62	MG	14	3125	1/1	0.79	0.23	60,60,60,60	0
61	K	14	3013	1/1	0.79	0.21	84,84,84,84	0
61	K	1H	3027	1/1	0.79	0.09	63,63,63,63	0
61	K	14	3062	1/1	0.79	0.14	76,76,76,76	0
62	MG	14	3195	1/1	0.79	0.25	53,53,53,53	0
62	MG	14	3244	1/1	0.79	0.17	64,64,64,64	0
62	MG	1G	1689	1/1	0.79	0.16	57,57,57,57	0
61	K	5E	201	1/1	0.79	0.12	76,76,76,76	0
62	MG	1G	1668	1/1	0.79	0.24	69,69,69,69	0
62	MG	1H	3176[B]	1/1	0.80	0.26	20,20,20,20	1
61	K	14	3088	1/1	0.80	0.14	98,98,98,98	0
61	K	39	302	1/1	0.80	0.09	74,74,74,74	0
61	K	1G	1632	1/1	0.80	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3176[A]	1/1	0.80	0.26	21,21,21,21	1
62	MG	1G	1688	1/1	0.80	0.17	65,65,65,65	0
61	K	13	1608	1/1	0.81	0.11	89,89,89,89	0
61	K	13	1606	1/1	0.81	0.20	57,57,57,57	0
61	K	1G	1631	1/1	0.81	0.17	86,86,86,86	0
61	K	2K	103	1/1	0.81	0.09	79,79,79,79	0
62	MG	13	1720	1/1	0.81	0.25	64,64,64,64	0
61	K	1H	3131	1/1	0.81	0.11	63,63,63,63	0
61	K	14	3092	1/1	0.82	0.16	106,106,106,106	0
62	MG	14	3228	1/1	0.82	0.16	58,58,58,58	0
62	MG	O8	101	1/1	0.82	0.23	60,60,60,60	0
61	K	1G	1622	1/1	0.82	0.09	74,74,74,74	0
62	MG	1H	3211	1/1	0.82	0.18	56,56,56,56	0
62	MG	16	208	1/1	0.82	0.13	44,44,44,44	0
62	MG	1H	3351	1/1	0.83	0.25	79,79,79,79	0
61	K	13	1615	1/1	0.83	0.09	90,90,90,90	0
61	K	29	301	1/1	0.83	0.10	86,86,86,86	0
61	K	1H	3036	1/1	0.83	0.13	60,60,60,60	0
62	MG	6E	201	1/1	0.83	0.24	62,62,62,62	0
62	MG	1G	1650	1/1	0.83	0.25	68,68,68,68	0
62	MG	14	3158	1/1	0.83	0.25	49,49,49,49	0
62	MG	14	3171	1/1	0.83	0.20	55,55,55,55	0
62	MG	14	3173	1/1	0.83	0.23	66,66,66,66	0
61	K	1H	3020	1/1	0.83	0.10	65,65,65,65	0
62	MG	1G	1663[A]	1/1	0.83	0.45	29,29,29,29	1
62	MG	14	3182	1/1	0.83	0.21	62,62,62,62	0
62	MG	1G	1663[B]	1/1	0.83	0.45	30,30,30,30	1
62	MG	14	3199	1/1	0.83	0.26	66,66,66,66	0
61	K	1H	3022	1/1	0.83	0.09	66,66,66,66	0
61	K	14	3070	1/1	0.83	0.08	92,92,92,92	0
62	MG	14	3248	1/1	0.83	0.38	60,60,60,60	0
62	MG	1G	1679	1/1	0.83	0.18	62,62,62,62	0
61	K	14	3072	1/1	0.83	0.09	85,85,85,85	0
61	K	1G	1627	1/1	0.83	0.16	92,92,92,92	0
62	MG	14	3276	1/1	0.83	0.21	52,52,52,52	0
62	MG	14	3336	1/1	0.83	0.11	78,78,78,78	0
62	MG	14	3176	1/1	0.84	0.29	69,69,69,69	0
62	MG	1H	3281	1/1	0.84	0.23	49,49,49,49	0
62	MG	1H	3325	1/1	0.84	0.23	50,50,50,50	0
62	MG	14	3120	1/1	0.84	0.17	44,44,44,44	0
61	K	13	1625	1/1	0.84	0.10	77,77,77,77	0
61	K	1G	1604	1/1	0.84	0.08	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	1H	3038	1/1	0.84	0.14	56,56,56,56	0
62	MG	1H	3359	1/1	0.84	0.27	62,62,62,62	0
61	K	14	3097	1/1	0.84	0.11	91,91,91,91	0
61	K	1G	1623	1/1	0.84	0.09	95,95,95,95	0
61	K	13	1610	1/1	0.84	0.09	103,103,103,103	0
62	MG	1H	3272	1/1	0.84	0.29	55,55,55,55	0
62	MG	7I	101	1/1	0.85	0.25	71,71,71,71	0
62	MG	1H	3360	1/1	0.85	0.09	28,28,28,28	0
62	MG	1H	3174	1/1	0.85	0.33	60,60,60,60	0
62	MG	1H	3381	1/1	0.85	0.18	39,39,39,39	0
61	K	14	3105	1/1	0.85	0.13	91,91,91,91	0
62	MG	14	3170	1/1	0.85	0.21	54,54,54,54	0
62	MG	13	1696	1/1	0.85	0.24	64,64,64,64	0
62	MG	1H	3183	1/1	0.85	0.14	47,47,47,47	0
62	MG	1G	1649	1/1	0.85	0.26	74,74,74,74	0
61	K	14	3006	1/1	0.85	0.11	106,106,106,106	0
61	K	1G	1607	1/1	0.85	0.14	87,87,87,87	0
62	MG	1H	3279	1/1	0.85	0.16	32,32,32,32	0
61	K	1H	3044	1/1	0.85	0.13	92,92,92,92	0
62	MG	1H	3286	1/1	0.85	0.28	48,48,48,48	0
62	MG	14	3214	1/1	0.85	0.24	66,66,66,66	0
62	MG	13	1719	1/1	0.85	0.32	63,63,63,63	0
62	MG	14	3242	1/1	0.85	0.28	65,65,65,65	0
62	MG	1G	1678	1/1	0.85	0.26	54,54,54,54	0
62	MG	1H	3328[A]	1/1	0.85	0.42	22,22,22,22	1
62	MG	1H	3328[B]	1/1	0.85	0.42	27,27,27,27	1
62	MG	1H	3329	1/1	0.85	0.25	63,63,63,63	0
62	MG	13	1664	1/1	0.85	0.21	57,57,57,57	0
62	MG	13	1672	1/1	0.85	0.22	49,49,49,49	0
61	K	14	3014	1/1	0.85	0.17	80,80,80,80	0
62	MG	1H	3182	1/1	0.86	0.18	49,49,49,49	0
61	K	1H	3005	1/1	0.86	0.12	100,100,100,100	0
62	MG	13	1702	1/1	0.86	0.21	60,60,60,60	0
62	MG	1H	3269	1/1	0.86	0.11	33,33,33,33	0
62	MG	14	3164	1/1	0.86	0.16	48,48,48,48	0
62	MG	1G	1646	1/1	0.86	0.14	66,66,66,66	0
62	MG	13	1703	1/1	0.86	0.17	49,49,49,49	0
61	K	13	1651	1/1	0.86	0.11	81,81,81,81	0
61	K	14	3034	1/1	0.86	0.12	86,86,86,86	0
62	MG	13	1714	1/1	0.86	0.32	83,83,83,83	0
61	K	13	1646	1/1	0.86	0.14	63,63,63,63	0
61	K	13	1649	1/1	0.86	0.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	14	3003	1/1	0.86	0.13	100,100,100,100	0
61	K	1G	1616	1/1	0.86	0.10	86,86,86,86	0
61	K	1H	3126	1/1	0.86	0.11	86,86,86,86	0
62	MG	1H	3155[A]	1/1	0.86	0.42	19,19,19,19	1
62	MG	14	3234	1/1	0.86	0.27	55,55,55,55	0
62	MG	14	3239	1/1	0.86	0.25	66,66,66,66	0
62	MG	1H	3155[B]	1/1	0.86	0.42	22,22,22,22	1
62	MG	1G	1684	1/1	0.86	0.13	79,79,79,79	0
62	MG	1H	3358	1/1	0.86	0.27	41,41,41,41	0
61	K	14	3077	1/1	0.86	0.11	73,73,73,73	0
61	K	14	3082	1/1	0.86	0.10	80,80,80,80	0
62	MG	1G	1697	1/1	0.86	0.26	63,63,63,63	0
62	MG	14	3268	1/1	0.86	0.14	36,36,36,36	0
62	MG	4L	101	1/1	0.86	0.21	79,79,79,79	0
61	K	13	1650	1/1	0.86	0.14	97,97,97,97	0
61	K	14	3102	1/1	0.87	0.13	76,76,76,76	0
62	MG	1G	1648	1/1	0.87	0.19	67,67,67,67	0
62	MG	1H	3315	1/1	0.87	0.15	43,43,43,43	0
62	MG	1H	3318	1/1	0.87	0.17	56,56,56,56	0
61	K	1H	3026	1/1	0.87	0.14	88,88,88,88	0
61	K	13	1641	1/1	0.87	0.08	84,84,84,84	0
62	MG	14	3174	1/1	0.87	0.19	38,38,38,38	0
62	MG	1H	3164	1/1	0.87	0.09	58,58,58,58	0
61	K	1G	1602	1/1	0.87	0.20	104,104,104,104	0
62	MG	1H	3332	1/1	0.87	0.20	48,48,48,48	0
62	MG	14	3181	1/1	0.87	0.18	49,49,49,49	0
62	MG	1H	3339	1/1	0.87	0.18	55,55,55,55	0
62	MG	14	3185	1/1	0.87	0.24	51,51,51,51	0
62	MG	14	3186	1/1	0.87	0.23	49,49,49,49	0
62	MG	13	1706	1/1	0.87	0.15	46,46,46,46	0
62	MG	1G	1680	1/1	0.87	0.17	50,50,50,50	0
62	MG	13	1707	1/1	0.87	0.22	58,58,58,58	0
62	MG	14	3215	1/1	0.87	0.14	45,45,45,45	0
62	MG	14	3221	1/1	0.87	0.10	52,52,52,52	0
61	K	13	1631	1/1	0.87	0.09	58,58,58,58	0
62	MG	13	1662	1/1	0.87	0.21	54,54,54,54	0
62	MG	1G	1686	1/1	0.87	0.28	75,75,75,75	0
61	K	14	3039	1/1	0.87	0.10	61,61,61,61	0
62	MG	1H	3213	1/1	0.87	0.10	25,25,25,25	0
62	MG	1H	3259	1/1	0.87	0.14	46,46,46,46	0
61	K	1H	3140	1/1	0.87	0.08	62,62,62,62	0
62	MG	14	3256	1/1	0.87	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	14	3010	1/1	0.87	0.07	58,58,58,58	0
61	K	14	3065	1/1	0.87	0.14	55,55,55,55	0
62	MG	14	3121	1/1	0.87	0.25	47,47,47,47	0
62	MG	13	1694	1/1	0.87	0.24	57,57,57,57	0
62	MG	1G	1641	1/1	0.87	0.27	64,64,64,64	0
62	MG	2K	104	1/1	0.88	0.26	48,48,48,48	0
62	MG	1H	3149	1/1	0.88	0.24	40,40,40,40	0
61	K	1H	3105	1/1	0.88	0.08	50,50,50,50	0
62	MG	1G	1692	1/1	0.88	0.30	72,72,72,72	0
61	K	1H	3125	1/1	0.88	0.12	64,64,64,64	0
62	MG	42	201	1/1	0.88	0.20	70,70,70,70	0
61	K	13	1603	1/1	0.88	0.07	75,75,75,75	0
62	MG	14	3119	1/1	0.88	0.17	49,49,49,49	0
62	MG	13	1680	1/1	0.88	0.21	49,49,49,49	0
61	K	1H	3128	1/1	0.88	0.10	64,64,64,64	0
61	K	1H	3023	1/1	0.88	0.08	63,63,63,63	0
61	K	14	3079	1/1	0.88	0.14	81,81,81,81	0
62	MG	1H	3367	1/1	0.88	0.09	35,35,35,35	0
61	K	1H	3138	1/1	0.88	0.12	62,62,62,62	0
62	MG	16	205	1/1	0.88	0.22	46,46,46,46	0
62	MG	1H	3187	1/1	0.88	0.11	30,30,30,30	0
61	K	14	3083	1/1	0.88	0.14	70,70,70,70	0
62	MG	31	303	1/1	0.88	0.17	37,37,37,37	0
61	K	14	3017	1/1	0.88	0.16	52,52,52,52	0
62	MG	P8	101	1/1	0.88	0.16	35,35,35,35	0
62	MG	1G	1639	1/1	0.88	0.17	69,69,69,69	0
62	MG	1H	3245	1/1	0.88	0.17	50,50,50,50	0
62	MG	1G	1643	1/1	0.88	0.21	62,62,62,62	0
