



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 02:44 AM UTC

PDB ID : 6QNR / pdb_00006qnr
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

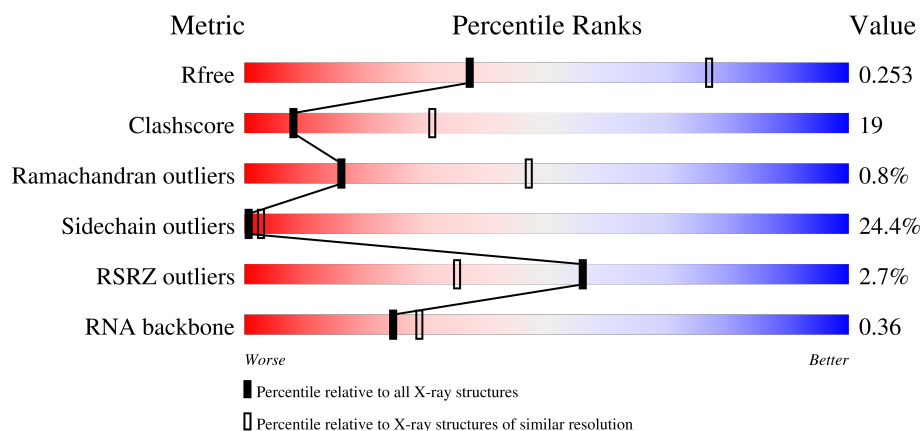
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

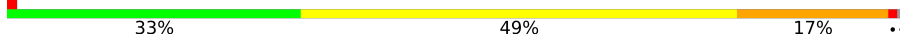
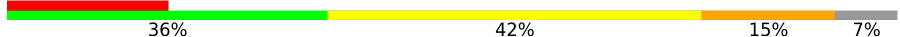
The reported resolution of this entry is 3.10 Å.

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 ≥ 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	 34% 49% 16% •
1	1G	1522	 33% 49% 17% ••
2	12	256	 18% 36% 42% 15% 7%
2	1E	256	 6% 44% 37% 11% 7%

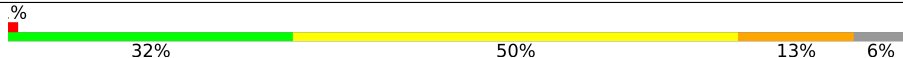
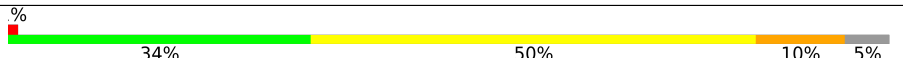
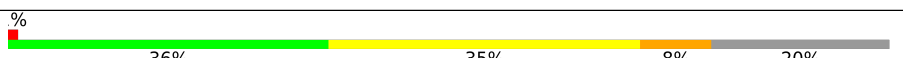
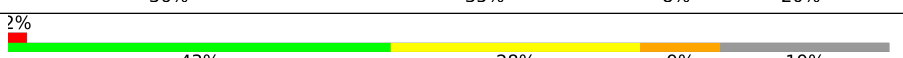
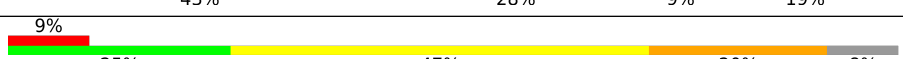
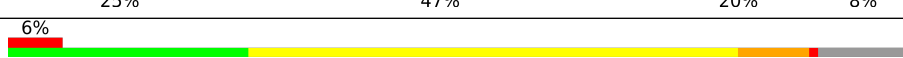
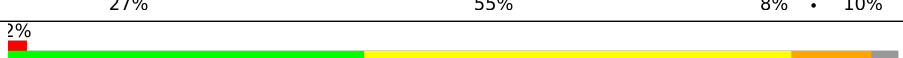
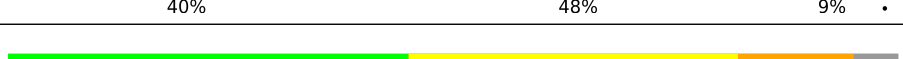
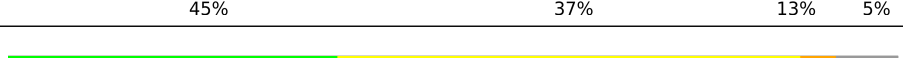
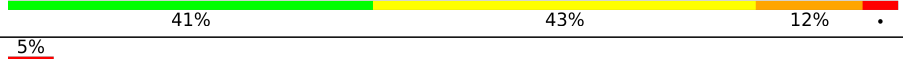
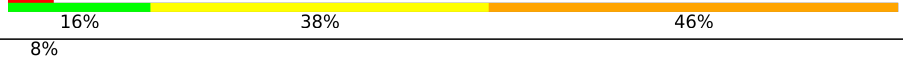
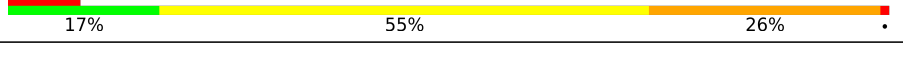
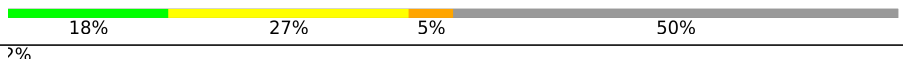
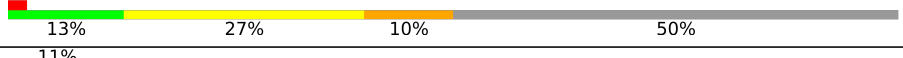
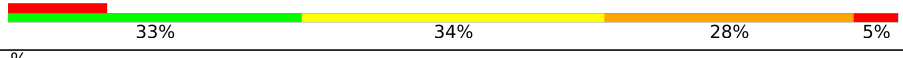
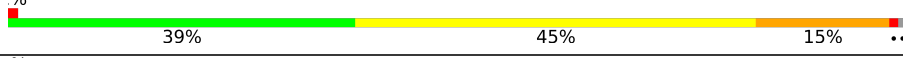
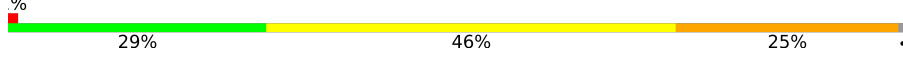
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

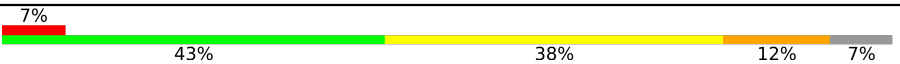
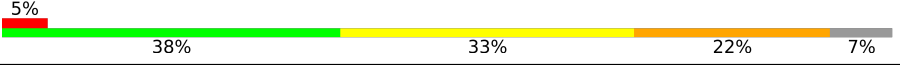
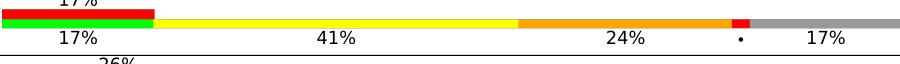
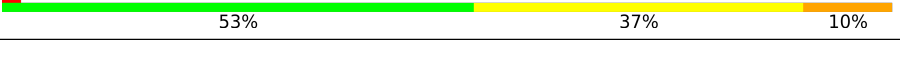
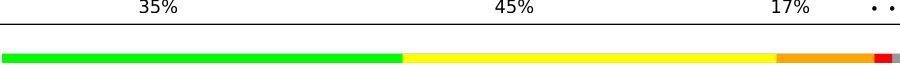
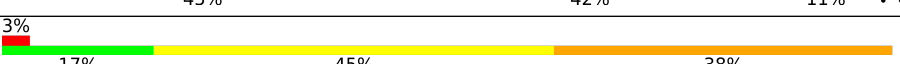
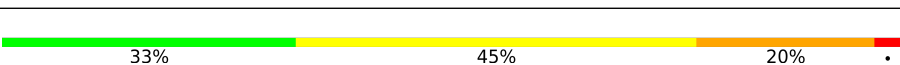
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Mol	Chain	Length	Quality of chain
42	A8	112	
43	75	146	
43	B8	146	
44	85	118	
44	C8	118	
45	95	101	
45	D8	101	
46	A5	113	
46	E8	113	
47	B5	96	
47	F8	96	
48	C5	110	
48	G8	110	
49	D5	206	
49	H8	206	
50	E5	85	
50	I8	85	
51	F5	98	
51	J8	98	
52	G5	72	
52	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	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 (CCD ID: 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 (CCD ID: 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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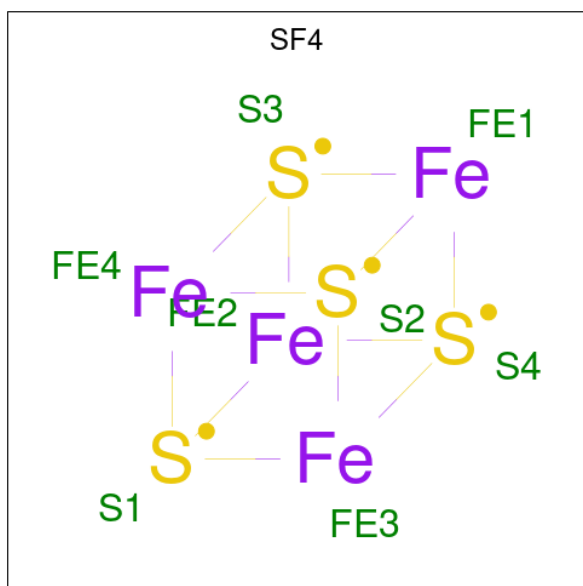
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	31	1	Total 1	Mg 1	0	0
62	41	1	Total 1	Mg 1	0	0
62	78	2	Total 2	Mg 2	0	0
62	C8	1	Total 1	Mg 1	0	0
62	F8	1	Total 1	Mg 1	0	0
62	I8	1	Total 1	Mg 1	0	0
62	J8	1	Total 1	Mg 1	0	0
62	L8	1	Total 1	Mg 1	0	0
62	N8	1	Total 1	Mg 1	0	0
62	O8	1	Total 1	Mg 1	0	0
62	P8	1	Total 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 (CCD ID: SF4) (formula: Fe_4S_4).



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 (CCD ID: 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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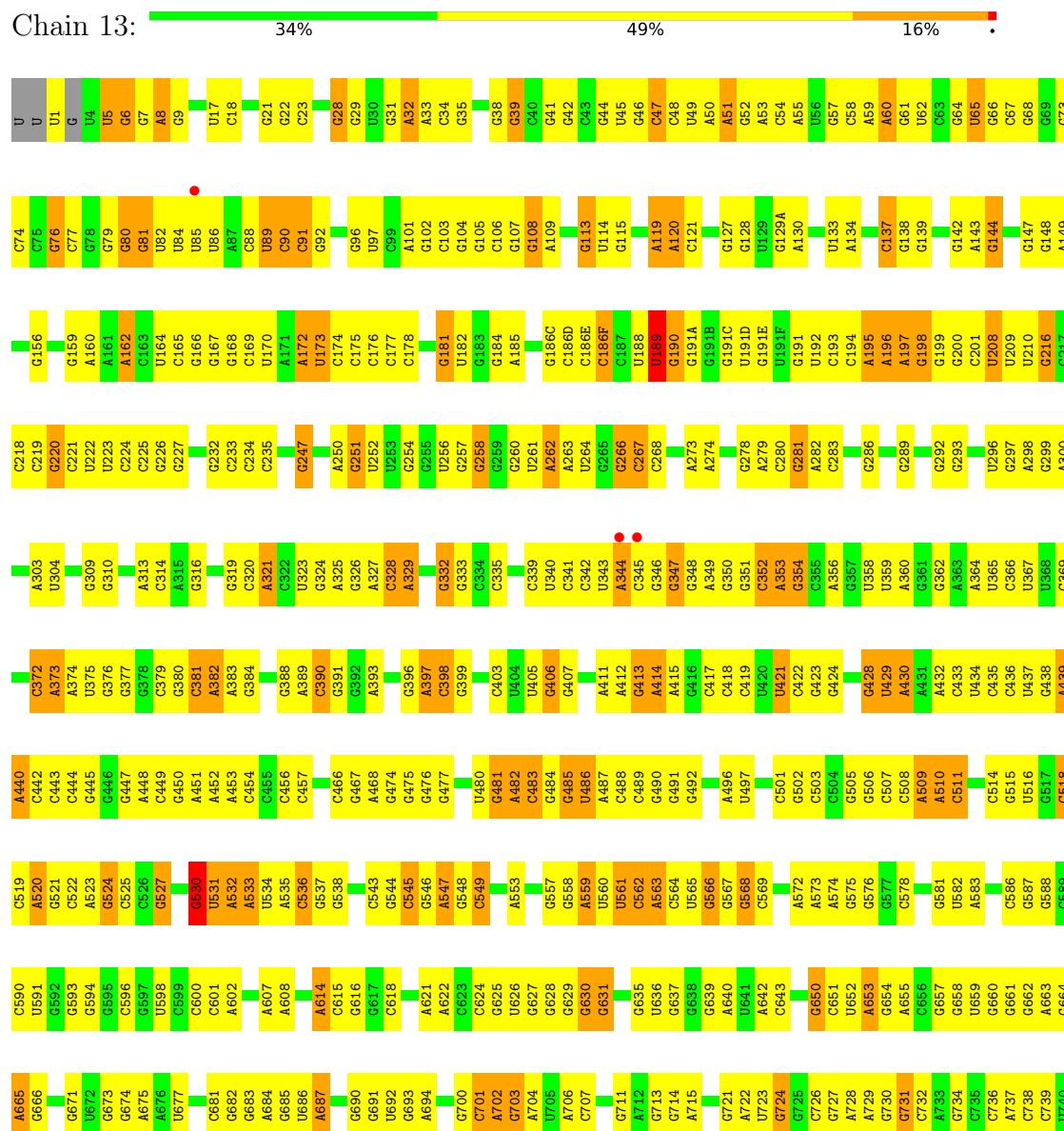
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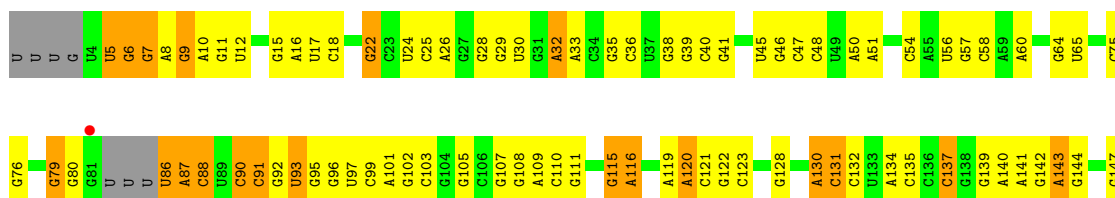
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	M5	6	Total	O	0	0
			6	6		

3 Residue-property plots

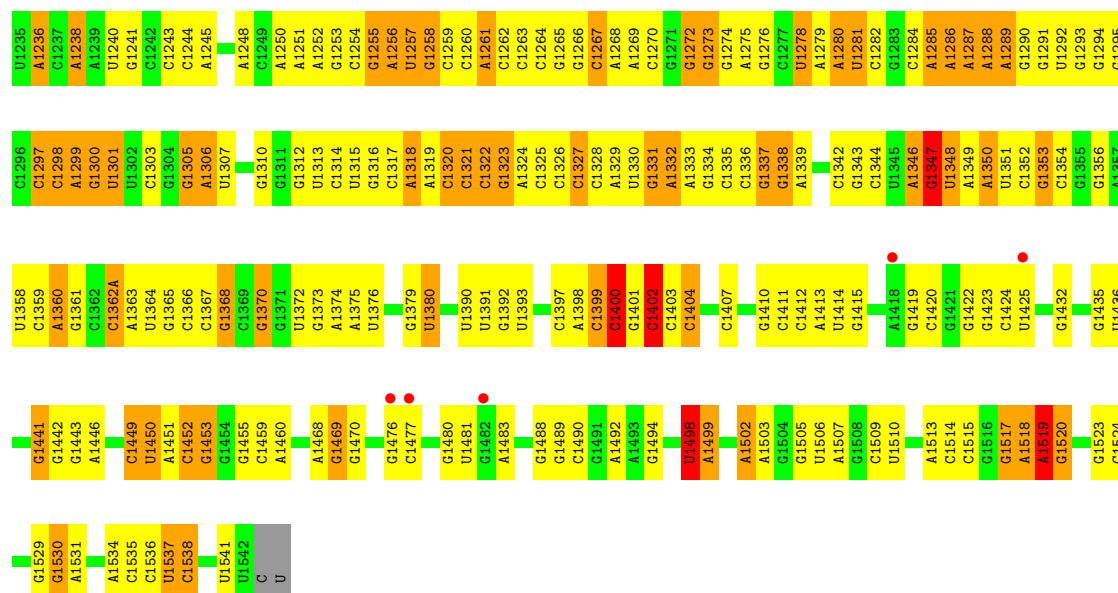
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

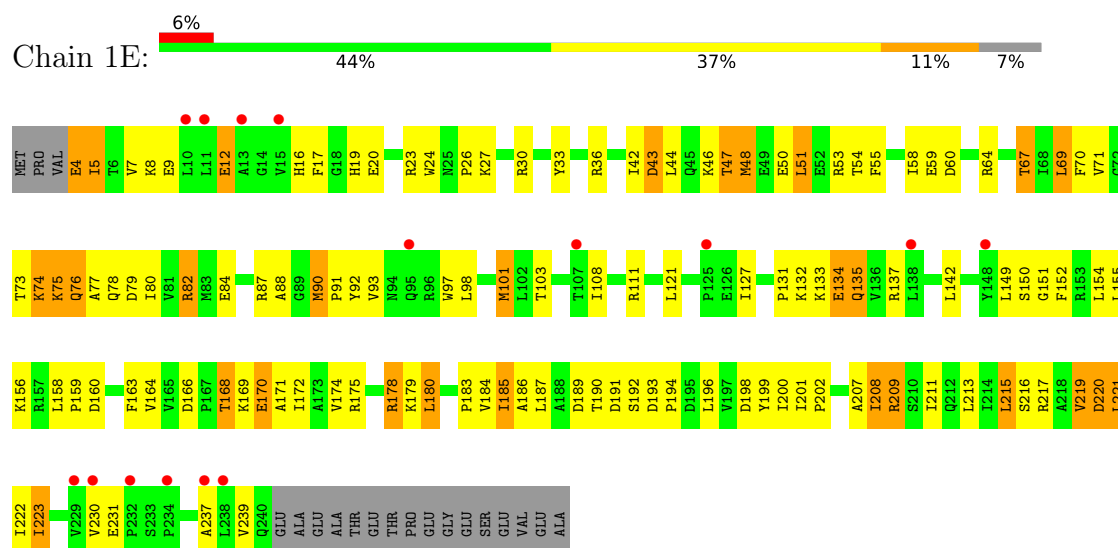




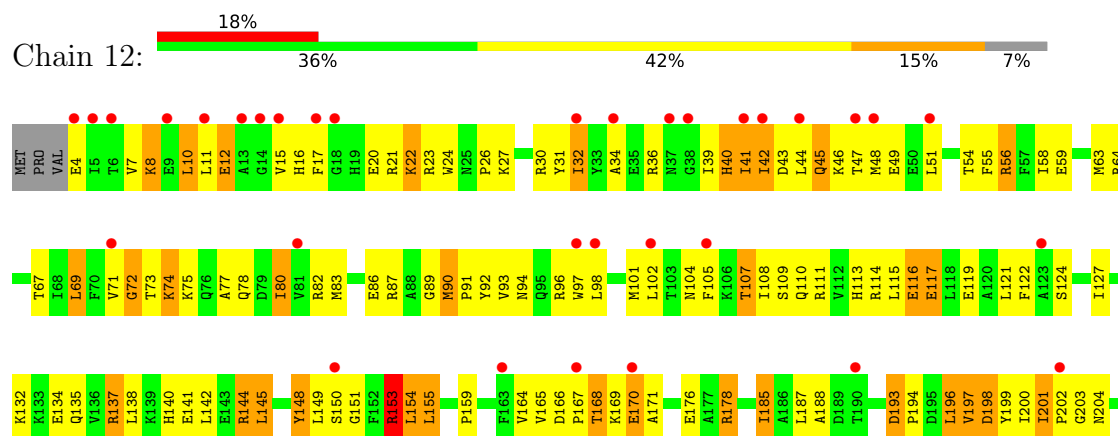
G1175	G1176	G1177	G1178	G1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	G1188	C1189	A1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	A1201	G1202	G1203	A1204	U1205	G1206	G1207	G1208	U1209	A1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	A1225	G1226	A1227	A1228	A1229	G1230	G1231	U1232	G1233	G1234																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C1038	C1039	C979	A978	C904	C826	U751	A687	G616	G537	A452	G377	U304	U208	C150	A151	A152	C153	C154	C155	G156	G157	G158	G159	A160	C163	U164	C165	G166	G167	G168	C169	C174	C175	C176	C177	C178	U180	C181	U182	G183	C184	A185	C186	C186A	C186B	G186C	C186D	C269	A270	C271	C272	A273	C277	G278	A279	C280	G281	U287	A288	G289	A195	A196	A197	G198	G199	G200	C201																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1108	C1109	A1176	G1177	C1111	C1112	C1113	C1116	G1117	C1118	C1119	G1120	U1121	G1186	G1187	A1188	C1189	G1190	A1191	G1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	C1200	U1135	A1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	A1146	C1147	A1213	C1214	G1215	G1216	C1217	A1151	A1152	C1153	G1154	G1155	G1156	C1157	U1158	A1159	G1160	C1161	C1162	A1167	A1169	U1170	G1171	C1172	G1173	C1174																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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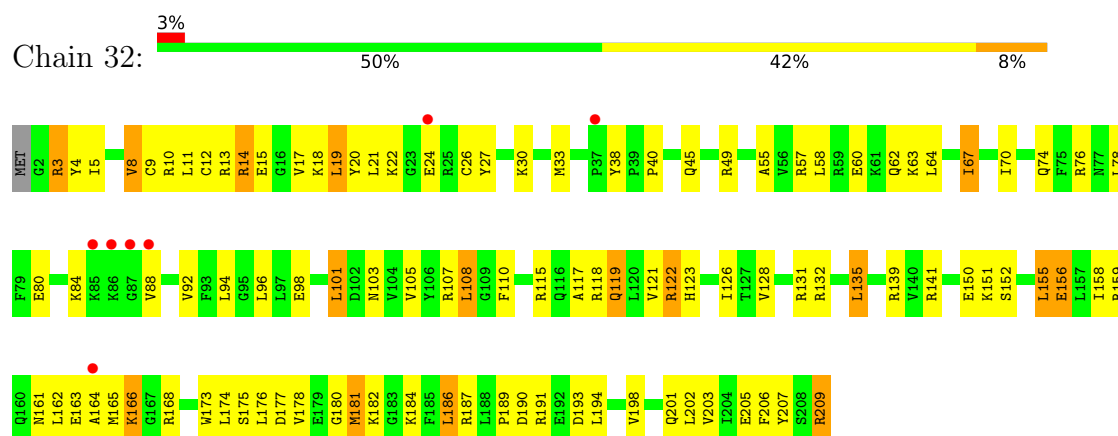
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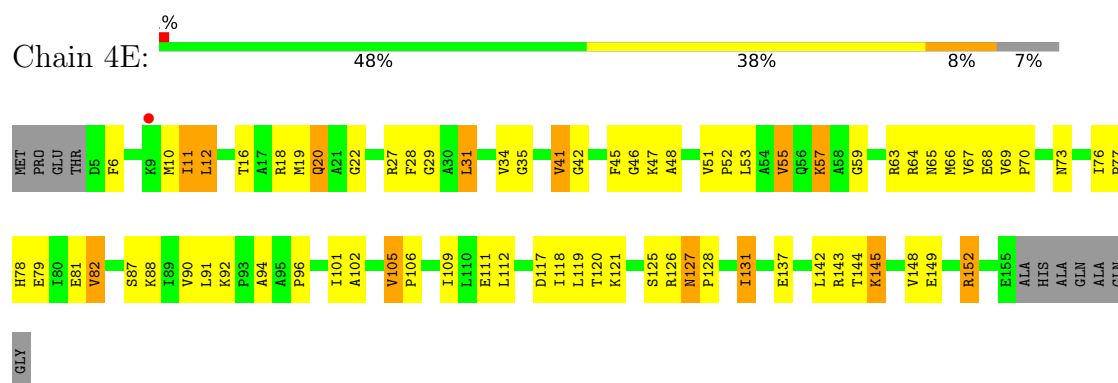
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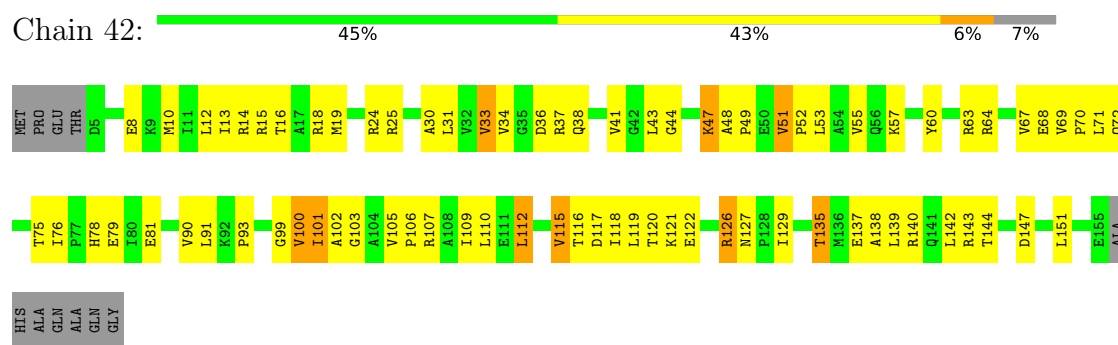
- Molecule 4: 30S ribosomal protein S4



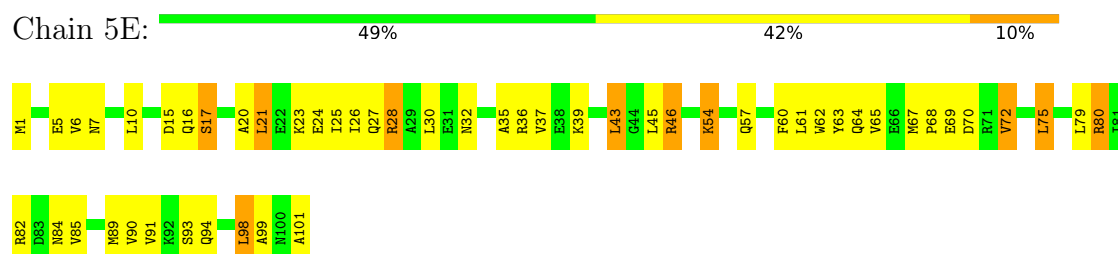
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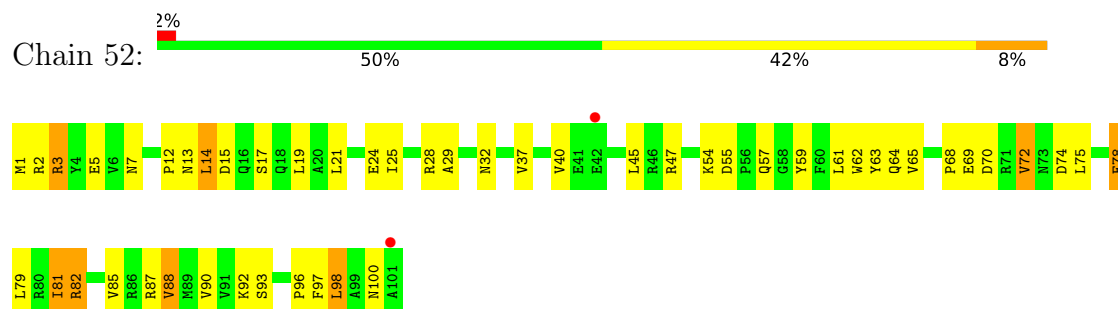
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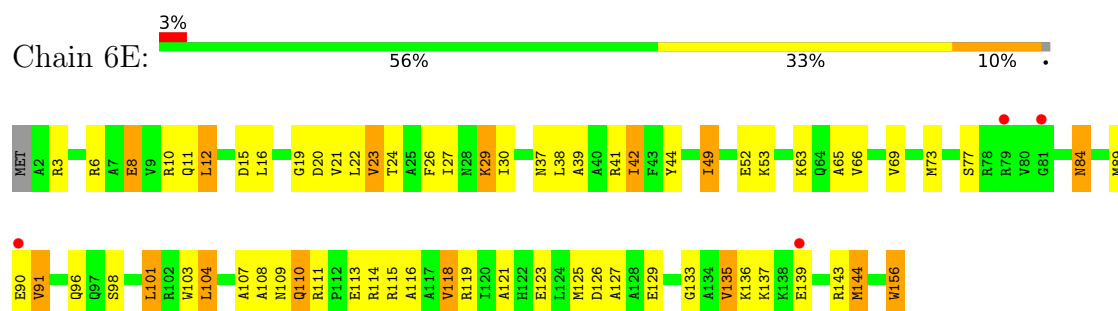
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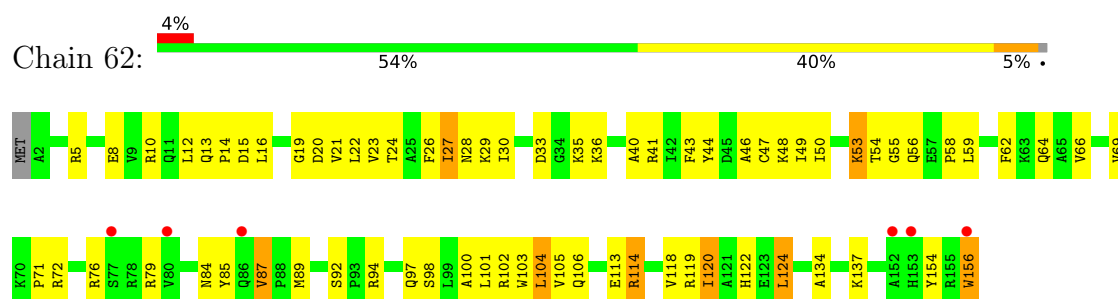
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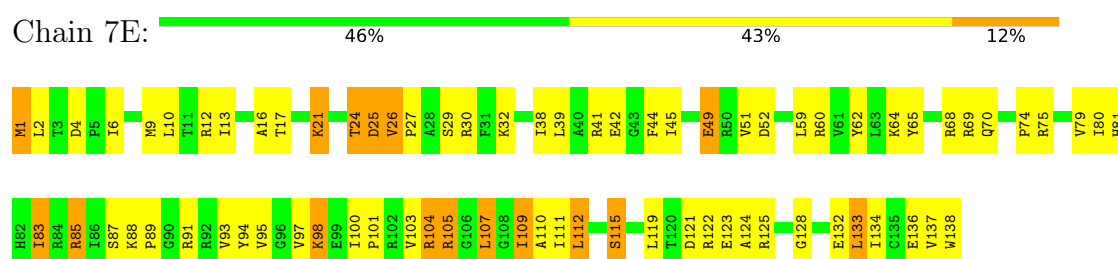
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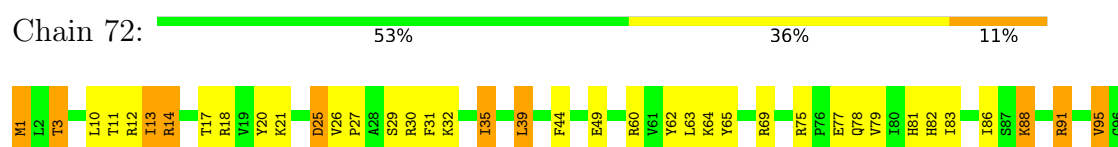
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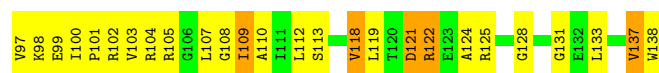


- Molecule 8: 30S ribosomal protein S8

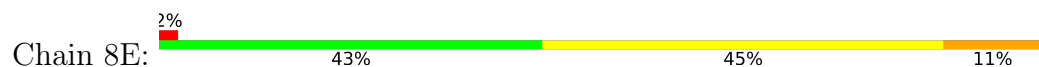


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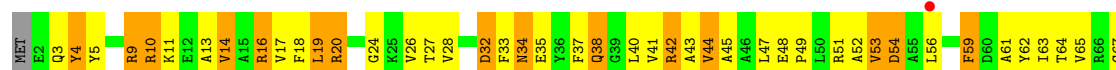




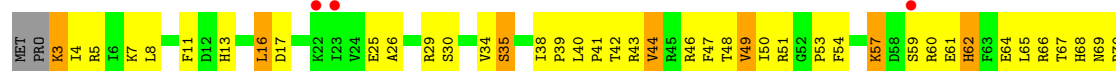
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

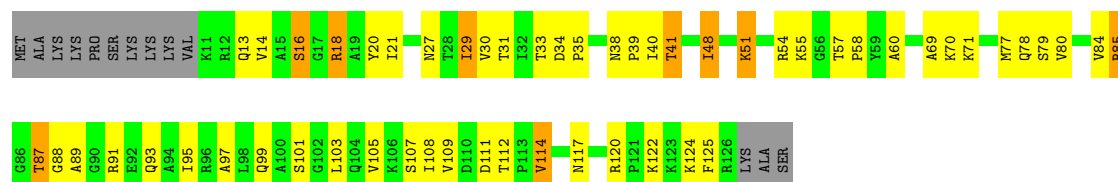


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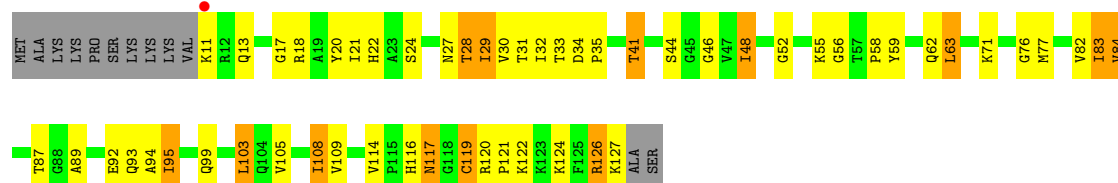


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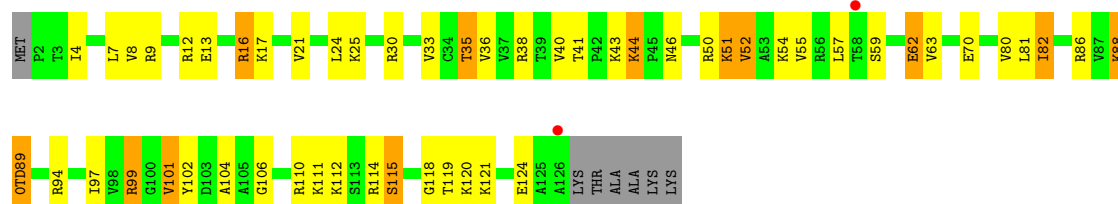




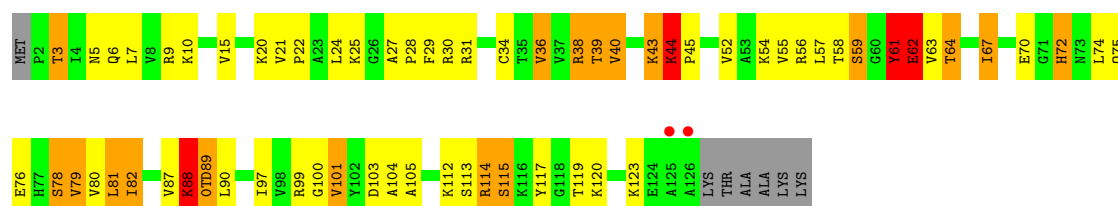
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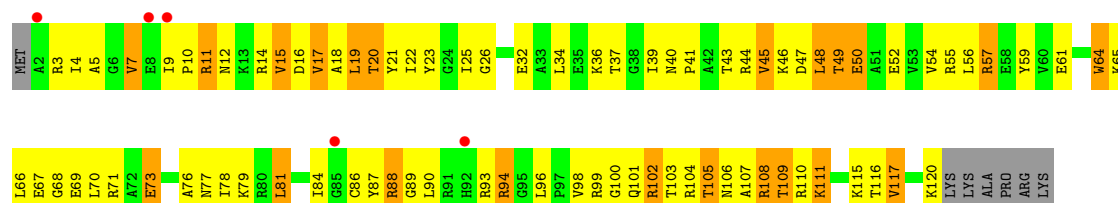
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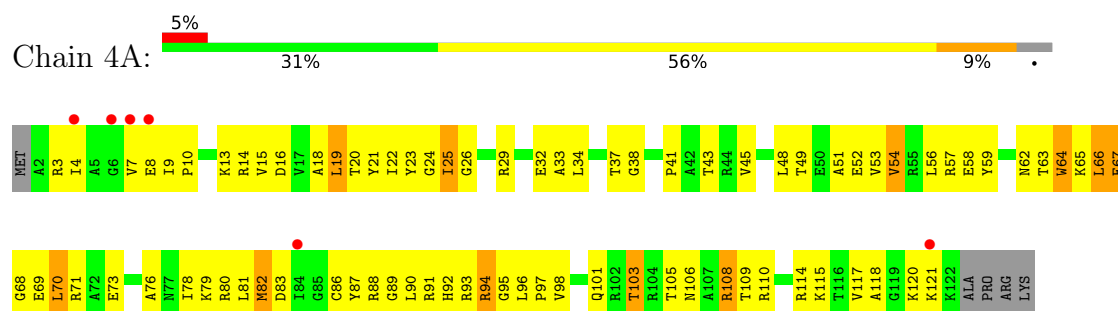
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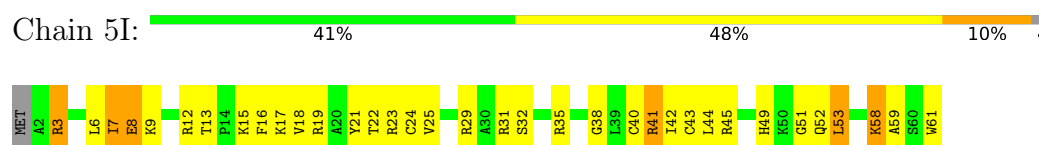
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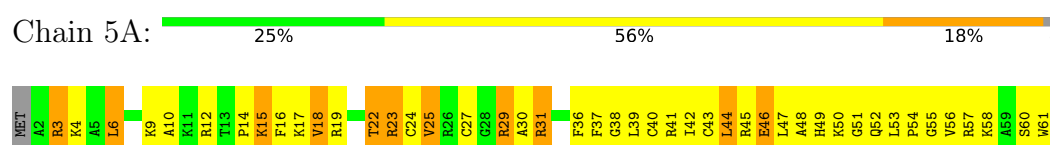
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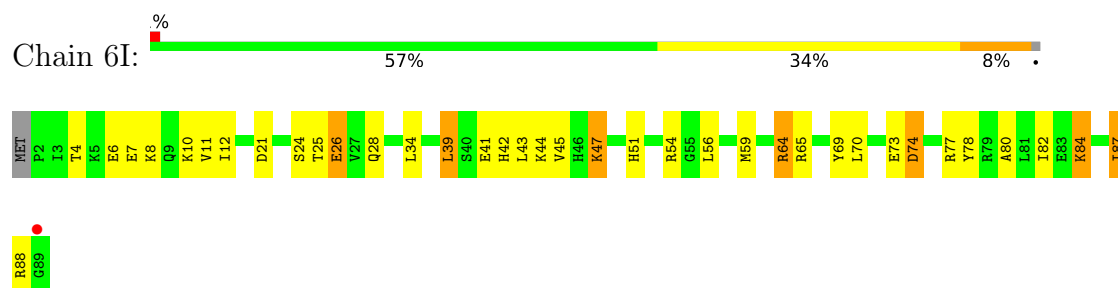
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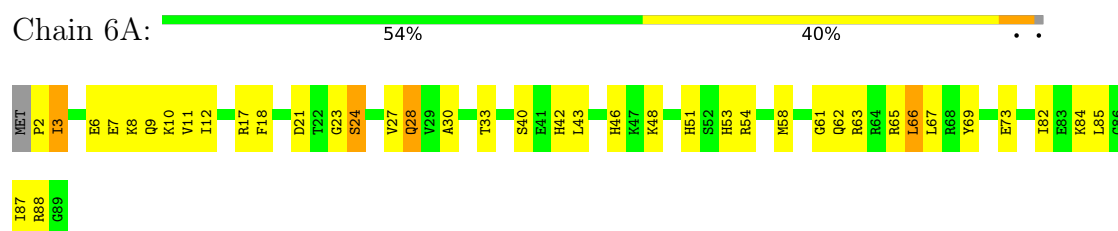
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

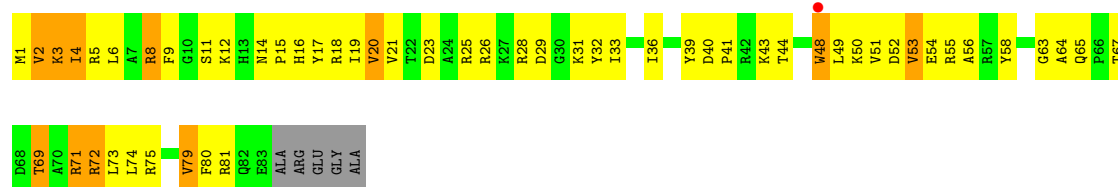


- Molecule 15: 30S ribosomal protein S15

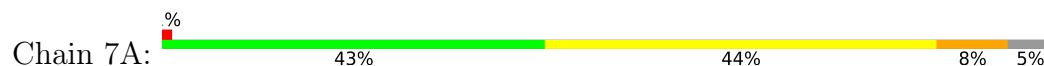


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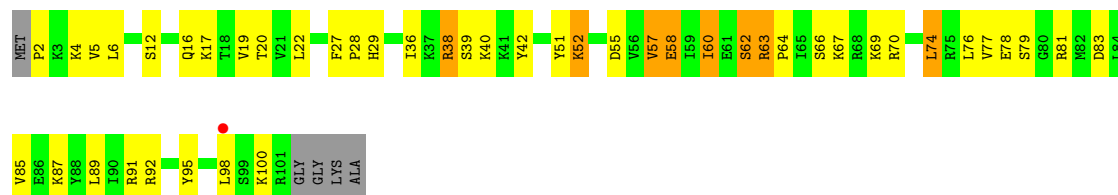




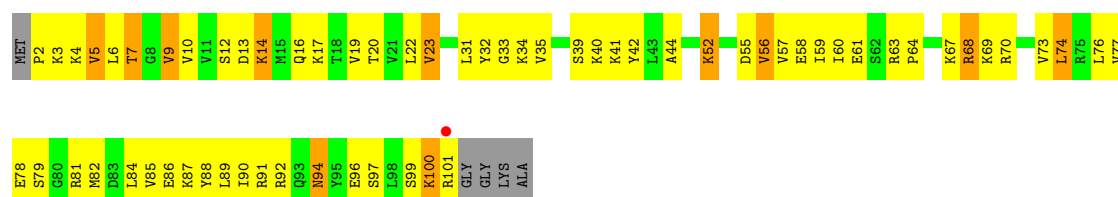
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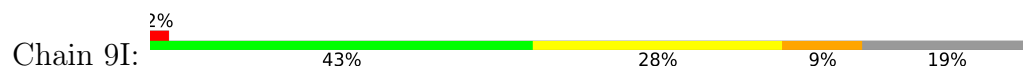
- Molecule 17: 30S ribosomal protein S17



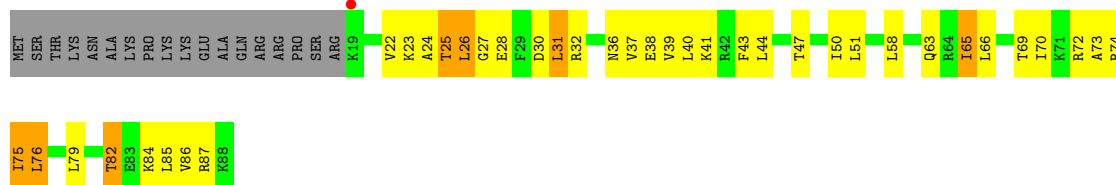
- Molecule 17: 30S ribosomal protein S17



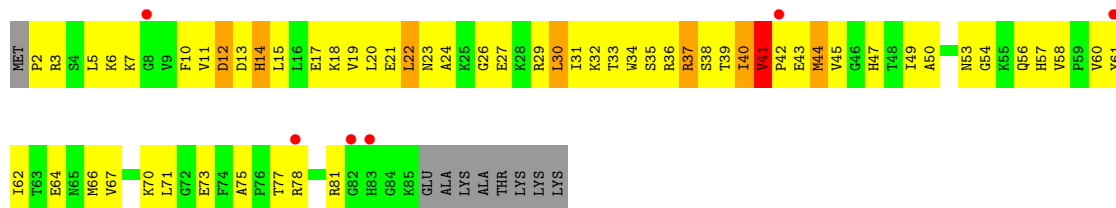
- Molecule 18: 30S ribosomal protein S18



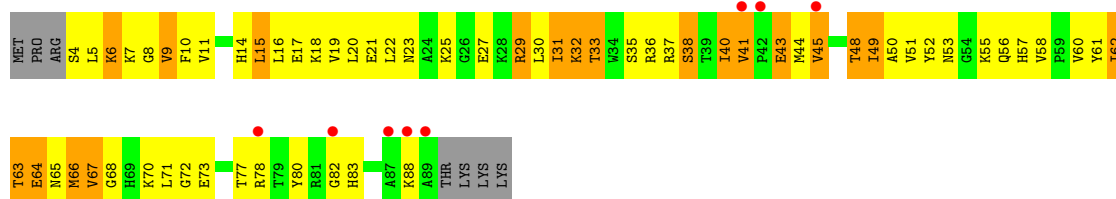
- Molecule 18: 30S ribosomal protein S18



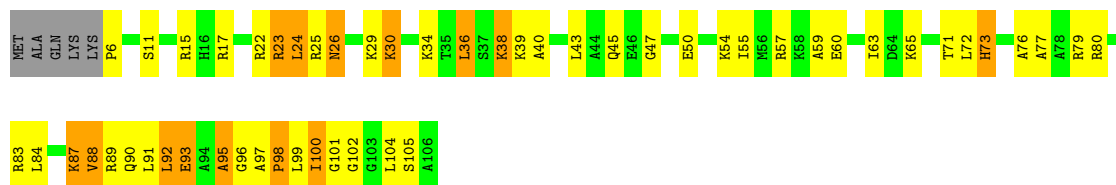
• Molecule 19: 30S ribosomal protein S19



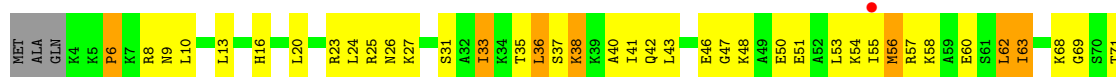
• Molecule 19: 30S ribosomal protein S19

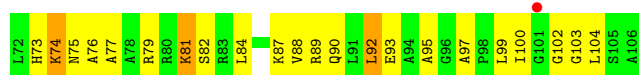


• Molecule 20: 30S ribosomal protein S20

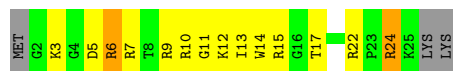


• Molecule 20: 30S ribosomal protein S20

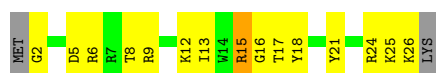




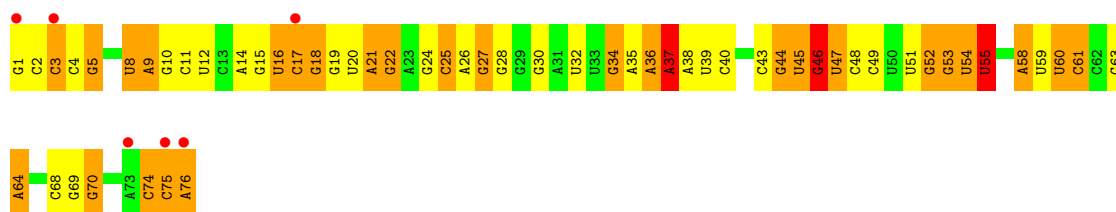
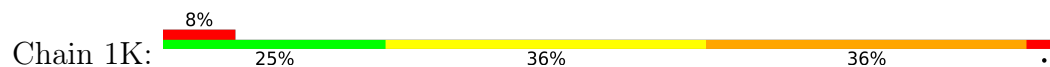
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



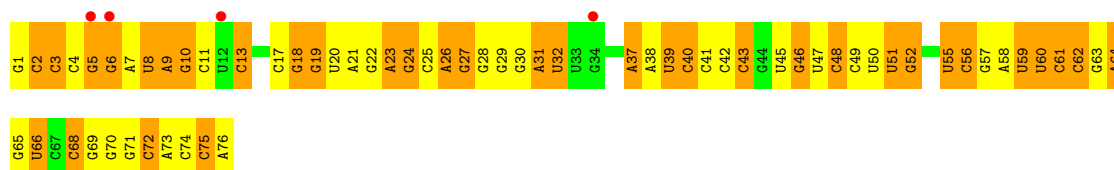
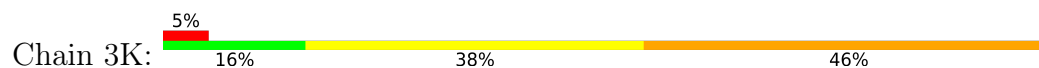
- Molecule 22: E. coli tRNAPhe



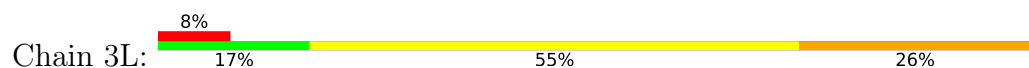
- Molecule 23: E. coli tRNAPhe

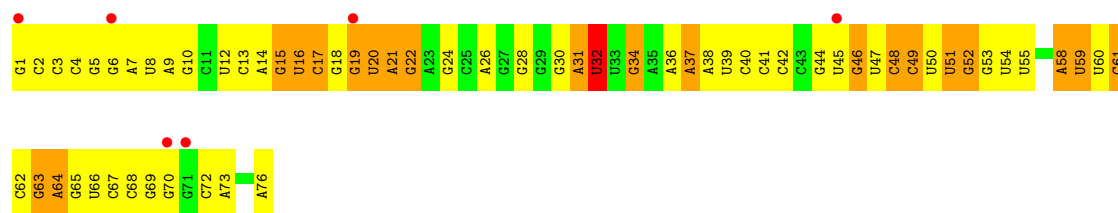


- Molecule 24: E. coli tRNAPhe



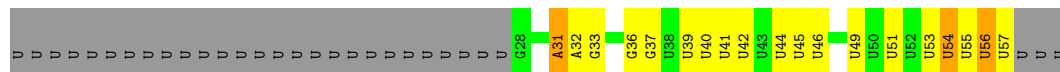
- Molecule 24: E. coli tRNAPhe





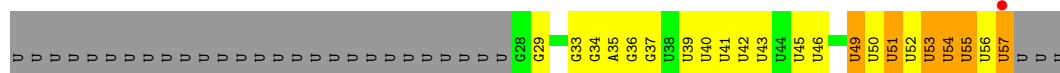
• Molecule 25: mRNA

Chain 4K: 18% 27% 5% 50%



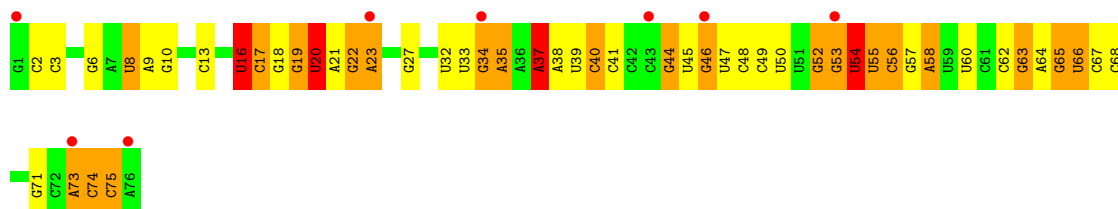
• Molecule 25: mRNA

Chain 4L: 2% 13% 27% 10% 50%



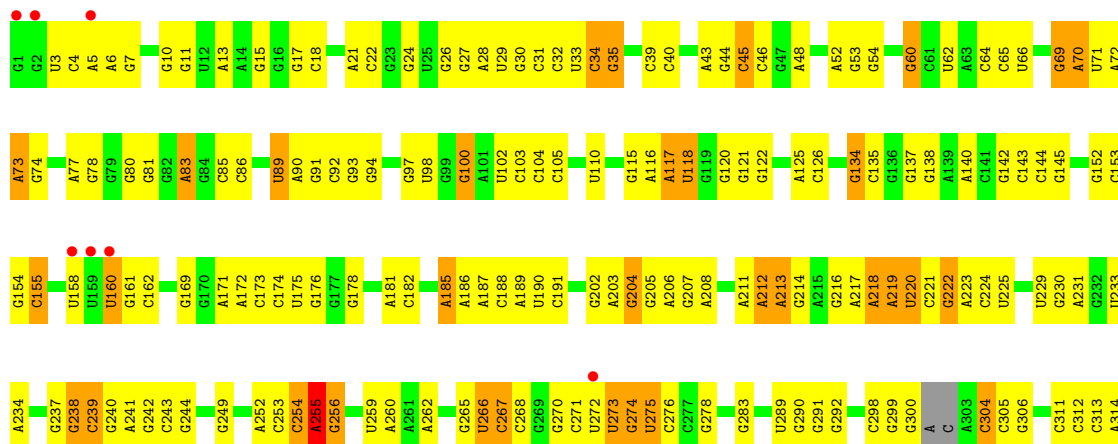
• Molecule 26: E. coli tRNAPhe

Chain 5K: 11% 33% 34% 28% 5%



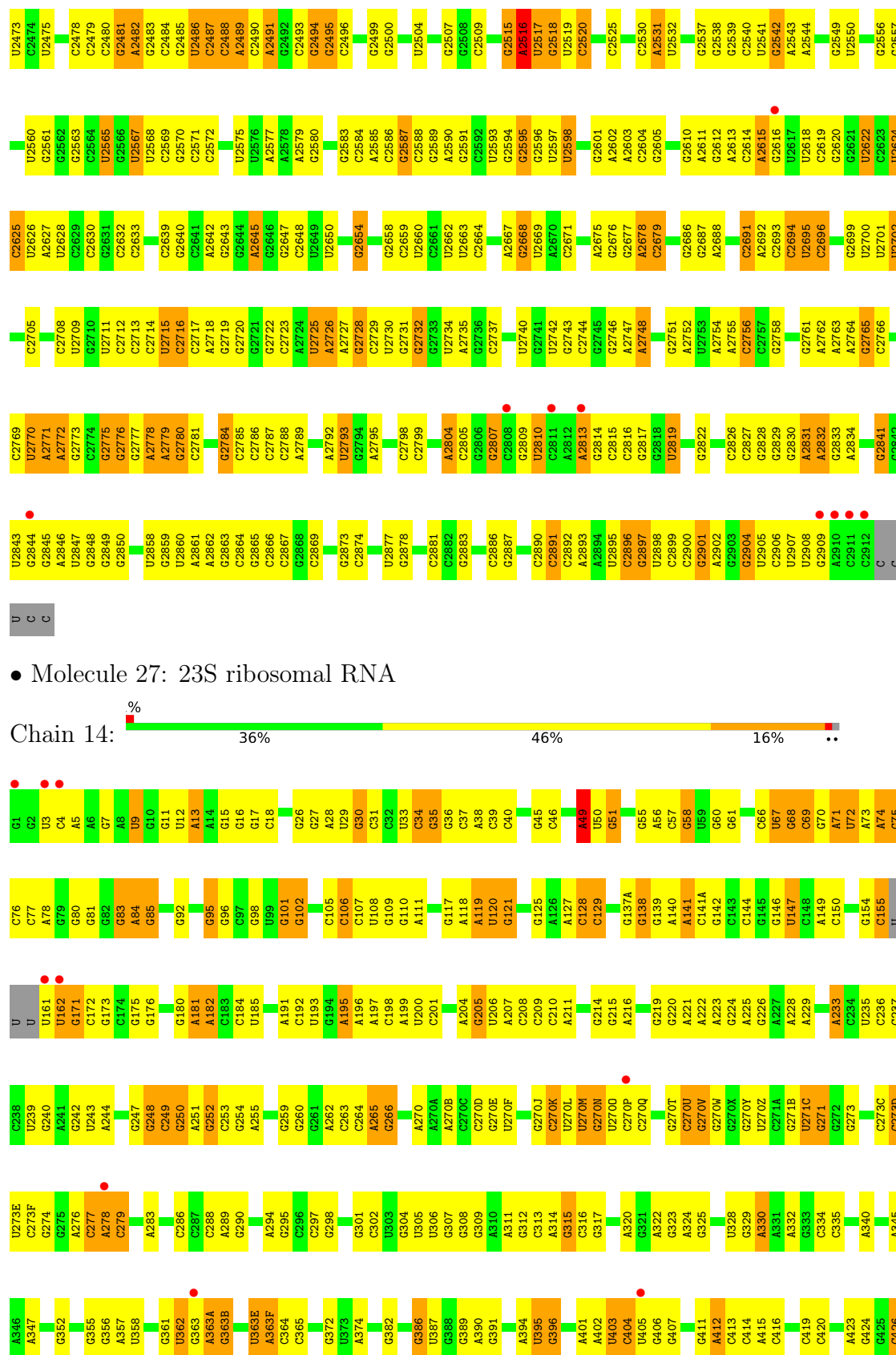
• Molecule 27: 23S ribosomal RNA

Chain 1H: % 39% 45% 15% ..



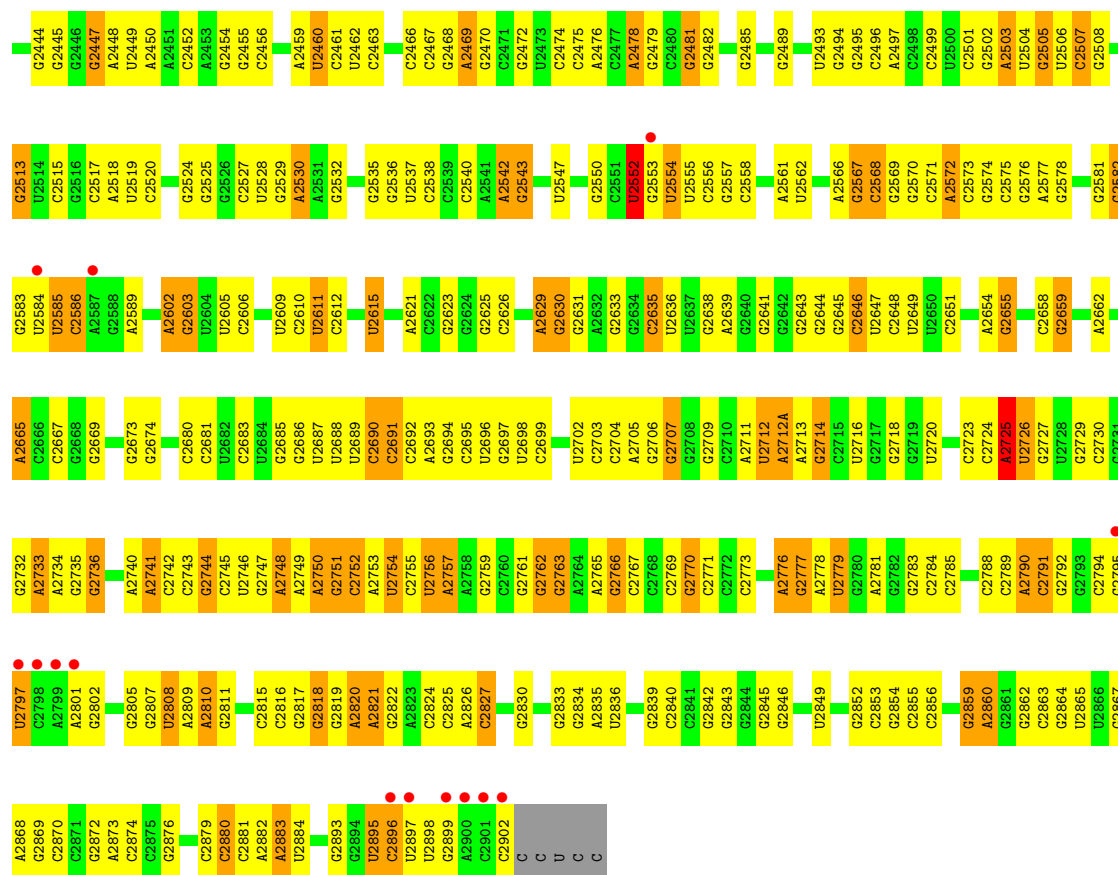
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G1384	C1298	G1146	G1218	A1145	G1083	A926	A926	A941	A770	G	U551	G477	G390	U318
U1387	G1299	G1147	G1219	G1146	C1085	G927	G927	G942	G773	C	U552	G478	G391	A319
A1388	A1300	U1148	A1220	U1148	G1089	G928	G928	C943	G774	G	C553	C480	C322	C322
A1389	G1303	C1149	U1221	C1149	C1090	G929	G929	C944	A775	G	A554	A481	C323	G323
C1392	G1306	U1150	A1223	A1150	G1091	G930	G930	C945	G776	•	A555	C482	A324	A324
G1395	G1307	C1151	C1224	U1151	G1092	G931	G931	C946	C777	•	C556	C483	C327	C327
A1396	C1308	U1152	C1225	G1153	A1093	C932	C932	A948	C778	•	C557	A484	G398	U328
U1399	A1309	G1094	C1226	G1154	G1094	C933	C933	G949	C779	•	A558	G628	A399	G329
G1402	A1312	U1155	G1229	U1155	A1095	A935	A935	A850	A782	•	U560	A487	G400	U330
G1403	G1313	C1156	G1230	C1156	C1096	C936	C936	G853	A783	•	C561	C488	U401	U331
U1404	U1314	G1157	G1231	U1157	A1097	C937	C937	C954	C784	•	A562	U412	U412	G332
A1406	A1315	U1158	G1232	G1158	C1098	C938	C938	C955	G787	•	C563	G490	G333	G333
A1407	A1316	U1159	G1233	U1159	G1099	G939	G939	U858	U788	•	G564	A493	G334	G334
G1408	C1317	U1160	A1235	U1160	C1100	C940	C940	U859	U788	•	C565	A494	A335	A335
G1411	G1415	G1161	G1236	G1161	A1101	A937	A937	C960	U792	•	C566	G495	A336	A336
G1416	G1416	C1168	G1237	C1168	G1102	A943	A943	A867	G793	•	C567	G496	A339	A339
G1417	G1417	A1170	G1238	A1170	C1103	C944	C944	A868	A794	•	C568	G497	C341	C341
G1418	G1418	U1177	G1239	U1177	U1105	A946	A946	A869	U795	•	C569	A498	U422	G340
G1419	G1419	G1172	A1240	G1172	G1106	A947	A947	U860	G796	•	C570	A498	U423	G341
G1422	G1422	A1173	G1241	A1173	U1107	A948	A948	U874	C797	•	A572	A505	G424	C344
G1423	G1423	A1174	C1246	A1174	U1108	C949	C949	U875	A798	•	A573	A506	G428	A345
G1426	G1426	U1175	G1247	U1175	C1109	C950	C950	U876	A799	•	G574	A507	A429	A346
G1427	G1427	G1176	G1248	G1176	G1110	C951	C951	U880	C802	•	U579	A508	A430	A347
G1428	G1428	U1177	A1250	U1177	U1111	A952	A952	U881	C803	•	U580	A509	U431	G348
G1429	G1429	G1178	U1251	U1178	C	G953	G953	U887	C804	•	U581	A510	U432	G352
G1430	G1430	U1179	G1252	U1179	U	A957	A957	C988	C805	•	U582	A511	U433	U353
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G1432	G1432	G1182	C1254	G1182	G	C959	C959	C992	G807	•	U586	A513	G435	A355
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G1434	G1434	G1184	A1256	G1184	G1118	C961	C961	C994	A809	•	C588	A515	A440	A357
G1435	G1435	G1185	U1257	G1185	G1119	A964	A964	U895	U810	•	C589	A516	C441	G358
G1436	G1436	G1186	U1258	G1186	U	A965	A965	U896	G811	•	U590	A517	C442	C359
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G1446	G1446	G1201	C1277	G1201	A1131	G992	G992	U909	G826	•	G601	A527	G458	G374
G1447	G1447	A1202	G1278	A1202	A1132	G993	G993	U910	U827	•	A602	A528	G459	C375
G1448	G1448	G1203	G1279	G1203	G1133	G994	G994	U911	G828	•	G603	A529	U462	G377
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G1450	G1450	C1205	A1281	C1205	G1135	G1000	G1000	C913	A830	•	C605	A531	U462	G379
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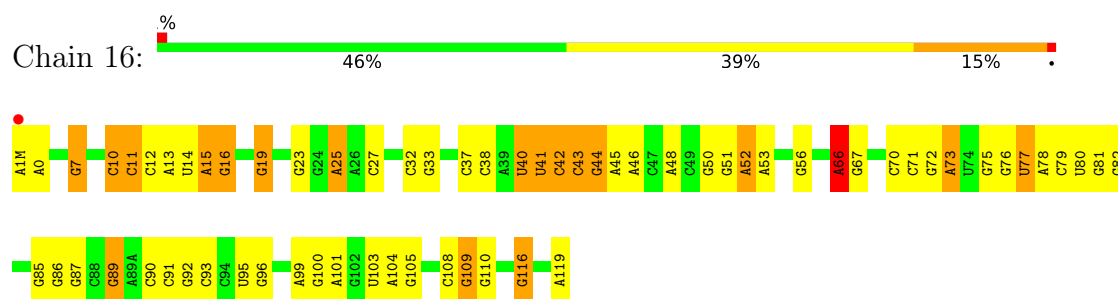


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G1344	A1288	G1185	G1122	A1064	G989	C914	G948	U779	G695	A643	A578	A505	A429
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G1346	C1270	G1187	G1126	G1056	C991	G916	C850	A781	C698	C645	C581	C510	U434
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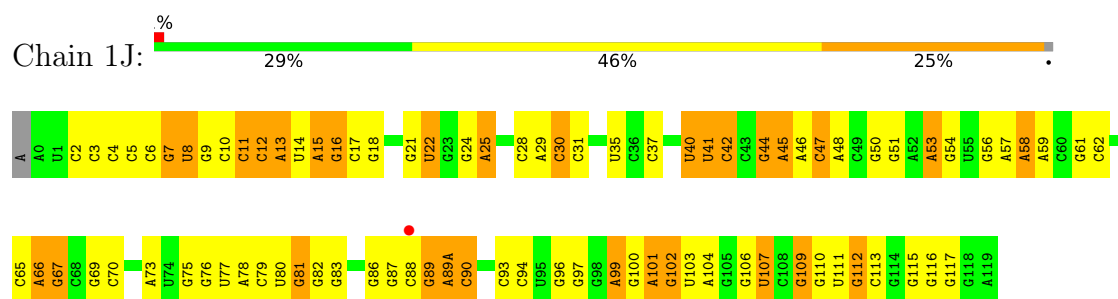
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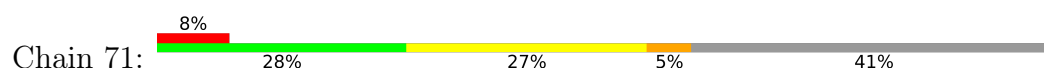
• Molecule 28: 5S ribosomal RNA