61	K	1H	3041	1/1	0.88	0.11	68,68,68,68	0
61	K	14	3038	1/1	0.88	0.08	92,92,92,92	0
61	K	13	1607	1/1	0.88	0.06	65,65,65,65	0
62	MG	14	3187	1/1	0.88	0.22	51,51,51,51	0
62	MG	14	3188	1/1	0.88	0.15	56,56,56,56	0
61	K	14	3042	1/1	0.88	0.08	51,51,51,51	0
62	MG	1G	1653	1/1	0.88	0.13	53,53,53,53	0
62	MG	13	1710	1/1	0.88	0.20	52,52,52,52	0
61	K	14	3052	1/1	0.88	0.10	76,76,76,76	0
62	MG	1H	3287	1/1	0.88	0.14	37,37,37,37	0
62	MG	1H	3290	1/1	0.88	0.12	38,38,38,38	0
62	MG	1G	1670	1/1	0.88	0.20	57,57,57,57	0
62	MG	14	3235	1/1	0.88	0.17	50,50,50,50	0
62	MG	1G	1672	1/1	0.88	0.25	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3303	1/1	0.88	0.20	46,46,46,46	0
62	MG	13	1718	1/1	0.88	0.25	55,55,55,55	0
62	MG	14	3245	1/1	0.88	0.20	36,36,36,36	0
61	K	1H	3046	1/1	0.88	0.11	72,72,72,72	0
61	K	1H	3088	1/1	0.88	0.07	50,50,50,50	0
62	MG	14	3251	1/1	0.88	0.15	45,45,45,45	0
62	MG	1G	1681	1/1	0.88	0.21	45,45,45,45	0
62	MG	1H	3326	1/1	0.88	0.23	60,60,60,60	0
62	MG	13	1653	1/1	0.88	0.21	67,67,67,67	0
62	MG	13	1654	1/1	0.88	0.18	42,42,42,42	0
62	MG	14	3270	1/1	0.88	0.20	66,66,66,66	0
61	K	14	3064	1/1	0.88	0.10	87,87,87,87	0
62	MG	1G	1687	1/1	0.88	0.18	67,67,67,67	0
62	MG	1J	202	1/1	0.88	0.10	83,83,83,83	0
62	MG	1G	1655	1/1	0.89	0.13	58,58,58,58	0
62	MG	1H	3264	1/1	0.89	0.26	55,55,55,55	0
61	K	13	1613	1/1	0.89	0.09	76,76,76,76	0
61	K	1H	3028	1/1	0.89	0.09	87,87,87,87	0
62	MG	1G	1667	1/1	0.89	0.23	42,42,42,42	0
62	MG	1H	3275	1/1	0.89	0.26	44,44,44,44	0
61	K	1H	3021	1/1	0.89	0.17	78,78,78,78	0
62	MG	1H	3280	1/1	0.89	0.17	86,86,86,86	0
61	K	1H	3135	1/1	0.89	0.14	82,82,82,82	0
61	K	14	3058	1/1	0.89	0.10	85,85,85,85	0
61	K	14	3087	1/1	0.89	0.11	74,74,74,74	0
62	MG	1H	3369	1/1	0.89	0.18	46,46,46,46	0
61	K	13	1635	1/1	0.89	0.12	95,95,95,95	0
62	MG	1H	3500	1/1	0.89	0.09	63,63,63,63	0
62	MG	1H	3517	1/1	0.89	0.10	26,26,26,26	0
62	MG	14	3197	1/1	0.89	0.17	48,48,48,48	0
62	MG	13	1665	1/1	0.89	0.14	51,51,51,51	0
62	MG	14	3207	1/1	0.89	0.29	62,62,62,62	0
62	MG	14	3213	1/1	0.89	0.18	40,40,40,40	0
62	MG	1G	1685	1/1	0.89	0.15	51,51,51,51	0
61	K	14	3091	1/1	0.89	0.14	78,78,78,78	0
62	MG	1H	3316	1/1	0.89	0.16	60,60,60,60	0
62	MG	14	3224	1/1	0.89	0.08	36,36,36,36	0
61	K	14	3020	1/1	0.89	0.07	64,64,64,64	0
62	MG	14	3231	1/1	0.89	0.11	39,39,39,39	0
62	MG	1H	3320[A]	1/1	0.89	0.22	8,8,8,8	1
62	MG	1H	3320[B]	1/1	0.89	0.22	9,9,9,9	1
62	MG	1H	3323	1/1	0.89	0.22	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1G	1640	1/1	0.89	0.28	51,51,51,51	0
62	MG	1H	3186	1/1	0.89	0.29	55,55,55,55	0
62	MG	2L	102	1/1	0.89	0.16	56,56,56,56	0
61	K	1H	3002	1/1	0.89	0.07	73,73,73,73	0
61	K	14	3101	1/1	0.89	0.07	76,76,76,76	0
62	MG	1G	1647	1/1	0.89	0.28	55,55,55,55	0
61	K	14	3035	1/1	0.89	0.09	83,83,83,83	0
61	K	13	1616	1/1	0.89	0.08	75,75,75,75	0
62	MG	1H	3331	1/1	0.89	0.08	54,54,54,54	0
62	MG	13	1697	1/1	0.89	0.19	45,45,45,45	0
62	MG	14	3143	1/1	0.89	0.12	39,39,39,39	0
62	MG	14	3153	1/1	0.89	0.18	51,51,51,51	0
62	MG	1G	1654	1/1	0.89	0.25	50,50,50,50	0
62	MG	14	3351	1/1	0.89	0.11	55,55,55,55	0
62	MG	14	3161	1/1	0.89	0.11	47,47,47,47	0
62	MG	1H	3221	1/1	0.90	0.15	34,34,34,34	0
62	MG	14	3165	1/1	0.90	0.13	45,45,45,45	0
62	MG	1H	3236	1/1	0.90	0.21	43,43,43,43	0
62	MG	1H	3338	1/1	0.90	0.10	43,43,43,43	0
62	MG	1H	3238	1/1	0.90	0.10	39,39,39,39	0
62	MG	13	1675	1/1	0.90	0.23	49,49,49,49	0
62	MG	13	1678	1/1	0.90	0.15	38,38,38,38	0
62	MG	1H	3263	1/1	0.90	0.09	36,36,36,36	0
62	MG	1H	3355	1/1	0.90	0.09	57,57,57,57	0
61	K	14	3094	1/1	0.90	0.09	86,86,86,86	0
62	MG	13	1722	1/1	0.90	0.10	52,52,52,52	0
62	MG	14	3184	1/1	0.90	0.20	48,48,48,48	0
62	MG	1G	1676	1/1	0.90	0.15	71,71,71,71	0
61	K	1H	3122	1/1	0.90	0.07	65,65,65,65	0
62	MG	1H	3362	1/1	0.90	0.28	64,64,64,64	0
61	K	13	1643	1/1	0.90	0.06	76,76,76,76	0
62	MG	1H	3364	1/1	0.90	0.20	58,58,58,58	0
62	MG	14	3196	1/1	0.90	0.12	59,59,59,59	0
62	MG	1H	3365	1/1	0.90	0.16	58,58,58,58	0
61	K	13	1636	1/1	0.90	0.10	70,70,70,70	0
61	K	14	3076	1/1	0.90	0.08	86,86,86,86	0
62	MG	14	3209	1/1	0.90	0.12	53,53,53,53	0
62	MG	1H	3370	1/1	0.90	0.28	61,61,61,61	0
62	MG	1H	3153	1/1	0.90	0.10	45,45,45,45	0
61	K	14	3005	1/1	0.90	0.13	82,82,82,82	0
62	MG	13	1701	1/1	0.90	0.27	69,69,69,69	0
62	MG	1H	3162	1/1	0.90	0.30	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	14	3078	1/1	0.90	0.09	81,81,81,81	0
62	MG	1H	3305	1/1	0.90	0.23	41,41,41,41	0
62	MG	14	3233	1/1	0.90	0.21	52,52,52,52	0
62	MG	1H	3165	1/1	0.90	0.12	40,40,40,40	0
62	MG	1G	1699	1/1	0.90	0.20	62,62,62,62	0
62	MG	41	202	1/1	0.90	0.12	55,55,55,55	0
62	MG	14	3241	1/1	0.90	0.21	59,59,59,59	0
61	K	1H	3008	1/1	0.90	0.08	65,65,65,65	0
61	K	1H	3072	1/1	0.90	0.11	53,53,53,53	0
62	MG	14	3115	1/1	0.90	0.13	42,42,42,42	0
62	MG	1H	3319	1/1	0.90	0.21	50,50,50,50	0
61	K	1H	3010	1/1	0.90	0.10	66,66,66,66	0
62	MG	13	1708	1/1	0.90	0.23	60,60,60,60	0
62	MG	14	3254	1/1	0.90	0.09	62,62,62,62	0
61	K	1H	3096	1/1	0.90	0.11	52,52,52,52	0
61	K	13	1618	1/1	0.90	0.09	85,85,85,85	0
61	K	1H	3108	1/1	0.90	0.09	76,76,76,76	0
62	MG	14	3267	1/1	0.90	0.09	44,44,44,44	0
62	MG	1H	3327	1/1	0.90	0.09	40,40,40,40	0
62	MG	14	3149	1/1	0.90	0.21	37,37,37,37	0
62	MG	14	3271	1/1	0.90	0.21	51,51,51,51	0
61	K	41	201	1/1	0.90	0.10	67,67,67,67	0
62	MG	14	3309	1/1	0.90	0.09	26,26,26,26	0
62	MG	14	3317	1/1	0.90	0.08	40,40,40,40	0
62	MG	14	3156	1/1	0.90	0.20	34,34,34,34	0
62	MG	1H	3212	1/1	0.90	0.09	44,44,44,44	0
61	K	14	3093	1/1	0.90	0.07	53,53,53,53	0
62	MG	1H	3246	1/1	0.91	0.19	35,35,35,35	0
62	MG	1H	3254	1/1	0.91	0.10	29,29,29,29	0
61	K	1G	1633	1/1	0.91	0.07	76,76,76,76	0
61	K	14	3084	1/1	0.91	0.08	73,73,73,73	0
61	K	1G	1635	1/1	0.91	0.17	91,91,91,91	0
61	K	13	1639	1/1	0.91	0.06	66,66,66,66	0
62	MG	1H	3270	1/1	0.91	0.08	42,42,42,42	0
61	K	14	3048	1/1	0.91	0.08	67,67,67,67	0
62	MG	1H	3147	1/1	0.91	0.18	54,54,54,54	0
62	MG	13	1686	1/1	0.91	0.08	34,34,34,34	0
62	MG	14	3189	1/1	0.91	0.07	50,50,50,50	0
62	MG	14	3190	1/1	0.91	0.17	77,77,77,77	0
62	MG	13	1688	1/1	0.91	0.20	56,56,56,56	0
61	K	52	201	1/1	0.91	0.08	76,76,76,76	0
61	K	13	1645	1/1	0.91	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3429	1/1	0.91	0.11	29,29,29,29	0
62	MG	1H	3157	1/1	0.91	0.18	49,49,49,49	0
61	K	1H	3091	1/1	0.91	0.06	64,64,64,64	0
62	MG	14	3212	1/1	0.91	0.23	44,44,44,44	0
62	MG	1H	3297	1/1	0.91	0.11	40,40,40,40	0
61	K	14	3096	1/1	0.91	0.07	70,70,70,70	0
62	MG	1G	1696	1/1	0.91	0.31	52,52,52,52	0
61	K	1H	3003	1/1	0.91	0.05	56,56,56,56	0
62	MG	1H	3171	1/1	0.91	0.17	30,30,30,30	0
62	MG	14	3225	1/1	0.91	0.09	47,47,47,47	0
61	K	1G	1608	1/1	0.91	0.06	80,80,80,80	0
62	MG	14	3230	1/1	0.91	0.18	54,54,54,54	0
61	K	14	3007	1/1	0.91	0.14	64,64,64,64	0
62	MG	13	1705	1/1	0.91	0.19	56,56,56,56	0
62	MG	14	3109	1/1	0.91	0.17	41,41,41,41	0
62	MG	1G	1638	1/1	0.91	0.15	46,46,46,46	0
62	MG	14	3118	1/1	0.91	0.26	58,58,58,58	0
61	K	1H	3132	1/1	0.91	0.10	87,87,87,87	0
61	K	1G	1617	1/1	0.91	0.07	63,63,63,63	0
62	MG	1H	3321	1/1	0.91	0.11	36,36,36,36	0
61	K	14	3071	1/1	0.91	0.17	77,77,77,77	0
61	K	13	1605	1/1	0.91	0.06	81,81,81,81	0
62	MG	1H	3196	1/1	0.91	0.16	40,40,40,40	0
62	MG	14	3139	1/1	0.91	0.15	41,41,41,41	0
62	MG	1H	3199	1/1	0.91	0.18	34,34,34,34	0
62	MG	14	3255	1/1	0.91	0.10	63,63,63,63	0
62	MG	14	3146	1/1	0.91	0.15	49,49,49,49	0
61	K	1K	101	1/1	0.91	0.06	83,83,83,83	0