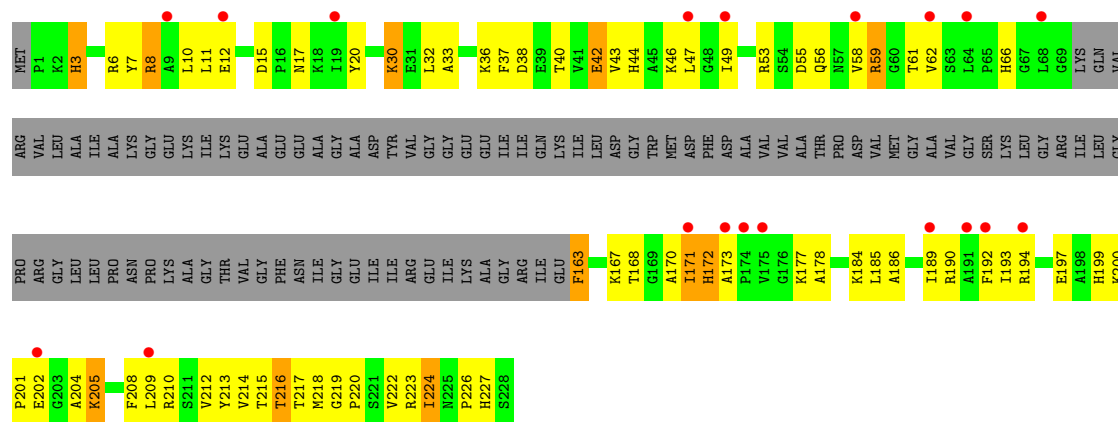


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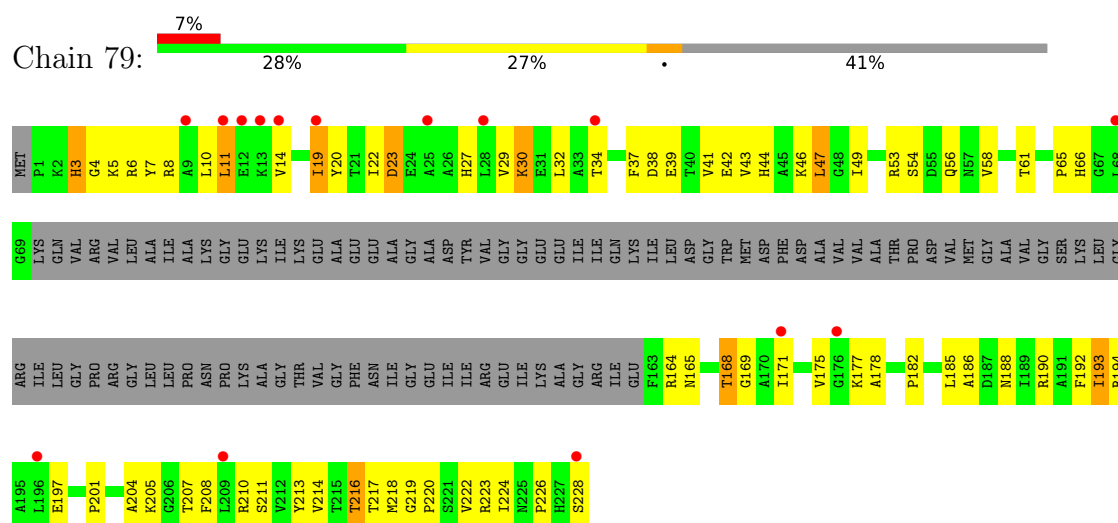


• Molecule 29: 50S ribosomal protein L1

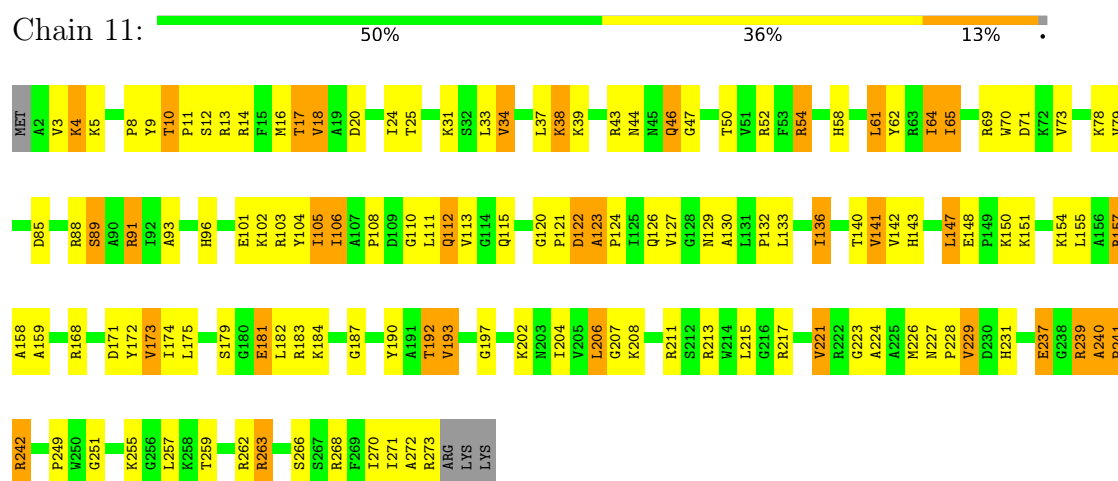




- Molecule 29: 50S ribosomal protein L1

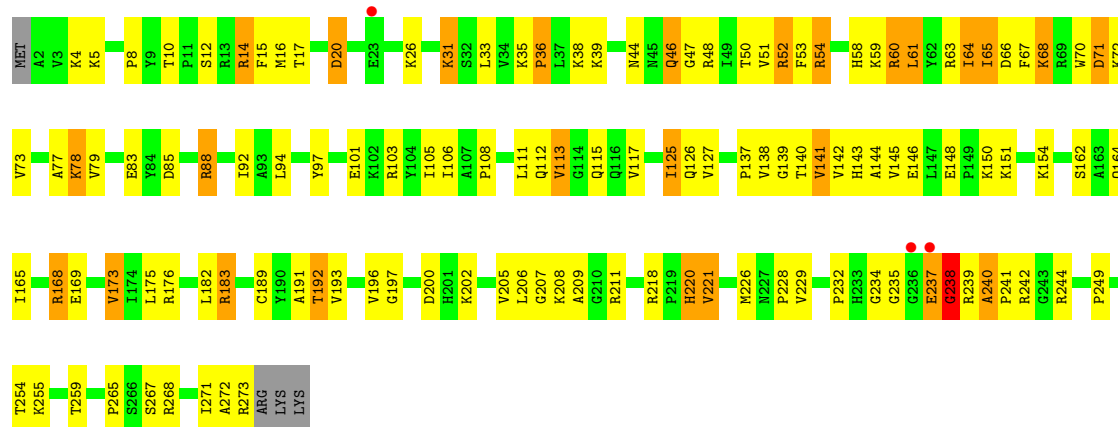


- Molecule 30: 50S ribosomal protein L2



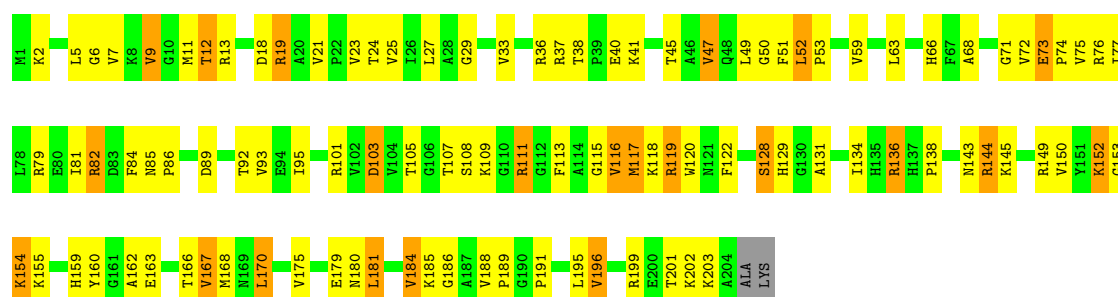
- Molecule 30: 50S ribosomal protein L2





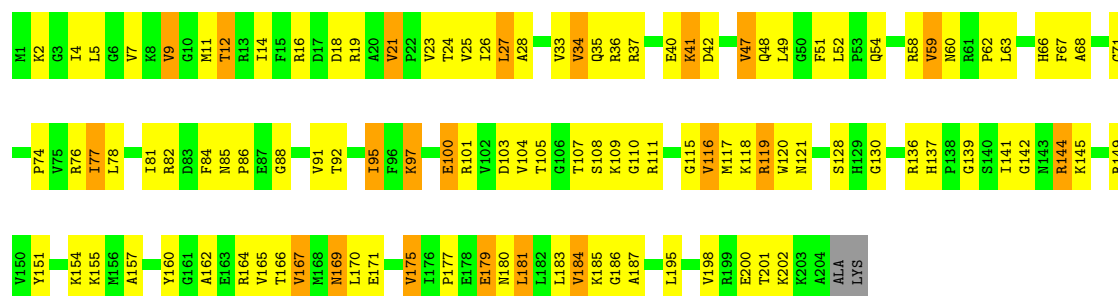
• Molecule 31: 50S ribosomal protein L3

Chain 21: 49% 40% 11%



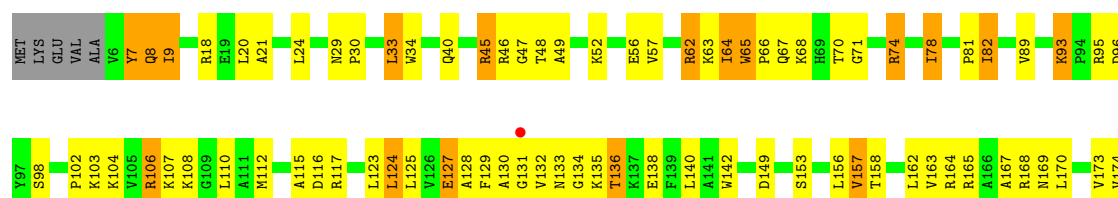
• Molecule 31: 50S ribosomal protein L3

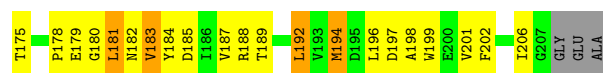
Chain 29: 46% 43% 10%



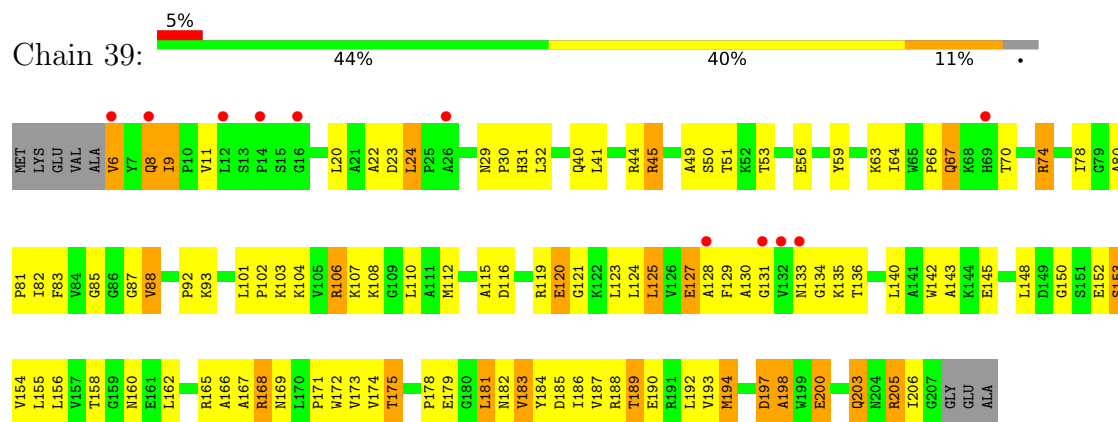
• Molecule 32: 50S ribosomal protein L4

Chain 31: 48% 38% 10%

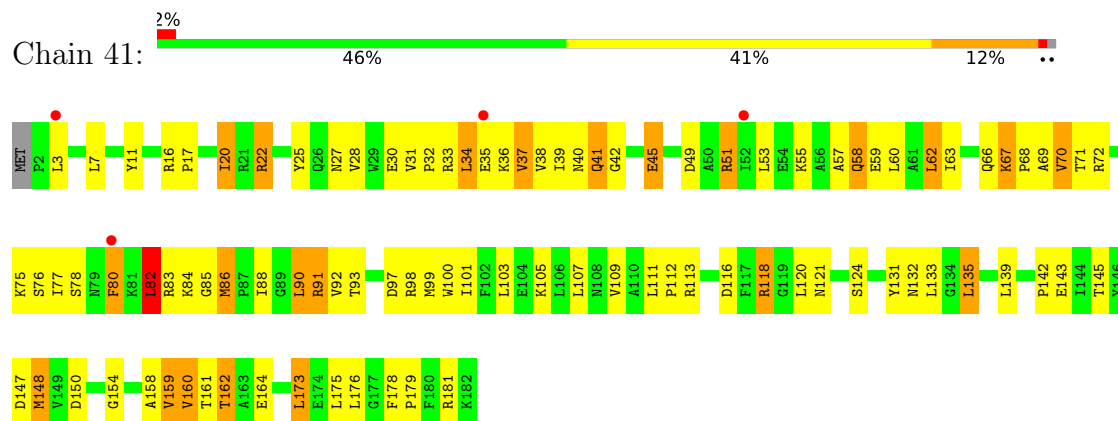




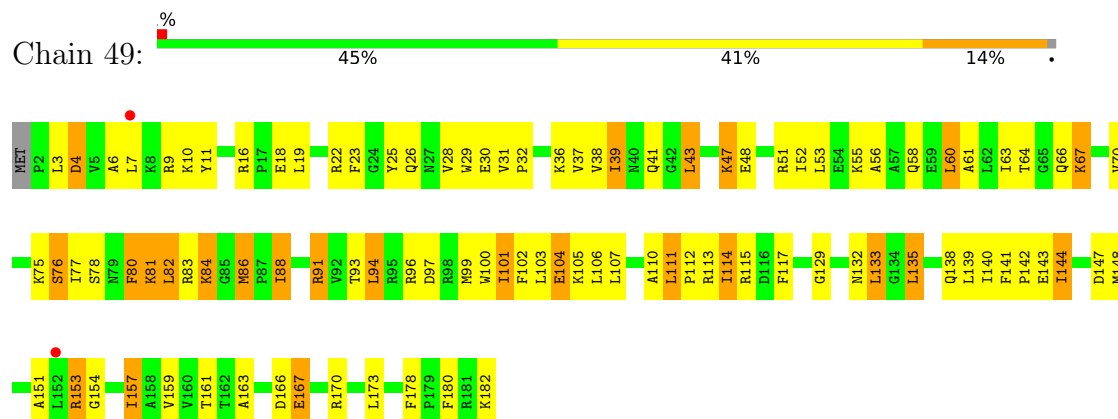
• Molecule 32: 50S ribosomal protein L4



• Molecule 33: 50S ribosomal protein L5

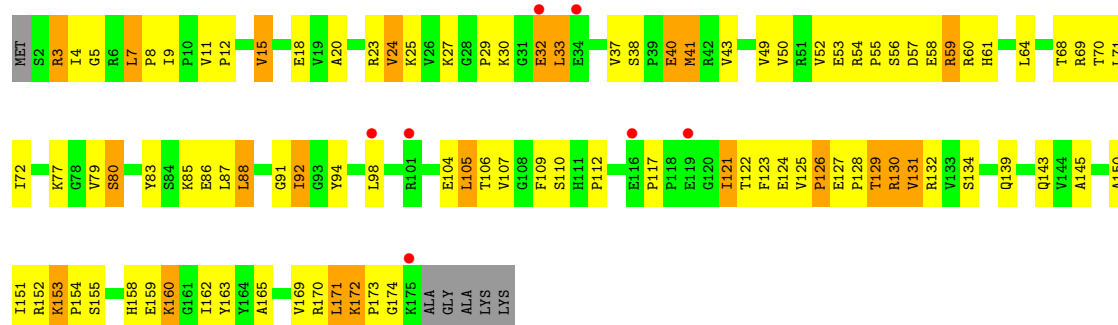


• Molecule 33: 50S ribosomal protein L5

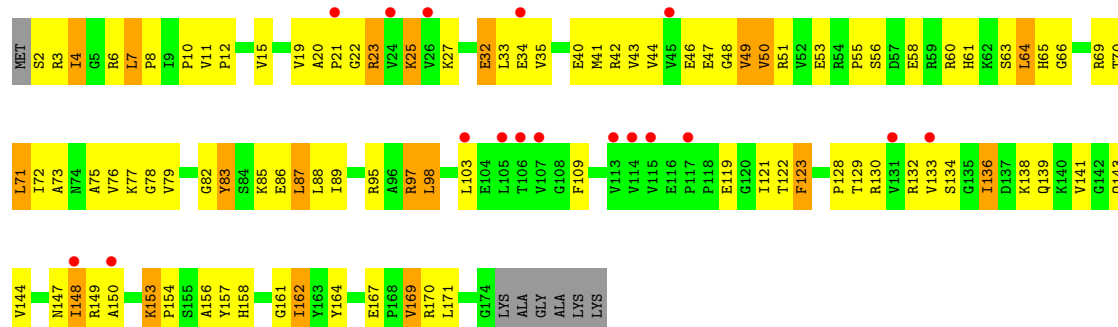
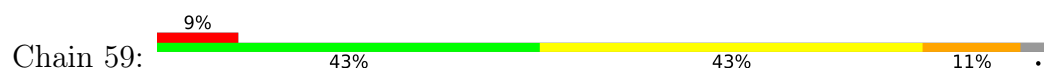


• Molecule 34: 50S ribosomal protein L6

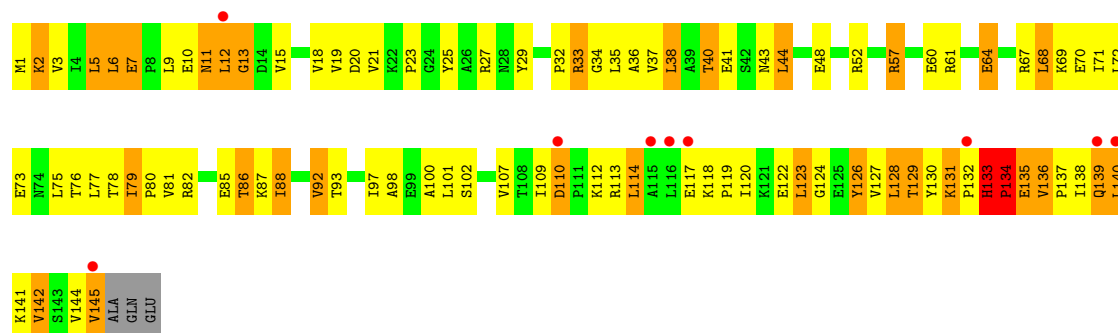




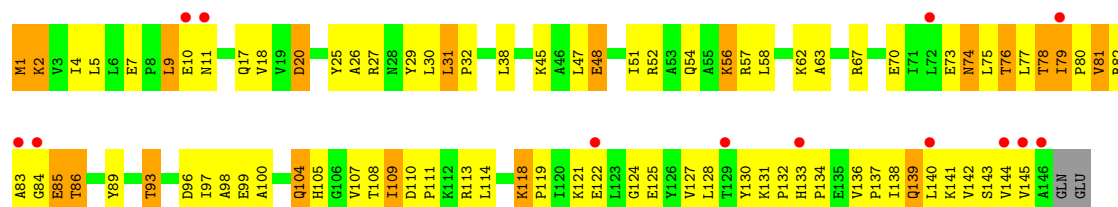
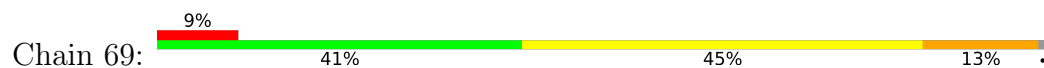
• Molecule 34: 50S ribosomal protein L6



• Molecule 35: 50S ribosomal protein L9

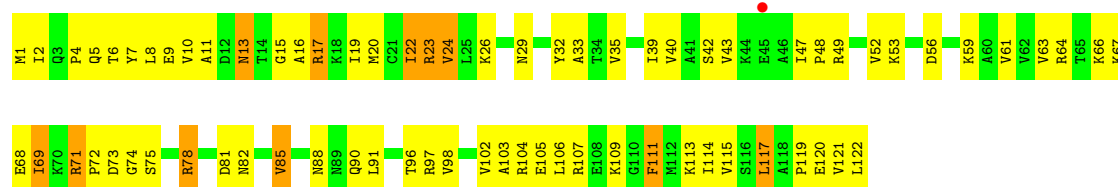


• Molecule 35: 50S ribosomal protein L9

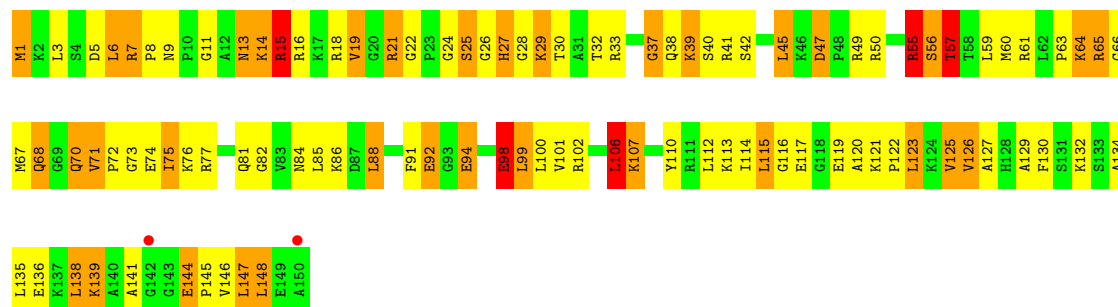


Chain 38:

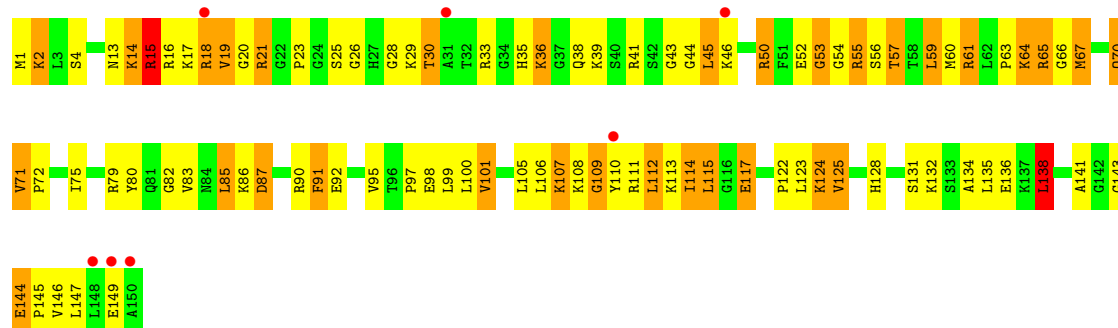




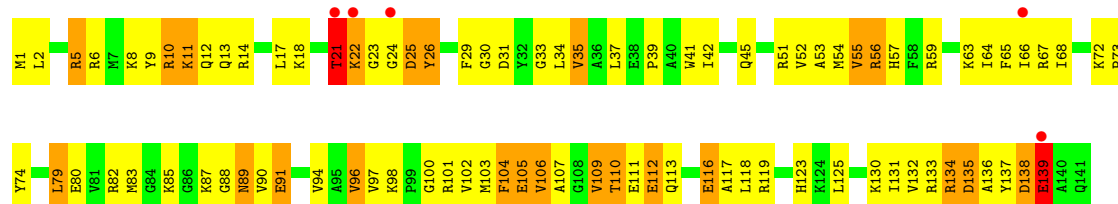
• Molecule 39: 50S ribosomal protein L15



• Molecule 39: 50S ribosomal protein L15

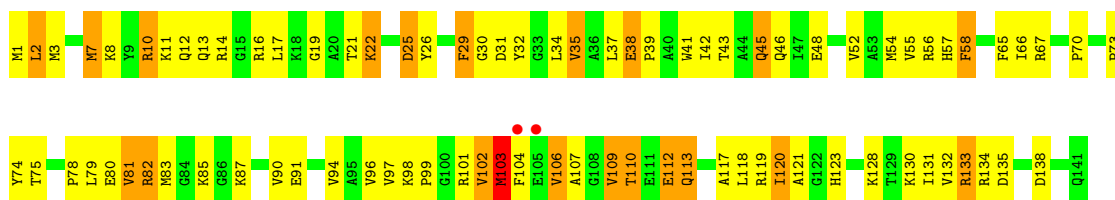


• Molecule 40: 50S ribosomal protein L16



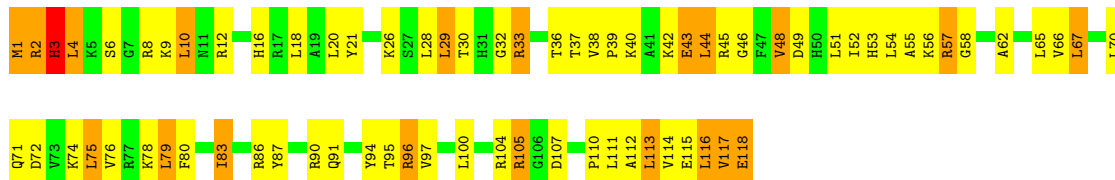
• Molecule 40: 50S ribosomal protein L16





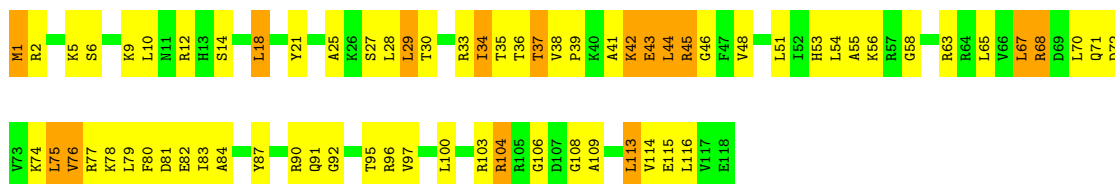
• Molecule 41: 50S ribosomal protein L17

Chain 98: 37% 45% 17%



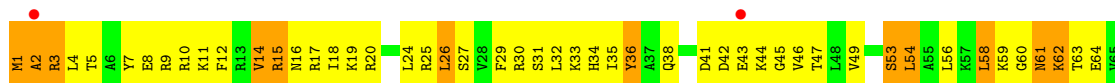
• Molecule 41: 50S ribosomal protein L17

Chain 55: 41% 47% 13%



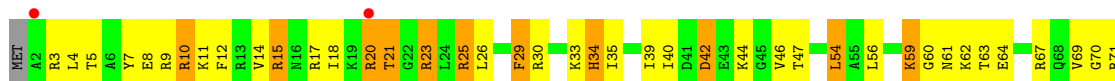
• Molecule 42: 50S ribosomal protein L18

Chain A8: 3% 32% 52% 14%

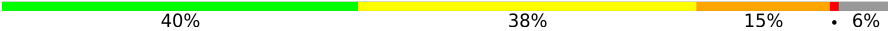


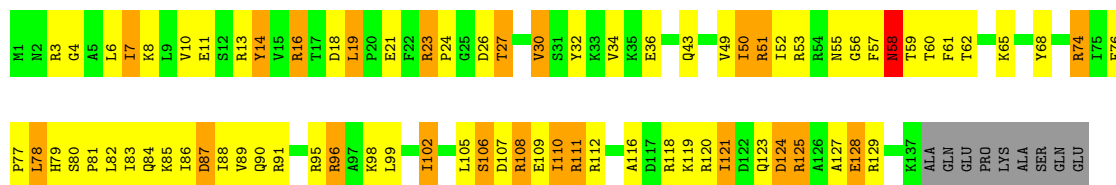
• Molecule 42: 50S ribosomal protein L18

Chain 65: 3% 41% 45% 13%



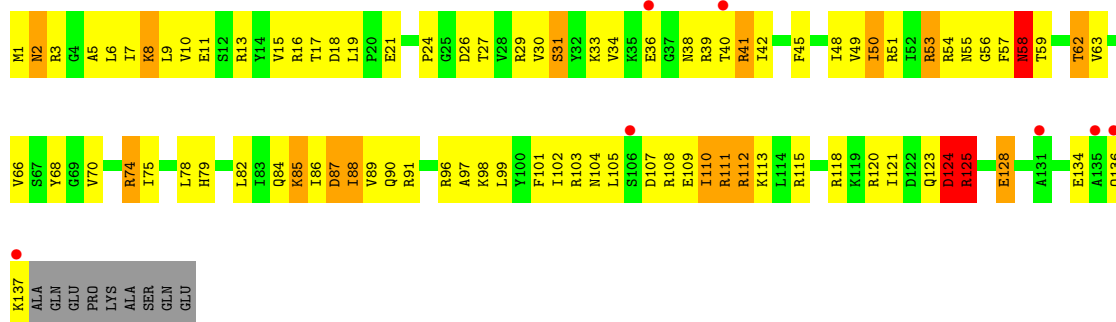
• Molecule 43: 50S ribosomal protein L19

Chain B8: 



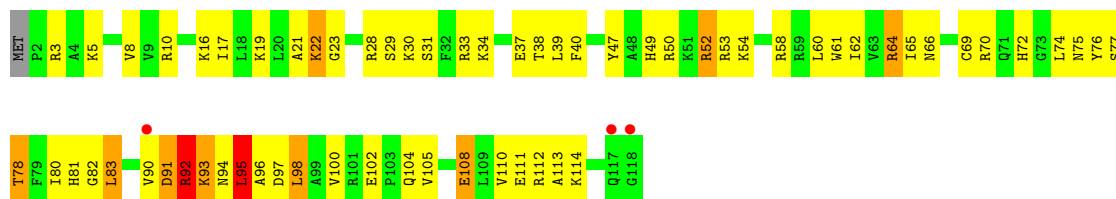
• Molecule 43: 50S ribosomal protein L19

Chain 75: 



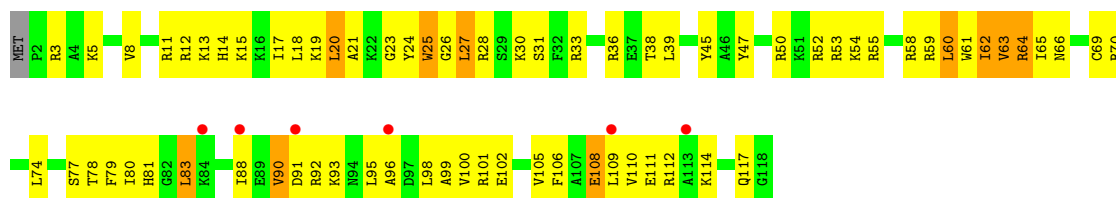
• Molecule 44: 50S ribosomal protein L20

Chain C8: 



• Molecule 44: 50S ribosomal protein L20

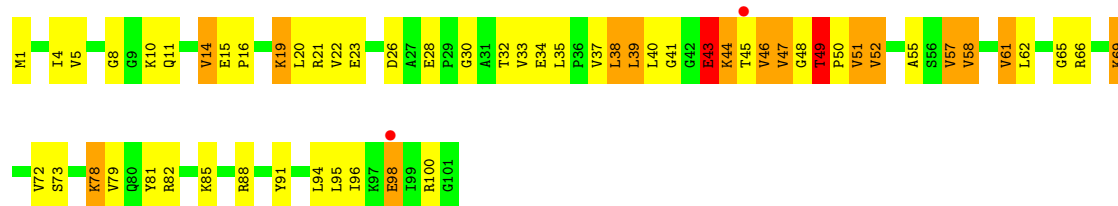
Chain 85: 



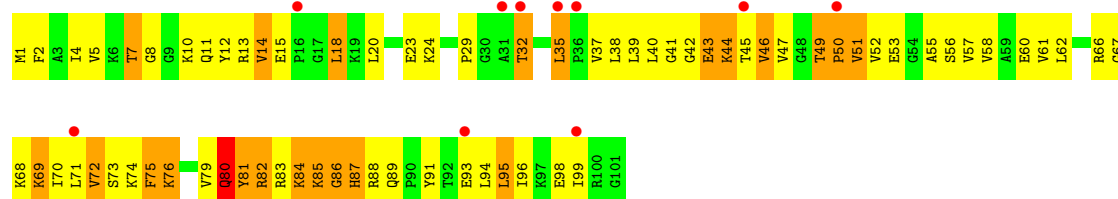
• Molecule 45: 50S ribosomal protein L21

Chain D8: 

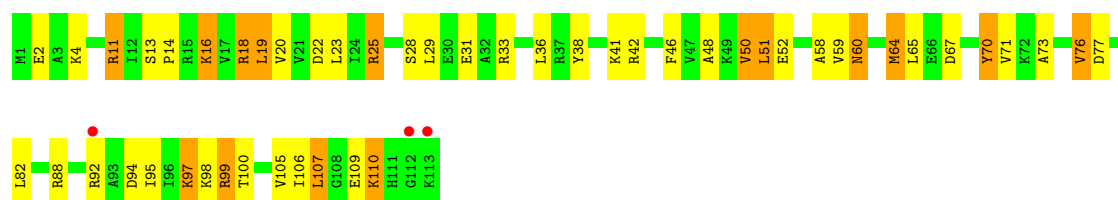




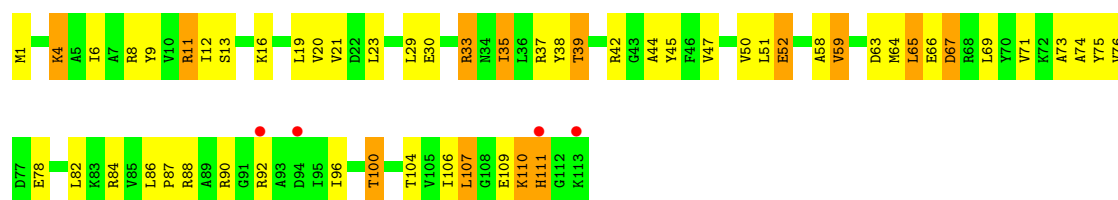
• Molecule 45: 50S ribosomal protein L21