61	K	1G	1625	1/1	0.91	0.09	108,108,108,108	0
62	MG	14	3155	1/1	0.91	0.16	38,38,38,38	0
62	MG	13	1711	1/1	0.91	0.25	55,55,55,55	0
62	MG	1H	3220	1/1	0.91	0.27	50,50,50,50	0
61	K	1H	3114	1/1	0.91	0.11	55,55,55,55	0
62	MG	1H	3334	1/1	0.91	0.09	43,43,43,43	0
62	MG	1G	1662	1/1	0.91	0.21	51,51,51,51	0
61	K	1H	3115	1/1	0.91	0.09	52,52,52,52	0
61	K	14	3080	1/1	0.91	0.09	79,79,79,79	0
62	MG	1H	3242	1/1	0.91	0.10	37,37,37,37	0
61	K	1H	3047	1/1	0.91	0.13	74,74,74,74	0
62	MG	1J	204	1/1	0.91	0.26	64,64,64,64	0
62	MG	29	302	1/1	0.91	0.16	38,38,38,38	0
62	MG	14	3166	1/1	0.92	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	1H	3050	1/1	0.92	0.14	53,53,53,53	0
61	K	1H	3051	1/1	0.92	0.10	49,49,49,49	0
61	K	13	1642	1/1	0.92	0.11	93,93,93,93	0
62	MG	13	1673	1/1	0.92	0.29	55,55,55,55	0
61	K	14	3041	1/1	0.92	0.09	66,66,66,66	0
62	MG	1G	1664	1/1	0.92	0.19	40,40,40,40	0
62	MG	1G	1666	1/1	0.92	0.30	46,46,46,46	0
62	MG	14	3178	1/1	0.92	0.24	53,53,53,53	0
61	K	1G	1605	1/1	0.92	0.06	92,92,92,92	0
62	MG	1H	3344	1/1	0.92	0.14	39,39,39,39	0
62	MG	1H	3346	1/1	0.92	0.17	55,55,55,55	0
62	MG	1H	3349	1/1	0.92	0.18	48,48,48,48	0
62	MG	1H	3350	1/1	0.92	0.15	25,25,25,25	0
62	MG	1H	3258	1/1	0.92	0.31	52,52,52,52	0
62	MG	1G	1677	1/1	0.92	0.20	57,57,57,57	0
62	MG	1H	3353	1/1	0.92	0.16	33,33,33,33	0
61	K	14	3043	1/1	0.92	0.09	80,80,80,80	0
62	MG	14	3194	1/1	0.92	0.19	54,54,54,54	0
61	K	14	3045	1/1	0.92	0.10	83,83,83,83	0
61	K	1H	3080	1/1	0.92	0.06	45,45,45,45	0
61	K	2K	101	1/1	0.92	0.17	62,62,62,62	0
62	MG	1H	3361	1/1	0.92	0.26	57,57,57,57	0
62	MG	14	3201	1/1	0.92	0.19	49,49,49,49	0
62	MG	14	3204	1/1	0.92	0.20	38,38,38,38	0
61	K	1H	3011	1/1	0.92	0.06	59,59,59,59	0
62	MG	13	1692	1/1	0.92	0.17	51,51,51,51	0
62	MG	13	1693	1/1	0.92	0.25	61,61,61,61	0
61	K	1H	3013	1/1	0.92	0.15	81,81,81,81	0
62	MG	13	1695	1/1	0.92	0.13	66,66,66,66	0
62	MG	1H	3163	1/1	0.92	0.25	55,55,55,55	0
62	MG	14	3217	1/1	0.92	0.13	69,69,69,69	0
62	MG	1H	3282	1/1	0.92	0.12	49,49,49,49	0
62	MG	14	3222	1/1	0.92	0.19	57,57,57,57	0
62	MG	1H	3372	1/1	0.92	0.12	31,31,31,31	0
62	MG	1H	3375	1/1	0.92	0.12	36,36,36,36	0
62	MG	1H	3376	1/1	0.92	0.16	54,54,54,54	0
61	K	14	3061	1/1	0.92	0.12	63,63,63,63	0
62	MG	1G	1718	1/1	0.92	0.09	39,39,39,39	0
61	K	14	3009	1/1	0.92	0.13	64,64,64,64	0
61	K	14	3098	1/1	0.92	0.08	67,67,67,67	0
61	K	1H	3004	1/1	0.92	0.11	88,88,88,88	0
62	MG	14	3236	1/1	0.92	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3298	1/1	0.92	0.07	28,28,28,28	0
61	K	14	3011	1/1	0.92	0.17	80,80,80,80	0
62	MG	14	3117	1/1	0.92	0.08	49,49,49,49	0
62	MG	16	209	1/1	0.92	0.36	59,59,59,59	0
61	K	14	3104	1/1	0.92	0.10	75,75,75,75	0
62	MG	1H	3311	1/1	0.92	0.12	47,47,47,47	0
61	K	1H	3045	1/1	0.92	0.12	59,59,59,59	0
62	MG	14	3122	1/1	0.92	0.19	49,49,49,49	0
61	K	14	3106	1/1	0.92	0.21	68,68,68,68	0
61	K	1H	3141	1/1	0.92	0.10	41,41,41,41	0
62	MG	14	3132	1/1	0.92	0.22	53,53,53,53	0
62	MG	14	3133	1/1	0.92	0.17	39,39,39,39	0
61	K	1H	3029	1/1	0.92	0.09	85,85,85,85	0
62	MG	1H	3195	1/1	0.92	0.19	37,37,37,37	0
61	K	1H	3144	1/1	0.92	0.17	56,56,56,56	0
61	K	45	201	1/1	0.92	0.14	90,90,90,90	0
62	MG	1H	3201	1/1	0.92	0.14	45,45,45,45	0
62	MG	14	3273	1/1	0.92	0.16	37,37,37,37	0
62	MG	14	3274	1/1	0.92	0.19	54,54,54,54	0
62	MG	14	3275	1/1	0.92	0.17	42,42,42,42	0
62	MG	1H	3202	1/1	0.92	0.18	45,45,45,45	0
61	K	14	3018	1/1	0.92	0.07	65,65,65,65	0
61	K	16	202	1/1	0.92	0.06	74,74,74,74	0
62	MG	14	3332	1/1	0.92	0.07	54,54,54,54	0
62	MG	13	1712	1/1	0.92	0.17	43,43,43,43	0
62	MG	14	3341	1/1	0.92	0.07	35,35,35,35	0
62	MG	14	3159	1/1	0.92	0.27	56,56,56,56	0
62	MG	14	3352	1/1	0.92	0.10	63,63,63,63	0
62	MG	14	3387	1/1	0.92	0.13	45,45,45,45	0
62	MG	13	1713	1/1	0.92	0.15	46,46,46,46	0
61	K	13	1647	1/1	0.92	0.05	50,50,50,50	0
62	MG	1H	3227	1/1	0.92	0.11	29,29,29,29	0
62	MG	14	3180	1/1	0.93	0.16	59,59,59,59	0
61	K	13	1634	1/1	0.93	0.10	90,90,90,90	0
61	K	13	1612	1/1	0.93	0.15	50,50,50,50	0
62	MG	1H	3179	1/1	0.93	0.19	30,30,30,30	0
61	K	1H	3134	1/1	0.93	0.11	54,54,54,54	0
61	K	1G	1611	1/1	0.93	0.11	86,86,86,86	0
62	MG	1H	3291	1/1	0.93	0.20	47,47,47,47	0
62	MG	1H	3368	1/1	0.93	0.26	44,44,44,44	0
62	MG	1G	1682	1/1	0.93	0.25	41,41,41,41	0
62	MG	1H	3294	1/1	0.93	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	14	3191	1/1	0.93	0.07	34,34,34,34	0
62	MG	14	3192	1/1	0.93	0.13	41,41,41,41	0
62	MG	13	1671	1/1	0.93	0.27	49,49,49,49	0
62	MG	1H	3371	1/1	0.93	0.07	31,31,31,31	0
61	K	14	3050	1/1	0.93	0.05	63,63,63,63	0
62	MG	1H	3373	1/1	0.93	0.21	43,43,43,43	0
61	K	1G	1614	1/1	0.93	0.07	86,86,86,86	0
61	K	1H	3098	1/1	0.93	0.07	41,41,41,41	0
62	MG	14	3202	1/1	0.93	0.17	42,42,42,42	0
61	K	14	3055	1/1	0.93	0.19	65,65,65,65	0
62	MG	1H	3399	1/1	0.93	0.09	24,24,24,24	0
62	MG	14	3208	1/1	0.93	0.22	58,58,58,58	0
62	MG	1H	3313	1/1	0.93	0.07	44,44,44,44	0
62	MG	13	1677	1/1	0.93	0.10	42,42,42,42	0
61	K	1H	3137	1/1	0.93	0.09	63,63,63,63	0
62	MG	1H	3539	1/1	0.93	0.07	66,66,66,66	0
61	K	1H	3031	1/1	0.93	0.10	39,39,39,39	0
62	MG	1G	1736	1/1	0.93	0.09	62,62,62,62	0
62	MG	14	3220	1/1	0.93	0.08	46,46,46,46	0
61	K	1H	3032	1/1	0.93	0.06	54,54,54,54	0
61	K	1H	3110	1/1	0.93	0.06	60,60,60,60	0
62	MG	13	1687	1/1	0.93	0.22	50,50,50,50	0
62	MG	14	3107	1/1	0.93	0.16	33,33,33,33	0
62	MG	13	1724	1/1	0.93	0.16	43,43,43,43	0
62	MG	14	3113	1/1	0.93	0.13	36,36,36,36	0
62	MG	13	1726	1/1	0.93	0.14	46,46,46,46	0
62	MG	78	201	1/1	0.93	0.13	38,38,38,38	0
62	MG	C8	201	1/1	0.93	0.12	44,44,44,44	0
62	MG	1H	3229	1/1	0.93	0.32	43,43,43,43	0
61	K	14	3099	1/1	0.93	0.06	67,67,67,67	0
62	MG	14	3237	1/1	0.93	0.06	96,96,96,96	0
62	MG	13	1689	1/1	0.93	0.19	53,53,53,53	0
62	MG	13	1690	1/1	0.93	0.07	51,51,51,51	0
62	MG	1H	3244	1/1	0.93	0.24	34,34,34,34	0
62	MG	14	3243	1/1	0.93	0.16	54,54,54,54	0
61	K	1H	3112	1/1	0.93	0.08	48,48,48,48	0
61	K	1G	1628	1/1	0.93	0.08	76,76,76,76	0
62	MG	1G	1644	1/1	0.93	0.12	59,59,59,59	0
62	MG	1H	3252	1/1	0.93	0.26	42,42,42,42	0
61	K	14	3103	1/1	0.93	0.10	70,70,70,70	0
62	MG	14	3140	1/1	0.93	0.15	47,47,47,47	0
62	MG	1H	3255	1/1	0.93	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3154	1/1	0.93	0.16	26,26,26,26	0
62	MG	14	3147	1/1	0.93	0.17	40,40,40,40	0
62	MG	14	3259	1/1	0.93	0.25	42,42,42,42	0
62	MG	1H	3340	1/1	0.93	0.10	48,48,48,48	0
62	MG	14	3264	1/1	0.93	0.15	45,45,45,45	0
62	MG	1G	1651	1/1	0.93	0.20	43,43,43,43	0
62	MG	14	3154	1/1	0.93	0.12	50,50,50,50	0
62	MG	1G	1652	1/1	0.93	0.12	17,17,17,17	0
61	K	13	1614	1/1	0.93	0.16	71,71,71,71	0
61	K	13	1638	1/1	0.93	0.06	56,56,56,56	0
61	K	1H	3025	1/1	0.93	0.08	53,53,53,53	0
62	MG	1G	1656	1/1	0.93	0.26	58,58,58,58	0
62	MG	14	3163	1/1	0.93	0.14	31,31,31,31	0
62	MG	1G	1659	1/1	0.93	0.29	64,64,64,64	0
61	K	1H	3014	1/1	0.93	0.07	60,60,60,60	0
62	MG	13	1699	1/1	0.93	0.10	43,43,43,43	0
61	K	1H	3086	1/1	0.93	0.05	66,66,66,66	0
62	MG	1H	3273	1/1	0.93	0.27	61,61,61,61	0
61	K	1H	3016	1/1	0.93	0.05	63,63,63,63	0
62	MG	1H	3277	1/1	0.93	0.17	42,42,42,42	0
62	MG	1H	3356	1/1	0.93	0.16	43,43,43,43	0
62	MG	14	3399	1/1	0.93	0.06	106,106,106,106	0
62	MG	1H	3278	1/1	0.93	0.14	28,28,28,28	0
61	K	14	3040	1/1	0.93	0.06	93,93,93,93	0
61	K	2A	201	1/1	0.93	0.06	70,70,70,70	0
62	MG	39	303	1/1	0.93	0.13	54,54,54,54	0
62	MG	14	3167	1/1	0.94	0.16	38,38,38,38	0
61	K	1H	3064	1/1	0.94	0.06	34,34,34,34	0