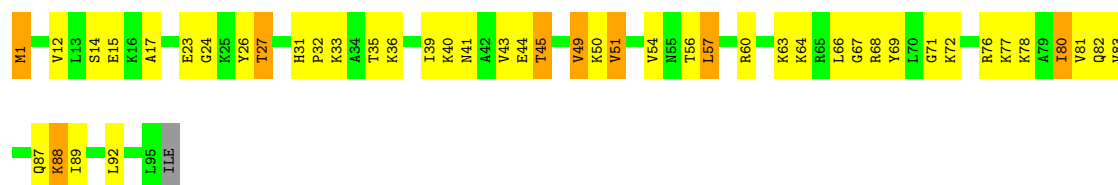
• Molecule 46: 50S ribosomal protein L22



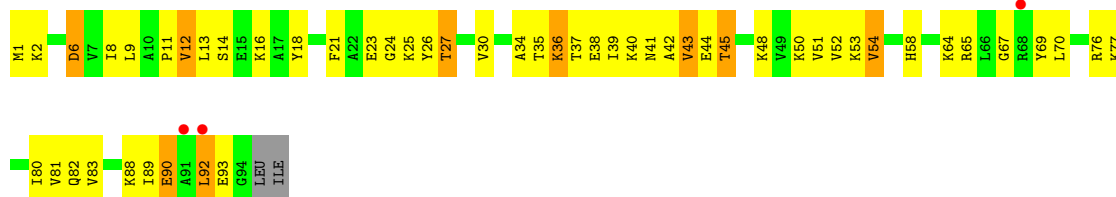
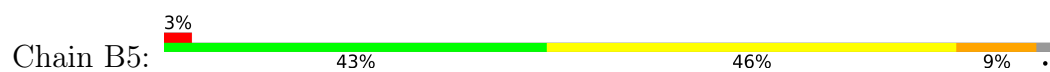
• Molecule 46: 50S ribosomal protein L22



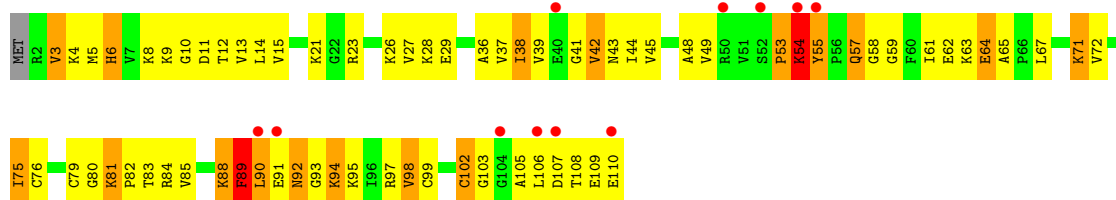
• Molecule 47: 50S ribosomal protein L23



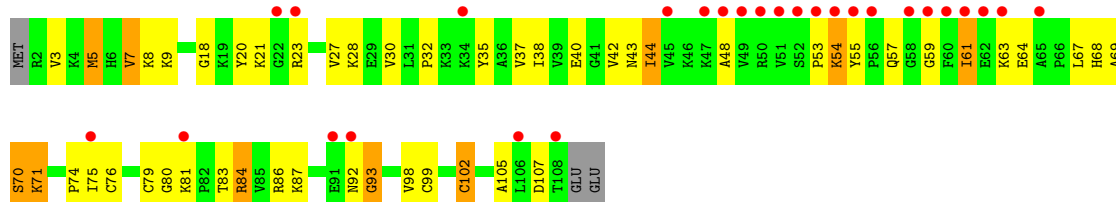
• Molecule 47: 50S ribosomal protein L23



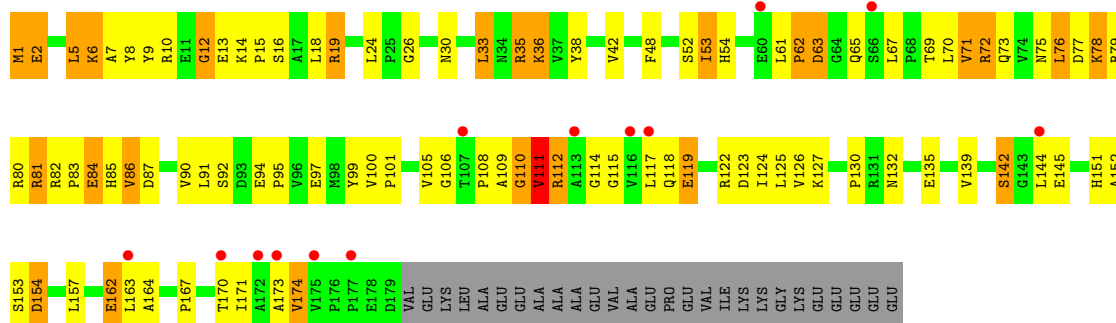
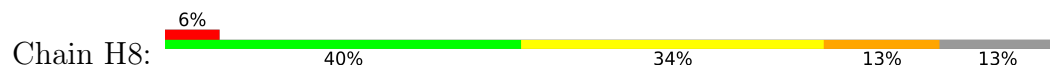
- Molecule 48: 50S ribosomal protein L24



- Molecule 48: 50S ribosomal protein L24

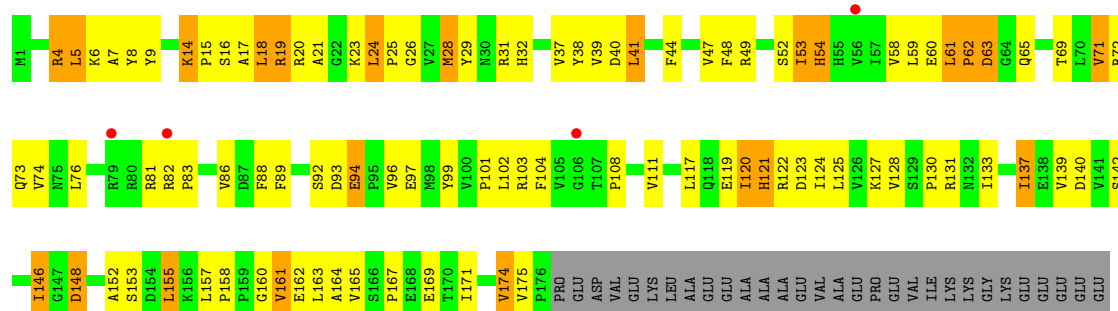


- Molecule 49: 50S ribosomal protein L25



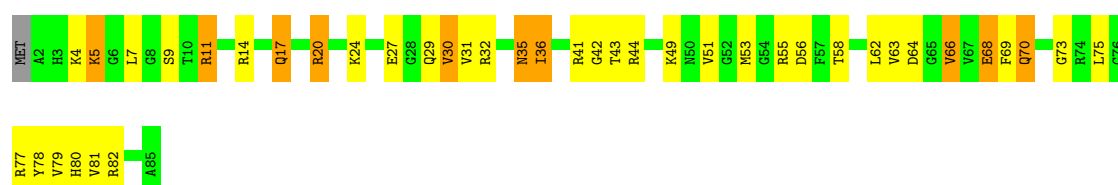
- Molecule 49: 50S ribosomal protein L25





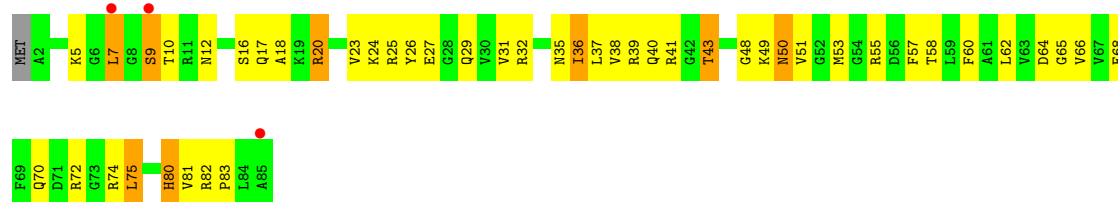
• Molecule 50: 50S ribosomal protein L27

Chain I8: 51% 36% 12%



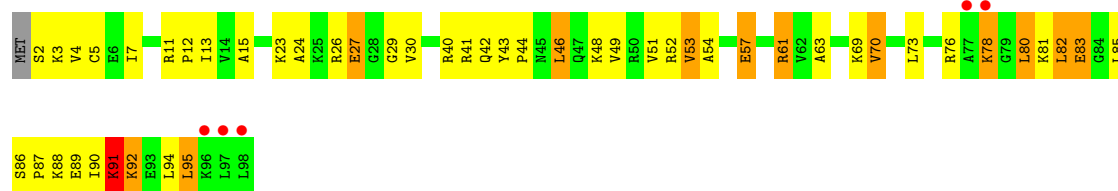
• Molecule 50: 50S ribosomal protein L27

Chain E5: 4% 44% 46% 9%



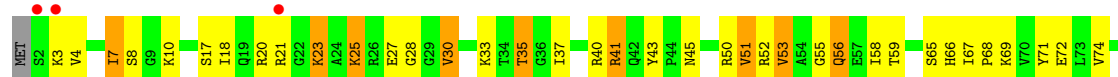
• Molecule 51: 50S ribosomal protein L28

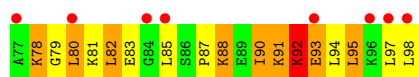
Chain J8: 5% 49% 37% 12%



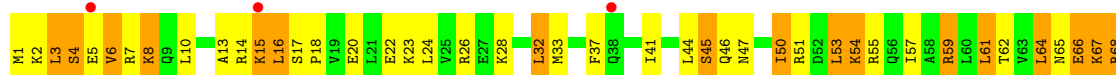
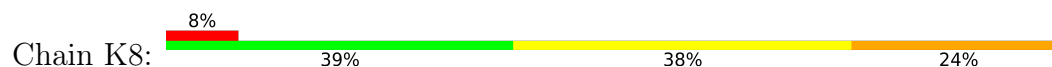
• Molecule 51: 50S ribosomal protein L28

Chain F5: 11% 44% 37% 17%

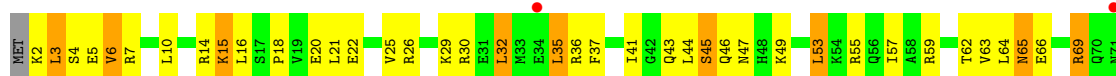




- Molecule 52: 50S ribosomal protein L29



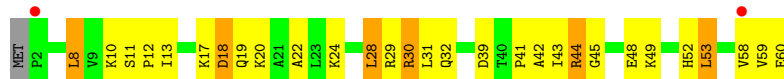
- Molecule 52: 50S ribosomal protein L29



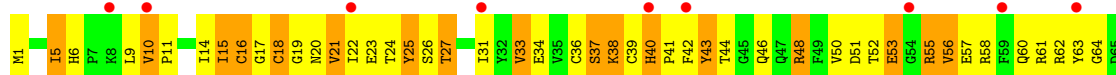
- Molecule 53: 50S ribosomal protein L30



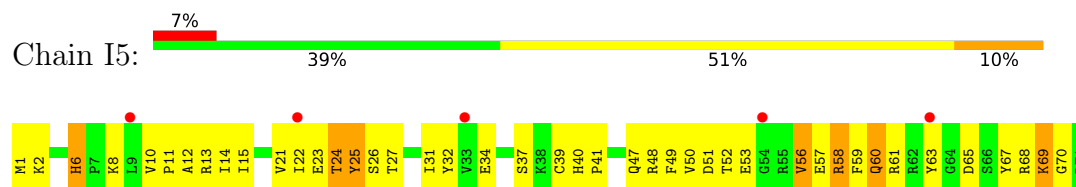
- Molecule 53: 50S ribosomal protein L30



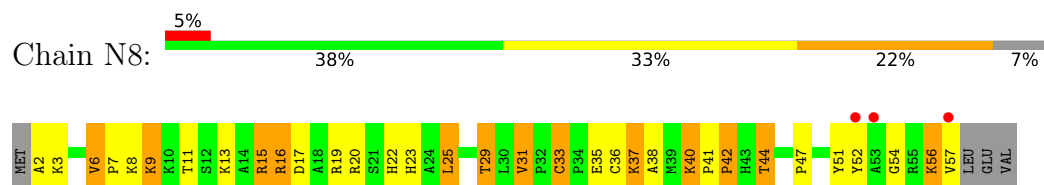
- Molecule 54: 50S ribosomal protein L31



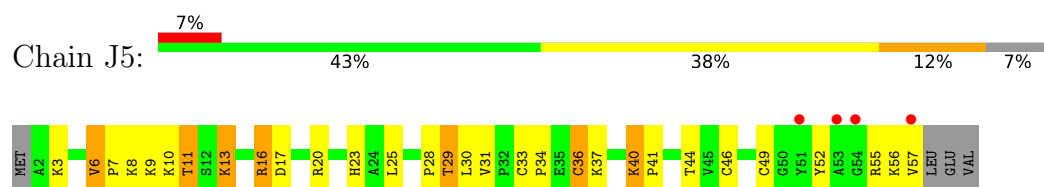
- Molecule 54: 50S ribosomal protein L31



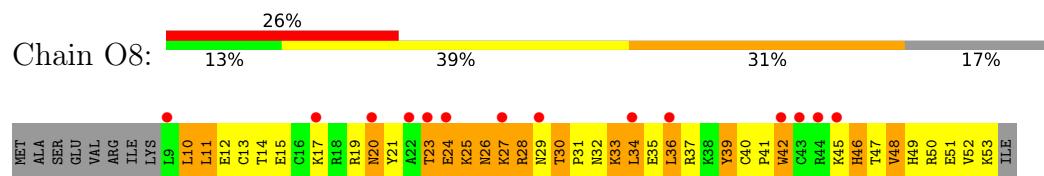
- Molecule 55: 50S ribosomal protein L32



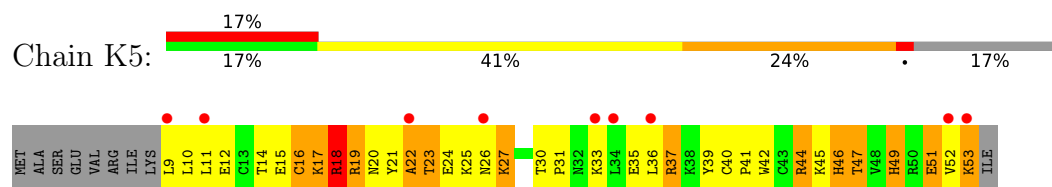
- Molecule 55: 50S ribosomal protein L32



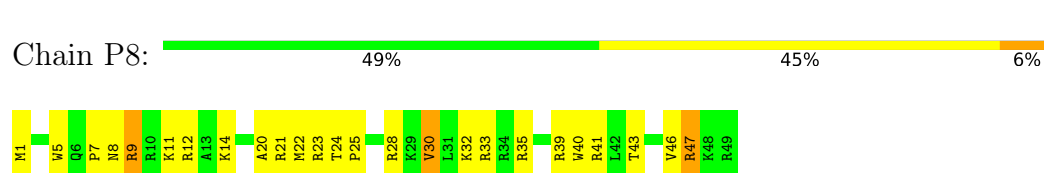
- Molecule 56: 50S ribosomal protein L33



- Molecule 56: 50S ribosomal protein L33

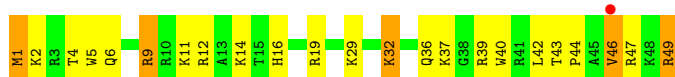


- Molecule 57: 50S ribosomal protein L34

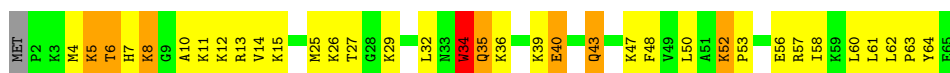


- Molecule 57: 50S ribosomal protein L34

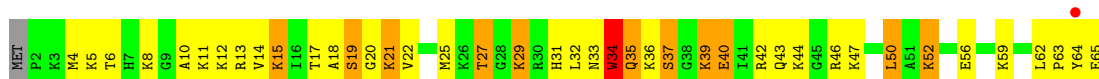




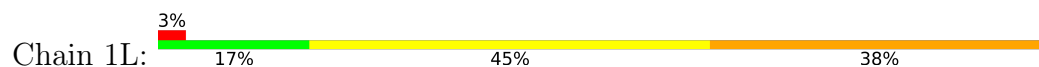
- Molecule 58: 50S ribosomal protein L35



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: E. coli tRNAPhe



- Molecule 60: E. coli tRNAPhe



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.196 , 0.253 0.197 , 0.253	Depositor DCC
R_{free} test set	34306 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 5MU, OMG, H2U, MG, 7MG, 5MC, OMU, MIA, 3AU, K, 4SU, SF4, 2MA, MA6, 0TD, PSU, ZN, OMC, 4OC, M2G, UR3

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	0.43	1/36175 (0.0%)	0.66	10/56452 (0.0%)
1	1G	0.38	1/36106 (0.0%)	0.63	6/56346 (0.0%)
2	12	0.31	0/1959	0.64	0/2642
2	1E	0.33	0/1959	0.58	0/2642
3	22	0.31	0/1636	0.59	0/2205
3	2E	0.38	0/1629	0.64	0/2195
4	32	0.41	0/1732	0.61	0/2318
4	3E	0.42	0/1732	0.62	0/2318
5	42	0.39	0/1171	0.60	0/1576
5	4E	0.47	0/1171	0.67	0/1576
6	52	0.40	0/855	0.60	0/1154
6	5E	0.42	0/855	0.61	0/1154
7	62	0.36	0/1275	0.53	0/1709
7	6E	0.39	0/1275	0.55	0/1709
8	72	0.33	0/1135	0.62	0/1527
8	7E	0.43	0/1135	0.66	0/1527
9	82	0.30	0/1022	0.55	0/1371
9	8E	0.34	0/1022	0.60	0/1371
10	1A	0.35	0/814	0.67	0/1095
10	1I	0.37	0/814	0.68	0/1095
11	2A	0.37	0/888	0.60	0/1198
11	2I	0.44	0/879	0.60	0/1187
12	3A	0.44	0/982	0.77	2/1313 (0.2%)
12	3I	0.56	0/982	0.86	0/1313
13	4A	0.32	0/974	0.62	0/1303
13	4I	0.38	0/956	0.67	0/1281
14	5A	0.37	0/500	0.70	0/664
14	5I	0.42	0/500	0.68	0/664
15	6A	0.39	0/744	0.53	0/992
15	6I	0.47	0/744	0.68	0/992
16	7A	0.43	0/721	0.63	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	7I	0.40	0/716	0.67	0/963
17	8A	0.38	0/847	0.64	0/1131
17	8I	0.42	0/847	0.68	0/1131
18	9A	0.44	0/578	0.78	1/768 (0.1%)
18	9I	0.46	0/589	0.79	0/782
19	AA	0.31	0/698	0.60	0/938
19	AI	0.38	0/689	0.77	1/926 (0.1%)
20	BA	0.38	0/778	0.68	1/1028 (0.1%)
20	BI	0.34	0/768	0.66	1/1014 (0.1%)
21	1B	0.33	0/221	0.53	0/288
21	1F	0.35	0/212	0.61	0/277
22	1K	0.35	1/1647 (0.1%)	0.55	0/2565
23	2K	0.51	0/1580	0.71	0/2459
24	3K	0.32	0/1739	0.54	0/2708
24	3L	0.31	0/1739	0.53	0/2708
25	4K	0.38	0/689	0.54	0/1069
25	4L	0.38	0/689	0.58	0/1069
26	5K	0.30	1/1629 (0.1%)	0.49	0/2538
27	14	0.48	0/69120	0.71	20/107900 (0.0%)
27	1H	0.62	0/69453	0.83	39/108417 (0.0%)
28	16	0.49	0/2928	0.73	1/4568 (0.0%)
28	1J	0.38	0/2906	0.64	0/4533
29	7I	0.21	0/1072	0.45	0/1447
29	79	0.23	0/1072	0.47	0/1447
30	11	0.70	0/2165	1.03	4/2919 (0.1%)
30	19	0.57	0/2165	0.89	8/2919 (0.3%)
31	21	0.58	0/1592	0.78	1/2149 (0.0%)
31	29	0.41	0/1592	0.65	0/2149
32	31	0.66	0/1620	0.88	0/2194
32	39	0.48	0/1620	0.75	0/2194
33	41	0.46	0/1498	0.71	1/2016 (0.0%)
33	49	0.32	0/1498	0.64	0/2016
34	51	0.43	0/1362	0.72	2/1841 (0.1%)
34	59	0.29	0/1353	0.59	0/1830
35	61	0.44	0/1146	0.82	0/1551
35	69	0.41	0/1151	0.68	0/1558
36	38	0.33	0/636	0.71	0/847
37	15	0.37	0/1131	0.65	0/1525
37	58	0.65	1/1131 (0.1%)	1.01	6/1525 (0.4%)
38	25	0.46	0/942	0.70	0/1269
38	68	0.62	0/942	0.83	0/1269
39	35	0.50	0/1161	0.94	3/1544 (0.2%)
39	78	0.66	0/1161	1.11	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	45	0.44	0/1142	0.73	0/1527
40	88	0.61	0/1171	0.90	1/1565 (0.1%)
41	55	0.46	0/981	0.70	0/1312
41	98	0.57	0/981	0.89	2/1312 (0.2%)
42	65	0.41	0/891	0.70	0/1187
42	A8	0.51	0/899	0.85	3/1197 (0.3%)
43	75	0.43	0/1155	0.67	0/1542
43	B8	0.59	0/1155	0.82	0/1542
44	85	0.42	0/981	0.66	0/1306
44	C8	0.63	0/981	0.90	0/1306
45	95	0.47	0/789	0.86	1/1057 (0.1%)
45	D8	0.56	0/789	0.81	0/1057
46	A5	0.51	0/910	0.67	0/1220
46	E8	0.65	0/910	0.88	0/1220
47	B5	0.51	0/756	0.74	0/1014
47	F8	0.65	0/761	0.93	2/1021 (0.2%)
48	C5	0.45	0/788	0.81	0/1059
48	G8	0.51	0/838	0.85	0/1121
49	D5	0.30	0/1435	0.60	0/1947
49	H8	0.42	0/1460	0.68	0/1982
50	E5	0.43	0/666	0.74	0/888
50	I8	0.71	0/670	0.96	0/892
51	F5	0.51	0/769	0.83	0/1022
51	J8	0.65	0/769	0.86	0/1022
52	G5	0.47	0/592	0.69	0/784
52	K8	0.59	0/600	0.75	0/794
53	H5	0.36	0/473	0.63	0/635
53	L8	0.53	0/473	0.76	0/635
54	I5	0.33	0/593	0.72	0/795
54	M8	0.42	0/593	0.77	0/795
55	J5	0.47	0/448	0.76	0/606
55	N8	0.53	0/448	0.81	0/606
56	K5	0.49	0/396	0.89	1/529 (0.2%)
56	O8	0.57	0/396	0.95	0/529
57	L5	0.59	0/437	0.76	0/575
57	P8	0.77	0/427	0.90	0/564
58	M5	0.51	0/514	0.88	0/679
58	Q8	0.65	0/514	0.94	0/679
59	1L	0.25	0/1717	0.48	0/2674
60	2L	0.39	0/1602	0.61	0/2493
All	All	0.49	5/326284 (0.0%)	0.73	117/488082 (0.0%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	58	136	GLU	CA-C	7.49	1.56	1.52
1	13	1498	UR3	O3'-P	5.93	1.62	1.56
1	1G	1498	UR3	O3'-P	5.65	1.61	1.56
22	1K	8	4SU	O3'-P	5.13	1.61	1.56
26	5K	8	4SU	O3'-P	5.11	1.61	1.56

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1H	2150	G	OP1-P-OP2	-13.82	78.15	119.60
27	1H	2150	G	O5'-P-OP2	-11.41	73.78	108.00
27	1H	2149	A	OP2-P-O3'	10.70	140.09	108.00
27	1H	2149	A	OP1-P-O3'	-9.79	78.64	108.00
27	1H	2015	G	C2'-C3'-O3'	8.49	122.24	109.50

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	903	0
1	1G	32526	0	16442	934	0
2	12	1924	0	1975	106	0
2	1E	1924	0	1975	97	0
3	22	1612	0	1677	95	0
3	2E	1605	0	1668	62	0
4	32	1702	0	1762	71	0
4	3E	1702	0	1764	96	0
5	42	1155	0	1212	55	0
5	4E	1155	0	1213	43	0
6	52	842	0	857	34	0
6	5E	842	0	857	35	0
7	62	1256	0	1296	52	0
7	6E	1256	0	1296	56	0
8	72	1115	0	1177	53	0
8	7E	1115	0	1177	55	0
9	82	1004	0	1032	80	0
9	8E	1004	0	1032	57	0
10	1A	801	0	849	61	0
10	1I	801	0	849	47	0
11	2A	873	0	894	44	0
11	2I	864	0	881	35	0
12	3A	977	0	1064	52	0
12	3I	977	0	1061	41	0
13	4A	964	0	1034	61	0
13	4I	946	0	1008	75	0
14	5A	491	0	530	52	0
14	5I	491	0	529	36	0
15	6A	733	0	771	26	0
15	6I	733	0	771	30	0
16	7A	705	0	725	39	0
16	7I	700	0	720	55	0
17	8A	834	0	904	56	0
17	8I	834	0	904	38	0
18	9A	573	0	644	29	0
18	9I	584	0	657	32	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	34	0
20	BA	776	0	856	53	0
20	BI	766	0	854	45	0
21	1B	217	0	234	14	0
21	1F	208	0	221	14	0
22	1K	1628	0	839	53	0
23	2K	1635	0	850	33	0
24	3K	1626	0	832	72	0
24	3L	1626	0	834	49	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	1525	0
27	1H	62245	0	31354	1497	1
28	16	2617	0	1327	64	0
28	1J	2598	0	1316	81	0
29	71	1049	0	1071	63	0
29	79	1049	0	1071	59	0
30	11	2115	0	2195	116	0
30	19	2115	0	2195	98	0
31	21	1559	0	1618	77	0
31	29	1559	0	1618	92	0
32	31	1585	0	1632	93	0
32	39	1585	0	1632	92	0
33	41	1473	0	1535	78	0
33	49	1473	0	1535	75	0
34	51	1336	0	1418	73	0
34	59	1327	0	1405	75	0
35	61	1131	0	1218	73	0
35	69	1136	0	1223	61	0
36	38	635	0	677	25	0
37	15	1104	0	1180	47	0
37	58	1104	0	1180	62	0
38	25	932	0	996	55	0
38	68	932	0	996	50	0
39	35	1144	0	1228	87	0
39	78	1144	0	1228	117	0
40	45	1121	0	1179	76	0
40	88	1150	0	1209	90	0
41	55	967	0	1033	63	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	67	0
43	75	1141	0	1202	66	0
43	B8	1141	0	1202	67	0
44	85	963	0	1022	66	0
44	C8	963	0	1022	62	0
45	95	778	0	852	66	0
45	D8	778	0	852	40	0
46	A5	899	0	964	34	0
46	E8	899	0	964	36	0
47	B5	742	0	803	40	0
47	F8	747	0	805	37	0
48	C5	776	0	820	30	0
48	G8	825	0	898	42	0
49	D5	1404	0	1437	76	0
49	H8	1428	0	1454	75	0
50	E5	657	0	677	41	0
50	I8	661	0	688	38	0
51	F5	762	0	848	41	0
51	J8	762	0	848	41	0
52	G5	590	0	643	36	0
52	K8	598	0	655	36	0
53	H5	468	0	518	31	0
53	L8	468	0	518	16	0
54	I5	580	0	577	42	0
54	M8	580	0	577	51	0
55	J5	434	0	454	25	0
55	N8	434	0	454	30	0
56	K5	389	0	404	32	0
56	O8	389	0	404	33	0
57	L5	429	0	480	16	0
57	P8	419	0	458	18	0
58	M5	506	0	567	53	0
58	Q8	506	0	567	35	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	67	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	9487	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 9487 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	44
2	1E	235/256 (92%)	176 (75%)	58 (25%)	1 (0%)	30	61
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%)	18	49
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	47
9	8E	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	47
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	44
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%)	10	37
20	BA	101/106 (95%)	80 (79%)	20 (20%)	1 (1%)	12	41
20	BI	99/106 (93%)	81 (82%)	17 (17%)	1 (1%)	12	41
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	32
31	21	202/206 (98%)	185 (92%)	16 (8%)	1 (0%)	24	57
31	29	202/206 (98%)	171 (85%)	31 (15%)	0	100	100
32	31	200/210 (95%)	177 (88%)	20 (10%)	3 (2%)	8	32
32	39	200/210 (95%)	168 (84%)	30 (15%)	2 (1%)	12	41
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%)	10	37
34	59	171/180 (95%)	122 (71%)	48 (28%)	1 (1%)	21	52
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	20
37	15	136/140 (97%)	113 (83%)	22 (16%)	1 (1%)	18	49

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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	47
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	44
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%)	6	28
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	25
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	11
49	D5	174/206 (84%)	125 (72%)	47 (27%)	2 (1%)	11	39
49	H8	177/206 (86%)	127 (72%)	48 (27%)	2 (1%)	11	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%)	11	39
51	J8	95/98 (97%)	74 (78%)	20 (21%)	1 (1%)	11	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	19
54	M8	69/71 (97%)	38 (55%)	28 (41%)	3 (4%)	2	12
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	11
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	47

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%)	149 (73%)	56 (27%)	0	1
2	1E	205/220 (93%)	158 (77%)	47 (23%)	1	4
3	22	160/188 (85%)	121 (76%)	39 (24%)	1	3
3	2E	159/188 (85%)	116 (73%)	43 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	145 (81%)	35 (19%)	1	7
4	3E	180/181 (99%)	137 (76%)	43 (24%)	1	3
5	42	116/123 (94%)	97 (84%)	19 (16%)	2	11
5	4E	116/123 (94%)	87 (75%)	29 (25%)	0	2
6	52	90/90 (100%)	74 (82%)	16 (18%)	2	9
6	5E	90/90 (100%)	72 (80%)	18 (20%)	1	6
7	62	126/127 (99%)	103 (82%)	23 (18%)	2	8
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	4
8	72	119/119 (100%)	97 (82%)	22 (18%)	1	8
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	5
9	82	97/99 (98%)	66 (68%)	31 (32%)	0	0
9	8E	97/99 (98%)	72 (74%)	25 (26%)	0	2
10	1A	89/92 (97%)	64 (72%)	25 (28%)	0	1
10	1I	89/92 (97%)	68 (76%)	21 (24%)	1	3
11	2A	89/99 (90%)	70 (79%)	19 (21%)	1	5
11	2I	88/99 (89%)	71 (81%)	17 (19%)	1	7
12	3A	103/108 (95%)	73 (71%)	30 (29%)	0	1
12	3I	103/108 (95%)	80 (78%)	23 (22%)	1	4
13	4A	97/101 (96%)	76 (78%)	21 (22%)	1	5
13	4I	95/101 (94%)	68 (72%)	27 (28%)	0	1
14	5A	49/50 (98%)	37 (76%)	12 (24%)	1	3
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	28
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	11
16	7A	72/74 (97%)	57 (79%)	15 (21%)	1	5
16	7I	72/74 (97%)	57 (79%)	15 (21%)	1	5
17	8A	95/97 (98%)	78 (82%)	17 (18%)	2	9
17	8I	95/97 (98%)	80 (84%)	15 (16%)	2	12
18	9A	61/77 (79%)	47 (77%)	14 (23%)	1	4
18	9I	62/77 (80%)	51 (82%)	11 (18%)	2	9
19	AA	73/80 (91%)	48 (66%)	25 (34%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	73/80 (91%)	47 (64%)	26 (36%)	0	0
20	BA	75/82 (92%)	61 (81%)	14 (19%)	1	7
20	BI	75/82 (92%)	60 (80%)	15 (20%)	1	6
21	1B	20/22 (91%)	17 (85%)	3 (15%)	3	13
21	1F	19/22 (86%)	17 (90%)	2 (10%)	6	26
29	71	111/181 (61%)	96 (86%)	15 (14%)	4	16
29	79	111/181 (61%)	93 (84%)	18 (16%)	2	11
30	11	214/218 (98%)	169 (79%)	45 (21%)	1	5
30	19	214/218 (98%)	167 (78%)	47 (22%)	1	4
31	21	164/166 (99%)	127 (77%)	37 (23%)	1	4
31	29	164/166 (99%)	127 (77%)	37 (23%)	1	4
32	31	161/166 (97%)	128 (80%)	33 (20%)	1	5
32	39	161/166 (97%)	125 (78%)	36 (22%)	1	4
33	41	155/156 (99%)	116 (75%)	39 (25%)	0	2
33	49	155/156 (99%)	116 (75%)	39 (25%)	0	2
34	51	145/148 (98%)	107 (74%)	38 (26%)	0	2
34	59	144/148 (97%)	112 (78%)	32 (22%)	1	4
35	61	122/124 (98%)	80 (66%)	42 (34%)	0	0
35	69	122/124 (98%)	89 (73%)	33 (27%)	0	2
36	38	66/135 (49%)	40 (61%)	26 (39%)	0	0
37	15	117/119 (98%)	86 (74%)	31 (26%)	0	2
37	58	117/119 (98%)	82 (70%)	35 (30%)	0	1
38	25	100/100 (100%)	76 (76%)	24 (24%)	1	3
38	68	100/100 (100%)	76 (76%)	24 (24%)	1	3
39	35	116/116 (100%)	75 (65%)	41 (35%)	0	0
39	78	116/116 (100%)	76 (66%)	40 (34%)	0	0
40	45	111/111 (100%)	83 (75%)	28 (25%)	0	2
40	88	113/111 (102%)	86 (76%)	27 (24%)	1	3
41	55	101/101 (100%)	78 (77%)	23 (23%)	1	4
41	98	101/101 (100%)	71 (70%)	30 (30%)	0	1
42	65	87/88 (99%)	68 (78%)	19 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	A8	88/88 (100%)	62 (70%)	26 (30%)	0	1
43	75	120/127 (94%)	83 (69%)	37 (31%)	0	0
43	B8	120/127 (94%)	85 (71%)	35 (29%)	0	1
44	85	93/94 (99%)	74 (80%)	19 (20%)	1	5
44	C8	93/94 (99%)	68 (73%)	25 (27%)	0	2
45	95	82/82 (100%)	55 (67%)	27 (33%)	0	0
45	D8	82/82 (100%)	52 (63%)	30 (37%)	0	0
46	A5	92/92 (100%)	67 (73%)	25 (27%)	0	1
46	E8	92/92 (100%)	71 (77%)	21 (23%)	1	4
47	B5	76/78 (97%)	56 (74%)	20 (26%)	0	2
47	F8	76/78 (97%)	59 (78%)	17 (22%)	1	4
48	C5	78/91 (86%)	58 (74%)	20 (26%)	0	2
48	G8	88/91 (97%)	57 (65%)	31 (35%)	0	0
49	D5	155/179 (87%)	120 (77%)	35 (23%)	1	4
49	H8	158/179 (88%)	118 (75%)	40 (25%)	0	2
50	E5	65/67 (97%)	49 (75%)	16 (25%)	1	3
50	I8	66/67 (98%)	50 (76%)	16 (24%)	1	3
51	F5	82/83 (99%)	59 (72%)	23 (28%)	0	1
51	J8	82/83 (99%)	62 (76%)	20 (24%)	1	3
52	G5	64/67 (96%)	52 (81%)	12 (19%)	1	7
52	K8	65/67 (97%)	42 (65%)	23 (35%)	0	0
53	H5	51/52 (98%)	41 (80%)	10 (20%)	1	6
53	L8	51/52 (98%)	40 (78%)	11 (22%)	1	5
54	I5	63/63 (100%)	54 (86%)	9 (14%)	3	14
54	M8	63/63 (100%)	43 (68%)	20 (32%)	0	0
55	J5	48/52 (92%)	35 (73%)	13 (27%)	0	2
55	N8	48/52 (92%)	33 (69%)	15 (31%)	0	0
56	K5	44/52 (85%)	29 (66%)	15 (34%)	0	0
56	O8	44/52 (85%)	25 (57%)	19 (43%)	0	0
57	L5	42/42 (100%)	30 (71%)	12 (29%)	0	1
57	P8	40/42 (95%)	30 (75%)	10 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	M5	52/55 (94%)	41 (79%)	11 (21%)	1	5
58	Q8	52/55 (94%)	41 (79%)	11 (21%)	1	5
All	All	9889/10493 (94%)	7477 (76%)	2412 (24%)	1	3