62	MG	1H	3146	1/1	0.94	0.23	38,38,38,38	0
62	MG	1G	1657	1/1	0.94	0.22	53,53,53,53	0
62	MG	1G	1658	1/1	0.94	0.22	46,46,46,46	0
62	MG	1H	3248	1/1	0.94	0.20	34,34,34,34	0
62	MG	1H	3345[A]	1/1	0.94	0.53	23,23,23,23	1
62	MG	1H	3345[B]	1/1	0.94	0.53	24,24,24,24	1
61	K	13	1623	1/1	0.94	0.05	56,56,56,56	0
62	MG	13	1691	1/1	0.94	0.20	50,50,50,50	0
61	K	1H	3073	1/1	0.94	0.10	56,56,56,56	0
61	K	1H	3009	1/1	0.94	0.08	64,64,64,64	0
61	K	1H	3121	1/1	0.94	0.10	62,62,62,62	0
61	K	1H	3081	1/1	0.94	0.09	49,49,49,49	0
61	K	14	3024	1/1	0.94	0.08	52,52,52,52	0
62	MG	1H	3357	1/1	0.94	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1G	1673	1/1	0.94	0.11	50,50,50,50	0
62	MG	1H	3266	1/1	0.94	0.08	39,39,39,39	0
62	MG	1H	3159	1/1	0.94	0.15	44,44,44,44	0
62	MG	1H	3161	1/1	0.94	0.19	55,55,55,55	0
62	MG	1H	3271	1/1	0.94	0.10	47,47,47,47	0
61	K	14	3025	1/1	0.94	0.07	50,50,50,50	0
61	K	14	3027	1/1	0.94	0.11	54,54,54,54	0
61	K	1G	1634	1/1	0.94	0.08	62,62,62,62	0
62	MG	1H	3276	1/1	0.94	0.18	44,44,44,44	0
62	MG	13	1652	1/1	0.94	0.14	43,43,43,43	0
62	MG	14	3200	1/1	0.94	0.27	52,52,52,52	0
61	K	1H	3082	1/1	0.94	0.05	46,46,46,46	0
61	K	1G	1636	1/1	0.94	0.11	78,78,78,78	0
62	MG	13	1659	1/1	0.94	0.10	56,56,56,56	0
61	K	1H	3030	1/1	0.94	0.05	73,73,73,73	0
61	K	13	1604	1/1	0.94	0.06	82,82,82,82	0
62	MG	1H	3285	1/1	0.94	0.17	43,43,43,43	0
62	MG	1H	3180	1/1	0.94	0.10	43,43,43,43	0
61	K	1H	3017	1/1	0.94	0.14	56,56,56,56	0
62	MG	1G	1691	1/1	0.94	0.23	64,64,64,64	0
61	K	BA	201	1/1	0.94	0.07	72,72,72,72	0
62	MG	14	3216	1/1	0.94	0.15	51,51,51,51	0
62	MG	1G	1695	1/1	0.94	0.15	72,72,72,72	0
61	K	1H	3095	1/1	0.94	0.07	58,58,58,58	0
61	K	1H	3034	1/1	0.94	0.10	66,66,66,66	0
62	MG	1G	1698	1/1	0.94	0.29	66,66,66,66	0
62	MG	14	3223	1/1	0.94	0.15	40,40,40,40	0
62	MG	1H	3437	1/1	0.94	0.09	51,51,51,51	0
62	MG	1G	1714	1/1	0.94	0.07	88,88,88,88	0
62	MG	14	3226	1/1	0.94	0.27	55,55,55,55	0
62	MG	1H	3457	1/1	0.94	0.10	25,25,25,25	0
62	MG	1H	3477	1/1	0.94	0.08	28,28,28,28	0
62	MG	1H	3488	1/1	0.94	0.10	35,35,35,35	0
62	MG	2L	101	1/1	0.94	0.11	58,58,58,58	0
62	MG	1H	3188	1/1	0.94	0.18	20,20,20,20	0
62	MG	1H	3189	1/1	0.94	0.14	41,41,41,41	0
62	MG	1H	3530	1/1	0.94	0.06	21,21,21,21	0
62	MG	14	3108	1/1	0.94	0.16	59,59,59,59	0
62	MG	1H	3192	1/1	0.94	0.10	37,37,37,37	0
62	MG	14	3112	1/1	0.94	0.08	44,44,44,44	0
62	MG	1H	3564	1/1	0.94	0.07	25,25,25,25	0
62	MG	14	3114	1/1	0.94	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3577	1/1	0.94	0.08	37,37,37,37	0
62	MG	16	204	1/1	0.94	0.18	39,39,39,39	0
62	MG	14	3247	1/1	0.94	0.10	47,47,47,47	0
61	K	14	3047	1/1	0.94	0.08	74,74,74,74	0
61	K	1H	3035	1/1	0.94	0.10	52,52,52,52	0
62	MG	1H	3197	1/1	0.94	0.07	30,30,30,30	0
62	MG	1H	3314	1/1	0.94	0.13	41,41,41,41	0
62	MG	13	1676	1/1	0.94	0.22	53,53,53,53	0
61	K	1H	3099	1/1	0.94	0.12	59,59,59,59	0
62	MG	13	1715	1/1	0.94	0.18	60,60,60,60	0
62	MG	14	3131	1/1	0.94	0.14	43,43,43,43	0
62	MG	1H	3203	1/1	0.94	0.10	26,26,26,26	0
62	MG	1H	3204	1/1	0.94	0.12	29,29,29,29	0
62	MG	14	3135	1/1	0.94	0.16	47,47,47,47	0
62	MG	1H	3207	1/1	0.94	0.21	38,38,38,38	0
61	K	14	3051	1/1	0.94	0.05	65,65,65,65	0
62	MG	13	1679	1/1	0.94	0.21	45,45,45,45	0
61	K	1H	3018	1/1	0.94	0.20	51,51,51,51	0
62	MG	14	3145	1/1	0.94	0.12	49,49,49,49	0
62	MG	1H	3214	1/1	0.94	0.21	41,41,41,41	0
62	MG	1G	1642	1/1	0.94	0.14	45,45,45,45	0
62	MG	14	3277	1/1	0.94	0.27	61,61,61,61	0
62	MG	14	3278	1/1	0.94	0.17	49,49,49,49	0
62	MG	14	3289	1/1	0.94	0.09	51,51,51,51	0
62	MG	13	1681	1/1	0.94	0.23	44,44,44,44	0
61	K	1G	1620	1/1	0.94	0.06	83,83,83,83	0
62	MG	14	3329	1/1	0.94	0.08	28,28,28,28	0
62	MG	1G	1645	1/1	0.94	0.12	62,62,62,62	0
62	MG	1H	3225	1/1	0.94	0.13	37,37,37,37	0
62	MG	13	1723	1/1	0.94	0.27	60,60,60,60	0
62	MG	14	3157	1/1	0.94	0.15	34,34,34,34	0
62	MG	1H	3228	1/1	0.94	0.20	31,31,31,31	0
62	MG	13	1685	1/1	0.94	0.20	45,45,45,45	0
61	K	1H	3139	1/1	0.94	0.06	64,64,64,64	0
62	MG	1H	3336	1/1	0.94	0.26	45,45,45,45	0
62	MG	13	1749	1/1	0.94	0.08	52,52,52,52	0
61	K	13	1621	1/1	0.94	0.09	61,61,61,61	0
61	K	14	3100	1/1	0.94	0.07	71,71,71,71	0
62	MG	1H	3160	1/1	0.95	0.12	29,29,29,29	0
62	MG	1G	1665	1/1	0.95	0.07	50,50,50,50	0
61	K	1H	3090	1/1	0.95	0.11	55,55,55,55	0
61	K	13	1630	1/1	0.95	0.05	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	14	3177	1/1	0.95	0.07	45,45,45,45	0
61	K	1H	3094	1/1	0.95	0.07	51,51,51,51	0
62	MG	14	3179	1/1	0.95	0.15	32,32,32,32	0
61	K	1H	3048	1/1	0.95	0.06	72,72,72,72	0
61	K	1H	3049	1/1	0.95	0.11	55,55,55,55	0
62	MG	1H	3166	1/1	0.95	0.11	41,41,41,41	0
62	MG	1H	3168	1/1	0.95	0.16	15,15,15,15	0
62	MG	1G	1675	1/1	0.95	0.19	65,65,65,65	0
61	K	2K	102	1/1	0.95	0.15	58,58,58,58	0
62	MG	1H	3172	1/1	0.95	0.17	31,31,31,31	0
61	K	13	1644	1/1	0.95	0.06	74,74,74,74	0
62	MG	1H	3175	1/1	0.95	0.12	31,31,31,31	0
61	K	14	3069	1/1	0.95	0.09	56,56,56,56	0
61	K	14	3015	1/1	0.95	0.05	47,47,47,47	0
62	MG	13	1704	1/1	0.95	0.21	56,56,56,56	0
61	K	1H	3058	1/1	0.95	0.09	43,43,43,43	0
62	MG	13	1657	1/1	0.95	0.19	38,38,38,38	0
62	MG	1H	3283	1/1	0.95	0.26	44,44,44,44	0
62	MG	1H	3284	1/1	0.95	0.06	36,36,36,36	0
61	K	1H	3059	1/1	0.95	0.05	19,19,19,19	0
62	MG	13	1660	1/1	0.95	0.06	39,39,39,39	0
61	K	1G	1629	1/1	0.95	0.07	88,88,88,88	0
62	MG	1H	3424	1/1	0.95	0.08	42,42,42,42	0
62	MG	1H	3288	1/1	0.95	0.14	44,44,44,44	0
62	MG	13	1663	1/1	0.95	0.14	47,47,47,47	0
62	MG	1H	3453	1/1	0.95	0.08	20,20,20,20	0
61	K	1G	1630	1/1	0.95	0.07	80,80,80,80	0
62	MG	14	3210	1/1	0.95	0.17	47,47,47,47	0
62	MG	14	3211	1/1	0.95	0.18	58,58,58,58	0
62	MG	1H	3473	1/1	0.95	0.08	19,19,19,19	0
61	K	1H	3109	1/1	0.95	0.05	57,57,57,57	0
62	MG	1H	3193	1/1	0.95	0.12	40,40,40,40	0
62	MG	1H	3489	1/1	0.95	0.09	57,57,57,57	0
62	MG	1G	1700	1/1	0.95	0.20	52,52,52,52	0
62	MG	1G	1707	1/1	0.95	0.06	62,62,62,62	0
62	MG	1G	1708	1/1	0.95	0.08	101,101,101,101	0
62	MG	13	1666	1/1	0.95	0.20	46,46,46,46	0
62	MG	1H	3506	1/1	0.95	0.08	15,15,15,15	0
62	MG	1H	3512	1/1	0.95	0.08	39,39,39,39	0
62	MG	1H	3299	1/1	0.95	0.13	47,47,47,47	0
62	MG	1H	3528	1/1	0.95	0.07	50,50,50,50	0
62	MG	1H	3300	1/1	0.95	0.30	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3301	1/1	0.95	0.18	41,41,41,41	0
62	MG	13	1669	1/1	0.95	0.13	34,34,34,34	0
61	K	1H	3037	1/1	0.95	0.15	70,70,70,70	0
62	MG	14	3232	1/1	0.95	0.27	63,63,63,63	0
61	K	14	3030	1/1	0.95	0.04	63,63,63,63	0
62	MG	14	3110	1/1	0.95	0.11	35,35,35,35	0
62	MG	13	1717	1/1	0.95	0.29	62,62,62,62	0
62	MG	16	206	1/1	0.95	0.10	52,52,52,52	0
61	K	14	3033	1/1	0.95	0.08	52,52,52,52	0
61	K	1H	3111	1/1	0.95	0.06	51,51,51,51	0
62	MG	14	3116	1/1	0.95	0.15	32,32,32,32	0
61	K	13	1602	1/1	0.95	0.10	72,72,72,72	0
61	K	14	3086	1/1	0.95	0.07	65,65,65,65	0
62	MG	1H	3209	1/1	0.95	0.21	52,52,52,52	0
61	K	13	1632	1/1	0.95	0.10	79,79,79,79	0
62	MG	14	3246	1/1	0.95	0.07	35,35,35,35	0
61	K	4I	201	1/1	0.95	0.06	71,71,71,71	0
62	MG	J8	101	1/1	0.95	0.15	32,32,32,32	0
62	MG	L8	101	1/1	0.95	0.08	38,38,38,38	0
61	K	1H	3118	1/1	0.95	0.05	56,56,56,56	0
62	MG	14	3128	1/1	0.95	0.17	28,28,28,28	0
61	K	13	1626	1/1	0.95	0.06	73,73,73,73	0
62	MG	1G	1637	1/1	0.95	0.13	55,55,55,55	0
62	MG	1H	3324	1/1	0.95	0.15	12,12,12,12	0
62	MG	13	1741	1/1	0.95	0.07	109,109,109,109	0
61	K	1H	3006	1/1	0.95	0.15	44,44,44,44	0
62	MG	14	3263	1/1	0.95	0.26	60,60,60,60	0
62	MG	14	3137	1/1	0.95	0.15	49,49,49,49	0
62	MG	14	3265	1/1	0.95	0.15	34,34,34,34	0
62	MG	13	1764	1/1	0.95	0.07	86,86,86,86	0
62	MG	1H	3226	1/1	0.95	0.22	40,40,40,40	0
62	MG	14	3269	1/1	0.95	0.16	68,68,68,68	0
62	MG	13	1682	1/1	0.95	0.17	33,33,33,33	0
62	MG	13	1683	1/1	0.95	0.11	39,39,39,39	0
62	MG	14	3272	1/1	0.95	0.19	61,61,61,61	0
61	K	4A	201	1/1	0.95	0.07	96,96,96,96	0
62	MG	1H	3230	1/1	0.95	0.23	39,39,39,39	0
62	MG	1H	3333	1/1	0.95	0.09	50,50,50,50	0
62	MG	1H	3232	1/1	0.95	0.16	43,43,43,43	0
62	MG	1H	3233	1/1	0.95	0.12	51,51,51,51	0
62	MG	1H	3234	1/1	0.95	0.21	39,39,39,39	0
61	K	14	3095	1/1	0.95	0.04	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	14	3292	1/1	0.95	0.09	29,29,29,29	0
62	MG	14	3295	1/1	0.95	0.07	50,50,50,50	0
62	MG	14	3305	1/1	0.95	0.07	40,40,40,40	0
61	K	14	3044	1/1	0.95	0.12	69,69,69,69	0
61	K	5A	101	1/1	0.95	0.06	82,82,82,82	0
62	MG	14	3325	1/1	0.95	0.07	30,30,30,30	0
62	MG	14	3326	1/1	0.95	0.07	40,40,40,40	0
62	MG	1H	3243	1/1	0.95	0.18	41,41,41,41	0
62	MG	1H	3151	1/1	0.95	0.20	41,41,41,41	0
62	MG	1H	3152	1/1	0.95	0.06	36,36,36,36	0
61	K	1H	3123	1/1	0.95	0.08	50,50,50,50	0
61	K	14	3001	1/1	0.95	0.08	76,76,76,76	0
62	MG	1H	3348	1/1	0.95	0.09	30,30,30,30	0
62	MG	14	3360	1/1	0.95	0.10	37,37,37,37	0
62	MG	14	3374	1/1	0.95	0.06	30,30,30,30	0
61	K	1H	3007	1/1	0.95	0.05	55,55,55,55	0
62	MG	14	3397	1/1	0.95	0.10	75,75,75,75	0
62	MG	14	3168	1/1	0.95	0.16	37,37,37,37	0
61	K	13	1627	1/1	0.95	0.04	46,46,46,46	0
62	MG	1J	203	1/1	0.95	0.17	48,48,48,48	0
61	K	1G	1612	1/1	0.95	0.05	58,58,58,58	0
62	MG	14	3172	1/1	0.95	0.17	26,26,26,26	0
61	K	1G	1613	1/1	0.95	0.06	63,63,63,63	0
62	MG	M5	101	1/1	0.95	0.07	84,84,84,84	0
62	MG	1H	3544	1/1	0.96	0.05	63,63,63,63	0
62	MG	14	3142	1/1	0.96	0.18	51,51,51,51	0
62	MG	1H	3549	1/1	0.96	0.10	60,60,60,60	0
62	MG	1H	3552	1/1	0.96	0.11	85,85,85,85	0
62	MG	1H	3554	1/1	0.96	0.05	77,77,77,77	0
62	MG	1H	3555	1/1	0.96	0.12	56,56,56,56	0
62	MG	14	3148	1/1	0.96	0.15	43,43,43,43	0
62	MG	1H	3556	1/1	0.96	0.14	47,47,47,47	0
62	MG	14	3150	1/1	0.96	0.09	29,29,29,29	0
62	MG	14	3152	1/1	0.96	0.14	32,32,32,32	0
61	K	1H	3133	1/1	0.96	0.09	61,61,61,61	0
62	MG	1H	3569	1/1	0.96	0.06	62,62,62,62	0
62	MG	1H	3576	1/1	0.96	0.09	69,69,69,69	0
62	MG	1H	3292	1/1	0.96	0.04	32,32,32,32	0
61	K	14	3068	1/1	0.96	0.05	61,61,61,61	0
62	MG	1H	3295	1/1	0.96	0.06	29,29,29,29	0
62	MG	1H	3296	1/1	0.96	0.05	32,32,32,32	0
62	MG	14	3160	1/1	0.96	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	16	207	1/1	0.96	0.16	43,43,43,43	0
62	MG	14	3162	1/1	0.96	0.10	46,46,46,46	0
62	MG	13	1716	1/1	0.96	0.08	37,37,37,37	0
61	K	1G	1621	1/1	0.96	0.04	76,76,76,76	0
61	K	1H	3100	1/1	0.96	0.05	44,44,44,44	0
62	MG	21	303	1/1	0.96	0.10	33,33,33,33	0
61	K	1H	3101	1/1	0.96	0.04	49,49,49,49	0
61	K	1H	3103	1/1	0.96	0.13	33,33,33,33	0
62	MG	14	3169	1/1	0.96	0.16	33,33,33,33	0
62	MG	1H	3302	1/1	0.96	0.12	29,29,29,29	0
62	MG	78	202	1/1	0.96	0.13	30,30,30,30	0
61	K	14	3074	1/1	0.96	0.11	73,73,73,73	0
62	MG	1H	3304	1/1	0.96	0.17	38,38,38,38	0
61	K	14	3019	1/1	0.96	0.08	40,40,40,40	0
62	MG	N8	101	1/1	0.96	0.14	41,41,41,41	0
62	MG	1H	3306	1/1	0.96	0.07	34,34,34,34	0
62	MG	1H	3308	1/1	0.96	0.04	27,27,27,27	0
62	MG	Q8	101[A]	1/1	0.96	0.49	13,13,13,13	1
62	MG	Q8	101[B]	1/1	0.96	0.49	11,11,11,11	1
62	MG	1H	3309	1/1	0.96	0.05	52,52,52,52	0
62	MG	1H	3310	1/1	0.96	0.04	18,18,18,18	0
61	K	1G	1626	1/1	0.96	0.04	67,67,67,67	0
62	MG	1H	3312	1/1	0.96	0.19	39,39,39,39	0
62	MG	14	3183	1/1	0.96	0.20	30,30,30,30	0
62	MG	1H	3205	1/1	0.96	0.15	33,33,33,33	0
62	MG	1H	3206	1/1	0.96	0.12	25,25,25,25	0
61	K	14	3022	1/1	0.96	0.12	50,50,50,50	0
62	MG	13	1725	1/1	0.96	0.27	58,58,58,58	0
62	MG	1H	3210	1/1	0.96	0.17	38,38,38,38	0
61	K	1H	3104	1/1	0.96	0.07	42,42,42,42	0
62	MG	13	1738	1/1	0.96	0.06	86,86,86,86	0
61	K	1H	3012	1/1	0.96	0.07	51,51,51,51	0
61	K	14	3081	1/1	0.96	0.07	54,54,54,54	0
62	MG	1H	3322	1/1	0.96	0.08	23,23,23,23	0
62	MG	1H	3216	1/1	0.96	0.15	34,34,34,34	0
62	MG	1H	3217	1/1	0.96	0.22	31,31,31,31	0
62	MG	13	1750	1/1	0.96	0.06	52,52,52,52	0
62	MG	14	3198	1/1	0.96	0.13	33,33,33,33	0
62	MG	13	1751	1/1	0.96	0.10	75,75,75,75	0
62	MG	1H	3222	1/1	0.96	0.14	32,32,32,32	0
62	MG	1H	3223	1/1	0.96	0.14	30,30,30,30	0
62	MG	1H	3224	1/1	0.96	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	14	3203	1/1	0.96	0.25	45,45,45,45	0
62	MG	13	1755	1/1	0.96	0.05	83,83,83,83	0
62	MG	14	3206	1/1	0.96	0.16	55,55,55,55	0
62	MG	1H	3330	1/1	0.96	0.21	45,45,45,45	0
62	MG	1G	1660	1/1	0.96	0.26	46,46,46,46	0
62	MG	13	1757	1/1	0.96	0.08	50,50,50,50	0
61	K	13	1609	1/1	0.96	0.06	57,57,57,57	0
62	MG	13	1767	1/1	0.96	0.08	70,70,70,70	0
62	MG	13	1770	1/1	0.96	0.06	71,71,71,71	0
61	K	14	3029	1/1	0.96	0.07	81,81,81,81	0
62	MG	1H	3231	1/1	0.96	0.26	43,43,43,43	0
61	K	1H	3074	1/1	0.96	0.10	34,34,34,34	0
61	K	14	3085	1/1	0.96	0.06	62,62,62,62	0
61	K	14	3032	1/1	0.96	0.13	53,53,53,53	0
62	MG	14	3218	1/1	0.96	0.12	60,60,60,60	0
62	MG	1G	1669	1/1	0.96	0.30	60,60,60,60	0
62	MG	1H	3235	1/1	0.96	0.07	42,42,42,42	0
61	K	1H	3077	1/1	0.96	0.09	47,47,47,47	0
62	MG	1H	3237	1/1	0.96	0.11	38,38,38,38	0
61	K	13	1640	1/1	0.96	0.04	60,60,60,60	0
62	MG	1H	3239	1/1	0.96	0.07	26,26,26,26	0
61	K	14	3089	1/1	0.96	0.06	64,64,64,64	0
61	K	1H	3024	1/1	0.96	0.07	59,59,59,59	0
62	MG	14	3229	1/1	0.96	0.06	48,48,48,48	0
61	K	14	3037	1/1	0.96	0.05	60,60,60,60	0
61	K	31	302	1/1	0.96	0.08	45,45,45,45	0
61	K	1H	3015	1/1	0.96	0.05	44,44,44,44	0
61	K	88	201	1/1	0.96	0.12	57,57,57,57	0
62	MG	1H	3250	1/1	0.96	0.12	38,38,38,38	0
61	K	13	1601	1/1	0.96	0.06	67,67,67,67	0
61	K	13	1624	1/1	0.96	0.09	59,59,59,59	0
61	K	1G	1603	1/1	0.96	0.10	62,62,62,62	0
62	MG	1H	3256	1/1	0.96	0.13	40,40,40,40	0
62	MG	14	3240	1/1	0.96	0.22	57,57,57,57	0
62	MG	1H	3257	1/1	0.96	0.14	40,40,40,40	0
61	K	1H	3120	1/1	0.96	0.05	60,60,60,60	0
61	K	13	1637	1/1	0.96	0.08	64,64,64,64	0
62	MG	1H	3260	1/1	0.96	0.05	24,24,24,24	0
62	MG	1H	3261	1/1	0.96	0.04	44,44,44,44	0
62	MG	1H	3262	1/1	0.96	0.25	46,46,46,46	0
61	K	14	3046	1/1	0.96	0.11	54,54,54,54	0
61	K	1H	3019	1/1	0.96	0.05	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3265	1/1	0.96	0.11	48,48,48,48	0
62	MG	14	3250	1/1	0.96	0.05	38,38,38,38	0
61	K	13	1633	1/1	0.96	0.06	55,55,55,55	0
62	MG	1H	3267	1/1	0.96	0.17	53,53,53,53	0
61	K	1G	1610	1/1	0.96	0.04	68,68,68,68	0
62	MG	13	1700	1/1	0.96	0.13	47,47,47,47	0
61	K	1H	3062	1/1	0.96	0.03	27,27,27,27	0
62	MG	1H	3377	1/1	0.96	0.12	26,26,26,26	0
62	MG	1G	1709	1/1	0.96	0.06	73,73,73,73	0
62	MG	14	3261	1/1	0.96	0.20	43,43,43,43	0
62	MG	14	3262	1/1	0.96	0.19	41,41,41,41	0
62	MG	1G	1711	1/1	0.96	0.07	97,97,97,97	0
62	MG	1G	1713	1/1	0.96	0.09	120,120,120,120	0
62	MG	1H	3379	1/1	0.96	0.26	47,47,47,47	0
62	MG	1H	3380	1/1	0.96	0.27	44,44,44,44	0
62	MG	1G	1721	1/1	0.96	0.05	45,45,45,45	0
62	MG	1G	1731	1/1	0.96	0.06	81,81,81,81	0
61	K	1H	3063	1/1	0.96	0.05	47,47,47,47	0
62	MG	1H	3382	1/1	0.96	0.07	13,13,13,13	0
62	MG	1H	3391	1/1	0.96	0.08	20,20,20,20	0
61	K	1J	201	1/1	0.96	0.05	81,81,81,81	0
62	MG	2L	103	1/1	0.96	0.17	45,45,45,45	0
62	MG	1H	3422	1/1	0.96	0.06	29,29,29,29	0
62	MG	1H	3274	1/1	0.96	0.07	31,31,31,31	0
61	K	1H	3097	1/1	0.96	0.06	25,25,25,25	0
61	K	39	301	1/1	0.96	0.08	75,75,75,75	0
62	MG	14	3280	1/1	0.96	0.08	45,45,45,45	0
61	K	14	3054	1/1	0.96	0.05	58,58,58,58	0