5 of 2412 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	49	64	THR
50	E5	10	THR
34	59	167	GLU
33	49	58	GLN
41	55	71	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
19	AA	23	ASN
43	75	58	ASN
30	19	96	HIS
35	69	74	ASN
46	A5	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1514/1522 (99%)	370 (24%)	51 (3%)
1	1G	1512/1522 (99%)	388 (25%)	48 (3%)
22	1K	75/76 (98%)	39 (52%)	0
23	2K	75/76 (98%)	22 (29%)	2 (2%)
24	3K	75/76 (98%)	39 (52%)	3 (4%)
24	3L	75/76 (98%)	37 (49%)	1 (1%)
25	4K	29/60 (48%)	8 (27%)	2 (6%)
25	4L	29/60 (48%)	12 (41%)	2 (6%)
26	5K	75/76 (98%)	36 (48%)	5 (6%)
27	14	2872/2917 (98%)	785 (27%)	65 (2%)
27	1H	2885/2917 (98%)	729 (25%)	77 (2%)
28	16	121/122 (99%)	27 (22%)	1 (0%)
28	1J	120/122 (98%)	39 (32%)	4 (3%)
59	1L	75/76 (98%)	35 (46%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
60	2L	75/76 (98%)	24 (32%)	0
All	All	9607/9774 (98%)	2590 (26%)	262 (2%)

5 of 2590 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
27	5MC	1H	1985	61,27	19,22,23	3.73	7 (36%)	26,32,35	1.45	3 (11%)
1	M2G	1G	966	1	24,27,28	2.86	8 (33%)	33,40,43	1.64	7 (21%)
27	PSU	1H	1934	27	18,21,22	1.13	2 (11%)	21,30,33	1.91	6 (28%)
27	5MU	14	1915	27	19,22,23	4.01	5 (26%)	27,32,35	3.45	9 (33%)
27	5MU	1H	1938	27	19,22,23	4.29	5 (26%)	27,32,35	3.91	10 (37%)
1	4OC	13	1402	62,1	20,23,24	2.87	8 (40%)	25,32,35	1.49	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	13	1207	61,1	23,26,27	2.80	9 (39%)	33,38,41	2.49	13 (39%)
59	PSU	1L	39	59	18,21,22	1.16	3 (16%)	21,30,33	2.18	7 (33%)
22	PSU	1K	32	61,22	18,21,22	1.12	1 (5%)	21,30,33	1.32	2 (9%)
26	PSU	5K	32	26	18,21,22	1.16	1 (5%)	21,30,33	1.81	4 (19%)
27	2MA	1H	2516	61,27	22,25,26	3.21	8 (36%)	32,37,40	2.15	9 (28%)
23	5MU	2K	54	23	19,22,23	3.80	5 (26%)	27,32,35	3.28	7 (25%)
60	5MU	2L	54	60	19,22,23	3.86	5 (26%)	27,32,35	3.13	10 (37%)
60	PSU	2L	55	60	18,21,22	1.37	2 (11%)	21,30,33	1.82	4 (19%)
1	M2G	13	966	1	24,27,28	2.69	9 (37%)	33,40,43	1.67	9 (27%)
22	4SU	1K	8	22	18,21,22	1.84	5 (27%)	25,30,33	2.38	6 (24%)
22	5MU	1K	54	22	19,22,23	3.92	5 (26%)	27,32,35	3.22	10 (37%)
23	PSU	2K	39	23	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
24	PSU	3L	39	24	18,21,22	1.20	1 (5%)	21,30,33	1.73	4 (19%)
1	5MC	13	1404	1	19,22,23	3.24	8 (42%)	26,32,35	1.20	1 (3%)
27	OMU	1H	2565	27,62	19,22,23	2.13	6 (31%)	25,31,34	2.51	10 (40%)
1	5MC	13	967	1	19,22,23	3.90	8 (42%)	26,32,35	1.09	1 (3%)
60	7MG	2L	46	60	23,26,27	3.21	6 (26%)	27,39,42	2.77	10 (37%)
60	3AU	2L	47	60	24,28,29	2.83	8 (33%)	30,40,43	2.02	8 (26%)
24	PSU	3K	39	24	18,21,22	1.20	1 (5%)	21,30,33	1.74	4 (19%)
27	OMC	14	1920	27	19,22,23	1.73	3 (15%)	25,31,34	1.11	1 (4%)
12	0TD	3I	89	12	8,9,10	2.12	1 (12%)	6,11,13	3.49	3 (50%)
23	3AU	2K	47	23	24,28,29	2.97	6 (25%)	30,40,43	1.81	7 (23%)
23	4SU	2K	8	23	18,21,22	1.81	4 (22%)	25,30,33	2.52	6 (24%)
23	PSU	2K	32	23	18,21,22	1.11	2 (11%)	21,30,33	1.98	5 (23%)
24	PSU	3L	32	24	18,21,22	1.18	2 (11%)	21,30,33	1.86	4 (19%)
26	5MU	5K	54	26	19,22,23	4.04	5 (26%)	27,32,35	3.15	9 (33%)
59	MIA	1L	37	59	28,31,32	2.21	4 (14%)	38,44,47	3.07	13 (34%)
60	PSU	2L	39	60	18,21,22	1.21	1 (5%)	21,30,33	1.79	4 (19%)
1	UR3	13	1498	1	19,22,23	2.75	5 (26%)	26,32,35	2.23	7 (26%)
27	5MC	14	1942	27	19,22,23	3.95	8 (42%)	26,32,35	1.34	5 (19%)
1	5MC	13	1400	1	19,22,23	3.86	8 (42%)	26,32,35	1.09	2 (7%)
12	0TD	3A	89	12	8,9,10	1.38	1 (12%)	6,11,13	1.75	2 (33%)
27	5MC	14	1962	61,27	19,22,23	3.62	8 (42%)	26,32,35	1.29	3 (11%)
26	4SU	5K	8	26	18,21,22	1.80	3 (16%)	25,30,33	2.51	5 (20%)
23	PSU	2K	55	23	18,21,22	1.27	1 (5%)	21,30,33	1.76	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	5MU	1H	1962	61,27	19,22,23	3.41	5 (26%)	27,32,35	4.32	10 (37%)
24	PSU	3K	32	24	18,21,22	1.07	1 (5%)	21,30,33	1.73	4 (19%)
27	PSU	1H	2618	27	18,21,22	1.30	3 (16%)	21,30,33	2.02	7 (33%)
27	2MA	14	2503	61,27,62	22,25,26	3.20	7 (31%)	32,37,40	2.37	10 (31%)
23	7MG	2K	46	23	23,26,27	3.02	7 (30%)	27,39,42	2.78	9 (33%)
1	5MC	13	1407	1	19,22,23	3.46	8 (42%)	26,32,35	1.09	2 (7%)
1	MA6	1G	1519	1	23,26,27	1.46	6 (26%)	33,38,41	2.69	11 (33%)
22	MIA	1K	37	22	28,31,32	2.14	4 (14%)	38,44,47	2.95	13 (34%)
22	7MG	1K	46	22	23,26,27	3.08	7 (30%)	27,39,42	2.83	9 (33%)
1	MA6	13	1518	1	23,26,27	1.31	5 (21%)	33,38,41	2.63	11 (33%)
1	5MC	1G	1400	1	19,22,23	4.03	8 (42%)	26,32,35	1.46	5 (19%)
27	PSU	14	1917	27	18,21,22	1.14	2 (11%)	21,30,33	1.76	5 (23%)
59	PSU	1L	32	59	18,21,22	1.03	1 (5%)	21,30,33	1.54	3 (14%)
26	MIA	5K	37	26	28,31,32	2.49	5 (17%)	38,44,47	3.38	16 (42%)
27	OMU	14	2552	27,62	19,22,23	2.46	6 (31%)	25,31,34	2.03	6 (24%)
60	4SU	2L	8	60	18,21,22	1.85	3 (16%)	25,30,33	2.26	6 (24%)
23	H2U	2K	16	23	18,21,22	1.93	4 (22%)	19,30,33	1.57	4 (21%)
1	PSU	13	516	62,1	18,21,22	0.92	1 (5%)	21,30,33	1.68	4 (19%)
27	5MU	14	1939	61,27	19,22,23	3.85	5 (26%)	27,32,35	3.43	9 (33%)
26	PSU	5K	55	26	18,21,22	1.18	1 (5%)	21,30,33	1.73	4 (19%)
27	PSU	14	1911	27	18,21,22	1.14	1 (5%)	21,30,33	1.61	4 (19%)
1	5MC	1G	1404	1	19,22,23	3.72	8 (42%)	26,32,35	1.50	3 (11%)
59	5MU	1L	54	59	19,22,23	3.92	5 (26%)	27,32,35	3.23	8 (29%)
27	5MC	1H	1965	27	19,22,23	3.41	8 (42%)	26,32,35	1.45	5 (19%)
1	4OC	1G	1402	62,1	20,23,24	2.63	7 (35%)	25,32,35	1.63	5 (20%)
26	H2U	5K	16	26	18,21,22	2.21	4 (22%)	19,30,33	1.64	4 (21%)
1	UR3	1G	1498	1	19,22,23	2.67	6 (31%)	26,32,35	2.06	5 (19%)
1	MA6	1G	1518	1	23,26,27	1.46	5 (21%)	33,38,41	2.57	12 (36%)
60	PSU	2L	32	60	18,21,22	1.05	1 (5%)	21,30,33	2.16	5 (23%)
23	H2U	2K	20	23	18,21,22	2.16	4 (22%)	19,30,33	1.55	3 (15%)
60	H2U	2L	16	60	18,21,22	2.15	4 (22%)	19,30,33	1.68	4 (21%)
27	PSU	14	2605	27	18,21,22	1.36	3 (16%)	21,30,33	2.20	7 (33%)
23	MIA	2K	37	23	28,31,32	2.30	4 (14%)	38,44,47	2.53	13 (34%)
1	5MC	1G	1407	1	19,22,23	3.54	8 (42%)	26,32,35	1.20	3 (11%)
60	MIA	2L	37	60	28,31,32	2.21	3 (10%)	38,44,47	2.90	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMG	14	2251	60,61,27	23,26,27	4.97	10 (43%)	32,38,41	4.60	17 (53%)
26	H2U	5K	20	26,28	18,21,22	2.38	4 (22%)	19,30,33	1.68	4 (21%)
1	MA6	13	1519	1	23,26,27	1.48	4 (17%)	33,38,41	3.02	13 (39%)
27	PSU	1H	1940	27	18,21,22	0.95	1 (5%)	21,30,33	1.70	4 (19%)
22	PSU	1K	39	22	18,21,22	1.08	1 (5%)	21,30,33	2.15	4 (19%)
1	7MG	1G	527	61,1	23,26,27	3.06	7 (30%)	27,39,42	2.86	9 (33%)
22	PSU	1K	55	22	18,21,22	1.18	1 (5%)	21,30,33	1.99	6 (28%)
24	MIA	3L	37	24	28,31,32	2.43	3 (10%)	38,44,47	3.29	14 (36%)
1	2MG	1G	1207	1	23,26,27	2.93	8 (34%)	33,38,41	2.30	12 (36%)
27	OMG	1H	2264	23,61,27	23,26,27	4.69	10 (43%)	32,38,41	4.45	17 (53%)
1	7MG	13	527	61,1	23,26,27	3.00	9 (39%)	27,39,42	2.79	8 (29%)
24	MIA	3K	37	25,24	28,31,32	2.42	4 (14%)	38,44,47	3.16	15 (39%)
26	PSU	5K	39	26	18,21,22	1.25	1 (5%)	21,30,33	1.89	5 (23%)
27	OMC	1H	1943	61,27	19,22,23	1.72	3 (15%)	25,31,34	1.33	4 (16%)
1	PSU	1G	516	62,1	18,21,22	1.20	1 (5%)	21,30,33	1.55	2 (9%)
1	5MC	1G	967	1	19,22,23	3.80	8 (42%)	26,32,35	1.14	2 (7%)

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
27	5MC	1H	1985	61,27	-	0/7/25/26	0/2/2/2
1	M2G	1G	966	1	-	0/11/29/30	0/3/3/3
27	PSU	1H	1934	27	-	0/7/25/26	0/2/2/2
27	5MU	14	1915	27	-	0/7/25/26	0/2/2/2
27	5MU	1H	1938	27	-	3/7/25/26	0/2/2/2
1	4OC	13	1402	62,1	-	2/9/29/30	0/2/2/2
1	2MG	13	1207	61,1	-	0/9/27/28	0/3/3/3
59	PSU	1L	39	59	-	0/7/25/26	0/2/2/2
22	PSU	1K	32	61,22	-	0/7/25/26	0/2/2/2
26	PSU	5K	32	26	-	0/7/25/26	0/2/2/2
27	2MA	1H	2516	61,27	-	2/7/25/26	0/3/3/3
23	5MU	2K	54	23	-	0/7/25/26	0/2/2/2
60	5MU	2L	54	60	-	2/7/25/26	0/2/2/2
60	PSU	2L	55	60	-	0/7/25/26	0/2/2/2
1	M2G	13	966	1	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	1K	8	22	-	1/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	39	23	-	0/7/25/26	0/2/2/2
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
1	5MC	13	1404	1	-	0/7/25/26	0/2/2/2
27	OMU	1H	2565	27,62	-	0/9/27/28	0/2/2/2
1	5MC	13	967	1	-	0/7/25/26	0/2/2/2
60	7MG	2L	46	60	-	2/7/37/38	0/3/3/3
60	3AU	2L	47	60	-	7/16/34/35	0/2/2/2
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
27	OMC	14	1920	27	-	2/9/27/28	0/2/2/2
12	0TD	3I	89	12	-	3/7/12/14	-
23	3AU	2K	47	23	-	7/16/34/35	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	32	23	-	0/7/25/26	0/2/2/2
24	PSU	3L	32	24	-	5/7/25/26	0/2/2/2
26	5MU	5K	54	26	-	2/7/25/26	0/2/2/2
59	MIA	1L	37	59	-	2/15/33/34	0/3/3/3
60	PSU	2L	39	60	-	0/7/25/26	0/2/2/2
1	UR3	13	1498	1	-	2/7/25/26	0/2/2/2
27	5MC	14	1942	27	-	0/7/25/26	0/2/2/2
1	5MC	13	1400	1	-	0/7/25/26	0/2/2/2
12	0TD	3A	89	12	-	4/7/12/14	-
27	5MC	14	1962	61,27	-	2/7/25/26	0/2/2/2
26	4SU	5K	8	26	-	2/7/25/26	0/2/2/2
23	PSU	2K	55	23	-	2/7/25/26	0/2/2/2
27	5MU	1H	1962	61,27	-	2/7/25/26	0/2/2/2
24	PSU	3K	32	24	-	2/7/25/26	0/2/2/2
27	PSU	1H	2618	27	-	0/7/25/26	0/2/2/2
27	2MA	14	2503	61,27,62	-	0/7/25/26	0/3/3/3
23	7MG	2K	46	23	-	0/7/37/38	0/3/3/3
1	5MC	13	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	1G	1519	1	-	2/11/29/30	0/3/3/3
22	MIA	1K	37	22	-	4/15/33/34	0/3/3/3
22	7MG	1K	46	22	-	2/7/37/38	0/3/3/3
1	MA6	13	1518	1	-	0/11/29/30	0/3/3/3
1	5MC	1G	1400	1	-	2/7/25/26	0/2/2/2
27	PSU	14	1917	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PSU	1L	32	59	-	0/7/25/26	0/2/2/2
26	MIA	5K	37	26	-	6/15/33/34	0/3/3/3
27	OMU	14	2552	27,62	-	4/9/27/28	0/2/2/2
60	4SU	2L	8	60	-	2/7/25/26	0/2/2/2
23	H2U	2K	16	23	-	0/7/38/39	0/2/2/2
1	PSU	13	516	62,1	-	0/7/25/26	0/2/2/2
27	5MU	14	1939	61,27	-	0/7/25/26	0/2/2/2
26	PSU	5K	55	26	-	2/7/25/26	0/2/2/2
27	PSU	14	1911	27	-	0/7/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/7/25/26	0/2/2/2
59	5MU	1L	54	59	-	0/7/25/26	0/2/2/2
27	5MC	1H	1965	27	-	0/7/25/26	0/2/2/2
1	4OC	1G	1402	62,1	-	2/9/29/30	0/2/2/2
26	H2U	5K	16	26	-	3/7/38/39	0/2/2/2
1	UR3	1G	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	1G	1518	1	-	4/11/29/30	0/3/3/3
60	PSU	2L	32	60	-	0/7/25/26	0/2/2/2
23	H2U	2K	20	23	-	4/7/38/39	0/2/2/2
60	H2U	2L	16	60	-	0/7/38/39	0/2/2/2
27	PSU	14	2605	27	-	0/7/25/26	0/2/2/2
23	MIA	2K	37	23	-	3/15/33/34	0/3/3/3
1	5MC	1G	1407	1	-	0/7/25/26	0/2/2/2
60	MIA	2L	37	60	-	4/15/33/34	0/3/3/3
27	OMG	14	2251	60,61,27	-	0/9/27/28	0/3/3/3
26	H2U	5K	20	26,28	-	5/7/38/39	0/2/2/2
1	MA6	13	1519	1	-	3/11/29/30	0/3/3/3
27	PSU	1H	1940	27	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
1	7MG	1G	527	61,1	-	2/7/37/38	0/3/3/3
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
24	MIA	3L	37	24	-	4/15/33/34	0/3/3/3
1	2MG	1G	1207	1	-	2/9/27/28	0/3/3/3
27	OMG	1H	2264	23,61,27	-	0/9/27/28	0/3/3/3
1	7MG	13	527	61,1	-	2/7/37/38	0/3/3/3
24	MIA	3K	37	25,24	-	8/15/33/34	0/3/3/3
26	PSU	5K	39	26	-	1/7/25/26	0/2/2/2
27	OMC	1H	1943	61,27	-	0/9/27/28	0/2/2/2
1	PSU	1G	516	62,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1G	967	1	-	0/7/25/26	0/2/2/2

The worst 5 of 425 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1H	1938	5MU	C2-N1	14.65	1.61	1.38
26	5K	54	5MU	C2-N1	13.23	1.59	1.38
27	14	1915	5MU	C2-N1	13.02	1.58	1.38
60	2L	54	5MU	C2-N1	12.79	1.58	1.38
59	1L	54	5MU	C2-N1	12.63	1.58	1.38

The worst 5 of 619 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1H	1962	5MU	C5-C4-N3	13.70	127.23	115.32
27	1H	2264	OMG	C6-C5-N7	13.24	154.38	130.29
27	1H	1938	5MU	C5-C4-N3	12.21	125.94	115.32
27	14	2251	OMG	C6-C5-N7	12.16	152.42	130.29
24	3L	37	MIA	C11-S10-C2	11.80	111.11	102.25

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	13	527	7MG	O4'-C4'-C5'-O5'
1	1G	1207	2MG	O4'-C4'-C5'-O5'
1	13	1402	4OC	O4'-C4'-C5'-O5'
1	1G	1402	4OC	O4'-C4'-C5'-O5'
1	1G	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

57 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1H	1985	5MC	1	0
27	14	1915	5MU	1	0
1	13	1402	4OC	1	0
1	13	1207	2MG	1	0
59	1L	39	PSU	1	0
27	1H	2516	2MA	3	0
23	2K	54	5MU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2L	54	5MU	4	0
1	13	966	M2G	1	0
22	1K	54	5MU	1	0
1	13	1404	5MC	1	0
27	1H	2565	OMU	3	0
1	13	967	5MC	1	0
24	3K	39	PSU	1	0
12	3I	89	0TD	1	0
24	3L	32	PSU	1	0
26	5K	54	5MU	1	0
59	1L	37	MIA	2	0
1	13	1498	UR3	4	0
27	14	1942	5MC	1	0
1	13	1400	5MC	1	0
12	3A	89	0TD	3	0
27	14	1962	5MC	2	0
23	2K	55	PSU	1	0
27	1H	1962	5MU	1	0
27	14	2503	2MA	2	0
23	2K	46	7MG	1	0
1	1G	1519	MA6	4	0
22	1K	37	MIA	2	0
22	1K	46	7MG	4	0
1	13	1518	MA6	2	0
1	1G	1400	5MC	1	0
26	5K	37	MIA	1	0
27	14	2552	OMU	4	0
60	2L	8	4SU	2	0
27	14	1939	5MU	2	0
26	5K	55	PSU	1	0
27	14	1911	PSU	1	0
1	1G	1404	5MC	1	0
1	1G	1402	4OC	2	0
26	5K	16	H2U	4	0
1	1G	1498	UR3	3	0
1	1G	1518	MA6	2	0
60	2L	32	PSU	1	0
23	2K	20	H2U	1	0
27	14	2251	OMG	2	0
26	5K	20	H2U	1	0
1	13	1519	MA6	2	0
27	1H	1940	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	55	PSU	4	0
24	3L	37	MIA	3	0
1	1G	1207	2MG	3	0
27	1H	2264	OMG	1	0
24	3K	37	MIA	3	0
27	1H	1943	OMC	2	0
1	1G	516	PSU	1	0
1	1G	967	5MC	2	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, 95th 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 ²)	Q<0.9
1	13	1504/1522 (98%)	-0.35	6 (0%) 88 76	28, 69, 150, 240	0
1	1G	1501/1522 (98%)	-0.29	9 (0%) 85 70	38, 81, 144, 248	0
2	12	237/256 (92%)	1.18	45 (18%) 3 1	85, 134, 165, 184	0
2	1E	237/256 (92%)	0.65	15 (6%) 26 14	67, 105, 146, 160	0
3	22	206/239 (86%)	0.49	5 (2%) 59 38	81, 109, 137, 144	0
3	2E	205/239 (85%)	0.39	4 (1%) 65 44	62, 81, 122, 145	0
4	32	208/209 (99%)	0.27	7 (3%) 48 28	58, 74, 95, 120	0
4	3E	208/209 (99%)	0.39	0 100 100	58, 77, 99, 108	0
5	42	151/162 (93%)	0.29	0 100 100	67, 84, 102, 133	0
5	4E	151/162 (93%)	0.15	1 (0%) 84 68	50, 67, 90, 113	0
6	52	101/101 (100%)	0.30	2 (1%) 65 44	53, 74, 90, 111	0
6	5E	101/101 (100%)	0.16	0 100 100	50, 73, 89, 106	0
7	62	155/156 (99%)	0.30	6 (3%) 43 24	78, 93, 131, 152	0
7	6E	155/156 (99%)	0.20	4 (2%) 57 36	66, 85, 109, 117	0
8	72	138/138 (100%)	0.06	0 100 100	64, 85, 96, 105	0
8	7E	138/138 (100%)	0.03	0 100 100	55, 72, 85, 97	0
9	82	127/128 (99%)	0.32	1 (0%) 82 65	78, 115, 132, 137	0
9	8E	127/128 (99%)	0.30	2 (1%) 70 49	57, 102, 119, 123	0
10	1A	99/105 (94%)	0.68	3 (3%) 52 31	86, 123, 142, 144	0
10	1I	99/105 (94%)	0.78	6 (6%) 27 15	52, 105, 131, 135	0
11	2A	117/129 (90%)	0.12	1 (0%) 81 63	50, 77, 104, 140	0
11	2I	116/129 (89%)	-0.06	0 100 100	42, 69, 94, 119	0
12	3A	124/132 (93%)	0.07	2 (1%) 70 49	49, 69, 95, 149	0
12	3I	124/132 (93%)	-0.10	2 (1%) 70 49	37, 47, 77, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	121/126 (96%)	0.43	6 (4%) 34 18	81, 118, 131, 141	0
13	4I	119/126 (94%)	0.50	5 (4%) 40 22	57, 92, 109, 118	0
14	5A	60/61 (98%)	0.16	0 100 100	83, 97, 121, 126	0
14	5I	60/61 (98%)	-0.05	0 100 100	61, 71, 85, 99	0
15	6A	88/89 (98%)	-0.11	0 100 100	53, 75, 94, 100	0
15	6I	88/89 (98%)	0.00	1 (1%) 78 59	44, 66, 90, 98	0
16	7A	84/88 (95%)	0.16	1 (1%) 76 58	59, 68, 86, 124	0
16	7I	83/88 (94%)	0.23	1 (1%) 76 58	63, 76, 99, 127	0
17	8A	100/105 (95%)	0.01	1 (1%) 79 61	57, 77, 94, 110	0
17	8I	100/105 (95%)	-0.09	1 (1%) 79 61	53, 69, 81, 87	0
18	9A	70/88 (79%)	0.22	1 (1%) 73 53	60, 75, 104, 126	0
18	9I	71/88 (80%)	0.14	2 (2%) 55 34	54, 69, 110, 127	0
19	AA	86/93 (92%)	0.73	8 (9%) 14 8	105, 131, 158, 170	0
19	AI	84/93 (90%)	0.70	6 (7%) 22 12	72, 96, 114, 119	0
20	BA	103/106 (97%)	0.16	2 (1%) 66 45	65, 84, 109, 116	0
20	BI	101/106 (95%)	-0.03	0 100 100	65, 83, 111, 123	0
21	1B	25/27 (92%)	0.10	0 100 100	94, 109, 123, 127	0
21	1F	24/27 (88%)	0.06	0 100 100	74, 85, 99, 110	0
22	1K	69/76 (90%)	0.60	6 (8%) 16 9	51, 163, 204, 219	0
23	2K	66/76 (86%)	-0.49	0 100 100	33, 59, 81, 131	0
24	3K	73/76 (96%)	0.81	4 (5%) 30 16	35, 200, 222, 230	0
24	3L	73/76 (96%)	0.79	6 (8%) 17 10	49, 197, 229, 238	0
25	4K	30/60 (50%)	0.36	0 100 100	43, 130, 219, 232	0
25	4L	30/60 (50%)	0.30	1 (3%) 49 29	61, 148, 218, 223	0
26	5K	68/76 (89%)	1.03	8 (11%) 9 5	80, 154, 180, 197	0
27	14	2865/2917 (98%)	-0.33	32 (1%) 78 59	27, 59, 194, 252	0
27	1H	2879/2917 (98%)	-0.60	32 (1%) 78 59	13, 37, 171, 243	0
28	16	122/122 (100%)	-0.75	1 (0%) 82 65	37, 55, 74, 146	0
28	1J	121/122 (99%)	-0.22	1 (0%) 82 65	65, 90, 118, 175	0
29	71	135/229 (58%)	1.22	19 (14%) 6 3	113, 202, 228, 236	0
29	79	135/229 (58%)	1.14	15 (11%) 10 5	131, 194, 215, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	11	272/276 (98%)	-0.36	0 100 100	14, 32, 47, 68	0
30	19	272/276 (98%)	-0.14	3 (1%) 78 59	25, 45, 61, 73	0
31	21	204/206 (99%)	-0.29	0 100 100	16, 46, 74, 97	0
31	29	204/206 (99%)	0.07	0 100 100	38, 72, 98, 111	0
32	31	202/210 (96%)	-0.25	1 (0%) 87 73	13, 42, 72, 99	0
32	39	202/210 (96%)	0.47	11 (5%) 31 17	30, 64, 95, 109	0
33	41	181/182 (99%)	0.23	4 (2%) 62 41	50, 66, 95, 111	0
33	49	181/182 (99%)	0.34	2 (1%) 78 59	82, 99, 124, 132	0
34	51	174/180 (96%)	0.47	7 (4%) 42 23	53, 76, 96, 117	0
34	59	173/180 (96%)	0.96	17 (9%) 13 7	135, 183, 220, 240	0
35	61	145/148 (97%)	0.65	9 (6%) 26 14	43, 96, 112, 126	0
35	69	146/148 (98%)	0.72	13 (8%) 15 8	52, 93, 116, 129	0
36	38	84/173 (48%)	1.60	22 (26%) 1 1	116, 159, 172, 180	0
37	15	138/140 (98%)	0.36	2 (1%) 73 53	51, 84, 109, 119	0
37	58	138/140 (98%)	0.07	5 (3%) 46 26	29, 46, 80, 92	0
38	25	122/122 (100%)	0.11	1 (0%) 82 65	43, 65, 83, 95	0
38	68	122/122 (100%)	-0.42	0 100 100	21, 40, 54, 64	0
39	35	150/150 (100%)	0.44	7 (4%) 36 19	35, 77, 106, 122	0
39	78	150/150 (100%)	-0.05	2 (1%) 75 56	19, 46, 81, 121	0
40	45	141/141 (100%)	0.18	2 (1%) 73 53	47, 85, 114, 163	0
40	88	141/141 (100%)	-0.02	5 (3%) 47 27	25, 44, 67, 91	5 (3%)
41	55	118/118 (100%)	-0.23	0 100 100	38, 57, 78, 93	0
41	98	118/118 (100%)	-0.31	0 100 100	24, 42, 61, 73	0
42	65	111/112 (99%)	0.53	3 (2%) 56 35	63, 89, 122, 132	0
42	A8	112/112 (100%)	0.13	3 (2%) 56 35	41, 55, 75, 94	0
43	75	137/146 (93%)	0.40	7 (5%) 33 18	57, 73, 145, 164	0
43	B8	137/146 (93%)	-0.12	0 100 100	32, 53, 104, 138	0
44	85	117/118 (99%)	0.46	6 (5%) 33 18	41, 78, 120, 134	0
44	C8	117/118 (99%)	-0.21	3 (2%) 57 36	20, 36, 63, 93	0
45	95	101/101 (100%)	1.07	10 (9%) 13 7	41, 94, 109, 125	0
45	D8	101/101 (100%)	0.13	2 (1%) 65 44	23, 57, 73, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	A5	113/113 (100%)	0.24	4 (3%) 47 27	37, 50, 93, 124	0
46	E8	113/113 (100%)	-0.17	3 (2%) 56 35	25, 35, 63, 104	0
47	B5	94/96 (97%)	0.11	3 (3%) 50 30	40, 58, 79, 106	0
47	F8	95/96 (98%)	-0.22	0 100 100	23, 36, 54, 74	0
48	C5	107/110 (97%)	1.41	27 (25%) 1 1	61, 81, 130, 140	0
48	G8	109/110 (99%)	0.60	11 (10%) 12 6	44, 71, 118, 137	0
49	D5	176/206 (85%)	0.62	4 (2%) 61 39	89, 130, 206, 210	0
49	H8	179/206 (86%)	0.72	13 (7%) 21 11	47, 85, 160, 171	0
50	E5	84/85 (98%)	0.06	3 (3%) 46 26	44, 65, 88, 110	0
50	I8	84/85 (98%)	-0.18	0 100 100	21, 38, 63, 81	0
51	F5	97/98 (98%)	0.50	11 (11%) 10 5	37, 57, 98, 111	0
51	J8	97/98 (98%)	0.02	5 (5%) 33 17	20, 41, 88, 114	0
52	G5	71/72 (98%)	0.43	3 (4%) 40 22	49, 69, 96, 122	0
52	K8	72/72 (100%)	0.14	6 (8%) 17 9	30, 47, 64, 82	0
53	H5	59/60 (98%)	0.35	2 (3%) 48 28	57, 76, 119, 122	0
53	L8	59/60 (98%)	-0.29	0 100 100	30, 44, 74, 93	0
54	I5	71/71 (100%)	0.88	5 (7%) 22 12	104, 142, 169, 174	0
54	M8	71/71 (100%)	1.32	14 (19%) 3 1	72, 115, 152, 158	0
55	J5	56/60 (93%)	0.44	4 (7%) 22 12	35, 63, 121, 129	0
55	N8	56/60 (93%)	0.11	3 (5%) 31 17	18, 47, 108, 114	0
56	K5	45/54 (83%)	1.46	9 (20%) 3 1	103, 136, 163, 169	0
56	O8	45/54 (83%)	1.48	14 (31%) 1 1	73, 103, 134, 144	0
57	L5	49/49 (100%)	-0.17	1 (2%) 65 44	28, 35, 77, 88	0
57	P8	49/49 (100%)	-0.51	0 100 100	15, 20, 50, 71	0
58	M5	64/65 (98%)	-0.03	1 (1%) 70 49	41, 51, 76, 94	0
58	Q8	64/65 (98%)	-0.48	0 100 100	21, 31, 41, 62	0
59	1L	72/76 (94%)	0.14	2 (2%) 55 34	80, 196, 235, 239	0
60	2L	67/76 (88%)	-0.43	0 100 100	52, 82, 113, 145	0
All	All	21491/22459 (95%)	-0.01	576 (2%) 56 35	13, 69, 169, 252	5 (0%)