62	MG	14	3111	1/1	0.96	0.09	32,32,32,32	0
62	MG	1H	3455	1/1	0.96	0.06	11,11,11,11	0
61	K	1H	3129	1/1	0.96	0.10	60,60,60,60	0
62	MG	14	3306	1/1	0.96	0.07	32,32,32,32	0
61	K	14	3056	1/1	0.96	0.06	56,56,56,56	0
62	MG	14	3313	1/1	0.96	0.06	33,33,33,33	0
62	MG	14	3314	1/1	0.96	0.07	28,28,28,28	0
62	MG	1H	3474	1/1	0.96	0.06	24,24,24,24	0
62	MG	14	3320	1/1	0.96	0.07	25,25,25,25	0
62	MG	1H	3181	1/1	0.96	0.21	36,36,36,36	0
61	K	14	3008	1/1	0.96	0.12	47,47,47,47	0
61	K	1G	1615	1/1	0.96	0.04	60,60,60,60	0
62	MG	1H	3496	1/1	0.96	0.09	48,48,48,48	0
62	MG	1H	3184	1/1	0.96	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3501	1/1	0.96	0.12	57,57,57,57	0
62	MG	1H	3503	1/1	0.96	0.07	29,29,29,29	0
62	MG	1H	3185	1/1	0.96	0.06	40,40,40,40	0
61	K	1H	3042	1/1	0.96	0.04	54,54,54,54	0
62	MG	14	3372	1/1	0.96	0.05	64,64,64,64	0
62	MG	14	3373	1/1	0.96	0.06	68,68,68,68	0
62	MG	1H	3514	1/1	0.96	0.08	53,53,53,53	0
62	MG	14	3380	1/1	0.96	0.07	76,76,76,76	0
62	MG	14	3386	1/1	0.96	0.13	61,61,61,61	0
62	MG	14	3129	1/1	0.96	0.07	34,34,34,34	0
62	MG	14	3394	1/1	0.96	0.13	61,61,61,61	0
62	MG	1H	3515	1/1	0.96	0.07	40,40,40,40	0
61	K	1H	3070	1/1	0.96	0.06	46,46,46,46	0
62	MG	1H	3519	1/1	0.96	0.17	25,25,25,25	0
62	MG	14	3134	1/1	0.96	0.17	34,34,34,34	0
61	K	1G	1618	1/1	0.96	0.14	79,79,79,79	0
62	MG	1H	3529	1/1	0.96	0.15	54,54,54,54	0
61	K	14	3066	1/1	0.96	0.04	64,64,64,64	0
62	MG	1H	3190	1/1	0.96	0.13	32,32,32,32	0
62	MG	1H	3516	1/1	0.97	0.06	21,21,21,21	0
62	MG	1H	3198	1/1	0.97	0.05	20,20,20,20	0
62	MG	14	3193	1/1	0.97	0.19	40,40,40,40	0
61	K	14	3073	1/1	0.97	0.05	60,60,60,60	0
62	MG	1H	3522	1/1	0.97	0.10	49,49,49,49	0
62	MG	1H	3526	1/1	0.97	0.09	21,21,21,21	0
62	MG	1G	1694	1/1	0.97	0.07	43,43,43,43	0
62	MG	1H	3200	1/1	0.97	0.13	36,36,36,36	0
62	MG	1H	3268	1/1	0.97	0.06	34,34,34,34	0
62	MG	1H	3335	1/1	0.97	0.22	40,40,40,40	0
62	MG	13	1769	1/1	0.97	0.08	54,54,54,54	0
62	MG	1H	3542	1/1	0.97	0.13	33,33,33,33	0
62	MG	1H	3337	1/1	0.97	0.04	23,23,23,23	0
62	MG	1G	1702	1/1	0.97	0.06	64,64,64,64	0
62	MG	14	3205	1/1	0.97	0.31	51,51,51,51	0
62	MG	1G	1703	1/1	0.97	0.04	81,81,81,81	0
62	MG	1H	3548	1/1	0.97	0.06	32,32,32,32	0
61	K	1H	3119	1/1	0.97	0.17	46,46,46,46	0
62	MG	1H	3550	1/1	0.97	0.07	64,64,64,64	0
62	MG	1H	3551	1/1	0.97	0.07	45,45,45,45	0
61	K	1H	3143	1/1	0.97	0.04	71,71,71,71	0
62	MG	1H	3553	1/1	0.97	0.07	60,60,60,60	0
61	K	1H	3054	1/1	0.97	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3341	1/1	0.97	0.09	24,24,24,24	0
62	MG	1G	1724	1/1	0.97	0.04	82,82,82,82	0
62	MG	1G	1726	1/1	0.97	0.06	49,49,49,49	0
61	K	1H	3056	1/1	0.97	0.04	37,37,37,37	0
62	MG	1G	1733	1/1	0.97	0.04	81,81,81,81	0
62	MG	14	3219	1/1	0.97	0.12	33,33,33,33	0
62	MG	1G	1735	1/1	0.97	0.08	88,88,88,88	0
62	MG	1H	3558	1/1	0.97	0.11	56,56,56,56	0
62	MG	1H	3563	1/1	0.97	0.07	75,75,75,75	0
61	K	2I	301	1/1	0.97	0.12	62,62,62,62	0
62	MG	1H	3566	1/1	0.97	0.10	37,37,37,37	0
62	MG	1H	3567	1/1	0.97	0.08	24,24,24,24	0
62	MG	13	1655	1/1	0.97	0.10	51,51,51,51	0
62	MG	14	3227	1/1	0.97	0.10	38,38,38,38	0
62	MG	1H	3208	1/1	0.97	0.07	37,37,37,37	0
62	MG	13	1656	1/1	0.97	0.09	49,49,49,49	0
62	MG	1H	3150	1/1	0.97	0.19	25,25,25,25	0
62	MG	1H	3347	1/1	0.97	0.06	38,38,38,38	0
61	K	1G	1624	1/1	0.97	0.05	60,60,60,60	0
62	MG	13	1658	1/1	0.97	0.13	36,36,36,36	0
61	K	1H	3076	1/1	0.97	0.05	50,50,50,50	0
61	K	13	1617	1/1	0.97	0.08	50,50,50,50	0
62	MG	1H	3215	1/1	0.97	0.15	40,40,40,40	0
62	MG	16	211	1/1	0.97	0.04	57,57,57,57	0
62	MG	14	3238	1/1	0.97	0.14	44,44,44,44	0
62	MG	16	215	1/1	0.97	0.05	52,52,52,52	0
62	MG	1H	3354	1/1	0.97	0.06	29,29,29,29	0
62	MG	13	1661	1/1	0.97	0.14	39,39,39,39	0
61	K	1H	3124	1/1	0.97	0.06	64,64,64,64	0
62	MG	1H	3218	1/1	0.97	0.13	28,28,28,28	0
62	MG	1H	3156	1/1	0.97	0.26	33,33,33,33	0
61	K	1H	3039	1/1	0.97	0.05	54,54,54,54	0
62	MG	I8	101	1/1	0.97	0.12	26,26,26,26	0
62	MG	14	3126	1/1	0.97	0.11	27,27,27,27	0
62	MG	1H	3158	1/1	0.97	0.07	57,57,57,57	0
61	K	1H	3061	1/1	0.97	0.04	43,43,43,43	0
62	MG	14	3130	1/1	0.97	0.03	38,38,38,38	0
61	K	14	3049	1/1	0.97	0.04	49,49,49,49	0
62	MG	14	3252	1/1	0.97	0.20	42,42,42,42	0
61	K	1H	3127	1/1	0.97	0.05	47,47,47,47	0
62	MG	13	1668	1/1	0.97	0.07	31,31,31,31	0
61	K	1H	3033	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3366	1/1	0.97	0.10	40,40,40,40	0
62	MG	14	3258	1/1	0.97	0.10	34,34,34,34	0
62	MG	13	1670	1/1	0.97	0.08	42,42,42,42	0
61	K	1H	3085	1/1	0.97	0.10	39,39,39,39	0
61	K	14	3090	1/1	0.97	0.04	64,64,64,64	0
62	MG	1H	3167	1/1	0.97	0.10	20,20,20,20	0
61	K	1G	1606	1/1	0.97	0.19	61,61,61,61	0
62	MG	1H	3169	1/1	0.97	0.14	15,15,15,15	0
62	MG	14	3144	1/1	0.97	0.07	36,36,36,36	0
62	MG	14	3266	1/1	0.97	0.04	38,38,38,38	0
62	MG	1H	3170	1/1	0.97	0.13	18,18,18,18	0
61	K	1H	3107	1/1	0.97	0.07	44,44,44,44	0
61	K	13	1619	1/1	0.97	0.19	58,58,58,58	0
61	K	1G	1609	1/1	0.97	0.04	91,91,91,91	0
62	MG	1H	3378	1/1	0.97	0.04	28,28,28,28	0
62	MG	1H	3307	1/1	0.97	0.06	25,25,25,25	0
62	MG	14	3151	1/1	0.97	0.10	26,26,26,26	0
61	K	13	1628	1/1	0.97	0.03	51,51,51,51	0
61	K	14	3059	1/1	0.97	0.09	48,48,48,48	0
62	MG	1H	3240	1/1	0.97	0.14	39,39,39,39	0
62	MG	1H	3383	1/1	0.97	0.05	18,18,18,18	0
61	K	14	3060	1/1	0.97	0.08	45,45,45,45	0
61	K	14	3026	1/1	0.97	0.03	35,35,35,35	0
62	MG	14	3282	1/1	0.97	0.06	48,48,48,48	0
62	MG	1H	3417	1/1	0.97	0.05	61,61,61,61	0
62	MG	14	3291	1/1	0.97	0.06	58,58,58,58	0
62	MG	1H	3419	1/1	0.97	0.08	27,27,27,27	0
62	MG	14	3293	1/1	0.97	0.07	60,60,60,60	0
62	MG	14	3294	1/1	0.97	0.06	51,51,51,51	0
61	K	1H	3089	1/1	0.97	0.03	36,36,36,36	0
62	MG	14	3301	1/1	0.97	0.06	38,38,38,38	0
62	MG	1H	3423	1/1	0.97	0.06	35,35,35,35	0
61	K	14	3063	1/1	0.97	0.04	57,57,57,57	0
62	MG	1H	3426	1/1	0.97	0.09	12,12,12,12	0
62	MG	1H	3428	1/1	0.97	0.04	23,23,23,23	0
61	K	14	3028	1/1	0.97	0.06	45,45,45,45	0
62	MG	1H	3247	1/1	0.97	0.15	21,21,21,21	0
62	MG	1H	3450	1/1	0.97	0.09	52,52,52,52	0
62	MG	1H	3317	1/1	0.97	0.23	52,52,52,52	0
61	K	1H	3065	1/1	0.97	0.14	30,30,30,30	0
62	MG	1H	3249	1/1	0.97	0.13	31,31,31,31	0
61	K	1H	3067	1/1	0.97	0.03	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	13	1622	1/1	0.97	0.05	61,61,61,61	0
62	MG	14	3340	1/1	0.97	0.06	26,26,26,26	0
62	MG	13	1747	1/1	0.97	0.06	32,32,32,32	0
62	MG	14	3343	1/1	0.97	0.07	50,50,50,50	0
62	MG	14	3347	1/1	0.97	0.06	27,27,27,27	0
62	MG	14	3348	1/1	0.97	0.06	30,30,30,30	0
62	MG	1H	3479	1/1	0.97	0.05	18,18,18,18	0
62	MG	1H	3484	1/1	0.97	0.07	16,16,16,16	0
62	MG	1H	3485	1/1	0.97	0.07	29,29,29,29	0
62	MG	14	3364	1/1	0.97	0.05	36,36,36,36	0
62	MG	14	3369	1/1	0.97	0.05	76,76,76,76	0
62	MG	14	3370	1/1	0.97	0.07	44,44,44,44	0
62	MG	14	3371	1/1	0.97	0.05	32,32,32,32	0
62	MG	13	1748	1/1	0.97	0.06	38,38,38,38	0
61	K	1H	3071	1/1	0.97	0.04	42,42,42,42	0
62	MG	1H	3490	1/1	0.97	0.04	32,32,32,32	0
62	MG	14	3375	1/1	0.97	0.06	84,84,84,84	0
61	K	1H	3116	1/1	0.97	0.05	61,61,61,61	0
62	MG	14	3381	1/1	0.97	0.07	56,56,56,56	0
62	MG	14	3383	1/1	0.97	0.09	51,51,51,51	0
62	MG	14	3385	1/1	0.97	0.05	58,58,58,58	0
62	MG	1H	3497	1/1	0.97	0.10	55,55,55,55	0
61	K	14	3002	1/1	0.97	0.06	69,69,69,69	0
62	MG	14	3389	1/1	0.97	0.05	45,45,45,45	0
62	MG	14	3392	1/1	0.97	0.08	75,75,75,75	0
62	MG	1H	3191	1/1	0.97	0.12	24,24,24,24	0
62	MG	13	1753	1/1	0.97	0.05	69,69,69,69	0
62	MG	1H	3504	1/1	0.97	0.10	20,20,20,20	0
61	K	19	301	1/1	0.97	0.13	52,52,52,52	0
62	MG	1H	3507	1/1	0.97	0.06	17,17,17,17	0
62	MG	1H	3508	1/1	0.97	0.06	22,22,22,22	0
61	K	14	3036	1/1	0.97	0.13	41,41,41,41	0
61	K	1H	3001	1/1	0.97	0.05	48,48,48,48	0
62	MG	13	1766	1/1	0.97	0.07	64,64,64,64	0
62	MG	1H	3454	1/1	0.98	0.06	23,23,23,23	0
62	MG	1H	3352	1/1	0.98	0.07	43,43,43,43	0
62	MG	1H	3148	1/1	0.98	0.14	35,35,35,35	0
62	MG	1H	3461	1/1	0.98	0.05	20,20,20,20	0
62	MG	1H	3462	1/1	0.98	0.05	27,27,27,27	0
62	MG	1H	3464	1/1	0.98	0.07	23,23,23,23	0
62	MG	1H	3466	1/1	0.98	0.06	22,22,22,22	0
62	MG	1H	3468	1/1	0.98	0.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	K	1H	3043	1/1	0.98	0.04	58,58,58,58	0
61	K	14	3031	1/1	0.98	0.03	29,29,29,29	0
62	MG	1H	3475	1/1	0.98	0.06	40,40,40,40	0
61	K	1H	3117	1/1	0.98	0.12	57,57,57,57	0
62	MG	1H	3478	1/1	0.98	0.12	44,44,44,44	0
62	MG	13	1727	1/1	0.98	0.08	60,60,60,60	0
62	MG	1H	3480	1/1	0.98	0.05	18,18,18,18	0
62	MG	1H	3481	1/1	0.98	0.05	21,21,21,21	0
62	MG	14	3127	1/1	0.98	0.10	30,30,30,30	0
62	MG	1H	3483	1/1	0.98	0.08	36,36,36,36	0
62	MG	13	1728	1/1	0.98	0.06	60,60,60,60	0
62	MG	13	1729	1/1	0.98	0.03	61,61,61,61	0
62	MG	13	1733	1/1	0.98	0.03	62,62,62,62	0
61	K	1H	3093	1/1	0.98	0.07	42,42,42,42	0
61	K	1H	3052	1/1	0.98	0.04	52,52,52,52	0
62	MG	1H	3493	1/1	0.98	0.08	27,27,27,27	0
62	MG	1H	3494	1/1	0.98	0.05	43,43,43,43	0
62	MG	1H	3495	1/1	0.98	0.07	48,48,48,48	0
62	MG	13	1744	1/1	0.98	0.05	19,19,19,19	0
62	MG	14	3138	1/1	0.98	0.08	31,31,31,31	0
61	K	1G	1619	1/1	0.98	0.07	74,74,74,74	0
62	MG	1H	3498	1/1	0.98	0.09	24,24,24,24	0
62	MG	14	3141	1/1	0.98	0.14	26,26,26,26	0
61	K	14	3057	1/1	0.98	0.06	54,54,54,54	0
61	K	1H	3106	1/1	0.98	0.07	59,59,59,59	0
62	MG	1H	3502	1/1	0.98	0.04	25,25,25,25	0
61	K	1H	3136	1/1	0.98	0.09	54,54,54,54	0
62	MG	1H	3241	1/1	0.98	0.16	30,30,30,30	0
61	K	14	3016	1/1	0.98	0.03	44,44,44,44	0
62	MG	13	1752	1/1	0.98	0.06	47,47,47,47	0
61	K	1H	3066	1/1	0.98	0.05	27,27,27,27	0
62	MG	1H	3510	1/1	0.98	0.04	19,19,19,19	0
62	MG	13	1667	1/1	0.98	0.10	29,29,29,29	0
62	MG	1H	3289	1/1	0.98	0.20	35,35,35,35	0
62	MG	1H	3374	1/1	0.98	0.04	28,28,28,28	0
62	MG	13	1756	1/1	0.98	0.09	63,63,63,63	0
61	K	1H	3084	1/1	0.98	0.16	47,47,47,47	0
62	MG	13	1758	1/1	0.98	0.03	76,76,76,76	0
62	MG	1H	3520	1/1	0.98	0.06	37,37,37,37	0
62	MG	1H	3293	1/1	0.98	0.23	40,40,40,40	0
62	MG	1H	3523	1/1	0.98	0.05	32,32,32,32	0
62	MG	1H	3524	1/1	0.98	0.05	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	13	1759	1/1	0.98	0.06	52,52,52,52	0
62	MG	13	1763	1/1	0.98	0.05	64,64,64,64	0
61	K	1H	3057	1/1	0.98	0.03	23,23,23,23	0
61	K	1H	3069	1/1	0.98	0.03	16,16,16,16	0
62	MG	1H	3532	1/1	0.98	0.06	56,56,56,56	0
62	MG	1H	3535	1/1	0.98	0.06	64,64,64,64	0
62	MG	1H	3536	1/1	0.98	0.04	23,23,23,23	0
62	MG	1H	3173	1/1	0.98	0.13	28,28,28,28	0
62	MG	14	3281	1/1	0.98	0.05	25,25,25,25	0
62	MG	1H	3540	1/1	0.98	0.07	50,50,50,50	0
62	MG	14	3288	1/1	0.98	0.04	39,39,39,39	0
62	MG	1H	3541	1/1	0.98	0.04	66,66,66,66	0
62	MG	14	3290	1/1	0.98	0.06	36,36,36,36	0
62	MG	1H	3387	1/1	0.98	0.05	16,16,16,16	0
62	MG	1H	3390	1/1	0.98	0.06	26,26,26,26	0
62	MG	1H	3546	1/1	0.98	0.05	61,61,61,61	0
62	MG	1H	3547	1/1	0.98	0.06	52,52,52,52	0
61	K	14	3021	1/1	0.98	0.04	41,41,41,41	0
62	MG	14	3298	1/1	0.98	0.05	32,32,32,32	0
62	MG	1H	3393	1/1	0.98	0.04	17,17,17,17	0
62	MG	14	3303	1/1	0.98	0.04	58,58,58,58	0
61	K	1H	3053	1/1	0.98	0.04	25,25,25,25	0
62	MG	1H	3400	1/1	0.98	0.08	20,20,20,20	0
62	MG	1G	1693	1/1	0.98	0.09	40,40,40,40	0
62	MG	14	3310	1/1	0.98	0.05	25,25,25,25	0
62	MG	14	3312	1/1	0.98	0.09	38,38,38,38	0
62	MG	1H	3405	1/1	0.98	0.08	16,16,16,16	0
62	MG	1H	3409	1/1	0.98	0.11	14,14,14,14	0
62	MG	14	3315	1/1	0.98	0.05	39,39,39,39	0
62	MG	1H	3411	1/1	0.98	0.04	20,20,20,20	0
62	MG	14	3318	1/1	0.98	0.06	35,35,35,35	0
62	MG	1H	3412	1/1	0.98	0.05	16,16,16,16	0
62	MG	14	3321	1/1	0.98	0.06	26,26,26,26	0
62	MG	14	3322	1/1	0.98	0.04	41,41,41,41	0
62	MG	1H	3413	1/1	0.98	0.04	49,49,49,49	0
62	MG	1H	3415	1/1	0.98	0.07	16,16,16,16	0
62	MG	14	3327	1/1	0.98	0.06	36,36,36,36	0
61	K	1H	3078	1/1	0.98	0.02	45,45,45,45	0
62	MG	14	3331	1/1	0.98	0.07	51,51,51,51	0
62	MG	3E	301	1/1	0.98	0.03	82,82,82,82	0
62	MG	1H	3420	1/1	0.98	0.06	20,20,20,20	0
62	MG	14	3339	1/1	0.98	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1G	1705	1/1	0.98	0.07	73,73,73,73	0
62	MG	1H	3177	1/1	0.98	0.19	29,29,29,29	0
62	MG	14	3342	1/1	0.98	0.06	32,32,32,32	0
62	MG	1H	3178	1/1	0.98	0.11	17,17,17,17	0
62	MG	14	3345	1/1	0.98	0.06	48,48,48,48	0
62	MG	1H	3570	1/1	0.98	0.05	50,50,50,50	0
62	MG	1H	3573	1/1	0.98	0.03	40,40,40,40	0
62	MG	14	3349	1/1	0.98	0.08	48,48,48,48	0
62	MG	14	3350	1/1	0.98	0.06	39,39,39,39	0
62	MG	1H	3219	1/1	0.98	0.23	31,31,31,31	0
62	MG	1H	3425	1/1	0.98	0.04	16,16,16,16	0
62	MG	14	3354	1/1	0.98	0.06	30,30,30,30	0
62	MG	14	3356	1/1	0.98	0.05	36,36,36,36	0
62	MG	14	3357	1/1	0.98	0.04	48,48,48,48	0
62	MG	14	3358	1/1	0.98	0.12	51,51,51,51	0
62	MG	14	3359	1/1	0.98	0.05	33,33,33,33	0
62	MG	1G	1716	1/1	0.98	0.04	70,70,70,70	0
62	MG	14	3361	1/1	0.98	0.05	48,48,48,48	0
62	MG	14	3362	1/1	0.98	0.04	68,68,68,68	0
61	K	1H	3113	1/1	0.98	0.03	30,30,30,30	0
62	MG	14	3365	1/1	0.98	0.06	28,28,28,28	0
62	MG	1G	1720	1/1	0.98	0.10	73,73,73,73	0
61	K	1H	3079	1/1	0.98	0.05	37,37,37,37	0
62	MG	1G	1723	1/1	0.98	0.07	59,59,59,59	0
61	K	1H	3102	1/1	0.98	0.04	51,51,51,51	0
62	MG	1G	1725	1/1	0.98	0.04	69,69,69,69	0
62	MG	1H	3430	1/1	0.98	0.04	54,54,54,54	0
62	MG	1G	1727	1/1	0.98	0.05	59,59,59,59	0
62	MG	14	3376	1/1	0.98	0.05	54,54,54,54	0
62	MG	14	3379	1/1	0.98	0.04	43,43,43,43	0
62	MG	1G	1728	1/1	0.98	0.07	50,50,50,50	0
62	MG	1G	1729	1/1	0.98	0.06	67,67,67,67	0
62	MG	14	3382	1/1	0.98	0.05	52,52,52,52	0
62	MG	1G	1730	1/1	0.98	0.05	78,78,78,78	0
62	MG	14	3384	1/1	0.98	0.08	47,47,47,47	0
62	MG	1H	3431	1/1	0.98	0.05	46,46,46,46	0
62	MG	1H	3436	1/1	0.98	0.06	57,57,57,57	0
62	MG	1G	1734	1/1	0.98	0.08	94,94,94,94	0
62	MG	14	3388	1/1	0.98	0.07	91,91,91,91	0
62	MG	1H	3145	1/1	0.98	0.15	17,17,17,17	0
62	MG	14	3390	1/1	0.98	0.04	79,79,79,79	0
62	MG	1H	3438	1/1	0.98	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	14	3393	1/1	0.98	0.08	63,63,63,63	0
62	MG	32	302	1/1	0.98	0.06	79,79,79,79	0
62	MG	14	3395	1/1	0.98	0.05	25,25,25,25	0
62	MG	14	3396	1/1	0.98	0.05	66,66,66,66	0
62	MG	16	214	1/1	0.98	0.05	57,57,57,57	0
62	MG	1H	3440	1/1	0.98	0.04	62,62,62,62	0
62	MG	1H	3443	1/1	0.98	0.08	42,42,42,42	0
62	MG	1H	3444	1/1	0.98	0.05	23,23,23,23	0
61	K	16	203	1/1	0.98	0.03	44,44,44,44	0
62	MG	1H	3451	1/1	0.98	0.04	82,82,82,82	0
62	MG	29	303	1/1	0.98	0.05	28,28,28,28	0
62	MG	1H	3452	1/1	0.98	0.04	68,68,68,68	0
61	K	1H	3130	1/1	0.98	0.07	61,61,61,61	0
62	MG	13	1746	1/1	0.99	0.04	37,37,37,37	0
62	MG	1H	3432	1/1	0.99	0.03	55,55,55,55	0
62	MG	14	3253	1/1	0.99	0.03	47,47,47,47	0
62	MG	1H	3518	1/1	0.99	0.04	37,37,37,37	0
62	MG	1H	3433	1/1	0.99	0.06	51,51,51,51	0
62	MG	1H	3434	1/1	0.99	0.07	46,46,46,46	0
62	MG	1H	3521	1/1	0.99	0.06	14,14,14,14	0
62	MG	1H	3435	1/1	0.99	0.05	46,46,46,46	0
61	K	11	301	1/1	0.99	0.06	31,31,31,31	0
61	K	1H	3055	1/1	0.99	0.06	31,31,31,31	0
62	MG	1H	3525	1/1	0.99	0.05	15,15,15,15	0
62	MG	1H	3342	1/1	0.99	0.20	27,27,27,27	0
62	MG	1H	3527	1/1	0.99	0.07	26,26,26,26	0
61	K	31	301	1/1	0.99	0.06	48,48,48,48	0