The worst 5 of 576 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	14	2797	U	6.8
32	39	133	ASN	6.5
45	95	36	PRO	6.4
27	14	2900	A	5.4
48	C5	61	ILE	5.1

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, 95th 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 ²)	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 oligosaccharides 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, 95th 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	0.11	0.62	55,55,55,55	1
62	MG	1H	3343[B]	1/1	0.11	0.62	68,68,68,68	1
62	MG	1G	1674	1/1	0.47	0.30	122,122,122,122	0
61	K	14	3053	1/1	0.55	0.19	102,102,102,102	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
62	MG	14	3175[A]	1/1	0.56	0.43	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	14	3175[B]	1/1	0.56	0.43	36,36,36,36	1
62	MG	14	3260	1/1	0.60	0.31	84,84,84,84	0
62	MG	13	1709[A]	1/1	0.63	0.45	40,40,40,40	1
62	MG	13	1709[B]	1/1	0.63	0.45	45,45,45,45	1
61	K	49	201	1/1	0.67	0.12	108,108,108,108	0
61	K	13	1611	1/1	0.69	0.19	114,114,114,114	0
61	K	14	3012	1/1	0.70	0.18	117,117,117,117	0
62	MG	13	1674	1/1	0.70	0.21	75,75,75,75	0
61	K	32	301	1/1	0.70	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	3040[B]	1/1	0.71	0.26	43,43,43,43	1
61	K	1G	1601	1/1	0.71	0.22	115,115,115,115	0
61	K	1H	3142	1/1	0.72	0.16	78,78,78,78	0
61	K	14	3004	1/1	0.72	0.12	81,81,81,81	0
62	MG	14	3257	1/1	0.74	0.31	65,65,65,65	0
61	K	13	1620	1/1	0.74	0.12	87,87,87,87	0
61	K	14	3067	1/1	0.75	0.17	70,70,70,70	0
62	MG	14	3249	1/1	0.75	0.18	62,62,62,62	0
62	MG	16	210	1/1	0.76	0.22	62,62,62,62	0
61	K	13	1648	1/1	0.76	0.10	71,71,71,71	0
62	MG	13	1698	1/1	0.76	0.29	84,84,84,84	0
62	MG	14	3125	1/1	0.77	0.23	60,60,60,60	0
62	MG	13	1721	1/1	0.77	0.21	99,99,99,99	0
62	MG	14	3124	1/1	0.77	0.13	58,58,58,58	0
61	K	39	302	1/1	0.78	0.09	74,74,74,74	0
62	MG	1G	1689	1/1	0.78	0.16	57,57,57,57	0
61	K	14	3062	1/1	0.78	0.14	76,76,76,76	0
61	K	14	3088	1/1	0.78	0.14	98,98,98,98	0
62	MG	14	3136	1/1	0.78	0.23	59,59,59,59	0
61	K	1G	1631	1/1	0.79	0.16	86,86,86,86	0
62	MG	1G	1668	1/1	0.79	0.24	69,69,69,69	0
62	MG	13	1720	1/1	0.79	0.26	64,64,64,64	0
62	MG	13	1684	1/1	0.79	0.27	73,73,73,73	0
61	K	BI	201	1/1	0.79	0.13	108,108,108,108	0
61	K	14	3013	1/1	0.79	0.21	84,84,84,84	0
62	MG	16	208	1/1	0.79	0.13	44,44,44,44	0
61	K	1G	1632	1/1	0.80	0.09	78,78,78,78	0
61	K	5E	201	1/1	0.80	0.12	76,76,76,76	0
62	MG	1G	1661	1/1	0.80	0.31	79,79,79,79	0
62	MG	14	3195	1/1	0.80	0.25	53,53,53,53	0
62	MG	1G	1690	1/1	0.80	0.33	74,74,74,74	0
62	MG	13	1706	1/1	0.80	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1H	3359	1/1	0.80	0.26	62,62,62,62	0
61	K	13	1608	1/1	0.81	0.11	89,89,89,89	0
61	K	2K	103	1/1	0.81	0.09	79,79,79,79	0
62	MG	1G	1679	1/1	0.81	0.18	62,62,62,62	0
61	K	1H	3020	1/1	0.81	0.10	65,65,65,65	0
62	MG	14	3182	1/1	0.81	0.21	62,62,62,62	0
62	MG	1H	3381	1/1	0.81	0.17	39,39,39,39	0
62	MG	1H	3176[A]	1/1	0.81	0.26	21,21,21,21	1
62	MG	1H	3176[B]	1/1	0.81	0.26	20,20,20,20	1
62	MG	1H	3211	1/1	0.81	0.18	56,56,56,56	0
61	K	1H	3027	1/1	0.82	0.09	63,63,63,63	0
62	MG	14	3228	1/1	0.82	0.16	58,58,58,58	0
62	MG	14	3244	1/1	0.82	0.17	64,64,64,64	0
62	MG	1G	1650	1/1	0.82	0.24	68,68,68,68	0
61	K	1G	1622	1/1	0.82	0.08	74,74,74,74	0
61	K	14	3092	1/1	0.82	0.16	106,106,106,106	0
61	K	13	1625	1/1	0.83	0.09	77,77,77,77	0
61	K	13	1615	1/1	0.83	0.10	90,90,90,90	0
61	K	14	3097	1/1	0.83	0.11	91,91,91,91	0
62	MG	1H	3325	1/1	0.83	0.23	50,50,50,50	0
61	K	29	301	1/1	0.83	0.09	86,86,86,86	0
61	K	13	1610	1/1	0.83	0.09	103,103,103,103	0
61	K	1H	3131	1/1	0.83	0.10	63,63,63,63	0
62	MG	14	3199	1/1	0.83	0.25	66,66,66,66	0
62	MG	1H	3363	1/1	0.83	0.12	56,56,56,56	0
62	MG	1G	1688	1/1	0.83	0.16	65,65,65,65	0
61	K	14	3070	1/1	0.83	0.08	92,92,92,92	0
62	MG	7I	101	1/1	0.83	0.24	71,71,71,71	0
62	MG	4L	101	1/1	0.83	0.20	79,79,79,79	0
62	MG	14	3174	1/1	0.84	0.19	38,38,38,38	0
61	K	1G	1623	1/1	0.84	0.09	95,95,95,95	0
61	K	1G	1627	1/1	0.84	0.15	92,92,92,92	0
62	MG	14	3176	1/1	0.84	0.28	69,69,69,69	0
62	MG	13	1702	1/1	0.84	0.20	60,60,60,60	0
62	MG	14	3185	1/1	0.84	0.23	51,51,51,51	0
61	K	14	3006	1/1	0.84	0.11	106,106,106,106	0
61	K	1G	1604	1/1	0.84	0.08	91,91,91,91	0
61	K	14	3072	1/1	0.84	0.09	85,85,85,85	0
62	MG	13	1672	1/1	0.84	0.22	49,49,49,49	0
62	MG	1H	3351	1/1	0.84	0.25	79,79,79,79	0
61	K	1H	3038	1/1	0.84	0.14	56,56,56,56	0
62	MG	14	3171	1/1	0.84	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	14	3276	1/1	0.84	0.19	52,52,52,52	0
62	MG	14	3336	1/1	0.84	0.11	78,78,78,78	0
62	MG	13	1703	1/1	0.85	0.16	49,49,49,49	0
61	K	1G	1607	1/1	0.85	0.14	87,87,87,87	0
61	K	1G	1616	1/1	0.85	0.10	86,86,86,86	0
61	K	1H	3022	1/1	0.85	0.08	66,66,66,66	0
62	MG	14	3164	1/1	0.85	0.14	48,48,48,48	0
62	MG	1H	3360	1/1	0.85	0.09	28,28,28,28	0
62	MG	14	3173	1/1	0.85	0.24	66,66,66,66	0
62	MG	13	1719	1/1	0.85	0.30	63,63,63,63	0
61	K	14	3014	1/1	0.85	0.17	80,80,80,80	0
61	K	1H	3026	1/1	0.85	0.14	88,88,88,88	0
61	K	1H	3140	1/1	0.85	0.08	62,62,62,62	0
62	MG	1H	3174	1/1	0.85	0.31	60,60,60,60	0
61	K	13	1646	1/1	0.85	0.14	63,63,63,63	0
62	MG	14	3187	1/1	0.85	0.22	51,51,51,51	0
61	K	1H	3005	1/1	0.85	0.12	100,100,100,100	0
61	K	1G	1602	1/1	0.85	0.20	104,104,104,104	0
62	MG	1H	3259	1/1	0.85	0.14	46,46,46,46	0
62	MG	1H	3269	1/1	0.85	0.11	33,33,33,33	0
62	MG	14	3245	1/1	0.85	0.19	36,36,36,36	0
62	MG	1H	3272	1/1	0.85	0.28	55,55,55,55	0
62	MG	1G	1684	1/1	0.85	0.14	79,79,79,79	0
62	MG	1H	3287	1/1	0.85	0.14	37,37,37,37	0
61	K	13	1606	1/1	0.85	0.20	57,57,57,57	0
62	MG	1H	3329	1/1	0.85	0.24	63,63,63,63	0
62	MG	O8	101	1/1	0.86	0.21	60,60,60,60	0
62	MG	1G	1641	1/1	0.86	0.27	64,64,64,64	0
62	MG	1G	1646	1/1	0.86	0.14	66,66,66,66	0
61	K	14	3003	1/1	0.86	0.13	100,100,100,100	0
62	MG	1H	3278	1/1	0.86	0.13	28,28,28,28	0
62	MG	1H	3279	1/1	0.86	0.13	32,32,32,32	0
61	K	14	3077	1/1	0.86	0.11	73,73,73,73	0
62	MG	1G	1678	1/1	0.86	0.26	54,54,54,54	0
61	K	14	3082	1/1	0.86	0.10	80,80,80,80	0
62	MG	13	1680	1/1	0.86	0.20	49,49,49,49	0
61	K	14	3034	1/1	0.86	0.12	86,86,86,86	0
62	MG	1H	3155[A]	1/1	0.86	0.42	19,19,19,19	1
62	MG	14	3214	1/1	0.86	0.24	66,66,66,66	0
62	MG	14	3221	1/1	0.86	0.10	52,52,52,52	0
62	MG	14	3224	1/1	0.86	0.08	36,36,36,36	0
62	MG	1H	3155[B]	1/1	0.86	0.42	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	13	1694	1/1	0.86	0.24	57,57,57,57	0
61	K	1H	3036	1/1	0.86	0.12	60,60,60,60	0
61	K	1H	3126	1/1	0.86	0.11	86,86,86,86	0
61	K	14	3105	1/1	0.86	0.12	91,91,91,91	0
61	K	13	1649	1/1	0.86	0.08	81,81,81,81	0
61	K	13	1651	1/1	0.86	0.11	81,81,81,81	0
62	MG	14	3158	1/1	0.86	0.24	49,49,49,49	0
61	K	14	3083	1/1	0.87	0.13	70,70,70,70	0
62	MG	1G	1640	1/1	0.87	0.28	51,51,51,51	0
62	MG	1H	3286	1/1	0.87	0.28	48,48,48,48	0
61	K	1H	3044	1/1	0.87	0.12	92,92,92,92	0
62	MG	1G	1649	1/1	0.87	0.26	74,74,74,74	0
62	MG	1H	3316	1/1	0.87	0.14	60,60,60,60	0
61	K	14	3064	1/1	0.87	0.10	87,87,87,87	0
62	MG	1G	1663[A]	1/1	0.87	0.45	29,29,29,29	1
62	MG	1G	1663[B]	1/1	0.87	0.45	30,30,30,30	1
61	K	14	3065	1/1	0.87	0.14	55,55,55,55	0
62	MG	1G	1672	1/1	0.87	0.24	66,66,66,66	0
62	MG	14	3186	1/1	0.87	0.23	49,49,49,49	0
62	MG	1H	3339	1/1	0.87	0.18	55,55,55,55	0
61	K	14	3102	1/1	0.87	0.13	76,76,76,76	0
61	K	13	1650	1/1	0.87	0.13	97,97,97,97	0
62	MG	1G	1680	1/1	0.87	0.17	50,50,50,50	0
62	MG	14	3215	1/1	0.87	0.14	45,45,45,45	0
61	K	1H	3128	1/1	0.87	0.10	64,64,64,64	0
62	MG	1H	3355	1/1	0.87	0.08	57,57,57,57	0
61	K	13	1631	1/1	0.87	0.09	58,58,58,58	0
62	MG	1G	1686	1/1	0.87	0.28	75,75,75,75	0
62	MG	13	1707	1/1	0.87	0.20	58,58,58,58	0
62	MG	14	3248	1/1	0.87	0.37	60,60,60,60	0
61	K	14	3039	1/1	0.87	0.10	61,61,61,61	0
62	MG	14	3256	1/1	0.87	0.19	67,67,67,67	0
62	MG	1H	3369	1/1	0.87	0.18	46,46,46,46	0
62	MG	13	1662	1/1	0.87	0.21	54,54,54,54	0
62	MG	14	3268	1/1	0.87	0.13	36,36,36,36	0
62	MG	13	1718	1/1	0.87	0.24	55,55,55,55	0
61	K	14	3010	1/1	0.87	0.07	58,58,58,58	0
62	MG	13	1696	1/1	0.88	0.25	64,64,64,64	0
62	MG	14	3119	1/1	0.88	0.17	49,49,49,49	0
62	MG	14	3120	1/1	0.88	0.15	44,44,44,44	0
61	K	14	3038	1/1	0.88	0.08	92,92,92,92	0
62	MG	1H	3187	1/1	0.88	0.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	1H	3041	1/1	0.88	0.11	68,68,68,68	0
62	MG	1H	3245	1/1	0.88	0.17	50,50,50,50	0
61	K	14	3042	1/1	0.88	0.08	51,51,51,51	0
62	MG	31	303	1/1	0.88	0.17	37,37,37,37	0
61	K	14	3052	1/1	0.88	0.10	76,76,76,76	0
61	K	13	1607	1/1	0.88	0.06	65,65,65,65	0
62	MG	1H	3275	1/1	0.88	0.25	44,44,44,44	0
61	K	1H	3088	1/1	0.88	0.08	50,50,50,50	0
61	K	1H	3105	1/1	0.88	0.08	50,50,50,50	0
62	MG	14	3181	1/1	0.88	0.18	49,49,49,49	0
62	MG	1H	3281	1/1	0.88	0.21	49,49,49,49	0
62	MG	1G	1653	1/1	0.88	0.12	53,53,53,53	0
62	MG	1G	1654	1/1	0.88	0.25	50,50,50,50	0
62	MG	13	1710	1/1	0.88	0.20	52,52,52,52	0
61	K	1H	3125	1/1	0.88	0.12	64,64,64,64	0
62	MG	1H	3305	1/1	0.88	0.22	41,41,41,41	0
62	MG	13	1654	1/1	0.88	0.17	42,42,42,42	0
62	MG	1G	1670	1/1	0.88	0.20	57,57,57,57	0
61	K	13	1603	1/1	0.88	0.07	75,75,75,75	0
62	MG	1H	3326	1/1	0.88	0.22	60,60,60,60	0
62	MG	1H	3327	1/1	0.88	0.08	40,40,40,40	0
62	MG	14	3234	1/1	0.88	0.25	55,55,55,55	0
62	MG	14	3242	1/1	0.88	0.28	65,65,65,65	0
62	MG	1H	3328[A]	1/1	0.88	0.43	22,22,22,22	1
62	MG	1H	3328[B]	1/1	0.88	0.43	27,27,27,27	1
61	K	13	1635	1/1	0.88	0.12	95,95,95,95	0
62	MG	6E	201	1/1	0.88	0.23	62,62,62,62	0
62	MG	14	3251	1/1	0.88	0.15	45,45,45,45	0
61	K	1H	3023	1/1	0.88	0.08	63,63,63,63	0
62	MG	1H	3149	1/1	0.88	0.23	40,40,40,40	0
61	K	1H	3138	1/1	0.88	0.12	62,62,62,62	0
61	K	14	3017	1/1	0.88	0.16	52,52,52,52	0
62	MG	14	3270	1/1	0.88	0.19	66,66,66,66	0
61	K	13	1641	1/1	0.88	0.07	84,84,84,84	0
62	MG	42	201	1/1	0.88	0.20	70,70,70,70	0
62	MG	1J	202	1/1	0.88	0.10	83,83,83,83	0
62	MG	1H	3315	1/1	0.89	0.15	43,43,43,43	0
62	MG	13	1708	1/1	0.89	0.23	60,60,60,60	0
62	MG	14	3153	1/1	0.89	0.18	51,51,51,51	0
62	MG	14	3155	1/1	0.89	0.15	38,38,38,38	0
62	MG	1G	1643	1/1	0.89	0.20	62,62,62,62	0
62	MG	14	3161	1/1	0.89	0.12	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	3320[A]	1/1	0.89	0.22	8,8,8,8	1
62	MG	14	3170	1/1	0.89	0.20	54,54,54,54	0
62	MG	1G	1647	1/1	0.89	0.26	55,55,55,55	0
62	MG	1H	3320[B]	1/1	0.89	0.22	9,9,9,9	1
62	MG	13	1665	1/1	0.89	0.14	51,51,51,51	0
62	MG	1H	3182	1/1	0.89	0.17	49,49,49,49	0
62	MG	1H	3183	1/1	0.89	0.13	47,47,47,47	0
62	MG	1G	1655	1/1	0.89	0.13	58,58,58,58	0
61	K	14	3091	1/1	0.89	0.13	78,78,78,78	0
62	MG	1H	3199	1/1	0.89	0.17	34,34,34,34	0
61	K	14	3035	1/1	0.89	0.09	83,83,83,83	0
62	MG	1H	3213	1/1	0.89	0.09	25,25,25,25	0
62	MG	1H	3238	1/1	0.89	0.09	39,39,39,39	0
62	MG	14	3188	1/1	0.89	0.15	56,56,56,56	0
61	K	1H	3135	1/1	0.89	0.14	82,82,82,82	0
62	MG	14	3196	1/1	0.89	0.12	59,59,59,59	0
61	K	14	3101	1/1	0.89	0.07	76,76,76,76	0
62	MG	14	3207	1/1	0.89	0.29	62,62,62,62	0
62	MG	14	3213	1/1	0.89	0.17	40,40,40,40	0
62	MG	1G	1676	1/1	0.89	0.15	71,71,71,71	0
62	MG	1H	3264	1/1	0.89	0.26	55,55,55,55	0
61	K	1H	3021	1/1	0.89	0.16	78,78,78,78	0
61	K	1H	3028	1/1	0.89	0.09	87,87,87,87	0
62	MG	13	1697	1/1	0.89	0.19	45,45,45,45	0
62	MG	14	3231	1/1	0.89	0.10	39,39,39,39	0
62	MG	1H	3365	1/1	0.89	0.17	58,58,58,58	0
62	MG	14	3241	1/1	0.89	0.20	59,59,59,59	0
62	MG	1H	3367	1/1	0.89	0.10	35,35,35,35	0
61	K	1H	3045	1/1	0.89	0.11	59,59,59,59	0
62	MG	2K	104	1/1	0.89	0.25	48,48,48,48	0
62	MG	1H	3500	1/1	0.89	0.09	63,63,63,63	0
62	MG	16	205	1/1	0.89	0.22	46,46,46,46	0
62	MG	1G	1697	1/1	0.89	0.25	63,63,63,63	0
61	K	1H	3046	1/1	0.89	0.11	72,72,72,72	0
62	MG	2L	102	1/1	0.89	0.16	56,56,56,56	0
61	K	14	3020	1/1	0.89	0.07	64,64,64,64	0
62	MG	14	3109	1/1	0.89	0.17	41,41,41,41	0
61	K	14	3087	1/1	0.89	0.11	74,74,74,74	0
61	K	13	1616	1/1	0.89	0.08	75,75,75,75	0
62	MG	14	3121	1/1	0.89	0.25	47,47,47,47	0
62	MG	14	3351	1/1	0.89	0.11	55,55,55,55	0
62	MG	1G	1639	1/1	0.89	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	41	201	1/1	0.90	0.10	67,67,67,67	0
62	MG	1H	3370	1/1	0.90	0.27	61,61,61,61	0
62	MG	1H	3372	1/1	0.90	0.11	31,31,31,31	0
62	MG	1H	3254	1/1	0.90	0.10	29,29,29,29	0
62	MG	13	1714	1/1	0.90	0.32	83,83,83,83	0
62	MG	14	3133	1/1	0.90	0.17	39,39,39,39	0
62	MG	1H	3517	1/1	0.90	0.10	26,26,26,26	0
62	MG	14	3143	1/1	0.90	0.12	39,39,39,39	0
62	MG	1H	3263	1/1	0.90	0.09	36,36,36,36	0
61	K	1H	3122	1/1	0.90	0.07	65,65,65,65	0
62	MG	13	1664	1/1	0.90	0.20	57,57,57,57	0
61	K	13	1618	1/1	0.90	0.09	85,85,85,85	0
62	MG	41	202	1/1	0.90	0.12	55,55,55,55	0
62	MG	14	3165	1/1	0.90	0.13	45,45,45,45	0
61	K	14	3084	1/1	0.90	0.08	73,73,73,73	0
62	MG	P8	101	1/1	0.90	0.15	35,35,35,35	0
62	MG	13	1722	1/1	0.90	0.10	52,52,52,52	0
62	MG	13	1673	1/1	0.90	0.28	55,55,55,55	0
62	MG	1H	3280	1/1	0.90	0.16	86,86,86,86	0
61	K	14	3005	1/1	0.90	0.12	82,82,82,82	0
62	MG	13	1675	1/1	0.90	0.23	49,49,49,49	0
62	MG	1H	3147	1/1	0.90	0.17	54,54,54,54	0
62	MG	1G	1648	1/1	0.90	0.19	67,67,67,67	0
62	MG	1H	3303	1/1	0.90	0.21	46,46,46,46	0
61	K	1H	3008	1/1	0.90	0.08	65,65,65,65	0
61	K	1H	3010	1/1	0.90	0.10	66,66,66,66	0
61	K	14	3058	1/1	0.90	0.10	85,85,85,85	0
62	MG	1H	3318	1/1	0.90	0.16	56,56,56,56	0
62	MG	1H	3162	1/1	0.90	0.30	58,58,58,58	0
62	MG	1H	3163	1/1	0.90	0.26	55,55,55,55	0
62	MG	1H	3321	1/1	0.90	0.11	36,36,36,36	0
62	MG	14	3209	1/1	0.90	0.12	53,53,53,53	0
62	MG	1G	1667	1/1	0.90	0.22	42,42,42,42	0
62	MG	1H	3164	1/1	0.90	0.08	58,58,58,58	0
62	MG	1H	3165	1/1	0.90	0.11	40,40,40,40	0
61	K	14	3093	1/1	0.90	0.07	53,53,53,53	0
61	K	14	3094	1/1	0.90	0.09	86,86,86,86	0
61	K	1H	3072	1/1	0.90	0.11	53,53,53,53	0
61	K	1H	3132	1/1	0.90	0.10	87,87,87,87	0
62	MG	14	3233	1/1	0.90	0.22	52,52,52,52	0
62	MG	1H	3332	1/1	0.90	0.20	48,48,48,48	0
62	MG	14	3235	1/1	0.90	0.17	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	14	3239	1/1	0.90	0.25	66,66,66,66	0
61	K	13	1613	1/1	0.90	0.08	76,76,76,76	0
61	K	1H	3091	1/1	0.90	0.06	64,64,64,64	0
61	K	1H	3002	1/1	0.90	0.07	73,73,73,73	0
62	MG	1H	3201	1/1	0.90	0.13	45,45,45,45	0
62	MG	1G	1685	1/1	0.90	0.15	51,51,51,51	0
61	K	1H	3108	1/1	0.90	0.09	76,76,76,76	0
62	MG	1H	3358	1/1	0.90	0.26	41,41,41,41	0
62	MG	14	3254	1/1	0.90	0.09	62,62,62,62	0
62	MG	1H	3212	1/1	0.90	0.09	44,44,44,44	0
61	K	14	3076	1/1	0.90	0.08	86,86,86,86	0
62	MG	1G	1692	1/1	0.90	0.30	72,72,72,72	0
62	MG	1H	3361	1/1	0.90	0.25	57,57,57,57	0
62	MG	1G	1699	1/1	0.90	0.20	62,62,62,62	0
62	MG	1H	3362	1/1	0.90	0.27	64,64,64,64	0
62	MG	1H	3221	1/1	0.90	0.15	34,34,34,34	0
62	MG	1H	3236	1/1	0.90	0.20	43,43,43,43	0
62	MG	13	1653	1/1	0.90	0.20	67,67,67,67	0
62	MG	29	302	1/1	0.90	0.15	38,38,38,38	0
62	MG	13	1701	1/1	0.91	0.27	69,69,69,69	0
62	MG	1H	3319	1/1	0.91	0.21	50,50,50,50	0
61	K	1H	3047	1/1	0.91	0.13	74,74,74,74	0
61	K	52	201	1/1	0.91	0.08	76,76,76,76	0
62	MG	13	1705	1/1	0.91	0.20	56,56,56,56	0
61	K	14	3098	1/1	0.91	0.08	67,67,67,67	0
61	K	13	1645	1/1	0.91	0.12	72,72,72,72	0
62	MG	1H	3195	1/1	0.91	0.18	37,37,37,37	0
61	K	14	3061	1/1	0.91	0.12	63,63,63,63	0
62	MG	1G	1662	1/1	0.91	0.22	51,51,51,51	0
61	K	13	1636	1/1	0.91	0.09	70,70,70,70	0
61	K	1G	1605	1/1	0.91	0.05	92,92,92,92	0
62	MG	14	3184	1/1	0.91	0.19	48,48,48,48	0
62	MG	1G	1664	1/1	0.91	0.19	40,40,40,40	0
62	MG	1H	3331	1/1	0.91	0.08	54,54,54,54	0
61	K	13	1639	1/1	0.91	0.06	66,66,66,66	0
62	MG	13	1711	1/1	0.91	0.25	55,55,55,55	0
62	MG	14	3194	1/1	0.91	0.17	54,54,54,54	0
62	MG	1H	3220	1/1	0.91	0.27	50,50,50,50	0
62	MG	13	1712	1/1	0.91	0.17	43,43,43,43	0
61	K	1G	1608	1/1	0.91	0.06	80,80,80,80	0
62	MG	14	3201	1/1	0.91	0.19	49,49,49,49	0
61	K	1H	3096	1/1	0.91	0.12	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	1H	3242	1/1	0.91	0.09	37,37,37,37	0
61	K	14	3071	1/1	0.91	0.16	77,77,77,77	0
61	K	1G	1617	1/1	0.91	0.06	63,63,63,63	0
62	MG	1H	3258	1/1	0.91	0.31	52,52,52,52	0
61	K	1K	101	1/1	0.91	0.05	83,83,83,83	0
61	K	13	1605	1/1	0.91	0.06	81,81,81,81	0
62	MG	1H	3364	1/1	0.91	0.19	58,58,58,58	0
62	MG	14	3230	1/1	0.91	0.18	54,54,54,54	0
61	K	14	3078	1/1	0.91	0.09	81,81,81,81	0
61	K	14	3080	1/1	0.91	0.08	79,79,79,79	0
62	MG	1H	3270	1/1	0.91	0.07	42,42,42,42	0
61	K	1G	1625	1/1	0.91	0.08	108,108,108,108	0
61	K	1H	3114	1/1	0.91	0.11	55,55,55,55	0
62	MG	13	1678	1/1	0.91	0.15	38,38,38,38	0
62	MG	1H	3429	1/1	0.91	0.11	29,29,29,29	0
62	MG	1H	3153	1/1	0.91	0.10	45,45,45,45	0
61	K	1H	3115	1/1	0.91	0.09	52,52,52,52	0
61	K	13	1643	1/1	0.91	0.05	76,76,76,76	0
62	MG	1H	3282	1/1	0.91	0.11	49,49,49,49	0
62	MG	1H	3157	1/1	0.91	0.18	49,49,49,49	0
61	K	1G	1633	1/1	0.91	0.07	76,76,76,76	0
62	MG	14	3255	1/1	0.91	0.09	63,63,63,63	0
62	MG	1H	3290	1/1	0.91	0.11	38,38,38,38	0
62	MG	1H	3297	1/1	0.91	0.12	40,40,40,40	0
62	MG	1H	3298	1/1	0.91	0.07	28,28,28,28	0
62	MG	14	3264	1/1	0.91	0.15	45,45,45,45	0
62	MG	14	3267	1/1	0.91	0.07	44,44,44,44	0
62	MG	1G	1638	1/1	0.91	0.15	46,46,46,46	0
62	MG	14	3139	1/1	0.91	0.15	41,41,41,41	0
61	K	1G	1635	1/1	0.91	0.17	91,91,91,91	0
62	MG	14	3309	1/1	0.91	0.09	26,26,26,26	0
62	MG	14	3317	1/1	0.91	0.07	40,40,40,40	0
62	MG	14	3149	1/1	0.91	0.19	37,37,37,37	0
61	K	14	3045	1/1	0.91	0.10	83,83,83,83	0
61	K	14	3048	1/1	0.91	0.07	67,67,67,67	0
62	MG	1J	204	1/1	0.91	0.25	64,64,64,64	0
62	MG	1H	3171	1/1	0.91	0.17	30,30,30,30	0
61	K	1H	3011	1/1	0.92	0.06	59,59,59,59	0
61	K	14	3007	1/1	0.92	0.14	64,64,64,64	0
62	MG	14	3156	1/1	0.92	0.18	34,34,34,34	0
62	MG	1H	3323	1/1	0.92	0.22	52,52,52,52	0
62	MG	14	3159	1/1	0.92	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1G	1644	1/1	0.92	0.12	59,59,59,59	0
62	MG	1H	3202	1/1	0.92	0.18	45,45,45,45	0
62	MG	1H	3207	1/1	0.92	0.18	38,38,38,38	0
61	K	14	3009	1/1	0.92	0.12	64,64,64,64	0
61	K	1H	3050	1/1	0.92	0.14	53,53,53,53	0
61	K	45	201	1/1	0.92	0.14	90,90,90,90	0
62	MG	1G	1652	1/1	0.92	0.12	17,17,17,17	0
62	MG	13	1713	1/1	0.92	0.15	46,46,46,46	0
61	K	14	3011	1/1	0.92	0.17	80,80,80,80	0
61	K	1G	1614	1/1	0.92	0.07	86,86,86,86	0
62	MG	14	3178	1/1	0.92	0.24	53,53,53,53	0
62	MG	1G	1656	1/1	0.92	0.25	58,58,58,58	0
62	MG	1H	3338	1/1	0.92	0.09	43,43,43,43	0
61	K	1H	3051	1/1	0.92	0.10	49,49,49,49	0
61	K	1H	3029	1/1	0.92	0.09	85,85,85,85	0
61	K	1H	3080	1/1	0.92	0.07	45,45,45,45	0
62	MG	1H	3344	1/1	0.92	0.14	39,39,39,39	0
62	MG	1G	1666	1/1	0.92	0.30	46,46,46,46	0
62	MG	14	3189	1/1	0.92	0.07	50,50,50,50	0
62	MG	14	3190	1/1	0.92	0.17	77,77,77,77	0
62	MG	1H	3346	1/1	0.92	0.16	55,55,55,55	0
62	MG	1H	3349	1/1	0.92	0.17	48,48,48,48	0
62	MG	1H	3350	1/1	0.92	0.16	25,25,25,25	0
62	MG	14	3197	1/1	0.92	0.16	48,48,48,48	0
62	MG	1H	3246	1/1	0.92	0.18	35,35,35,35	0
62	MG	1H	3353	1/1	0.92	0.15	33,33,33,33	0
62	MG	14	3204	1/1	0.92	0.19	38,38,38,38	0
61	K	14	3018	1/1	0.92	0.07	65,65,65,65	0
62	MG	14	3208	1/1	0.92	0.20	58,58,58,58	0
62	MG	1G	1677	1/1	0.92	0.20	57,57,57,57	0
62	MG	14	3212	1/1	0.92	0.22	44,44,44,44	0
62	MG	13	1726	1/1	0.92	0.14	46,46,46,46	0
61	K	14	3079	1/1	0.92	0.13	81,81,81,81	0
61	K	1H	3013	1/1	0.92	0.15	81,81,81,81	0
62	MG	1G	1681	1/1	0.92	0.19	45,45,45,45	0
62	MG	14	3222	1/1	0.92	0.19	57,57,57,57	0
61	K	1H	3016	1/1	0.92	0.06	63,63,63,63	0
62	MG	14	3225	1/1	0.92	0.08	47,47,47,47	0
61	K	13	1647	1/1	0.92	0.05	50,50,50,50	0
61	K	1H	3141	1/1	0.92	0.10	41,41,41,41	0
61	K	1H	3003	1/1	0.92	0.05	56,56,56,56	0
62	MG	1H	3154	1/1	0.92	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1G	1687	1/1	0.92	0.16	67,67,67,67	0
62	MG	13	1690	1/1	0.92	0.06	51,51,51,51	0
62	MG	14	3236	1/1	0.92	0.23	50,50,50,50	0
62	MG	1H	3368	1/1	0.92	0.25	44,44,44,44	0
62	MG	13	1692	1/1	0.92	0.17	51,51,51,51	0
62	MG	1G	1691	1/1	0.92	0.23	64,64,64,64	0
62	MG	13	1693	1/1	0.92	0.26	61,61,61,61	0
62	MG	1G	1696	1/1	0.92	0.28	52,52,52,52	0
61	K	14	3041	1/1	0.92	0.09	66,66,66,66	0
62	MG	13	1695	1/1	0.92	0.13	66,66,66,66	0
61	K	1H	3144	1/1	0.92	0.17	56,56,56,56	0
62	MG	2L	101	1/1	0.92	0.10	58,58,58,58	0
61	K	14	3043	1/1	0.92	0.09	80,80,80,80	0
61	K	16	202	1/1	0.92	0.06	74,74,74,74	0
62	MG	14	3107	1/1	0.92	0.15	33,33,33,33	0
62	MG	14	3259	1/1	0.92	0.24	42,42,42,42	0
61	K	1H	3004	1/1	0.92	0.11	88,88,88,88	0
62	MG	14	3115	1/1	0.92	0.12	42,42,42,42	0
61	K	14	3096	1/1	0.92	0.06	70,70,70,70	0
62	MG	16	209	1/1	0.92	0.35	59,59,59,59	0
61	K	1H	3110	1/1	0.92	0.06	60,60,60,60	0
62	MG	14	3271	1/1	0.92	0.19	51,51,51,51	0
62	MG	14	3275	1/1	0.92	0.15	42,42,42,42	0
61	K	13	1642	1/1	0.92	0.10	93,93,93,93	0
61	K	2K	101	1/1	0.92	0.16	62,62,62,62	0
62	MG	14	3132	1/1	0.92	0.22	53,53,53,53	0
62	MG	78	201	1/1	0.92	0.11	38,38,38,38	0
62	MG	1H	3186	1/1	0.92	0.28	55,55,55,55	0
61	K	13	1614	1/1	0.92	0.16	71,71,71,71	0
61	K	14	3104	1/1	0.92	0.10	75,75,75,75	0
62	MG	1H	3196	1/1	0.92	0.15	40,40,40,40	0
62	MG	39	303	1/1	0.92	0.12	54,54,54,54	0
62	MG	13	1671	1/1	0.93	0.26	49,49,49,49	0
62	MG	1H	3244	1/1	0.93	0.24	34,34,34,34	0
61	K	1H	3025	1/1	0.93	0.08	53,53,53,53	0
62	MG	14	3191	1/1	0.93	0.07	34,34,34,34	0
61	K	13	1638	1/1	0.93	0.06	56,56,56,56	0
61	K	1G	1611	1/1	0.93	0.11	86,86,86,86	0
61	K	1H	3031	1/1	0.93	0.10	39,39,39,39	0
62	MG	13	1677	1/1	0.93	0.11	42,42,42,42	0
61	K	14	3103	1/1	0.93	0.10	70,70,70,70	0
62	MG	13	1679	1/1	0.93	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	14	3202	1/1	0.93	0.17	42,42,42,42	0
62	MG	1G	1736	1/1	0.93	0.08	62,62,62,62	0
62	MG	1H	3334	1/1	0.93	0.07	43,43,43,43	0
62	MG	1H	3266	1/1	0.93	0.07	39,39,39,39	0
61	K	1H	3098	1/1	0.93	0.07	41,41,41,41	0
62	MG	1G	1642	1/1	0.93	0.14	45,45,45,45	0
62	MG	13	1681	1/1	0.93	0.23	44,44,44,44	0
61	K	14	3055	1/1	0.93	0.19	65,65,65,65	0
62	MG	1G	1645	1/1	0.93	0.12	62,62,62,62	0
62	MG	14	3118	1/1	0.93	0.26	58,58,58,58	0
62	MG	13	1685	1/1	0.93	0.20	45,45,45,45	0
62	MG	1H	3277	1/1	0.93	0.17	42,42,42,42	0
62	MG	13	1686	1/1	0.93	0.07	34,34,34,34	0
62	MG	14	3122	1/1	0.93	0.19	49,49,49,49	0
62	MG	13	1688	1/1	0.93	0.19	56,56,56,56	0
61	K	14	3106	1/1	0.93	0.20	68,68,68,68	0
62	MG	1G	1651	1/1	0.93	0.20	43,43,43,43	0
61	K	2A	201	1/1	0.93	0.06	70,70,70,70	0
61	K	1H	3032	1/1	0.93	0.06	54,54,54,54	0
62	MG	1H	3283	1/1	0.93	0.25	44,44,44,44	0
62	MG	14	3140	1/1	0.93	0.15	47,47,47,47	0
62	MG	1H	3197	1/1	0.93	0.07	30,30,30,30	0
62	MG	14	3146	1/1	0.93	0.14	49,49,49,49	0
62	MG	14	3147	1/1	0.93	0.17	40,40,40,40	0
62	MG	13	1724	1/1	0.93	0.15	43,43,43,43	0
61	K	1H	3035	1/1	0.93	0.10	52,52,52,52	0
62	MG	14	3154	1/1	0.93	0.12	50,50,50,50	0
62	MG	1H	3291	1/1	0.93	0.20	47,47,47,47	0
62	MG	1H	3294	1/1	0.93	0.19	59,59,59,59	0
62	MG	13	1749	1/1	0.93	0.08	52,52,52,52	0
61	K	13	1612	1/1	0.93	0.15	50,50,50,50	0
61	K	1H	3134	1/1	0.93	0.10	54,54,54,54	0
62	MG	14	3163	1/1	0.93	0.14	31,31,31,31	0
61	K	1H	3112	1/1	0.93	0.08	48,48,48,48	0
62	MG	1H	3313	1/1	0.93	0.07	44,44,44,44	0
62	MG	1H	3146	1/1	0.93	0.19	38,38,38,38	0
62	MG	1H	3371	1/1	0.93	0.07	31,31,31,31	0
61	K	14	3040	1/1	0.93	0.06	93,93,93,93	0
62	MG	1H	3373	1/1	0.93	0.21	43,43,43,43	0
62	MG	14	3274	1/1	0.93	0.18	54,54,54,54	0
62	MG	1H	3375	1/1	0.93	0.11	36,36,36,36	0
62	MG	1H	3376	1/1	0.93	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	14	3278	1/1	0.93	0.17	49,49,49,49	0
62	MG	13	1699	1/1	0.93	0.10	43,43,43,43	0
62	MG	1H	3228	1/1	0.93	0.20	31,31,31,31	0
62	MG	14	3332	1/1	0.93	0.07	54,54,54,54	0
62	MG	1H	3457	1/1	0.93	0.10	25,25,25,25	0
62	MG	14	3341	1/1	0.93	0.07	35,35,35,35	0
62	MG	1H	3229	1/1	0.93	0.30	43,43,43,43	0
62	MG	14	3352	1/1	0.93	0.10	63,63,63,63	0
62	MG	14	3387	1/1	0.93	0.13	45,45,45,45	0
61	K	1G	1628	1/1	0.93	0.08	76,76,76,76	0
62	MG	1H	3539	1/1	0.93	0.07	66,66,66,66	0
62	MG	1H	3577	1/1	0.93	0.08	37,37,37,37	0
61	K	1H	3086	1/1	0.93	0.05	66,66,66,66	0
61	K	1H	3095	1/1	0.94	0.07	58,58,58,58	0
61	K	13	1604	1/1	0.94	0.06	82,82,82,82	0
61	K	1G	1620	1/1	0.94	0.06	83,83,83,83	0
62	MG	1H	3273	1/1	0.94	0.25	61,61,61,61	0
61	K	1H	3137	1/1	0.94	0.09	63,63,63,63	0
62	MG	1H	3276	1/1	0.94	0.15	44,44,44,44	0
62	MG	14	3177	1/1	0.94	0.08	45,45,45,45	0
61	K	1H	3034	1/1	0.94	0.09	66,66,66,66	0
62	MG	14	3180	1/1	0.94	0.15	59,59,59,59	0
61	K	1H	3139	1/1	0.94	0.06	64,64,64,64	0
62	MG	1G	1673	1/1	0.94	0.11	50,50,50,50	0
61	K	14	3069	1/1	0.94	0.09	56,56,56,56	0
61	K	1H	3099	1/1	0.94	0.12	59,59,59,59	0
62	MG	13	1652	1/1	0.94	0.13	43,43,43,43	0
61	K	13	1627	1/1	0.94	0.04	46,46,46,46	0
61	K	1H	3014	1/1	0.94	0.07	60,60,60,60	0
61	K	14	3024	1/1	0.94	0.08	52,52,52,52	0
61	K	14	3025	1/1	0.94	0.07	50,50,50,50	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	3292	1/1	0.94	0.04	32,32,32,32	0
62	MG	1H	3399	1/1	0.94	0.09	24,24,24,24	0
62	MG	1H	3192	1/1	0.94	0.10	37,37,37,37	0
62	MG	1H	3437	1/1	0.94	0.08	51,51,51,51	0
62	MG	1H	3453	1/1	0.94	0.07	20,20,20,20	0
61	K	1H	3037	1/1	0.94	0.15	70,70,70,70	0
62	MG	1H	3488	1/1	0.94	0.10	35,35,35,35	0
62	MG	13	1669	1/1	0.94	0.13	34,34,34,34	0
61	K	1H	3064	1/1	0.94	0.06	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	1695	1/1	0.94	0.15	72,72,72,72	0
61	K	13	1621	1/1	0.94	0.08	61,61,61,61	0
62	MG	1H	3564	1/1	0.94	0.07	25,25,25,25	0
62	MG	1G	1698	1/1	0.94	0.29	66,66,66,66	0
61	K	1G	1636	1/1	0.94	0.11	78,78,78,78	0
62	MG	14	3217	1/1	0.94	0.13	69,69,69,69	0
62	MG	1G	1718	1/1	0.94	0.08	39,39,39,39	0
62	MG	16	204	1/1	0.94	0.18	39,39,39,39	0
62	MG	14	3223	1/1	0.94	0.15	40,40,40,40	0
61	K	1H	3073	1/1	0.94	0.10	56,56,56,56	0
62	MG	16	207	1/1	0.94	0.15	43,43,43,43	0
62	MG	14	3226	1/1	0.94	0.26	55,55,55,55	0
62	MG	1H	3203	1/1	0.94	0.10	26,26,26,26	0
61	K	1H	3121	1/1	0.94	0.10	62,62,62,62	0
62	MG	13	1676	1/1	0.94	0.22	53,53,53,53	0
62	MG	14	3232	1/1	0.94	0.26	63,63,63,63	0
62	MG	14	3108	1/1	0.94	0.16	59,59,59,59	0
61	K	1H	3017	1/1	0.94	0.14	56,56,56,56	0
62	MG	14	3112	1/1	0.94	0.07	44,44,44,44	0
62	MG	14	3114	1/1	0.94	0.07	33,33,33,33	0
62	MG	14	3237	1/1	0.94	0.05	96,96,96,96	0
61	K	BA	201	1/1	0.94	0.07	72,72,72,72	0
62	MG	14	3117	1/1	0.94	0.07	49,49,49,49	0
62	MG	1H	3214	1/1	0.94	0.21	41,41,41,41	0
62	MG	14	3243	1/1	0.94	0.16	54,54,54,54	0
62	MG	C8	201	1/1	0.94	0.12	44,44,44,44	0
61	K	14	3044	1/1	0.94	0.11	69,69,69,69	0
62	MG	14	3247	1/1	0.94	0.10	47,47,47,47	0
62	MG	13	1723	1/1	0.94	0.26	60,60,60,60	0
62	MG	1H	3225	1/1	0.94	0.12	37,37,37,37	0
61	K	1H	3081	1/1	0.94	0.09	49,49,49,49	0
61	K	14	3047	1/1	0.94	0.08	74,74,74,74	0
62	MG	14	3131	1/1	0.94	0.14	43,43,43,43	0
62	MG	1H	3233	1/1	0.94	0.11	51,51,51,51	0
62	MG	1H	3234	1/1	0.94	0.21	39,39,39,39	0
62	MG	14	3135	1/1	0.94	0.16	47,47,47,47	0
62	MG	13	1682	1/1	0.94	0.16	33,33,33,33	0
61	K	1H	3082	1/1	0.94	0.05	46,46,46,46	0
61	K	14	3050	1/1	0.94	0.05	63,63,63,63	0
62	MG	1H	3336	1/1	0.94	0.25	45,45,45,45	0
61	K	14	3051	1/1	0.94	0.05	65,65,65,65	0
62	MG	13	1687	1/1	0.94	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	14	3273	1/1	0.94	0.17	37,37,37,37	0
61	K	1H	3018	1/1	0.94	0.19	51,51,51,51	0
62	MG	1H	3248	1/1	0.94	0.19	34,34,34,34	0
62	MG	1H	3252	1/1	0.94	0.26	42,42,42,42	0
62	MG	14	3277	1/1	0.94	0.27	61,61,61,61	0
61	K	14	3099	1/1	0.94	0.05	67,67,67,67	0
62	MG	14	3289	1/1	0.94	0.09	51,51,51,51	0
62	MG	1H	3151	1/1	0.94	0.19	41,41,41,41	0
62	MG	14	3157	1/1	0.94	0.15	34,34,34,34	0
62	MG	13	1691	1/1	0.94	0.20	50,50,50,50	0
61	K	14	3100	1/1	0.94	0.06	71,71,71,71	0
61	K	1H	3009	1/1	0.94	0.08	64,64,64,64	0
62	MG	1G	1658	1/1	0.94	0.22	46,46,46,46	0
62	MG	1G	1659	1/1	0.94	0.29	64,64,64,64	0
62	MG	14	3360	1/1	0.94	0.10	37,37,37,37	0
61	K	13	1623	1/1	0.94	0.05	56,56,56,56	0
62	MG	14	3397	1/1	0.94	0.09	75,75,75,75	0
62	MG	14	3399	1/1	0.94	0.06	106,106,106,106	0
62	MG	14	3166	1/1	0.94	0.10	58,58,58,58	0
62	MG	14	3167	1/1	0.94	0.15	38,38,38,38	0
62	MG	14	3168	1/1	0.94	0.16	37,37,37,37	0
62	MG	1H	3356	1/1	0.94	0.14	43,43,43,43	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	3304	1/1	0.95	0.17	38,38,38,38	0
62	MG	14	3162	1/1	0.95	0.10	46,46,46,46	0
61	K	1H	3133	1/1	0.95	0.09	61,61,61,61	0
62	MG	1H	3311	1/1	0.95	0.11	47,47,47,47	0
62	MG	1H	3312	1/1	0.95	0.18	39,39,39,39	0
61	K	1H	3094	1/1	0.95	0.07	51,51,51,51	0
62	MG	1H	3314	1/1	0.95	0.13	41,41,41,41	0
62	MG	1H	3193	1/1	0.95	0.12	40,40,40,40	0
61	K	14	3066	1/1	0.95	0.04	64,64,64,64	0
61	K	1H	3048	1/1	0.95	0.06	72,72,72,72	0
62	MG	14	3172	1/1	0.95	0.17	26,26,26,26	0
62	MG	13	1657	1/1	0.95	0.20	38,38,38,38	0
62	MG	13	1659	1/1	0.95	0.10	56,56,56,56	0
61	K	14	3015	1/1	0.95	0.05	47,47,47,47	0
62	MG	13	1663	1/1	0.95	0.14	47,47,47,47	0
62	MG	1H	3322	1/1	0.95	0.08	23,23,23,23	0
61	K	1H	3049	1/1	0.95	0.11	55,55,55,55	0
62	MG	1H	3324	1/1	0.95	0.15	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1H	3204	1/1	0.95	0.11	29,29,29,29	0
61	K	13	1637	1/1	0.95	0.08	64,64,64,64	0
62	MG	1H	3210	1/1	0.95	0.17	38,38,38,38	0
62	MG	1G	1657	1/1	0.95	0.22	53,53,53,53	0
62	MG	13	1717	1/1	0.95	0.29	62,62,62,62	0
62	MG	13	1666	1/1	0.95	0.20	46,46,46,46	0
61	K	2K	102	1/1	0.95	0.15	58,58,58,58	0
61	K	14	3022	1/1	0.95	0.12	50,50,50,50	0
61	K	1G	1630	1/1	0.95	0.07	80,80,80,80	0
62	MG	1H	3333	1/1	0.95	0.09	50,50,50,50	0
61	K	1H	3058	1/1	0.95	0.09	43,43,43,43	0
62	MG	14	3192	1/1	0.95	0.13	41,41,41,41	0
62	MG	1G	1665	1/1	0.95	0.07	50,50,50,50	0
62	MG	1H	3222	1/1	0.95	0.14	32,32,32,32	0
62	MG	1H	3223	1/1	0.95	0.13	30,30,30,30	0
61	K	14	3027	1/1	0.95	0.11	54,54,54,54	0
62	MG	1H	3340	1/1	0.95	0.10	48,48,48,48	0
62	MG	14	3200	1/1	0.95	0.25	52,52,52,52	0
62	MG	1H	3226	1/1	0.95	0.21	40,40,40,40	0
62	MG	1H	3227	1/1	0.95	0.08	29,29,29,29	0
61	K	14	3029	1/1	0.95	0.07	81,81,81,81	0
62	MG	14	3206	1/1	0.95	0.16	55,55,55,55	0
62	MG	1G	1675	1/1	0.95	0.19	65,65,65,65	0
62	MG	1H	3345[A]	1/1	0.95	0.50	23,23,23,23	1
62	MG	1H	3345[B]	1/1	0.95	0.50	24,24,24,24	1
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	13	1725	1/1	0.95	0.27	58,58,58,58	0
62	MG	1H	3232	1/1	0.95	0.16	43,43,43,43	0
61	K	14	3030	1/1	0.95	0.04	63,63,63,63	0
62	MG	13	1741	1/1	0.95	0.07	109,109,109,109	0
62	MG	14	3216	1/1	0.95	0.15	51,51,51,51	0
62	MG	1G	1682	1/1	0.95	0.25	41,41,41,41	0
62	MG	14	3218	1/1	0.95	0.12	60,60,60,60	0
62	MG	14	3220	1/1	0.95	0.07	46,46,46,46	0
61	K	14	3033	1/1	0.95	0.08	52,52,52,52	0
62	MG	13	1764	1/1	0.95	0.07	86,86,86,86	0
61	K	1H	3059	1/1	0.95	0.05	19,19,19,19	0
62	MG	1H	3357	1/1	0.95	0.17	28,28,28,28	0
61	K	14	3086	1/1	0.95	0.07	65,65,65,65	0
61	K	1H	3109	1/1	0.95	0.05	57,57,57,57	0
61	K	14	3037	1/1	0.95	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
61	K	14	3089	1/1	0.95	0.06	64,64,64,64	0
61	K	1G	1634	1/1	0.95	0.08	62,62,62,62	0
61	K	1H	3062	1/1	0.95	0.03	27,27,27,27	0
62	MG	1H	3255	1/1	0.95	0.17	47,47,47,47	0
62	MG	1H	3152	1/1	0.95	0.06	36,36,36,36	0
61	K	13	1644	1/1	0.95	0.06	74,74,74,74	0
62	MG	1H	3262	1/1	0.95	0.23	46,46,46,46	0
61	K	13	1632	1/1	0.95	0.11	79,79,79,79	0
61	K	14	3095	1/1	0.95	0.04	64,64,64,64	0
62	MG	1G	1700	1/1	0.95	0.20	52,52,52,52	0
62	MG	1G	1708	1/1	0.95	0.08	101,101,101,101	0
62	MG	1G	1714	1/1	0.95	0.06	88,88,88,88	0
62	MG	13	1689	1/1	0.95	0.20	53,53,53,53	0
61	K	13	1634	1/1	0.95	0.09	90,90,90,90	0
62	MG	1H	3159	1/1	0.95	0.14	44,44,44,44	0
62	MG	1H	3271	1/1	0.95	0.10	47,47,47,47	0
62	MG	1H	3160	1/1	0.95	0.11	29,29,29,29	0
62	MG	1H	3380	1/1	0.95	0.27	44,44,44,44	0
62	MG	1H	3161	1/1	0.95	0.18	55,55,55,55	0
61	K	1H	3118	1/1	0.95	0.06	56,56,56,56	0
62	MG	1H	3424	1/1	0.95	0.08	42,42,42,42	0
62	MG	14	3110	1/1	0.95	0.11	35,35,35,35	0
61	K	4A	201	1/1	0.95	0.07	96,96,96,96	0
62	MG	14	3113	1/1	0.95	0.13	36,36,36,36	0
62	MG	14	3261	1/1	0.95	0.20	43,43,43,43	0
62	MG	14	3263	1/1	0.95	0.26	60,60,60,60	0
61	K	5A	101	1/1	0.95	0.06	82,82,82,82	0
61	K	1H	3120	1/1	0.95	0.05	60,60,60,60	0
62	MG	1H	3168	1/1	0.95	0.16	15,15,15,15	0
62	MG	14	3269	1/1	0.95	0.16	68,68,68,68	0
62	MG	1H	3473	1/1	0.95	0.08	19,19,19,19	0
61	K	14	3001	1/1	0.95	0.08	76,76,76,76	0
62	MG	14	3272	1/1	0.95	0.18	61,61,61,61	0
62	MG	1H	3489	1/1	0.95	0.09	57,57,57,57	0
62	MG	1H	3172	1/1	0.95	0.17	31,31,31,31	0
62	MG	1H	3506	1/1	0.95	0.08	15,15,15,15	0
62	MG	1H	3515	1/1	0.95	0.07	40,40,40,40	0
61	K	4I	201	1/1	0.95	0.06	71,71,71,71	0
62	MG	1H	3530	1/1	0.95	0.06	21,21,21,21	0
62	MG	1H	3175	1/1	0.95	0.12	31,31,31,31	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	14	3305	1/1	0.95	0.06	40,40,40,40	0
62	MG	1H	3284	1/1	0.95	0.06	36,36,36,36	0
62	MG	1H	3285	1/1	0.95	0.16	43,43,43,43	0
62	MG	14	3326	1/1	0.95	0.07	40,40,40,40	0
62	MG	14	3329	1/1	0.95	0.07	28,28,28,28	0
61	K	13	1630	1/1	0.95	0.05	66,66,66,66	0
61	K	1H	3030	1/1	0.95	0.05	73,73,73,73	0
62	MG	14	3340	1/1	0.95	0.06	26,26,26,26	0
62	MG	16	206	1/1	0.95	0.10	52,52,52,52	0
62	MG	1H	3179	1/1	0.95	0.17	30,30,30,30	0
62	MG	14	3145	1/1	0.95	0.11	49,49,49,49	0
62	MG	1H	3180	1/1	0.95	0.10	43,43,43,43	0
62	MG	14	3374	1/1	0.95	0.06	30,30,30,30	0
61	K	1H	3006	1/1	0.95	0.15	44,44,44,44	0
61	K	1G	1612	1/1	0.95	0.05	58,58,58,58	0
62	MG	1H	3295	1/1	0.95	0.06	29,29,29,29	0
61	K	1H	3007	1/1	0.95	0.05	55,55,55,55	0
61	K	1H	3090	1/1	0.95	0.11	55,55,55,55	0
62	MG	1H	3299	1/1	0.95	0.13	47,47,47,47	0
62	MG	1H	3301	1/1	0.95	0.17	41,41,41,41	0
62	MG	M5	101	1/1	0.95	0.07	84,84,84,84	0
61	K	1H	3015	1/1	0.96	0.05	44,44,44,44	0
62	MG	1H	3247	1/1	0.96	0.14	21,21,21,21	0
61	K	1H	3024	1/1	0.96	0.07	59,59,59,59	0
62	MG	1H	3250	1/1	0.96	0.11	38,38,38,38	0
62	MG	14	3169	1/1	0.96	0.16	33,33,33,33	0
62	MG	13	1704	1/1	0.96	0.21	56,56,56,56	0
61	K	1H	3063	1/1	0.96	0.05	47,47,47,47	0
61	K	31	302	1/1	0.96	0.08	45,45,45,45	0
62	MG	1H	3256	1/1	0.96	0.12	40,40,40,40	0
62	MG	1H	3257	1/1	0.96	0.14	40,40,40,40	0
61	K	14	3074	1/1	0.96	0.11	73,73,73,73	0
61	K	13	1622	1/1	0.96	0.05	61,61,61,61	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
61	K	14	3032	1/1	0.96	0.13	53,53,53,53	0
62	MG	14	3179	1/1	0.96	0.15	32,32,32,32	0
62	MG	1H	3347	1/1	0.96	0.05	38,38,38,38	0
62	MG	1H	3348	1/1	0.96	0.08	30,30,30,30	0
61	K	88	201	1/1	0.96	0.12	57,57,57,57	0
62	MG	14	3183	1/1	0.96	0.19	30,30,30,30	0
61	K	1H	3070	1/1	0.96	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1G	1660	1/1	0.96	0.25	46,46,46,46	0
61	K	13	1602	1/1	0.96	0.11	72,72,72,72	0
62	MG	1H	3267	1/1	0.96	0.18	53,53,53,53	0
61	K	14	3081	1/1	0.96	0.07	54,54,54,54	0
62	MG	1H	3181	1/1	0.96	0.19	36,36,36,36	0
61	K	1G	1603	1/1	0.96	0.10	62,62,62,62	0
61	K	1H	3123	1/1	0.96	0.08	50,50,50,50	0
62	MG	13	1715	1/1	0.96	0.17	60,60,60,60	0
62	MG	1H	3274	1/1	0.96	0.07	31,31,31,31	0
61	K	1H	3124	1/1	0.96	0.06	64,64,64,64	0
62	MG	1G	1669	1/1	0.96	0.30	60,60,60,60	0
61	K	14	3085	1/1	0.96	0.06	62,62,62,62	0
62	MG	14	3198	1/1	0.96	0.13	33,33,33,33	0
61	K	1H	3097	1/1	0.96	0.06	25,25,25,25	0
62	MG	1H	3190	1/1	0.96	0.13	32,32,32,32	0
61	K	13	1624	1/1	0.96	0.08	59,59,59,59	0
61	K	1H	3074	1/1	0.96	0.10	34,34,34,34	0
62	MG	14	3203	1/1	0.96	0.24	45,45,45,45	0
61	K	1H	3100	1/1	0.96	0.05	44,44,44,44	0
61	K	1G	1613	1/1	0.96	0.06	63,63,63,63	0
61	K	1H	3101	1/1	0.96	0.04	49,49,49,49	0
61	K	1G	1615	1/1	0.96	0.03	60,60,60,60	0
61	K	1H	3103	1/1	0.96	0.13	33,33,33,33	0
62	MG	13	1738	1/1	0.96	0.06	86,86,86,86	0
61	K	14	3008	1/1	0.96	0.12	47,47,47,47	0
62	MG	1H	3288	1/1	0.96	0.12	44,44,44,44	0
62	MG	1H	3379	1/1	0.96	0.25	47,47,47,47	0
62	MG	13	1747	1/1	0.96	0.06	32,32,32,32	0
62	MG	1H	3205	1/1	0.96	0.15	33,33,33,33	0
62	MG	1H	3391	1/1	0.96	0.07	20,20,20,20	0
62	MG	1H	3206	1/1	0.96	0.12	25,25,25,25	0
62	MG	1H	3422	1/1	0.96	0.06	29,29,29,29	0
62	MG	13	1683	1/1	0.96	0.11	39,39,39,39	0
62	MG	13	1750	1/1	0.96	0.06	52,52,52,52	0
62	MG	1H	3296	1/1	0.96	0.05	32,32,32,32	0
62	MG	13	1757	1/1	0.96	0.08	50,50,50,50	0
61	K	1H	3104	1/1	0.96	0.07	42,42,42,42	0
62	MG	13	1770	1/1	0.96	0.06	71,71,71,71	0
62	MG	1H	3474	1/1	0.96	0.06	24,24,24,24	0
62	MG	1H	3477	1/1	0.96	0.06	28,28,28,28	0
62	MG	14	3229	1/1	0.96	0.06	48,48,48,48	0
62	MG	1H	3300	1/1	0.96	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	1G	1618	1/1	0.96	0.14	79,79,79,79	0
62	MG	1G	1707	1/1	0.96	0.06	62,62,62,62	0
62	MG	1H	3496	1/1	0.96	0.08	48,48,48,48	0
62	MG	1G	1713	1/1	0.96	0.09	120,120,120,120	0
62	MG	1H	3302	1/1	0.96	0.12	29,29,29,29	0
61	K	1H	3077	1/1	0.96	0.09	47,47,47,47	0
62	MG	1G	1721	1/1	0.96	0.05	45,45,45,45	0
62	MG	1G	1731	1/1	0.96	0.05	81,81,81,81	0
62	MG	14	3240	1/1	0.96	0.22	57,57,57,57	0
62	MG	1H	3507	1/1	0.96	0.06	17,17,17,17	0
62	MG	1H	3512	1/1	0.96	0.07	39,39,39,39	0
62	MG	1H	3514	1/1	0.96	0.08	53,53,53,53	0
61	K	14	3054	1/1	0.96	0.05	58,58,58,58	0
62	MG	2L	103	1/1	0.96	0.18	45,45,45,45	0
62	MG	14	3246	1/1	0.96	0.06	35,35,35,35	0
61	K	1G	1621	1/1	0.96	0.04	76,76,76,76	0
62	MG	1H	3528	1/1	0.96	0.07	50,50,50,50	0
62	MG	1H	3529	1/1	0.96	0.14	54,54,54,54	0
62	MG	14	3250	1/1	0.96	0.05	38,38,38,38	0
62	MG	1H	3307	1/1	0.96	0.05	25,25,25,25	0
61	K	14	3056	1/1	0.96	0.06	56,56,56,56	0
62	MG	1H	3544	1/1	0.96	0.05	63,63,63,63	0
62	MG	1H	3549	1/1	0.96	0.10	60,60,60,60	0
62	MG	1H	3551	1/1	0.96	0.07	45,45,45,45	0
62	MG	1H	3555	1/1	0.96	0.12	56,56,56,56	0
62	MG	14	3116	1/1	0.96	0.15	32,32,32,32	0
62	MG	1H	3556	1/1	0.96	0.15	47,47,47,47	0
62	MG	14	3262	1/1	0.96	0.18	41,41,41,41	0
62	MG	1H	3224	1/1	0.96	0.14	35,35,35,35	0
62	MG	1H	3566	1/1	0.96	0.10	37,37,37,37	0
62	MG	14	3265	1/1	0.96	0.15	34,34,34,34	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
61	K	1H	3019	1/1	0.96	0.05	60,60,60,60	0
62	MG	1H	3150	1/1	0.96	0.19	25,25,25,25	0
61	K	13	1609	1/1	0.96	0.06	57,57,57,57	0
62	MG	14	3128	1/1	0.96	0.17	28,28,28,28	0
62	MG	14	3129	1/1	0.96	0.07	34,34,34,34	0
61	K	13	1601	1/1	0.96	0.05	67,67,67,67	0
61	K	1G	1626	1/1	0.96	0.04	67,67,67,67	0
62	MG	1H	3230	1/1	0.96	0.23	39,39,39,39	0
62	MG	1H	3231	1/1	0.96	0.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	1H	3111	1/1	0.96	0.06	51,51,51,51	0
62	MG	14	3280	1/1	0.96	0.08	45,45,45,45	0
62	MG	14	3137	1/1	0.96	0.14	49,49,49,49	0
62	MG	21	303	1/1	0.96	0.10	33,33,33,33	0
61	K	1J	201	1/1	0.96	0.05	81,81,81,81	0
62	MG	14	3301	1/1	0.96	0.06	38,38,38,38	0
62	MG	14	3142	1/1	0.96	0.18	51,51,51,51	0
62	MG	14	3306	1/1	0.96	0.07	32,32,32,32	0
61	K	19	301	1/1	0.96	0.13	52,52,52,52	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	3235	1/1	0.96	0.06	42,42,42,42	0
62	MG	14	3320	1/1	0.96	0.06	25,25,25,25	0
62	MG	14	3325	1/1	0.96	0.06	30,30,30,30	0
62	MG	78	202	1/1	0.96	0.13	30,30,30,30	0
61	K	13	1640	1/1	0.96	0.04	60,60,60,60	0
62	MG	14	3148	1/1	0.96	0.14	43,43,43,43	0
62	MG	I8	101	1/1	0.96	0.11	26,26,26,26	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
62	MG	J8	101	1/1	0.96	0.14	32,32,32,32	0
62	MG	L8	101	1/1	0.96	0.07	38,38,38,38	0
61	K	39	301	1/1	0.96	0.07	75,75,75,75	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	3239	1/1	0.96	0.06	26,26,26,26	0
62	MG	14	3380	1/1	0.96	0.06	76,76,76,76	0
62	MG	14	3381	1/1	0.96	0.07	56,56,56,56	0
62	MG	14	3386	1/1	0.96	0.12	61,61,61,61	0
62	MG	Q8	101[A]	1/1	0.96	0.49	13,13,13,13	1
62	MG	14	3394	1/1	0.96	0.12	61,61,61,61	0
62	MG	Q8	101[B]	1/1	0.96	0.49	11,11,11,11	1
61	K	1G	1629	1/1	0.96	0.06	88,88,88,88	0
62	MG	14	3160	1/1	0.96	0.04	38,38,38,38	0
62	MG	1H	3243	1/1	0.96	0.17	41,41,41,41	0
62	MG	13	1700	1/1	0.96	0.13	47,47,47,47	0
61	K	14	3068	1/1	0.96	0.05	61,61,61,61	0
62	MG	1H	3330	1/1	0.96	0.20	45,45,45,45	0
61	K	14	3073	1/1	0.97	0.06	60,60,60,60	0
62	MG	1H	3426	1/1	0.97	0.10	12,12,12,12	0
62	MG	1H	3428	1/1	0.97	0.04	23,23,23,23	0
61	K	14	3036	1/1	0.97	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	1H	3143	1/1	0.97	0.04	71,71,71,71	0
62	MG	1H	3450	1/1	0.97	0.09	52,52,52,52	0
61	K	1H	3042	1/1	0.97	0.04	54,54,54,54	0
62	MG	1H	3455	1/1	0.97	0.06	11,11,11,11	0
62	MG	14	3193	1/1	0.97	0.18	40,40,40,40	0
62	MG	13	1655	1/1	0.97	0.10	51,51,51,51	0