62	MG	1H	3441	1/1	0.99	0.06	61,61,61,61	0
62	MG	1H	3442	1/1	0.99	0.04	56,56,56,56	0
62	MG	1H	3531	1/1	0.99	0.09	21,21,21,21	0
61	K	1H	3092	1/1	0.99	0.06	37,37,37,37	0
62	MG	1G	1671	1/1	0.99	0.29	46,46,46,46	0
62	MG	1H	3533	1/1	0.99	0.04	49,49,49,49	0
62	MG	1H	3534	1/1	0.99	0.03	27,27,27,27	0
61	K	14	3023	1/1	0.99	0.07	60,60,60,60	0
62	MG	1H	3445	1/1	0.99	0.03	50,50,50,50	0
62	MG	1H	3537	1/1	0.99	0.04	54,54,54,54	0
62	MG	1H	3538	1/1	0.99	0.04	27,27,27,27	0
62	MG	1H	3446	1/1	0.99	0.04	48,48,48,48	0
62	MG	1H	3447	1/1	0.99	0.04	19,19,19,19	0
62	MG	1H	3448	1/1	0.99	0.07	57,57,57,57	0
62	MG	14	3279	1/1	0.99	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3449	1/1	0.99	0.05	15,15,15,15	0
62	MG	1H	3543	1/1	0.99	0.06	48,48,48,48	0
61	K	1H	3060	1/1	0.99	0.04	34,34,34,34	0
62	MG	14	3283	1/1	0.99	0.03	21,21,21,21	0
62	MG	14	3284	1/1	0.99	0.05	34,34,34,34	0
62	MG	14	3285	1/1	0.99	0.06	30,30,30,30	0
62	MG	14	3286	1/1	0.99	0.05	25,25,25,25	0
62	MG	1H	3545	1/1	0.99	0.04	45,45,45,45	0
61	K	1H	3075	1/1	0.99	0.03	28,28,28,28	0
62	MG	13	1754	1/1	0.99	0.05	35,35,35,35	0
61	K	1H	3087	1/1	0.99	0.02	31,31,31,31	0
61	K	14	3075	1/1	0.99	0.03	36,36,36,36	0
62	MG	1H	3384	1/1	0.99	0.04	11,11,11,11	0
62	MG	1H	3456	1/1	0.99	0.12	14,14,14,14	0
62	MG	1H	3386	1/1	0.99	0.03	31,31,31,31	0
62	MG	14	3296	1/1	0.99	0.04	35,35,35,35	0
62	MG	1H	3459	1/1	0.99	0.04	15,15,15,15	0
62	MG	14	3299	1/1	0.99	0.03	48,48,48,48	0
62	MG	1H	3460	1/1	0.99	0.03	11,11,11,11	0
62	MG	14	3302	1/1	0.99	0.06	29,29,29,29	0
62	MG	13	1730	1/1	0.99	0.06	76,76,76,76	0
62	MG	14	3304	1/1	0.99	0.03	63,63,63,63	0
62	MG	1H	3389	1/1	0.99	0.03	13,13,13,13	0
62	MG	1H	3557	1/1	0.99	0.02	22,22,22,22	0
62	MG	14	3307	1/1	0.99	0.09	36,36,36,36	0
62	MG	14	3308	1/1	0.99	0.03	77,77,77,77	0
62	MG	1H	3463	1/1	0.99	0.04	17,17,17,17	0
62	MG	1H	3559	1/1	0.99	0.07	15,15,15,15	0
62	MG	14	3311	1/1	0.99	0.03	31,31,31,31	0
62	MG	1H	3560	1/1	0.99	0.08	13,13,13,13	0
62	MG	1H	3561	1/1	0.99	0.03	38,38,38,38	0
62	MG	1H	3562	1/1	0.99	0.04	31,31,31,31	0
62	MG	1G	1701	1/1	0.99	0.03	45,45,45,45	0
62	MG	1H	3251	1/1	0.99	0.16	39,39,39,39	0
62	MG	1H	3465	1/1	0.99	0.04	21,21,21,21	0
62	MG	1G	1704	1/1	0.99	0.03	66,66,66,66	0
62	MG	1H	3565	1/1	0.99	0.05	25,25,25,25	0
62	MG	13	1732	1/1	0.99	0.04	51,51,51,51	0
62	MG	14	3323	1/1	0.99	0.04	56,56,56,56	0
62	MG	14	3324	1/1	0.99	0.03	43,43,43,43	0
62	MG	1H	3467	1/1	0.99	0.04	44,44,44,44	0
62	MG	1H	3568	1/1	0.99	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1G	1710	1/1	0.99	0.03	59,59,59,59	0
62	MG	1H	3392	1/1	0.99	0.04	51,51,51,51	0
62	MG	14	3330	1/1	0.99	0.05	39,39,39,39	0
62	MG	1G	1712	1/1	0.99	0.03	81,81,81,81	0
62	MG	1H	3469	1/1	0.99	0.04	13,13,13,13	0
62	MG	14	3333	1/1	0.99	0.06	62,62,62,62	0
62	MG	14	3334	1/1	0.99	0.04	33,33,33,33	0
62	MG	14	3335	1/1	0.99	0.03	70,70,70,70	0
62	MG	1H	3571	1/1	0.99	0.05	26,26,26,26	0
62	MG	14	3337	1/1	0.99	0.03	83,83,83,83	0
62	MG	14	3338	1/1	0.99	0.04	34,34,34,34	0
62	MG	1G	1715	1/1	0.99	0.04	39,39,39,39	0
62	MG	1H	3572	1/1	0.99	0.05	25,25,25,25	0
62	MG	1G	1717	1/1	0.99	0.04	67,67,67,67	0
62	MG	1H	3470	1/1	0.99	0.05	24,24,24,24	0
62	MG	1G	1719	1/1	0.99	0.15	66,66,66,66	0
62	MG	1H	3575	1/1	0.99	0.03	17,17,17,17	0
62	MG	14	3346	1/1	0.99	0.07	52,52,52,52	0
62	MG	1H	3471	1/1	0.99	0.05	56,56,56,56	0
62	MG	1G	1722	1/1	0.99	0.07	46,46,46,46	0
62	MG	1H	3472	1/1	0.99	0.03	17,17,17,17	0
62	MG	1H	3253	1/1	0.99	0.23	41,41,41,41	0
62	MG	1H	3394	1/1	0.99	0.03	11,11,11,11	0
62	MG	1H	3395	1/1	0.99	0.04	23,23,23,23	0
62	MG	14	3353	1/1	0.99	0.11	62,62,62,62	0
62	MG	1H	3476	1/1	0.99	0.05	15,15,15,15	0
62	MG	14	3355	1/1	0.99	0.07	39,39,39,39	0
62	MG	1H	3397	1/1	0.99	0.04	17,17,17,17	0
62	MG	1H	3398	1/1	0.99	0.07	52,52,52,52	0
61	K	13	1629	1/1	0.99	0.03	50,50,50,50	0
62	MG	13	1760	1/1	0.99	0.02	65,65,65,65	0
62	MG	1G	1732	1/1	0.99	0.04	83,83,83,83	0
62	MG	16	212	1/1	0.99	0.04	36,36,36,36	0
62	MG	16	213	1/1	0.99	0.04	41,41,41,41	0
62	MG	14	3363	1/1	0.99	0.03	26,26,26,26	0
62	MG	1H	3403	1/1	0.99	0.03	27,27,27,27	0
62	MG	1H	3482	1/1	0.99	0.03	45,45,45,45	0
62	MG	14	3366	1/1	0.99	0.04	55,55,55,55	0
62	MG	14	3367	1/1	0.99	0.04	70,70,70,70	0
62	MG	1H	3404	1/1	0.99	0.02	43,43,43,43	0
62	MG	13	1761	1/1	0.99	0.06	86,86,86,86	0
62	MG	1H	3407	1/1	0.99	0.02	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3486	1/1	0.99	0.04	36,36,36,36	0
62	MG	1H	3487	1/1	0.99	0.07	41,41,41,41	0
62	MG	13	1762	1/1	0.99	0.03	52,52,52,52	0
62	MG	F8	101	1/1	0.99	0.15	32,32,32,32	0
62	MG	13	1734	1/1	0.99	0.08	41,41,41,41	0
62	MG	14	3377	1/1	0.99	0.04	59,59,59,59	0
62	MG	14	3378	1/1	0.99	0.04	57,57,57,57	0
62	MG	13	1735	1/1	0.99	0.04	35,35,35,35	0
62	MG	1H	3491	1/1	0.99	0.12	42,42,42,42	0
62	MG	1H	3492	1/1	0.99	0.03	63,63,63,63	0
62	MG	1H	3194	1/1	0.99	0.04	14,14,14,14	0
62	MG	1H	3414	1/1	0.99	0.05	39,39,39,39	0
62	MG	13	1765	1/1	0.99	0.04	73,73,73,73	0
62	MG	1H	3416	1/1	0.99	0.05	69,69,69,69	0
62	MG	13	1736	1/1	0.99	0.04	44,44,44,44	0
62	MG	1H	3418	1/1	0.99	0.03	29,29,29,29	0
62	MG	1H	3499	1/1	0.99	0.04	32,32,32,32	0
62	MG	13	1737	1/1	0.99	0.07	65,65,65,65	0
62	MG	13	1768	1/1	0.99	0.04	78,78,78,78	0
62	MG	14	3391	1/1	0.99	0.03	81,81,81,81	0
62	MG	1H	3421	1/1	0.99	0.06	36,36,36,36	0
61	K	16	201	1/1	0.99	0.02	55,55,55,55	0
62	MG	14	3123	1/1	0.99	0.03	36,36,36,36	0
62	MG	13	1739	1/1	0.99	0.05	30,30,30,30	0
62	MG	1H	3505	1/1	0.99	0.04	16,16,16,16	0
61	K	1H	3068	1/1	0.99	0.04	29,29,29,29	0
62	MG	14	3398	1/1	0.99	0.10	47,47,47,47	0
62	MG	13	1742	1/1	0.99	0.03	60,60,60,60	0
62	MG	14	3400	1/1	0.99	0.04	63,63,63,63	0
62	MG	13	1743	1/1	0.99	0.04	54,54,54,54	0
62	MG	1H	3509	1/1	0.99	0.03	27,27,27,27	0
62	MG	1H	3427	1/1	0.99	0.07	36,36,36,36	0
62	MG	1J	205	1/1	0.99	0.06	68,68,68,68	0
61	K	1H	3083	1/1	0.99	0.03	54,54,54,54	0
62	MG	1H	3513	1/1	0.99	0.11	30,30,30,30	0
62	MG	2K	105	1/1	0.99	0.06	45,45,45,45	0
62	MG	13	1745	1/1	0.99	0.04	39,39,39,39	0
62	MG	M5	102	1/1	0.99	0.08	58,58,58,58	0
63	SF4	3E	302	8/8	0.99	0.07	56,57,68,71	0
63	SF4	32	303	8/8	0.99	0.03	57,68,76,85	0
64	ZN	5I	101	1/1	0.99	0.02	70,70,70,70	0
62	MG	14	3316	1/1	1.00	0.02	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	MG	1H	3406	1/1	1.00	0.02	14,14,14,14	0
62	MG	14	3297	1/1	1.00	0.03	28,28,28,28	0
62	MG	14	3319	1/1	1.00	0.03	27,27,27,27	0
62	MG	13	1740	1/1	1.00	0.04	33,33,33,33	0
62	MG	14	3368	1/1	1.00	0.06	29,29,29,29	0
62	MG	14	3344	1/1	1.00	0.03	31,31,31,31	0
62	MG	1H	3574	1/1	1.00	0.08	24,24,24,24	0
62	MG	14	3300	1/1	1.00	0.03	61,61,61,61	0
62	MG	1H	3408	1/1	1.00	0.01	29,29,29,29	0
62	MG	11	302	1/1	1.00	0.04	14,14,14,14	0
62	MG	21	302	1/1	1.00	0.03	14,14,14,14	0
62	MG	1H	3439	1/1	1.00	0.04	53,53,53,53	0
62	MG	1H	3511	1/1	1.00	0.03	26,26,26,26	0
62	MG	14	3328	1/1	1.00	0.02	25,25,25,25	0
62	MG	13	1731	1/1	1.00	0.06	38,38,38,38	0
62	MG	14	3287	1/1	1.00	0.02	39,39,39,39	0
62	MG	1H	3410	1/1	1.00	0.02	16,16,16,16	0
62	MG	1H	3401	1/1	1.00	0.03	16,16,16,16	0
62	MG	1H	3402	1/1	1.00	0.02	23,23,23,23	0
62	MG	1G	1706	1/1	1.00	0.03	43,43,43,43	0
62	MG	1H	3396	1/1	1.00	0.03	16,16,16,16	0
62	MG	1H	3388	1/1	1.00	0.02	15,15,15,15	0
62	MG	1H	3385	1/1	1.00	0.02	20,20,20,20	0
62	MG	1H	3458	1/1	1.00	0.04	21,21,21,21	0
64	ZN	5A	102	1/1	1.00	0.02	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.