62	MG	1H	3306	1/1	0.97	0.07	34,34,34,34	0
62	MG	1H	3156	1/1	0.97	0.25	33,33,33,33	0
62	MG	1H	3475	1/1	0.97	0.06	40,40,40,40	0
62	MG	1H	3308	1/1	0.97	0.04	27,27,27,27	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	13	1656	1/1	0.97	0.09	49,49,49,49	0
61	K	1H	3089	1/1	0.97	0.03	36,36,36,36	0
62	MG	13	1658	1/1	0.97	0.13	36,36,36,36	0
61	K	21	301	1/1	0.97	0.12	62,62,62,62	0
62	MG	14	3205	1/1	0.97	0.31	51,51,51,51	0
62	MG	1H	3501	1/1	0.97	0.11	57,57,57,57	0
62	MG	1H	3503	1/1	0.97	0.07	29,29,29,29	0
62	MG	1H	3504	1/1	0.97	0.10	20,20,20,20	0
62	MG	1G	1694	1/1	0.97	0.08	43,43,43,43	0
62	MG	13	1660	1/1	0.97	0.05	39,39,39,39	0
62	MG	13	1661	1/1	0.97	0.14	39,39,39,39	0
62	MG	1H	3508	1/1	0.97	0.06	22,22,22,22	0
62	MG	1H	3317	1/1	0.97	0.23	52,52,52,52	0
61	K	1H	3107	1/1	0.97	0.07	44,44,44,44	0
62	MG	1H	3237	1/1	0.97	0.10	38,38,38,38	0
62	MG	1G	1702	1/1	0.97	0.06	64,64,64,64	0
62	MG	1H	3516	1/1	0.97	0.06	21,21,21,21	0
61	K	1G	1624	1/1	0.97	0.05	60,60,60,60	0
62	MG	14	3219	1/1	0.97	0.12	33,33,33,33	0
62	MG	1G	1709	1/1	0.97	0.05	73,73,73,73	0
62	MG	1G	1711	1/1	0.97	0.07	97,97,97,97	0
62	MG	1H	3519	1/1	0.97	0.16	25,25,25,25	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	1H	3166	1/1	0.97	0.09	41,41,41,41	0
62	MG	1G	1724	1/1	0.97	0.04	82,82,82,82	0
62	MG	14	3227	1/1	0.97	0.09	38,38,38,38	0
62	MG	1G	1726	1/1	0.97	0.06	49,49,49,49	0
62	MG	1H	3240	1/1	0.97	0.14	39,39,39,39	0
62	MG	1G	1733	1/1	0.97	0.04	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1G	1735	1/1	0.97	0.07	88,88,88,88	0
62	MG	1H	3167	1/1	0.97	0.10	20,20,20,20	0
61	K	1H	3071	1/1	0.97	0.04	42,42,42,42	0
62	MG	1H	3169	1/1	0.97	0.14	15,15,15,15	0
62	MG	1H	3548	1/1	0.97	0.06	32,32,32,32	0
62	MG	1H	3170	1/1	0.97	0.13	18,18,18,18	0
61	K	1H	3127	1/1	0.97	0.05	47,47,47,47	0
62	MG	14	3238	1/1	0.97	0.13	44,44,44,44	0
62	MG	1H	3552	1/1	0.97	0.11	85,85,85,85	0
62	MG	1H	3554	1/1	0.97	0.05	77,77,77,77	0
61	K	1H	3012	1/1	0.97	0.06	51,51,51,51	0
61	K	14	3046	1/1	0.97	0.11	54,54,54,54	0
62	MG	1H	3563	1/1	0.97	0.07	75,75,75,75	0
62	MG	1H	3249	1/1	0.97	0.12	31,31,31,31	0
62	MG	13	1670	1/1	0.97	0.08	42,42,42,42	0
62	MG	1H	3567	1/1	0.97	0.08	24,24,24,24	0
61	K	1H	3129	1/1	0.97	0.09	60,60,60,60	0
62	MG	13	1716	1/1	0.97	0.07	37,37,37,37	0
61	K	1H	3054	1/1	0.97	0.05	27,27,27,27	0
61	K	14	3049	1/1	0.97	0.03	49,49,49,49	0
61	K	1H	3033	1/1	0.97	0.06	36,36,36,36	0
62	MG	14	3252	1/1	0.97	0.20	42,42,42,42	0
62	MG	1H	3335	1/1	0.97	0.22	40,40,40,40	0
61	K	14	3090	1/1	0.97	0.04	64,64,64,64	0
62	MG	1H	3337	1/1	0.97	0.03	23,23,23,23	0
61	K	1H	3076	1/1	0.97	0.05	50,50,50,50	0
62	MG	14	3258	1/1	0.97	0.09	34,34,34,34	0
62	MG	14	3126	1/1	0.97	0.11	27,27,27,27	0
62	MG	1H	3184	1/1	0.97	0.18	40,40,40,40	0
62	MG	16	211	1/1	0.97	0.04	57,57,57,57	0
62	MG	16	215	1/1	0.97	0.05	52,52,52,52	0
62	MG	1H	3185	1/1	0.97	0.05	40,40,40,40	0
62	MG	1H	3341	1/1	0.97	0.09	24,24,24,24	0
62	MG	14	3134	1/1	0.97	0.16	34,34,34,34	0
62	MG	14	3266	1/1	0.97	0.04	38,38,38,38	0
61	K	1G	1606	1/1	0.97	0.18	61,61,61,61	0
61	K	1H	3039	1/1	0.97	0.05	54,54,54,54	0
61	K	14	3019	1/1	0.97	0.08	40,40,40,40	0
62	MG	1H	3265	1/1	0.97	0.10	48,48,48,48	0
61	K	1H	3061	1/1	0.97	0.03	43,43,43,43	0
61	K	1G	1609	1/1	0.97	0.04	91,91,91,91	0
62	MG	1H	3268	1/1	0.97	0.06	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	14	3144	1/1	0.97	0.07	36,36,36,36	0
62	MG	N8	101	1/1	0.97	0.12	41,41,41,41	0
62	MG	1H	3191	1/1	0.97	0.12	24,24,24,24	0
61	K	14	3057	1/1	0.97	0.06	54,54,54,54	0
61	K	1G	1610	1/1	0.97	0.04	68,68,68,68	0
61	K	14	3059	1/1	0.97	0.08	48,48,48,48	0
62	MG	14	3282	1/1	0.97	0.06	48,48,48,48	0
62	MG	13	1748	1/1	0.97	0.06	38,38,38,38	0
62	MG	14	3290	1/1	0.97	0.06	36,36,36,36	0
62	MG	14	3291	1/1	0.97	0.06	58,58,58,58	0
62	MG	14	3151	1/1	0.97	0.10	26,26,26,26	0
62	MG	14	3293	1/1	0.97	0.07	60,60,60,60	0
62	MG	14	3294	1/1	0.97	0.05	51,51,51,51	0
62	MG	1H	3354	1/1	0.97	0.06	29,29,29,29	0
61	K	14	3060	1/1	0.97	0.08	45,45,45,45	0
61	K	1H	3136	1/1	0.97	0.08	54,54,54,54	0
62	MG	1H	3200	1/1	0.97	0.12	36,36,36,36	0
62	MG	13	1751	1/1	0.97	0.09	75,75,75,75	0
62	MG	13	1753	1/1	0.97	0.04	69,69,69,69	0
62	MG	13	1755	1/1	0.97	0.05	83,83,83,83	0
61	K	14	3026	1/1	0.97	0.03	35,35,35,35	0
61	K	14	3063	1/1	0.97	0.04	57,57,57,57	0
62	MG	13	1767	1/1	0.97	0.08	70,70,70,70	0
62	MG	13	1769	1/1	0.97	0.08	54,54,54,54	0
62	MG	1H	3208	1/1	0.97	0.07	37,37,37,37	0
62	MG	1H	3366	1/1	0.97	0.10	40,40,40,40	0
62	MG	1H	3209	1/1	0.97	0.20	52,52,52,52	0
61	K	1H	3116	1/1	0.97	0.05	61,61,61,61	0
61	K	14	3028	1/1	0.97	0.06	45,45,45,45	0
62	MG	14	3343	1/1	0.97	0.07	50,50,50,50	0
62	MG	14	3347	1/1	0.97	0.05	27,27,27,27	0
62	MG	14	3348	1/1	0.97	0.05	30,30,30,30	0
61	K	13	1628	1/1	0.97	0.03	51,51,51,51	0
62	MG	1H	3289	1/1	0.97	0.20	35,35,35,35	0
61	K	1H	3119	1/1	0.97	0.17	46,46,46,46	0
62	MG	14	3364	1/1	0.97	0.05	36,36,36,36	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
61	K	14	3031	1/1	0.97	0.03	29,29,29,29	0
62	MG	1H	3215	1/1	0.97	0.14	40,40,40,40	0
62	MG	1H	3216	1/1	0.97	0.15	34,34,34,34	0
62	MG	14	3375	1/1	0.97	0.06	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1H	3377	1/1	0.97	0.12	26,26,26,26	0
62	MG	1H	3217	1/1	0.97	0.22	31,31,31,31	0
62	MG	14	3383	1/1	0.97	0.09	51,51,51,51	0
62	MG	1H	3218	1/1	0.97	0.13	28,28,28,28	0
61	K	1H	3001	1/1	0.97	0.05	48,48,48,48	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	3382	1/1	0.97	0.07	13,13,13,13	0
62	MG	1H	3383	1/1	0.97	0.05	18,18,18,18	0
62	MG	1H	3390	1/1	0.97	0.05	26,26,26,26	0
61	K	1H	3085	1/1	0.97	0.10	39,39,39,39	0
62	MG	1J	203	1/1	0.97	0.16	48,48,48,48	0
61	K	13	1617	1/1	0.97	0.08	50,50,50,50	0
62	MG	1H	3419	1/1	0.97	0.08	27,27,27,27	0
61	K	14	3002	1/1	0.97	0.06	69,69,69,69	0
62	MG	1H	3423	1/1	0.97	0.06	35,35,35,35	0
62	MG	1H	3443	1/1	0.98	0.07	42,42,42,42	0
62	MG	1H	3444	1/1	0.98	0.04	23,23,23,23	0
61	K	1H	3057	1/1	0.98	0.03	23,23,23,23	0
62	MG	1H	3451	1/1	0.98	0.04	82,82,82,82	0
62	MG	1H	3452	1/1	0.98	0.04	68,68,68,68	0
62	MG	14	3111	1/1	0.98	0.07	32,32,32,32	0
61	K	13	1619	1/1	0.98	0.18	58,58,58,58	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	13	1727	1/1	0.98	0.08	60,60,60,60	0
62	MG	1H	3461	1/1	0.98	0.05	20,20,20,20	0
62	MG	1H	3464	1/1	0.98	0.07	23,23,23,23	0
62	MG	1H	3466	1/1	0.98	0.05	22,22,22,22	0
62	MG	13	1728	1/1	0.98	0.05	60,60,60,60	0
61	K	13	1633	1/1	0.98	0.05	55,55,55,55	0
61	K	1H	3052	1/1	0.98	0.04	52,52,52,52	0
62	MG	13	1744	1/1	0.98	0.05	19,19,19,19	0
62	MG	14	3123	1/1	0.98	0.04	36,36,36,36	0
62	MG	1H	3478	1/1	0.98	0.12	44,44,44,44	0
62	MG	1H	3158	1/1	0.98	0.07	57,57,57,57	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
61	K	1H	3106	1/1	0.98	0.06	59,59,59,59	0
62	MG	14	3130	1/1	0.98	0.03	38,38,38,38	0
62	MG	1H	3485	1/1	0.98	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	1H	3053	1/1	0.98	0.04	25,25,25,25	0
61	K	1H	3043	1/1	0.98	0.03	58,58,58,58	0
62	MG	1H	3490	1/1	0.98	0.04	32,32,32,32	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	14	3138	1/1	0.98	0.08	31,31,31,31	0
61	K	1H	3093	1/1	0.98	0.07	42,42,42,42	0
62	MG	1H	3497	1/1	0.98	0.10	55,55,55,55	0
62	MG	14	3141	1/1	0.98	0.14	26,26,26,26	0
62	MG	1H	3498	1/1	0.98	0.08	24,24,24,24	0
61	K	1H	3056	1/1	0.98	0.04	37,37,37,37	0
62	MG	1H	3241	1/1	0.98	0.16	30,30,30,30	0
62	MG	1H	3502	1/1	0.98	0.04	25,25,25,25	0
62	MG	13	1752	1/1	0.98	0.06	47,47,47,47	0
61	K	16	203	1/1	0.98	0.03	44,44,44,44	0
61	K	1H	3078	1/1	0.98	0.02	45,45,45,45	0
62	MG	13	1756	1/1	0.98	0.09	63,63,63,63	0
61	K	1H	3079	1/1	0.98	0.05	37,37,37,37	0
62	MG	1H	3510	1/1	0.98	0.04	19,19,19,19	0
62	MG	13	1758	1/1	0.98	0.03	76,76,76,76	0
62	MG	13	1763	1/1	0.98	0.05	64,64,64,64	0
61	K	14	3016	1/1	0.98	0.03	44,44,44,44	0
62	MG	13	1766	1/1	0.98	0.07	64,64,64,64	0
62	MG	1H	3374	1/1	0.98	0.04	28,28,28,28	0
62	MG	1H	3173	1/1	0.98	0.13	28,28,28,28	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	0.04	32,32,32,32	0
62	MG	1H	3524	1/1	0.98	0.04	16,16,16,16	0
62	MG	13	1667	1/1	0.98	0.10	29,29,29,29	0
62	MG	1H	3378	1/1	0.98	0.04	28,28,28,28	0
62	MG	13	1668	1/1	0.98	0.07	31,31,31,31	0
61	K	1H	3130	1/1	0.98	0.07	61,61,61,61	0
62	MG	1H	3532	1/1	0.98	0.06	56,56,56,56	0
62	MG	14	3281	1/1	0.98	0.05	25,25,25,25	0
62	MG	1H	3535	1/1	0.98	0.06	64,64,64,64	0
62	MG	14	3288	1/1	0.98	0.04	39,39,39,39	0
62	MG	1H	3536	1/1	0.98	0.04	23,23,23,23	0
62	MG	3E	301	1/1	0.98	0.03	82,82,82,82	0
62	MG	1H	3541	1/1	0.98	0.04	66,66,66,66	0
62	MG	1H	3542	1/1	0.98	0.13	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	3177	1/1	0.98	0.19	29,29,29,29	0
62	MG	1H	3547	1/1	0.98	0.06	52,52,52,52	0
61	K	1G	1619	1/1	0.98	0.06	74,74,74,74	0
62	MG	1H	3387	1/1	0.98	0.05	16,16,16,16	0
62	MG	14	3303	1/1	0.98	0.03	58,58,58,58	0
62	MG	1H	3550	1/1	0.98	0.07	64,64,64,64	0
62	MG	1H	3219	1/1	0.98	0.22	31,31,31,31	0
61	K	1H	3113	1/1	0.98	0.03	30,30,30,30	0
62	MG	14	3310	1/1	0.98	0.04	25,25,25,25	0
62	MG	14	3312	1/1	0.98	0.10	38,38,38,38	0
62	MG	1H	3553	1/1	0.98	0.06	60,60,60,60	0
62	MG	1G	1693	1/1	0.98	0.09	40,40,40,40	0
62	MG	14	3315	1/1	0.98	0.04	39,39,39,39	0
62	MG	1H	3393	1/1	0.98	0.04	17,17,17,17	0
62	MG	14	3318	1/1	0.98	0.06	35,35,35,35	0
61	K	1H	3065	1/1	0.98	0.14	30,30,30,30	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	3405	1/1	0.98	0.08	16,16,16,16	0
62	MG	1H	3558	1/1	0.98	0.09	56,56,56,56	0
62	MG	14	3327	1/1	0.98	0.05	36,36,36,36	0
62	MG	1H	3409	1/1	0.98	0.11	14,14,14,14	0
62	MG	14	3331	1/1	0.98	0.07	51,51,51,51	0
62	MG	1H	3411	1/1	0.98	0.04	20,20,20,20	0
62	MG	1H	3412	1/1	0.98	0.05	16,16,16,16	0
62	MG	14	3339	1/1	0.98	0.09	29,29,29,29	0
62	MG	1H	3413	1/1	0.98	0.04	49,49,49,49	0
62	MG	1G	1703	1/1	0.98	0.04	81,81,81,81	0
62	MG	14	3342	1/1	0.98	0.05	32,32,32,32	0
62	MG	1G	1705	1/1	0.98	0.07	73,73,73,73	0
62	MG	14	3345	1/1	0.98	0.06	48,48,48,48	0
62	MG	1H	3415	1/1	0.98	0.07	16,16,16,16	0
62	MG	1H	3570	1/1	0.98	0.05	50,50,50,50	0
62	MG	14	3349	1/1	0.98	0.07	48,48,48,48	0
62	MG	14	3350	1/1	0.98	0.06	39,39,39,39	0
62	MG	1H	3573	1/1	0.98	0.03	40,40,40,40	0
62	MG	1H	3417	1/1	0.98	0.05	61,61,61,61	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	K	14	3021	1/1	0.98	0.04	41,41,41,41	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
62	MG	1H	3420	1/1	0.98	0.06	20,20,20,20	0
62	MG	14	3365	1/1	0.98	0.06	28,28,28,28	0
62	MG	14	3369	1/1	0.98	0.05	76,76,76,76	0
62	MG	1G	1716	1/1	0.98	0.04	70,70,70,70	0
61	K	1H	3067	1/1	0.98	0.03	53,53,53,53	0
62	MG	1G	1720	1/1	0.98	0.11	73,73,73,73	0
62	MG	1H	3148	1/1	0.98	0.14	35,35,35,35	0
62	MG	1G	1723	1/1	0.98	0.07	59,59,59,59	0
61	K	1H	3069	1/1	0.98	0.03	16,16,16,16	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	1725	1/1	0.98	0.04	69,69,69,69	0
61	K	1H	3117	1/1	0.98	0.12	57,57,57,57	0
62	MG	14	3382	1/1	0.98	0.05	52,52,52,52	0
62	MG	1G	1727	1/1	0.98	0.05	59,59,59,59	0
62	MG	14	3384	1/1	0.98	0.08	47,47,47,47	0
62	MG	14	3385	1/1	0.98	0.05	58,58,58,58	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	3388	1/1	0.98	0.07	91,91,91,91	0
62	MG	1G	1730	1/1	0.98	0.05	78,78,78,78	0
62	MG	14	3390	1/1	0.98	0.04	79,79,79,79	0
61	K	1H	3084	1/1	0.98	0.16	47,47,47,47	0
62	MG	14	3393	1/1	0.98	0.08	63,63,63,63	0
62	MG	1H	3309	1/1	0.98	0.04	52,52,52,52	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	1G	1734	1/1	0.98	0.07	94,94,94,94	0
62	MG	1H	3430	1/1	0.98	0.04	54,54,54,54	0
62	MG	16	214	1/1	0.98	0.05	57,57,57,57	0
62	MG	32	302	1/1	0.98	0.05	79,79,79,79	0
62	MG	1H	3431	1/1	0.98	0.04	46,46,46,46	0
62	MG	1H	3436	1/1	0.98	0.05	57,57,57,57	0
62	MG	1H	3310	1/1	0.98	0.04	18,18,18,18	0
62	MG	1H	3438	1/1	0.98	0.07	74,74,74,74	0
62	MG	16	213	1/1	0.99	0.04	41,41,41,41	0
62	MG	1H	3468	1/1	0.99	0.04	24,24,24,24	0
62	MG	1H	3469	1/1	0.99	0.04	13,13,13,13	0
62	MG	1H	3470	1/1	0.99	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1H	3471	1/1	0.99	0.05	56,56,56,56	0
62	MG	1H	3472	1/1	0.99	0.03	17,17,17,17	0
62	MG	2K	105	1/1	0.99	0.06	45,45,45,45	0
62	MG	1H	3145	1/1	0.99	0.12	17,17,17,17	0
62	MG	13	1739	1/1	0.99	0.05	30,30,30,30	0
62	MG	F8	101	1/1	0.99	0.14	32,32,32,32	0
62	MG	1H	3476	1/1	0.99	0.05	15,15,15,15	0
62	MG	1H	3342	1/1	0.99	0.18	27,27,27,27	0
61	K	1H	3087	1/1	0.99	0.02	31,31,31,31	0
62	MG	1H	3384	1/1	0.99	0.04	11,11,11,11	0
62	MG	1H	3480	1/1	0.99	0.05	18,18,18,18	0
62	MG	14	3253	1/1	0.99	0.03	47,47,47,47	0
62	MG	1H	3386	1/1	0.99	0.03	31,31,31,31	0
62	MG	1H	3482	1/1	0.99	0.03	45,45,45,45	0
62	MG	13	1742	1/1	0.99	0.03	60,60,60,60	0
62	MG	1H	3389	1/1	0.99	0.03	13,13,13,13	0
62	MG	13	1743	1/1	0.99	0.04	54,54,54,54	0
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
61	K	11	301	1/1	0.99	0.06	31,31,31,31	0
62	MG	1H	3392	1/1	0.99	0.04	51,51,51,51	0
62	MG	13	1745	1/1	0.99	0.04	39,39,39,39	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	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	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
62	MG	13	1746	1/1	0.99	0.04	37,37,37,37	0
62	MG	1H	3400	1/1	0.99	0.07	20,20,20,20	0
62	MG	1H	3499	1/1	0.99	0.03	32,32,32,32	0
62	MG	1H	3403	1/1	0.99	0.03	27,27,27,27	0
62	MG	1H	3404	1/1	0.99	0.02	43,43,43,43	0
61	K	14	3075	1/1	0.99	0.03	36,36,36,36	0
62	MG	1H	3407	1/1	0.99	0.02	16,16,16,16	0
61	K	13	1629	1/1	0.99	0.03	50,50,50,50	0
62	MG	1H	3505	1/1	0.99	0.04	16,16,16,16	0
62	MG	14	3279	1/1	0.99	0.06	22,22,22,22	0
61	K	31	301	1/1	0.99	0.06	48,48,48,48	0
61	K	1H	3075	1/1	0.99	0.03	28,28,28,28	0
61	K	1H	3055	1/1	0.99	0.06	31,31,31,31	0
62	MG	14	3283	1/1	0.99	0.03	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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	3509	1/1	0.99	0.03	27,27,27,27	0
62	MG	1H	3414	1/1	0.99	0.05	39,39,39,39	0
62	MG	1H	3511	1/1	0.99	0.02	26,26,26,26	0
61	K	14	3023	1/1	0.99	0.07	60,60,60,60	0
62	MG	1H	3513	1/1	0.99	0.11	30,30,30,30	0
62	MG	1H	3416	1/1	0.99	0.05	69,69,69,69	0
62	MG	1H	3194	1/1	0.99	0.04	14,14,14,14	0
61	K	1H	3083	1/1	0.99	0.03	54,54,54,54	0
62	MG	14	3296	1/1	0.99	0.03	35,35,35,35	0
62	MG	14	3298	1/1	0.99	0.04	32,32,32,32	0
62	MG	14	3299	1/1	0.99	0.03	48,48,48,48	0
62	MG	13	1754	1/1	0.99	0.05	35,35,35,35	0
62	MG	14	3302	1/1	0.99	0.06	29,29,29,29	0
62	MG	1H	3518	1/1	0.99	0.04	37,37,37,37	0
62	MG	14	3304	1/1	0.99	0.03	63,63,63,63	0
62	MG	1G	1671	1/1	0.99	0.29	46,46,46,46	0
62	MG	1H	3421	1/1	0.99	0.06	36,36,36,36	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
61	K	1H	3092	1/1	0.99	0.06	37,37,37,37	0
62	MG	1H	3521	1/1	0.99	0.06	14,14,14,14	0
62	MG	14	3311	1/1	0.99	0.03	31,31,31,31	0
62	MG	1H	3198	1/1	0.99	0.04	20,20,20,20	0
61	K	1H	3102	1/1	0.99	0.03	51,51,51,51	0
62	MG	1H	3425	1/1	0.99	0.04	16,16,16,16	0
62	MG	1H	3525	1/1	0.99	0.05	15,15,15,15	0
61	K	1H	3066	1/1	0.99	0.05	27,27,27,27	0
62	MG	1H	3527	1/1	0.99	0.07	26,26,26,26	0
62	MG	1H	3427	1/1	0.99	0.07	36,36,36,36	0
61	K	1H	3060	1/1	0.99	0.04	34,34,34,34	0
62	MG	13	1759	1/1	0.99	0.06	52,52,52,52	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	3531	1/1	0.99	0.07	21,21,21,21	0
62	MG	13	1761	1/1	0.99	0.05	86,86,86,86	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
62	MG	14	3330	1/1	0.99	0.05	39,39,39,39	0
62	MG	13	1762	1/1	0.99	0.03	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	1H	3432	1/1	0.99	0.03	55,55,55,55	0
62	MG	14	3333	1/1	0.99	0.05	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	3537	1/1	0.99	0.04	54,54,54,54	0
62	MG	14	3337	1/1	0.99	0.03	83,83,83,83	0
62	MG	1H	3538	1/1	0.99	0.04	27,27,27,27	0
62	MG	1H	3433	1/1	0.99	0.06	51,51,51,51	0
62	MG	1H	3540	1/1	0.99	0.07	50,50,50,50	0
62	MG	1H	3434	1/1	0.99	0.06	46,46,46,46	0
62	MG	1H	3435	1/1	0.99	0.05	46,46,46,46	0
62	MG	1H	3543	1/1	0.99	0.06	48,48,48,48	0
62	MG	14	3346	1/1	0.99	0.07	52,52,52,52	0
61	K	16	201	1/1	0.99	0.02	55,55,55,55	0
62	MG	1H	3546	1/1	0.99	0.05	61,61,61,61	0
62	MG	13	1729	1/1	0.99	0.03	61,61,61,61	0
62	MG	13	1765	1/1	0.99	0.04	73,73,73,73	0
62	MG	1H	3440	1/1	0.99	0.04	62,62,62,62	0
62	MG	1G	1701	1/1	0.99	0.03	45,45,45,45	0
62	MG	14	3353	1/1	0.99	0.11	62,62,62,62	0
62	MG	1H	3441	1/1	0.99	0.06	61,61,61,61	0
62	MG	14	3355	1/1	0.99	0.07	39,39,39,39	0
62	MG	1H	3442	1/1	0.99	0.04	56,56,56,56	0
62	MG	13	1730	1/1	0.99	0.06	76,76,76,76	0
62	MG	13	1732	1/1	0.99	0.04	51,51,51,51	0
62	MG	1H	3445	1/1	0.99	0.03	50,50,50,50	0
62	MG	1H	3446	1/1	0.99	0.04	48,48,48,48	0
62	MG	1G	1710	1/1	0.99	0.03	59,59,59,59	0
62	MG	1H	3447	1/1	0.99	0.04	19,19,19,19	0
62	MG	14	3363	1/1	0.99	0.03	26,26,26,26	0
62	MG	1G	1712	1/1	0.99	0.03	81,81,81,81	0
62	MG	1H	3557	1/1	0.99	0.02	22,22,22,22	0
62	MG	14	3366	1/1	0.99	0.03	55,55,55,55	0
62	MG	14	3367	1/1	0.99	0.04	70,70,70,70	0
62	MG	1H	3448	1/1	0.99	0.07	57,57,57,57	0
62	MG	1G	1715	1/1	0.99	0.04	39,39,39,39	0
62	MG	1H	3559	1/1	0.99	0.07	15,15,15,15	0
62	MG	1G	1717	1/1	0.99	0.04	67,67,67,67	0
62	MG	1H	3560	1/1	0.99	0.08	13,13,13,13	0
62	MG	1G	1719	1/1	0.99	0.15	66,66,66,66	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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	1G	1722	1/1	0.99	0.07	46,46,46,46	0
62	MG	1H	3449	1/1	0.99	0.06	15,15,15,15	0
62	MG	13	1768	1/1	0.99	0.03	78,78,78,78	0
62	MG	1H	3565	1/1	0.99	0.05	25,25,25,25	0
62	MG	13	1733	1/1	0.99	0.03	62,62,62,62	0
62	MG	1H	3251	1/1	0.99	0.15	39,39,39,39	0
62	MG	1H	3568	1/1	0.99	0.09	34,34,34,34	0
62	MG	13	1734	1/1	0.99	0.07	41,41,41,41	0
62	MG	1H	3253	1/1	0.99	0.23	41,41,41,41	0
62	MG	1H	3571	1/1	0.99	0.05	26,26,26,26	0
62	MG	1G	1732	1/1	0.99	0.03	83,83,83,83	0
62	MG	1H	3572	1/1	0.99	0.04	25,25,25,25	0
62	MG	14	3391	1/1	0.99	0.03	81,81,81,81	0
62	MG	13	1735	1/1	0.99	0.03	35,35,35,35	0
62	MG	1H	3575	1/1	0.99	0.03	17,17,17,17	0
62	MG	1H	3456	1/1	0.99	0.12	14,14,14,14	0
62	MG	13	1736	1/1	0.99	0.04	44,44,44,44	0
62	MG	1H	3459	1/1	0.99	0.04	15,15,15,15	0
62	MG	13	1737	1/1	0.99	0.07	65,65,65,65	0
62	MG	14	3398	1/1	0.99	0.10	47,47,47,47	0
62	MG	1H	3462	1/1	0.99	0.05	27,27,27,27	0
62	MG	14	3400	1/1	0.99	0.03	63,63,63,63	0
62	MG	1H	3463	1/1	0.99	0.03	17,17,17,17	0
61	K	1H	3068	1/1	0.99	0.04	29,29,29,29	0
62	MG	1H	3465	1/1	0.99	0.04	21,21,21,21	0
62	MG	1J	205	1/1	0.99	0.05	68,68,68,68	0
62	MG	1H	3178	1/1	0.99	0.10	17,17,17,17	0
62	MG	29	303	1/1	0.99	0.05	28,28,28,28	0
62	MG	1H	3467	1/1	0.99	0.03	44,44,44,44	0
62	MG	16	212	1/1	0.99	0.04	36,36,36,36	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	1H	3406	1/1	1.00	0.02	14,14,14,14	0
62	MG	1H	3418	1/1	1.00	0.03	29,29,29,29	0
62	MG	14	3300	1/1	1.00	0.03	61,61,61,61	0
62	MG	1G	1704	1/1	1.00	0.03	66,66,66,66	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	MG	1G	1706	1/1	1.00	0.03	43,43,43,43	0
62	MG	1H	3458	1/1	1.00	0.04	21,21,21,21	0
62	MG	1H	3408	1/1	1.00	0.01	29,29,29,29	0
62	MG	1H	3460	1/1	1.00	0.03	11,11,11,11	0
62	MG	1H	3388	1/1	1.00	0.02	15,15,15,15	0
62	MG	1H	3410	1/1	1.00	0.02	16,16,16,16	0
62	MG	13	1760	1/1	1.00	0.02	65,65,65,65	0
62	MG	1H	3401	1/1	1.00	0.03	16,16,16,16	0
62	MG	14	3338	1/1	1.00	0.03	34,34,34,34	0
62	MG	14	3368	1/1	1.00	0.06	29,29,29,29	0
62	MG	14	3287	1/1	1.00	0.02	39,39,39,39	0
62	MG	1H	3402	1/1	1.00	0.02	23,23,23,23	0
62	MG	11	302	1/1	1.00	0.04	14,14,14,14	0
62	MG	21	302	1/1	1.00	0.02	14,14,14,14	0
62	MG	1H	3385	1/1	1.00	0.02	20,20,20,20	0
62	MG	14	3344	1/1	1.00	0.03	31,31,31,31	0
62	MG	14	3316	1/1	1.00	0.02	34,34,34,34	0
62	MG	1H	3574	1/1	1.00	0.08	24,24,24,24	0
62	MG	1H	3439	1/1	1.00	0.04	53,53,53,53	0
62	MG	14	3319	1/1	1.00	0.03	27,27,27,27	0
62	MG	1H	3396	1/1	1.00	0.03	16,16,16,16	0
62	MG	13	1740	1/1	1.00	0.03	33,33,33,33	0
62	MG	1H	3545	1/1	1.00	0.04	45,45,45,45	0
62	MG	14	3297	1/1	1.00	0.02	28,28,28,28	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.